Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:24 PM UTC

PDB ID	:	1QZV / pdb_00001qzv
Title	:	Crystal structure of plant photosystem I
Authors	:	Ben-Shem, A.; Frolow, F.; Nelson, N.
Deposited on	:	2003-09-18
Resolution	:	4.44 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

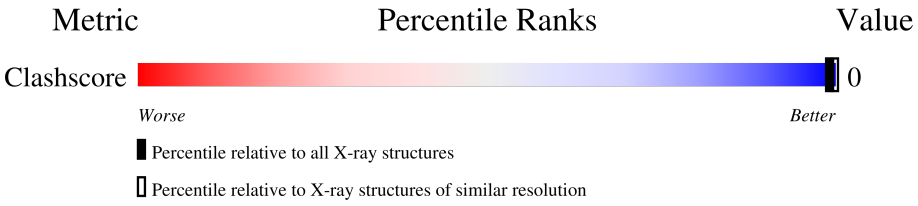
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 4.44 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	1140 (4.98-3.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	726	100%
1	P	726	100%
2	B	732	100%
2	Q	732	100%
3	C	80	100%
3	R	80	100%
4	D	154	100%
4	S	154	100%
5	E	64	100%
5	T	64	100%

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Mol	Chain	Length	Quality of chain
6	F	154	100%
6	U	154	100%
7	G	74	100%
7	V	74	100%
8	H	52	100%
8	W	52	100%
9	I	30	100%
9	Y	30	100%
10	J	41	100%
10	Z	41	100%
11	5	42	100%
11	K	42	100%
12	6	135	100%
12	L	135	100%
13	1	109	100%
13	7	109	100%
14	2	115	98%
14	8	115	98%
15	3	117	100%
15	9	117	100%
16	0	119	100%
16	4	119	100%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
17	CLA	0	1011	X	-	-	-
17	CLA	0	1012	X	-	-	-
17	CLA	0	1013	X	-	-	-
17	CLA	0	1014	X	-	-	-
17	CLA	0	1015	X	-	-	-
17	CLA	0	1016	X	-	-	-
17	CLA	0	1017	X	-	-	-
17	CLA	0	1021	X	-	-	-
17	CLA	0	1022	X	-	-	-
17	CLA	0	1023	X	-	-	-
17	CLA	0	1025	X	-	-	-
17	CLA	0	1026	X	-	-	-
17	CLA	0	1031	X	-	-	-
17	CLA	0	1032	X	-	-	-
17	CLA	0	1033	X	-	-	-
17	CLA	0	8002	X	-	-	-
17	CLA	1	1011	X	-	-	-
17	CLA	1	1012	X	-	-	-
17	CLA	1	1013	X	-	-	-
17	CLA	1	1014	X	-	-	-
17	CLA	1	1015	X	-	-	-
17	CLA	1	1016	X	-	-	-
17	CLA	1	1017	X	-	-	-
17	CLA	1	1021	X	-	-	-
17	CLA	1	1022	X	-	-	-
17	CLA	1	1023	X	-	-	-
17	CLA	1	1025	X	-	-	-
17	CLA	1	1026	X	-	-	-
17	CLA	1	1031	X	-	-	-
17	CLA	2	1011	X	-	-	-
17	CLA	2	1012	X	-	-	-
17	CLA	2	1013	X	-	-	-
17	CLA	2	1014	X	-	-	-
17	CLA	2	1015	X	-	-	-
17	CLA	2	1016	X	-	-	-
17	CLA	2	1017	X	-	-	-
17	CLA	2	1021	X	-	-	-
17	CLA	2	1022	X	-	-	-
17	CLA	2	1023	X	-	-	-
17	CLA	2	1025	X	-	-	-
17	CLA	2	1026	X	-	-	-
17	CLA	2	1031	X	-	-	-
17	CLA	2	1033	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
17	CLA	2	4007	X	-	-	-
17	CLA	3	1011	X	-	-	-
17	CLA	3	1012	X	-	-	-
17	CLA	3	1014	X	-	-	-
17	CLA	3	1015	X	-	-	-
17	CLA	3	1016	X	-	-	-
17	CLA	3	1017	X	-	-	-
17	CLA	3	1021	X	-	-	-
17	CLA	3	1022	X	-	-	-
17	CLA	3	1025	X	-	-	-
17	CLA	3	1026	X	-	-	-
17	CLA	3	1031	X	-	-	-
17	CLA	3	1032	X	-	-	-
17	CLA	3	1033	X	-	-	-
17	CLA	3	1041	X	-	-	-
17	CLA	4	1011	X	-	-	-
17	CLA	4	1012	X	-	-	-
17	CLA	4	1013	X	-	-	-
17	CLA	4	1014	X	-	-	-
17	CLA	4	1015	X	-	-	-
17	CLA	4	1016	X	-	-	-
17	CLA	4	1017	X	-	-	-
17	CLA	4	1021	X	-	-	-
17	CLA	4	1022	X	-	-	-
17	CLA	4	1023	X	-	-	-
17	CLA	4	1025	X	-	-	-
17	CLA	4	1026	X	-	-	-
17	CLA	4	1031	X	-	-	-
17	CLA	4	1032	X	-	-	-
17	CLA	4	1033	X	-	-	-
17	CLA	4	4002	X	-	-	-
17	CLA	5	5401	X	-	-	-
17	CLA	5	5403	X	-	-	-
17	CLA	5	5404	X	-	-	-
17	CLA	6	5501	X	-	-	-
17	CLA	6	5503	X	-	-	-
17	CLA	6	5504	X	-	-	-
17	CLA	7	1011	X	-	-	-
17	CLA	7	1012	X	-	-	-
17	CLA	7	1013	X	-	-	-
17	CLA	7	1014	X	-	-	-
17	CLA	7	1015	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
17	CLA	7	1016	X	-	-	-
17	CLA	7	1017	X	-	-	-
17	CLA	7	1021	X	-	-	-
17	CLA	7	1022	X	-	-	-
17	CLA	7	1023	X	-	-	-
17	CLA	7	1025	X	-	-	-
17	CLA	7	1026	X	-	-	-
17	CLA	7	1031	X	-	-	-
17	CLA	8	1011	X	-	-	-
17	CLA	8	1012	X	-	-	-
17	CLA	8	1013	X	-	-	-
17	CLA	8	1014	X	-	-	-
17	CLA	8	1015	X	-	-	-
17	CLA	8	1016	X	-	-	-
17	CLA	8	1017	X	-	-	-
17	CLA	8	1021	X	-	-	-
17	CLA	8	1022	X	-	-	-
17	CLA	8	1023	X	-	-	-
17	CLA	8	1025	X	-	-	-
17	CLA	8	1026	X	-	-	-
17	CLA	8	1031	X	-	-	-
17	CLA	8	1033	X	-	-	-
17	CLA	8	8007	X	-	-	-
17	CLA	9	1011	X	-	-	-
17	CLA	9	1012	X	-	-	-
17	CLA	9	1014	X	-	-	-
17	CLA	9	1015	X	-	-	-
17	CLA	9	1016	X	-	-	-
17	CLA	9	1017	X	-	-	-
17	CLA	9	1021	X	-	-	-
17	CLA	9	1022	X	-	-	-
17	CLA	9	1025	X	-	-	-
17	CLA	9	1026	X	-	-	-
17	CLA	9	1031	X	-	-	-
17	CLA	9	1032	X	-	-	-
17	CLA	9	1033	X	-	-	-
17	CLA	9	1041	X	-	-	-
17	CLA	A	1011	X	-	-	-
17	CLA	A	1012	X	-	-	-
17	CLA	A	1013	X	-	-	-
17	CLA	A	1102	X	-	-	-
17	CLA	A	1103	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
17	CLA	A	1104	X	-	-	-
17	CLA	A	1105	X	-	-	-
17	CLA	A	1106	X	-	-	-
17	CLA	A	1107	X	-	-	-
17	CLA	A	1108	X	-	-	-
17	CLA	A	1109	X	-	-	-
17	CLA	A	1110	X	-	-	-
17	CLA	A	1111	X	-	-	-
17	CLA	A	1112	X	-	-	-
17	CLA	A	1113	X	-	-	-
17	CLA	A	1114	X	-	-	-
17	CLA	A	1115	X	-	-	-
17	CLA	A	1116	X	-	-	-
17	CLA	A	1117	X	-	-	-
17	CLA	A	1118	X	-	-	-
17	CLA	A	1119	X	-	-	-
17	CLA	A	1120	X	-	-	-
17	CLA	A	1121	X	-	-	-
17	CLA	A	1122	X	-	-	-
17	CLA	A	1123	X	-	-	-
17	CLA	A	1124	X	-	-	-
17	CLA	A	1125	X	-	-	-
17	CLA	A	1126	X	-	-	-
17	CLA	A	1127	X	-	-	-
17	CLA	A	1128	X	-	-	-
17	CLA	A	1129	X	-	-	-
17	CLA	A	1131	X	-	-	-
17	CLA	A	1132	X	-	-	-
17	CLA	A	1133	X	-	-	-
17	CLA	A	1134	X	-	-	-
17	CLA	A	1135	X	-	-	-
17	CLA	A	1136	X	-	-	-
17	CLA	A	1137	X	-	-	-
17	CLA	A	1138	X	-	-	-
17	CLA	A	1139	X	-	-	-
17	CLA	A	1140	X	-	-	-
17	CLA	A	1402	X	-	-	-
17	CLA	A	1901	X	-	-	-
17	CLA	A	4009	X	-	-	-
17	CLA	A	4010	X	-	-	-
17	CLA	B	1021	X	-	-	-
17	CLA	B	1022	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
17	CLA	B	1023	X	-	-	-
17	CLA	B	1130	X	-	-	-
17	CLA	B	1201	X	-	-	-
17	CLA	B	1202	X	-	-	-
17	CLA	B	1203	X	-	-	-
17	CLA	B	1204	X	-	-	-
17	CLA	B	1205	X	-	-	-
17	CLA	B	1206	X	-	-	-
17	CLA	B	1207	X	-	-	-
17	CLA	B	1208	X	-	-	-
17	CLA	B	1209	X	-	-	-
17	CLA	B	1210	X	-	-	-
17	CLA	B	1211	X	-	-	-
17	CLA	B	1212	X	-	-	-
17	CLA	B	1213	X	-	-	-
17	CLA	B	1214	X	-	-	-
17	CLA	B	1215	X	-	-	-
17	CLA	B	1216	X	-	-	-
17	CLA	B	1217	X	-	-	-
17	CLA	B	1218	X	-	-	-
17	CLA	B	1219	X	-	-	-
17	CLA	B	1220	X	-	-	-
17	CLA	B	1221	X	-	-	-
17	CLA	B	1222	X	-	-	-
17	CLA	B	1223	X	-	-	-
17	CLA	B	1224	X	-	-	-
17	CLA	B	1225	X	-	-	-
17	CLA	B	1226	X	-	-	-
17	CLA	B	1227	X	-	-	-
17	CLA	B	1228	X	-	-	-
17	CLA	B	1230	X	-	-	-
17	CLA	B	1231	X	-	-	-
17	CLA	B	1232	X	-	-	-
17	CLA	B	1234	X	-	-	-
17	CLA	B	1235	X	-	-	-
17	CLA	B	1236	X	-	-	-
17	CLA	B	1237	X	-	-	-
17	CLA	B	1238	X	-	-	-
17	CLA	B	1239	X	-	-	-
17	CLA	B	1240	X	-	-	-
17	CLA	B	1241	X	-	-	-
17	CLA	B	1242	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
17	CLA	B	4001	X	-	-	-
17	CLA	F	1229	X	-	-	-
17	CLA	F	1301	X	-	-	-
17	CLA	F	4003	X	-	-	-
17	CLA	F	4004	X	-	-	-
17	CLA	F	4005	X	-	-	-
17	CLA	F	4006	X	-	-	-
17	CLA	G	1233	X	-	-	-
17	CLA	G	1701	X	-	-	-
17	CLA	H	1801	X	-	-	-
17	CLA	J	1101	X	-	-	-
17	CLA	J	1302	X	-	-	-
17	CLA	J	4008	X	-	-	-
17	CLA	K	1401	X	-	-	-
17	CLA	K	1403	X	-	-	-
17	CLA	K	1404	X	-	-	-
17	CLA	L	1501	X	-	-	-
17	CLA	L	1503	X	-	-	-
17	CLA	L	1504	X	-	-	-
17	CLA	P	5011	X	-	-	-
17	CLA	P	5012	X	-	-	-
17	CLA	P	5013	X	-	-	-
17	CLA	P	5102	X	-	-	-
17	CLA	P	5103	X	-	-	-
17	CLA	P	5104	X	-	-	-
17	CLA	P	5105	X	-	-	-
17	CLA	P	5106	X	-	-	-
17	CLA	P	5107	X	-	-	-
17	CLA	P	5108	X	-	-	-
17	CLA	P	5109	X	-	-	-
17	CLA	P	5110	X	-	-	-
17	CLA	P	5111	X	-	-	-
17	CLA	P	5112	X	-	-	-
17	CLA	P	5113	X	-	-	-
17	CLA	P	5114	X	-	-	-
17	CLA	P	5115	X	-	-	-
17	CLA	P	5116	X	-	-	-
17	CLA	P	5117	X	-	-	-
17	CLA	P	5118	X	-	-	-
17	CLA	P	5119	X	-	-	-
17	CLA	P	5120	X	-	-	-
17	CLA	P	5121	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
17	CLA	P	5122	X	-	-	-
17	CLA	P	5123	X	-	-	-
17	CLA	P	5124	X	-	-	-
17	CLA	P	5125	X	-	-	-
17	CLA	P	5126	X	-	-	-
17	CLA	P	5127	X	-	-	-
17	CLA	P	5128	X	-	-	-
17	CLA	P	5129	X	-	-	-
17	CLA	P	5131	X	-	-	-
17	CLA	P	5132	X	-	-	-
17	CLA	P	5133	X	-	-	-
17	CLA	P	5134	X	-	-	-
17	CLA	P	5135	X	-	-	-
17	CLA	P	5136	X	-	-	-
17	CLA	P	5137	X	-	-	-
17	CLA	P	5138	X	-	-	-
17	CLA	P	5139	X	-	-	-
17	CLA	P	5140	X	-	-	-
17	CLA	P	5402	X	-	-	-
17	CLA	P	5901	X	-	-	-
17	CLA	P	8009	X	-	-	-
17	CLA	P	8010	X	-	-	-
17	CLA	Q	5021	X	-	-	-
17	CLA	Q	5022	X	-	-	-
17	CLA	Q	5023	X	-	-	-
17	CLA	Q	5130	X	-	-	-
17	CLA	Q	5201	X	-	-	-
17	CLA	Q	5202	X	-	-	-
17	CLA	Q	5203	X	-	-	-
17	CLA	Q	5204	X	-	-	-
17	CLA	Q	5205	X	-	-	-
17	CLA	Q	5206	X	-	-	-
17	CLA	Q	5207	X	-	-	-
17	CLA	Q	5208	X	-	-	-
17	CLA	Q	5209	X	-	-	-
17	CLA	Q	5210	X	-	-	-
17	CLA	Q	5211	X	-	-	-
17	CLA	Q	5212	X	-	-	-
17	CLA	Q	5213	X	-	-	-
17	CLA	Q	5214	X	-	-	-
17	CLA	Q	5215	X	-	-	-
17	CLA	Q	5216	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
17	CLA	Q	5217	X	-	-	-
17	CLA	Q	5218	X	-	-	-
17	CLA	Q	5219	X	-	-	-
17	CLA	Q	5220	X	-	-	-
17	CLA	Q	5221	X	-	-	-
17	CLA	Q	5222	X	-	-	-
17	CLA	Q	5223	X	-	-	-
17	CLA	Q	5224	X	-	-	-
17	CLA	Q	5225	X	-	-	-
17	CLA	Q	5226	X	-	-	-
17	CLA	Q	5227	X	-	-	-
17	CLA	Q	5228	X	-	-	-
17	CLA	Q	5230	X	-	-	-
17	CLA	Q	5231	X	-	-	-
17	CLA	Q	5232	X	-	-	-
17	CLA	Q	5234	X	-	-	-
17	CLA	Q	5235	X	-	-	-
17	CLA	Q	5236	X	-	-	-
17	CLA	Q	5237	X	-	-	-
17	CLA	Q	5238	X	-	-	-
17	CLA	Q	5239	X	-	-	-
17	CLA	Q	5240	X	-	-	-
17	CLA	Q	5241	X	-	-	-
17	CLA	Q	5242	X	-	-	-
17	CLA	Q	8001	X	-	-	-
17	CLA	U	5229	X	-	-	-
17	CLA	U	5301	X	-	-	-
17	CLA	U	8003	X	-	-	-
17	CLA	U	8004	X	-	-	-
17	CLA	U	8005	X	-	-	-
17	CLA	U	8006	X	-	-	-
17	CLA	V	5233	X	-	-	-
17	CLA	V	5701	X	-	-	-
17	CLA	W	5801	X	-	-	-
17	CLA	Z	5101	X	-	-	-
17	CLA	Z	5302	X	-	-	-
17	CLA	Z	8008	X	-	-	-

2 Entry composition (i)

There are 19 unique types of molecules in this entry. The entry contains 13938 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called PLANT PHOTOSYSTEM I: SUBUNIT PSAA.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
1	A	726	Total C 726 726	0	0	726
1	P	726	Total C 726 726	0	0	726

- Molecule 2 is a protein called PLANT PHOTOSYSTEM I: SUBUNIT PSAB.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
2	B	732	Total C 732 732	0	0	732
2	Q	732	Total C 732 732	0	0	732

- Molecule 3 is a protein called PLANT PHOTOSYSTEM I: SUBUNIT PSAC.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
3	C	80	Total C 80 80	0	0	80
3	R	80	Total C 80 80	0	0	80

- Molecule 4 is a protein called PLANT PHOTOSYSTEM I: SUBUNIT PSAD.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
4	D	154	Total C 154 154	0	0	154
4	S	154	Total C 154 154	0	0	154

- Molecule 5 is a protein called PLANT PHOTOSYSTEM I: SUBUNIT PSAE.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
5	E	64	Total C 64 64	0	0	64
5	T	64	Total C 64 64	0	0	64

- Molecule 6 is a protein called PLANT PHOTOSYSTEM I: SUBUNIT PSAF.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
6	F	154	Total C 154 154	0	0	154
6	U	154	Total C 154 154	0	0	154

- Molecule 7 is a protein called PLANT PHOTOSYSTEM I: SUBUNIT PSAG.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
7	G	74	Total C 74 74	0	0	74
7	V	74	Total C 74 74	0	0	74

- Molecule 8 is a protein called PLANT PHOTOSYSTEM I: SUBUNIT PSAH.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
8	H	52	Total C 52 52	0	0	52
8	W	52	Total C 52 52	0	0	52

- Molecule 9 is a protein called PLANT PHOTOSYSTEM I: SUBUNIT PSAI.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
9	I	30	Total C 30 30	0	0	30
9	Y	30	Total C 30 30	0	0	30

- Molecule 10 is a protein called PLANT PHOTOSYSTEM I: SUBUNIT PSAJ.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
10	J	41	Total C 41 41	0	0	41

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
10	Z	41	Total C 41 41	0	0	41

- Molecule 11 is a protein called PLANT PHOTOSYSTEM I: SUBUNIT PSAK.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
11	K	42	Total C 42 42	0	0	42
11	5	42	Total C 42 42	0	0	42

- Molecule 12 is a protein called PLANT PHOTOSYSTEM I: SUBUNIT PSAL.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
12	L	135	Total C 135 135	0	0	135
12	6	135	Total C 135 135	0	0	135

- Molecule 13 is a protein called PLANT LIGHT HARVESTING COMPLEX I(LHCI): SUBUNIT LHCA1.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
13	1	109	Total C 109 109	0	0	109
13	7	109	Total C 109 109	0	0	109

- Molecule 14 is a protein called PLANT LIGHT HARVESTING COMPLEX I(LHCI): SUBUNIT LHCA2.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
14	2	115	Total C 115 115	0	0	115
14	8	115	Total C 115 115	0	0	115

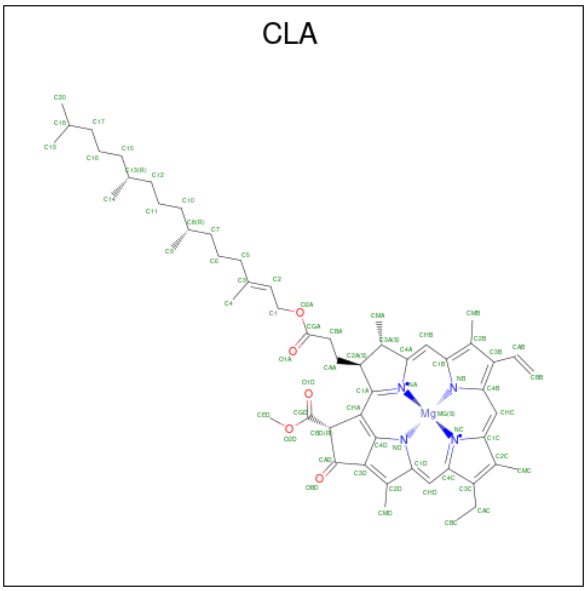
- Molecule 15 is a protein called PLANT LIGHT HARVESTING COMPLEX I(LHCI): SUBUNIT LHCA3.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
15	3	117	Total C 117 117	0	0	117
15	9	117	Total C 117 117	0	0	117

- Molecule 16 is a protein called PLANT LIGHT HARVESTING COMPLEX I(LHCI): SUBUNIT LHCA4.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
16	4	119	Total C 119 119	0	0	119
16	0	119	Total C 119 119	0	0	119

- Molecule 17 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	A	1	Total C Mg N 25 20 1 4	0	0
17	A	1	Total C Mg N 25 20 1 4	0	0
17	A	1	Total C Mg N 25 20 1 4	0	0
17	A	1	Total C Mg N 25 20 1 4	0	0
17	A	1	Total C Mg N 25 20 1 4	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
17	A	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	A	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	A	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	A	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	A	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	A	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	A	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	A	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	A	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	A	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	A	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	A	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	A	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	A	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	A	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	A	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	A	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	A	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	A	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	A	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	A	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	A	1	Total	C	Mg	N	0	0
			25	20	1	4		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
17	A	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	A	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	A	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	A	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	A	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	A	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	A	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	A	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	A	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	A	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	A	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	A	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	A	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	A	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	A	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	A	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	A	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	A	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	A	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	A	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	B	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	B	1	Total	C	Mg	N	0	0
			25	20	1	4		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
17	B	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	B	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	B	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	B	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	B	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	B	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	B	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	B	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	B	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	B	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	B	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	B	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	B	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	B	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	B	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	B	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	B	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	B	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	B	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	B	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	B	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	B	1	Total	C	Mg	N	0	0
			25	20	1	4		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
17	B	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	B	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	B	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	B	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	B	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	B	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	B	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	B	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	B	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	B	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	B	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	B	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	B	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	B	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	B	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	B	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	B	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	B	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	B	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	B	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	B	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	B	1	Total	C	Mg	N	0	0
			25	20	1	4		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
17	B	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	F	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	F	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	F	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	F	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	F	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	F	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	G	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	G	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	H	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	J	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	J	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	J	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	K	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	K	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	K	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	L	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	L	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	L	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	L	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	1	1	Total	C	Mg	N	0	0
			25	20	1	4		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
17	1	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	1	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	1	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	1	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	1	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	1	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	1	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	1	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	1	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	1	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	1	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	1	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	1	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	2	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	2	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	2	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	2	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	2	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	2	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	2	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	2	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	2	1	Total	C	Mg	N	0	0
			25	20	1	4		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
17	2	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	2	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	2	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	2	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	2	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	2	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	3	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	3	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	3	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	3	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	3	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	3	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	3	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	3	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	3	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	3	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	3	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	3	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	3	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	4	1	Total	C	Mg	N	0	0
			25	20	1	4		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
17	4	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	4	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	4	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	4	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	4	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	4	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	4	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	4	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	4	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	4	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	4	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	4	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	4	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	4	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	4	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	4	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	4	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	4	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	P	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	P	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	P	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	P	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	P	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	P	1	Total	C	Mg	N	0	0
			25	20	1	4		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
17	P	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	P	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	P	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	P	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	P	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	P	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	P	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	P	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	P	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	P	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	P	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	P	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	P	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	P	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	P	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	P	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	P	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	P	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	P	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	P	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	P	1	Total	C	Mg	N	0	0
			25	20	1	4		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
17	P	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	P	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	P	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	P	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	P	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	P	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	P	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	P	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	P	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	P	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	P	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	P	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	P	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	P	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	P	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	P	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	P	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	P	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	P	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	Q	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	Q	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	Q	1	Total	C	Mg	N	0	0
			25	20	1	4		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
17	Q	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	Q	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	Q	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	Q	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	Q	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	Q	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	Q	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	Q	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	Q	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	Q	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	Q	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	Q	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	Q	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	Q	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	Q	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	Q	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	Q	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	Q	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	Q	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	Q	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	Q	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	Q	1	Total	C	Mg	N	0	0
			25	20	1	4		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
17	Q	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	Q	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	Q	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	Q	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	Q	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	Q	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	Q	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	Q	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	Q	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	Q	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	Q	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	Q	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	Q	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	Q	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	Q	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	Q	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	Q	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	Q	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	Q	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	Q	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	Q	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	Q	1	Total	C	Mg	N	0	0
			25	20	1	4		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
17	U	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	U	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	U	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	U	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	U	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	U	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	V	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	V	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	W	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	Z	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	Z	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	Z	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	5	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	5	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	5	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	6	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	6	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	6	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	6	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	7	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	7	1	Total	C	Mg	N	0	0
			25	20	1	4		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
17	7	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	7	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	7	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	7	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	7	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	7	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	7	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	7	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	7	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	7	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	7	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	8	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	8	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	8	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	8	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	8	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	8	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	8	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	8	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	8	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	8	1	Total	C	Mg	N	0	0
			25	20	1	4		

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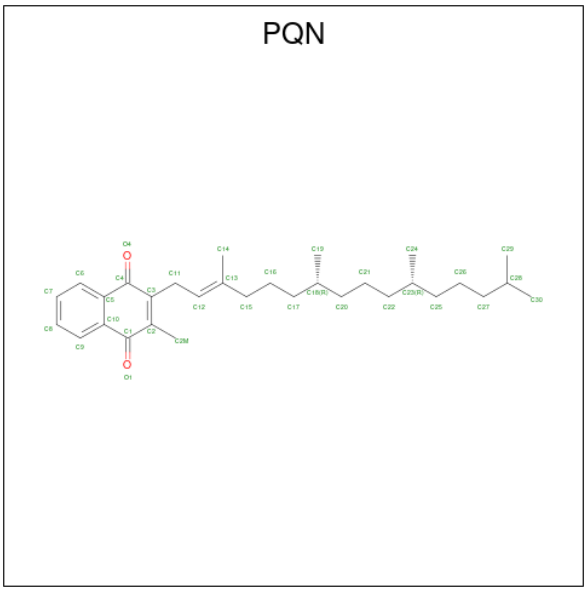
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
17	8	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	8	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	8	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	8	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	8	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	9	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	9	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	9	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	9	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	9	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	9	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	9	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	9	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	9	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	9	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	9	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	9	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	9	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	9	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	0	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	0	1	Total	C	Mg	N	0	0
			25	20	1	4		

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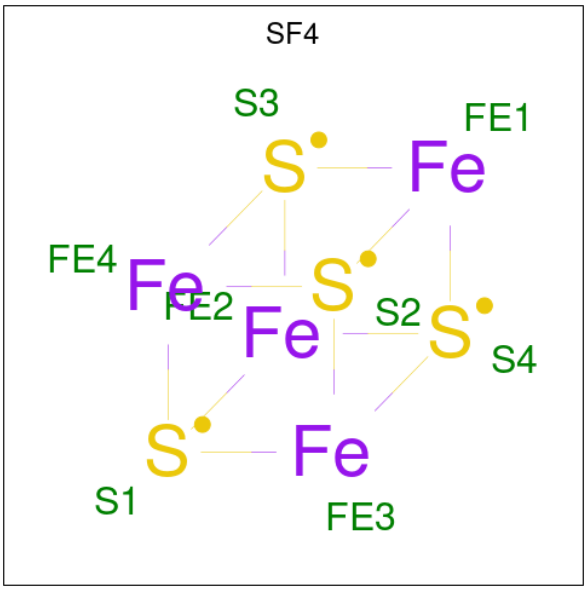
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
17	0	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	0	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	0	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	0	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	0	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	0	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	0	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	0	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	0	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	0	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	0	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	0	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	0	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	0	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	0	1	Total	C	Mg	N	0	0
			25	20	1	4		

- Molecule 18 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	A	1	Total C O 13 11 2	0	0
18	B	1	Total C O 13 11 2	0	0
18	P	1	Total C O 13 11 2	0	0
18	Q	1	Total C O 13 11 2	0	0

- Molecule 19 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
19	A	1	Total	Fe	S	0	0
			8	4	4		
19	C	1	Total	Fe	S	0	0
			8	4	4		
19	C	1	Total	Fe	S	0	0
			8	4	4		
19	P	1	Total	Fe	S	0	0
			8	4	4		
19	R	1	Total	Fe	S	0	0
			8	4	4		
19	R	1	Total	Fe	S	0	0
			8	4	4		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

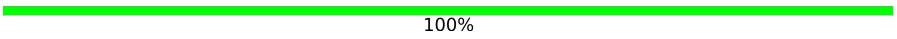
Note EDS was not executed.

• Molecule 1: PLANT PHOTOSYSTEM I: SUBUNIT PSAA

Chain A: 

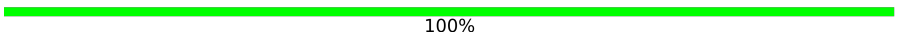
There are no outlier residues recorded for this chain.

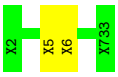
• Molecule 1: PLANT PHOTOSYSTEM I: SUBUNIT PSAA

Chain P: 

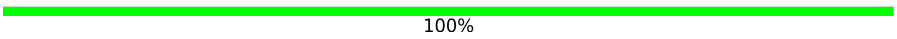
There are no outlier residues recorded for this chain.

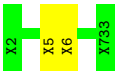
• Molecule 2: PLANT PHOTOSYSTEM I: SUBUNIT PSAB

Chain B: 

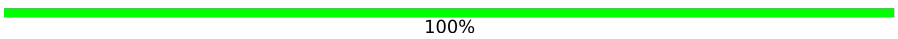


• Molecule 2: PLANT PHOTOSYSTEM I: SUBUNIT PSAB

Chain Q: 

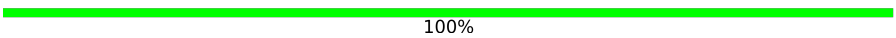


• Molecule 3: PLANT PHOTOSYSTEM I: SUBUNIT PSAC

Chain C: 

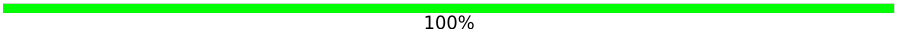
There are no outlier residues recorded for this chain.

• Molecule 3: PLANT PHOTOSYSTEM I: SUBUNIT PSAC

Chain R: 

There are no outlier residues recorded for this chain.

• Molecule 4: PLANT PHOTOSYSTEM I: SUBUNIT PSAD

Chain D: 

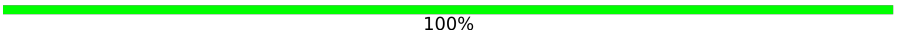
There are no outlier residues recorded for this chain.

• Molecule 4: PLANT PHOTOSYSTEM I: SUBUNIT PSAD

Chain S: 

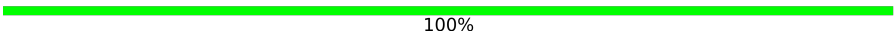
There are no outlier residues recorded for this chain.

• Molecule 5: PLANT PHOTOSYSTEM I: SUBUNIT PSAE

Chain E: 

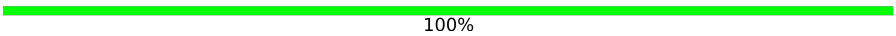
There are no outlier residues recorded for this chain.

• Molecule 5: PLANT PHOTOSYSTEM I: SUBUNIT PSAE

Chain T: 

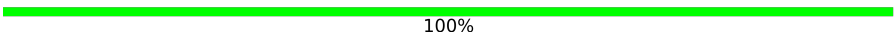
There are no outlier residues recorded for this chain.

• Molecule 6: PLANT PHOTOSYSTEM I: SUBUNIT PSAF

Chain F: 

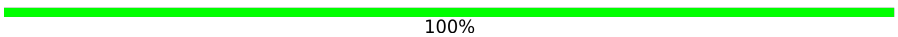
There are no outlier residues recorded for this chain.

• Molecule 6: PLANT PHOTOSYSTEM I: SUBUNIT PSAF

Chain U: 

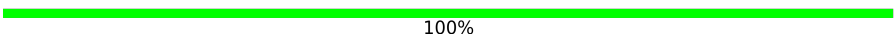
There are no outlier residues recorded for this chain.

• Molecule 7: PLANT PHOTOSYSTEM I: SUBUNIT PSAG

Chain G: 

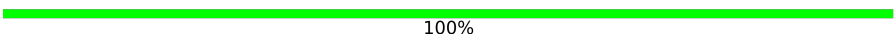
There are no outlier residues recorded for this chain.

• Molecule 7: PLANT PHOTOSYSTEM I: SUBUNIT PSAG

Chain V: 

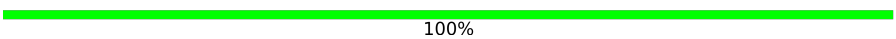
There are no outlier residues recorded for this chain.

• Molecule 8: PLANT PHOTOSYSTEM I: SUBUNIT PSAH

Chain H: 

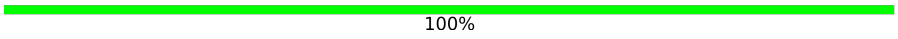
There are no outlier residues recorded for this chain.

• Molecule 8: PLANT PHOTOSYSTEM I: SUBUNIT PSAH

Chain W: 

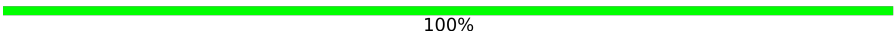
There are no outlier residues recorded for this chain.

• Molecule 9: PLANT PHOTOSYSTEM I: SUBUNIT PSAI

Chain I: 

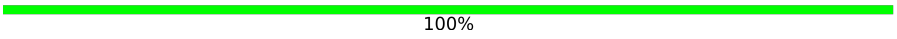
There are no outlier residues recorded for this chain.

• Molecule 9: PLANT PHOTOSYSTEM I: SUBUNIT PSAI

Chain Y: 

There are no outlier residues recorded for this chain.

• Molecule 10: PLANT PHOTOSYSTEM I: SUBUNIT PSAJ

Chain J: 

There are no outlier residues recorded for this chain.

• Molecule 10: PLANT PHOTOSYSTEM I: SUBUNIT PSAJ

Chain Z: 

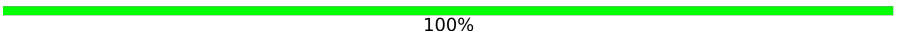
There are no outlier residues recorded for this chain.

• Molecule 11: PLANT PHOTOSYSTEM I: SUBUNIT PSAK

Chain K: 

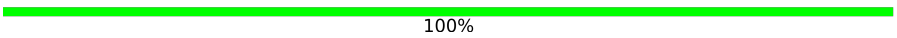
There are no outlier residues recorded for this chain.

• Molecule 11: PLANT PHOTOSYSTEM I: SUBUNIT PSAK

Chain 5: 

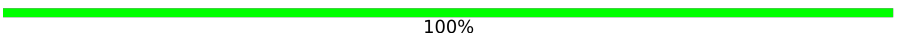
There are no outlier residues recorded for this chain.

• Molecule 12: PLANT PHOTOSYSTEM I: SUBUNIT PSAL

Chain L: 

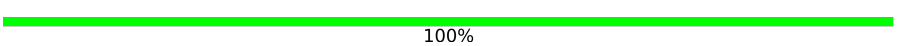
There are no outlier residues recorded for this chain.

• Molecule 12: PLANT PHOTOSYSTEM I: SUBUNIT PSAL

Chain 6: 

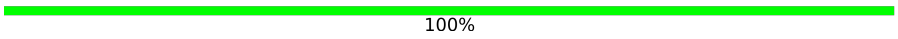
There are no outlier residues recorded for this chain.

• Molecule 13: PLANT LIGHT HARVESTING COMPLEX I(LHCI): SUBUNIT LHCA1

Chain 1: 

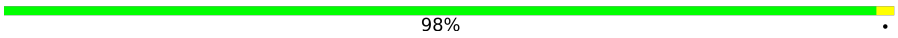
There are no outlier residues recorded for this chain.

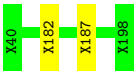
• Molecule 13: PLANT LIGHT HARVESTING COMPLEX I(LHCI): SUBUNIT LHCA1

Chain 7: 

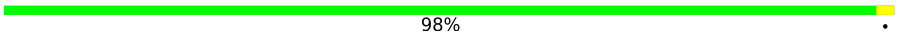
There are no outlier residues recorded for this chain.

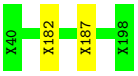
• Molecule 14: PLANT LIGHT HARVESTING COMPLEX I(LHCI): SUBUNIT LHCA2

Chain 2: 

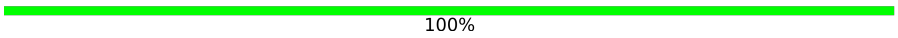


• Molecule 14: PLANT LIGHT HARVESTING COMPLEX I(LHCI): SUBUNIT LHCA2

Chain 8: 

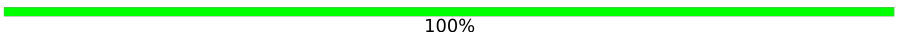


• Molecule 15: PLANT LIGHT HARVESTING COMPLEX I(LHCI): SUBUNIT LHCA3

Chain 3: 

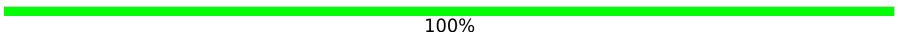
There are no outlier residues recorded for this chain.

• Molecule 15: PLANT LIGHT HARVESTING COMPLEX I(LHCI): SUBUNIT LHCA3

Chain 9: 

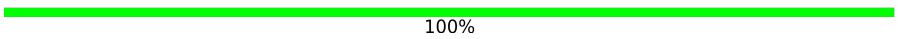
There are no outlier residues recorded for this chain.

• Molecule 16: PLANT LIGHT HARVESTING COMPLEX I(LHCI): SUBUNIT LHCA4

Chain 4: 

There are no outlier residues recorded for this chain.

• Molecule 16: PLANT LIGHT HARVESTING COMPLEX I(LHCI): SUBUNIT LHCA4

Chain 0: 

There are no outlier residues recorded for this chain.

4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	182.28Å 190.38Å 220.25Å 90.00° 90.48° 90.00°	Depositor
Resolution (Å)	50.00 – 4.44	Depositor
% Data completeness (in resolution range)	99.6 (50.00-4.44)	Depositor
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
Refinement program	REFMAC 5.0	Depositor
R, R_{free}	0.410 , 0.420	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	13938	wwPDB-VP
Average B, all atoms (Å^2)	105.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PQN, CLA, SF4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

There are no protein, RNA or DNA chains available to summarize Z scores of covalent bonds and angles.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	726	0	0	0	0
1	P	726	0	0	0	0
2	B	732	0	0	1	0
2	Q	732	0	0	1	0
3	C	80	0	0	0	0
3	R	80	0	0	0	0
4	D	154	0	0	0	0
4	S	154	0	0	0	0
5	E	64	0	0	0	0
5	T	64	0	0	0	0
6	F	154	0	0	0	0
6	U	154	0	0	0	0
7	G	74	0	0	0	0
7	V	74	0	0	0	0
8	H	52	0	0	0	0
8	W	52	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	I	30	0	0	0	0
9	Y	30	0	0	0	0
10	J	41	0	0	0	0
10	Z	41	0	0	0	0
11	5	42	0	0	0	0
11	K	42	0	0	0	0
12	6	135	0	0	0	0
12	L	135	0	0	0	0
13	1	109	0	0	0	0
13	7	109	0	0	0	0
14	2	115	0	0	1	0
14	8	115	0	0	1	0
15	3	117	0	0	0	0
15	9	117	0	0	0	0
16	0	119	0	0	0	0
16	4	119	0	0	0	0
17	0	400	0	48	0	0
17	1	325	0	39	0	0
17	2	375	0	45	0	0
17	3	350	0	42	0	0
17	4	400	0	48	0	0
17	5	75	0	9	0	0
17	6	100	0	12	0	0
17	7	325	0	39	0	0
17	8	375	0	45	0	0
17	9	350	0	42	0	0
17	A	1125	0	135	0	0
17	B	1125	0	135	0	0
17	F	150	0	18	0	0
17	G	50	0	6	0	0
17	H	25	0	3	0	0
17	J	75	0	9	0	0
17	K	75	0	9	0	0
17	L	100	0	12	0	0
17	P	1125	0	135	0	0
17	Q	1125	0	135	0	0
17	U	150	0	18	0	0
17	V	50	0	6	0	0
17	W	25	0	3	0	0
17	Z	75	0	9	0	0
18	A	13	0	7	0	0
18	B	13	0	7	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	P	13	0	7	0	0
18	Q	13	0	7	0	0
19	A	8	0	0	0	0
19	C	16	0	0	0	0
19	P	8	0	0	0	0
19	R	16	0	0	0	0
All	All	13938	0	1030	4	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 0.

All (4) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:8:182:UNK:CA	14:8:187:UNK:CA	2.92	0.48
14:2:182:UNK:CA	14:2:187:UNK:CA	2.92	0.47
2:B:5:UNK:CA	2:B:6:UNK:CA	2.97	0.42
2:Q:5:UNK:CA	2:Q:6:UNK:CA	2.97	0.42

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains (i)

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

344 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
17	CLA	9	1033	-	24,32,73	2.08	6 (25%)	31,54,113	3.05	7 (22%)
19	SF4	C	3003	-	0,12,12	-	-	-		
17	CLA	4	1031	-	24,32,73	2.08	7 (29%)	31,54,113	3.06	7 (22%)
17	CLA	Q	5221	-	24,32,73	2.42	9 (37%)	31,54,113	3.15	7 (22%)
17	CLA	V	5701	-	24,32,73	2.08	6 (25%)	31,54,113	3.04	7 (22%)
17	CLA	3	1022	-	24,32,73	2.09	6 (25%)	31,54,113	3.06	7 (22%)
17	CLA	J	1101	-	24,32,73	2.08	6 (25%)	31,54,113	3.04	7 (22%)
17	CLA	Q	5220	-	24,32,73	2.19	7 (29%)	31,54,113	2.88	7 (22%)
17	CLA	0	1017	-	24,32,73	2.07	6 (25%)	31,54,113	3.02	7 (22%)
17	CLA	P	5901	-	24,32,73	2.41	8 (33%)	31,54,113	4.25	11 (35%)
17	CLA	7	1021	-	24,32,73	2.86	7 (29%)	31,54,113	3.02	7 (22%)
17	CLA	4	1023	-	24,32,73	2.07	6 (25%)	31,54,113	3.01	7 (22%)
17	CLA	B	1241	-	24,32,73	2.09	6 (25%)	31,54,113	3.03	7 (22%)
17	CLA	Q	5242	-	24,32,73	2.08	6 (25%)	31,54,113	3.01	7 (22%)
17	CLA	3	1033	-	24,32,73	2.08	6 (25%)	31,54,113	3.05	7 (22%)
17	CLA	Q	5022	-	24,32,73	2.38	9 (37%)	31,54,113	3.04	8 (25%)
17	CLA	A	1132	-	24,32,73	1.82	7 (29%)	31,54,113	2.83	7 (22%)
17	CLA	Z	5302	-	24,32,73	2.57	8 (33%)	31,54,113	4.24	9 (29%)
17	CLA	2	1026	-	24,32,73	2.08	6 (25%)	31,54,113	3.05	7 (22%)
17	CLA	9	1032	-	24,32,73	2.09	6 (25%)	31,54,113	3.06	7 (22%)
17	CLA	7	1012	-	24,32,73	2.08	6 (25%)	31,54,113	3.02	7 (22%)
17	CLA	6	5503	-	24,32,73	2.13	7 (29%)	31,54,113	2.78	6 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
17	CLA	Q	5204	-	24,32,73	2.00	9 (37%)	31,54,113	3.21	8 (25%)
17	CLA	7	1026	-	24,32,73	2.08	6 (25%)	31,54,113	3.05	7 (22%)
19	SF4	A	3001	-	0,12,12	-	-	-		
17	CLA	Q	5231	-	24,32,73	2.11	9 (37%)	31,54,113	3.03	7 (22%)
17	CLA	A	1129	-	24,32,73	1.92	8 (33%)	31,54,113	3.05	9 (29%)
17	CLA	A	1138	-	24,32,73	2.01	7 (29%)	31,54,113	2.91	8 (25%)
17	CLA	8	1031	-	24,32,73	2.08	6 (25%)	31,54,113	3.02	7 (22%)
17	CLA	4	4002	-	24,32,73	2.08	6 (25%)	31,54,113	3.06	7 (22%)
17	CLA	Q	5211	-	24,32,73	1.97	7 (29%)	31,54,113	2.89	6 (19%)
17	CLA	7	1022	-	24,32,73	2.08	6 (25%)	31,54,113	3.04	7 (22%)
17	CLA	3	1016	-	24,32,73	2.07	6 (25%)	31,54,113	3.01	7 (22%)
17	CLA	A	4009	-	24,32,73	2.09	6 (25%)	31,54,113	3.04	7 (22%)
17	CLA	K	1404	-	24,32,73	2.09	6 (25%)	31,54,113	3.05	7 (22%)
17	CLA	P	5139	-	24,32,73	2.04	7 (29%)	31,54,113	2.79	6 (19%)
17	CLA	K	1403	-	24,32,73	2.08	6 (25%)	31,54,113	3.03	7 (22%)
17	CLA	9	1012	-	24,32,73	2.08	6 (25%)	31,54,113	3.05	7 (22%)
17	CLA	9	1025	-	24,32,73	2.07	6 (25%)	31,54,113	3.03	7 (22%)
17	CLA	4	1032	-	24,32,73	2.08	6 (25%)	31,54,113	3.04	7 (22%)
17	CLA	U	5229	-	24,32,73	1.98	8 (33%)	31,54,113	2.94	7 (22%)
17	CLA	Q	5234	-	24,32,73	2.25	8 (33%)	31,54,113	2.94	6 (19%)
17	CLA	B	1021	-	24,32,73	2.16	8 (33%)	31,54,113	2.94	6 (19%)
17	CLA	B	4001	-	24,32,73	2.08	6 (25%)	31,54,113	3.04	7 (22%)
17	CLA	0	1032	-	24,32,73	2.07	6 (25%)	31,54,113	3.06	7 (22%)
17	CLA	2	1022	-	24,32,73	2.08	6 (25%)	31,54,113	3.03	7 (22%)
17	CLA	4	1011	-	24,32,73	2.09	6 (25%)	31,54,113	3.05	7 (22%)
17	CLA	A	1114	-	24,32,73	2.01	8 (33%)	31,54,113	2.94	7 (22%)
17	CLA	Q	5202	-	24,32,73	2.11	6 (25%)	31,54,113	2.98	6 (19%)
17	CLA	2	1017	-	24,32,73	2.09	6 (25%)	31,54,113	3.03	7 (22%)
17	CLA	1	1025	-	24,32,73	2.08	6 (25%)	31,54,113	3.04	7 (22%)
17	CLA	P	5102	-	24,32,73	2.02	7 (29%)	31,54,113	2.94	7 (22%)
17	CLA	Q	5212	-	24,32,73	2.14	8 (33%)	31,54,113	2.84	7 (22%)
17	CLA	1	1013	-	24,32,73	2.08	6 (25%)	31,54,113	3.03	7 (22%)
17	CLA	1	1031	-	24,32,73	2.07	6 (25%)	31,54,113	3.03	7 (22%)
17	CLA	P	5131	-	24,32,73	1.97	5 (20%)	31,54,113	2.92	8 (25%)
17	CLA	0	1022	-	24,32,73	2.09	6 (25%)	31,54,113	3.06	7 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
17	CLA	1	1014	-	24,32,73	2.08	6 (25%)	31,54,113	3.03	7 (22%)
17	CLA	7	1013	-	24,32,73	2.09	6 (25%)	31,54,113	3.03	7 (22%)
17	CLA	W	5801	-	24,32,73	2.08	6 (25%)	31,54,113	3.03	7 (22%)
17	CLA	8	1033	-	24,32,73	2.09	6 (25%)	31,54,113	3.02	7 (22%)
17	CLA	J	1302	-	24,32,73	2.57	8 (33%)	31,54,113	4.24	9 (29%)
17	CLA	P	5125	-	24,32,73	2.21	8 (33%)	31,54,113	3.14	8 (25%)
17	CLA	5	5401	-	24,32,73	2.15	8 (33%)	31,54,113	2.84	8 (25%)
17	CLA	7	1017	-	24,32,73	2.09	6 (25%)	31,54,113	3.05	7 (22%)
17	CLA	A	1133	-	24,32,73	1.87	8 (33%)	31,54,113	2.94	8 (25%)
17	CLA	P	8009	-	24,32,73	2.09	6 (25%)	31,54,113	3.03	7 (22%)
17	CLA	7	1031	-	24,32,73	2.07	6 (25%)	31,54,113	3.02	7 (22%)
17	CLA	Q	5236	-	24,32,73	2.12	7 (29%)	31,54,113	2.80	7 (22%)
17	CLA	B	1211	-	24,32,73	1.98	7 (29%)	31,54,113	2.88	6 (19%)
17	CLA	V	5233	-	24,32,73	2.08	8 (33%)	31,54,113	2.98	6 (19%)
17	CLA	A	1108	-	24,32,73	2.45	5 (20%)	31,54,113	3.78	10 (32%)
17	CLA	A	1012	-	24,32,73	2.33	7 (29%)	31,54,113	3.10	8 (25%)
17	CLA	9	1021	-	24,32,73	2.08	6 (25%)	31,54,113	3.03	8 (25%)
17	CLA	B	1236	-	24,32,73	2.12	7 (29%)	31,54,113	2.79	7 (22%)
17	CLA	9	1031	-	24,32,73	2.08	6 (25%)	31,54,113	3.03	7 (22%)
17	CLA	Q	8001	-	24,32,73	2.08	6 (25%)	31,54,113	3.04	7 (22%)
17	CLA	A	1125	-	24,32,73	2.20	8 (33%)	31,54,113	3.15	8 (25%)
17	CLA	7	1015	-	24,32,73	2.09	7 (29%)	31,54,113	3.05	7 (22%)
17	CLA	3	1015	-	24,32,73	2.08	6 (25%)	31,54,113	3.04	7 (22%)
17	CLA	P	8010	-	24,32,73	2.09	6 (25%)	31,54,113	3.05	7 (22%)
17	CLA	A	1102	-	24,32,73	2.02	7 (29%)	31,54,113	2.95	7 (22%)
17	CLA	B	1237	-	24,32,73	1.85	8 (33%)	31,54,113	2.90	7 (22%)
17	CLA	B	1217	-	24,32,73	2.09	8 (33%)	31,54,113	3.05	7 (22%)
18	PQN	P	6001	-	14,14,34	4.54	13 (92%)	20,20,45	0.99	1 (5%)
17	CLA	4	1017	-	24,32,73	2.08	6 (25%)	31,54,113	3.03	7 (22%)
18	PQN	Q	6002	-	14,14,34	4.40	13 (92%)	20,20,45	1.04	2 (10%)
17	CLA	2	1033	-	24,32,73	2.09	6 (25%)	31,54,113	3.01	7 (22%)
17	CLA	P	5123	-	24,32,73	2.34	7 (29%)	31,54,113	3.09	8 (25%)
17	CLA	A	1118	-	24,32,73	2.10	8 (33%)	31,54,113	3.18	8 (25%)
17	CLA	A	1013	-	24,32,73	2.11	8 (33%)	31,54,113	2.70	9 (29%)
17	CLA	A	1120	-	24,32,73	2.01	8 (33%)	31,54,113	2.95	7 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
17	CLA	P	5012	-	24,32,73	2.33	7 (29%)	31,54,113	3.09	8 (25%)
17	CLA	0	1016	-	24,32,73	2.08	6 (25%)	31,54,113	3.03	8 (25%)
17	CLA	4	1026	-	24,32,73	2.08	6 (25%)	31,54,113	3.04	7 (22%)
17	CLA	B	1224	-	24,32,73	2.24	8 (33%)	31,54,113	2.95	8 (25%)
17	CLA	P	5133	-	24,32,73	1.87	8 (33%)	31,54,113	2.94	8 (25%)
17	CLA	A	1105	-	24,32,73	2.17	7 (29%)	31,54,113	2.75	7 (22%)
17	CLA	P	5137	-	24,32,73	2.57	7 (29%)	31,54,113	3.86	9 (29%)
17	CLA	B	1215	-	24,32,73	1.91	6 (25%)	31,54,113	2.97	7 (22%)
17	CLA	Q	5216	-	24,32,73	2.03	8 (33%)	31,54,113	2.76	7 (22%)
17	CLA	B	1204	-	24,32,73	2.00	8 (33%)	31,54,113	3.21	8 (25%)
17	CLA	A	1104	-	24,32,73	2.24	9 (37%)	31,54,113	2.99	7 (22%)
17	CLA	B	1130	-	24,32,73	1.99	7 (29%)	31,54,113	3.09	7 (22%)
17	CLA	P	5117	-	24,32,73	1.92	6 (25%)	31,54,113	2.82	9 (29%)
17	CLA	G	1233	-	24,32,73	2.09	8 (33%)	31,54,113	3.00	6 (19%)
17	CLA	8	1025	-	24,32,73	2.09	6 (25%)	31,54,113	3.01	7 (22%)
17	CLA	2	1023	-	24,32,73	2.08	6 (25%)	31,54,113	3.02	7 (22%)
17	CLA	7	1011	-	24,32,73	2.09	6 (25%)	31,54,113	3.05	7 (22%)
17	CLA	A	1113	-	24,32,73	2.38	8 (33%)	31,54,113	4.10	11 (35%)
17	CLA	K	1401	-	24,32,73	2.16	8 (33%)	31,54,113	2.84	8 (25%)
17	CLA	6	5501	-	24,32,73	2.31	8 (33%)	31,54,113	2.72	8 (25%)
17	CLA	B	1239	-	24,32,73	1.77	6 (25%)	31,54,113	2.93	6 (19%)
17	CLA	B	1201	-	24,32,73	1.97	7 (29%)	31,54,113	2.94	8 (25%)
17	CLA	A	1103	-	24,32,73	1.99	7 (29%)	31,54,113	3.21	8 (25%)
17	CLA	8	1014	-	24,32,73	2.08	6 (25%)	31,54,113	3.04	7 (22%)
17	CLA	L	1502	-	24,32,73	2.12	7 (29%)	31,54,113	2.88	8 (25%)
17	CLA	Q	5225	-	24,32,73	2.13	7 (29%)	31,54,113	2.53	8 (25%)
17	CLA	9	1026	-	24,32,73	2.08	6 (25%)	31,54,113	3.04	7 (22%)
17	CLA	3	1041	-	24,32,73	2.08	6 (25%)	31,54,113	3.04	7 (22%)
17	CLA	P	5126	-	24,32,73	2.15	6 (25%)	31,54,113	2.91	7 (22%)
17	CLA	L	1503	-	24,32,73	2.12	7 (29%)	31,54,113	2.78	6 (19%)
17	CLA	8	1021	-	24,32,73	2.08	6 (25%)	31,54,113	3.01	7 (22%)
17	CLA	0	1012	-	24,32,73	2.10	6 (25%)	31,54,113	3.05	7 (22%)
17	CLA	4	1021	-	24,32,73	2.07	6 (25%)	31,54,113	3.01	7 (22%)
17	CLA	9	1014	-	24,32,73	2.08	6 (25%)	31,54,113	3.05	7 (22%)
17	CLA	A	1123	-	24,32,73	2.33	7 (29%)	31,54,113	3.09	8 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
17	CLA	P	5140	-	24,32,73	1.90	6 (25%)	31,54,113	2.97	7 (22%)
17	CLA	A	1110	-	24,32,73	1.99	5 (20%)	31,54,113	3.09	8 (25%)
17	CLA	8	1012	-	24,32,73	2.09	6 (25%)	31,54,113	3.05	7 (22%)
19	SF4	R	7003	-	0,12,12	-	-	-		
17	CLA	P	5121	-	24,32,73	2.15	8 (33%)	31,54,113	2.73	6 (19%)
17	CLA	P	5122	-	24,32,73	1.93	8 (33%)	31,54,113	2.95	7 (22%)
17	CLA	A	1121	-	24,32,73	2.16	8 (33%)	31,54,113	2.72	6 (19%)
17	CLA	7	1023	-	24,32,73	2.08	6 (25%)	31,54,113	3.02	7 (22%)
17	CLA	1	1022	-	24,32,73	2.08	6 (25%)	31,54,113	3.05	7 (22%)
17	CLA	4	1016	-	24,32,73	2.07	6 (25%)	31,54,113	3.04	7 (22%)
17	CLA	1	1015	-	24,32,73	2.08	6 (25%)	31,54,113	3.04	7 (22%)
17	CLA	P	5109	-	24,32,73	2.00	8 (33%)	31,54,113	2.81	7 (22%)
17	CLA	B	1228	-	24,32,73	2.04	8 (33%)	31,54,113	3.03	9 (29%)
17	CLA	A	1901	-	24,32,73	2.41	8 (33%)	31,54,113	4.26	11 (35%)
17	CLA	Q	5021	-	24,32,73	2.15	8 (33%)	31,54,113	2.93	6 (19%)
17	CLA	2	1021	-	24,32,73	2.07	6 (25%)	31,54,113	3.00	7 (22%)
17	CLA	2	4007	-	24,32,73	2.09	6 (25%)	31,54,113	3.03	7 (22%)
17	CLA	3	1032	-	24,32,73	2.09	6 (25%)	31,54,113	3.06	7 (22%)
17	CLA	P	5106	-	24,32,73	1.96	6 (25%)	31,54,113	2.91	7 (22%)
17	CLA	Q	5205	-	24,32,73	2.09	7 (29%)	31,54,113	2.64	6 (19%)
17	CLA	A	1119	-	24,32,73	1.99	7 (29%)	31,54,113	2.92	8 (25%)
17	CLA	P	5129	-	24,32,73	1.91	8 (33%)	31,54,113	3.05	9 (29%)
17	CLA	A	1402	-	24,32,73	2.28	7 (29%)	31,54,113	3.07	6 (19%)
17	CLA	B	1205	-	24,32,73	2.09	7 (29%)	31,54,113	2.64	6 (19%)
17	CLA	B	1221	-	24,32,73	2.43	9 (37%)	31,54,113	3.15	7 (22%)
17	CLA	P	5107	-	24,32,73	1.94	7 (29%)	31,54,113	2.95	8 (25%)
17	CLA	P	5114	-	24,32,73	2.02	8 (33%)	31,54,113	2.94	7 (22%)
17	CLA	P	5136	-	24,32,73	2.20	8 (33%)	31,54,113	2.70	8 (25%)
17	CLA	2	1011	-	24,32,73	2.08	6 (25%)	31,54,113	3.05	7 (22%)
17	CLA	P	5127	-	24,32,73	2.10	7 (29%)	31,54,113	2.86	6 (19%)
17	CLA	Q	5217	-	24,32,73	2.09	8 (33%)	31,54,113	3.05	7 (22%)
17	CLA	8	1013	-	24,32,73	2.08	6 (25%)	31,54,113	3.04	7 (22%)
17	CLA	2	1016	-	24,32,73	2.08	6 (25%)	31,54,113	3.05	7 (22%)
17	CLA	P	5132	-	24,32,73	1.82	7 (29%)	31,54,113	2.83	7 (22%)
17	CLA	Q	5240	-	24,32,73	2.08	6 (25%)	31,54,113	3.02	7 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
17	CLA	U	8003	-	24,32,73	2.07	6 (25%)	31,54,113	3.03	7 (22%)
17	CLA	Q	5215	-	24,32,73	1.92	6 (25%)	31,54,113	2.98	7 (22%)
17	CLA	Q	5213	-	24,32,73	2.12	7 (29%)	31,54,113	2.76	8 (25%)
17	CLA	B	1235	-	24,32,73	2.12	8 (33%)	31,54,113	2.90	7 (22%)
17	CLA	P	5138	-	24,32,73	2.01	7 (29%)	31,54,113	2.91	8 (25%)
17	CLA	A	1109	-	24,32,73	2.00	8 (33%)	31,54,113	2.80	7 (22%)
17	CLA	G	1701	-	24,32,73	2.08	6 (25%)	31,54,113	3.04	7 (22%)
17	CLA	3	1031	-	24,32,73	2.08	6 (25%)	31,54,113	3.03	7 (22%)
17	CLA	A	1127	-	24,32,73	2.11	7 (29%)	31,54,113	2.84	6 (19%)
17	CLA	P	5128	-	24,32,73	2.35	7 (29%)	31,54,113	2.71	8 (25%)
17	CLA	7	1016	-	24,32,73	2.08	6 (25%)	31,54,113	3.02	7 (22%)
17	CLA	B	1223	-	24,32,73	2.31	8 (33%)	31,54,113	3.13	8 (25%)
17	CLA	P	5111	-	24,32,73	2.07	8 (33%)	31,54,113	3.19	8 (25%)
17	CLA	B	1222	-	24,32,73	1.94	6 (25%)	31,54,113	2.93	6 (19%)
17	CLA	A	1140	-	24,32,73	1.90	6 (25%)	31,54,113	2.97	7 (22%)
17	CLA	P	5116	-	24,32,73	2.16	7 (29%)	31,54,113	2.97	7 (22%)
17	CLA	0	8002	-	24,32,73	2.09	6 (25%)	31,54,113	3.08	8 (25%)
17	CLA	B	1219	-	24,32,73	2.40	8 (33%)	31,54,113	3.99	9 (29%)
17	CLA	P	5110	-	24,32,73	1.99	5 (20%)	31,54,113	3.11	8 (25%)
17	CLA	P	5120	-	24,32,73	2.02	8 (33%)	31,54,113	2.95	7 (22%)
17	CLA	1	1026	-	24,32,73	2.08	6 (25%)	31,54,113	3.04	7 (22%)
17	CLA	A	1115	-	24,32,73	2.17	8 (33%)	31,54,113	2.61	8 (25%)
17	CLA	Q	5228	-	24,32,73	2.05	8 (33%)	31,54,113	3.04	9 (29%)
17	CLA	Q	5222	-	24,32,73	1.95	7 (29%)	31,54,113	2.93	6 (19%)
17	CLA	B	1214	-	24,32,73	2.05	8 (33%)	31,54,113	2.91	7 (22%)
17	CLA	B	1232	-	24,32,73	2.22	8 (33%)	31,54,113	2.90	7 (22%)
17	CLA	Q	5207	-	24,32,73	2.35	8 (33%)	31,54,113	3.03	6 (19%)
17	CLA	Z	8008	-	24,32,73	2.08	6 (25%)	31,54,113	3.04	7 (22%)
17	CLA	Q	5232	-	24,32,73	2.21	8 (33%)	31,54,113	2.89	7 (22%)
17	CLA	9	1017	-	24,32,73	2.08	6 (25%)	31,54,113	3.03	7 (22%)
17	CLA	1	1023	-	24,32,73	2.09	6 (25%)	31,54,113	3.03	7 (22%)
17	CLA	B	1242	-	24,32,73	2.09	6 (25%)	31,54,113	3.02	7 (22%)
17	CLA	0	1014	-	24,32,73	2.07	6 (25%)	31,54,113	3.02	7 (22%)
17	CLA	Q	5239	-	24,32,73	1.77	6 (25%)	31,54,113	2.93	6 (19%)
17	CLA	P	5011	-	24,32,73	2.16	9 (37%)	31,54,113	2.96	5 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
17	CLA	U	8004	-	24,32,73	2.08	6 (25%)	31,54,113	3.03	7 (22%)
17	CLA	A	1131	-	24,32,73	1.97	5 (20%)	31,54,113	2.92	8 (25%)
17	CLA	A	1112	-	24,32,73	2.24	8 (33%)	31,54,113	2.85	8 (25%)
17	CLA	0	1023	-	24,32,73	2.07	6 (25%)	31,54,113	3.01	8 (25%)
17	CLA	8	1022	-	24,32,73	2.08	6 (25%)	31,54,113	3.02	7 (22%)
17	CLA	Z	5101	-	24,32,73	2.08	6 (25%)	31,54,113	3.04	7 (22%)
17	CLA	Q	5209	-	24,32,73	2.10	8 (33%)	31,54,113	2.97	7 (22%)
17	CLA	8	1023	-	24,32,73	2.08	6 (25%)	31,54,113	3.02	7 (22%)
17	CLA	Q	5203	-	24,32,73	2.20	7 (29%)	31,54,113	2.94	7 (22%)
17	CLA	0	1013	-	24,32,73	2.07	6 (25%)	31,54,113	3.01	7 (22%)
17	CLA	B	1227	-	24,32,73	1.96	7 (29%)	31,54,113	3.00	9 (29%)
17	CLA	A	1107	-	24,32,73	1.94	7 (29%)	31,54,113	2.96	8 (25%)
17	CLA	A	1122	-	24,32,73	1.93	8 (33%)	31,54,113	2.94	7 (22%)
17	CLA	B	1234	-	24,32,73	2.25	8 (33%)	31,54,113	2.94	6 (19%)
17	CLA	B	1231	-	24,32,73	2.12	9 (37%)	31,54,113	3.06	7 (22%)
17	CLA	9	1022	-	24,32,73	2.09	6 (25%)	31,54,113	3.05	7 (22%)
17	CLA	B	1022	-	24,32,73	2.38	9 (37%)	31,54,113	3.05	8 (25%)
17	CLA	B	1226	-	24,32,73	2.12	7 (29%)	31,54,113	2.77	8 (25%)
17	CLA	Q	5130	-	24,32,73	2.00	7 (29%)	31,54,113	3.10	7 (22%)
17	CLA	Q	5223	-	24,32,73	2.31	8 (33%)	31,54,113	3.13	8 (25%)
17	CLA	U	8006	-	24,32,73	2.08	6 (25%)	31,54,113	3.04	7 (22%)
17	CLA	P	5134	-	24,32,73	2.04	8 (33%)	31,54,113	3.00	8 (25%)
17	CLA	Q	5226	-	24,32,73	2.13	7 (29%)	31,54,113	2.76	8 (25%)
17	CLA	Q	5227	-	24,32,73	1.96	7 (29%)	31,54,113	3.00	9 (29%)
17	CLA	Q	5206	-	24,32,73	1.97	4 (16%)	31,54,113	2.98	7 (22%)
17	CLA	B	1240	-	24,32,73	2.08	6 (25%)	31,54,113	3.03	7 (22%)
17	CLA	F	4006	-	24,32,73	2.08	6 (25%)	31,54,113	3.04	7 (22%)
17	CLA	0	1021	-	24,32,73	2.07	6 (25%)	31,54,113	3.00	7 (22%)
17	CLA	0	1031	-	24,32,73	2.09	7 (29%)	31,54,113	3.06	7 (22%)
17	CLA	B	1023	-	24,32,73	2.30	11 (45%)	31,54,113	2.99	9 (29%)
17	CLA	B	1216	-	24,32,73	2.03	8 (33%)	31,54,113	2.76	7 (22%)
17	CLA	Q	5208	-	24,32,73	2.04	8 (33%)	31,54,113	2.80	7 (22%)
17	CLA	A	4010	-	24,32,73	2.08	6 (25%)	31,54,113	3.04	7 (22%)
17	CLA	B	1212	-	24,32,73	2.13	7 (29%)	31,54,113	2.82	7 (22%)
17	CLA	8	1015	-	24,32,73	2.08	6 (25%)	31,54,113	3.03	8 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
18	PQN	A	2001	-	14,14,34	4.55	13 (92%)	20,20,45	0.99	1 (5%)
17	CLA	1	1011	-	24,32,73	2.09	6 (25%)	31,54,113	3.05	7 (22%)
17	CLA	P	5115	-	24,32,73	2.17	8 (33%)	31,54,113	2.62	8 (25%)
17	CLA	Q	5023	-	24,32,73	2.30	11 (45%)	31,54,113	3.00	9 (29%)
17	CLA	A	1126	-	24,32,73	2.15	6 (25%)	31,54,113	2.91	7 (22%)
17	CLA	B	1210	-	24,32,73	2.39	8 (33%)	31,54,113	3.03	8 (25%)
19	SF4	C	3002	-	0,12,12	-	-	-		
17	CLA	8	1016	-	24,32,73	2.08	6 (25%)	31,54,113	3.04	7 (22%)
17	CLA	B	1220	-	24,32,73	2.19	7 (29%)	31,54,113	2.87	7 (22%)
17	CLA	3	1025	-	24,32,73	2.08	6 (25%)	31,54,113	3.04	7 (22%)
17	CLA	Q	5224	-	24,32,73	2.24	7 (29%)	31,54,113	2.94	8 (25%)
17	CLA	B	1225	-	24,32,73	2.13	7 (29%)	31,54,113	2.52	8 (25%)
17	CLA	P	5135	-	24,32,73	2.20	7 (29%)	31,54,113	3.05	7 (22%)
17	CLA	8	1026	-	24,32,73	2.08	6 (25%)	31,54,113	3.04	7 (22%)
17	CLA	3	1014	-	24,32,73	2.09	6 (25%)	31,54,113	3.04	7 (22%)
17	CLA	0	1025	-	24,32,73	2.07	6 (25%)	31,54,113	3.01	7 (22%)
17	CLA	U	8005	-	24,32,73	2.09	6 (25%)	31,54,113	3.04	7 (22%)
17	CLA	A	1124	-	24,32,73	1.82	6 (25%)	31,54,113	2.81	7 (22%)
17	CLA	7	1025	-	24,32,73	2.07	6 (25%)	31,54,113	3.04	7 (22%)
17	CLA	9	1016	-	24,32,73	2.08	6 (25%)	31,54,113	3.01	8 (25%)
17	CLA	B	1208	-	24,32,73	2.04	8 (33%)	31,54,113	2.80	7 (22%)
17	CLA	A	1134	-	24,32,73	2.04	8 (33%)	31,54,113	3.01	8 (25%)
17	CLA	P	5112	-	24,32,73	2.24	8 (33%)	31,54,113	2.84	8 (25%)
17	CLA	P	5113	-	24,32,73	2.39	8 (33%)	31,54,113	4.10	11 (35%)
17	CLA	8	1011	-	24,32,73	2.08	6 (25%)	31,54,113	3.03	7 (22%)
17	CLA	F	1301	-	24,32,73	2.23	7 (29%)	31,54,113	2.87	6 (19%)
17	CLA	2	1012	-	24,32,73	2.08	6 (25%)	31,54,113	3.04	7 (22%)
17	CLA	3	1012	-	24,32,73	2.08	6 (25%)	31,54,113	3.05	7 (22%)
19	SF4	R	7002	-	0,12,12	-	-	-		
17	CLA	F	1229	-	24,32,73	1.97	8 (33%)	31,54,113	2.92	7 (22%)
17	CLA	P	5108	-	24,32,73	2.45	5 (20%)	31,54,113	3.77	10 (32%)
17	CLA	3	1026	-	24,32,73	2.08	6 (25%)	31,54,113	3.04	7 (22%)
17	CLA	A	1135	-	24,32,73	2.20	7 (29%)	31,54,113	3.07	7 (22%)
17	CLA	P	5124	-	24,32,73	1.82	6 (25%)	31,54,113	2.82	7 (22%)
17	CLA	2	1031	-	24,32,73	2.08	6 (25%)	31,54,113	3.02	7 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
17	CLA	F	4004	-	24,32,73	2.08	6 (25%)	31,54,113	3.04	7 (22%)
17	CLA	F	4003	-	24,32,73	2.08	6 (25%)	31,54,113	3.04	7 (22%)
17	CLA	0	1033	-	24,32,73	2.08	6 (25%)	31,54,113	3.04	7 (22%)
17	CLA	1	1017	-	24,32,73	2.08	6 (25%)	31,54,113	3.04	7 (22%)
17	CLA	4	1025	-	24,32,73	2.08	6 (25%)	31,54,113	3.02	7 (22%)
17	CLA	B	1203	-	24,32,73	2.19	7 (29%)	31,54,113	2.92	7 (22%)
17	CLA	B	1230	-	24,32,73	1.97	8 (33%)	31,54,113	2.87	7 (22%)
17	CLA	Q	5241	-	24,32,73	2.09	6 (25%)	31,54,113	3.05	7 (22%)
17	CLA	Q	5219	-	24,32,73	2.39	8 (33%)	31,54,113	3.98	9 (29%)
17	CLA	7	1014	-	24,32,73	2.07	6 (25%)	31,54,113	3.01	7 (22%)
17	CLA	Q	5214	-	24,32,73	2.06	8 (33%)	31,54,113	2.92	7 (22%)
17	CLA	5	5403	-	24,32,73	2.09	6 (25%)	31,54,113	3.03	7 (22%)
17	CLA	Q	5218	-	24,32,73	2.16	7 (29%)	31,54,113	3.02	9 (29%)
17	CLA	0	1015	-	24,32,73	2.10	6 (25%)	31,54,113	3.04	7 (22%)
17	CLA	9	1015	-	24,32,73	2.08	6 (25%)	31,54,113	3.03	7 (22%)
17	CLA	P	5118	-	24,32,73	2.10	8 (33%)	31,54,113	3.18	9 (29%)
17	CLA	B	1213	-	24,32,73	2.12	7 (29%)	31,54,113	2.77	8 (25%)
17	CLA	4	1012	-	24,32,73	2.10	6 (25%)	31,54,113	3.05	7 (22%)
17	CLA	F	4005	-	24,32,73	2.08	6 (25%)	31,54,113	3.04	7 (22%)
18	PQN	B	2002	-	14,14,34	4.40	13 (92%)	20,20,45	1.04	2 (10%)
17	CLA	L	1501	-	24,32,73	2.31	8 (33%)	31,54,113	2.71	8 (25%)
17	CLA	A	1128	-	24,32,73	2.34	7 (29%)	31,54,113	2.69	8 (25%)
17	CLA	B	1202	-	24,32,73	2.11	6 (25%)	31,54,113	2.98	6 (19%)
17	CLA	2	1025	-	24,32,73	2.09	6 (25%)	31,54,113	3.01	7 (22%)
17	CLA	J	4008	-	24,32,73	2.08	6 (25%)	31,54,113	3.04	7 (22%)
17	CLA	8	1017	-	24,32,73	2.09	6 (25%)	31,54,113	3.03	7 (22%)
17	CLA	B	1207	-	24,32,73	2.35	8 (33%)	31,54,113	3.02	6 (19%)
17	CLA	P	5103	-	24,32,73	1.99	7 (29%)	31,54,113	3.22	8 (25%)
17	CLA	P	5013	-	24,32,73	2.11	8 (33%)	31,54,113	2.69	8 (25%)
17	CLA	B	1206	-	24,32,73	1.97	4 (16%)	31,54,113	2.98	7 (22%)
17	CLA	3	1011	-	24,32,73	2.09	6 (25%)	31,54,113	3.04	7 (22%)
17	CLA	1	1021	-	24,32,73	2.86	7 (29%)	31,54,113	3.03	7 (22%)
17	CLA	U	5301	-	24,32,73	2.23	7 (29%)	31,54,113	2.88	6 (19%)
17	CLA	0	1011	-	24,32,73	2.09	6 (25%)	31,54,113	3.04	7 (22%)
17	CLA	A	1137	-	24,32,73	2.57	8 (33%)	31,54,113	3.85	9 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
17	CLA	9	1011	-	24,32,73	2.09	6 (25%)	31,54,113	3.05	7 (22%)
17	CLA	8	8007	-	24,32,73	2.09	6 (25%)	31,54,113	3.04	7 (22%)
17	CLA	H	1801	-	24,32,73	2.08	6 (25%)	31,54,113	3.03	7 (22%)
17	CLA	A	1117	-	24,32,73	1.92	6 (25%)	31,54,113	2.83	9 (29%)
17	CLA	Q	5210	-	24,32,73	2.39	8 (33%)	31,54,113	3.03	8 (25%)
17	CLA	3	1017	-	24,32,73	2.08	6 (25%)	31,54,113	3.03	7 (22%)
17	CLA	P	5119	-	24,32,73	2.00	7 (29%)	31,54,113	2.91	8 (25%)
17	CLA	A	1139	-	24,32,73	2.04	7 (29%)	31,54,113	2.79	6 (19%)
17	CLA	Q	5238	-	24,32,73	1.96	7 (29%)	31,54,113	2.80	8 (25%)
17	CLA	6	5504	-	24,32,73	2.08	6 (25%)	31,54,113	3.03	7 (22%)
17	CLA	1	1016	-	24,32,73	2.08	6 (25%)	31,54,113	3.02	7 (22%)
17	CLA	4	1013	-	24,32,73	2.07	6 (25%)	31,54,113	3.03	7 (22%)
17	CLA	A	1136	-	24,32,73	2.19	8 (33%)	31,54,113	2.70	8 (25%)
17	CLA	A	1111	-	24,32,73	2.06	8 (33%)	31,54,113	3.18	8 (25%)
17	CLA	A	1011	-	24,32,73	2.15	9 (37%)	31,54,113	2.96	5 (16%)
17	CLA	Q	5230	-	24,32,73	1.97	8 (33%)	31,54,113	2.87	7 (22%)
19	SF4	P	7001	-	0,12,12	-	-	-		
17	CLA	4	1022	-	24,32,73	2.09	6 (25%)	31,54,113	3.05	7 (22%)
17	CLA	1	1012	-	24,32,73	2.08	6 (25%)	31,54,113	3.03	7 (22%)
17	CLA	Q	5237	-	24,32,73	1.85	8 (33%)	31,54,113	2.91	7 (22%)
17	CLA	4	1015	-	24,32,73	2.09	6 (25%)	31,54,113	3.04	7 (22%)
17	CLA	0	1026	-	24,32,73	2.08	6 (25%)	31,54,113	3.03	7 (22%)
17	CLA	5	5404	-	24,32,73	2.09	6 (25%)	31,54,113	3.06	7 (22%)
17	CLA	P	5105	-	24,32,73	2.17	7 (29%)	31,54,113	2.74	7 (22%)
17	CLA	Q	5201	-	24,32,73	1.96	7 (29%)	31,54,113	2.95	8 (25%)
17	CLA	Q	5235	-	24,32,73	2.11	8 (33%)	31,54,113	2.90	7 (22%)
17	CLA	B	1209	-	24,32,73	2.10	8 (33%)	31,54,113	2.98	7 (22%)
17	CLA	9	1041	-	24,32,73	2.09	6 (25%)	31,54,113	3.02	7 (22%)
17	CLA	B	1238	-	24,32,73	1.97	7 (29%)	31,54,113	2.79	8 (25%)
17	CLA	A	1106	-	24,32,73	1.96	6 (25%)	31,54,113	2.90	7 (22%)
17	CLA	P	5402	-	24,32,73	2.28	7 (29%)	31,54,113	3.06	6 (19%)
17	CLA	3	1021	-	24,32,73	2.09	6 (25%)	31,54,113	3.02	7 (22%)
17	CLA	A	1116	-	24,32,73	2.16	7 (29%)	31,54,113	2.98	7 (22%)
17	CLA	2	1015	-	24,32,73	2.08	6 (25%)	31,54,113	3.03	7 (22%)
17	CLA	2	1013	-	24,32,73	2.08	6 (25%)	31,54,113	3.03	7 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
17	CLA	6	5502	-	24,32,73	2.12	7 (29%)	31,54,113	2.90	8 (25%)
17	CLA	2	1014	-	24,32,73	2.07	6 (25%)	31,54,113	3.03	8 (25%)
17	CLA	4	1014	-	24,32,73	2.07	6 (25%)	31,54,113	3.03	7 (22%)
17	CLA	L	1504	-	24,32,73	2.08	6 (25%)	31,54,113	3.03	7 (22%)
17	CLA	B	1218	-	24,32,73	2.16	7 (29%)	31,54,113	3.04	9 (29%)
17	CLA	P	5104	-	24,32,73	2.24	9 (37%)	31,54,113	2.99	7 (22%)
17	CLA	4	1033	-	24,32,73	2.08	6 (25%)	31,54,113	3.04	7 (22%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	9	1033	-	1/1/4/20	-	-
19	SF4	C	3003	-	-	-	0/6/5/5
17	CLA	4	1031	-	1/1/4/20	-	-
17	CLA	Q	5221	-	1/1/4/20	-	-
17	CLA	V	5701	-	1/1/4/20	-	-
17	CLA	3	1022	-	1/1/4/20	-	-
17	CLA	J	1101	-	1/1/4/20	-	-
17	CLA	Q	5220	-	1/1/4/20	-	-
17	CLA	0	1017	-	1/1/4/20	-	-
17	CLA	P	5901	-	1/1/4/20	-	-
17	CLA	7	1021	-	1/1/4/20	-	-
17	CLA	4	1023	-	1/1/4/20	-	-
17	CLA	B	1241	-	1/1/4/20	-	-
17	CLA	Q	5242	-	1/1/4/20	-	-
17	CLA	3	1033	-	1/1/4/20	-	-
17	CLA	Q	5022	-	1/1/4/20	-	-
17	CLA	A	1132	-	1/1/4/20	-	-
17	CLA	Z	5302	-	1/1/4/20	-	-
17	CLA	2	1026	-	1/1/4/20	-	-
17	CLA	9	1032	-	1/1/4/20	-	-
17	CLA	7	1012	-	1/1/4/20	-	-
17	CLA	6	5503	-	1/1/4/20	-	-
17	CLA	Q	5204	-	1/1/4/20	-	-
17	CLA	7	1026	-	1/1/4/20	-	-
19	SF4	A	3001	-	-	-	0/6/5/5
17	CLA	Q	5231	-	1/1/4/20	-	-
17	CLA	A	1129	-	1/1/4/20	-	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	A	1138	-	1/1/4/20	-	-
17	CLA	8	1031	-	1/1/4/20	-	-
17	CLA	4	4002	-	1/1/4/20	-	-
17	CLA	Q	5211	-	1/1/4/20	-	-
17	CLA	7	1022	-	1/1/4/20	-	-
17	CLA	3	1016	-	1/1/4/20	-	-
17	CLA	A	4009	-	1/1/4/20	-	-
17	CLA	K	1404	-	1/1/4/20	-	-
17	CLA	P	5139	-	1/1/4/20	-	-
17	CLA	K	1403	-	1/1/4/20	-	-
17	CLA	9	1012	-	1/1/4/20	-	-
17	CLA	9	1025	-	1/1/4/20	-	-
17	CLA	4	1032	-	1/1/4/20	-	-
17	CLA	U	5229	-	1/1/4/20	-	-
17	CLA	Q	5234	-	1/1/4/20	-	-
17	CLA	B	1021	-	1/1/4/20	-	-
17	CLA	B	4001	-	1/1/4/20	-	-
17	CLA	0	1032	-	1/1/4/20	-	-
17	CLA	2	1022	-	1/1/4/20	-	-
17	CLA	4	1011	-	1/1/4/20	-	-
17	CLA	A	1114	-	1/1/4/20	-	-
17	CLA	Q	5202	-	1/1/4/20	-	-
17	CLA	2	1017	-	1/1/4/20	-	-
17	CLA	1	1025	-	1/1/4/20	-	-
17	CLA	P	5102	-	1/1/4/20	-	-
17	CLA	Q	5212	-	1/1/4/20	-	-
17	CLA	1	1013	-	1/1/4/20	-	-
17	CLA	1	1031	-	1/1/4/20	-	-
17	CLA	P	5131	-	1/1/4/20	-	-
17	CLA	0	1022	-	1/1/4/20	-	-
17	CLA	1	1014	-	1/1/4/20	-	-
17	CLA	7	1013	-	1/1/4/20	-	-
17	CLA	W	5801	-	1/1/4/20	-	-
17	CLA	8	1033	-	1/1/4/20	-	-
17	CLA	J	1302	-	1/1/4/20	-	-
17	CLA	P	5125	-	1/1/4/20	-	-
17	CLA	5	5401	-	1/1/4/20	-	-
17	CLA	7	1017	-	1/1/4/20	-	-
17	CLA	A	1133	-	1/1/4/20	-	-
17	CLA	P	8009	-	1/1/4/20	-	-
17	CLA	7	1031	-	1/1/4/20	-	-
17	CLA	Q	5236	-	1/1/4/20	-	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	B	1211	-	1/1/4/20	-	-
17	CLA	V	5233	-	1/1/4/20	-	-
17	CLA	A	1108	-	1/1/4/20	-	-
17	CLA	A	1012	-	1/1/4/20	-	-
17	CLA	9	1021	-	1/1/4/20	-	-
17	CLA	B	1236	-	1/1/4/20	-	-
17	CLA	9	1031	-	1/1/4/20	-	-
17	CLA	Q	8001	-	1/1/4/20	-	-
17	CLA	A	1125	-	1/1/4/20	-	-
17	CLA	7	1015	-	1/1/4/20	-	-
17	CLA	3	1015	-	1/1/4/20	-	-
17	CLA	P	8010	-	1/1/4/20	-	-
17	CLA	A	1102	-	1/1/4/20	-	-
17	CLA	B	1237	-	1/1/4/20	-	-
17	CLA	B	1217	-	1/1/4/20	-	-
18	PQN	P	6001	-	-	-	0/2/2/2
17	CLA	4	1017	-	1/1/4/20	-	-
18	PQN	Q	6002	-	-	-	0/2/2/2
17	CLA	2	1033	-	1/1/4/20	-	-
17	CLA	P	5123	-	1/1/4/20	-	-
17	CLA	A	1118	-	1/1/4/20	-	-
17	CLA	A	1013	-	1/1/4/20	-	-
17	CLA	A	1120	-	1/1/4/20	-	-
17	CLA	P	5012	-	1/1/4/20	-	-
17	CLA	0	1016	-	1/1/4/20	-	-
17	CLA	4	1026	-	1/1/4/20	-	-
17	CLA	B	1224	-	1/1/4/20	-	-
17	CLA	P	5133	-	1/1/4/20	-	-
17	CLA	A	1105	-	1/1/4/20	-	-
17	CLA	P	5137	-	1/1/4/20	-	-
17	CLA	B	1215	-	1/1/4/20	-	-
17	CLA	Q	5216	-	1/1/4/20	-	-
17	CLA	B	1204	-	1/1/4/20	-	-
17	CLA	A	1104	-	1/1/4/20	-	-
17	CLA	B	1130	-	1/1/4/20	-	-
17	CLA	P	5117	-	1/1/4/20	-	-
17	CLA	G	1233	-	1/1/4/20	-	-
17	CLA	8	1025	-	1/1/4/20	-	-
17	CLA	2	1023	-	1/1/4/20	-	-
17	CLA	7	1011	-	1/1/4/20	-	-
17	CLA	A	1113	-	1/1/4/20	-	-
17	CLA	K	1401	-	1/1/4/20	-	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	6	5501	-	1/1/4/20	-	-
17	CLA	B	1239	-	1/1/4/20	-	-
17	CLA	B	1201	-	1/1/4/20	-	-
17	CLA	A	1103	-	1/1/4/20	-	-
17	CLA	8	1014	-	1/1/4/20	-	-
17	CLA	Q	5225	-	1/1/4/20	-	-
17	CLA	9	1026	-	1/1/4/20	-	-
17	CLA	3	1041	-	1/1/4/20	-	-
17	CLA	P	5126	-	1/1/4/20	-	-
17	CLA	L	1503	-	1/1/4/20	-	-
17	CLA	8	1021	-	1/1/4/20	-	-
17	CLA	0	1012	-	1/1/4/20	-	-
17	CLA	4	1021	-	1/1/4/20	-	-
17	CLA	9	1014	-	1/1/4/20	-	-
17	CLA	A	1123	-	1/1/4/20	-	-
17	CLA	P	5140	-	1/1/4/20	-	-
17	CLA	A	1110	-	1/1/4/20	-	-
17	CLA	8	1012	-	1/1/4/20	-	-
19	SF4	R	7003	-	-	-	0/6/5/5
17	CLA	P	5121	-	1/1/4/20	-	-
17	CLA	P	5122	-	1/1/4/20	-	-
17	CLA	A	1121	-	1/1/4/20	-	-
17	CLA	7	1023	-	1/1/4/20	-	-
17	CLA	1	1022	-	1/1/4/20	-	-
17	CLA	4	1016	-	1/1/4/20	-	-
17	CLA	1	1015	-	1/1/4/20	-	-
17	CLA	P	5109	-	1/1/4/20	-	-
17	CLA	B	1228	-	1/1/4/20	-	-
17	CLA	A	1901	-	1/1/4/20	-	-
17	CLA	Q	5021	-	1/1/4/20	-	-
17	CLA	2	1021	-	1/1/4/20	-	-
17	CLA	2	4007	-	1/1/4/20	-	-
17	CLA	3	1032	-	1/1/4/20	-	-
17	CLA	P	5106	-	1/1/4/20	-	-
17	CLA	Q	5205	-	1/1/4/20	-	-
17	CLA	A	1119	-	1/1/4/20	-	-
17	CLA	P	5129	-	1/1/4/20	-	-
17	CLA	A	1402	-	1/1/4/20	-	-
17	CLA	B	1205	-	1/1/4/20	-	-
17	CLA	B	1221	-	1/1/4/20	-	-
17	CLA	P	5107	-	1/1/4/20	-	-
17	CLA	P	5114	-	1/1/4/20	-	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	P	5136	-	1/1/4/20	-	-
17	CLA	2	1011	-	1/1/4/20	-	-
17	CLA	P	5127	-	1/1/4/20	-	-
17	CLA	Q	5217	-	1/1/4/20	-	-
17	CLA	8	1013	-	1/1/4/20	-	-
17	CLA	2	1016	-	1/1/4/20	-	-
17	CLA	P	5132	-	1/1/4/20	-	-
17	CLA	Q	5240	-	1/1/4/20	-	-
17	CLA	U	8003	-	1/1/4/20	-	-
17	CLA	Q	5215	-	1/1/4/20	-	-
17	CLA	Q	5213	-	1/1/4/20	-	-
17	CLA	B	1235	-	1/1/4/20	-	-
17	CLA	P	5138	-	1/1/4/20	-	-
17	CLA	A	1109	-	1/1/4/20	-	-
17	CLA	G	1701	-	1/1/4/20	-	-
17	CLA	3	1031	-	1/1/4/20	-	-
17	CLA	A	1127	-	1/1/4/20	-	-
17	CLA	P	5128	-	1/1/4/20	-	-
17	CLA	7	1016	-	1/1/4/20	-	-
17	CLA	B	1223	-	1/1/4/20	-	-
17	CLA	P	5111	-	1/1/4/20	-	-
17	CLA	B	1222	-	1/1/4/20	-	-
17	CLA	A	1140	-	1/1/4/20	-	-
17	CLA	P	5116	-	1/1/4/20	-	-
17	CLA	0	8002	-	1/1/4/20	-	-
17	CLA	B	1219	-	1/1/4/20	-	-
17	CLA	P	5110	-	1/1/4/20	-	-
17	CLA	P	5120	-	1/1/4/20	-	-
17	CLA	1	1026	-	1/1/4/20	-	-
17	CLA	A	1115	-	1/1/4/20	-	-
17	CLA	Q	5228	-	1/1/4/20	-	-
17	CLA	Q	5222	-	1/1/4/20	-	-
17	CLA	B	1214	-	1/1/4/20	-	-
17	CLA	B	1232	-	1/1/4/20	-	-
17	CLA	Q	5207	-	1/1/4/20	-	-
17	CLA	Z	8008	-	1/1/4/20	-	-
17	CLA	Q	5232	-	1/1/4/20	-	-
17	CLA	9	1017	-	1/1/4/20	-	-
17	CLA	1	1023	-	1/1/4/20	-	-
17	CLA	B	1242	-	1/1/4/20	-	-
17	CLA	0	1014	-	1/1/4/20	-	-
17	CLA	Q	5239	-	1/1/4/20	-	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	P	5011	-	1/1/4/20	-	-
17	CLA	U	8004	-	1/1/4/20	-	-
17	CLA	A	1131	-	1/1/4/20	-	-
17	CLA	A	1112	-	1/1/4/20	-	-
17	CLA	0	1023	-	1/1/4/20	-	-
17	CLA	8	1022	-	1/1/4/20	-	-
17	CLA	Z	5101	-	1/1/4/20	-	-
17	CLA	Q	5209	-	1/1/4/20	-	-
17	CLA	8	1023	-	1/1/4/20	-	-
17	CLA	Q	5203	-	1/1/4/20	-	-
17	CLA	0	1013	-	1/1/4/20	-	-
17	CLA	B	1227	-	1/1/4/20	-	-
17	CLA	A	1107	-	1/1/4/20	-	-
17	CLA	A	1122	-	1/1/4/20	-	-
17	CLA	B	1234	-	1/1/4/20	-	-
17	CLA	B	1231	-	1/1/4/20	-	-
17	CLA	9	1022	-	1/1/4/20	-	-
17	CLA	B	1022	-	1/1/4/20	-	-
17	CLA	B	1226	-	1/1/4/20	-	-
17	CLA	Q	5130	-	1/1/4/20	-	-
17	CLA	Q	5223	-	1/1/4/20	-	-
17	CLA	U	8006	-	1/1/4/20	-	-
17	CLA	P	5134	-	1/1/4/20	-	-
17	CLA	Q	5226	-	1/1/4/20	-	-
17	CLA	Q	5227	-	1/1/4/20	-	-
17	CLA	Q	5206	-	1/1/4/20	-	-
17	CLA	B	1240	-	1/1/4/20	-	-
17	CLA	F	4006	-	1/1/4/20	-	-
17	CLA	0	1021	-	1/1/4/20	-	-
17	CLA	0	1031	-	1/1/4/20	-	-
17	CLA	B	1023	-	1/1/4/20	-	-
17	CLA	B	1216	-	1/1/4/20	-	-
17	CLA	Q	5208	-	1/1/4/20	-	-
17	CLA	A	4010	-	1/1/4/20	-	-
17	CLA	B	1212	-	1/1/4/20	-	-
17	CLA	8	1015	-	1/1/4/20	-	-
18	PQN	A	2001	-	-	-	0/2/2/2
17	CLA	1	1011	-	1/1/4/20	-	-
17	CLA	P	5115	-	1/1/4/20	-	-
17	CLA	Q	5023	-	1/1/4/20	-	-
17	CLA	A	1126	-	1/1/4/20	-	-
17	CLA	B	1210	-	1/1/4/20	-	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	SF4	C	3002	-	-	-	0/6/5/5
17	CLA	8	1016	-	1/1/4/20	-	-
17	CLA	B	1220	-	1/1/4/20	-	-
17	CLA	3	1025	-	1/1/4/20	-	-
17	CLA	Q	5224	-	1/1/4/20	-	-
17	CLA	B	1225	-	1/1/4/20	-	-
17	CLA	P	5135	-	1/1/4/20	-	-
17	CLA	8	1026	-	1/1/4/20	-	-
17	CLA	3	1014	-	1/1/4/20	-	-
17	CLA	0	1025	-	1/1/4/20	-	-
17	CLA	U	8005	-	1/1/4/20	-	-
17	CLA	A	1124	-	1/1/4/20	-	-
17	CLA	7	1025	-	1/1/4/20	-	-
17	CLA	9	1016	-	1/1/4/20	-	-
17	CLA	B	1208	-	1/1/4/20	-	-
17	CLA	A	1134	-	1/1/4/20	-	-
17	CLA	P	5112	-	1/1/4/20	-	-
17	CLA	P	5113	-	1/1/4/20	-	-
17	CLA	8	1011	-	1/1/4/20	-	-
17	CLA	F	1301	-	1/1/4/20	-	-
17	CLA	2	1012	-	1/1/4/20	-	-
17	CLA	3	1012	-	1/1/4/20	-	-
19	SF4	R	7002	-	-	-	0/6/5/5
17	CLA	F	1229	-	1/1/4/20	-	-
17	CLA	P	5108	-	1/1/4/20	-	-
17	CLA	3	1026	-	1/1/4/20	-	-
17	CLA	A	1135	-	1/1/4/20	-	-
17	CLA	P	5124	-	1/1/4/20	-	-
17	CLA	2	1031	-	1/1/4/20	-	-
17	CLA	F	4004	-	1/1/4/20	-	-
17	CLA	F	4003	-	1/1/4/20	-	-
17	CLA	0	1033	-	1/1/4/20	-	-
17	CLA	1	1017	-	1/1/4/20	-	-
17	CLA	4	1025	-	1/1/4/20	-	-
17	CLA	B	1203	-	1/1/4/20	-	-
17	CLA	B	1230	-	1/1/4/20	-	-
17	CLA	Q	5241	-	1/1/4/20	-	-
17	CLA	Q	5219	-	1/1/4/20	-	-
17	CLA	7	1014	-	1/1/4/20	-	-
17	CLA	Q	5214	-	1/1/4/20	-	-
17	CLA	5	5403	-	1/1/4/20	-	-
17	CLA	Q	5218	-	1/1/4/20	-	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	0	1015	-	1/1/4/20	-	-
17	CLA	9	1015	-	1/1/4/20	-	-
17	CLA	P	5118	-	1/1/4/20	-	-
17	CLA	B	1213	-	1/1/4/20	-	-
17	CLA	4	1012	-	1/1/4/20	-	-
17	CLA	F	4005	-	1/1/4/20	-	-
18	PQN	B	2002	-	-	-	0/2/2/2
17	CLA	L	1501	-	1/1/4/20	-	-
17	CLA	A	1128	-	1/1/4/20	-	-
17	CLA	B	1202	-	1/1/4/20	-	-
17	CLA	2	1025	-	1/1/4/20	-	-
17	CLA	J	4008	-	1/1/4/20	-	-
17	CLA	8	1017	-	1/1/4/20	-	-
17	CLA	B	1207	-	1/1/4/20	-	-
17	CLA	P	5103	-	1/1/4/20	-	-
17	CLA	P	5013	-	1/1/4/20	-	-
17	CLA	B	1206	-	1/1/4/20	-	-
17	CLA	3	1011	-	1/1/4/20	-	-
17	CLA	1	1021	-	1/1/4/20	-	-
17	CLA	U	5301	-	1/1/4/20	-	-
17	CLA	0	1011	-	1/1/4/20	-	-
17	CLA	A	1137	-	1/1/4/20	-	-
17	CLA	9	1011	-	1/1/4/20	-	-
17	CLA	8	8007	-	1/1/4/20	-	-
17	CLA	H	1801	-	1/1/4/20	-	-
17	CLA	A	1117	-	1/1/4/20	-	-
17	CLA	Q	5210	-	1/1/4/20	-	-
17	CLA	3	1017	-	1/1/4/20	-	-
17	CLA	P	5119	-	1/1/4/20	-	-
17	CLA	A	1139	-	1/1/4/20	-	-
17	CLA	Q	5238	-	1/1/4/20	-	-
17	CLA	6	5504	-	1/1/4/20	-	-
17	CLA	1	1016	-	1/1/4/20	-	-
17	CLA	4	1013	-	1/1/4/20	-	-
17	CLA	A	1136	-	1/1/4/20	-	-
17	CLA	A	1111	-	1/1/4/20	-	-
17	CLA	A	1011	-	1/1/4/20	-	-
17	CLA	Q	5230	-	1/1/4/20	-	-
19	SF4	P	7001	-	-	-	0/6/5/5
17	CLA	4	1022	-	1/1/4/20	-	-
17	CLA	1	1012	-	1/1/4/20	-	-
17	CLA	Q	5237	-	1/1/4/20	-	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	4	1015	-	1/1/4/20	-	-
17	CLA	0	1026	-	1/1/4/20	-	-
17	CLA	5	5404	-	1/1/4/20	-	-
17	CLA	P	5105	-	1/1/4/20	-	-
17	CLA	Q	5201	-	1/1/4/20	-	-
17	CLA	Q	5235	-	1/1/4/20	-	-
17	CLA	B	1209	-	1/1/4/20	-	-
17	CLA	9	1041	-	1/1/4/20	-	-
17	CLA	B	1238	-	1/1/4/20	-	-
17	CLA	A	1106	-	1/1/4/20	-	-
17	CLA	P	5402	-	1/1/4/20	-	-
17	CLA	3	1021	-	1/1/4/20	-	-
17	CLA	A	1116	-	1/1/4/20	-	-
17	CLA	2	1015	-	1/1/4/20	-	-
17	CLA	2	1013	-	1/1/4/20	-	-
17	CLA	2	1014	-	1/1/4/20	-	-
17	CLA	4	1014	-	1/1/4/20	-	-
17	CLA	L	1504	-	1/1/4/20	-	-
17	CLA	B	1218	-	1/1/4/20	-	-
17	CLA	P	5104	-	1/1/4/20	-	-
17	CLA	4	1033	-	1/1/4/20	-	-

All (2320) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	2001	PQN	O1-C1	9.05	1.42	1.23
18	P	6001	PQN	O1-C1	9.02	1.42	1.23
17	1	1021	CLA	MG-NA	8.83	2.27	2.06
17	7	1021	CLA	MG-NA	8.79	2.27	2.06
18	Q	6002	PQN	O1-C1	8.59	1.41	1.23
18	A	2001	PQN	O4-C4	8.56	1.42	1.24
18	B	2002	PQN	O1-C1	8.56	1.41	1.23
18	P	6001	PQN	O4-C4	8.56	1.42	1.24
18	Q	6002	PQN	O4-C4	8.26	1.42	1.24
18	B	2002	PQN	O4-C4	8.26	1.42	1.24
17	A	1137	CLA	MG-NA	7.45	2.24	2.06
17	P	5137	CLA	MG-NA	7.45	2.24	2.06
17	P	5123	CLA	MG-NA	7.41	2.23	2.06
17	A	1123	CLA	MG-NA	7.40	2.23	2.06
17	Z	5302	CLA	MG-NA	7.27	2.23	2.06
17	J	1302	CLA	MG-NA	7.25	2.23	2.06
17	B	1221	CLA	MG-NA	7.17	2.23	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	Q	5221	CLA	MG-NA	7.17	2.23	2.06
17	A	1108	CLA	MG-NA	7.16	2.23	2.06
17	P	5108	CLA	MG-NA	7.15	2.23	2.06
17	Q	5210	CLA	MG-NA	7.09	2.23	2.06
17	B	1210	CLA	MG-NA	7.06	2.23	2.06
17	A	1901	CLA	MG-NA	6.91	2.22	2.06
17	P	5901	CLA	MG-NA	6.89	2.22	2.06
17	P	5012	CLA	MG-NA	6.88	2.22	2.06
17	A	1012	CLA	MG-NA	6.87	2.22	2.06
17	Q	5207	CLA	MG-NA	6.76	2.22	2.06
17	B	1207	CLA	MG-NA	6.74	2.22	2.06
17	6	5501	CLA	MG-NA	6.73	2.22	2.06
17	Q	5206	CLA	MG-NA	6.72	2.22	2.06
17	B	1206	CLA	MG-NA	6.71	2.22	2.06
17	L	1501	CLA	MG-NA	6.70	2.22	2.06
17	A	1113	CLA	MG-NA	6.67	2.22	2.06
17	P	5113	CLA	MG-NA	6.66	2.22	2.06
17	P	5402	CLA	MG-NA	6.63	2.22	2.06
17	A	1402	CLA	MG-NA	6.62	2.22	2.06
17	P	5131	CLA	MG-NA	6.58	2.21	2.06
17	A	1131	CLA	MG-NA	6.57	2.21	2.06
17	B	1219	CLA	MG-NA	6.55	2.21	2.06
17	Q	5219	CLA	MG-NA	6.54	2.21	2.06
17	B	1234	CLA	MG-NA	6.51	2.21	2.06
17	Q	5234	CLA	MG-NA	6.51	2.21	2.06
17	P	5126	CLA	MG-NA	6.51	2.21	2.06
17	A	1126	CLA	MG-NA	6.49	2.21	2.06
17	Q	5225	CLA	MG-NA	6.49	2.21	2.06
17	B	1225	CLA	MG-NA	6.45	2.21	2.06
17	B	1224	CLA	MG-NA	6.44	2.21	2.06
17	A	1112	CLA	MG-NA	6.44	2.21	2.06
17	Q	5224	CLA	MG-NA	6.43	2.21	2.06
17	P	5112	CLA	MG-NA	6.42	2.21	2.06
17	P	5127	CLA	MG-NA	6.39	2.21	2.06
17	B	1232	CLA	MG-NA	6.37	2.21	2.06
17	A	1121	CLA	MG-NA	6.37	2.21	2.06
17	A	1127	CLA	MG-NA	6.37	2.21	2.06
17	A	1135	CLA	MG-NA	6.36	2.21	2.06
17	P	5135	CLA	MG-NA	6.36	2.21	2.06
17	Q	5232	CLA	MG-NA	6.36	2.21	2.06
17	B	1238	CLA	MG-NA	6.35	2.21	2.06
17	B	1236	CLA	MG-NA	6.35	2.21	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	P	5121	CLA	MG-NA	6.35	2.21	2.06
17	Q	5236	CLA	MG-NA	6.35	2.21	2.06
17	Q	5238	CLA	MG-NA	6.35	2.21	2.06
17	B	1213	CLA	MG-NA	6.29	2.21	2.06
17	P	5128	CLA	MG-NA	6.28	2.21	2.06
17	Q	5213	CLA	MG-NA	6.28	2.21	2.06
17	A	1115	CLA	MG-NA	6.27	2.21	2.06
17	Q	5220	CLA	MG-NA	6.27	2.21	2.06
17	P	5115	CLA	MG-NA	6.26	2.21	2.06
17	B	1220	CLA	MG-NA	6.26	2.21	2.06
17	A	1128	CLA	MG-NA	6.26	2.21	2.06
17	P	5116	CLA	MG-NA	6.23	2.21	2.06
17	A	1116	CLA	MG-NA	6.23	2.21	2.06
17	Q	5223	CLA	MG-NA	6.22	2.21	2.06
17	B	1223	CLA	MG-NA	6.22	2.21	2.06
17	A	1011	CLA	MG-NA	6.20	2.21	2.06
17	P	5011	CLA	MG-NA	6.20	2.21	2.06
17	7	1021	CLA	MG-NB	6.20	2.18	2.05
17	1	1021	CLA	MG-NB	6.17	2.18	2.05
17	Q	5202	CLA	MG-NA	6.15	2.20	2.06
17	P	5105	CLA	MG-NA	6.14	2.20	2.06
17	B	1202	CLA	MG-NA	6.14	2.20	2.06
17	P	5139	CLA	MG-NA	6.14	2.20	2.06
17	A	1139	CLA	MG-NA	6.13	2.20	2.06
17	Q	5021	CLA	MG-NA	6.13	2.20	2.06
17	A	1105	CLA	MG-NA	6.13	2.20	2.06
17	B	1021	CLA	MG-NA	6.12	2.20	2.06
17	B	1203	CLA	MG-NA	6.11	2.20	2.06
17	Q	5203	CLA	MG-NA	6.10	2.20	2.06
17	Q	5226	CLA	MG-NA	6.07	2.20	2.06
17	P	5102	CLA	MG-NA	6.05	2.20	2.06
17	A	1102	CLA	MG-NA	6.05	2.20	2.06
17	B	1226	CLA	MG-NA	6.03	2.20	2.06
17	A	1104	CLA	MG-NA	6.03	2.20	2.06
17	P	5104	CLA	MG-NA	6.00	2.20	2.06
17	7	1013	CLA	MG-NA	6.00	2.20	2.06
17	9	1011	CLA	MG-NA	6.00	2.20	2.06
17	6	5503	CLA	MG-NA	5.99	2.20	2.06
17	3	1025	CLA	MG-NA	5.99	2.20	2.06
17	3	1032	CLA	MG-NA	5.99	2.20	2.06
17	3	1011	CLA	MG-NA	5.99	2.20	2.06
17	Q	5212	CLA	MG-NA	5.99	2.20	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	L	1503	CLA	MG-NA	5.99	2.20	2.06
17	7	1011	CLA	MG-NA	5.99	2.20	2.06
17	0	1015	CLA	MG-NA	5.99	2.20	2.06
17	1	1013	CLA	MG-NA	5.98	2.20	2.06
17	0	1032	CLA	MG-NA	5.98	2.20	2.06
17	9	1032	CLA	MG-NA	5.97	2.20	2.06
17	2	1025	CLA	MG-NA	5.97	2.20	2.06
17	4	1032	CLA	MG-NA	5.97	2.20	2.06
17	1	1011	CLA	MG-NA	5.97	2.20	2.06
17	8	1026	CLA	MG-NA	5.97	2.20	2.06
17	8	1033	CLA	MG-NA	5.97	2.20	2.06
17	8	8007	CLA	MG-NA	5.97	2.20	2.06
17	8	1016	CLA	MG-NA	5.97	2.20	2.06
17	B	1212	CLA	MG-NA	5.97	2.20	2.06
17	4	1015	CLA	MG-NA	5.97	2.20	2.06
17	9	1033	CLA	MG-NA	5.97	2.20	2.06
17	8	1025	CLA	MG-NA	5.97	2.20	2.06
17	0	8002	CLA	MG-NA	5.97	2.20	2.06
17	9	1025	CLA	MG-NA	5.97	2.20	2.06
17	0	1012	CLA	MG-NA	5.96	2.20	2.06
17	3	1022	CLA	MG-NA	5.96	2.20	2.06
17	9	1031	CLA	MG-NA	5.96	2.20	2.06
17	2	1026	CLA	MG-NA	5.96	2.20	2.06
17	9	1022	CLA	MG-NA	5.96	2.20	2.06
17	1	1031	CLA	MG-NA	5.96	2.20	2.06
17	0	1031	CLA	MG-NA	5.96	2.20	2.06
17	2	1022	CLA	MG-NA	5.96	2.20	2.06
17	K	1401	CLA	MG-NA	5.96	2.20	2.06
17	9	1012	CLA	MG-NA	5.96	2.20	2.06
17	8	1022	CLA	MG-NA	5.96	2.20	2.06
17	4	1012	CLA	MG-NA	5.96	2.20	2.06
17	8	1014	CLA	MG-NA	5.96	2.20	2.06
17	2	1033	CLA	MG-NA	5.96	2.20	2.06
17	4	1031	CLA	MG-NA	5.96	2.20	2.06
17	9	1017	CLA	MG-NA	5.96	2.20	2.06
17	2	1016	CLA	MG-NA	5.96	2.20	2.06
17	Z	5101	CLA	MG-NA	5.96	2.20	2.06
17	4	4002	CLA	MG-NA	5.96	2.20	2.06
17	B	1242	CLA	MG-NA	5.95	2.20	2.06
17	8	1031	CLA	MG-NA	5.95	2.20	2.06
17	0	1011	CLA	MG-NA	5.95	2.20	2.06
17	1	1022	CLA	MG-NA	5.95	2.20	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	2	4007	CLA	MG-NA	5.95	2.20	2.06
17	5	5401	CLA	MG-NA	5.95	2.20	2.06
17	7	1031	CLA	MG-NA	5.95	2.20	2.06
17	3	1015	CLA	MG-NA	5.95	2.20	2.06
17	7	1015	CLA	MG-NA	5.95	2.20	2.06
17	3	1012	CLA	MG-NA	5.95	2.20	2.06
17	4	1011	CLA	MG-NA	5.95	2.20	2.06
17	F	4006	CLA	MG-NA	5.95	2.20	2.06
17	6	5504	CLA	MG-NA	5.95	2.20	2.06
17	W	5801	CLA	MG-NA	5.95	2.20	2.06
17	3	1033	CLA	MG-NA	5.95	2.20	2.06
17	A	4009	CLA	MG-NA	5.95	2.20	2.06
17	3	1031	CLA	MG-NA	5.95	2.20	2.06
17	1	1014	CLA	MG-NA	5.94	2.20	2.06
17	1	1026	CLA	MG-NA	5.94	2.20	2.06
17	1	1015	CLA	MG-NA	5.94	2.20	2.06
17	U	8006	CLA	MG-NA	5.94	2.20	2.06
17	5	5403	CLA	MG-NA	5.94	2.20	2.06
17	G	1701	CLA	MG-NA	5.94	2.20	2.06
17	9	1015	CLA	MG-NA	5.94	2.20	2.06
17	2	1011	CLA	MG-NA	5.94	2.20	2.06
17	4	1033	CLA	MG-NA	5.94	2.20	2.06
17	0	1023	CLA	MG-NA	5.94	2.20	2.06
17	3	1017	CLA	MG-NA	5.94	2.20	2.06
17	V	5701	CLA	MG-NA	5.94	2.20	2.06
17	1	1017	CLA	MG-NA	5.93	2.20	2.06
17	2	1017	CLA	MG-NA	5.93	2.20	2.06
17	P	8009	CLA	MG-NA	5.93	2.20	2.06
17	7	1016	CLA	MG-NA	5.93	2.20	2.06
17	Q	5241	CLA	MG-NA	5.93	2.20	2.06
17	U	8005	CLA	MG-NA	5.93	2.20	2.06
17	J	1101	CLA	MG-NA	5.93	2.20	2.06
17	3	1014	CLA	MG-NA	5.93	2.20	2.06
17	3	1021	CLA	MG-NA	5.93	2.20	2.06
17	4	1022	CLA	MG-NA	5.93	2.20	2.06
17	0	1022	CLA	MG-NA	5.93	2.20	2.06
17	4	1023	CLA	MG-NA	5.93	2.20	2.06
17	U	8004	CLA	MG-NA	5.93	2.20	2.06
17	A	4010	CLA	MG-NA	5.93	2.20	2.06
17	2	1031	CLA	MG-NA	5.93	2.20	2.06
17	L	1504	CLA	MG-NA	5.93	2.20	2.06
17	5	5404	CLA	MG-NA	5.93	2.20	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	F	4005	CLA	MG-NA	5.93	2.20	2.06
17	Q	5240	CLA	MG-NA	5.93	2.20	2.06
17	9	1026	CLA	MG-NA	5.93	2.20	2.06
17	9	1021	CLA	MG-NA	5.93	2.20	2.06
17	1	1012	CLA	MG-NA	5.93	2.20	2.06
17	B	1240	CLA	MG-NA	5.93	2.20	2.06
17	J	4008	CLA	MG-NA	5.93	2.20	2.06
17	K	1404	CLA	MG-NA	5.93	2.20	2.06
17	3	1026	CLA	MG-NA	5.93	2.20	2.06
17	H	1801	CLA	MG-NA	5.93	2.20	2.06
17	7	1022	CLA	MG-NA	5.93	2.20	2.06
17	8	1013	CLA	MG-NA	5.93	2.20	2.06
17	K	1403	CLA	MG-NA	5.93	2.20	2.06
17	2	1014	CLA	MG-NA	5.93	2.20	2.06
17	F	4003	CLA	MG-NA	5.92	2.20	2.06
17	0	1026	CLA	MG-NA	5.92	2.20	2.06
17	8	1011	CLA	MG-NA	5.92	2.20	2.06
17	9	1016	CLA	MG-NA	5.92	2.20	2.06
17	B	1241	CLA	MG-NA	5.92	2.20	2.06
17	P	8010	CLA	MG-NA	5.92	2.20	2.06
17	7	1017	CLA	MG-NA	5.92	2.20	2.06
17	8	1012	CLA	MG-NA	5.92	2.20	2.06
17	B	4001	CLA	MG-NA	5.92	2.20	2.06
17	7	1012	CLA	MG-NA	5.92	2.20	2.06
17	1	1016	CLA	MG-NA	5.92	2.20	2.06
17	1	1023	CLA	MG-NA	5.92	2.20	2.06
17	F	4004	CLA	MG-NA	5.92	2.20	2.06
17	Q	5242	CLA	MG-NA	5.92	2.20	2.06
17	8	1021	CLA	MG-NA	5.92	2.20	2.06
17	4	1017	CLA	MG-NA	5.92	2.20	2.06
17	Q	8001	CLA	MG-NA	5.92	2.20	2.06
17	2	1012	CLA	MG-NA	5.91	2.20	2.06
17	7	1026	CLA	MG-NA	5.91	2.20	2.06
17	7	1014	CLA	MG-NA	5.91	2.20	2.06
17	2	1013	CLA	MG-NA	5.91	2.20	2.06
17	0	1033	CLA	MG-NA	5.91	2.20	2.06
17	4	1026	CLA	MG-NA	5.91	2.20	2.06
17	8	1017	CLA	MG-NA	5.91	2.20	2.06
17	P	5114	CLA	MG-NA	5.91	2.20	2.06
17	3	1041	CLA	MG-NA	5.91	2.20	2.06
17	Z	8008	CLA	MG-NA	5.90	2.20	2.06
17	3	1016	CLA	MG-NA	5.90	2.20	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	U	8003	CLA	MG-NA	5.90	2.20	2.06
17	2	1021	CLA	MG-NA	5.90	2.20	2.06
17	2	1023	CLA	MG-NA	5.90	2.20	2.06
17	7	1023	CLA	MG-NA	5.90	2.20	2.06
17	1	1025	CLA	MG-NA	5.90	2.20	2.06
17	9	1014	CLA	MG-NA	5.89	2.20	2.06
17	9	1041	CLA	MG-NA	5.89	2.20	2.06
17	A	1114	CLA	MG-NA	5.89	2.20	2.06
17	4	1014	CLA	MG-NA	5.89	2.20	2.06
17	4	1013	CLA	MG-NA	5.89	2.20	2.06
17	0	1014	CLA	MG-NA	5.88	2.20	2.06
17	2	1015	CLA	MG-NA	5.88	2.20	2.06
17	0	1016	CLA	MG-NA	5.88	2.20	2.06
17	0	1017	CLA	MG-NA	5.88	2.20	2.06
17	0	1021	CLA	MG-NA	5.88	2.20	2.06
17	7	1025	CLA	MG-NA	5.88	2.20	2.06
17	4	1021	CLA	MG-NA	5.87	2.20	2.06
17	0	1013	CLA	MG-NA	5.87	2.20	2.06
17	8	1015	CLA	MG-NA	5.87	2.20	2.06
17	8	1023	CLA	MG-NA	5.87	2.20	2.06
17	4	1016	CLA	MG-NA	5.86	2.20	2.06
17	4	1025	CLA	MG-NA	5.86	2.20	2.06
17	Q	5022	CLA	MG-NA	5.84	2.20	2.06
17	0	1025	CLA	MG-NA	5.84	2.20	2.06
17	G	1233	CLA	MG-NA	5.83	2.20	2.06
17	B	1022	CLA	MG-NA	5.83	2.20	2.06
17	Q	5208	CLA	MG-NA	5.82	2.20	2.06
17	P	5117	CLA	MG-NA	5.82	2.20	2.06
17	A	1117	CLA	MG-NA	5.82	2.20	2.06
17	V	5233	CLA	MG-NA	5.81	2.20	2.06
17	U	5301	CLA	MG-NA	5.81	2.20	2.06
17	B	1208	CLA	MG-NA	5.81	2.20	2.06
17	B	1218	CLA	MG-NA	5.80	2.20	2.06
17	F	1301	CLA	MG-NA	5.80	2.20	2.06
17	Q	5216	CLA	MG-NA	5.79	2.20	2.06
18	A	2001	PQN	C2M-C2	-5.78	1.36	1.50
17	B	1216	CLA	MG-NA	5.78	2.20	2.06
18	P	6001	PQN	C2M-C2	-5.78	1.36	1.50
17	B	1211	CLA	MG-NA	5.78	2.20	2.06
17	Q	5218	CLA	MG-NA	5.77	2.20	2.06
17	Q	5211	CLA	MG-NA	5.77	2.20	2.06
17	B	1217	CLA	MG-NA	5.74	2.19	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	A	1125	CLA	MG-NA	5.74	2.19	2.06
17	P	5125	CLA	MG-NA	5.72	2.19	2.06
17	Q	5217	CLA	MG-NA	5.72	2.19	2.06
18	Q	6002	PQN	C3-C2	5.71	1.46	1.35
17	A	1136	CLA	MG-NA	5.70	2.19	2.06
17	P	5136	CLA	MG-NA	5.69	2.19	2.06
18	B	2002	PQN	C3-C2	5.69	1.46	1.35
18	A	2001	PQN	C3-C2	5.68	1.46	1.35
17	Q	5215	CLA	MG-NA	5.68	2.19	2.06
17	B	1215	CLA	MG-NA	5.66	2.19	2.06
18	P	6001	PQN	C3-C2	5.66	1.46	1.35
17	P	5134	CLA	MG-NA	5.63	2.19	2.06
17	P	5111	CLA	MG-NA	5.63	2.19	2.06
17	A	1134	CLA	MG-NA	5.63	2.19	2.06
17	A	1111	CLA	MG-NA	5.61	2.19	2.06
17	A	1120	CLA	MG-NA	5.57	2.19	2.06
17	Q	5209	CLA	MG-NA	5.56	2.19	2.06
17	A	1118	CLA	MG-NA	5.55	2.19	2.06
18	Q	6002	PQN	C2M-C2	-5.55	1.37	1.50
18	B	2002	PQN	C2M-C2	-5.55	1.37	1.50
17	P	5120	CLA	MG-NA	5.55	2.19	2.06
17	B	1209	CLA	MG-NA	5.54	2.19	2.06
17	P	5118	CLA	MG-NA	5.54	2.19	2.06
17	A	1107	CLA	MG-NA	5.51	2.19	2.06
17	P	5107	CLA	MG-NA	5.50	2.19	2.06
17	Q	5201	CLA	MG-NA	5.49	2.19	2.06
17	B	1205	CLA	MG-NA	5.49	2.19	2.06
17	B	1201	CLA	MG-NA	5.49	2.19	2.06
17	Q	5205	CLA	MG-NA	5.46	2.19	2.06
17	A	1122	CLA	MG-NA	5.45	2.19	2.06
17	L	1502	CLA	MG-NA	5.45	2.19	2.06
17	6	5502	CLA	MG-NA	5.45	2.19	2.06
17	P	5122	CLA	MG-NA	5.45	2.19	2.06
17	Q	5227	CLA	MG-NA	5.43	2.19	2.06
17	B	1227	CLA	MG-NA	5.43	2.19	2.06
17	B	1222	CLA	MG-NA	5.40	2.19	2.06
17	Q	5222	CLA	MG-NA	5.39	2.19	2.06
17	Q	5228	CLA	MG-NA	5.35	2.19	2.06
17	A	1119	CLA	MG-NA	5.35	2.19	2.06
17	P	5119	CLA	MG-NA	5.33	2.18	2.06
17	B	1228	CLA	MG-NA	5.33	2.18	2.06
17	P	5109	CLA	MG-NA	5.33	2.18	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	P	5110	CLA	MG-NA	5.33	2.18	2.06
17	A	1110	CLA	MG-NA	5.32	2.18	2.06
17	A	1109	CLA	MG-NA	5.31	2.18	2.06
17	P	5106	CLA	MG-NA	5.29	2.18	2.06
17	P	5133	CLA	MG-NA	5.29	2.18	2.06
17	A	1133	CLA	MG-NA	5.29	2.18	2.06
17	A	1013	CLA	MG-NA	5.28	2.18	2.06
17	A	1106	CLA	MG-NA	5.28	2.18	2.06
17	P	5013	CLA	MG-NA	5.26	2.18	2.06
17	B	1230	CLA	MG-NA	5.24	2.18	2.06
17	Q	5230	CLA	MG-NA	5.23	2.18	2.06
17	B	1214	CLA	MG-NA	5.21	2.18	2.06
17	Q	5214	CLA	MG-NA	5.20	2.18	2.06
17	U	5229	CLA	MG-NA	5.19	2.18	2.06
17	F	1229	CLA	MG-NA	5.17	2.18	2.06
17	Q	5023	CLA	MG-NA	5.17	2.18	2.06
17	A	1140	CLA	MG-NA	5.17	2.18	2.06
17	P	5140	CLA	MG-NA	5.16	2.18	2.06
17	B	1023	CLA	MG-NA	5.16	2.18	2.06
17	B	1231	CLA	MG-NA	5.14	2.18	2.06
17	P	5108	CLA	MG-NB	5.14	2.16	2.05
17	A	1103	CLA	MG-NA	5.12	2.18	2.06
17	P	5103	CLA	MG-NA	5.10	2.18	2.06
17	Q	5231	CLA	MG-NA	5.10	2.18	2.06
17	A	1108	CLA	MG-NB	5.10	2.15	2.05
17	P	5138	CLA	MG-NA	5.08	2.18	2.06
17	A	1138	CLA	MG-NA	5.07	2.18	2.06
17	A	1137	CLA	MG-NC	5.04	2.18	2.06
17	P	5137	CLA	MG-NC	5.04	2.18	2.06
17	J	1302	CLA	MG-NB	5.03	2.15	2.05
17	Z	5302	CLA	MG-NB	5.01	2.15	2.05
17	A	1129	CLA	MG-NA	4.98	2.18	2.06
17	7	1021	CLA	MG-ND	-4.98	1.95	2.05
17	1	1021	CLA	MG-ND	-4.97	1.95	2.05
17	P	5129	CLA	MG-NA	4.96	2.18	2.06
17	P	5132	CLA	MG-NA	4.92	2.18	2.06
17	A	1132	CLA	MG-NA	4.91	2.17	2.06
17	B	1023	CLA	C3B-C4B	4.90	1.50	1.40
17	P	5124	CLA	MG-NA	4.88	2.17	2.06
17	Q	5023	CLA	C3B-C4B	4.88	1.50	1.40
17	Q	5130	CLA	MG-NA	4.85	2.17	2.06
17	Q	5237	CLA	MG-NA	4.85	2.17	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	Q	5239	CLA	MG-NA	4.85	2.17	2.06
17	B	1237	CLA	MG-NA	4.85	2.17	2.06
17	B	1239	CLA	MG-NA	4.84	2.17	2.06
17	A	1124	CLA	MG-NA	4.84	2.17	2.06
17	B	1235	CLA	MG-NA	4.84	2.17	2.06
17	Q	5235	CLA	MG-NA	4.82	2.17	2.06
17	B	1130	CLA	MG-NA	4.82	2.17	2.06
17	A	1113	CLA	MG-NB	4.80	2.15	2.05
17	P	5113	CLA	MG-NB	4.79	2.15	2.05
17	A	1108	CLA	MG-NC	4.67	2.17	2.06
17	B	1210	CLA	MG-NB	4.67	2.15	2.05
17	Q	5210	CLA	MG-NB	4.66	2.15	2.05
17	P	5108	CLA	MG-NC	4.65	2.17	2.06
17	A	1103	CLA	MG-NB	4.65	2.15	2.05
17	P	5103	CLA	MG-NB	4.63	2.15	2.05
17	Q	5219	CLA	MG-NB	4.61	2.14	2.05
17	Q	5204	CLA	MG-NA	4.61	2.17	2.06
17	Q	5203	CLA	MG-NB	4.61	2.14	2.05
17	B	1219	CLA	MG-NB	4.61	2.14	2.05
17	B	1204	CLA	MG-NA	4.61	2.17	2.06
17	B	1203	CLA	MG-NB	4.59	2.14	2.05
17	B	1202	CLA	MG-NB	4.55	2.14	2.05
17	Q	5202	CLA	MG-NB	4.55	2.14	2.05
17	B	1232	CLA	C3B-C4B	4.54	1.49	1.40
17	Q	5232	CLA	C3B-C4B	4.52	1.49	1.40
17	B	1022	CLA	MG-NC	4.52	2.17	2.06
17	P	5128	CLA	MG-NB	4.51	2.14	2.05
17	Q	5022	CLA	MG-NC	4.51	2.17	2.06
17	P	5128	CLA	C3B-C4B	4.50	1.49	1.40
17	A	1128	CLA	C3B-C4B	4.49	1.49	1.40
17	A	1128	CLA	MG-NB	4.46	2.14	2.05
17	Q	5207	CLA	MG-NB	4.43	2.14	2.05
17	B	1207	CLA	MG-NB	4.42	2.14	2.05
17	B	1224	CLA	MG-NC	4.33	2.16	2.06
17	P	5137	CLA	MG-NB	4.32	2.14	2.05
17	Q	5224	CLA	MG-NC	4.31	2.16	2.06
17	A	1137	CLA	MG-NB	4.30	2.14	2.05
17	Q	5212	CLA	C3B-C4B	4.29	1.49	1.40
17	B	1212	CLA	C3B-C4B	4.27	1.49	1.40
17	P	5136	CLA	C3B-C4B	4.25	1.49	1.40
17	A	1136	CLA	C3B-C4B	4.25	1.49	1.40
17	P	5115	CLA	C3B-C4B	4.24	1.49	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	P	5112	CLA	C3B-C4B	4.24	1.49	1.40
17	A	1115	CLA	C3B-C4B	4.24	1.49	1.40
17	A	1112	CLA	C3B-C4B	4.23	1.49	1.40
17	A	1135	CLA	MG-NB	4.22	2.14	2.05
17	B	1223	CLA	MG-NB	4.21	2.14	2.05
17	Q	5022	CLA	C3B-C4B	4.20	1.49	1.40
17	B	1022	CLA	C3B-C4B	4.20	1.49	1.40
17	P	5118	CLA	C3B-C4B	4.20	1.49	1.40
17	A	1118	CLA	C3B-C4B	4.20	1.49	1.40
17	2	1017	CLA	C3B-C4B	4.19	1.49	1.40
17	P	5135	CLA	MG-NB	4.19	2.14	2.05
17	Q	5223	CLA	MG-NB	4.18	2.14	2.05
17	0	1016	CLA	C3B-C4B	4.17	1.49	1.40
17	P	5125	CLA	C3B-C4B	4.17	1.49	1.40
17	8	1025	CLA	C3B-C4B	4.17	1.49	1.40
17	U	8005	CLA	C3B-C4B	4.17	1.49	1.40
17	0	1022	CLA	C3B-C4B	4.16	1.49	1.40
17	B	1221	CLA	C3B-C4B	4.16	1.49	1.40
17	4	1015	CLA	C3B-C4B	4.16	1.49	1.40
17	8	1017	CLA	C3B-C4B	4.16	1.49	1.40
17	4	1026	CLA	C3B-C4B	4.16	1.49	1.40
17	A	1125	CLA	C3B-C4B	4.15	1.49	1.40
17	2	1022	CLA	C3B-C4B	4.15	1.49	1.40
17	Q	5224	CLA	C3B-C4B	4.15	1.49	1.40
17	B	1224	CLA	C3B-C4B	4.15	1.49	1.40
17	8	1022	CLA	C3B-C4B	4.15	1.49	1.40
17	1	1023	CLA	C3B-C4B	4.15	1.49	1.40
17	0	1015	CLA	C3B-C4B	4.15	1.49	1.40
17	4	1011	CLA	C3B-C4B	4.15	1.49	1.40
17	5	5404	CLA	C3B-C4B	4.15	1.49	1.40
17	K	1404	CLA	C3B-C4B	4.15	1.49	1.40
17	B	1205	CLA	MG-NB	4.15	2.14	2.05
17	4	1022	CLA	C3B-C4B	4.15	1.49	1.40
17	Q	5221	CLA	C3B-C4B	4.15	1.49	1.40
17	Q	5242	CLA	C3B-C4B	4.15	1.49	1.40
17	Q	5205	CLA	MG-NB	4.14	2.14	2.05
17	4	1031	CLA	C3B-C4B	4.14	1.49	1.40
17	8	1033	CLA	C3B-C4B	4.14	1.49	1.40
17	7	1011	CLA	C3B-C4B	4.14	1.49	1.40
17	9	1011	CLA	C3B-C4B	4.14	1.49	1.40
17	F	4005	CLA	C3B-C4B	4.14	1.49	1.40
17	4	1016	CLA	C3B-C4B	4.14	1.49	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	9	1041	CLA	C3B-C4B	4.14	1.49	1.40
17	1	1011	CLA	C3B-C4B	4.14	1.49	1.40
17	0	1026	CLA	C3B-C4B	4.14	1.49	1.40
17	4	1033	CLA	C3B-C4B	4.14	1.49	1.40
17	P	8010	CLA	C3B-C4B	4.14	1.49	1.40
17	9	1026	CLA	C3B-C4B	4.14	1.49	1.40
17	9	1032	CLA	C3B-C4B	4.13	1.49	1.40
17	B	1242	CLA	C3B-C4B	4.13	1.49	1.40
17	7	1017	CLA	C3B-C4B	4.13	1.49	1.40
17	Z	8008	CLA	C3B-C4B	4.13	1.49	1.40
17	0	1032	CLA	C3B-C4B	4.13	1.49	1.40
17	3	1041	CLA	C3B-C4B	4.13	1.49	1.40
17	4	1032	CLA	C3B-C4B	4.13	1.49	1.40
17	0	1031	CLA	C3B-C4B	4.13	1.49	1.40
17	2	1025	CLA	C3B-C4B	4.13	1.49	1.40
17	A	1402	CLA	MG-NB	4.13	2.14	2.05
17	P	5402	CLA	MG-NB	4.13	2.14	2.05
17	1	1017	CLA	C3B-C4B	4.13	1.49	1.40
17	3	1021	CLA	C3B-C4B	4.13	1.49	1.40
17	0	1011	CLA	C3B-C4B	4.13	1.49	1.40
17	3	1016	CLA	C3B-C4B	4.13	1.49	1.40
17	3	1026	CLA	C3B-C4B	4.12	1.49	1.40
17	3	1032	CLA	C3B-C4B	4.12	1.49	1.40
17	8	1011	CLA	C3B-C4B	4.12	1.49	1.40
17	F	4004	CLA	C3B-C4B	4.12	1.49	1.40
17	3	1011	CLA	C3B-C4B	4.12	1.49	1.40
17	B	1241	CLA	C3B-C4B	4.12	1.49	1.40
17	9	1022	CLA	C3B-C4B	4.12	1.49	1.40
17	K	1403	CLA	C3B-C4B	4.12	1.49	1.40
17	3	1022	CLA	C3B-C4B	4.12	1.49	1.40
17	9	1016	CLA	C3B-C4B	4.12	1.49	1.40
17	H	1801	CLA	C3B-C4B	4.12	1.49	1.40
17	A	4010	CLA	C3B-C4B	4.12	1.49	1.40
17	5	5403	CLA	C3B-C4B	4.12	1.49	1.40
17	2	1033	CLA	C3B-C4B	4.12	1.49	1.40
17	0	8002	CLA	C3B-C4B	4.12	1.49	1.40
17	7	1013	CLA	C3B-C4B	4.12	1.49	1.40
17	2	4007	CLA	C3B-C4B	4.11	1.49	1.40
17	2	1013	CLA	C3B-C4B	4.11	1.49	1.40
17	7	1016	CLA	C3B-C4B	4.11	1.49	1.40
17	U	8004	CLA	C3B-C4B	4.11	1.49	1.40
17	7	1025	CLA	C3B-C4B	4.11	1.49	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	J	4008	CLA	C3B-C4B	4.11	1.49	1.40
17	4	1012	CLA	C3B-C4B	4.11	1.49	1.40
17	8	8007	CLA	C3B-C4B	4.11	1.49	1.40
17	3	1015	CLA	C3B-C4B	4.11	1.49	1.40
17	J	1101	CLA	C3B-C4B	4.11	1.49	1.40
17	2	1031	CLA	C3B-C4B	4.11	1.49	1.40
17	W	5801	CLA	C3B-C4B	4.11	1.49	1.40
17	1	1016	CLA	C3B-C4B	4.11	1.49	1.40
17	1	1013	CLA	C3B-C4B	4.11	1.49	1.40
17	1	1021	CLA	C3B-C4B	4.11	1.49	1.40
17	2	1011	CLA	C3B-C4B	4.11	1.49	1.40
17	1	1022	CLA	C3B-C4B	4.11	1.49	1.40
17	8	1013	CLA	C3B-C4B	4.11	1.49	1.40
17	0	1033	CLA	C3B-C4B	4.11	1.49	1.40
17	6	5504	CLA	C3B-C4B	4.11	1.49	1.40
17	0	1012	CLA	C3B-C4B	4.11	1.49	1.40
17	Z	5101	CLA	C3B-C4B	4.11	1.49	1.40
17	7	1023	CLA	C3B-C4B	4.11	1.49	1.40
17	0	1025	CLA	C3B-C4B	4.11	1.49	1.40
17	Q	5241	CLA	C3B-C4B	4.11	1.49	1.40
17	8	1023	CLA	C3B-C4B	4.11	1.49	1.40
17	9	1033	CLA	C3B-C4B	4.10	1.49	1.40
17	7	1022	CLA	C3B-C4B	4.10	1.49	1.40
17	9	1015	CLA	C3B-C4B	4.10	1.49	1.40
17	1	1012	CLA	C3B-C4B	4.10	1.49	1.40
17	8	1015	CLA	C3B-C4B	4.10	1.49	1.40
17	7	1021	CLA	C3B-C4B	4.10	1.49	1.40
17	8	1031	CLA	C3B-C4B	4.10	1.49	1.40
17	B	1235	CLA	C3B-C4B	4.10	1.49	1.40
17	V	5701	CLA	C3B-C4B	4.10	1.49	1.40
17	9	1021	CLA	C3B-C4B	4.10	1.49	1.40
17	8	1016	CLA	C3B-C4B	4.10	1.49	1.40
17	2	1015	CLA	C3B-C4B	4.10	1.49	1.40
17	G	1701	CLA	C3B-C4B	4.10	1.49	1.40
17	1	1025	CLA	C3B-C4B	4.10	1.49	1.40
17	0	1014	CLA	C3B-C4B	4.10	1.49	1.40
17	4	1013	CLA	C3B-C4B	4.10	1.49	1.40
17	2	1023	CLA	C3B-C4B	4.10	1.49	1.40
17	4	1021	CLA	C3B-C4B	4.10	1.49	1.40
17	Q	5240	CLA	C3B-C4B	4.10	1.49	1.40
17	4	1025	CLA	C3B-C4B	4.10	1.49	1.40
17	8	1021	CLA	C3B-C4B	4.10	1.49	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	3	1033	CLA	C3B-C4B	4.10	1.48	1.40
17	7	1012	CLA	C3B-C4B	4.09	1.48	1.40
17	B	1240	CLA	C3B-C4B	4.09	1.48	1.40
17	F	4006	CLA	C3B-C4B	4.09	1.48	1.40
17	2	1012	CLA	C3B-C4B	4.09	1.48	1.40
17	7	1031	CLA	C3B-C4B	4.09	1.48	1.40
17	9	1017	CLA	C3B-C4B	4.09	1.48	1.40
17	1	1015	CLA	C3B-C4B	4.09	1.48	1.40
17	P	8009	CLA	C3B-C4B	4.09	1.48	1.40
17	3	1017	CLA	C3B-C4B	4.09	1.48	1.40
17	0	1021	CLA	C3B-C4B	4.09	1.48	1.40
17	8	1012	CLA	C3B-C4B	4.09	1.48	1.40
17	9	1031	CLA	C3B-C4B	4.09	1.48	1.40
17	4	1023	CLA	C3B-C4B	4.09	1.48	1.40
17	4	4002	CLA	C3B-C4B	4.09	1.48	1.40
17	4	1014	CLA	C3B-C4B	4.09	1.48	1.40
17	A	4009	CLA	C3B-C4B	4.09	1.48	1.40
17	0	1013	CLA	C3B-C4B	4.09	1.48	1.40
17	3	1012	CLA	C3B-C4B	4.09	1.48	1.40
17	B	4001	CLA	C3B-C4B	4.08	1.48	1.40
17	3	1014	CLA	C3B-C4B	4.08	1.48	1.40
17	U	8006	CLA	C3B-C4B	4.08	1.48	1.40
17	2	1016	CLA	C3B-C4B	4.08	1.48	1.40
17	L	1504	CLA	C3B-C4B	4.08	1.48	1.40
17	7	1015	CLA	C3B-C4B	4.08	1.48	1.40
17	3	1031	CLA	C3B-C4B	4.08	1.48	1.40
17	2	1026	CLA	C3B-C4B	4.08	1.48	1.40
17	2	1021	CLA	C3B-C4B	4.08	1.48	1.40
17	8	1014	CLA	C3B-C4B	4.08	1.48	1.40
17	0	1017	CLA	C3B-C4B	4.08	1.48	1.40
17	1	1014	CLA	C3B-C4B	4.07	1.48	1.40
17	2	1014	CLA	C3B-C4B	4.07	1.48	1.40
17	7	1014	CLA	C3B-C4B	4.07	1.48	1.40
17	9	1014	CLA	C3B-C4B	4.07	1.48	1.40
17	P	5013	CLA	MG-NB	4.07	2.13	2.05
17	8	1026	CLA	C3B-C4B	4.06	1.48	1.40
17	Q	5235	CLA	C3B-C4B	4.06	1.48	1.40
17	B	1219	CLA	C3B-C4B	4.06	1.48	1.40
17	1	1031	CLA	C3B-C4B	4.06	1.48	1.40
17	Q	5219	CLA	C3B-C4B	4.06	1.48	1.40
17	A	1013	CLA	MG-NB	4.06	2.13	2.05
17	Q	5218	CLA	C3B-C4B	4.06	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	3	1025	CLA	C3B-C4B	4.06	1.48	1.40
17	0	1023	CLA	C3B-C4B	4.06	1.48	1.40
17	Q	8001	CLA	C3B-C4B	4.05	1.48	1.40
17	B	1218	CLA	C3B-C4B	4.05	1.48	1.40
17	9	1012	CLA	C3B-C4B	4.05	1.48	1.40
17	4	1017	CLA	C3B-C4B	4.05	1.48	1.40
17	Q	5228	CLA	C3B-C4B	4.05	1.48	1.40
17	J	1302	CLA	MG-NC	4.04	2.15	2.06
17	A	1140	CLA	C3B-C4B	4.04	1.48	1.40
17	1	1026	CLA	C3B-C4B	4.04	1.48	1.40
17	7	1026	CLA	C3B-C4B	4.03	1.48	1.40
17	A	1012	CLA	MG-NC	4.03	2.15	2.06
17	Z	5302	CLA	MG-NC	4.03	2.15	2.06
17	B	1228	CLA	C3B-C4B	4.02	1.48	1.40
17	9	1025	CLA	C3B-C4B	4.02	1.48	1.40
17	F	4003	CLA	C3B-C4B	4.02	1.48	1.40
17	U	5229	CLA	C3B-C4B	4.02	1.48	1.40
17	Q	5213	CLA	C3B-C4B	4.01	1.48	1.40
17	P	5140	CLA	C3B-C4B	4.01	1.48	1.40
17	A	1126	CLA	MG-NC	4.01	2.15	2.06
17	P	5012	CLA	MG-NC	4.01	2.15	2.06
17	B	1221	CLA	MG-NB	4.01	2.13	2.05
17	Q	5220	CLA	C3B-C4B	4.00	1.48	1.40
17	P	5126	CLA	MG-NC	4.00	2.15	2.06
17	Q	5221	CLA	MG-NB	4.00	2.13	2.05
17	P	5901	CLA	C3B-C4B	4.00	1.48	1.40
17	U	8003	CLA	C3B-C4B	4.00	1.48	1.40
17	P	5129	CLA	C3B-C4B	3.99	1.48	1.40
17	F	1301	CLA	C3B-C4B	3.99	1.48	1.40
17	Q	5214	CLA	C3B-C4B	3.99	1.48	1.40
17	F	1229	CLA	C3B-C4B	3.99	1.48	1.40
17	A	1901	CLA	C3B-C4B	3.99	1.48	1.40
17	B	1213	CLA	C3B-C4B	3.98	1.48	1.40
17	B	1214	CLA	C3B-C4B	3.98	1.48	1.40
17	A	1104	CLA	MG-NB	3.98	2.13	2.05
17	B	1220	CLA	C3B-C4B	3.98	1.48	1.40
17	P	5125	CLA	MG-NB	3.97	2.13	2.05
17	Q	5204	CLA	C3B-C4B	3.97	1.48	1.40
17	B	1204	CLA	C3B-C4B	3.97	1.48	1.40
17	P	5901	CLA	MG-NC	3.97	2.15	2.06
17	A	1125	CLA	MG-NB	3.97	2.13	2.05
17	B	1234	CLA	C3B-C4B	3.96	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	P	5123	CLA	C3B-C4B	3.96	1.48	1.40
17	A	1123	CLA	C3B-C4B	3.96	1.48	1.40
17	U	5301	CLA	C3B-C4B	3.96	1.48	1.40
17	A	1901	CLA	MG-NC	3.95	2.15	2.06
17	A	1129	CLA	C3B-C4B	3.95	1.48	1.40
17	Q	5234	CLA	C3B-C4B	3.95	1.48	1.40
17	P	5104	CLA	MG-NB	3.95	2.13	2.05
17	6	5501	CLA	C3B-C4B	3.94	1.48	1.40
17	P	5119	CLA	C3B-C4B	3.94	1.48	1.40
17	L	1501	CLA	C3B-C4B	3.94	1.48	1.40
17	P	5113	CLA	MG-NC	3.93	2.15	2.06
17	A	1119	CLA	C3B-C4B	3.93	1.48	1.40
17	B	1231	CLA	C3B-C4B	3.92	1.48	1.40
17	P	5138	CLA	C3B-C4B	3.92	1.48	1.40
17	Q	5231	CLA	C3B-C4B	3.92	1.48	1.40
17	A	1113	CLA	MG-NC	3.91	2.15	2.06
17	A	1138	CLA	C3B-C4B	3.90	1.48	1.40
17	A	1120	CLA	C3B-C4B	3.90	1.48	1.40
17	A	1901	CLA	MG-NB	3.89	2.13	2.05
17	P	5120	CLA	C3B-C4B	3.89	1.48	1.40
17	P	5901	CLA	MG-NB	3.89	2.13	2.05
17	B	1209	CLA	C3B-C4B	3.88	1.48	1.40
17	Q	5209	CLA	C3B-C4B	3.88	1.48	1.40
17	B	1206	CLA	MG-NC	3.85	2.15	2.06
17	Q	5206	CLA	MG-NC	3.84	2.15	2.06
17	P	5134	CLA	C3B-C4B	3.83	1.48	1.40
17	A	1116	CLA	C3B-C4B	3.82	1.48	1.40
17	A	1134	CLA	C3B-C4B	3.82	1.48	1.40
17	P	5116	CLA	C3B-C4B	3.82	1.48	1.40
17	Q	5223	CLA	C3B-C4B	3.81	1.48	1.40
17	G	1233	CLA	C3B-C4B	3.81	1.48	1.40
17	A	1106	CLA	C3B-C4B	3.81	1.48	1.40
17	V	5233	CLA	C3B-C4B	3.81	1.48	1.40
17	B	1223	CLA	C3B-C4B	3.81	1.48	1.40
17	P	5106	CLA	C3B-C4B	3.80	1.48	1.40
17	A	1110	CLA	C3B-C4B	3.80	1.48	1.40
17	A	1121	CLA	C3B-C4B	3.80	1.48	1.40
17	B	1207	CLA	C2B-C1B	3.79	1.48	1.40
17	Q	5207	CLA	C2B-C1B	3.79	1.48	1.40
17	Q	5130	CLA	C2B-C1B	3.79	1.48	1.40
17	P	5121	CLA	C3B-C4B	3.79	1.48	1.40
17	B	1130	CLA	C2B-C1B	3.78	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	K	1401	CLA	C3B-C4B	3.78	1.48	1.40
17	6	5502	CLA	C3B-C4B	3.78	1.48	1.40
17	L	1502	CLA	C3B-C4B	3.77	1.48	1.40
17	5	5401	CLA	C3B-C4B	3.77	1.48	1.40
17	P	5110	CLA	C3B-C4B	3.77	1.48	1.40
17	B	1022	CLA	MG-NB	3.76	2.13	2.05
17	Q	5022	CLA	MG-NB	3.76	2.13	2.05
17	Q	5234	CLA	MG-NB	3.75	2.13	2.05
17	P	5135	CLA	C2B-C1B	3.75	1.48	1.40
17	A	1135	CLA	C2B-C1B	3.74	1.48	1.40
17	P	5402	CLA	C3B-C4B	3.74	1.48	1.40
17	B	1234	CLA	MG-NB	3.73	2.13	2.05
17	P	5115	CLA	MG-NB	3.72	2.13	2.05
17	A	1115	CLA	MG-NB	3.71	2.13	2.05
17	A	1402	CLA	C3B-C4B	3.71	1.48	1.40
18	Q	6002	PQN	C10-C5	3.70	1.46	1.40
17	6	5503	CLA	C3B-C4B	3.69	1.48	1.40
17	B	1201	CLA	C3B-C4B	3.69	1.48	1.40
17	P	5104	CLA	C3B-C4B	3.69	1.48	1.40
17	A	1011	CLA	CHA-C4D	3.69	1.47	1.38
17	6	5502	CLA	MG-NB	3.68	2.13	2.05
17	J	1302	CLA	C3B-C4B	3.68	1.48	1.40
17	Z	5302	CLA	C3B-C4B	3.68	1.48	1.40
17	Q	5217	CLA	C3B-C4B	3.67	1.48	1.40
17	Q	5201	CLA	C3B-C4B	3.67	1.48	1.40
17	Q	5216	CLA	C3B-C4B	3.67	1.48	1.40
17	P	5011	CLA	CHA-C4D	3.67	1.47	1.38
17	A	1136	CLA	MG-NB	3.67	2.13	2.05
17	P	5136	CLA	MG-NB	3.67	2.13	2.05
17	B	1216	CLA	C3B-C4B	3.67	1.48	1.40
17	L	1503	CLA	C3B-C4B	3.66	1.48	1.40
17	B	1217	CLA	C3B-C4B	3.66	1.48	1.40
18	B	2002	PQN	C10-C5	3.66	1.46	1.40
17	L	1502	CLA	MG-NB	3.66	2.13	2.05
17	A	1104	CLA	C3B-C4B	3.65	1.48	1.40
17	P	5013	CLA	C3B-C4B	3.65	1.48	1.40
17	B	1205	CLA	C3B-C4B	3.65	1.48	1.40
17	Q	5205	CLA	C3B-C4B	3.64	1.48	1.40
17	Q	5214	CLA	MG-NB	3.61	2.13	2.05
17	P	5105	CLA	C3B-C4B	3.61	1.47	1.40
17	P	5109	CLA	C3B-C4B	3.61	1.47	1.40
17	A	1013	CLA	C3B-C4B	3.61	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	P	5114	CLA	C3B-C4B	3.61	1.47	1.40
17	A	1109	CLA	C3B-C4B	3.60	1.47	1.40
17	A	1114	CLA	C3B-C4B	3.60	1.47	1.40
17	B	1214	CLA	MG-NB	3.59	2.12	2.05
17	B	1219	CLA	MG-NC	3.59	2.14	2.06
17	A	1105	CLA	C3B-C4B	3.58	1.47	1.40
17	B	1208	CLA	C3B-C4B	3.58	1.47	1.40
17	Q	5208	CLA	C3B-C4B	3.57	1.47	1.40
17	Q	5219	CLA	MG-NC	3.56	2.14	2.06
17	B	1210	CLA	C3B-C4B	3.55	1.47	1.40
17	Q	5210	CLA	C3B-C4B	3.55	1.47	1.40
17	Q	5227	CLA	C3B-C4B	3.54	1.47	1.40
17	P	5011	CLA	C2B-C1B	3.52	1.47	1.40
17	Q	5130	CLA	C3B-C4B	3.52	1.47	1.40
17	B	1021	CLA	MG-NC	3.52	2.14	2.06
17	B	1227	CLA	C3B-C4B	3.50	1.47	1.40
17	B	1130	CLA	C3B-C4B	3.49	1.47	1.40
17	Q	5021	CLA	MG-NC	3.48	2.14	2.06
17	A	1126	CLA	C3B-C4B	3.48	1.47	1.40
17	B	1230	CLA	C3B-C4B	3.47	1.47	1.40
17	Q	5207	CLA	C3B-C4B	3.47	1.47	1.40
17	A	1011	CLA	C2B-C1B	3.47	1.47	1.40
17	P	5126	CLA	C3B-C4B	3.47	1.47	1.40
17	B	1231	CLA	C2B-C1B	3.46	1.47	1.40
17	Q	5230	CLA	C3B-C4B	3.45	1.47	1.40
17	B	1207	CLA	C3B-C4B	3.45	1.47	1.40
17	P	5111	CLA	C3B-C4B	3.45	1.47	1.40
17	K	1401	CLA	MG-NB	3.45	2.12	2.05
17	5	5401	CLA	MG-NB	3.45	2.12	2.05
17	A	1111	CLA	C3B-C4B	3.44	1.47	1.40
17	Q	5203	CLA	C2B-C1B	3.43	1.47	1.40
17	P	5105	CLA	MG-NB	3.43	2.12	2.05
17	B	1210	CLA	MG-NC	3.42	2.14	2.06
17	Q	5231	CLA	C2B-C1B	3.42	1.47	1.40
17	A	1105	CLA	MG-NB	3.42	2.12	2.05
17	A	1135	CLA	MG-NC	3.42	2.14	2.06
17	Q	5235	CLA	CHC-C1C	3.41	1.45	1.38
17	P	5135	CLA	MG-NC	3.41	2.14	2.06
17	B	1231	CLA	MG-NB	3.41	2.12	2.05
17	B	1235	CLA	CHC-C1C	3.41	1.45	1.38
17	Q	5231	CLA	MG-NB	3.41	2.12	2.05
17	Q	5203	CLA	C3B-C4B	3.40	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	B	1203	CLA	C2B-C1B	3.39	1.47	1.40
17	A	1012	CLA	MG-NB	3.39	2.12	2.05
17	B	1237	CLA	C3B-C4B	3.39	1.47	1.40
17	Q	5210	CLA	MG-NC	3.39	2.14	2.06
17	F	1301	CLA	C2B-C1B	3.38	1.47	1.40
17	Q	5237	CLA	C3B-C4B	3.38	1.47	1.40
17	B	1226	CLA	MG-NC	3.38	2.14	2.06
17	Q	5023	CLA	MG-NC	3.38	2.14	2.06
17	A	1127	CLA	MG-NC	3.37	2.14	2.06
17	B	1023	CLA	MG-NC	3.37	2.14	2.06
17	U	5301	CLA	C2B-C1B	3.37	1.47	1.40
17	P	5012	CLA	MG-NB	3.35	2.12	2.05
17	Q	5226	CLA	MG-NC	3.35	2.14	2.06
17	B	1203	CLA	C3B-C4B	3.35	1.47	1.40
17	P	5127	CLA	MG-NC	3.35	2.14	2.06
17	P	5012	CLA	C3B-C4B	3.34	1.47	1.40
17	P	5137	CLA	C3B-C4B	3.34	1.47	1.40
17	A	1137	CLA	C3B-C4B	3.34	1.47	1.40
17	A	1012	CLA	C3B-C4B	3.33	1.47	1.40
17	P	5107	CLA	C3B-C4B	3.33	1.47	1.40
17	9	1022	CLA	MG-NB	3.32	2.12	2.05
17	B	1230	CLA	MG-NB	3.32	2.12	2.05
17	Q	5230	CLA	MG-NB	3.31	2.12	2.05
17	0	1015	CLA	MG-NB	3.31	2.12	2.05
17	P	5111	CLA	C2B-C1B	3.31	1.47	1.40
17	A	1402	CLA	C2B-C1B	3.31	1.47	1.40
17	0	1011	CLA	MG-NB	3.31	2.12	2.05
17	P	5402	CLA	C2B-C1B	3.30	1.47	1.40
17	A	1111	CLA	MG-NB	3.30	2.12	2.05
17	0	1012	CLA	MG-NB	3.30	2.12	2.05
17	7	1015	CLA	MG-NB	3.29	2.12	2.05
17	A	1107	CLA	C3B-C4B	3.29	1.47	1.40
17	B	1236	CLA	MG-NC	3.29	2.14	2.06
17	5	5403	CLA	MG-NB	3.29	2.12	2.05
17	Q	5236	CLA	MG-NC	3.29	2.14	2.06
17	L	1501	CLA	CHC-C1C	3.29	1.45	1.38
17	1	1022	CLA	MG-NB	3.29	2.12	2.05
17	8	1012	CLA	MG-NB	3.29	2.12	2.05
17	4	1022	CLA	MG-NB	3.28	2.12	2.05
17	A	1124	CLA	C3B-C4B	3.28	1.47	1.40
17	Q	5225	CLA	C3B-C4B	3.28	1.47	1.40
17	P	5111	CLA	MG-NB	3.28	2.12	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	A	1111	CLA	C2B-C1B	3.28	1.47	1.40
17	K	1403	CLA	MG-NB	3.28	2.12	2.05
17	8	1033	CLA	MG-NB	3.28	2.12	2.05
17	B	1223	CLA	C2B-C1B	3.28	1.47	1.40
17	7	1022	CLA	MG-NB	3.28	2.12	2.05
17	9	1012	CLA	MG-NB	3.28	2.12	2.05
17	B	1225	CLA	C3B-C4B	3.28	1.47	1.40
18	B	2002	PQN	C6-C5	3.27	1.44	1.39
17	P	8010	CLA	MG-NB	3.27	2.12	2.05
17	9	1014	CLA	MG-NB	3.27	2.12	2.05
17	6	5501	CLA	CHC-C1C	3.27	1.44	1.38
17	9	1033	CLA	MG-NB	3.27	2.12	2.05
17	3	1022	CLA	MG-NB	3.27	2.12	2.05
17	Q	5223	CLA	C2B-C1B	3.27	1.47	1.40
17	3	1033	CLA	MG-NB	3.27	2.12	2.05
17	4	1011	CLA	MG-NB	3.27	2.12	2.05
17	L	1501	CLA	MG-NB	3.27	2.12	2.05
17	4	1012	CLA	MG-NB	3.27	2.12	2.05
17	P	5108	CLA	C3B-C4B	3.27	1.47	1.40
17	1	1015	CLA	MG-NB	3.27	2.12	2.05
17	A	4009	CLA	MG-NB	3.27	2.12	2.05
17	7	1023	CLA	MG-NB	3.27	2.12	2.05
17	A	4010	CLA	MG-NB	3.26	2.12	2.05
18	Q	6002	PQN	C6-C5	3.26	1.44	1.39
17	P	5124	CLA	C3B-C4B	3.26	1.47	1.40
17	0	1022	CLA	MG-NB	3.26	2.12	2.05
17	2	1025	CLA	MG-NB	3.26	2.12	2.05
17	Q	5212	CLA	MG-NB	3.26	2.12	2.05
17	7	1012	CLA	MG-NB	3.26	2.12	2.05
17	4	1015	CLA	MG-NB	3.26	2.12	2.05
17	B	1211	CLA	C3B-C4B	3.26	1.47	1.40
17	A	1102	CLA	C3B-C4B	3.26	1.47	1.40
17	B	1205	CLA	C2B-C1B	3.26	1.47	1.40
17	P	5102	CLA	C3B-C4B	3.26	1.47	1.40
17	Q	5205	CLA	MG-NC	3.25	2.14	2.06
17	8	1011	CLA	MG-NB	3.25	2.12	2.05
17	8	1015	CLA	MG-NB	3.25	2.12	2.05
17	Q	5222	CLA	C3B-C4B	3.25	1.47	1.40
17	K	1404	CLA	MG-NB	3.25	2.12	2.05
17	0	1023	CLA	MG-NB	3.25	2.12	2.05
17	3	1012	CLA	MG-NB	3.25	2.12	2.05
17	5	5404	CLA	MG-NB	3.25	2.12	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	Q	5023	CLA	CHC-C1C	3.25	1.44	1.38
17	4	1023	CLA	MG-NB	3.25	2.12	2.05
17	P	5113	CLA	C3B-C4B	3.25	1.47	1.40
17	P	8009	CLA	MG-NB	3.25	2.12	2.05
17	9	1016	CLA	MG-NB	3.25	2.12	2.05
17	2	1021	CLA	MG-NB	3.25	2.12	2.05
17	3	1016	CLA	MG-NB	3.25	2.12	2.05
17	6	5501	CLA	MG-NB	3.25	2.12	2.05
17	A	1108	CLA	C3B-C4B	3.24	1.47	1.40
17	B	1021	CLA	C3B-C4B	3.24	1.47	1.40
17	F	1301	CLA	MG-NC	3.24	2.14	2.06
17	B	1212	CLA	MG-NB	3.24	2.12	2.05
17	7	1013	CLA	MG-NB	3.24	2.12	2.05
17	3	1014	CLA	MG-NB	3.24	2.12	2.05
17	4	1031	CLA	MG-NB	3.24	2.12	2.05
17	P	5133	CLA	C3B-C4B	3.24	1.47	1.40
17	Q	5021	CLA	C3B-C4B	3.24	1.47	1.40
17	4	1026	CLA	MG-NB	3.24	2.12	2.05
17	3	1031	CLA	MG-NB	3.24	2.12	2.05
17	0	1017	CLA	MG-NB	3.24	2.12	2.05
17	2	1015	CLA	MG-NB	3.24	2.12	2.05
17	2	1033	CLA	MG-NB	3.24	2.12	2.05
17	A	1113	CLA	C3B-C4B	3.24	1.47	1.40
17	A	1133	CLA	C3B-C4B	3.24	1.47	1.40
17	P	5125	CLA	C2B-C1B	3.24	1.47	1.40
17	F	4003	CLA	MG-NB	3.24	2.12	2.05
17	2	1023	CLA	MG-NB	3.24	2.12	2.05
17	0	1031	CLA	MG-NB	3.24	2.12	2.05
17	2	4007	CLA	MG-NB	3.24	2.12	2.05
17	4	1017	CLA	MG-NB	3.24	2.12	2.05
17	P	5136	CLA	C2B-C1B	3.24	1.47	1.40
17	3	1041	CLA	MG-NB	3.24	2.12	2.05
17	W	5801	CLA	MG-NB	3.24	2.12	2.05
17	9	1015	CLA	MG-NB	3.24	2.12	2.05
17	Q	8001	CLA	MG-NB	3.23	2.12	2.05
17	1	1012	CLA	MG-NB	3.23	2.12	2.05
17	1	1023	CLA	MG-NB	3.23	2.12	2.05
17	9	1011	CLA	MG-NB	3.23	2.12	2.05
17	Q	5205	CLA	C2B-C1B	3.23	1.47	1.40
17	7	1026	CLA	MG-NB	3.23	2.12	2.05
17	7	1025	CLA	MG-NB	3.23	2.12	2.05
17	8	1013	CLA	MG-NB	3.23	2.12	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	8	1023	CLA	MG-NB	3.23	2.12	2.05
17	L	1504	CLA	MG-NB	3.23	2.12	2.05
17	Q	5211	CLA	C3B-C4B	3.23	1.47	1.40
17	Q	5208	CLA	MG-NB	3.23	2.12	2.05
17	U	8003	CLA	MG-NB	3.23	2.12	2.05
17	B	1222	CLA	C3B-C4B	3.23	1.47	1.40
17	2	1012	CLA	MG-NB	3.23	2.12	2.05
17	P	5137	CLA	C2B-C1B	3.23	1.47	1.40
17	2	1013	CLA	MG-NB	3.23	2.12	2.05
17	6	5504	CLA	MG-NB	3.23	2.12	2.05
17	4	1025	CLA	MG-NB	3.23	2.12	2.05
17	B	1241	CLA	MG-NB	3.23	2.12	2.05
17	8	1021	CLA	MG-NB	3.23	2.12	2.05
17	B	1023	CLA	CHC-C1C	3.23	1.44	1.38
17	8	8007	CLA	MG-NB	3.23	2.12	2.05
17	8	1025	CLA	MG-NB	3.23	2.12	2.05
17	1	1025	CLA	MG-NB	3.23	2.12	2.05
17	3	1015	CLA	MG-NB	3.23	2.12	2.05
17	B	1225	CLA	MG-NC	3.23	2.13	2.06
17	1	1017	CLA	MG-NB	3.23	2.12	2.05
17	Q	5241	CLA	MG-NB	3.23	2.12	2.05
17	U	5301	CLA	MG-NC	3.23	2.13	2.06
17	J	1101	CLA	MG-NB	3.23	2.12	2.05
17	3	1032	CLA	MG-NB	3.23	2.12	2.05
17	8	1016	CLA	MG-NB	3.23	2.12	2.05
17	9	1031	CLA	MG-NB	3.23	2.12	2.05
17	7	1017	CLA	MG-NB	3.22	2.12	2.05
17	B	1205	CLA	MG-NC	3.22	2.13	2.06
17	9	1032	CLA	MG-NB	3.22	2.12	2.05
17	1	1026	CLA	MG-NB	3.22	2.12	2.05
17	9	1026	CLA	MG-NB	3.22	2.12	2.05
17	0	1026	CLA	MG-NB	3.22	2.12	2.05
17	A	1125	CLA	C2B-C1B	3.22	1.47	1.40
17	B	1226	CLA	MG-NB	3.22	2.12	2.05
17	2	1011	CLA	MG-NB	3.22	2.12	2.05
17	Q	5218	CLA	CHC-C1C	3.22	1.44	1.38
17	1	1013	CLA	MG-NB	3.22	2.12	2.05
17	9	1041	CLA	MG-NB	3.22	2.12	2.05
17	2	1026	CLA	MG-NB	3.22	2.12	2.05
17	4	1033	CLA	MG-NB	3.22	2.12	2.05
17	9	1017	CLA	MG-NB	3.22	2.12	2.05
17	Q	5225	CLA	MG-NC	3.22	2.13	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	3	1011	CLA	MG-NB	3.22	2.12	2.05
17	3	1026	CLA	MG-NB	3.22	2.12	2.05
17	7	1031	CLA	MG-NB	3.22	2.12	2.05
17	0	1033	CLA	MG-NB	3.22	2.12	2.05
17	2	1016	CLA	MG-NB	3.22	2.12	2.05
17	B	1242	CLA	MG-NB	3.22	2.12	2.05
17	7	1016	CLA	MG-NB	3.22	2.12	2.05
17	B	1219	CLA	C2B-C1B	3.22	1.47	1.40
17	8	1026	CLA	MG-NB	3.22	2.12	2.05
17	G	1701	CLA	MG-NB	3.22	2.12	2.05
17	1	1011	CLA	MG-NB	3.22	2.12	2.05
17	2	1014	CLA	MG-NB	3.21	2.12	2.05
17	B	1218	CLA	CHC-C1C	3.21	1.44	1.38
17	4	1013	CLA	MG-NB	3.21	2.12	2.05
17	3	1021	CLA	MG-NB	3.21	2.12	2.05
17	A	1136	CLA	C2B-C1B	3.21	1.47	1.40
17	F	4006	CLA	MG-NB	3.21	2.12	2.05
17	U	8004	CLA	MG-NB	3.21	2.12	2.05
17	7	1011	CLA	MG-NB	3.21	2.12	2.05
17	2	1017	CLA	MG-NB	3.21	2.12	2.05
17	J	4008	CLA	MG-NB	3.21	2.12	2.05
17	B	4001	CLA	MG-NB	3.21	2.12	2.05
17	F	4004	CLA	MG-NB	3.21	2.12	2.05
17	4	1021	CLA	MG-NB	3.21	2.12	2.05
17	Q	5226	CLA	MG-NB	3.21	2.12	2.05
17	1	1016	CLA	MG-NB	3.21	2.12	2.05
17	3	1025	CLA	MG-NB	3.20	2.12	2.05
17	U	8005	CLA	MG-NB	3.20	2.12	2.05
17	B	1208	CLA	MG-NB	3.20	2.12	2.05
17	4	1016	CLA	MG-NB	3.20	2.12	2.05
17	0	1025	CLA	MG-NB	3.20	2.12	2.05
17	4	1032	CLA	MG-NB	3.20	2.12	2.05
17	0	1016	CLA	MG-NB	3.20	2.12	2.05
17	H	1801	CLA	MG-NB	3.20	2.12	2.05
17	4	4002	CLA	MG-NB	3.20	2.12	2.05
17	8	1017	CLA	MG-NB	3.20	2.12	2.05
17	1	1031	CLA	MG-NB	3.20	2.12	2.05
17	V	5701	CLA	MG-NB	3.20	2.12	2.05
17	8	1014	CLA	MG-NB	3.20	2.12	2.05
17	A	1137	CLA	C2B-C1B	3.20	1.47	1.40
17	1	1014	CLA	MG-NB	3.20	2.12	2.05
17	Z	5101	CLA	MG-NB	3.20	2.12	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	4	1014	CLA	MG-NB	3.19	2.12	2.05
17	B	1240	CLA	MG-NB	3.19	2.12	2.05
17	Q	5242	CLA	MG-NB	3.19	2.12	2.05
17	0	1013	CLA	MG-NB	3.19	2.12	2.05
17	9	1021	CLA	MG-NB	3.19	2.12	2.05
17	0	1014	CLA	MG-NB	3.19	2.12	2.05
17	Q	5240	CLA	MG-NB	3.19	2.12	2.05
17	3	1017	CLA	MG-NB	3.19	2.12	2.05
17	F	4005	CLA	MG-NB	3.19	2.12	2.05
17	Z	8008	CLA	MG-NB	3.19	2.12	2.05
17	0	1021	CLA	MG-NB	3.19	2.12	2.05
17	U	8006	CLA	MG-NB	3.19	2.12	2.05
17	Q	5235	CLA	MG-NB	3.19	2.12	2.05
17	A	1105	CLA	MG-NC	3.18	2.13	2.06
17	2	1031	CLA	MG-NB	3.18	2.12	2.05
17	A	1118	CLA	C2B-C1B	3.18	1.47	1.40
17	P	5123	CLA	MG-NB	3.18	2.12	2.05
17	Q	5219	CLA	C2B-C1B	3.18	1.47	1.40
17	7	1014	CLA	MG-NB	3.18	2.12	2.05
17	A	1138	CLA	MG-NB	3.18	2.12	2.05
17	9	1025	CLA	MG-NB	3.18	2.12	2.05
18	P	6001	PQN	C10-C5	3.18	1.45	1.40
17	A	1123	CLA	MG-NB	3.18	2.12	2.05
17	0	8002	CLA	MG-NB	3.18	2.12	2.05
17	L	1501	CLA	MG-NC	3.18	2.13	2.06
17	8	1031	CLA	MG-NB	3.18	2.12	2.05
17	2	1022	CLA	MG-NB	3.17	2.12	2.05
17	A	1128	CLA	CHC-C1C	3.17	1.44	1.38
17	B	1236	CLA	C3B-C4B	3.17	1.47	1.40
17	0	1032	CLA	MG-NB	3.17	2.12	2.05
18	A	2001	PQN	C10-C5	3.17	1.45	1.40
17	B	1235	CLA	MG-NB	3.16	2.12	2.05
17	P	5105	CLA	MG-NC	3.16	2.13	2.06
17	P	5138	CLA	MG-NB	3.16	2.12	2.05
18	P	6001	PQN	C6-C5	3.16	1.44	1.39
18	A	2001	PQN	C6-C5	3.15	1.44	1.39
17	8	1022	CLA	MG-NB	3.15	2.12	2.05
17	Q	5220	CLA	MG-NB	3.15	2.12	2.05
17	P	5118	CLA	C2B-C1B	3.15	1.47	1.40
17	P	5128	CLA	CHC-C1C	3.15	1.44	1.38
17	6	5501	CLA	MG-NC	3.14	2.13	2.06
17	Q	5236	CLA	C3B-C4B	3.14	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	B	1220	CLA	MG-NB	3.14	2.12	2.05
17	L	1503	CLA	MG-NB	3.14	2.12	2.05
17	V	5233	CLA	C2B-C1B	3.12	1.46	1.40
17	B	1209	CLA	MG-NB	3.12	2.12	2.05
17	6	5503	CLA	MG-NB	3.12	2.12	2.05
17	B	1209	CLA	C2B-C1B	3.12	1.46	1.40
17	L	1502	CLA	C2B-C1B	3.11	1.46	1.40
17	Q	5209	CLA	MG-NB	3.11	2.12	2.05
17	Q	5202	CLA	C2B-C1B	3.11	1.46	1.40
17	G	1233	CLA	C2B-C1B	3.10	1.46	1.40
17	B	1202	CLA	C2B-C1B	3.10	1.46	1.40
17	6	5502	CLA	C2B-C1B	3.10	1.46	1.40
17	6	5501	CLA	C2B-C1B	3.10	1.46	1.40
17	A	1109	CLA	C2B-C1B	3.09	1.46	1.40
17	Q	5209	CLA	C2B-C1B	3.09	1.46	1.40
17	A	1901	CLA	CHC-C1C	3.09	1.44	1.38
17	P	5901	CLA	CHC-C1C	3.08	1.44	1.38
17	B	1204	CLA	C2B-C1B	3.08	1.46	1.40
17	P	5134	CLA	C2B-C1B	3.08	1.46	1.40
17	6	5502	CLA	CHC-C1C	3.08	1.44	1.38
17	A	1134	CLA	C2B-C1B	3.07	1.46	1.40
17	L	1502	CLA	CHC-C1C	3.07	1.44	1.38
17	P	5109	CLA	C2B-C1B	3.07	1.46	1.40
17	Q	5210	CLA	C2B-C1B	3.07	1.46	1.40
17	A	1105	CLA	C2B-C1B	3.06	1.46	1.40
17	Q	5204	CLA	C2B-C1B	3.06	1.46	1.40
17	Q	5236	CLA	MG-NB	3.06	2.11	2.05
17	Q	5218	CLA	MG-NB	3.06	2.11	2.05
17	B	1210	CLA	C2B-C1B	3.06	1.46	1.40
17	P	5138	CLA	CHC-C1C	3.06	1.44	1.38
17	L	1501	CLA	C2B-C1B	3.05	1.46	1.40
17	A	1138	CLA	CHC-C1C	3.05	1.44	1.38
17	P	5110	CLA	C2B-C1B	3.05	1.46	1.40
17	P	5106	CLA	CHC-C1C	3.05	1.44	1.38
17	P	5105	CLA	C2B-C1B	3.05	1.46	1.40
17	F	1301	CLA	MG-NB	3.05	2.11	2.05
17	U	5301	CLA	MG-NB	3.05	2.11	2.05
17	B	1236	CLA	MG-NB	3.05	2.11	2.05
17	A	1110	CLA	C2B-C1B	3.04	1.46	1.40
17	P	5139	CLA	MG-NB	3.03	2.11	2.05
17	P	5116	CLA	MG-NB	3.03	2.11	2.05
17	A	1116	CLA	MG-NC	3.03	2.13	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	P	5013	CLA	C2B-C1B	3.03	1.46	1.40
17	A	1013	CLA	C2B-C1B	3.03	1.46	1.40
17	B	1218	CLA	MG-NB	3.03	2.11	2.05
17	P	5116	CLA	MG-NC	3.02	2.13	2.06
17	A	1106	CLA	CHC-C1C	3.02	1.44	1.38
17	A	1104	CLA	C2B-C1B	3.02	1.46	1.40
17	A	1131	CLA	MG-NC	3.01	2.13	2.06
17	B	1221	CLA	CHC-C1C	3.01	1.44	1.38
17	A	1138	CLA	C2B-C1B	3.01	1.46	1.40
17	A	1139	CLA	MG-NB	3.00	2.11	2.05
17	P	5138	CLA	C2B-C1B	3.00	1.46	1.40
17	A	1112	CLA	CHC-C1C	3.00	1.44	1.38
17	A	1109	CLA	MG-NB	3.00	2.11	2.05
17	B	1223	CLA	MG-NC	3.00	2.13	2.06
17	P	5131	CLA	MG-NC	3.00	2.13	2.06
17	P	5104	CLA	C2B-C1B	3.00	1.46	1.40
17	Q	5217	CLA	C2B-C1B	3.00	1.46	1.40
17	Q	5223	CLA	MG-NC	3.00	2.13	2.06
18	A	2001	PQN	C2-C1	-3.00	1.44	1.48
17	Q	5226	CLA	C2B-C1B	2.99	1.46	1.40
17	A	1012	CLA	C3D-C2D	2.99	1.42	1.35
17	A	1116	CLA	MG-NB	2.99	2.11	2.05
17	P	5112	CLA	CHC-C1C	2.99	1.44	1.38
17	P	5109	CLA	MG-NB	2.99	2.11	2.05
17	B	1217	CLA	C2B-C1B	2.99	1.46	1.40
17	B	1224	CLA	CHC-C1C	2.99	1.44	1.38
17	P	5122	CLA	C3B-C4B	2.99	1.46	1.40
17	Q	5221	CLA	CHC-C1C	2.99	1.44	1.38
17	P	5125	CLA	CHC-C1C	2.99	1.44	1.38
17	P	5117	CLA	C3B-C4B	2.99	1.46	1.40
17	Q	5238	CLA	C2B-C1B	2.98	1.46	1.40
17	A	1117	CLA	C3B-C4B	2.98	1.46	1.40
17	P	5012	CLA	C3D-C2D	2.98	1.42	1.35
17	A	1121	CLA	MG-NB	2.98	2.11	2.05
17	Q	5231	CLA	CHC-C1C	2.98	1.44	1.38
17	B	1022	CLA	C3D-C2D	2.98	1.42	1.35
17	Q	5224	CLA	CHC-C1C	2.98	1.44	1.38
17	P	5112	CLA	C2B-C1B	2.98	1.46	1.40
17	P	5113	CLA	C2B-C1B	2.98	1.46	1.40
17	Q	5022	CLA	C3D-C2D	2.98	1.42	1.35
17	P	5121	CLA	MG-NB	2.98	2.11	2.05
17	B	1230	CLA	C2B-C1B	2.97	1.46	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	B	1231	CLA	CHC-C1C	2.97	1.44	1.38
17	Q	5212	CLA	MG-NC	2.97	2.13	2.06
17	A	1122	CLA	C3B-C4B	2.97	1.46	1.40
17	Q	5230	CLA	C2B-C1B	2.97	1.46	1.40
17	Q	5023	CLA	MG-NB	2.97	2.11	2.05
17	A	1125	CLA	CHC-C1C	2.96	1.44	1.38
17	B	1238	CLA	C2B-C1B	2.96	1.46	1.40
17	B	1023	CLA	MG-NB	2.96	2.11	2.05
17	B	1225	CLA	MG-NB	2.96	2.11	2.05
17	Q	5212	CLA	CHC-C1C	2.96	1.44	1.38
17	B	1201	CLA	MG-NB	2.96	2.11	2.05
17	Q	5130	CLA	MG-NC	2.96	2.13	2.06
17	B	1226	CLA	C2B-C1B	2.96	1.46	1.40
17	B	1212	CLA	MG-NC	2.96	2.13	2.06
17	B	1130	CLA	MG-NC	2.95	2.13	2.06
17	Q	5225	CLA	MG-NB	2.95	2.11	2.05
17	Q	5201	CLA	MG-NB	2.95	2.11	2.05
17	B	1222	CLA	C2B-C1B	2.95	1.46	1.40
17	Q	5222	CLA	C2B-C1B	2.95	1.46	1.40
17	A	1112	CLA	C2B-C1B	2.95	1.46	1.40
17	P	5103	CLA	C3B-C4B	2.94	1.46	1.40
17	K	1401	CLA	C2B-C1B	2.94	1.46	1.40
17	B	1216	CLA	MG-NC	2.94	2.13	2.06
17	B	1212	CLA	CHC-C1C	2.94	1.44	1.38
18	P	6001	PQN	C2-C1	-2.94	1.44	1.48
17	5	5401	CLA	C2B-C1B	2.94	1.46	1.40
17	A	1113	CLA	C2B-C1B	2.93	1.46	1.40
17	P	5131	CLA	C2B-C1B	2.93	1.46	1.40
17	Q	5232	CLA	CHC-C1C	2.93	1.44	1.38
17	B	1218	CLA	C2B-C1B	2.92	1.46	1.40
17	A	1131	CLA	C2B-C1B	2.92	1.46	1.40
17	P	5121	CLA	MG-NC	2.92	2.13	2.06
17	A	1103	CLA	C3B-C4B	2.92	1.46	1.40
17	P	5126	CLA	C2B-C1B	2.92	1.46	1.40
17	B	1232	CLA	CHC-C1C	2.92	1.44	1.38
17	Q	5220	CLA	CHC-C1C	2.92	1.44	1.38
17	Q	5218	CLA	C2B-C1B	2.92	1.46	1.40
17	P	5118	CLA	CHC-C1C	2.92	1.44	1.38
17	Q	5216	CLA	MG-NC	2.91	2.13	2.06
17	Q	5023	CLA	C2B-C1B	2.91	1.46	1.40
17	B	1220	CLA	CHC-C1C	2.91	1.44	1.38
17	A	1121	CLA	MG-NC	2.91	2.13	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	B	1234	CLA	C2B-C1B	2.91	1.46	1.40
17	Q	5234	CLA	CHC-C1C	2.91	1.44	1.38
17	A	1126	CLA	C2B-C1B	2.91	1.46	1.40
17	B	1023	CLA	C2B-C1B	2.91	1.46	1.40
17	P	5123	CLA	CHC-C1C	2.91	1.44	1.38
17	Q	5234	CLA	C2B-C1B	2.91	1.46	1.40
17	Q	5202	CLA	C3B-C4B	2.90	1.46	1.40
17	P	5119	CLA	CHC-C1C	2.90	1.44	1.38
17	P	5128	CLA	C2B-C1B	2.90	1.46	1.40
17	A	1119	CLA	CHC-C1C	2.90	1.44	1.38
17	B	1226	CLA	C3B-C4B	2.89	1.46	1.40
17	A	1118	CLA	CHC-C1C	2.88	1.44	1.38
17	A	1128	CLA	C2B-C1B	2.88	1.46	1.40
17	6	5503	CLA	CHC-C1C	2.88	1.44	1.38
17	A	1115	CLA	C2B-C1B	2.88	1.46	1.40
17	A	1139	CLA	C3B-C4B	2.88	1.46	1.40
17	B	1234	CLA	CHC-C1C	2.87	1.44	1.38
17	B	1207	CLA	MG-NC	2.87	2.13	2.06
17	Q	5226	CLA	C3B-C4B	2.87	1.46	1.40
17	P	5115	CLA	C2B-C1B	2.87	1.46	1.40
17	B	1202	CLA	C3B-C4B	2.87	1.46	1.40
17	A	1123	CLA	CHC-C1C	2.87	1.44	1.38
17	P	5139	CLA	C3B-C4B	2.87	1.46	1.40
17	Q	5207	CLA	MG-NC	2.85	2.13	2.06
17	B	1217	CLA	MG-NB	2.85	2.11	2.05
17	A	1134	CLA	MG-NB	2.85	2.11	2.05
17	Q	5021	CLA	C2B-C1B	2.85	1.46	1.40
17	Q	5204	CLA	C3D-C2D	2.85	1.41	1.35
17	L	1503	CLA	CHC-C1C	2.84	1.44	1.38
17	B	1215	CLA	C3B-C4B	2.84	1.46	1.40
17	P	5127	CLA	C3D-C2D	2.84	1.41	1.35
17	A	1127	CLA	C3D-C2D	2.84	1.41	1.35
17	A	1123	CLA	C2B-C1B	2.83	1.46	1.40
17	Q	5215	CLA	C3B-C4B	2.83	1.46	1.40
17	A	1120	CLA	CHC-C1C	2.83	1.44	1.38
17	Q	5213	CLA	C3D-C2D	2.82	1.41	1.35
17	P	5120	CLA	CHC-C1C	2.82	1.44	1.38
17	Q	5217	CLA	MG-NB	2.82	2.11	2.05
17	B	1204	CLA	C3D-C2D	2.82	1.41	1.35
17	P	5123	CLA	C2B-C1B	2.82	1.46	1.40
17	A	1107	CLA	MG-NC	2.82	2.13	2.06
17	P	5012	CLA	CHC-C1C	2.82	1.44	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	A	1139	CLA	C2B-C1B	2.82	1.46	1.40
17	K	1401	CLA	MG-NC	2.81	2.13	2.06
17	B	1021	CLA	C2B-C1B	2.81	1.46	1.40
17	4	1012	CLA	C2B-C1B	2.81	1.46	1.40
17	Q	5235	CLA	MG-NC	2.81	2.12	2.06
17	P	5117	CLA	C3D-C2D	2.80	1.41	1.35
17	P	5134	CLA	MG-NB	2.80	2.11	2.05
17	5	5401	CLA	MG-NC	2.80	2.12	2.06
17	A	1012	CLA	CHC-C1C	2.80	1.44	1.38
17	P	5139	CLA	C2B-C1B	2.80	1.46	1.40
17	P	5107	CLA	MG-NC	2.80	2.12	2.06
17	B	1213	CLA	C3D-C2D	2.80	1.41	1.35
17	P	5140	CLA	C2B-C1B	2.80	1.46	1.40
17	B	1235	CLA	MG-NC	2.80	2.12	2.06
17	B	1211	CLA	MG-NB	2.80	2.11	2.05
17	P	5135	CLA	C3B-C4B	2.79	1.46	1.40
17	A	1103	CLA	C2B-C1B	2.79	1.46	1.40
17	A	1117	CLA	C3D-C2D	2.79	1.41	1.35
17	A	1140	CLA	C2B-C1B	2.78	1.46	1.40
17	J	1302	CLA	CHC-C1C	2.78	1.44	1.38
17	Q	5220	CLA	C2B-C1B	2.78	1.46	1.40
17	Q	5211	CLA	MG-NB	2.78	2.11	2.05
17	B	1220	CLA	C2B-C1B	2.77	1.46	1.40
17	P	5103	CLA	C2B-C1B	2.77	1.46	1.40
17	P	5120	CLA	MG-NB	2.77	2.11	2.05
17	A	1135	CLA	C3B-C4B	2.77	1.46	1.40
18	P	6001	PQN	C8-C9	2.77	1.43	1.38
17	P	5121	CLA	C2B-C1B	2.77	1.46	1.40
17	B	1215	CLA	C2B-C1B	2.76	1.46	1.40
17	0	1012	CLA	C2B-C1B	2.76	1.46	1.40
17	A	1129	CLA	CHC-C1C	2.76	1.43	1.38
17	Z	5302	CLA	CHC-C1C	2.76	1.43	1.38
17	A	1121	CLA	C2B-C1B	2.76	1.46	1.40
17	P	5118	CLA	MG-NB	2.76	2.11	2.05
17	Q	5221	CLA	MG-NC	2.76	2.12	2.06
17	V	5701	CLA	C2B-C1B	2.75	1.46	1.40
17	A	1136	CLA	CHC-C1C	2.75	1.43	1.38
17	A	1127	CLA	C2B-C1B	2.75	1.46	1.40
17	A	1118	CLA	MG-NB	2.75	2.11	2.05
17	0	1022	CLA	C2B-C1B	2.75	1.46	1.40
17	0	1021	CLA	C2B-C1B	2.75	1.46	1.40
17	B	1208	CLA	C2B-C1B	2.75	1.46	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	3	1032	CLA	C2B-C1B	2.75	1.46	1.40
17	B	1234	CLA	C3D-C2D	2.75	1.41	1.35
17	P	5402	CLA	C3D-C2D	2.75	1.41	1.35
17	U	5229	CLA	MG-NC	2.75	2.12	2.06
17	P	5127	CLA	C2B-C1B	2.75	1.46	1.40
17	5	5403	CLA	C2B-C1B	2.75	1.46	1.40
17	0	1015	CLA	C2B-C1B	2.75	1.46	1.40
17	A	1116	CLA	C2B-C1B	2.74	1.46	1.40
17	1	1014	CLA	C2B-C1B	2.74	1.46	1.40
17	G	1233	CLA	MG-NB	2.74	2.11	2.05
18	A	2001	PQN	C8-C9	2.74	1.43	1.38
17	A	1128	CLA	MG-NC	2.74	2.12	2.06
17	A	1112	CLA	MG-NB	2.74	2.11	2.05
17	A	1402	CLA	C3D-C2D	2.74	1.41	1.35
17	A	1120	CLA	MG-NB	2.74	2.11	2.05
17	4	4002	CLA	C2B-C1B	2.74	1.46	1.40
17	8	1017	CLA	C2B-C1B	2.74	1.46	1.40
17	9	1032	CLA	C2B-C1B	2.74	1.46	1.40
17	Q	5228	CLA	CHC-C1C	2.74	1.43	1.38
17	Q	5215	CLA	C2B-C1B	2.74	1.46	1.40
17	8	1026	CLA	C2B-C1B	2.74	1.46	1.40
17	2	1017	CLA	C2B-C1B	2.74	1.46	1.40
17	W	5801	CLA	C2B-C1B	2.74	1.46	1.40
17	B	1221	CLA	MG-NC	2.73	2.12	2.06
17	Q	5238	CLA	MG-NC	2.73	2.12	2.06
17	B	1228	CLA	CHC-C1C	2.73	1.43	1.38
17	P	5129	CLA	CHC-C1C	2.73	1.43	1.38
17	9	1014	CLA	C2B-C1B	2.73	1.46	1.40
17	F	1229	CLA	MG-NC	2.73	2.12	2.06
17	9	1033	CLA	C2B-C1B	2.73	1.46	1.40
17	B	1238	CLA	MG-NC	2.73	2.12	2.06
17	Q	5235	CLA	C2B-C1B	2.73	1.46	1.40
17	Q	5021	CLA	MG-NB	2.73	2.11	2.05
17	P	5136	CLA	CHC-C1C	2.73	1.43	1.38
17	0	1013	CLA	C2B-C1B	2.73	1.46	1.40
17	P	5102	CLA	CHC-C1C	2.73	1.43	1.38
17	4	1013	CLA	C2B-C1B	2.73	1.46	1.40
17	Q	5234	CLA	C3D-C2D	2.73	1.41	1.35
17	P	5128	CLA	MG-NC	2.73	2.12	2.06
17	B	1021	CLA	MG-NB	2.73	2.11	2.05
17	2	4007	CLA	C2B-C1B	2.73	1.46	1.40
17	Q	8001	CLA	C2B-C1B	2.73	1.46	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	P	5112	CLA	MG-NB	2.73	2.11	2.05
17	V	5233	CLA	MG-NB	2.73	2.11	2.05
17	3	1014	CLA	C2B-C1B	2.73	1.46	1.40
17	5	5404	CLA	C2B-C1B	2.73	1.46	1.40
17	L	1503	CLA	MG-NC	2.73	2.12	2.06
17	1	1023	CLA	C2B-C1B	2.73	1.46	1.40
17	P	5116	CLA	C2B-C1B	2.73	1.46	1.40
17	6	5503	CLA	MG-NC	2.72	2.12	2.06
17	B	1213	CLA	C2B-C1B	2.72	1.46	1.40
17	B	4001	CLA	C2B-C1B	2.72	1.46	1.40
17	G	1701	CLA	C2B-C1B	2.72	1.46	1.40
17	Q	5241	CLA	C2B-C1B	2.72	1.46	1.40
17	F	4006	CLA	C2B-C1B	2.72	1.46	1.40
17	K	1403	CLA	C2B-C1B	2.72	1.46	1.40
17	4	1022	CLA	C2B-C1B	2.72	1.46	1.40
17	4	1033	CLA	C2B-C1B	2.72	1.46	1.40
17	7	1017	CLA	C2B-C1B	2.72	1.46	1.40
17	4	1021	CLA	C2B-C1B	2.72	1.46	1.40
17	1	1011	CLA	C2B-C1B	2.72	1.46	1.40
17	A	1102	CLA	CHC-C1C	2.72	1.43	1.38
17	4	1015	CLA	C2B-C1B	2.72	1.46	1.40
17	7	1012	CLA	C2B-C1B	2.72	1.46	1.40
17	8	8007	CLA	C2B-C1B	2.72	1.46	1.40
17	K	1404	CLA	C2B-C1B	2.72	1.46	1.40
17	B	1221	CLA	C2B-C1B	2.72	1.46	1.40
17	0	8002	CLA	C2B-C1B	2.72	1.46	1.40
17	3	1017	CLA	C2B-C1B	2.72	1.46	1.40
17	Q	5213	CLA	C2B-C1B	2.72	1.46	1.40
17	7	1014	CLA	C2B-C1B	2.71	1.46	1.40
17	2	1026	CLA	C2B-C1B	2.71	1.46	1.40
17	B	1241	CLA	C2B-C1B	2.71	1.46	1.40
17	A	1139	CLA	MG-NC	2.71	2.12	2.06
17	H	1801	CLA	C2B-C1B	2.71	1.46	1.40
17	Q	5228	CLA	C2B-C1B	2.71	1.46	1.40
17	A	1137	CLA	CHC-C1C	2.71	1.43	1.38
17	P	5137	CLA	CHC-C1C	2.71	1.43	1.38
17	B	1235	CLA	C2B-C1B	2.71	1.46	1.40
17	0	1033	CLA	C2B-C1B	2.71	1.46	1.40
17	A	1140	CLA	CHC-C1C	2.71	1.43	1.38
17	U	5301	CLA	CHC-C1C	2.71	1.43	1.38
17	P	5139	CLA	MG-NC	2.71	2.12	2.06
17	7	1023	CLA	C2B-C1B	2.71	1.46	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	2	1011	CLA	C2B-C1B	2.71	1.46	1.40
17	3	1012	CLA	C2B-C1B	2.71	1.46	1.40
17	8	1011	CLA	C2B-C1B	2.70	1.46	1.40
17	Q	5226	CLA	C3D-C2D	2.70	1.41	1.35
17	8	1033	CLA	C2B-C1B	2.70	1.46	1.40
17	1	1031	CLA	C2B-C1B	2.70	1.46	1.40
17	4	1011	CLA	C2B-C1B	2.70	1.46	1.40
17	9	1031	CLA	C2B-C1B	2.70	1.46	1.40
17	1	1017	CLA	C2B-C1B	2.70	1.46	1.40
17	6	5503	CLA	C3D-C2D	2.70	1.41	1.35
17	7	1031	CLA	C2B-C1B	2.70	1.46	1.40
17	8	1022	CLA	C2B-C1B	2.70	1.46	1.40
17	Q	5208	CLA	C2B-C1B	2.70	1.46	1.40
17	Z	8008	CLA	C2B-C1B	2.70	1.46	1.40
17	B	1242	CLA	C2B-C1B	2.70	1.46	1.40
17	Q	5224	CLA	MG-NB	2.70	2.11	2.05
17	F	1301	CLA	CHC-C1C	2.70	1.43	1.38
17	9	1017	CLA	C2B-C1B	2.70	1.46	1.40
17	L	1504	CLA	C2B-C1B	2.70	1.46	1.40
17	3	1033	CLA	C2B-C1B	2.70	1.46	1.40
17	Q	5221	CLA	C2B-C1B	2.70	1.46	1.40
17	B	1224	CLA	MG-NB	2.70	2.11	2.05
17	Q	5021	CLA	C3D-C2D	2.70	1.41	1.35
17	A	1114	CLA	MG-NC	2.70	2.12	2.06
17	2	1033	CLA	C2B-C1B	2.70	1.46	1.40
17	J	1101	CLA	C2B-C1B	2.69	1.46	1.40
17	4	1017	CLA	C2B-C1B	2.69	1.46	1.40
17	2	1022	CLA	C2B-C1B	2.69	1.46	1.40
17	7	1011	CLA	C2B-C1B	2.69	1.46	1.40
17	3	1031	CLA	C2B-C1B	2.69	1.46	1.40
17	P	5133	CLA	C2B-C1B	2.69	1.46	1.40
17	0	1011	CLA	C2B-C1B	2.69	1.46	1.40
17	1	1025	CLA	C2B-C1B	2.69	1.46	1.40
17	0	1017	CLA	C2B-C1B	2.69	1.46	1.40
17	4	1014	CLA	C2B-C1B	2.69	1.46	1.40
17	8	1021	CLA	C2B-C1B	2.69	1.46	1.40
17	8	1023	CLA	C2B-C1B	2.69	1.46	1.40
17	J	4008	CLA	C2B-C1B	2.69	1.46	1.40
17	3	1011	CLA	C2B-C1B	2.69	1.46	1.40
17	U	8004	CLA	C2B-C1B	2.69	1.46	1.40
18	B	2002	PQN	C8-C9	2.69	1.43	1.38
17	A	4009	CLA	C2B-C1B	2.69	1.46	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	A	4010	CLA	C2B-C1B	2.69	1.46	1.40
17	P	5140	CLA	CHC-C1C	2.69	1.43	1.38
17	2	1013	CLA	C2B-C1B	2.69	1.46	1.40
17	P	5114	CLA	MG-NC	2.69	2.12	2.06
17	F	4003	CLA	C2B-C1B	2.69	1.46	1.40
17	9	1012	CLA	C2B-C1B	2.69	1.46	1.40
17	1	1013	CLA	C2B-C1B	2.69	1.46	1.40
17	8	1013	CLA	C2B-C1B	2.69	1.46	1.40
17	8	1016	CLA	C2B-C1B	2.69	1.46	1.40
17	B	1021	CLA	C3D-C2D	2.69	1.41	1.35
17	4	1026	CLA	C2B-C1B	2.69	1.46	1.40
17	7	1025	CLA	C2B-C1B	2.69	1.46	1.40
17	7	1026	CLA	C2B-C1B	2.68	1.46	1.40
17	Z	5101	CLA	C2B-C1B	2.68	1.46	1.40
17	9	1011	CLA	C2B-C1B	2.68	1.46	1.40
17	2	1012	CLA	C2B-C1B	2.68	1.46	1.40
17	9	1026	CLA	C2B-C1B	2.68	1.46	1.40
17	1	1026	CLA	C2B-C1B	2.68	1.46	1.40
17	9	1025	CLA	C2B-C1B	2.68	1.46	1.40
17	1	1016	CLA	C2B-C1B	2.68	1.46	1.40
17	2	1023	CLA	C2B-C1B	2.68	1.46	1.40
18	Q	6002	PQN	C8-C9	2.68	1.43	1.38
17	Q	5242	CLA	C2B-C1B	2.68	1.46	1.40
17	U	8006	CLA	C2B-C1B	2.68	1.46	1.40
17	B	1226	CLA	C3D-C2D	2.68	1.41	1.35
17	2	1016	CLA	C2B-C1B	2.68	1.46	1.40
17	2	1021	CLA	C2B-C1B	2.68	1.46	1.40
17	Q	5239	CLA	C2B-C1B	2.68	1.46	1.40
17	0	1031	CLA	C2B-C1B	2.68	1.46	1.40
17	0	1032	CLA	C2B-C1B	2.68	1.46	1.40
17	L	1503	CLA	C3D-C2D	2.68	1.41	1.35
17	2	1031	CLA	C2B-C1B	2.68	1.46	1.40
17	4	1025	CLA	C2B-C1B	2.68	1.46	1.40
17	4	1032	CLA	C2B-C1B	2.68	1.46	1.40
17	0	1026	CLA	C2B-C1B	2.68	1.46	1.40
17	9	1015	CLA	C2B-C1B	2.68	1.46	1.40
17	J	1302	CLA	C2B-C1B	2.68	1.46	1.40
17	2	1025	CLA	C2B-C1B	2.68	1.46	1.40
17	0	1016	CLA	C2B-C1B	2.68	1.46	1.40
17	F	4004	CLA	C2B-C1B	2.68	1.46	1.40
17	6	5504	CLA	C2B-C1B	2.68	1.46	1.40
17	9	1021	CLA	C2B-C1B	2.68	1.46	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	A	1102	CLA	MG-NB	2.68	2.11	2.05
17	3	1021	CLA	C2B-C1B	2.68	1.46	1.40
17	Z	5302	CLA	C2B-C1B	2.68	1.46	1.40
17	4	1031	CLA	C2B-C1B	2.67	1.46	1.40
17	7	1015	CLA	C2B-C1B	2.67	1.46	1.40
17	3	1015	CLA	C2B-C1B	2.67	1.46	1.40
17	7	1013	CLA	C2B-C1B	2.67	1.46	1.40
17	3	1041	CLA	C2B-C1B	2.67	1.46	1.40
17	9	1041	CLA	C2B-C1B	2.67	1.46	1.40
17	1	1012	CLA	C2B-C1B	2.67	1.46	1.40
17	4	1016	CLA	C2B-C1B	2.67	1.46	1.40
17	0	1014	CLA	C2B-C1B	2.67	1.46	1.40
17	B	1240	CLA	C2B-C1B	2.67	1.46	1.40
17	1	1015	CLA	C2B-C1B	2.67	1.46	1.40
17	8	1025	CLA	C2B-C1B	2.67	1.46	1.40
17	A	1133	CLA	C2B-C1B	2.67	1.46	1.40
17	8	1031	CLA	C2B-C1B	2.67	1.46	1.40
17	0	1025	CLA	C2B-C1B	2.67	1.46	1.40
17	B	1239	CLA	C2B-C1B	2.66	1.46	1.40
17	A	1124	CLA	MG-NB	2.66	2.11	2.05
17	B	1228	CLA	C2B-C1B	2.66	1.46	1.40
17	P	5127	CLA	C3B-C4B	2.66	1.46	1.40
17	8	1012	CLA	C2B-C1B	2.66	1.46	1.40
17	P	5102	CLA	MG-NB	2.66	2.11	2.05
17	B	1213	CLA	MG-NB	2.66	2.11	2.05
17	8	1015	CLA	C2B-C1B	2.66	1.46	1.40
17	B	1236	CLA	C2B-C1B	2.66	1.46	1.40
17	3	1026	CLA	C2B-C1B	2.66	1.46	1.40
17	1	1021	CLA	C2B-C1B	2.66	1.45	1.40
17	3	1025	CLA	C2B-C1B	2.66	1.45	1.40
17	7	1022	CLA	C2B-C1B	2.66	1.45	1.40
17	B	1201	CLA	C2B-C1B	2.66	1.45	1.40
17	U	8003	CLA	C2B-C1B	2.66	1.45	1.40
17	B	1201	CLA	CHC-C1C	2.66	1.43	1.38
17	4	1023	CLA	C2B-C1B	2.66	1.45	1.40
17	Q	5210	CLA	C3D-C2D	2.65	1.41	1.35
17	Q	5228	CLA	CHB-C1B	-2.65	1.32	1.39
17	U	8005	CLA	C2B-C1B	2.65	1.45	1.40
17	A	1127	CLA	C3B-C4B	2.65	1.45	1.40
17	2	1015	CLA	C2B-C1B	2.65	1.45	1.40
17	P	5124	CLA	MG-NB	2.65	2.11	2.05
17	P	8009	CLA	C2B-C1B	2.65	1.45	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	P	8010	CLA	C2B-C1B	2.65	1.45	1.40
17	Q	5240	CLA	C2B-C1B	2.65	1.45	1.40
17	F	1301	CLA	C3D-C2D	2.64	1.41	1.35
17	Q	5236	CLA	C2B-C1B	2.64	1.45	1.40
17	7	1016	CLA	C2B-C1B	2.64	1.45	1.40
17	2	1014	CLA	C2B-C1B	2.64	1.45	1.40
17	3	1022	CLA	C2B-C1B	2.64	1.45	1.40
17	7	1021	CLA	C2B-C1B	2.64	1.45	1.40
17	P	5135	CLA	CHB-C4A	2.64	1.43	1.36
17	0	1023	CLA	C2B-C1B	2.64	1.45	1.40
17	B	1228	CLA	CHB-C1B	-2.64	1.32	1.39
17	Q	5213	CLA	MG-NB	2.64	2.11	2.05
17	P	5117	CLA	MG-NB	2.64	2.11	2.05
17	3	1016	CLA	C2B-C1B	2.64	1.45	1.40
17	8	1014	CLA	C2B-C1B	2.64	1.45	1.40
17	9	1016	CLA	C2B-C1B	2.63	1.45	1.40
18	B	2002	PQN	C9-C10	2.63	1.43	1.39
17	Q	5201	CLA	C2B-C1B	2.63	1.45	1.40
17	P	5114	CLA	C2B-C1B	2.63	1.45	1.40
17	P	5126	CLA	MG-NB	2.63	2.11	2.05
17	Q	5205	CLA	CHB-C1B	-2.63	1.32	1.39
17	B	1205	CLA	CHB-C1B	-2.63	1.32	1.39
17	1	1022	CLA	C2B-C1B	2.63	1.45	1.40
17	A	1132	CLA	C2B-C1B	2.63	1.45	1.40
17	B	1210	CLA	C3D-C2D	2.63	1.41	1.35
17	9	1022	CLA	C2B-C1B	2.63	1.45	1.40
17	A	1136	CLA	MG-NC	2.63	2.12	2.06
17	A	1113	CLA	C3D-C2D	2.63	1.41	1.35
17	F	4005	CLA	C2B-C1B	2.63	1.45	1.40
17	U	5301	CLA	C3D-C2D	2.62	1.41	1.35
17	A	1106	CLA	MG-NB	2.62	2.11	2.05
17	Q	5201	CLA	CHC-C1C	2.62	1.43	1.38
17	P	5113	CLA	C3D-C2D	2.62	1.41	1.35
17	A	1114	CLA	C2B-C1B	2.61	1.45	1.40
17	A	1135	CLA	CHB-C4A	2.61	1.43	1.36
17	A	1117	CLA	MG-NB	2.61	2.11	2.05
17	P	5106	CLA	MG-NB	2.61	2.11	2.05
17	Q	5232	CLA	MG-NC	2.61	2.12	2.06
17	A	1103	CLA	CHC-C1C	2.61	1.43	1.38
17	P	5136	CLA	MG-NC	2.61	2.12	2.06
17	Q	5223	CLA	CHC-C1C	2.60	1.43	1.38
17	Q	5222	CLA	MG-NB	2.60	2.10	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	B	1232	CLA	MG-NC	2.60	2.12	2.06
18	P	6001	PQN	C8-C7	2.60	1.44	1.38
17	A	1126	CLA	MG-NB	2.60	2.10	2.05
17	A	1109	CLA	MG-NC	2.60	2.12	2.06
17	P	5109	CLA	MG-NC	2.60	2.12	2.06
18	Q	6002	PQN	C5-C4	-2.60	1.43	1.48
18	B	2002	PQN	C5-C4	-2.60	1.43	1.48
18	Q	6002	PQN	C9-C10	2.60	1.43	1.39
17	P	5132	CLA	C2B-C1B	2.59	1.45	1.40
17	B	1223	CLA	CHC-C1C	2.59	1.43	1.38
17	Q	5227	CLA	C2B-C1B	2.59	1.45	1.40
17	P	5103	CLA	CHC-C1C	2.59	1.43	1.38
18	A	2001	PQN	C8-C7	2.59	1.43	1.38
17	P	5115	CLA	MG-NC	2.59	2.12	2.06
17	A	1106	CLA	C2B-C1B	2.59	1.45	1.40
17	B	1214	CLA	CHC-C1C	2.59	1.43	1.38
17	B	1227	CLA	C2B-C1B	2.58	1.45	1.40
17	A	1105	CLA	CHC-C1C	2.58	1.43	1.38
17	P	5105	CLA	CHC-C1C	2.58	1.43	1.38
18	A	2001	PQN	C7-C6	2.58	1.43	1.38
18	A	2001	PQN	C10-C1	-2.58	1.43	1.48
17	P	5106	CLA	C2B-C1B	2.58	1.45	1.40
18	P	6001	PQN	C10-C1	-2.58	1.43	1.48
17	A	1115	CLA	MG-NC	2.58	2.12	2.06
17	P	5011	CLA	MG-NC	2.57	2.12	2.06
17	A	1011	CLA	MG-NC	2.57	2.12	2.06
17	B	1215	CLA	MG-NB	2.57	2.10	2.05
17	A	1124	CLA	MG-NC	2.57	2.12	2.06
17	P	5013	CLA	CHB-C1B	-2.57	1.33	1.39
17	Q	5214	CLA	CHC-C1C	2.57	1.43	1.38
17	Q	5211	CLA	MG-NC	2.57	2.12	2.06
17	Q	5215	CLA	MG-NB	2.56	2.10	2.05
17	P	5901	CLA	C2B-C1B	2.56	1.45	1.40
17	A	1111	CLA	MG-NC	2.56	2.12	2.06
17	A	1013	CLA	CHB-C1B	-2.56	1.33	1.39
17	Q	5232	CLA	MG-NB	2.55	2.10	2.05
18	P	6001	PQN	C7-C6	2.55	1.43	1.38
17	P	5124	CLA	MG-NC	2.55	2.12	2.06
17	U	5229	CLA	MG-NB	2.55	2.10	2.05
17	P	5012	CLA	C2B-C1B	2.55	1.45	1.40
17	B	1222	CLA	MG-NB	2.54	2.10	2.05
17	A	1012	CLA	C2B-C1B	2.54	1.45	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	B	1212	CLA	C2B-C1B	2.54	1.45	1.40
17	A	1901	CLA	C2B-C1B	2.54	1.45	1.40
17	Q	5203	CLA	MG-NC	2.54	2.12	2.06
17	A	1129	CLA	CHB-C1B	-2.54	1.33	1.39
17	B	1211	CLA	MG-NC	2.54	2.12	2.06
17	P	5129	CLA	CHB-C1B	-2.54	1.33	1.39
17	A	1116	CLA	CHC-C1C	2.54	1.43	1.38
17	P	5132	CLA	MG-NC	2.53	2.12	2.06
17	Q	5224	CLA	C2B-C1B	2.53	1.45	1.40
17	P	5104	CLA	MG-NC	2.53	2.12	2.06
17	P	5111	CLA	MG-NC	2.53	2.12	2.06
17	B	1203	CLA	MG-NC	2.53	2.12	2.06
17	P	5116	CLA	CHC-C1C	2.53	1.43	1.38
17	A	1132	CLA	MG-NC	2.53	2.12	2.06
17	B	1232	CLA	MG-NB	2.53	2.10	2.05
17	P	5122	CLA	C2B-C1B	2.53	1.45	1.40
17	Q	5212	CLA	C2B-C1B	2.53	1.45	1.40
17	Q	5227	CLA	MG-NB	2.52	2.10	2.05
17	A	1119	CLA	CHB-C1B	-2.52	1.33	1.39
17	L	1503	CLA	C2B-C1B	2.52	1.45	1.40
17	Q	5237	CLA	C3D-C2D	2.52	1.41	1.35
17	6	5503	CLA	C2B-C1B	2.52	1.45	1.40
17	A	1132	CLA	C3B-C4B	2.52	1.45	1.40
17	Q	5214	CLA	C2B-C1B	2.52	1.45	1.40
17	B	1224	CLA	C2B-C1B	2.52	1.45	1.40
17	P	5119	CLA	CHB-C1B	-2.52	1.33	1.39
17	B	1227	CLA	MG-NB	2.52	2.10	2.05
17	F	1229	CLA	MG-NB	2.52	2.10	2.05
17	P	5132	CLA	C3B-C4B	2.52	1.45	1.40
17	A	1122	CLA	C2B-C1B	2.52	1.45	1.40
17	A	1011	CLA	C3B-C4B	2.51	1.45	1.40
17	P	5125	CLA	MG-NC	2.51	2.12	2.06
17	A	1125	CLA	MG-NC	2.51	2.12	2.06
17	P	5011	CLA	C3B-C4B	2.51	1.45	1.40
17	B	1237	CLA	C3D-C2D	2.50	1.41	1.35
17	A	1104	CLA	MG-NC	2.50	2.12	2.06
17	Q	5023	CLA	C3D-C2D	2.50	1.41	1.35
17	Q	5023	CLA	CHB-C1B	-2.50	1.33	1.39
17	P	5128	CLA	C3D-C2D	2.49	1.41	1.35
17	F	1229	CLA	CHC-C1C	2.49	1.43	1.38
17	B	1023	CLA	CHB-C1B	-2.49	1.33	1.39
17	P	5136	CLA	C3D-C2D	2.49	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	B	1239	CLA	C3B-C4B	2.49	1.45	1.40
17	B	1023	CLA	C3D-C2D	2.49	1.40	1.35
18	B	2002	PQN	C8-C7	2.48	1.43	1.38
17	A	1136	CLA	C3D-C2D	2.48	1.40	1.35
17	F	1229	CLA	C2B-C1B	2.48	1.45	1.40
17	B	1214	CLA	C2B-C1B	2.48	1.45	1.40
17	Q	5209	CLA	C3D-C2D	2.48	1.40	1.35
17	P	5112	CLA	C3D-C2D	2.48	1.40	1.35
18	A	2001	PQN	C9-C10	2.47	1.43	1.39
17	Q	5204	CLA	CHB-C1B	-2.47	1.33	1.39
17	A	1112	CLA	C3D-C2D	2.47	1.40	1.35
17	Q	5223	CLA	CHB-C4A	2.47	1.42	1.36
17	B	1204	CLA	CHB-C1B	-2.47	1.33	1.39
17	A	1137	CLA	C3D-C2D	2.47	1.40	1.35
17	Q	5130	CLA	C3D-C2D	2.47	1.40	1.35
17	Q	5228	CLA	MG-NB	2.47	2.10	2.05
18	P	6001	PQN	C5-C4	-2.47	1.44	1.48
17	Q	5239	CLA	C3B-C4B	2.47	1.45	1.40
17	B	1130	CLA	C3D-C2D	2.47	1.40	1.35
17	B	1202	CLA	C3D-C2D	2.47	1.40	1.35
17	Q	5202	CLA	C3D-C2D	2.47	1.40	1.35
17	Q	5217	CLA	CHC-C1C	2.47	1.43	1.38
18	Q	6002	PQN	C8-C7	2.46	1.43	1.38
17	U	5229	CLA	C2B-C1B	2.46	1.45	1.40
17	Q	5219	CLA	C3D-C2D	2.46	1.40	1.35
17	Q	5230	CLA	CHB-C4A	2.46	1.42	1.36
18	A	2001	PQN	C5-C4	-2.46	1.44	1.48
17	P	5134	CLA	C3D-C2D	2.46	1.40	1.35
17	B	1228	CLA	MG-NB	2.46	2.10	2.05
18	P	6001	PQN	C9-C10	2.46	1.43	1.39
17	A	1128	CLA	C3D-C2D	2.46	1.40	1.35
17	B	1220	CLA	C3D-C2D	2.46	1.40	1.35
17	Q	5216	CLA	C3D-C2D	2.46	1.40	1.35
17	B	1227	CLA	CHC-C1C	2.46	1.43	1.38
17	Q	5220	CLA	C3D-C2D	2.46	1.40	1.35
17	Q	5207	CLA	C3D-C2D	2.46	1.40	1.35
17	U	5229	CLA	CHC-C1C	2.46	1.43	1.38
17	A	1134	CLA	C3D-C2D	2.46	1.40	1.35
17	P	5104	CLA	CHC-C1C	2.46	1.43	1.38
17	B	1230	CLA	CHB-C4A	2.46	1.42	1.36
17	B	1223	CLA	CHB-C4A	2.45	1.42	1.36
17	B	1217	CLA	CHC-C1C	2.45	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	Q	5227	CLA	CHC-C1C	2.45	1.43	1.38
17	P	5117	CLA	MG-NC	2.45	2.12	2.06
17	A	1117	CLA	MG-NC	2.45	2.12	2.06
17	P	5134	CLA	CHC-C1C	2.45	1.43	1.38
17	Q	5220	CLA	MG-NC	2.45	2.12	2.06
17	A	1134	CLA	CHC-C1C	2.45	1.43	1.38
17	B	1022	CLA	MG-ND	-2.45	2.00	2.05
17	P	5137	CLA	C3D-C2D	2.45	1.40	1.35
17	P	5124	CLA	CHB-C1B	-2.44	1.33	1.39
17	A	1108	CLA	C2B-C1B	2.44	1.45	1.40
17	P	5120	CLA	C2B-C1B	2.44	1.45	1.40
17	Q	5022	CLA	MG-ND	-2.44	2.00	2.05
17	P	5111	CLA	C3D-C2D	2.44	1.40	1.35
17	L	1501	CLA	C3D-C2D	2.44	1.40	1.35
17	B	1207	CLA	C3D-C2D	2.44	1.40	1.35
17	B	1219	CLA	C3D-C2D	2.44	1.40	1.35
17	B	1209	CLA	C3D-C2D	2.44	1.40	1.35
17	P	5139	CLA	CHB-C4A	2.44	1.42	1.36
17	A	1139	CLA	CHB-C4A	2.44	1.42	1.36
17	P	5013	CLA	MG-NC	2.43	2.12	2.06
17	A	1120	CLA	C2B-C1B	2.43	1.45	1.40
17	P	5133	CLA	MG-NC	2.43	2.12	2.06
17	Q	5239	CLA	MG-NC	2.43	2.12	2.06
17	B	1232	CLA	C2B-C1B	2.43	1.45	1.40
17	B	1216	CLA	C3D-C2D	2.43	1.40	1.35
17	B	1204	CLA	MG-NB	2.43	2.10	2.05
17	A	1133	CLA	MG-NC	2.43	2.12	2.06
17	B	1219	CLA	CHC-C1C	2.43	1.43	1.38
17	A	1124	CLA	CHB-C1B	-2.43	1.33	1.39
17	A	1102	CLA	C2B-C1B	2.43	1.45	1.40
17	B	1239	CLA	MG-NC	2.43	2.12	2.06
17	B	1220	CLA	MG-NC	2.43	2.12	2.06
17	P	5110	CLA	C3D-C2D	2.43	1.40	1.35
17	P	5108	CLA	C2B-C1B	2.43	1.45	1.40
17	Q	5214	CLA	MG-NC	2.43	2.12	2.06
17	P	5114	CLA	MG-NB	2.42	2.10	2.05
17	B	1216	CLA	MG-NB	2.42	2.10	2.05
17	A	1013	CLA	MG-NC	2.42	2.12	2.06
17	A	1104	CLA	CHC-C1C	2.42	1.43	1.38
17	B	1214	CLA	MG-NC	2.42	2.12	2.06
17	L	1502	CLA	CHB-C1B	-2.42	1.33	1.39
17	P	5102	CLA	C2B-C1B	2.42	1.45	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	A	1110	CLA	C3D-C2D	2.42	1.40	1.35
17	Q	5223	CLA	C3D-C2D	2.42	1.40	1.35
17	A	1124	CLA	C2B-C1B	2.42	1.45	1.40
17	6	5502	CLA	CHB-C1B	-2.42	1.33	1.39
17	6	5501	CLA	C3D-C2D	2.41	1.40	1.35
17	Q	5204	CLA	MG-NB	2.41	2.10	2.05
17	P	5901	CLA	C3D-C2D	2.41	1.40	1.35
17	Q	5222	CLA	MG-NC	2.41	2.12	2.06
17	A	1111	CLA	C3D-C2D	2.41	1.40	1.35
17	Q	5219	CLA	CHC-C1C	2.41	1.43	1.38
17	B	1223	CLA	C3D-C2D	2.40	1.40	1.35
17	B	1232	CLA	C3D-C2D	2.40	1.40	1.35
18	B	2002	PQN	C2-C1	-2.40	1.44	1.48
17	A	1114	CLA	MG-NB	2.40	2.10	2.05
17	P	5120	CLA	C3D-C2D	2.40	1.40	1.35
17	A	1901	CLA	C3D-C2D	2.40	1.40	1.35
17	P	5124	CLA	C2B-C1B	2.40	1.45	1.40
18	Q	6002	PQN	C2-C1	-2.40	1.44	1.48
17	A	1110	CLA	MG-NB	2.40	2.10	2.05
17	A	1138	CLA	CHB-C1B	-2.40	1.33	1.39
17	B	1021	CLA	CHB-C1B	-2.40	1.33	1.39
17	Q	5232	CLA	C2B-C1B	2.40	1.45	1.40
17	P	5138	CLA	CHB-C1B	-2.39	1.33	1.39
17	Q	5216	CLA	MG-NB	2.39	2.10	2.05
17	Q	5232	CLA	C3D-C2D	2.39	1.40	1.35
17	B	1222	CLA	MG-NC	2.39	2.12	2.06
17	A	1115	CLA	CHC-C1C	2.39	1.43	1.38
17	4	1012	CLA	CHB-C1B	-2.39	1.33	1.39
17	B	1221	CLA	C3D-C2D	2.39	1.40	1.35
17	P	5122	CLA	MG-NB	2.39	2.10	2.05
17	P	5110	CLA	MG-NB	2.39	2.10	2.05
17	B	1209	CLA	CHC-C1C	2.39	1.43	1.38
17	B	1214	CLA	CHB-C1B	-2.39	1.33	1.39
17	B	1228	CLA	C3D-C2D	2.38	1.40	1.35
17	P	5112	CLA	MG-NC	2.38	2.11	2.06
17	Q	5209	CLA	CHC-C1C	2.38	1.43	1.38
17	P	5115	CLA	CHC-C1C	2.38	1.43	1.38
17	A	1120	CLA	C3D-C2D	2.38	1.40	1.35
17	B	1209	CLA	CHB-C4A	2.38	1.42	1.36
17	A	1122	CLA	MG-NB	2.38	2.10	2.05
17	Q	5225	CLA	C2B-C1B	2.38	1.45	1.40
17	Q	5021	CLA	CHB-C1B	-2.38	1.33	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	Q	5022	CLA	CHC-C1C	2.38	1.43	1.38
17	A	1013	CLA	C3D-C2D	2.38	1.40	1.35
17	0	1012	CLA	CHB-C1B	-2.37	1.33	1.39
17	A	1129	CLA	C2B-C1B	2.37	1.45	1.40
17	A	1112	CLA	MG-NC	2.37	2.11	2.06
17	Q	5214	CLA	CHB-C1B	-2.37	1.33	1.39
17	Q	5228	CLA	C3D-C2D	2.37	1.40	1.35
17	B	1208	CLA	CHB-C1B	-2.37	1.33	1.39
17	A	1116	CLA	C3D-C2D	2.37	1.40	1.35
17	Q	5221	CLA	C3D-C2D	2.37	1.40	1.35
17	9	1011	CLA	CHB-C1B	-2.36	1.33	1.39
17	Q	5213	CLA	MG-NC	2.36	2.11	2.06
17	B	1022	CLA	CHC-C1C	2.36	1.43	1.38
17	5	5401	CLA	C3D-C2D	2.36	1.40	1.35
17	B	1208	CLA	MG-NC	2.36	2.11	2.06
17	Q	5208	CLA	MG-NC	2.36	2.11	2.06
17	Q	5208	CLA	CHB-C1B	-2.35	1.33	1.39
17	P	5013	CLA	C3D-C2D	2.35	1.40	1.35
17	B	1213	CLA	MG-NC	2.35	2.11	2.06
17	9	1017	CLA	CHB-C1B	-2.35	1.33	1.39
17	B	1221	CLA	CHB-C1B	-2.35	1.33	1.39
17	Q	5209	CLA	CHB-C4A	2.35	1.42	1.36
17	P	5129	CLA	C2B-C1B	2.35	1.45	1.40
17	Q	5206	CLA	C2B-C1B	2.35	1.45	1.40
17	Q	5217	CLA	C3D-C2D	2.35	1.40	1.35
17	0	8002	CLA	CHB-C1B	-2.35	1.33	1.39
17	B	1225	CLA	C2B-C1B	2.35	1.45	1.40
17	K	1401	CLA	C3D-C2D	2.35	1.40	1.35
17	Q	5207	CLA	MG-ND	-2.35	2.01	2.05
17	3	1011	CLA	CHB-C1B	-2.35	1.33	1.39
17	B	1207	CLA	MG-ND	-2.35	2.01	2.05
17	P	8009	CLA	CHB-C1B	-2.35	1.33	1.39
17	P	5116	CLA	C3D-C2D	2.34	1.40	1.35
17	A	1102	CLA	MG-NC	2.34	2.11	2.06
17	4	4002	CLA	CHB-C1B	-2.34	1.33	1.39
17	0	1015	CLA	CHB-C1B	-2.34	1.33	1.39
17	A	1127	CLA	CHB-C4A	2.34	1.42	1.36
17	V	5701	CLA	CHB-C1B	-2.34	1.33	1.39
17	0	1031	CLA	CHB-C1B	-2.34	1.33	1.39
17	A	1119	CLA	C3D-C2D	2.34	1.40	1.35
17	B	1231	CLA	C3D-C2D	2.34	1.40	1.35
17	P	5123	CLA	MG-NC	2.33	2.11	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	A	4009	CLA	CHB-C1B	-2.33	1.33	1.39
17	P	5115	CLA	CHB-C1B	-2.33	1.33	1.39
17	J	1302	CLA	C3D-C2D	2.33	1.40	1.35
17	Q	5239	CLA	MG-NB	2.33	2.10	2.05
17	Q	5231	CLA	C3D-C2D	2.33	1.40	1.35
17	2	1015	CLA	CHB-C1B	-2.33	1.33	1.39
17	3	1017	CLA	CHB-C1B	-2.33	1.33	1.39
17	7	1012	CLA	CHB-C1B	-2.33	1.33	1.39
17	B	1206	CLA	C2B-C1B	2.33	1.45	1.40
17	B	1236	CLA	CHC-C1C	2.33	1.43	1.38
17	P	5102	CLA	MG-NC	2.33	2.11	2.06
17	Q	5213	CLA	CHC-C1C	2.33	1.43	1.38
17	A	1106	CLA	CHB-C1B	-2.33	1.33	1.39
17	8	1025	CLA	CHB-C1B	-2.33	1.33	1.39
17	Q	5236	CLA	CHB-C1B	-2.33	1.33	1.39
17	8	1011	CLA	CHB-C1B	-2.33	1.33	1.39
17	1	1016	CLA	CHB-C1B	-2.33	1.33	1.39
17	4	1015	CLA	CHB-C1B	-2.33	1.33	1.39
17	B	1204	CLA	MG-NC	2.33	2.11	2.06
17	Q	5236	CLA	CHC-C1C	2.33	1.43	1.38
17	Q	5221	CLA	CHB-C1B	-2.33	1.33	1.39
17	P	5119	CLA	MG-NB	2.33	2.10	2.05
17	P	5106	CLA	CHB-C1B	-2.33	1.33	1.39
17	1	1026	CLA	CHB-C1B	-2.32	1.33	1.39
17	6	5501	CLA	C2C-C1C	2.32	1.48	1.43
17	2	1025	CLA	CHB-C1B	-2.32	1.33	1.39
17	3	1014	CLA	CHB-C1B	-2.32	1.33	1.39
17	9	1041	CLA	CHB-C1B	-2.32	1.33	1.39
17	2	1011	CLA	CHB-C1B	-2.32	1.33	1.39
17	9	1032	CLA	CHB-C1B	-2.32	1.33	1.39
17	P	5112	CLA	CHB-C1B	-2.32	1.33	1.39
17	B	1239	CLA	MG-NB	2.32	2.10	2.05
17	P	5140	CLA	MG-NB	2.32	2.10	2.05
17	A	1115	CLA	CHB-C1B	-2.32	1.33	1.39
17	B	4001	CLA	CHB-C1B	-2.32	1.33	1.39
17	A	1122	CLA	CHC-C1C	2.32	1.43	1.38
17	Q	8001	CLA	CHB-C1B	-2.32	1.33	1.39
17	P	5127	CLA	CHB-C4A	2.32	1.42	1.36
17	0	1013	CLA	CHB-C1B	-2.32	1.33	1.39
17	G	1701	CLA	CHB-C1B	-2.32	1.33	1.39
17	3	1041	CLA	CHB-C1B	-2.32	1.33	1.39
17	8	1031	CLA	CHB-C1B	-2.32	1.33	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	B	1236	CLA	CHB-C1B	-2.32	1.33	1.39
17	Q	5201	CLA	MG-NC	2.32	2.11	2.06
17	B	1218	CLA	C3D-C2D	2.32	1.40	1.35
17	A	1123	CLA	MG-NC	2.32	2.11	2.06
17	B	1201	CLA	MG-NC	2.32	2.11	2.06
17	A	1132	CLA	C3D-C2D	2.32	1.40	1.35
17	2	1031	CLA	CHB-C1B	-2.32	1.33	1.39
17	Q	5204	CLA	MG-NC	2.32	2.11	2.06
17	7	1016	CLA	CHB-C1B	-2.32	1.33	1.39
17	P	5113	CLA	CHB-C4A	2.32	1.42	1.36
17	8	1015	CLA	CHB-C1B	-2.32	1.33	1.39
17	L	1502	CLA	C3D-C2D	2.31	1.40	1.35
17	1	1025	CLA	CHB-C1B	-2.31	1.33	1.39
17	Q	5235	CLA	CHB-C1B	-2.31	1.33	1.39
17	B	1241	CLA	CHB-C1B	-2.31	1.33	1.39
17	8	1026	CLA	CHB-C1B	-2.31	1.33	1.39
17	J	4008	CLA	CHB-C1B	-2.31	1.33	1.39
17	Q	5240	CLA	CHB-C1B	-2.31	1.33	1.39
17	0	1025	CLA	CHB-C1B	-2.31	1.33	1.39
17	4	1031	CLA	CHB-C1B	-2.31	1.33	1.39
17	B	1235	CLA	CHB-C1B	-2.31	1.33	1.39
17	L	1501	CLA	C2C-C1C	2.31	1.48	1.43
17	G	1233	CLA	CHB-C4A	2.31	1.42	1.36
17	0	1016	CLA	CHB-C1B	-2.31	1.33	1.39
17	3	1032	CLA	CHB-C1B	-2.31	1.33	1.39
17	2	1033	CLA	CHB-C1B	-2.31	1.33	1.39
17	4	1025	CLA	CHB-C1B	-2.31	1.33	1.39
17	Q	5237	CLA	MG-NB	2.31	2.10	2.05
17	P	8010	CLA	CHB-C1B	-2.31	1.33	1.39
17	2	1026	CLA	CHB-C1B	-2.31	1.33	1.39
17	A	1127	CLA	MG-NB	2.31	2.10	2.05
17	P	5127	CLA	MG-NB	2.31	2.10	2.05
17	P	5119	CLA	C3D-C2D	2.31	1.40	1.35
17	4	1011	CLA	CHB-C1B	-2.31	1.33	1.39
17	B	1237	CLA	MG-NB	2.31	2.10	2.05
17	4	1016	CLA	CHB-C1B	-2.31	1.33	1.39
17	Z	8008	CLA	CHB-C1B	-2.31	1.33	1.39
17	B	1210	CLA	CHB-C1B	-2.31	1.33	1.39
17	8	1033	CLA	CHB-C1B	-2.31	1.33	1.39
17	A	1140	CLA	MG-NB	2.31	2.10	2.05
17	4	1017	CLA	CHB-C1B	-2.31	1.33	1.39
17	4	1033	CLA	CHB-C1B	-2.31	1.33	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	5	5404	CLA	CHB-C1B	-2.31	1.33	1.39
17	Q	5230	CLA	MG-NC	2.31	2.11	2.06
17	3	1021	CLA	CHB-C1B	-2.31	1.33	1.39
17	4	1026	CLA	CHB-C1B	-2.31	1.33	1.39
17	8	1017	CLA	CHB-C1B	-2.31	1.33	1.39
17	0	1014	CLA	CHB-C1B	-2.31	1.33	1.39
17	B	1217	CLA	C3D-C2D	2.31	1.40	1.35
17	A	4010	CLA	CHB-C1B	-2.31	1.33	1.39
17	B	1240	CLA	CHB-C1B	-2.31	1.33	1.39
17	2	1012	CLA	CHB-C1B	-2.31	1.33	1.39
17	3	1026	CLA	CHB-C1B	-2.31	1.33	1.39
17	B	1217	CLA	CHB-C4A	2.31	1.42	1.36
17	U	8003	CLA	CHB-C1B	-2.31	1.33	1.39
17	P	5107	CLA	CHC-C1C	2.31	1.43	1.38
17	0	1033	CLA	CHB-C1B	-2.31	1.33	1.39
17	G	1233	CLA	MG-NC	2.31	2.11	2.06
17	P	5119	CLA	MG-NC	2.31	2.11	2.06
17	7	1025	CLA	CHB-C1B	-2.30	1.33	1.39
17	P	5132	CLA	C3D-C2D	2.30	1.40	1.35
17	Q	5215	CLA	MG-NC	2.30	2.11	2.06
17	8	1023	CLA	CHB-C1B	-2.30	1.33	1.39
17	Z	5302	CLA	C3D-C2D	2.30	1.40	1.35
17	A	1112	CLA	CHB-C1B	-2.30	1.33	1.39
17	F	4003	CLA	CHB-C1B	-2.30	1.33	1.39
17	7	1026	CLA	CHB-C1B	-2.30	1.33	1.39
17	9	1021	CLA	CHB-C1B	-2.30	1.33	1.39
17	V	5233	CLA	CHB-C4A	2.30	1.42	1.36
17	9	1014	CLA	CHB-C1B	-2.30	1.33	1.39
17	9	1026	CLA	CHB-C1B	-2.30	1.33	1.39
17	B	1216	CLA	C2B-C1B	2.30	1.45	1.40
17	U	8004	CLA	CHB-C1B	-2.30	1.33	1.39
17	K	1404	CLA	CHB-C1B	-2.30	1.33	1.39
17	B	1211	CLA	CHC-C1C	2.30	1.43	1.38
17	Q	5210	CLA	CHB-C1B	-2.30	1.33	1.39
17	9	1022	CLA	CHB-C1B	-2.30	1.33	1.39
17	F	4004	CLA	CHB-C1B	-2.30	1.33	1.39
17	L	1504	CLA	CHB-C1B	-2.30	1.33	1.39
17	2	1017	CLA	CHB-C1B	-2.30	1.33	1.39
17	3	1022	CLA	CHB-C1B	-2.30	1.33	1.39
17	B	1213	CLA	CHC-C1C	2.30	1.43	1.38
17	6	5502	CLA	C3D-C2D	2.30	1.40	1.35
17	Q	5241	CLA	CHB-C1B	-2.30	1.33	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	U	8005	CLA	CHB-C1B	-2.30	1.33	1.39
17	9	1031	CLA	CHB-C1B	-2.30	1.33	1.39
17	4	1022	CLA	CHB-C1B	-2.30	1.33	1.39
17	U	8006	CLA	CHB-C1B	-2.30	1.33	1.39
17	J	1101	CLA	CHB-C1B	-2.30	1.33	1.39
17	7	1023	CLA	CHB-C1B	-2.30	1.33	1.39
17	A	1107	CLA	CHC-C1C	2.30	1.43	1.38
17	A	1119	CLA	MG-NC	2.30	2.11	2.06
17	2	1023	CLA	CHB-C1B	-2.30	1.33	1.39
17	B	1230	CLA	MG-NC	2.30	2.11	2.06
17	F	4006	CLA	CHB-C1B	-2.30	1.33	1.39
17	Q	5216	CLA	C2B-C1B	2.29	1.45	1.40
17	4	1014	CLA	CHB-C1B	-2.29	1.33	1.39
17	H	1801	CLA	CHB-C1B	-2.29	1.33	1.39
17	1	1023	CLA	CHB-C1B	-2.29	1.33	1.39
17	W	5801	CLA	CHB-C1B	-2.29	1.33	1.39
17	P	5122	CLA	CHC-C1C	2.29	1.43	1.38
17	A	1119	CLA	MG-NB	2.29	2.10	2.05
17	4	1013	CLA	CHB-C1B	-2.29	1.33	1.39
17	Q	5217	CLA	CHB-C4A	2.29	1.42	1.36
17	1	1012	CLA	CHB-C1B	-2.29	1.33	1.39
17	1	1022	CLA	CHB-C1B	-2.29	1.33	1.39
17	0	1022	CLA	CHB-C1B	-2.29	1.33	1.39
17	0	1011	CLA	CHB-C1B	-2.29	1.33	1.39
17	0	1026	CLA	CHB-C1B	-2.29	1.33	1.39
17	F	4005	CLA	CHB-C1B	-2.29	1.33	1.39
17	9	1025	CLA	CHB-C1B	-2.29	1.33	1.39
17	4	1021	CLA	CHB-C1B	-2.29	1.33	1.39
17	Q	5218	CLA	C3D-C2D	2.29	1.40	1.35
17	2	1013	CLA	CHB-C1B	-2.29	1.33	1.39
17	K	1401	CLA	CHC-C1C	2.29	1.43	1.38
17	V	5233	CLA	MG-NC	2.29	2.11	2.06
17	Q	5216	CLA	CHC-C1C	2.29	1.43	1.38
17	1	1011	CLA	CHB-C1B	-2.29	1.33	1.39
17	B	1216	CLA	CHC-C1C	2.29	1.43	1.38
17	1	1021	CLA	CHB-C1B	-2.29	1.33	1.39
17	B	1242	CLA	CHB-C1B	-2.29	1.33	1.39
17	A	1113	CLA	CHB-C4A	2.29	1.42	1.36
17	A	1104	CLA	MG-ND	-2.29	2.01	2.05
17	2	1016	CLA	CHB-C1B	-2.28	1.33	1.39
17	7	1021	CLA	CHB-C1B	-2.28	1.33	1.39
17	8	1022	CLA	CHB-C1B	-2.28	1.33	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	0	1017	CLA	CHB-C1B	-2.28	1.33	1.39
17	7	1017	CLA	CHB-C1B	-2.28	1.33	1.39
17	B	1215	CLA	MG-NC	2.28	2.11	2.06
17	1	1014	CLA	CHB-C1B	-2.28	1.33	1.39
17	7	1013	CLA	CHB-C1B	-2.28	1.33	1.39
17	P	5139	CLA	C3D-C2D	2.28	1.40	1.35
17	B	1237	CLA	C2B-C1B	2.28	1.45	1.40
17	4	1023	CLA	CHB-C1B	-2.28	1.33	1.39
17	1	1013	CLA	CHB-C1B	-2.28	1.33	1.39
17	8	1012	CLA	CHB-C1B	-2.28	1.33	1.39
17	9	1016	CLA	CHB-C1B	-2.28	1.33	1.39
17	7	1022	CLA	CHB-C1B	-2.28	1.33	1.39
17	3	1031	CLA	CHB-C1B	-2.28	1.33	1.39
17	Q	5211	CLA	CHC-C1C	2.28	1.43	1.38
17	3	1016	CLA	CHB-C1B	-2.28	1.33	1.39
17	4	1032	CLA	CHB-C1B	-2.28	1.33	1.39
17	Q	5237	CLA	C2B-C1B	2.28	1.45	1.40
17	2	1014	CLA	CHB-C1B	-2.28	1.33	1.39
17	3	1025	CLA	CHB-C1B	-2.28	1.33	1.39
17	Q	5214	CLA	C3D-C2D	2.28	1.40	1.35
17	6	5504	CLA	CHB-C1B	-2.28	1.33	1.39
17	V	5233	CLA	C3D-C2D	2.28	1.40	1.35
17	3	1015	CLA	CHB-C1B	-2.28	1.33	1.39
17	B	1130	CLA	CHB-C4A	2.27	1.42	1.36
17	3	1033	CLA	CHB-C1B	-2.27	1.33	1.39
17	0	1023	CLA	CHB-C1B	-2.27	1.33	1.39
17	J	1302	CLA	CHB-C4A	2.27	1.42	1.36
17	A	1104	CLA	C3D-C2D	2.27	1.40	1.35
17	1	1017	CLA	CHB-C1B	-2.27	1.33	1.39
17	1	1031	CLA	CHB-C1B	-2.27	1.33	1.39
17	8	1013	CLA	CHB-C1B	-2.27	1.33	1.39
17	A	1123	CLA	C3D-C2D	2.27	1.40	1.35
17	2	1021	CLA	CHB-C1B	-2.27	1.33	1.39
17	K	1403	CLA	CHB-C1B	-2.27	1.33	1.39
17	0	1021	CLA	CHB-C1B	-2.27	1.33	1.39
17	P	5123	CLA	C3D-C2D	2.27	1.40	1.35
17	8	1016	CLA	CHB-C1B	-2.27	1.33	1.39
17	P	5109	CLA	C3D-C2D	2.27	1.40	1.35
17	8	1021	CLA	CHB-C1B	-2.27	1.33	1.39
17	Q	5242	CLA	CHB-C1B	-2.27	1.33	1.39
17	Z	5101	CLA	CHB-C1B	-2.27	1.33	1.39
17	7	1011	CLA	CHB-C1B	-2.27	1.33	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	A	1129	CLA	MG-NB	2.27	2.10	2.05
17	Q	5130	CLA	CHB-C4A	2.27	1.42	1.36
17	Z	5302	CLA	CHB-C4A	2.27	1.42	1.36
17	G	1233	CLA	C3D-C2D	2.27	1.40	1.35
17	P	5133	CLA	C3D-C2D	2.27	1.40	1.35
17	8	8007	CLA	CHB-C1B	-2.27	1.33	1.39
17	9	1033	CLA	CHB-C1B	-2.27	1.33	1.39
17	P	5104	CLA	C3D-C2D	2.27	1.40	1.35
17	A	1109	CLA	C3D-C2D	2.27	1.40	1.35
17	1	1015	CLA	CHB-C1B	-2.26	1.33	1.39
17	2	1022	CLA	CHB-C1B	-2.26	1.33	1.39
17	5	5403	CLA	CHB-C1B	-2.26	1.33	1.39
17	7	1014	CLA	CHB-C1B	-2.26	1.33	1.39
17	A	1139	CLA	C3D-C2D	2.26	1.40	1.35
17	3	1012	CLA	CHB-C1B	-2.26	1.33	1.39
17	9	1015	CLA	CHB-C1B	-2.26	1.33	1.39
17	P	5104	CLA	MG-ND	-2.26	2.01	2.05
17	9	1012	CLA	CHB-C1B	-2.26	1.33	1.39
17	B	1227	CLA	CHB-C1B	-2.26	1.33	1.39
17	Q	5210	CLA	CHC-C1C	2.26	1.42	1.38
17	8	1014	CLA	CHB-C1B	-2.26	1.33	1.39
17	Q	5218	CLA	MG-NC	2.26	2.11	2.06
17	A	1103	CLA	CHB-C1B	-2.25	1.33	1.39
17	9	1025	CLA	CHC-C1C	2.25	1.42	1.38
17	5	5401	CLA	CHC-C1C	2.25	1.42	1.38
17	Q	5224	CLA	C3D-C2D	2.25	1.40	1.35
17	0	1032	CLA	CHB-C1B	-2.25	1.33	1.39
17	7	1031	CLA	CHB-C1B	-2.25	1.33	1.39
17	P	5122	CLA	MG-NC	2.25	2.11	2.06
17	P	5103	CLA	CHB-C1B	-2.25	1.33	1.39
17	P	5107	CLA	C2B-C1B	2.25	1.45	1.40
17	Q	5217	CLA	MG-NC	2.25	2.11	2.06
17	8	1033	CLA	CHC-C1C	2.25	1.42	1.38
17	A	1122	CLA	MG-NC	2.25	2.11	2.06
17	2	4007	CLA	CHB-C1B	-2.24	1.33	1.39
17	7	1015	CLA	CHB-C1B	-2.24	1.33	1.39
17	B	1235	CLA	C3D-C2D	2.24	1.40	1.35
17	B	1214	CLA	C3D-C2D	2.24	1.40	1.35
17	B	1218	CLA	MG-NC	2.24	2.11	2.06
17	B	1210	CLA	CHC-C1C	2.24	1.42	1.38
17	B	1224	CLA	C3D-C2D	2.24	1.40	1.35
17	8	1031	CLA	CHC-C1C	2.24	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	P	5136	CLA	CHB-C1B	-2.24	1.34	1.39
17	Q	5235	CLA	C3D-C2D	2.24	1.40	1.35
17	0	8002	CLA	CHC-C1C	2.23	1.42	1.38
17	B	1231	CLA	CHB-C1B	-2.23	1.34	1.39
17	B	1232	CLA	CHB-C1B	-2.23	1.34	1.39
17	B	1228	CLA	MG-NC	2.23	2.11	2.06
17	A	1133	CLA	C3D-C2D	2.23	1.40	1.35
17	P	5129	CLA	MG-NB	2.23	2.10	2.05
17	Q	5227	CLA	CHB-C1B	-2.23	1.34	1.39
17	Q	5232	CLA	CHB-C1B	-2.23	1.34	1.39
17	A	1132	CLA	CHB-C1B	-2.23	1.34	1.39
17	0	1023	CLA	CHC-C1C	2.23	1.42	1.38
17	7	1026	CLA	CHC-C1C	2.23	1.42	1.38
17	2	1033	CLA	CHC-C1C	2.22	1.42	1.38
17	U	8006	CLA	CHC-C1C	2.22	1.42	1.38
17	B	1217	CLA	MG-NC	2.22	2.11	2.06
17	Q	5228	CLA	MG-NC	2.22	2.11	2.06
17	1	1026	CLA	CHC-C1C	2.22	1.42	1.38
17	B	1208	CLA	CHC-C1C	2.22	1.42	1.38
17	2	1031	CLA	CHC-C1C	2.22	1.42	1.38
18	B	2002	PQN	C7-C6	2.22	1.42	1.38
17	B	1242	CLA	CHC-C1C	2.22	1.42	1.38
17	Q	5208	CLA	CHC-C1C	2.22	1.42	1.38
17	A	1011	CLA	MG-NB	2.22	2.10	2.05
17	9	1016	CLA	CHC-C1C	2.22	1.42	1.38
17	0	1022	CLA	CHC-C1C	2.22	1.42	1.38
17	B	1238	CLA	MG-NB	2.22	2.10	2.05
17	P	5132	CLA	CHB-C1B	-2.22	1.34	1.39
17	A	1136	CLA	CHB-C1B	-2.21	1.34	1.39
17	Q	5231	CLA	CHB-C1B	-2.21	1.34	1.39
17	4	1022	CLA	CHC-C1C	2.21	1.42	1.38
17	7	1017	CLA	CHC-C1C	2.21	1.42	1.38
17	9	1021	CLA	CHC-C1C	2.21	1.42	1.38
17	9	1014	CLA	CHC-C1C	2.21	1.42	1.38
17	3	1025	CLA	CHC-C1C	2.21	1.42	1.38
17	8	1015	CLA	CHC-C1C	2.21	1.42	1.38
17	0	1011	CLA	CHC-C1C	2.21	1.42	1.38
17	B	1023	CLA	CHD-C1D	2.21	1.44	1.38
17	B	1237	CLA	C3C-C4C	2.21	1.48	1.43
17	Q	5237	CLA	C3C-C4C	2.21	1.48	1.43
18	Q	6002	PQN	C7-C6	2.21	1.42	1.38
17	B	1241	CLA	CHC-C1C	2.21	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	2	1022	CLA	CHC-C1C	2.21	1.42	1.38
17	P	5011	CLA	MG-NB	2.20	2.10	2.05
17	2	1014	CLA	CHC-C1C	2.20	1.42	1.38
17	A	1132	CLA	MG-NB	2.20	2.10	2.05
17	3	1021	CLA	CHC-C1C	2.20	1.42	1.38
17	P	5122	CLA	CHB-C1B	-2.20	1.34	1.39
17	3	1014	CLA	CHC-C1C	2.20	1.42	1.38
17	4	1011	CLA	CHC-C1C	2.20	1.42	1.38
17	P	5132	CLA	MG-NB	2.20	2.10	2.05
17	B	1238	CLA	C3B-C4B	2.20	1.45	1.40
17	9	1041	CLA	CHC-C1C	2.20	1.42	1.38
17	A	1107	CLA	C2B-C1B	2.20	1.45	1.40
17	Q	5211	CLA	CHB-C1B	-2.20	1.34	1.39
17	4	1025	CLA	CHC-C1C	2.20	1.42	1.38
17	B	1240	CLA	CHC-C1C	2.20	1.42	1.38
17	Q	5241	CLA	CHC-C1C	2.20	1.42	1.38
17	0	1025	CLA	CHC-C1C	2.20	1.42	1.38
17	Q	5238	CLA	MG-NB	2.20	2.10	2.05
17	F	4006	CLA	CHC-C1C	2.20	1.42	1.38
17	P	5111	CLA	CHB-C1B	-2.20	1.34	1.39
17	Q	5242	CLA	CHC-C1C	2.20	1.42	1.38
17	P	5134	CLA	CHB-C4A	2.20	1.42	1.36
17	8	1012	CLA	CHC-C1C	2.19	1.42	1.38
17	8	1017	CLA	CHC-C1C	2.19	1.42	1.38
17	4	4002	CLA	CHC-C1C	2.19	1.42	1.38
17	4	1023	CLA	CHC-C1C	2.19	1.42	1.38
17	A	1111	CLA	CHB-C1B	-2.19	1.34	1.39
17	Q	5023	CLA	CHD-C1D	2.19	1.44	1.38
17	Z	8008	CLA	CHC-C1C	2.19	1.42	1.38
17	Q	5216	CLA	CHB-C1B	-2.19	1.34	1.39
17	1	1017	CLA	CHC-C1C	2.19	1.42	1.38
17	P	5113	CLA	CHC-C1C	2.19	1.42	1.38
17	A	1113	CLA	CHC-C1C	2.19	1.42	1.38
17	3	1016	CLA	CHC-C1C	2.19	1.42	1.38
17	8	1025	CLA	CHC-C1C	2.19	1.42	1.38
17	0	1015	CLA	CHC-C1C	2.19	1.42	1.38
17	1	1023	CLA	CHC-C1C	2.19	1.42	1.38
17	8	1014	CLA	CHC-C1C	2.19	1.42	1.38
17	3	1011	CLA	CHC-C1C	2.19	1.42	1.38
17	8	1022	CLA	CHC-C1C	2.19	1.42	1.38
17	L	1504	CLA	CHC-C1C	2.18	1.42	1.38
17	A	1122	CLA	CHB-C1B	-2.18	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	Q	5238	CLA	C3B-C4B	2.18	1.45	1.40
17	2	1015	CLA	CHC-C1C	2.18	1.42	1.38
17	B	1216	CLA	CHB-C1B	-2.18	1.34	1.39
17	G	1233	CLA	CHC-C1C	2.18	1.42	1.38
17	7	1021	CLA	CHC-C1C	2.18	1.42	1.38
17	A	1134	CLA	MG-NC	2.18	2.11	2.06
17	U	8005	CLA	CHC-C1C	2.18	1.42	1.38
17	4	1017	CLA	CHC-C1C	2.18	1.42	1.38
17	0	1017	CLA	CHC-C1C	2.18	1.42	1.38
17	J	4008	CLA	CHC-C1C	2.18	1.42	1.38
17	7	1023	CLA	CHC-C1C	2.18	1.42	1.38
17	1	1021	CLA	CHC-C1C	2.18	1.42	1.38
17	B	1211	CLA	CHB-C1B	-2.18	1.34	1.39
17	P	5114	CLA	C3D-C2D	2.18	1.40	1.35
17	Q	5240	CLA	CHC-C1C	2.18	1.42	1.38
17	A	1114	CLA	C3D-C2D	2.18	1.40	1.35
17	Q	5201	CLA	C3D-C2D	2.18	1.40	1.35
17	A	1134	CLA	CHB-C4A	2.18	1.42	1.36
17	P	8009	CLA	CHC-C1C	2.18	1.42	1.38
17	3	1022	CLA	CHC-C1C	2.18	1.42	1.38
17	9	1017	CLA	CHC-C1C	2.18	1.42	1.38
17	F	4005	CLA	CHC-C1C	2.18	1.42	1.38
17	H	1801	CLA	CHC-C1C	2.18	1.42	1.38
17	A	1121	CLA	C3D-C2D	2.17	1.40	1.35
17	P	5121	CLA	C3D-C2D	2.17	1.40	1.35
17	5	5403	CLA	CHC-C1C	2.17	1.42	1.38
17	8	1013	CLA	CHC-C1C	2.17	1.42	1.38
17	P	8010	CLA	CHC-C1C	2.17	1.42	1.38
17	U	8004	CLA	CHC-C1C	2.17	1.42	1.38
17	3	1033	CLA	CHC-C1C	2.17	1.42	1.38
17	6	5504	CLA	CHC-C1C	2.17	1.42	1.38
17	A	1107	CLA	MG-NB	2.17	2.10	2.05
17	K	1401	CLA	CHB-C1B	-2.17	1.34	1.39
17	2	4007	CLA	CHC-C1C	2.17	1.42	1.38
17	9	1033	CLA	CHC-C1C	2.17	1.42	1.38
17	0	1021	CLA	CHC-C1C	2.17	1.42	1.38
17	G	1701	CLA	CHC-C1C	2.17	1.42	1.38
17	V	5701	CLA	CHC-C1C	2.17	1.42	1.38
17	B	1209	CLA	MG-NC	2.17	2.11	2.06
17	2	1026	CLA	CHC-C1C	2.17	1.42	1.38
17	8	1026	CLA	CHC-C1C	2.17	1.42	1.38
17	Q	5226	CLA	CHB-C4A	2.17	1.42	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	3	1031	CLA	CHC-C1C	2.17	1.42	1.38
17	4	1015	CLA	CHC-C1C	2.17	1.42	1.38
17	A	4010	CLA	CHC-C1C	2.17	1.42	1.38
17	3	1015	CLA	CHC-C1C	2.17	1.42	1.38
17	P	5109	CLA	CHB-C1B	-2.17	1.34	1.39
17	A	4009	CLA	CHC-C1C	2.17	1.42	1.38
17	2	1017	CLA	CHC-C1C	2.17	1.42	1.38
17	P	5134	CLA	MG-NC	2.17	2.11	2.06
17	A	1109	CLA	CHB-C1B	-2.17	1.34	1.39
17	2	1016	CLA	CHC-C1C	2.17	1.42	1.38
17	B	1202	CLA	MG-NC	2.17	2.11	2.06
17	7	1031	CLA	CHC-C1C	2.17	1.42	1.38
17	3	1041	CLA	CHC-C1C	2.17	1.42	1.38
17	Q	5205	CLA	CHC-C1C	2.16	1.42	1.38
17	2	1012	CLA	CHC-C1C	2.16	1.42	1.38
17	A	1011	CLA	CHC-C1C	2.16	1.42	1.38
17	1	1031	CLA	CHC-C1C	2.16	1.42	1.38
17	P	5011	CLA	CHC-C1C	2.16	1.42	1.38
17	9	1012	CLA	CHC-C1C	2.16	1.42	1.38
17	3	1012	CLA	CHC-C1C	2.16	1.42	1.38
17	2	1025	CLA	CHC-C1C	2.16	1.42	1.38
17	V	5233	CLA	CHC-C1C	2.16	1.42	1.38
17	9	1011	CLA	CHC-C1C	2.16	1.42	1.38
17	2	1023	CLA	CHC-C1C	2.16	1.42	1.38
17	7	1013	CLA	CHC-C1C	2.16	1.42	1.38
17	B	1201	CLA	C3D-C2D	2.16	1.40	1.35
17	Q	5202	CLA	MG-NC	2.16	2.11	2.06
17	Q	5023	CLA	C2C-C1C	2.16	1.48	1.43
17	Q	5130	CLA	MG-NB	2.16	2.10	2.05
17	F	4003	CLA	CHC-C1C	2.16	1.42	1.38
17	B	1023	CLA	C2C-C1C	2.16	1.48	1.43
17	J	1101	CLA	CHC-C1C	2.16	1.42	1.38
17	1	1012	CLA	CHC-C1C	2.16	1.42	1.38
17	W	5801	CLA	CHC-C1C	2.16	1.42	1.38
17	9	1031	CLA	CHC-C1C	2.16	1.42	1.38
17	F	1229	CLA	C3D-C2D	2.16	1.40	1.35
17	P	5126	CLA	CHB-C1B	-2.16	1.34	1.39
17	5	5401	CLA	CHB-C1B	-2.16	1.34	1.39
17	B	1226	CLA	CHB-C4A	2.16	1.42	1.36
17	7	1022	CLA	CHC-C1C	2.16	1.42	1.38
17	9	1022	CLA	CHC-C1C	2.16	1.42	1.38
17	P	5402	CLA	MG-NC	2.16	2.11	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	P	5402	CLA	CHB-C4A	2.15	1.42	1.36
17	3	1017	CLA	CHC-C1C	2.15	1.42	1.38
17	Z	5101	CLA	CHC-C1C	2.15	1.42	1.38
17	8	1016	CLA	CHC-C1C	2.15	1.42	1.38
17	A	1402	CLA	CHB-C4A	2.15	1.42	1.36
17	A	1402	CLA	MG-NC	2.15	2.11	2.06
17	7	1011	CLA	CHC-C1C	2.15	1.42	1.38
17	B	1130	CLA	MG-NB	2.15	2.10	2.05
17	F	4004	CLA	CHC-C1C	2.15	1.42	1.38
17	Q	5023	CLA	C3C-C4C	2.15	1.48	1.43
17	U	8003	CLA	CHC-C1C	2.15	1.42	1.38
17	8	8007	CLA	CHC-C1C	2.15	1.42	1.38
17	B	1222	CLA	C3D-C2D	2.15	1.40	1.35
17	B	1205	CLA	CHC-C1C	2.15	1.42	1.38
17	K	1404	CLA	CHC-C1C	2.15	1.42	1.38
17	K	1403	CLA	CHC-C1C	2.15	1.42	1.38
17	Q	8001	CLA	CHC-C1C	2.15	1.42	1.38
17	0	1026	CLA	CHC-C1C	2.15	1.42	1.38
17	8	1023	CLA	CHC-C1C	2.15	1.42	1.38
17	B	4001	CLA	CHC-C1C	2.15	1.42	1.38
17	2	1021	CLA	CHC-C1C	2.15	1.42	1.38
17	4	1014	CLA	CHC-C1C	2.15	1.42	1.38
17	1	1013	CLA	CHC-C1C	2.15	1.42	1.38
17	Q	5230	CLA	CHC-C1C	2.14	1.42	1.38
17	7	1015	CLA	CHC-C1C	2.14	1.42	1.38
17	Q	5209	CLA	MG-NC	2.14	2.11	2.06
17	A	1126	CLA	CHB-C1B	-2.14	1.34	1.39
17	1	1011	CLA	CHC-C1C	2.14	1.42	1.38
17	Q	5222	CLA	C3D-C2D	2.14	1.40	1.35
17	8	1021	CLA	CHC-C1C	2.14	1.42	1.38
17	7	1016	CLA	CHC-C1C	2.14	1.42	1.38
17	1	1022	CLA	CHC-C1C	2.14	1.42	1.38
17	0	1012	CLA	CHC-C1C	2.14	1.42	1.38
17	U	5229	CLA	C3D-C2D	2.14	1.40	1.35
17	2	1013	CLA	CHC-C1C	2.14	1.42	1.38
17	B	1234	CLA	MG-NC	2.14	2.11	2.06
17	3	1032	CLA	CHC-C1C	2.14	1.42	1.38
17	4	1021	CLA	CHC-C1C	2.14	1.42	1.38
17	0	1033	CLA	CHC-C1C	2.14	1.42	1.38
17	P	5118	CLA	C3D-C2D	2.14	1.40	1.35
17	A	1133	CLA	CHC-C1C	2.14	1.42	1.38
17	B	1230	CLA	CHC-C1C	2.14	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	A	1121	CLA	CHC-C1C	2.14	1.42	1.38
17	7	1012	CLA	CHC-C1C	2.14	1.42	1.38
17	P	5107	CLA	MG-NB	2.14	2.10	2.05
17	4	1012	CLA	CHC-C1C	2.14	1.42	1.38
17	4	1033	CLA	CHC-C1C	2.14	1.42	1.38
17	5	5404	CLA	CHC-C1C	2.14	1.42	1.38
17	4	1026	CLA	CHC-C1C	2.13	1.42	1.38
17	Q	5237	CLA	MG-NC	2.13	2.11	2.06
17	Q	5204	CLA	CHD-C1D	2.13	1.43	1.38
17	0	1016	CLA	CHC-C1C	2.13	1.42	1.38
17	0	1013	CLA	CHC-C1C	2.13	1.42	1.38
17	Q	5212	CLA	CHB-C1B	-2.13	1.34	1.39
17	1	1015	CLA	CHC-C1C	2.13	1.42	1.38
17	0	1031	CLA	CHC-C1C	2.13	1.42	1.38
17	A	1118	CLA	C3D-C2D	2.13	1.40	1.35
17	Q	5234	CLA	MG-NC	2.13	2.11	2.06
17	1	1025	CLA	CHC-C1C	2.13	1.42	1.38
17	9	1032	CLA	CHC-C1C	2.13	1.42	1.38
17	1	1016	CLA	CHC-C1C	2.13	1.42	1.38
17	B	1023	CLA	C3C-C4C	2.13	1.48	1.43
17	4	1013	CLA	CHC-C1C	2.13	1.42	1.38
17	P	5140	CLA	MG-NC	2.13	2.11	2.06
17	7	1025	CLA	CHC-C1C	2.13	1.42	1.38
17	A	1140	CLA	MG-NC	2.12	2.11	2.06
17	Q	5203	CLA	C3D-C2D	2.12	1.40	1.35
17	B	1203	CLA	C3D-C2D	2.12	1.40	1.35
17	0	1032	CLA	CHC-C1C	2.12	1.42	1.38
17	4	1016	CLA	CHC-C1C	2.12	1.42	1.38
17	B	1204	CLA	CHD-C1D	2.12	1.43	1.38
17	4	1031	CLA	CHC-C1C	2.12	1.42	1.38
17	9	1015	CLA	CHC-C1C	2.12	1.42	1.38
17	A	1901	CLA	CHB-C1B	-2.12	1.34	1.39
17	A	1125	CLA	C3D-C2D	2.12	1.40	1.35
17	P	5131	CLA	C3B-C4B	2.12	1.44	1.40
17	B	1234	CLA	CHB-C4A	2.12	1.42	1.36
17	P	5121	CLA	CHC-C1C	2.11	1.42	1.38
17	8	1011	CLA	CHC-C1C	2.11	1.42	1.38
17	Q	5227	CLA	C3D-C2D	2.11	1.40	1.35
17	P	5125	CLA	C3D-C2D	2.11	1.40	1.35
18	Q	6002	PQN	C10-C1	-2.11	1.44	1.48
17	3	1026	CLA	CHC-C1C	2.11	1.42	1.38
17	B	1237	CLA	MG-NC	2.11	2.11	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	0	1014	CLA	CHC-C1C	2.11	1.42	1.38
17	B	1238	CLA	C3D-C2D	2.11	1.40	1.35
17	A	1118	CLA	CHB-C4A	2.11	1.41	1.36
17	2	1011	CLA	CHC-C1C	2.11	1.42	1.38
17	A	1131	CLA	C3B-C4B	2.10	1.44	1.40
17	A	1114	CLA	CHB-C1B	-2.10	1.34	1.39
17	4	1032	CLA	CHC-C1C	2.10	1.42	1.38
17	P	5133	CLA	CHC-C1C	2.10	1.42	1.38
17	B	1212	CLA	CHB-C1B	-2.10	1.34	1.39
17	P	5129	CLA	MG-NC	2.10	2.11	2.06
17	A	1129	CLA	MG-NC	2.10	2.11	2.06
17	A	1129	CLA	C3D-C2D	2.10	1.40	1.35
17	P	5901	CLA	CHB-C1B	-2.10	1.34	1.39
17	Q	5234	CLA	CHB-C4A	2.10	1.41	1.36
17	P	5115	CLA	C3D-C2D	2.10	1.40	1.35
17	A	1013	CLA	CHC-C1C	2.10	1.42	1.38
17	B	1022	CLA	C2B-C1B	2.10	1.44	1.40
17	Q	5022	CLA	C2B-C1B	2.09	1.44	1.40
17	Q	5238	CLA	C3D-C2D	2.09	1.40	1.35
17	P	5111	CLA	CHC-C1C	2.09	1.42	1.38
17	A	1107	CLA	MG-ND	-2.09	2.01	2.05
17	9	1026	CLA	CHC-C1C	2.09	1.42	1.38
17	P	5114	CLA	CHB-C1B	-2.09	1.34	1.39
17	P	5107	CLA	MG-ND	-2.09	2.01	2.05
17	1	1014	CLA	CHC-C1C	2.09	1.42	1.38
17	A	1111	CLA	CHC-C1C	2.09	1.42	1.38
17	Q	5206	CLA	C3D-C2D	2.09	1.40	1.35
17	A	1011	CLA	MG-ND	-2.09	2.01	2.05
17	P	5131	CLA	MG-NB	2.09	2.09	2.05
17	P	5118	CLA	CHB-C4A	2.09	1.41	1.36
17	B	1021	CLA	CHB-C4A	2.09	1.41	1.36
17	P	5125	CLA	CHB-C4A	2.09	1.41	1.36
17	B	1206	CLA	C3D-C2D	2.09	1.40	1.35
17	A	1138	CLA	MG-NC	2.09	2.11	2.06
17	P	5120	CLA	MG-NC	2.08	2.11	2.06
17	B	1227	CLA	C3D-C2D	2.08	1.40	1.35
17	P	5129	CLA	C3D-C2D	2.08	1.40	1.35
17	Q	5022	CLA	CHB-C1B	-2.08	1.34	1.39
17	A	1125	CLA	CHB-C4A	2.08	1.41	1.36
17	A	1131	CLA	MG-NB	2.08	2.09	2.05
17	A	1115	CLA	C3D-C2D	2.08	1.40	1.35
18	B	2002	PQN	C10-C1	-2.08	1.44	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	A	1135	CLA	C3C-C4C	2.08	1.48	1.43
17	P	5011	CLA	CHB-C4A	2.08	1.41	1.36
17	P	5102	CLA	MG-ND	-2.08	2.01	2.05
17	P	5138	CLA	MG-NC	2.08	2.11	2.06
17	P	5114	CLA	CHC-C1C	2.07	1.42	1.38
17	A	1122	CLA	C3D-C2D	2.07	1.40	1.35
17	B	1237	CLA	CHB-C1B	-2.07	1.34	1.39
17	B	1211	CLA	C2B-C1B	2.07	1.44	1.40
17	A	1114	CLA	CHC-C1C	2.07	1.42	1.38
17	A	1011	CLA	CHB-C4A	2.07	1.41	1.36
17	Q	5021	CLA	CHB-C4A	2.07	1.41	1.36
17	A	1102	CLA	MG-ND	-2.06	2.01	2.05
17	A	1104	CLA	CHA-C4D	2.06	1.43	1.38
17	B	1022	CLA	CHB-C1B	-2.06	1.34	1.39
17	P	5013	CLA	CHC-C1C	2.06	1.42	1.38
17	P	5105	CLA	CHB-C4A	2.06	1.41	1.36
17	P	5122	CLA	C3D-C2D	2.06	1.40	1.35
17	A	1120	CLA	MG-NC	2.06	2.11	2.06
17	Q	5208	CLA	C3D-C2D	2.06	1.40	1.35
17	Q	5219	CLA	CHB-C4A	2.06	1.41	1.36
17	U	5229	CLA	CHB-C1B	-2.05	1.34	1.39
17	B	1215	CLA	C3D-C2D	2.05	1.40	1.35
17	B	1231	CLA	CHB-C4A	2.05	1.41	1.36
17	P	5109	CLA	CHC-C1C	2.05	1.42	1.38
17	P	5011	CLA	MG-ND	-2.05	2.01	2.05
17	Q	5225	CLA	C3D-C2D	2.05	1.40	1.35
17	7	1014	CLA	CHC-C1C	2.05	1.42	1.38
17	Q	5237	CLA	CHB-C1B	-2.05	1.34	1.39
17	A	1118	CLA	MG-ND	-2.05	2.01	2.05
17	Q	5211	CLA	C2B-C1B	2.05	1.44	1.40
17	Q	5215	CLA	C3D-C2D	2.05	1.40	1.35
17	Q	5203	CLA	CHD-C1D	2.05	1.43	1.38
17	Q	5231	CLA	CHB-C4A	2.05	1.41	1.36
17	B	1207	CLA	CHB-C4A	2.05	1.41	1.36
17	B	1208	CLA	C3D-C2D	2.04	1.40	1.35
17	A	1105	CLA	CHB-C4A	2.04	1.41	1.36
17	P	5118	CLA	MG-ND	-2.04	2.01	2.05
17	P	5117	CLA	C2B-C1B	2.04	1.44	1.40
17	B	1239	CLA	CHB-C4A	2.04	1.41	1.36
17	P	5104	CLA	CHA-C4D	2.04	1.43	1.38
17	A	1117	CLA	C2B-C1B	2.04	1.44	1.40
17	Q	5238	CLA	C3C-C4C	2.04	1.47	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	P	5135	CLA	C3C-C4C	2.04	1.47	1.43
17	A	1133	CLA	CHB-C4A	2.04	1.41	1.36
17	F	1229	CLA	CHB-C1B	-2.04	1.34	1.39
17	Q	5230	CLA	C3D-C2D	2.04	1.39	1.35
17	B	1230	CLA	C3D-C2D	2.04	1.39	1.35
17	A	1109	CLA	CHC-C1C	2.03	1.42	1.38
17	B	1221	CLA	C2C-C1C	2.03	1.47	1.43
17	Q	5225	CLA	CHB-C1B	-2.03	1.34	1.39
17	Q	5221	CLA	C2C-C1C	2.03	1.47	1.43
17	B	1225	CLA	C3D-C2D	2.03	1.39	1.35
17	P	5133	CLA	MG-NB	2.03	2.09	2.05
17	P	5133	CLA	CHB-C4A	2.03	1.41	1.36
17	B	1219	CLA	CHB-C4A	2.03	1.41	1.36
17	Q	5239	CLA	CHB-C4A	2.03	1.41	1.36
17	Q	5207	CLA	CHB-C4A	2.02	1.41	1.36
17	B	1231	CLA	MG-NC	2.02	2.11	2.06
17	B	1238	CLA	C3C-C4C	2.02	1.47	1.43
17	A	1103	CLA	C3D-C2D	2.02	1.39	1.35
17	B	1224	CLA	C2C-C1C	2.02	1.47	1.43
17	B	1203	CLA	CHD-C1D	2.02	1.43	1.38
17	0	1031	CLA	C3D-C2D	2.02	1.39	1.35
17	Q	5231	CLA	MG-NC	2.02	2.11	2.06
17	A	1137	CLA	CHB-C4A	2.02	1.41	1.36
17	P	5103	CLA	C3D-C2D	2.02	1.39	1.35
17	P	5121	CLA	CHB-C1B	-2.02	1.34	1.39
17	Q	5204	CLA	CHB-C4A	2.01	1.41	1.36
17	A	1133	CLA	MG-NB	2.01	2.09	2.05
17	Q	5222	CLA	CHC-C1C	2.01	1.42	1.38
17	Q	5212	CLA	C3D-C2D	2.01	1.39	1.35
17	A	1121	CLA	CHB-C1B	-2.01	1.34	1.39
17	7	1015	CLA	C3D-C2D	2.01	1.39	1.35
17	P	5120	CLA	CHB-C1B	-2.01	1.34	1.39
17	B	1225	CLA	CHB-C1B	-2.01	1.34	1.39
17	A	1120	CLA	CHB-C1B	-2.00	1.34	1.39
17	4	1031	CLA	C3D-C2D	2.00	1.39	1.35

All (2439) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	Z	5302	CLA	C4A-NA-C1A	16.56	114.24	106.68
17	J	1302	CLA	C4A-NA-C1A	16.52	114.22	106.68
17	A	1901	CLA	C4A-NA-C1A	16.16	114.05	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	P	5901	CLA	C4A-NA-C1A	16.12	114.03	106.68
17	A	1113	CLA	C4A-NA-C1A	15.33	113.67	106.68
17	P	5113	CLA	C4A-NA-C1A	15.24	113.63	106.68
17	B	1219	CLA	C4A-NA-C1A	14.98	113.52	106.68
17	Q	5219	CLA	C4A-NA-C1A	14.89	113.47	106.68
17	A	1108	CLA	C4A-NA-C1A	13.61	112.89	106.68
17	P	5103	CLA	C4A-NA-C1A	13.59	112.88	106.68
17	A	1103	CLA	C4A-NA-C1A	13.55	112.86	106.68
17	P	5108	CLA	C4A-NA-C1A	13.53	112.85	106.68
17	P	5137	CLA	C4A-NA-C1A	13.13	112.67	106.68
17	A	1137	CLA	C4A-NA-C1A	13.11	112.66	106.68
17	A	1135	CLA	C4A-NA-C1A	12.97	112.60	106.68
17	P	5111	CLA	C4A-NA-C1A	12.96	112.59	106.68
17	A	1111	CLA	C4A-NA-C1A	12.95	112.59	106.68
17	P	5135	CLA	C4A-NA-C1A	12.85	112.54	106.68
17	Q	5130	CLA	C4A-NA-C1A	12.83	112.53	106.68
17	Q	5204	CLA	C4A-NA-C1A	12.77	112.50	106.68
17	B	1204	CLA	C4A-NA-C1A	12.77	112.50	106.68
17	B	1130	CLA	C4A-NA-C1A	12.74	112.49	106.68
17	A	1402	CLA	C4A-NA-C1A	12.67	112.46	106.68
17	Q	5223	CLA	C4A-NA-C1A	12.61	112.43	106.68
17	B	1223	CLA	C4A-NA-C1A	12.60	112.43	106.68
17	P	5123	CLA	C4A-NA-C1A	12.60	112.43	106.68
17	A	1123	CLA	C4A-NA-C1A	12.56	112.41	106.68
17	P	5402	CLA	C4A-NA-C1A	12.56	112.41	106.68
17	B	1202	CLA	C4A-NA-C1A	12.49	112.38	106.68
17	Q	5202	CLA	C4A-NA-C1A	12.49	112.38	106.68
17	B	1239	CLA	C4A-NA-C1A	12.39	112.33	106.68
17	Q	5239	CLA	C4A-NA-C1A	12.36	112.32	106.68
17	A	1125	CLA	C4A-NA-C1A	12.34	112.31	106.68
17	P	5125	CLA	C4A-NA-C1A	12.29	112.29	106.68
17	P	5110	CLA	C4A-NA-C1A	12.28	112.28	106.68
17	B	1206	CLA	C4A-NA-C1A	12.23	112.26	106.68
17	Q	5206	CLA	C4A-NA-C1A	12.21	112.25	106.68
17	A	1110	CLA	C4A-NA-C1A	12.19	112.24	106.68
17	Q	5207	CLA	C4A-NA-C1A	12.18	112.23	106.68
17	0	8002	CLA	C4A-NA-C1A	12.18	112.23	106.68
17	B	1221	CLA	C4A-NA-C1A	12.17	112.23	106.68
17	Q	5221	CLA	C4A-NA-C1A	12.16	112.23	106.68
17	B	1207	CLA	C4A-NA-C1A	12.09	112.19	106.68
17	4	4002	CLA	C4A-NA-C1A	12.07	112.19	106.68
17	0	1032	CLA	C4A-NA-C1A	12.03	112.17	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	2	1016	CLA	C4A-NA-C1A	12.02	112.16	106.68
17	1	1022	CLA	C4A-NA-C1A	12.01	112.16	106.68
17	5	5404	CLA	C4A-NA-C1A	12.01	112.16	106.68
17	B	1217	CLA	C4A-NA-C1A	12.01	112.16	106.68
17	3	1032	CLA	C4A-NA-C1A	12.01	112.16	106.68
17	8	1016	CLA	C4A-NA-C1A	12.01	112.16	106.68
17	8	1014	CLA	C4A-NA-C1A	12.00	112.15	106.68
17	9	1033	CLA	C4A-NA-C1A	12.00	112.15	106.68
17	0	1022	CLA	C4A-NA-C1A	11.98	112.15	106.68
17	9	1012	CLA	C4A-NA-C1A	11.98	112.14	106.68
17	4	1022	CLA	C4A-NA-C1A	11.98	112.14	106.68
17	7	1011	CLA	C4A-NA-C1A	11.97	112.14	106.68
17	8	1026	CLA	C4A-NA-C1A	11.97	112.14	106.68
17	3	1022	CLA	C4A-NA-C1A	11.97	112.14	106.68
17	1	1011	CLA	C4A-NA-C1A	11.95	112.13	106.68
17	9	1032	CLA	C4A-NA-C1A	11.95	112.13	106.68
17	4	1031	CLA	C4A-NA-C1A	11.95	112.13	106.68
17	U	8005	CLA	C4A-NA-C1A	11.95	112.13	106.68
17	7	1015	CLA	C4A-NA-C1A	11.95	112.13	106.68
17	Q	5210	CLA	C4A-NA-C1A	11.95	112.13	106.68
17	B	1210	CLA	C4A-NA-C1A	11.94	112.13	106.68
17	2	1014	CLA	C4A-NA-C1A	11.94	112.13	106.68
17	4	1032	CLA	C4A-NA-C1A	11.94	112.13	106.68
17	Q	5217	CLA	C4A-NA-C1A	11.94	112.13	106.68
17	0	1015	CLA	C4A-NA-C1A	11.94	112.13	106.68
17	7	1017	CLA	C4A-NA-C1A	11.94	112.12	106.68
17	8	1022	CLA	C4A-NA-C1A	11.93	112.12	106.68
17	3	1012	CLA	C4A-NA-C1A	11.93	112.12	106.68
17	3	1025	CLA	C4A-NA-C1A	11.93	112.12	106.68
17	7	1026	CLA	C4A-NA-C1A	11.93	112.12	106.68
17	F	4005	CLA	C4A-NA-C1A	11.93	112.12	106.68
17	8	1013	CLA	C4A-NA-C1A	11.93	112.12	106.68
17	2	1026	CLA	C4A-NA-C1A	11.93	112.12	106.68
17	Z	5101	CLA	C4A-NA-C1A	11.93	112.12	106.68
17	7	1022	CLA	C4A-NA-C1A	11.93	112.12	106.68
17	1	1015	CLA	C4A-NA-C1A	11.92	112.12	106.68
17	2	1011	CLA	C4A-NA-C1A	11.92	112.12	106.68
17	2	1022	CLA	C4A-NA-C1A	11.92	112.12	106.68
17	9	1011	CLA	C4A-NA-C1A	11.92	112.12	106.68
17	K	1404	CLA	C4A-NA-C1A	11.92	112.11	106.68
17	9	1025	CLA	C4A-NA-C1A	11.92	112.11	106.68
17	3	1026	CLA	C4A-NA-C1A	11.91	112.11	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	3	1033	CLA	C4A-NA-C1A	11.91	112.11	106.68
17	B	1231	CLA	C4A-NA-C1A	11.91	112.11	106.68
17	F	4003	CLA	C4A-NA-C1A	11.91	112.11	106.68
17	2	1031	CLA	C4A-NA-C1A	11.91	112.11	106.68
17	4	1015	CLA	C4A-NA-C1A	11.91	112.11	106.68
17	Q	5241	CLA	C4A-NA-C1A	11.91	112.11	106.68
17	8	1031	CLA	C4A-NA-C1A	11.91	112.11	106.68
17	9	1022	CLA	C4A-NA-C1A	11.91	112.11	106.68
17	4	1011	CLA	C4A-NA-C1A	11.90	112.11	106.68
17	0	1011	CLA	C4A-NA-C1A	11.90	112.11	106.68
17	J	4008	CLA	C4A-NA-C1A	11.90	112.11	106.68
17	0	1031	CLA	C4A-NA-C1A	11.90	112.11	106.68
17	1	1031	CLA	C4A-NA-C1A	11.90	112.11	106.68
17	F	4004	CLA	C4A-NA-C1A	11.90	112.11	106.68
17	G	1701	CLA	C4A-NA-C1A	11.90	112.11	106.68
17	Z	8008	CLA	C4A-NA-C1A	11.90	112.11	106.68
17	3	1014	CLA	C4A-NA-C1A	11.89	112.10	106.68
17	H	1801	CLA	C4A-NA-C1A	11.89	112.10	106.68
17	9	1014	CLA	C4A-NA-C1A	11.89	112.10	106.68
17	A	4009	CLA	C4A-NA-C1A	11.88	112.10	106.68
17	1	1025	CLA	C4A-NA-C1A	11.88	112.10	106.68
17	3	1015	CLA	C4A-NA-C1A	11.88	112.10	106.68
17	U	8006	CLA	C4A-NA-C1A	11.88	112.10	106.68
17	F	4006	CLA	C4A-NA-C1A	11.88	112.10	106.68
17	8	8007	CLA	C4A-NA-C1A	11.88	112.10	106.68
17	1	1026	CLA	C4A-NA-C1A	11.88	112.10	106.68
17	J	1101	CLA	C4A-NA-C1A	11.87	112.09	106.68
17	4	1033	CLA	C4A-NA-C1A	11.87	112.09	106.68
17	7	1025	CLA	C4A-NA-C1A	11.87	112.09	106.68
17	9	1026	CLA	C4A-NA-C1A	11.87	112.09	106.68
17	3	1011	CLA	C4A-NA-C1A	11.87	112.09	106.68
17	8	1012	CLA	C4A-NA-C1A	11.87	112.09	106.68
17	1	1017	CLA	C4A-NA-C1A	11.87	112.09	106.68
17	4	1016	CLA	C4A-NA-C1A	11.86	112.09	106.68
17	P	8010	CLA	C4A-NA-C1A	11.86	112.09	106.68
17	2	1013	CLA	C4A-NA-C1A	11.86	112.09	106.68
17	3	1041	CLA	C4A-NA-C1A	11.86	112.09	106.68
17	5	5403	CLA	C4A-NA-C1A	11.85	112.09	106.68
17	0	1033	CLA	C4A-NA-C1A	11.85	112.09	106.68
17	1	1021	CLA	C4A-NA-C1A	11.85	112.08	106.68
17	W	5801	CLA	C4A-NA-C1A	11.85	112.08	106.68
17	8	1011	CLA	C4A-NA-C1A	11.85	112.08	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	4	1017	CLA	C4A-NA-C1A	11.85	112.08	106.68
17	K	1403	CLA	C4A-NA-C1A	11.85	112.08	106.68
17	V	5701	CLA	C4A-NA-C1A	11.85	112.08	106.68
17	4	1026	CLA	C4A-NA-C1A	11.84	112.08	106.68
17	B	1240	CLA	C4A-NA-C1A	11.84	112.08	106.68
17	9	1021	CLA	C4A-NA-C1A	11.84	112.08	106.68
17	1	1014	CLA	C4A-NA-C1A	11.84	112.08	106.68
17	3	1017	CLA	C4A-NA-C1A	11.83	112.08	106.68
17	6	5504	CLA	C4A-NA-C1A	11.83	112.08	106.68
17	7	1031	CLA	C4A-NA-C1A	11.83	112.08	106.68
17	8	1023	CLA	C4A-NA-C1A	11.83	112.08	106.68
17	2	4007	CLA	C4A-NA-C1A	11.83	112.08	106.68
17	B	1242	CLA	C4A-NA-C1A	11.82	112.07	106.68
17	L	1504	CLA	C4A-NA-C1A	11.82	112.07	106.68
17	2	1023	CLA	C4A-NA-C1A	11.82	112.07	106.68
17	P	8009	CLA	C4A-NA-C1A	11.82	112.07	106.68
17	B	4001	CLA	C4A-NA-C1A	11.82	112.07	106.68
17	2	1015	CLA	C4A-NA-C1A	11.82	112.07	106.68
17	3	1031	CLA	C4A-NA-C1A	11.82	112.07	106.68
17	8	1017	CLA	C4A-NA-C1A	11.82	112.07	106.68
17	0	1016	CLA	C4A-NA-C1A	11.82	112.07	106.68
17	1	1013	CLA	C4A-NA-C1A	11.81	112.07	106.68
17	2	1017	CLA	C4A-NA-C1A	11.81	112.07	106.68
17	1	1012	CLA	C4A-NA-C1A	11.81	112.07	106.68
17	U	8004	CLA	C4A-NA-C1A	11.81	112.07	106.68
17	7	1021	CLA	C4A-NA-C1A	11.81	112.07	106.68
17	A	4010	CLA	C4A-NA-C1A	11.81	112.06	106.68
17	7	1013	CLA	C4A-NA-C1A	11.81	112.06	106.68
17	2	1012	CLA	C4A-NA-C1A	11.80	112.06	106.68
17	4	1013	CLA	C4A-NA-C1A	11.80	112.06	106.68
17	7	1012	CLA	C4A-NA-C1A	11.80	112.06	106.68
17	3	1021	CLA	C4A-NA-C1A	11.80	112.06	106.68
17	4	1023	CLA	C4A-NA-C1A	11.80	112.06	106.68
17	Q	5231	CLA	C4A-NA-C1A	11.80	112.06	106.68
17	9	1015	CLA	C4A-NA-C1A	11.80	112.06	106.68
17	9	1031	CLA	C4A-NA-C1A	11.80	112.06	106.68
17	Q	5242	CLA	C4A-NA-C1A	11.80	112.06	106.68
17	U	8003	CLA	C4A-NA-C1A	11.79	112.06	106.68
17	B	1234	CLA	C4A-NA-C1A	11.79	112.06	106.68
17	1	1016	CLA	C4A-NA-C1A	11.79	112.06	106.68
17	Q	8001	CLA	C4A-NA-C1A	11.79	112.06	106.68
17	9	1017	CLA	C4A-NA-C1A	11.79	112.06	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	7	1016	CLA	C4A-NA-C1A	11.79	112.06	106.68
17	0	1026	CLA	C4A-NA-C1A	11.79	112.06	106.68
17	0	1017	CLA	C4A-NA-C1A	11.78	112.06	106.68
17	4	1014	CLA	C4A-NA-C1A	11.78	112.05	106.68
17	A	1118	CLA	C4A-NA-C1A	11.78	112.05	106.68
17	9	1041	CLA	C4A-NA-C1A	11.77	112.05	106.68
17	B	1224	CLA	C4A-NA-C1A	11.77	112.05	106.68
17	4	1012	CLA	C4A-NA-C1A	11.77	112.05	106.68
17	A	1140	CLA	C4A-NA-C1A	11.77	112.05	106.68
17	2	1025	CLA	C4A-NA-C1A	11.77	112.05	106.68
17	P	5140	CLA	C4A-NA-C1A	11.77	112.05	106.68
17	0	1023	CLA	C4A-NA-C1A	11.77	112.05	106.68
17	B	1241	CLA	C4A-NA-C1A	11.77	112.05	106.68
17	1	1023	CLA	C4A-NA-C1A	11.76	112.05	106.68
17	8	1015	CLA	C4A-NA-C1A	11.76	112.04	106.68
17	8	1025	CLA	C4A-NA-C1A	11.76	112.04	106.68
17	Q	5234	CLA	C4A-NA-C1A	11.76	112.04	106.68
17	P	5118	CLA	C4A-NA-C1A	11.75	112.04	106.68
17	A	1104	CLA	C4A-NA-C1A	11.74	112.04	106.68
17	G	1233	CLA	C4A-NA-C1A	11.74	112.03	106.68
17	3	1016	CLA	C4A-NA-C1A	11.73	112.03	106.68
17	P	5012	CLA	C4A-NA-C1A	11.73	112.03	106.68
17	7	1023	CLA	C4A-NA-C1A	11.73	112.03	106.68
17	4	1025	CLA	C4A-NA-C1A	11.72	112.03	106.68
17	Q	5240	CLA	C4A-NA-C1A	11.72	112.03	106.68
17	7	1014	CLA	C4A-NA-C1A	11.72	112.03	106.68
17	0	1012	CLA	C4A-NA-C1A	11.72	112.03	106.68
17	0	1013	CLA	C4A-NA-C1A	11.72	112.03	106.68
17	B	1021	CLA	C4A-NA-C1A	11.72	112.02	106.68
17	Q	5224	CLA	C4A-NA-C1A	11.72	112.02	106.68
17	4	1021	CLA	C4A-NA-C1A	11.71	112.02	106.68
17	9	1016	CLA	C4A-NA-C1A	11.70	112.02	106.68
17	0	1021	CLA	C4A-NA-C1A	11.70	112.02	106.68
17	P	5104	CLA	C4A-NA-C1A	11.69	112.01	106.68
17	8	1033	CLA	C4A-NA-C1A	11.69	112.01	106.68
17	0	1014	CLA	C4A-NA-C1A	11.69	112.01	106.68
17	A	1012	CLA	C4A-NA-C1A	11.68	112.01	106.68
17	8	1021	CLA	C4A-NA-C1A	11.68	112.01	106.68
17	2	1033	CLA	C4A-NA-C1A	11.67	112.00	106.68
17	Q	5021	CLA	C4A-NA-C1A	11.65	112.00	106.68
17	V	5233	CLA	C4A-NA-C1A	11.65	111.99	106.68
17	0	1025	CLA	C4A-NA-C1A	11.64	111.99	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	2	1021	CLA	C4A-NA-C1A	11.64	111.99	106.68
17	A	1134	CLA	C4A-NA-C1A	11.60	111.97	106.68
17	P	5134	CLA	C4A-NA-C1A	11.60	111.97	106.68
17	Q	5209	CLA	C4A-NA-C1A	11.59	111.97	106.68
17	A	1129	CLA	C4A-NA-C1A	11.58	111.96	106.68
17	U	5301	CLA	C4A-NA-C1A	11.58	111.96	106.68
17	F	1301	CLA	C4A-NA-C1A	11.58	111.96	106.68
17	A	1114	CLA	C4A-NA-C1A	11.57	111.96	106.68
17	B	1209	CLA	C4A-NA-C1A	11.57	111.96	106.68
17	Q	5203	CLA	C4A-NA-C1A	11.57	111.96	106.68
17	P	5114	CLA	C4A-NA-C1A	11.56	111.95	106.68
17	P	5129	CLA	C4A-NA-C1A	11.55	111.95	106.68
17	B	1203	CLA	C4A-NA-C1A	11.54	111.94	106.68
17	B	1218	CLA	C4A-NA-C1A	11.52	111.94	106.68
17	P	5131	CLA	C4A-NA-C1A	11.49	111.92	106.68
17	A	1131	CLA	C4A-NA-C1A	11.45	111.90	106.68
17	A	1107	CLA	C4A-NA-C1A	11.44	111.90	106.68
17	P	5107	CLA	C4A-NA-C1A	11.42	111.89	106.68
17	Q	5218	CLA	C4A-NA-C1A	11.42	111.89	106.68
17	Q	5214	CLA	C4A-NA-C1A	11.41	111.88	106.68
17	Q	5212	CLA	C4A-NA-C1A	11.41	111.88	106.68
17	Q	5228	CLA	C4A-NA-C1A	11.39	111.88	106.68
17	A	1133	CLA	C4A-NA-C1A	11.39	111.87	106.68
17	B	1212	CLA	C4A-NA-C1A	11.35	111.86	106.68
17	B	1214	CLA	C4A-NA-C1A	11.34	111.85	106.68
17	B	1228	CLA	C4A-NA-C1A	11.32	111.84	106.68
17	P	5133	CLA	C4A-NA-C1A	11.31	111.84	106.68
17	Q	5201	CLA	C4A-NA-C1A	11.31	111.84	106.68
17	P	5137	CLA	C1C-NC-C4C	11.30	111.83	106.68
17	B	1201	CLA	C4A-NA-C1A	11.28	111.82	106.68
17	P	5106	CLA	C4A-NA-C1A	11.27	111.82	106.68
17	P	5124	CLA	C4A-NA-C1A	11.26	111.82	106.68
17	A	1106	CLA	C4A-NA-C1A	11.26	111.81	106.68
17	A	1137	CLA	C1C-NC-C4C	11.24	111.81	106.68
17	P	5127	CLA	C4A-NA-C1A	11.23	111.80	106.68
17	A	1102	CLA	C4A-NA-C1A	11.22	111.80	106.68
17	B	1222	CLA	C4A-NA-C1A	11.17	111.78	106.68
17	A	1124	CLA	C4A-NA-C1A	11.17	111.77	106.68
17	P	5102	CLA	C4A-NA-C1A	11.15	111.77	106.68
17	P	5109	CLA	C4A-NA-C1A	11.14	111.76	106.68
17	A	1127	CLA	C4A-NA-C1A	11.14	111.76	106.68
17	Q	5222	CLA	C4A-NA-C1A	11.13	111.76	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	U	5229	CLA	C4A-NA-C1A	11.10	111.74	106.68
17	Q	5235	CLA	C4A-NA-C1A	11.09	111.74	106.68
17	P	5138	CLA	C4A-NA-C1A	11.09	111.74	106.68
17	A	1122	CLA	C4A-NA-C1A	11.08	111.74	106.68
17	Q	5215	CLA	C4A-NA-C1A	11.08	111.74	106.68
17	A	1138	CLA	C4A-NA-C1A	11.08	111.73	106.68
17	P	5122	CLA	C4A-NA-C1A	11.08	111.73	106.68
17	B	1235	CLA	C4A-NA-C1A	11.06	111.73	106.68
17	Q	5211	CLA	C4A-NA-C1A	11.06	111.73	106.68
17	A	1120	CLA	C4A-NA-C1A	11.05	111.72	106.68
17	B	1211	CLA	C4A-NA-C1A	11.05	111.72	106.68
17	Q	5230	CLA	C4A-NA-C1A	11.03	111.71	106.68
17	A	1109	CLA	C4A-NA-C1A	11.03	111.71	106.68
17	F	1229	CLA	C4A-NA-C1A	11.02	111.71	106.68
17	B	1230	CLA	C4A-NA-C1A	11.00	111.70	106.68
17	B	1215	CLA	C4A-NA-C1A	11.00	111.70	106.68
17	Q	5237	CLA	C4A-NA-C1A	11.00	111.70	106.68
17	P	5120	CLA	C4A-NA-C1A	10.99	111.69	106.68
17	Q	5227	CLA	C4A-NA-C1A	10.98	111.69	106.68
17	B	1227	CLA	C4A-NA-C1A	10.98	111.69	106.68
17	B	1237	CLA	C4A-NA-C1A	10.96	111.68	106.68
17	Q	5236	CLA	C4A-NA-C1A	10.92	111.66	106.68
17	A	1901	CLA	C1C-NC-C4C	10.91	111.66	106.68
17	A	1116	CLA	C4A-NA-C1A	10.90	111.65	106.68
17	P	5116	CLA	C4A-NA-C1A	10.87	111.64	106.68
17	B	1236	CLA	C4A-NA-C1A	10.84	111.62	106.68
17	P	5139	CLA	C4A-NA-C1A	10.83	111.62	106.68
17	6	5502	CLA	C4A-NA-C1A	10.83	111.62	106.68
17	A	1139	CLA	C4A-NA-C1A	10.80	111.61	106.68
17	P	5901	CLA	C1C-NC-C4C	10.79	111.60	106.68
17	A	1117	CLA	C4A-NA-C1A	10.75	111.58	106.68
17	A	1105	CLA	C4A-NA-C1A	10.75	111.58	106.68
17	P	5117	CLA	C4A-NA-C1A	10.75	111.58	106.68
17	P	5132	CLA	C4A-NA-C1A	10.74	111.58	106.68
17	A	1011	CLA	C4A-NA-C1A	10.73	111.58	106.68
17	A	1132	CLA	C4A-NA-C1A	10.73	111.58	106.68
17	P	5011	CLA	C4A-NA-C1A	10.73	111.58	106.68
17	P	5105	CLA	C4A-NA-C1A	10.72	111.57	106.68
17	L	1502	CLA	C4A-NA-C1A	10.71	111.56	106.68
17	K	1401	CLA	C4A-NA-C1A	10.69	111.55	106.68
17	5	5401	CLA	C4A-NA-C1A	10.66	111.54	106.68
17	A	1119	CLA	C4A-NA-C1A	10.64	111.53	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	Q	5216	CLA	C4A-NA-C1A	10.64	111.53	106.68
17	P	5113	CLA	C1C-NC-C4C	10.63	111.53	106.68
17	B	1216	CLA	C4A-NA-C1A	10.62	111.53	106.68
17	Q	5220	CLA	C4A-NA-C1A	10.62	111.52	106.68
17	P	5119	CLA	C4A-NA-C1A	10.59	111.51	106.68
17	A	1113	CLA	C1C-NC-C4C	10.58	111.51	106.68
17	B	1220	CLA	C4A-NA-C1A	10.57	111.50	106.68
17	B	1232	CLA	C4A-NA-C1A	10.55	111.49	106.68
17	B	1208	CLA	C4A-NA-C1A	10.53	111.48	106.68
17	Q	5232	CLA	C4A-NA-C1A	10.53	111.48	106.68
17	B	1022	CLA	C4A-NA-C1A	10.53	111.48	106.68
17	Q	5022	CLA	C4A-NA-C1A	10.51	111.47	106.68
17	A	1126	CLA	C4A-NA-C1A	10.50	111.47	106.68
17	P	5126	CLA	C4A-NA-C1A	10.50	111.47	106.68
17	Q	5208	CLA	C4A-NA-C1A	10.49	111.46	106.68
17	B	1023	CLA	C4A-NA-C1A	10.47	111.46	106.68
17	Q	5023	CLA	C4A-NA-C1A	10.47	111.46	106.68
17	A	1112	CLA	C4A-NA-C1A	10.44	111.44	106.68
17	Q	5238	CLA	C4A-NA-C1A	10.44	111.44	106.68
17	B	1238	CLA	C4A-NA-C1A	10.43	111.44	106.68
17	L	1503	CLA	C4A-NA-C1A	10.38	111.41	106.68
17	6	5503	CLA	C4A-NA-C1A	10.38	111.41	106.68
17	P	5112	CLA	C4A-NA-C1A	10.37	111.41	106.68
17	B	1213	CLA	C4A-NA-C1A	10.15	111.31	106.68
17	Q	5213	CLA	C4A-NA-C1A	10.15	111.31	106.68
17	Q	5205	CLA	C4A-NA-C1A	10.14	111.30	106.68
17	B	1205	CLA	C4A-NA-C1A	10.13	111.30	106.68
17	A	1013	CLA	C4A-NA-C1A	10.08	111.28	106.68
17	P	5121	CLA	C4A-NA-C1A	10.06	111.27	106.68
17	A	1121	CLA	C4A-NA-C1A	10.00	111.24	106.68
17	P	5013	CLA	C4A-NA-C1A	9.98	111.23	106.68
17	P	5136	CLA	C4A-NA-C1A	9.93	111.21	106.68
17	A	1136	CLA	C4A-NA-C1A	9.91	111.20	106.68
17	Q	5219	CLA	C1C-NC-C4C	9.91	111.20	106.68
17	A	1108	CLA	C1C-NC-C4C	9.90	111.20	106.68
17	P	5108	CLA	C1C-NC-C4C	9.89	111.19	106.68
17	B	1219	CLA	C1C-NC-C4C	9.88	111.19	106.68
17	6	5501	CLA	C4A-NA-C1A	9.82	111.16	106.68
17	P	5115	CLA	C4A-NA-C1A	9.74	111.12	106.68
17	L	1501	CLA	C4A-NA-C1A	9.73	111.12	106.68
17	A	1115	CLA	C4A-NA-C1A	9.72	111.11	106.68
17	Q	5226	CLA	C4A-NA-C1A	9.68	111.10	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	P	5128	CLA	C4A-NA-C1A	9.65	111.08	106.68
17	B	1226	CLA	C4A-NA-C1A	9.63	111.07	106.68
17	A	1128	CLA	C4A-NA-C1A	9.56	111.04	106.68
17	Z	5302	CLA	C1C-NC-C4C	9.14	110.85	106.68
17	J	1302	CLA	C1C-NC-C4C	9.11	110.83	106.68
17	Q	5225	CLA	C4A-NA-C1A	8.92	110.75	106.68
17	B	1225	CLA	C4A-NA-C1A	8.86	110.72	106.68
17	P	5011	CLA	CHA-C4D-ND	8.65	137.06	124.84
17	A	1011	CLA	CHA-C4D-ND	8.63	137.03	124.84
17	J	1302	CLA	C1B-NB-C4B	7.88	111.84	106.31
17	Z	5302	CLA	C1B-NB-C4B	7.85	111.82	106.31
17	P	5901	CLA	CHA-C4D-ND	7.76	135.81	124.84
17	A	1901	CLA	CHA-C4D-ND	7.75	135.79	124.84
17	J	1302	CLA	CHA-C4D-ND	7.66	135.66	124.84
17	Z	5302	CLA	CHA-C4D-ND	7.63	135.61	124.84
17	B	1022	CLA	C1C-NC-C4C	7.56	110.13	106.68
17	Q	5022	CLA	C1C-NC-C4C	7.55	110.12	106.68
17	Q	5023	CLA	C1C-NC-C4C	7.49	110.09	106.68
17	Q	5219	CLA	CHA-C4D-ND	7.42	135.32	124.84
17	B	1219	CLA	CHA-C4D-ND	7.40	135.29	124.84
17	B	1023	CLA	C1C-NC-C4C	7.35	110.03	106.68
17	P	5137	CLA	CHA-C4D-ND	7.26	135.09	124.84
17	A	1137	CLA	CHA-C4D-ND	7.26	135.09	124.84
17	P	5113	CLA	C1B-NB-C4B	7.13	111.31	106.31
17	A	1113	CLA	C1B-NB-C4B	7.12	111.31	106.31
17	A	1104	CLA	CHA-C4D-ND	7.12	134.89	124.84
17	A	1108	CLA	CHA-C4D-ND	7.11	134.89	124.84
17	P	5118	CLA	C1C-NC-C4C	7.11	109.92	106.68
17	P	5104	CLA	CHA-C4D-ND	7.11	134.88	124.84
17	P	5108	CLA	CHA-C4D-ND	7.10	134.87	124.84
17	A	1118	CLA	C1C-NC-C4C	7.09	109.91	106.68
17	Q	5223	CLA	CHA-C4D-ND	7.07	134.83	124.84
17	P	5102	CLA	CHA-C4D-ND	7.06	134.82	124.84
17	A	1102	CLA	CHA-C4D-ND	7.06	134.81	124.84
17	B	1223	CLA	CHA-C4D-ND	7.05	134.80	124.84
17	B	1226	CLA	CHA-C4D-ND	7.05	134.80	124.84
17	P	5118	CLA	CHA-C4D-ND	7.03	134.77	124.84
17	Q	5226	CLA	CHA-C4D-ND	7.02	134.76	124.84
17	A	1118	CLA	CHA-C4D-ND	7.00	134.73	124.84
17	P	5113	CLA	CHA-C4D-ND	7.00	134.72	124.84
17	A	1113	CLA	CHA-C4D-ND	6.98	134.70	124.84
17	B	1222	CLA	CHA-C4D-ND	6.97	134.69	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	B	1207	CLA	CHA-C4D-ND	6.96	134.68	124.84
17	Q	5207	CLA	CHA-C4D-ND	6.94	134.64	124.84
17	Q	5222	CLA	CHA-C4D-ND	6.94	134.64	124.84
17	A	1123	CLA	CHA-C4D-ND	6.91	134.60	124.84
17	Q	5217	CLA	CHA-C4D-ND	6.91	134.59	124.84
17	B	1217	CLA	CHA-C4D-ND	6.90	134.59	124.84
17	P	5123	CLA	CHA-C4D-ND	6.90	134.58	124.84
17	A	1126	CLA	C1C-NC-C4C	6.88	109.82	106.68
17	P	5126	CLA	C1C-NC-C4C	6.88	109.82	106.68
17	B	1213	CLA	CHA-C4D-ND	6.88	134.56	124.84
17	A	1116	CLA	C1C-NC-C4C	6.86	109.81	106.68
17	Q	5218	CLA	CHA-C4D-ND	6.85	134.52	124.84
17	B	1218	CLA	CHA-C4D-ND	6.85	134.51	124.84
17	B	1130	CLA	CHA-C4D-ND	6.84	134.51	124.84
17	P	5125	CLA	CHA-C4D-ND	6.84	134.51	124.84
17	B	1211	CLA	CHA-C4D-ND	6.84	134.50	124.84
17	Q	5130	CLA	CHA-C4D-ND	6.84	134.50	124.84
17	9	1022	CLA	CHA-C4D-ND	6.84	134.50	124.84
17	A	1125	CLA	CHA-C4D-ND	6.83	134.49	124.84
17	Q	5213	CLA	CHA-C4D-ND	6.83	134.49	124.84
17	Q	5021	CLA	CHA-C4D-ND	6.83	134.49	124.84
17	P	5116	CLA	C1C-NC-C4C	6.83	109.80	106.68
17	0	1031	CLA	CHA-C4D-ND	6.83	134.48	124.84
17	0	1014	CLA	CHA-C4D-ND	6.82	134.48	124.84
17	P	5127	CLA	CHA-C4D-ND	6.82	134.47	124.84
17	Q	5211	CLA	CHA-C4D-ND	6.81	134.47	124.84
17	A	1107	CLA	CHA-C4D-ND	6.81	134.46	124.84
17	A	1139	CLA	CHA-C4D-ND	6.81	134.46	124.84
17	P	5107	CLA	CHA-C4D-ND	6.81	134.46	124.84
17	A	1127	CLA	CHA-C4D-ND	6.80	134.45	124.84
17	3	1016	CLA	CHA-C4D-ND	6.80	134.44	124.84
17	0	8002	CLA	CHA-C4D-ND	6.80	134.44	124.84
17	B	1021	CLA	CHA-C4D-ND	6.80	134.44	124.84
17	4	1014	CLA	CHA-C4D-ND	6.80	134.44	124.84
17	9	1016	CLA	CHA-C4D-ND	6.80	134.44	124.84
17	P	5121	CLA	CHA-C4D-ND	6.79	134.44	124.84
17	9	1026	CLA	CHA-C4D-ND	6.79	134.43	124.84
17	0	1017	CLA	CHA-C4D-ND	6.79	134.43	124.84
17	A	1121	CLA	CHA-C4D-ND	6.79	134.43	124.84
17	B	1221	CLA	CHA-C4D-ND	6.79	134.43	124.84
17	3	1022	CLA	CHA-C4D-ND	6.79	134.43	124.84
17	4	1031	CLA	CHA-C4D-ND	6.79	134.43	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	8	1033	CLA	CHA-C4D-ND	6.79	134.43	124.84
17	4	4002	CLA	CHA-C4D-ND	6.79	134.43	124.84
17	4	1011	CLA	CHA-C4D-ND	6.79	134.43	124.84
17	0	1023	CLA	CHA-C4D-ND	6.79	134.42	124.84
17	2	1033	CLA	CHA-C4D-ND	6.78	134.42	124.84
17	U	8006	CLA	CHA-C4D-ND	6.78	134.41	124.84
17	0	1012	CLA	CHA-C4D-ND	6.78	134.41	124.84
17	P	5139	CLA	CHA-C4D-ND	6.78	134.41	124.84
17	B	1227	CLA	CHA-C4D-ND	6.77	134.41	124.84
17	1	1021	CLA	CHA-C4D-ND	6.77	134.41	124.84
17	0	1032	CLA	CHA-C4D-ND	6.77	134.40	124.84
17	4	1012	CLA	CHA-C4D-ND	6.77	134.40	124.84
17	0	1026	CLA	CHA-C4D-ND	6.77	134.40	124.84
17	G	1233	CLA	CHA-C4D-ND	6.77	134.40	124.84
17	9	1011	CLA	CHA-C4D-ND	6.77	134.40	124.84
17	3	1026	CLA	CHA-C4D-ND	6.77	134.40	124.84
17	Q	5221	CLA	CHA-C4D-ND	6.77	134.40	124.84
17	4	1017	CLA	CHA-C4D-ND	6.77	134.40	124.84
17	3	1015	CLA	CHA-C4D-ND	6.76	134.39	124.84
17	7	1021	CLA	CHA-C4D-ND	6.76	134.39	124.84
17	Q	8001	CLA	CHA-C4D-ND	6.76	134.39	124.84
17	A	4010	CLA	CHA-C4D-ND	6.76	134.39	124.84
17	4	1021	CLA	CHA-C4D-ND	6.76	134.39	124.84
17	4	1023	CLA	CHA-C4D-ND	6.76	134.38	124.84
17	8	1015	CLA	CHA-C4D-ND	6.76	134.38	124.84
17	9	1031	CLA	CHA-C4D-ND	6.76	134.38	124.84
17	A	1122	CLA	CHA-C4D-ND	6.76	134.38	124.84
17	W	5801	CLA	CHA-C4D-ND	6.76	134.38	124.84
17	4	1032	CLA	CHA-C4D-ND	6.75	134.38	124.84
17	9	1032	CLA	CHA-C4D-ND	6.75	134.38	124.84
17	0	1011	CLA	CHA-C4D-ND	6.75	134.38	124.84
17	3	1031	CLA	CHA-C4D-ND	6.75	134.38	124.84
17	B	1240	CLA	CHA-C4D-ND	6.75	134.38	124.84
17	2	1012	CLA	CHA-C4D-ND	6.75	134.38	124.84
17	V	5233	CLA	CHA-C4D-ND	6.75	134.38	124.84
17	3	1017	CLA	CHA-C4D-ND	6.75	134.37	124.84
17	1	1017	CLA	CHA-C4D-ND	6.75	134.37	124.84
17	P	5122	CLA	CHA-C4D-ND	6.75	134.37	124.84
17	Q	5227	CLA	CHA-C4D-ND	6.75	134.37	124.84
17	P	5120	CLA	CHA-C4D-ND	6.75	134.37	124.84
17	8	1012	CLA	CHA-C4D-ND	6.75	134.37	124.84
17	3	1032	CLA	CHA-C4D-ND	6.74	134.37	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	0	1022	CLA	CHA-C4D-ND	6.74	134.37	124.84
17	1	1025	CLA	CHA-C4D-ND	6.74	134.36	124.84
17	2	1025	CLA	CHA-C4D-ND	6.74	134.36	124.84
17	U	8004	CLA	CHA-C4D-ND	6.74	134.36	124.84
17	2	1011	CLA	CHA-C4D-ND	6.74	134.36	124.84
17	7	1015	CLA	CHA-C4D-ND	6.74	134.36	124.84
17	7	1025	CLA	CHA-C4D-ND	6.74	134.36	124.84
17	8	1011	CLA	CHA-C4D-ND	6.74	134.36	124.84
17	0	1021	CLA	CHA-C4D-ND	6.74	134.36	124.84
17	B	1228	CLA	CHA-C4D-ND	6.74	134.36	124.84
17	4	1015	CLA	CHA-C4D-ND	6.74	134.36	124.84
17	F	4006	CLA	CHA-C4D-ND	6.74	134.36	124.84
17	G	1701	CLA	CHA-C4D-ND	6.74	134.36	124.84
17	9	1021	CLA	CHA-C4D-ND	6.74	134.36	124.84
17	K	1404	CLA	CHA-C4D-ND	6.74	134.36	124.84
17	4	1026	CLA	CHA-C4D-ND	6.74	134.36	124.84
17	P	8010	CLA	CHA-C4D-ND	6.74	134.36	124.84
17	2	1021	CLA	CHA-C4D-ND	6.74	134.36	124.84
17	3	1011	CLA	CHA-C4D-ND	6.74	134.36	124.84
17	7	1017	CLA	CHA-C4D-ND	6.74	134.36	124.84
17	P	5128	CLA	CHA-C4D-ND	6.74	134.36	124.84
17	7	1011	CLA	CHA-C4D-ND	6.74	134.36	124.84
17	B	4001	CLA	CHA-C4D-ND	6.74	134.35	124.84
17	J	1101	CLA	CHA-C4D-ND	6.74	134.35	124.84
17	4	1033	CLA	CHA-C4D-ND	6.74	134.35	124.84
17	9	1015	CLA	CHA-C4D-ND	6.74	134.35	124.84
17	F	4004	CLA	CHA-C4D-ND	6.73	134.35	124.84
17	2	1026	CLA	CHA-C4D-ND	6.73	134.35	124.84
17	2	1023	CLA	CHA-C4D-ND	6.73	134.35	124.84
17	Q	5228	CLA	CHA-C4D-ND	6.73	134.35	124.84
17	H	1801	CLA	CHA-C4D-ND	6.73	134.35	124.84
17	L	1504	CLA	CHA-C4D-ND	6.73	134.35	124.84
17	P	5012	CLA	CHA-C4D-ND	6.73	134.35	124.84
17	K	1403	CLA	CHA-C4D-ND	6.73	134.35	124.84
17	0	1016	CLA	CHA-C4D-ND	6.73	134.35	124.84
17	Q	5242	CLA	CHA-C4D-ND	6.73	134.35	124.84
17	4	1013	CLA	CHA-C4D-ND	6.73	134.34	124.84
17	4	1022	CLA	CHA-C4D-ND	6.73	134.34	124.84
17	9	1017	CLA	CHA-C4D-ND	6.73	134.34	124.84
17	0	1033	CLA	CHA-C4D-ND	6.73	134.34	124.84
17	1	1012	CLA	CHA-C4D-ND	6.73	134.34	124.84
17	8	1026	CLA	CHA-C4D-ND	6.73	134.34	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	A	4009	CLA	CHA-C4D-ND	6.73	134.34	124.84
17	1	1026	CLA	CHA-C4D-ND	6.73	134.34	124.84
17	2	1015	CLA	CHA-C4D-ND	6.73	134.34	124.84
17	5	5403	CLA	CHA-C4D-ND	6.73	134.34	124.84
17	8	1023	CLA	CHA-C4D-ND	6.73	134.34	124.84
17	V	5701	CLA	CHA-C4D-ND	6.73	134.34	124.84
17	1	1015	CLA	CHA-C4D-ND	6.73	134.34	124.84
17	A	1128	CLA	CHA-C4D-ND	6.72	134.34	124.84
17	A	1132	CLA	CHA-C4D-ND	6.72	134.34	124.84
17	1	1016	CLA	CHA-C4D-ND	6.72	134.34	124.84
17	P	5132	CLA	CHA-C4D-ND	6.72	134.34	124.84
17	8	1021	CLA	CHA-C4D-ND	6.72	134.34	124.84
17	U	8003	CLA	CHA-C4D-ND	6.72	134.34	124.84
17	Z	8008	CLA	CHA-C4D-ND	6.72	134.34	124.84
17	3	1041	CLA	CHA-C4D-ND	6.72	134.34	124.84
17	7	1031	CLA	CHA-C4D-ND	6.72	134.34	124.84
17	1	1011	CLA	CHA-C4D-ND	6.72	134.33	124.84
17	9	1025	CLA	CHA-C4D-ND	6.72	134.33	124.84
17	F	4005	CLA	CHA-C4D-ND	6.72	134.33	124.84
17	8	1014	CLA	CHA-C4D-ND	6.72	134.33	124.84
17	2	1031	CLA	CHA-C4D-ND	6.72	134.33	124.84
17	1	1014	CLA	CHA-C4D-ND	6.72	134.33	124.84
17	2	1014	CLA	CHA-C4D-ND	6.72	134.33	124.84
17	3	1012	CLA	CHA-C4D-ND	6.72	134.33	124.84
17	8	8007	CLA	CHA-C4D-ND	6.72	134.33	124.84
17	0	1015	CLA	CHA-C4D-ND	6.72	134.33	124.84
17	7	1012	CLA	CHA-C4D-ND	6.72	134.32	124.84
17	6	5504	CLA	CHA-C4D-ND	6.71	134.32	124.84
17	7	1023	CLA	CHA-C4D-ND	6.71	134.32	124.84
17	B	1242	CLA	CHA-C4D-ND	6.71	134.32	124.84
17	2	4007	CLA	CHA-C4D-ND	6.71	134.32	124.84
17	4	1025	CLA	CHA-C4D-ND	6.71	134.32	124.84
17	U	8005	CLA	CHA-C4D-ND	6.71	134.32	124.84
17	8	1025	CLA	CHA-C4D-ND	6.71	134.32	124.84
17	J	4008	CLA	CHA-C4D-ND	6.71	134.32	124.84
17	7	1026	CLA	CHA-C4D-ND	6.71	134.32	124.84
17	B	1241	CLA	CHA-C4D-ND	6.71	134.32	124.84
17	Q	5240	CLA	CHA-C4D-ND	6.71	134.32	124.84
17	0	1013	CLA	CHA-C4D-ND	6.71	134.32	124.84
17	A	1012	CLA	CHA-C4D-ND	6.71	134.32	124.84
17	1	1031	CLA	CHA-C4D-ND	6.71	134.32	124.84
17	1	1023	CLA	CHA-C4D-ND	6.71	134.32	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	3	1014	CLA	CHA-C4D-ND	6.71	134.32	124.84
17	4	1016	CLA	CHA-C4D-ND	6.71	134.32	124.84
17	Q	5241	CLA	CHA-C4D-ND	6.71	134.32	124.84
17	9	1014	CLA	CHA-C4D-ND	6.71	134.32	124.84
17	A	1120	CLA	CHA-C4D-ND	6.71	134.31	124.84
17	1	1013	CLA	CHA-C4D-ND	6.71	134.31	124.84
17	7	1016	CLA	CHA-C4D-ND	6.71	134.31	124.84
17	Q	5232	CLA	CHA-C4D-ND	6.71	134.31	124.84
17	1	1022	CLA	CHA-C4D-ND	6.70	134.31	124.84
17	A	1116	CLA	CHA-C4D-ND	6.70	134.31	124.84
17	3	1021	CLA	CHA-C4D-ND	6.70	134.31	124.84
17	F	4003	CLA	CHA-C4D-ND	6.70	134.31	124.84
17	2	1016	CLA	CHA-C4D-ND	6.70	134.31	124.84
17	P	5116	CLA	CHA-C4D-ND	6.70	134.31	124.84
17	2	1022	CLA	CHA-C4D-ND	6.70	134.31	124.84
17	2	1013	CLA	CHA-C4D-ND	6.70	134.30	124.84
17	5	5401	CLA	CHA-C4D-ND	6.70	134.30	124.84
17	5	5404	CLA	CHA-C4D-ND	6.70	134.30	124.84
17	9	1012	CLA	CHA-C4D-ND	6.70	134.30	124.84
17	3	1025	CLA	CHA-C4D-ND	6.70	134.30	124.84
17	Z	5101	CLA	CHA-C4D-ND	6.70	134.30	124.84
17	P	8009	CLA	CHA-C4D-ND	6.70	134.30	124.84
17	B	1232	CLA	CHA-C4D-ND	6.70	134.30	124.84
17	3	1033	CLA	CHA-C4D-ND	6.70	134.30	124.84
17	9	1033	CLA	CHA-C4D-ND	6.70	134.30	124.84
17	9	1041	CLA	CHA-C4D-ND	6.69	134.30	124.84
17	Q	5022	CLA	CHA-C4D-ND	6.69	134.29	124.84
17	7	1013	CLA	CHA-C4D-ND	6.69	134.29	124.84
17	2	1017	CLA	CHA-C4D-ND	6.69	134.29	124.84
17	B	1022	CLA	CHA-C4D-ND	6.69	134.29	124.84
17	8	1017	CLA	CHA-C4D-ND	6.69	134.29	124.84
17	8	1031	CLA	CHA-C4D-ND	6.69	134.29	124.84
17	K	1401	CLA	CHA-C4D-ND	6.69	134.28	124.84
17	8	1016	CLA	CHA-C4D-ND	6.69	134.28	124.84
17	Q	5203	CLA	CHA-C4D-ND	6.68	134.28	124.84
17	7	1014	CLA	CHA-C4D-ND	6.68	134.28	124.84
17	7	1022	CLA	CHA-C4D-ND	6.68	134.28	124.84
17	B	1215	CLA	CHA-C4D-ND	6.68	134.27	124.84
17	B	1210	CLA	CHA-C4D-ND	6.68	134.27	124.84
17	8	1013	CLA	CHA-C4D-ND	6.68	134.27	124.84
17	0	1025	CLA	CHA-C4D-ND	6.68	134.27	124.84
17	A	1110	CLA	CHA-C4D-ND	6.67	134.27	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	Q	5215	CLA	CHA-C4D-ND	6.67	134.26	124.84
17	Q	5201	CLA	CHA-C4D-ND	6.67	134.26	124.84
17	Q	5210	CLA	CHA-C4D-ND	6.67	134.25	124.84
17	8	1022	CLA	CHA-C4D-ND	6.66	134.25	124.84
17	B	1201	CLA	CHA-C4D-ND	6.66	134.25	124.84
17	P	5110	CLA	CHA-C4D-ND	6.66	134.25	124.84
17	Q	5230	CLA	CHA-C4D-ND	6.65	134.24	124.84
17	B	1203	CLA	CHA-C4D-ND	6.65	134.24	124.84
17	B	1230	CLA	CHA-C4D-ND	6.65	134.23	124.84
17	A	1402	CLA	CHA-C4D-ND	6.64	134.22	124.84
17	U	5301	CLA	CHA-C4D-ND	6.64	134.22	124.84
17	B	1204	CLA	C1C-NC-C4C	6.64	109.71	106.68
17	F	1301	CLA	CHA-C4D-ND	6.64	134.21	124.84
17	Q	5238	CLA	CHA-C4D-ND	6.63	134.21	124.84
17	B	1238	CLA	CHA-C4D-ND	6.63	134.21	124.84
17	Q	5204	CLA	C1C-NC-C4C	6.63	109.70	106.68
17	B	1208	CLA	CHA-C4D-ND	6.63	134.20	124.84
17	B	1023	CLA	CHA-C4D-ND	6.62	134.20	124.84
17	Q	5208	CLA	CHA-C4D-ND	6.62	134.19	124.84
17	B	1212	CLA	CHA-C4D-ND	6.62	134.19	124.84
17	P	5112	CLA	CHA-C4D-ND	6.62	134.19	124.84
17	P	5402	CLA	CHA-C4D-ND	6.62	134.19	124.84
17	A	1112	CLA	CHA-C4D-ND	6.62	134.18	124.84
17	B	1231	CLA	C1C-NC-C4C	6.61	109.70	106.68
17	Q	5212	CLA	CHA-C4D-ND	6.61	134.18	124.84
17	Q	5236	CLA	CHA-C4D-ND	6.61	134.18	124.84
17	B	1236	CLA	CHA-C4D-ND	6.61	134.18	124.84
17	U	5229	CLA	CHA-C4D-ND	6.60	134.16	124.84
17	P	5105	CLA	CHA-C4D-ND	6.60	134.16	124.84
17	A	1131	CLA	CHA-C4D-ND	6.59	134.15	124.84
17	A	1105	CLA	CHA-C4D-ND	6.59	134.15	124.84
17	Q	5023	CLA	CHA-C4D-ND	6.59	134.15	124.84
17	A	1114	CLA	CHA-C4D-ND	6.59	134.14	124.84
17	P	5114	CLA	CHA-C4D-ND	6.59	134.14	124.84
17	A	1103	CLA	CHA-C4D-ND	6.58	134.13	124.84
17	L	1501	CLA	CHA-C4D-ND	6.58	134.13	124.84
17	P	5131	CLA	CHA-C4D-ND	6.58	134.13	124.84
17	F	1229	CLA	CHA-C4D-ND	6.58	134.13	124.84
17	Q	5204	CLA	CHA-C4D-ND	6.58	134.13	124.84
17	B	1204	CLA	CHA-C4D-ND	6.56	134.11	124.84
17	6	5501	CLA	CHA-C4D-ND	6.56	134.11	124.84
17	P	5103	CLA	CHA-C4D-ND	6.56	134.10	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	B	1234	CLA	CHA-C4D-ND	6.56	134.10	124.84
17	A	1134	CLA	CHA-C4D-ND	6.55	134.10	124.84
17	Q	5234	CLA	CHA-C4D-ND	6.55	134.10	124.84
17	A	1126	CLA	CHA-C4D-ND	6.54	134.08	124.84
17	Q	5209	CLA	CHA-C4D-ND	6.54	134.07	124.84
17	B	1209	CLA	CHA-C4D-ND	6.54	134.07	124.84
17	P	5126	CLA	CHA-C4D-ND	6.53	134.07	124.84
17	B	1235	CLA	C1C-NC-C4C	6.53	109.66	106.68
17	Q	5235	CLA	C1C-NC-C4C	6.53	109.66	106.68
17	B	1220	CLA	CHA-C4D-ND	6.52	134.05	124.84
17	P	5134	CLA	CHA-C4D-ND	6.51	134.04	124.84
17	A	1119	CLA	CHA-C4D-ND	6.51	134.03	124.84
17	Q	5214	CLA	CHA-C4D-ND	6.50	134.03	124.84
17	Q	5220	CLA	CHA-C4D-ND	6.50	134.01	124.84
17	6	5502	CLA	C1C-NC-C4C	6.49	109.64	106.68
17	P	5119	CLA	C1C-NC-C4C	6.49	109.64	106.68
17	A	1117	CLA	CHA-C4D-ND	6.48	134.00	124.84
17	P	5111	CLA	CHA-C4D-ND	6.48	133.99	124.84
17	P	5119	CLA	CHA-C4D-ND	6.48	133.99	124.84
17	P	5133	CLA	CHA-C4D-ND	6.48	133.99	124.84
17	Q	5231	CLA	C1C-NC-C4C	6.47	109.63	106.68
17	A	1133	CLA	CHA-C4D-ND	6.47	133.98	124.84
17	B	1214	CLA	CHA-C4D-ND	6.47	133.97	124.84
17	B	1206	CLA	CHA-C4D-ND	6.47	133.97	124.84
17	P	5117	CLA	CHA-C4D-ND	6.46	133.97	124.84
17	P	5108	CLA	C1B-NB-C4B	6.46	110.84	106.31
17	P	5129	CLA	C1C-NC-C4C	6.46	109.62	106.68
17	A	1129	CLA	CHA-C4D-ND	6.46	133.96	124.84
17	Q	5227	CLA	C1C-NC-C4C	6.46	109.62	106.68
17	Q	5206	CLA	CHA-C4D-ND	6.45	133.95	124.84
17	B	1228	CLA	C1C-NC-C4C	6.45	109.62	106.68
17	B	1227	CLA	C1C-NC-C4C	6.45	109.62	106.68
17	P	5129	CLA	CHA-C4D-ND	6.45	133.94	124.84
17	A	1111	CLA	CHA-C4D-ND	6.44	133.94	124.84
17	A	1129	CLA	C1C-NC-C4C	6.44	109.62	106.68
17	Q	5228	CLA	C1C-NC-C4C	6.44	109.62	106.68
17	L	1503	CLA	CHA-C4D-ND	6.44	133.93	124.84
17	A	1115	CLA	CHA-C4D-ND	6.44	133.93	124.84
17	B	1219	CLA	C1B-NB-C4B	6.43	110.83	106.31
17	B	1225	CLA	CHA-C4D-ND	6.43	133.93	124.84
17	A	1119	CLA	C1C-NC-C4C	6.43	109.61	106.68
17	P	5135	CLA	CHA-C4D-ND	6.43	133.92	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	A	1013	CLA	CHA-C4D-ND	6.42	133.91	124.84
17	Q	5225	CLA	CHA-C4D-ND	6.42	133.91	124.84
17	A	1108	CLA	C1B-NB-C4B	6.42	110.82	106.31
17	P	5115	CLA	CHA-C4D-ND	6.42	133.91	124.84
17	A	1140	CLA	CHA-C4D-ND	6.42	133.91	124.84
17	6	5503	CLA	CHA-C4D-ND	6.42	133.91	124.84
17	Q	5231	CLA	CHA-C4D-ND	6.42	133.90	124.84
17	B	1231	CLA	CHA-C4D-ND	6.41	133.89	124.84
17	Q	5220	CLA	C1C-NC-C4C	6.41	109.60	106.68
17	A	1135	CLA	CHA-C4D-ND	6.40	133.88	124.84
17	Q	5219	CLA	C1B-NB-C4B	6.39	110.79	106.31
17	P	5013	CLA	CHA-C4D-ND	6.39	133.86	124.84
17	P	5140	CLA	CHA-C4D-ND	6.38	133.86	124.84
17	L	1502	CLA	C1C-NC-C4C	6.38	109.59	106.68
17	Q	5216	CLA	CHA-C4D-ND	6.35	133.81	124.84
17	A	1106	CLA	CHA-C4D-ND	6.34	133.79	124.84
17	P	5106	CLA	CHA-C4D-ND	6.33	133.79	124.84
17	B	1216	CLA	CHA-C4D-ND	6.33	133.79	124.84
17	B	1220	CLA	C1C-NC-C4C	6.33	109.57	106.68
17	B	1205	CLA	CHA-C4D-ND	6.30	133.74	124.84
17	P	5124	CLA	CHA-C4D-ND	6.29	133.73	124.84
17	A	1124	CLA	CHA-C4D-ND	6.28	133.72	124.84
17	Q	5205	CLA	CHA-C4D-ND	6.28	133.71	124.84
17	6	5502	CLA	CHA-C4D-ND	6.28	133.71	124.84
17	P	5138	CLA	CHA-C4D-ND	6.28	133.71	124.84
17	P	5136	CLA	CHA-C4D-ND	6.28	133.70	124.84
17	L	1502	CLA	CHA-C4D-ND	6.27	133.69	124.84
17	B	1215	CLA	C1C-NC-C4C	6.26	109.54	106.68
17	A	1138	CLA	CHA-C4D-ND	6.26	133.69	124.84
17	Q	5215	CLA	C1C-NC-C4C	6.26	109.54	106.68
17	Q	5202	CLA	CHA-C4D-ND	6.25	133.67	124.84
17	A	1109	CLA	CHA-C4D-ND	6.24	133.66	124.84
17	A	1136	CLA	CHA-C4D-ND	6.24	133.66	124.84
17	B	1202	CLA	CHA-C4D-ND	6.23	133.64	124.84
17	A	1901	CLA	C1B-NB-C4B	6.23	110.68	106.31
17	P	5109	CLA	CHA-C4D-ND	6.22	133.63	124.84
17	P	5901	CLA	C1B-NB-C4B	6.21	110.67	106.31
17	Q	5223	CLA	C1B-NB-C4B	6.18	110.65	106.31
17	B	1223	CLA	C1B-NB-C4B	6.18	110.65	106.31
17	B	1237	CLA	CHA-C4D-ND	6.17	133.55	124.84
17	Q	5237	CLA	CHA-C4D-ND	6.14	133.51	124.84
17	Q	5235	CLA	CHA-C4D-ND	6.13	133.50	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	Q	5237	CLA	C1C-NC-C4C	6.12	109.47	106.68
17	U	5229	CLA	C1C-NC-C4C	6.12	109.47	106.68
17	B	1235	CLA	CHA-C4D-ND	6.10	133.45	124.84
17	F	1229	CLA	C1C-NC-C4C	6.08	109.45	106.68
17	P	5138	CLA	C1C-NC-C4C	6.08	109.45	106.68
17	Q	5224	CLA	CHA-C4D-ND	6.06	133.39	124.84
17	B	1232	CLA	C1C-NC-C4C	6.05	109.44	106.68
17	B	1237	CLA	C1C-NC-C4C	6.05	109.44	106.68
17	P	5137	CLA	C1B-NB-C4B	6.05	110.56	106.31
17	P	5120	CLA	C1C-NC-C4C	6.05	109.44	106.68
17	B	1224	CLA	CHA-C4D-ND	6.04	133.37	124.84
17	A	1138	CLA	C1C-NC-C4C	6.00	109.42	106.68
17	A	1137	CLA	C1B-NB-C4B	5.99	110.51	106.31
17	A	1120	CLA	C1C-NC-C4C	5.97	109.40	106.68
17	Q	5232	CLA	C1C-NC-C4C	5.97	109.40	106.68
17	A	1112	CLA	C1C-NC-C4C	5.96	109.40	106.68
17	P	5122	CLA	C1C-NC-C4C	5.96	109.40	106.68
17	P	5112	CLA	C1C-NC-C4C	5.94	109.39	106.68
17	P	5106	CLA	C1C-NC-C4C	5.93	109.38	106.68
17	A	1122	CLA	C1C-NC-C4C	5.92	109.38	106.68
17	A	1012	CLA	C1C-NC-C4C	5.91	109.38	106.68
17	A	1106	CLA	C1C-NC-C4C	5.91	109.37	106.68
17	A	1134	CLA	C1C-NC-C4C	5.87	109.36	106.68
17	B	1218	CLA	C1C-NC-C4C	5.87	109.36	106.68
17	P	5134	CLA	C1C-NC-C4C	5.85	109.35	106.68
17	P	5125	CLA	C1B-NB-C4B	5.85	110.42	106.31
17	Q	5218	CLA	C1C-NC-C4C	5.84	109.34	106.68
17	P	5012	CLA	C1C-NC-C4C	5.83	109.34	106.68
17	B	1239	CLA	CHA-C4D-ND	5.83	133.07	124.84
17	A	1125	CLA	C1B-NB-C4B	5.82	110.40	106.31
17	Q	5239	CLA	CHA-C4D-ND	5.81	133.04	124.84
17	P	5110	CLA	C1C-NC-C4C	5.80	109.33	106.68
17	Q	5201	CLA	C1C-NC-C4C	5.76	109.31	106.68
17	Q	5207	CLA	C1B-NB-C4B	5.74	110.34	106.31
17	A	1110	CLA	C1C-NC-C4C	5.73	109.30	106.68
17	B	1207	CLA	C1B-NB-C4B	5.69	110.31	106.31
17	B	1201	CLA	C1C-NC-C4C	5.67	109.27	106.68
17	B	1209	CLA	C1C-NC-C4C	5.65	109.25	106.68
17	P	5133	CLA	C1C-NC-C4C	5.63	109.25	106.68
17	Q	5209	CLA	C1C-NC-C4C	5.61	109.24	106.68
17	B	1214	CLA	C1C-NC-C4C	5.60	109.23	106.68
17	A	1133	CLA	C1C-NC-C4C	5.60	109.23	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	Q	5214	CLA	C1C-NC-C4C	5.58	109.23	106.68
17	Q	5211	CLA	C1C-NC-C4C	5.58	109.23	106.68
17	A	1136	CLA	C1C-NC-C4C	5.56	109.22	106.68
17	B	1208	CLA	C1C-NC-C4C	5.55	109.21	106.68
17	6	5503	CLA	C1C-NC-C4C	5.55	109.21	106.68
17	Q	5208	CLA	C1C-NC-C4C	5.55	109.21	106.68
17	G	1233	CLA	C1C-NC-C4C	5.55	109.21	106.68
17	V	5233	CLA	C1C-NC-C4C	5.54	109.21	106.68
17	P	5102	CLA	C1C-NC-C4C	5.53	109.20	106.68
17	Q	5217	CLA	C1C-NC-C4C	5.53	109.20	106.68
17	L	1503	CLA	C1C-NC-C4C	5.52	109.20	106.68
17	P	5136	CLA	C1C-NC-C4C	5.52	109.20	106.68
17	A	1102	CLA	C1C-NC-C4C	5.51	109.19	106.68
17	B	1221	CLA	C1C-NC-C4C	5.50	109.19	106.68
17	Q	5221	CLA	C1C-NC-C4C	5.49	109.18	106.68
17	4	1012	CLA	C1B-NB-C4B	5.47	110.15	106.31
17	B	1217	CLA	C1C-NC-C4C	5.47	109.17	106.68
17	B	1211	CLA	C1C-NC-C4C	5.46	109.17	106.68
17	Q	5221	CLA	C1B-NB-C4B	5.46	110.14	106.31
17	0	1031	CLA	C1B-NB-C4B	5.45	110.14	106.31
17	9	1014	CLA	C1B-NB-C4B	5.45	110.13	106.31
17	4	1031	CLA	C1B-NB-C4B	5.43	110.12	106.31
17	Q	5202	CLA	C1B-NB-C4B	5.43	110.12	106.31
17	8	8007	CLA	C1B-NB-C4B	5.42	110.11	106.31
17	B	1221	CLA	C1B-NB-C4B	5.42	110.11	106.31
17	0	1012	CLA	C1B-NB-C4B	5.42	110.11	106.31
17	5	5404	CLA	C1B-NB-C4B	5.42	110.11	106.31
17	7	1025	CLA	C1B-NB-C4B	5.42	110.11	106.31
17	9	1011	CLA	C1B-NB-C4B	5.41	110.11	106.31
17	B	1202	CLA	C1B-NB-C4B	5.41	110.11	106.31
17	0	1022	CLA	C1B-NB-C4B	5.41	110.11	106.31
17	A	1011	CLA	C3D-C4D-CHA	-5.41	113.12	125.20
17	8	1033	CLA	C1B-NB-C4B	5.41	110.11	106.31
17	P	5011	CLA	C3D-C4D-CHA	-5.40	113.14	125.20
17	3	1014	CLA	C1B-NB-C4B	5.40	110.10	106.31
17	4	1011	CLA	C1B-NB-C4B	5.40	110.10	106.31
17	7	1013	CLA	C1B-NB-C4B	5.40	110.10	106.31
17	9	1012	CLA	C1B-NB-C4B	5.40	110.10	106.31
17	0	1011	CLA	C1B-NB-C4B	5.39	110.10	106.31
17	Q	5241	CLA	C1B-NB-C4B	5.39	110.10	106.31
17	1	1025	CLA	C1B-NB-C4B	5.39	110.09	106.31
17	8	1012	CLA	C1B-NB-C4B	5.39	110.09	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	2	4007	CLA	C1B-NB-C4B	5.39	110.09	106.31
17	8	1011	CLA	C1B-NB-C4B	5.39	110.09	106.31
17	9	1026	CLA	C1B-NB-C4B	5.39	110.09	106.31
17	4	1022	CLA	C1B-NB-C4B	5.39	110.09	106.31
17	3	1012	CLA	C1B-NB-C4B	5.38	110.09	106.31
17	K	1403	CLA	C1B-NB-C4B	5.38	110.09	106.31
17	0	1015	CLA	C1B-NB-C4B	5.38	110.09	106.31
17	3	1033	CLA	C1B-NB-C4B	5.38	110.08	106.31
17	K	1404	CLA	C1B-NB-C4B	5.38	110.08	106.31
17	B	1210	CLA	C1B-NB-C4B	5.37	110.08	106.31
17	2	1017	CLA	C1B-NB-C4B	5.37	110.08	106.31
17	4	1026	CLA	C1B-NB-C4B	5.37	110.08	106.31
17	Q	8001	CLA	C1B-NB-C4B	5.37	110.08	106.31
17	9	1033	CLA	C1B-NB-C4B	5.37	110.08	106.31
17	3	1026	CLA	C1B-NB-C4B	5.37	110.08	106.31
17	3	1011	CLA	C1B-NB-C4B	5.37	110.08	106.31
17	2	1012	CLA	C1B-NB-C4B	5.36	110.08	106.31
17	4	1015	CLA	C1B-NB-C4B	5.36	110.08	106.31
17	9	1022	CLA	C1B-NB-C4B	5.36	110.08	106.31
17	1	1023	CLA	C1B-NB-C4B	5.36	110.07	106.31
17	7	1011	CLA	C1B-NB-C4B	5.36	110.07	106.31
17	7	1023	CLA	C1B-NB-C4B	5.36	110.07	106.31
17	3	1032	CLA	C1B-NB-C4B	5.35	110.07	106.31
17	P	8010	CLA	C1B-NB-C4B	5.35	110.07	106.31
17	0	1026	CLA	C1B-NB-C4B	5.35	110.07	106.31
17	9	1017	CLA	C1B-NB-C4B	5.35	110.07	106.31
17	P	5402	CLA	C1B-NB-C4B	5.35	110.07	106.31
17	Q	5210	CLA	C1B-NB-C4B	5.35	110.07	106.31
17	8	1017	CLA	C1B-NB-C4B	5.35	110.07	106.31
17	9	1032	CLA	C1B-NB-C4B	5.35	110.06	106.31
17	2	1011	CLA	C1B-NB-C4B	5.35	110.06	106.31
17	7	1026	CLA	C1B-NB-C4B	5.35	110.06	106.31
17	1	1011	CLA	C1B-NB-C4B	5.34	110.06	106.31
17	1	1026	CLA	C1B-NB-C4B	5.34	110.06	106.31
17	9	1031	CLA	C1B-NB-C4B	5.34	110.06	106.31
17	A	4010	CLA	C1B-NB-C4B	5.34	110.06	106.31
17	1	1022	CLA	C1B-NB-C4B	5.34	110.06	106.31
17	B	1241	CLA	C1B-NB-C4B	5.34	110.06	106.31
17	4	1025	CLA	C1B-NB-C4B	5.34	110.06	106.31
17	0	8002	CLA	C1B-NB-C4B	5.34	110.06	106.31
17	4	1033	CLA	C1B-NB-C4B	5.34	110.06	106.31
17	0	1025	CLA	C1B-NB-C4B	5.34	110.06	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	4	4002	CLA	C1B-NB-C4B	5.34	110.06	106.31
17	5	5403	CLA	C1B-NB-C4B	5.34	110.06	106.31
17	B	1236	CLA	C1C-NC-C4C	5.34	109.11	106.68
17	W	5801	CLA	C1B-NB-C4B	5.34	110.06	106.31
17	8	1025	CLA	C1B-NB-C4B	5.33	110.06	106.31
17	G	1701	CLA	C1B-NB-C4B	5.33	110.05	106.31
17	2	1025	CLA	C1B-NB-C4B	5.33	110.05	106.31
17	7	1022	CLA	C1B-NB-C4B	5.33	110.05	106.31
17	F	4003	CLA	C1B-NB-C4B	5.33	110.05	106.31
17	L	1504	CLA	C1B-NB-C4B	5.33	110.05	106.31
17	V	5701	CLA	C1B-NB-C4B	5.33	110.05	106.31
17	B	4001	CLA	C1B-NB-C4B	5.33	110.05	106.31
17	1	1013	CLA	C1B-NB-C4B	5.33	110.05	106.31
17	2	1033	CLA	C1B-NB-C4B	5.32	110.05	106.31
17	0	1033	CLA	C1B-NB-C4B	5.32	110.05	106.31
17	3	1022	CLA	C1B-NB-C4B	5.32	110.05	106.31
17	4	1023	CLA	C1B-NB-C4B	5.32	110.05	106.31
17	7	1015	CLA	C1B-NB-C4B	5.32	110.05	106.31
17	3	1041	CLA	C1B-NB-C4B	5.32	110.04	106.31
17	Q	5236	CLA	C1C-NC-C4C	5.31	109.10	106.68
17	A	4009	CLA	C1B-NB-C4B	5.31	110.04	106.31
17	B	1226	CLA	C1B-NB-C4B	5.31	110.04	106.31
17	3	1017	CLA	C1B-NB-C4B	5.31	110.04	106.31
17	J	1101	CLA	C1B-NB-C4B	5.31	110.04	106.31
17	7	1016	CLA	C1B-NB-C4B	5.31	110.04	106.31
17	U	8004	CLA	C1B-NB-C4B	5.31	110.04	106.31
17	1	1017	CLA	C1B-NB-C4B	5.31	110.03	106.31
17	7	1031	CLA	C1B-NB-C4B	5.31	110.03	106.31
17	1	1014	CLA	C1B-NB-C4B	5.30	110.03	106.31
17	6	5504	CLA	C1B-NB-C4B	5.30	110.03	106.31
17	8	1013	CLA	C1B-NB-C4B	5.30	110.03	106.31
17	0	1014	CLA	C1B-NB-C4B	5.30	110.03	106.31
17	B	1242	CLA	C1B-NB-C4B	5.30	110.03	106.31
17	P	5140	CLA	C1C-NC-C4C	5.30	109.10	106.68
17	0	1016	CLA	C1B-NB-C4B	5.30	110.03	106.31
17	7	1017	CLA	C1B-NB-C4B	5.30	110.03	106.31
17	U	8003	CLA	C1B-NB-C4B	5.29	110.03	106.31
17	2	1026	CLA	C1B-NB-C4B	5.29	110.03	106.31
17	3	1031	CLA	C1B-NB-C4B	5.29	110.03	106.31
17	Q	5203	CLA	C1B-NB-C4B	5.29	110.03	106.31
17	8	1015	CLA	C1B-NB-C4B	5.29	110.03	106.31
17	A	1140	CLA	C1C-NC-C4C	5.29	109.09	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	2	1013	CLA	C1B-NB-C4B	5.29	110.02	106.31
17	9	1041	CLA	C1B-NB-C4B	5.29	110.02	106.31
17	0	1023	CLA	C1B-NB-C4B	5.29	110.02	106.31
17	H	1801	CLA	C1B-NB-C4B	5.29	110.02	106.31
17	4	1016	CLA	C1B-NB-C4B	5.29	110.02	106.31
17	4	1014	CLA	C1B-NB-C4B	5.29	110.02	106.31
17	3	1015	CLA	C1B-NB-C4B	5.28	110.02	106.31
17	U	8005	CLA	C1B-NB-C4B	5.28	110.02	106.31
17	Q	5226	CLA	C1B-NB-C4B	5.28	110.02	106.31
17	7	1012	CLA	C1B-NB-C4B	5.28	110.02	106.31
17	8	1023	CLA	C1B-NB-C4B	5.28	110.02	106.31
17	P	8009	CLA	C1B-NB-C4B	5.28	110.02	106.31
17	A	1402	CLA	C1B-NB-C4B	5.28	110.02	106.31
17	J	4008	CLA	C1B-NB-C4B	5.28	110.02	106.31
17	4	1013	CLA	C1B-NB-C4B	5.28	110.01	106.31
17	0	1013	CLA	C1B-NB-C4B	5.28	110.01	106.31
17	4	1021	CLA	C1B-NB-C4B	5.27	110.01	106.31
17	Q	5240	CLA	C1B-NB-C4B	5.27	110.01	106.31
17	Q	5242	CLA	C1B-NB-C4B	5.27	110.01	106.31
17	8	1022	CLA	C1B-NB-C4B	5.27	110.01	106.31
17	1	1015	CLA	C1B-NB-C4B	5.27	110.01	106.31
17	F	4006	CLA	C1B-NB-C4B	5.27	110.01	106.31
17	1	1016	CLA	C1B-NB-C4B	5.27	110.01	106.31
17	1	1031	CLA	C1B-NB-C4B	5.27	110.01	106.31
17	8	1016	CLA	C1B-NB-C4B	5.27	110.01	106.31
17	B	1240	CLA	C1B-NB-C4B	5.27	110.01	106.31
17	F	4004	CLA	C1B-NB-C4B	5.27	110.01	106.31
17	2	1015	CLA	C1B-NB-C4B	5.27	110.01	106.31
17	Z	5101	CLA	C1B-NB-C4B	5.27	110.01	106.31
17	0	1021	CLA	C1B-NB-C4B	5.27	110.01	106.31
17	3	1021	CLA	C1B-NB-C4B	5.27	110.01	106.31
17	1	1012	CLA	C1B-NB-C4B	5.27	110.01	106.31
17	2	1022	CLA	C1B-NB-C4B	5.27	110.01	106.31
17	3	1025	CLA	C1B-NB-C4B	5.27	110.01	106.31
17	8	1021	CLA	C1B-NB-C4B	5.26	110.00	106.31
17	2	1021	CLA	C1B-NB-C4B	5.26	110.00	106.31
17	8	1026	CLA	C1B-NB-C4B	5.26	110.00	106.31
17	9	1015	CLA	C1B-NB-C4B	5.26	110.00	106.31
17	2	1023	CLA	C1B-NB-C4B	5.25	110.00	106.31
17	2	1016	CLA	C1B-NB-C4B	5.25	110.00	106.31
17	Z	8008	CLA	C1B-NB-C4B	5.25	110.00	106.31
17	F	4005	CLA	C1B-NB-C4B	5.25	110.00	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	7	1021	CLA	C1B-NB-C4B	5.25	109.99	106.31
17	4	1017	CLA	C1B-NB-C4B	5.24	109.99	106.31
17	0	1017	CLA	C1B-NB-C4B	5.24	109.99	106.31
17	Q	5230	CLA	C1C-NC-C4C	5.24	109.07	106.68
17	9	1025	CLA	C1B-NB-C4B	5.24	109.99	106.31
17	P	5114	CLA	C1C-NC-C4C	5.24	109.07	106.68
17	3	1016	CLA	C1B-NB-C4B	5.24	109.99	106.31
17	4	1032	CLA	C1B-NB-C4B	5.23	109.98	106.31
17	U	8006	CLA	C1B-NB-C4B	5.23	109.98	106.31
17	A	1121	CLA	C1C-NC-C4C	5.23	109.07	106.68
17	P	5121	CLA	C1C-NC-C4C	5.23	109.07	106.68
17	0	1032	CLA	C1B-NB-C4B	5.23	109.98	106.31
17	P	5123	CLA	C1B-NB-C4B	5.23	109.98	106.31
17	1	1021	CLA	C1B-NB-C4B	5.22	109.98	106.31
17	A	1114	CLA	C1C-NC-C4C	5.22	109.06	106.68
17	A	1132	CLA	C1C-NC-C4C	5.22	109.06	106.68
17	K	1401	CLA	C1C-NC-C4C	5.22	109.06	106.68
17	B	1203	CLA	C1B-NB-C4B	5.22	109.97	106.31
17	2	1031	CLA	C1B-NB-C4B	5.21	109.97	106.31
17	B	1230	CLA	C1C-NC-C4C	5.21	109.06	106.68
17	7	1014	CLA	C1B-NB-C4B	5.21	109.97	106.31
17	9	1021	CLA	C1B-NB-C4B	5.21	109.97	106.31
17	9	1016	CLA	C1B-NB-C4B	5.21	109.97	106.31
17	A	1123	CLA	C1B-NB-C4B	5.20	109.96	106.31
17	5	5401	CLA	C1C-NC-C4C	5.20	109.05	106.68
17	B	1216	CLA	C1C-NC-C4C	5.20	109.05	106.68
17	P	5111	CLA	C1C-NC-C4C	5.19	109.05	106.68
17	P	5013	CLA	C1C-NC-C4C	5.19	109.05	106.68
17	2	1014	CLA	C1B-NB-C4B	5.19	109.95	106.31
17	Q	5216	CLA	C1C-NC-C4C	5.18	109.04	106.68
17	A	1111	CLA	C1C-NC-C4C	5.18	109.04	106.68
17	Q	5222	CLA	C1C-NC-C4C	5.18	109.04	106.68
17	8	1031	CLA	C1B-NB-C4B	5.17	109.94	106.31
17	P	5132	CLA	C1C-NC-C4C	5.16	109.03	106.68
17	B	1222	CLA	C1C-NC-C4C	5.15	109.03	106.68
17	A	1012	CLA	C1B-NB-C4B	5.15	109.92	106.31
17	8	1014	CLA	C1B-NB-C4B	5.14	109.92	106.31
17	A	1013	CLA	C1C-NC-C4C	5.12	109.02	106.68
17	A	1131	CLA	C1C-NC-C4C	5.08	109.00	106.68
17	B	1213	CLA	C1C-NC-C4C	5.08	109.00	106.68
17	P	5012	CLA	C1B-NB-C4B	5.07	109.87	106.31
17	Q	5213	CLA	C1C-NC-C4C	5.06	108.99	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	L	1501	CLA	C1C-NC-C4C	5.05	108.98	106.68
17	6	5501	CLA	C1C-NC-C4C	5.05	108.98	106.68
17	P	5131	CLA	C1C-NC-C4C	5.02	108.97	106.68
17	A	1128	CLA	C1C-NC-C4C	5.02	108.97	106.68
17	B	1224	CLA	C1C-NC-C4C	5.00	108.96	106.68
17	P	5128	CLA	C1C-NC-C4C	5.00	108.96	106.68
17	Q	5239	CLA	C1C-NC-C4C	5.00	108.96	106.68
17	B	1021	CLA	C1C-NC-C4C	4.99	108.95	106.68
17	P	5111	CLA	C1B-NB-C4B	4.99	109.81	106.31
17	P	5124	CLA	C1C-NC-C4C	4.96	108.94	106.68
17	A	1111	CLA	C1B-NB-C4B	4.95	109.79	106.31
17	B	1130	CLA	C1B-NB-C4B	4.93	109.77	106.31
17	P	5125	CLA	C1C-NC-C4C	4.93	108.93	106.68
17	A	1124	CLA	C1C-NC-C4C	4.93	108.93	106.68
17	Q	5238	CLA	C1C-NC-C4C	4.92	108.92	106.68
17	A	1125	CLA	C1C-NC-C4C	4.92	108.92	106.68
17	Q	5021	CLA	C1C-NC-C4C	4.92	108.92	106.68
17	Q	5130	CLA	C1B-NB-C4B	4.91	109.76	106.31
17	A	1117	CLA	C1C-NC-C4C	4.91	108.92	106.68
17	Q	5224	CLA	C1C-NC-C4C	4.91	108.92	106.68
17	0	1012	CLA	C1C-NC-C4C	4.90	108.92	106.68
17	P	5109	CLA	C1C-NC-C4C	4.89	108.91	106.68
17	B	1239	CLA	C1C-NC-C4C	4.89	108.91	106.68
17	4	1012	CLA	C1C-NC-C4C	4.89	108.91	106.68
17	A	1109	CLA	C1C-NC-C4C	4.86	108.90	106.68
17	A	1104	CLA	C1B-NB-C4B	4.85	109.72	106.31
17	B	1238	CLA	C1C-NC-C4C	4.85	108.89	106.68
17	P	5104	CLA	C1B-NB-C4B	4.84	109.71	106.31
17	A	1107	CLA	C1C-NC-C4C	4.82	108.88	106.68
17	P	5117	CLA	C1C-NC-C4C	4.82	108.88	106.68
17	8	1012	CLA	C1C-NC-C4C	4.79	108.87	106.68
17	A	1103	CLA	C1B-NB-C4B	4.79	109.67	106.31
17	A	1135	CLA	C1B-NB-C4B	4.77	109.66	106.31
17	P	5103	CLA	C1B-NB-C4B	4.76	109.65	106.31
17	P	5107	CLA	C1C-NC-C4C	4.75	108.85	106.68
17	V	5701	CLA	C1C-NC-C4C	4.74	108.84	106.68
17	P	5135	CLA	C1B-NB-C4B	4.73	109.63	106.31
17	0	1032	CLA	C1C-NC-C4C	4.72	108.83	106.68
17	Q	5241	CLA	C1C-NC-C4C	4.70	108.82	106.68
17	F	4005	CLA	C1C-NC-C4C	4.69	108.82	106.68
17	2	1012	CLA	C1C-NC-C4C	4.69	108.82	106.68
17	P	8010	CLA	C1C-NC-C4C	4.69	108.82	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	7	1026	CLA	C1C-NC-C4C	4.69	108.82	106.68
17	B	1241	CLA	C1C-NC-C4C	4.68	108.81	106.68
17	1	1017	CLA	C1C-NC-C4C	4.67	108.81	106.68
17	4	1032	CLA	C1C-NC-C4C	4.67	108.81	106.68
17	9	1032	CLA	C1C-NC-C4C	4.67	108.81	106.68
17	U	8005	CLA	C1C-NC-C4C	4.66	108.81	106.68
17	U	8004	CLA	C1C-NC-C4C	4.66	108.81	106.68
17	4	1016	CLA	C1C-NC-C4C	4.66	108.81	106.68
17	2	1016	CLA	C1C-NC-C4C	4.65	108.80	106.68
17	Z	8008	CLA	C1C-NC-C4C	4.65	108.80	106.68
17	F	4004	CLA	C1C-NC-C4C	4.65	108.80	106.68
17	2	1011	CLA	C1C-NC-C4C	4.65	108.80	106.68
17	A	4010	CLA	C1C-NC-C4C	4.65	108.80	106.68
17	G	1701	CLA	C1C-NC-C4C	4.65	108.80	106.68
17	3	1031	CLA	C1C-NC-C4C	4.65	108.80	106.68
17	3	1041	CLA	C1C-NC-C4C	4.65	108.80	106.68
17	4	1013	CLA	C1C-NC-C4C	4.65	108.80	106.68
17	4	1026	CLA	C1C-NC-C4C	4.65	108.80	106.68
17	3	1022	CLA	C1C-NC-C4C	4.65	108.80	106.68
17	B	1234	CLA	C1C-NC-C4C	4.64	108.80	106.68
17	1	1014	CLA	C1C-NC-C4C	4.64	108.80	106.68
17	3	1032	CLA	C1C-NC-C4C	4.64	108.80	106.68
17	B	4001	CLA	C1C-NC-C4C	4.64	108.80	106.68
17	L	1504	CLA	C1C-NC-C4C	4.64	108.80	106.68
17	A	4009	CLA	C1C-NC-C4C	4.64	108.80	106.68
17	K	1404	CLA	C1C-NC-C4C	4.64	108.80	106.68
17	P	8009	CLA	C1C-NC-C4C	4.64	108.80	106.68
17	0	1033	CLA	C1C-NC-C4C	4.64	108.80	106.68
17	Q	5022	CLA	C1B-NB-C4B	4.64	109.56	106.31
17	F	4006	CLA	C1C-NC-C4C	4.64	108.79	106.68
17	Q	5234	CLA	C1C-NC-C4C	4.64	108.79	106.68
17	B	1225	CLA	C1C-NC-C4C	4.63	108.79	106.68
17	2	1026	CLA	C1C-NC-C4C	4.63	108.79	106.68
17	0	1014	CLA	C1C-NC-C4C	4.63	108.79	106.68
17	Q	8001	CLA	C1C-NC-C4C	4.63	108.79	106.68
17	7	1017	CLA	C1C-NC-C4C	4.63	108.79	106.68
17	1	1011	CLA	C1C-NC-C4C	4.62	108.79	106.68
17	1	1012	CLA	C1C-NC-C4C	4.62	108.79	106.68
17	3	1033	CLA	C1C-NC-C4C	4.62	108.79	106.68
17	Q	5225	CLA	C1C-NC-C4C	4.62	108.79	106.68
17	0	1013	CLA	C1C-NC-C4C	4.62	108.79	106.68
17	B	1022	CLA	C1B-NB-C4B	4.62	109.56	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	U	8003	CLA	C1C-NC-C4C	4.62	108.79	106.68
17	8	1015	CLA	C1C-NC-C4C	4.62	108.79	106.68
17	7	1013	CLA	C1C-NC-C4C	4.62	108.78	106.68
17	8	1017	CLA	C1C-NC-C4C	4.62	108.78	106.68
17	9	1021	CLA	C1C-NC-C4C	4.62	108.78	106.68
17	Q	5240	CLA	C1C-NC-C4C	4.61	108.78	106.68
17	9	1022	CLA	C1C-NC-C4C	4.61	108.78	106.68
17	9	1025	CLA	C1C-NC-C4C	4.61	108.78	106.68
17	9	1011	CLA	C1C-NC-C4C	4.61	108.78	106.68
17	J	4008	CLA	C1C-NC-C4C	4.61	108.78	106.68
17	1	1015	CLA	C1C-NC-C4C	4.61	108.78	106.68
17	6	5504	CLA	C1C-NC-C4C	4.61	108.78	106.68
17	7	1023	CLA	C1C-NC-C4C	4.61	108.78	106.68
17	9	1031	CLA	C1C-NC-C4C	4.61	108.78	106.68
17	B	1240	CLA	C1C-NC-C4C	4.61	108.78	106.68
17	3	1011	CLA	C1C-NC-C4C	4.61	108.78	106.68
17	9	1015	CLA	C1C-NC-C4C	4.61	108.78	106.68
17	4	1011	CLA	C1C-NC-C4C	4.60	108.78	106.68
17	A	1137	CLA	C3D-C4D-CHA	-4.60	114.93	125.20
17	P	5137	CLA	C3D-C4D-CHA	-4.60	114.93	125.20
17	J	1101	CLA	C1C-NC-C4C	4.60	108.78	106.68
17	5	5404	CLA	C1C-NC-C4C	4.60	108.78	106.68
17	0	1016	CLA	C1C-NC-C4C	4.60	108.78	106.68
17	4	1033	CLA	C1C-NC-C4C	4.60	108.78	106.68
17	B	1205	CLA	C3D-C4D-CHA	-4.60	114.94	125.20
17	B	1226	CLA	C3D-C4D-CHA	-4.60	114.94	125.20
17	7	1012	CLA	C1C-NC-C4C	4.59	108.78	106.68
17	7	1014	CLA	C1C-NC-C4C	4.59	108.78	106.68
17	3	1025	CLA	C1C-NC-C4C	4.59	108.77	106.68
17	8	1016	CLA	C1C-NC-C4C	4.59	108.77	106.68
17	1	1026	CLA	C1C-NC-C4C	4.59	108.77	106.68
17	2	1013	CLA	C1C-NC-C4C	4.59	108.77	106.68
17	A	1105	CLA	C1C-NC-C4C	4.58	108.77	106.68
17	2	1015	CLA	C1C-NC-C4C	4.58	108.77	106.68
17	3	1021	CLA	C1C-NC-C4C	4.58	108.77	106.68
17	U	8006	CLA	C1C-NC-C4C	4.58	108.77	106.68
17	1	1023	CLA	C1C-NC-C4C	4.58	108.77	106.68
17	4	1014	CLA	C1C-NC-C4C	4.58	108.77	106.68
17	4	1017	CLA	C1C-NC-C4C	4.58	108.77	106.68
17	Q	5205	CLA	C3D-C4D-CHA	-4.58	114.97	125.20
17	0	1025	CLA	C1C-NC-C4C	4.58	108.77	106.68
17	B	1023	CLA	C3D-C4D-CHA	-4.58	114.98	125.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	Q	5226	CLA	C3D-C4D-CHA	-4.57	114.99	125.20
17	9	1026	CLA	C1C-NC-C4C	4.57	108.77	106.68
17	A	1131	CLA	C3D-C4D-CHA	-4.57	114.99	125.20
17	9	1014	CLA	C1C-NC-C4C	4.57	108.76	106.68
17	P	5131	CLA	C3D-C4D-CHA	-4.57	115.00	125.20
17	8	1013	CLA	C1C-NC-C4C	4.57	108.76	106.68
17	9	1041	CLA	C1C-NC-C4C	4.57	108.76	106.68
17	0	1022	CLA	C1C-NC-C4C	4.57	108.76	106.68
17	F	4003	CLA	C1C-NC-C4C	4.56	108.76	106.68
17	3	1017	CLA	C1C-NC-C4C	4.56	108.76	106.68
17	Q	5023	CLA	C3D-C4D-CHA	-4.56	115.01	125.20
17	1	1025	CLA	C1C-NC-C4C	4.56	108.76	106.68
17	0	1031	CLA	C1C-NC-C4C	4.56	108.76	106.68
17	4	4002	CLA	C1C-NC-C4C	4.56	108.76	106.68
17	8	8007	CLA	C1C-NC-C4C	4.56	108.76	106.68
17	9	1017	CLA	C1C-NC-C4C	4.56	108.76	106.68
17	0	1026	CLA	C1C-NC-C4C	4.56	108.76	106.68
17	B	1213	CLA	C3D-C4D-CHA	-4.56	115.03	125.20
17	3	1012	CLA	C1C-NC-C4C	4.55	108.76	106.68
17	7	1015	CLA	C1C-NC-C4C	4.55	108.76	106.68
17	0	1011	CLA	C1C-NC-C4C	4.55	108.76	106.68
17	Q	5213	CLA	C3D-C4D-CHA	-4.55	115.03	125.20
17	4	1031	CLA	C1C-NC-C4C	4.55	108.76	106.68
17	Z	5101	CLA	C1C-NC-C4C	4.55	108.76	106.68
17	8	1014	CLA	C1C-NC-C4C	4.55	108.76	106.68
17	B	1234	CLA	C1B-NB-C4B	4.55	109.51	106.31
17	U	5229	CLA	C3D-C4D-CHA	-4.55	115.04	125.20
17	7	1021	CLA	C1C-NC-C4C	4.55	108.75	106.68
17	1	1021	CLA	C1C-NC-C4C	4.55	108.75	106.68
17	H	1801	CLA	C1C-NC-C4C	4.54	108.75	106.68
17	1	1013	CLA	C1C-NC-C4C	4.54	108.75	106.68
17	3	1015	CLA	C1C-NC-C4C	4.54	108.75	106.68
17	B	1238	CLA	C3D-C4D-CHA	-4.54	115.05	125.20
17	F	1229	CLA	C3D-C4D-CHA	-4.54	115.06	125.20
17	P	5105	CLA	C1C-NC-C4C	4.54	108.75	106.68
17	7	1011	CLA	C1C-NC-C4C	4.54	108.75	106.68
17	0	1017	CLA	C1C-NC-C4C	4.54	108.75	106.68
17	4	1015	CLA	C1C-NC-C4C	4.54	108.75	106.68
17	8	1026	CLA	C1C-NC-C4C	4.54	108.75	106.68
17	B	1211	CLA	C3D-C4D-CHA	-4.53	115.07	125.20
17	B	1215	CLA	C3D-C4D-CHA	-4.53	115.08	125.20
17	P	5121	CLA	C3D-C4D-CHA	-4.53	115.08	125.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	Q	5215	CLA	C3D-C4D-CHA	-4.53	115.08	125.20
17	A	1121	CLA	C3D-C4D-CHA	-4.53	115.08	125.20
17	6	5501	CLA	C3D-C4D-CHA	-4.53	115.08	125.20
17	2	1021	CLA	C1C-NC-C4C	4.53	108.75	106.68
17	7	1025	CLA	C1C-NC-C4C	4.53	108.75	106.68
17	8	1021	CLA	C1C-NC-C4C	4.53	108.75	106.68
17	Q	5238	CLA	C3D-C4D-CHA	-4.53	115.08	125.20
17	L	1501	CLA	C3D-C4D-CHA	-4.53	115.09	125.20
17	2	1017	CLA	C1C-NC-C4C	4.53	108.75	106.68
17	2	1023	CLA	C1C-NC-C4C	4.53	108.75	106.68
17	W	5801	CLA	C1C-NC-C4C	4.53	108.75	106.68
17	7	1022	CLA	C1C-NC-C4C	4.53	108.75	106.68
17	9	1012	CLA	C1C-NC-C4C	4.53	108.75	106.68
17	4	1022	CLA	C1C-NC-C4C	4.52	108.74	106.68
17	8	1011	CLA	C1C-NC-C4C	4.52	108.74	106.68
17	Q	5210	CLA	C3D-C4D-CHA	-4.52	115.10	125.20
17	1	1016	CLA	C1C-NC-C4C	4.52	108.74	106.68
17	Q	5211	CLA	C3D-C4D-CHA	-4.52	115.10	125.20
17	B	1210	CLA	C3D-C4D-CHA	-4.52	115.11	125.20
17	A	1139	CLA	C1C-NC-C4C	4.52	108.74	106.68
17	4	1025	CLA	C1C-NC-C4C	4.52	108.74	106.68
17	8	1023	CLA	C1C-NC-C4C	4.52	108.74	106.68
17	A	1140	CLA	C3D-C4D-CHA	-4.52	115.11	125.20
17	K	1403	CLA	C1C-NC-C4C	4.52	108.74	106.68
17	Q	5021	CLA	C3D-C4D-CHA	-4.52	115.11	125.20
17	2	1033	CLA	C1C-NC-C4C	4.52	108.74	106.68
17	7	1016	CLA	C1C-NC-C4C	4.52	108.74	106.68
17	Q	5234	CLA	C1B-NB-C4B	4.52	109.48	106.31
17	P	5140	CLA	C3D-C4D-CHA	-4.51	115.12	125.20
17	1	1031	CLA	C1C-NC-C4C	4.51	108.74	106.68
17	A	1126	CLA	C3D-C4D-CHA	-4.51	115.12	125.20
17	3	1026	CLA	C1C-NC-C4C	4.50	108.73	106.68
17	5	5403	CLA	C1C-NC-C4C	4.50	108.73	106.68
17	B	1021	CLA	C3D-C4D-CHA	-4.50	115.14	125.20
17	P	5115	CLA	C3D-C4D-CHA	-4.50	115.14	125.20
17	0	8002	CLA	C1C-NC-C4C	4.50	108.73	106.68
17	A	1115	CLA	C3D-C4D-CHA	-4.50	115.15	125.20
17	2	1014	CLA	C1C-NC-C4C	4.50	108.73	106.68
17	A	1119	CLA	C3D-C4D-CHA	-4.50	115.16	125.20
17	P	5126	CLA	C3D-C4D-CHA	-4.50	115.16	125.20
17	1	1022	CLA	C1C-NC-C4C	4.50	108.73	106.68
17	3	1014	CLA	C1C-NC-C4C	4.50	108.73	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	4	1021	CLA	C1C-NC-C4C	4.50	108.73	106.68
17	Q	5236	CLA	C3D-C4D-CHA	-4.49	115.17	125.20
17	9	1016	CLA	C1C-NC-C4C	4.49	108.73	106.68
17	Q	5201	CLA	C3D-C4D-CHA	-4.49	115.17	125.20
17	B	1201	CLA	C3D-C4D-CHA	-4.49	115.18	125.20
17	B	1236	CLA	C3D-C4D-CHA	-4.48	115.19	125.20
17	Q	5242	CLA	C1C-NC-C4C	4.48	108.72	106.68
17	P	5118	CLA	C1B-NB-C4B	4.48	109.46	106.31
17	Q	5212	CLA	C1C-NC-C4C	4.48	108.72	106.68
17	2	4007	CLA	C1C-NC-C4C	4.48	108.72	106.68
17	P	5139	CLA	C1C-NC-C4C	4.48	108.72	106.68
17	8	1033	CLA	C1C-NC-C4C	4.48	108.72	106.68
17	9	1033	CLA	C1C-NC-C4C	4.48	108.72	106.68
17	0	1015	CLA	C1C-NC-C4C	4.47	108.72	106.68
17	Q	5202	CLA	C3D-C4D-CHA	-4.47	115.21	125.20
17	3	1016	CLA	C1C-NC-C4C	4.47	108.72	106.68
17	P	5119	CLA	C3D-C4D-CHA	-4.47	115.22	125.20
17	B	1230	CLA	C3D-C4D-CHA	-4.47	115.22	125.20
17	Q	5230	CLA	C3D-C4D-CHA	-4.47	115.22	125.20
17	7	1031	CLA	C1C-NC-C4C	4.47	108.72	106.68
17	A	1118	CLA	C1B-NB-C4B	4.47	109.45	106.31
17	A	1103	CLA	C3D-C4D-CHA	-4.47	115.23	125.20
17	Q	5206	CLA	C3D-C4D-CHA	-4.47	115.23	125.20
17	B	1202	CLA	C3D-C4D-CHA	-4.46	115.23	125.20
17	B	1206	CLA	C3D-C4D-CHA	-4.46	115.23	125.20
17	A	1108	CLA	C3D-C4D-CHA	-4.46	115.23	125.20
17	A	1123	CLA	C3D-C4D-CHA	-4.46	115.23	125.20
17	P	5102	CLA	C3D-C4D-CHA	-4.46	115.24	125.20
17	A	1122	CLA	C3D-C4D-CHA	-4.46	115.24	125.20
17	8	1031	CLA	C1C-NC-C4C	4.46	108.71	106.68
17	2	1025	CLA	C1C-NC-C4C	4.46	108.71	106.68
17	A	1102	CLA	C3D-C4D-CHA	-4.45	115.25	125.20
17	P	5108	CLA	C3D-C4D-CHA	-4.45	115.26	125.20
17	P	5128	CLA	C3D-C4D-CHA	-4.45	115.26	125.20
17	B	1242	CLA	C1C-NC-C4C	4.45	108.71	106.68
17	P	5132	CLA	C3D-C4D-CHA	-4.45	115.26	125.20
17	Q	5203	CLA	C3D-C4D-CHA	-4.45	115.26	125.20
17	5	5401	CLA	C3D-C4D-CHA	-4.45	115.26	125.20
17	P	5123	CLA	C3D-C4D-CHA	-4.45	115.26	125.20
17	Q	5224	CLA	C3D-C4D-CHA	-4.45	115.26	125.20
17	P	5122	CLA	C3D-C4D-CHA	-4.45	115.26	125.20
17	P	5103	CLA	C3D-C4D-CHA	-4.45	115.26	125.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	B	1234	CLA	C3D-C4D-CHA	-4.45	115.26	125.20
17	Q	5234	CLA	C3D-C4D-CHA	-4.45	115.27	125.20
17	2	1031	CLA	C1C-NC-C4C	4.45	108.71	106.68
17	B	1221	CLA	C3D-C4D-CHA	-4.44	115.28	125.20
17	P	5115	CLA	C1C-NC-C4C	4.44	108.71	106.68
17	B	1203	CLA	C3D-C4D-CHA	-4.44	115.28	125.20
17	A	1132	CLA	C3D-C4D-CHA	-4.44	115.28	125.20
17	B	1224	CLA	C3D-C4D-CHA	-4.44	115.29	125.20
17	A	1128	CLA	C3D-C4D-CHA	-4.44	115.29	125.20
17	U	8003	CLA	C3D-C4D-CHA	-4.44	115.29	125.20
17	0	1031	CLA	C3D-C4D-CHA	-4.44	115.29	125.20
17	K	1401	CLA	C3D-C4D-CHA	-4.43	115.30	125.20
17	Q	5221	CLA	C3D-C4D-CHA	-4.43	115.30	125.20
17	9	1022	CLA	C3D-C4D-CHA	-4.43	115.30	125.20
17	4	1031	CLA	C3D-C4D-CHA	-4.43	115.31	125.20
17	J	1302	CLA	C4D-ND-C1D	4.43	109.42	106.31
17	0	1021	CLA	C1C-NC-C4C	4.43	108.70	106.68
17	8	1023	CLA	C3D-C4D-CHA	-4.43	115.32	125.20
17	A	4009	CLA	C3D-C4D-CHA	-4.42	115.32	125.20
17	P	5012	CLA	C3D-C4D-CHA	-4.42	115.32	125.20
17	9	1031	CLA	C3D-C4D-CHA	-4.42	115.33	125.20
17	A	1115	CLA	C1C-NC-C4C	4.42	108.70	106.68
17	3	1022	CLA	C3D-C4D-CHA	-4.42	115.33	125.20
17	2	1023	CLA	C3D-C4D-CHA	-4.42	115.33	125.20
17	3	1016	CLA	C3D-C4D-CHA	-4.42	115.33	125.20
17	4	1017	CLA	C3D-C4D-CHA	-4.42	115.33	125.20
17	U	8006	CLA	C3D-C4D-CHA	-4.42	115.33	125.20
17	3	1031	CLA	C3D-C4D-CHA	-4.42	115.34	125.20
17	Q	5232	CLA	C3D-C4D-CHA	-4.42	115.34	125.20
17	1	1021	CLA	C3D-C4D-CHA	-4.42	115.34	125.20
17	4	1021	CLA	C3D-C4D-CHA	-4.42	115.34	125.20
17	Q	8001	CLA	C3D-C4D-CHA	-4.42	115.34	125.20
17	A	1012	CLA	C3D-C4D-CHA	-4.41	115.34	125.20
17	0	1014	CLA	C3D-C4D-CHA	-4.41	115.34	125.20
17	0	1021	CLA	C3D-C4D-CHA	-4.41	115.34	125.20
17	Q	5237	CLA	C3D-C4D-CHA	-4.41	115.34	125.20
17	8	1021	CLA	C3D-C4D-CHA	-4.41	115.34	125.20
17	0	1016	CLA	C3D-C4D-CHA	-4.41	115.34	125.20
17	P	5110	CLA	C1B-NB-C4B	4.41	109.41	106.31
17	2	1021	CLA	C3D-C4D-CHA	-4.41	115.35	125.20
17	4	1025	CLA	C3D-C4D-CHA	-4.41	115.35	125.20
17	8	1025	CLA	C1C-NC-C4C	4.41	108.69	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	Q	5204	CLA	C3D-C4D-CHA	-4.41	115.35	125.20
17	9	1011	CLA	C3D-C4D-CHA	-4.41	115.35	125.20
17	Q	5241	CLA	C3D-C4D-CHA	-4.41	115.35	125.20
17	7	1021	CLA	C3D-C4D-CHA	-4.41	115.35	125.20
17	8	8007	CLA	C3D-C4D-CHA	-4.41	115.35	125.20
17	A	4010	CLA	C3D-C4D-CHA	-4.41	115.35	125.20
17	4	1013	CLA	C3D-C4D-CHA	-4.41	115.35	125.20
17	F	4003	CLA	C3D-C4D-CHA	-4.41	115.36	125.20
17	P	8010	CLA	C3D-C4D-CHA	-4.41	115.36	125.20
17	0	1017	CLA	C3D-C4D-CHA	-4.41	115.36	125.20
17	B	1232	CLA	C3D-C4D-CHA	-4.41	115.36	125.20
17	B	4001	CLA	C3D-C4D-CHA	-4.41	115.36	125.20
17	A	1105	CLA	C3D-C4D-CHA	-4.41	115.36	125.20
17	3	1014	CLA	C3D-C4D-CHA	-4.41	115.36	125.20
17	P	8009	CLA	C3D-C4D-CHA	-4.41	115.36	125.20
17	7	1022	CLA	C3D-C4D-CHA	-4.41	115.36	125.20
17	B	1241	CLA	C3D-C4D-CHA	-4.41	115.36	125.20
17	7	1017	CLA	C3D-C4D-CHA	-4.41	115.36	125.20
17	9	1016	CLA	C3D-C4D-CHA	-4.41	115.36	125.20
17	B	1237	CLA	C3D-C4D-CHA	-4.41	115.36	125.20
17	1	1025	CLA	C3D-C4D-CHA	-4.41	115.36	125.20
17	Z	8008	CLA	C3D-C4D-CHA	-4.41	115.36	125.20
17	0	1025	CLA	C3D-C4D-CHA	-4.41	115.36	125.20
17	9	1012	CLA	C3D-C4D-CHA	-4.41	115.36	125.20
17	W	5801	CLA	C3D-C4D-CHA	-4.40	115.36	125.20
17	2	4007	CLA	C3D-C4D-CHA	-4.40	115.37	125.20
17	9	1014	CLA	C3D-C4D-CHA	-4.40	115.37	125.20
17	P	5105	CLA	C3D-C4D-CHA	-4.40	115.37	125.20
17	3	1012	CLA	C3D-C4D-CHA	-4.40	115.37	125.20
17	2	1011	CLA	C3D-C4D-CHA	-4.40	115.37	125.20
17	H	1801	CLA	C3D-C4D-CHA	-4.40	115.37	125.20
17	Z	5101	CLA	C3D-C4D-CHA	-4.40	115.37	125.20
17	4	1023	CLA	C3D-C4D-CHA	-4.40	115.37	125.20
17	4	1026	CLA	C3D-C4D-CHA	-4.40	115.37	125.20
17	3	1026	CLA	C3D-C4D-CHA	-4.40	115.38	125.20
17	9	1026	CLA	C3D-C4D-CHA	-4.40	115.38	125.20
17	F	4006	CLA	C3D-C4D-CHA	-4.40	115.38	125.20
17	8	1011	CLA	C3D-C4D-CHA	-4.40	115.38	125.20
17	0	8002	CLA	C3D-C4D-CHA	-4.40	115.38	125.20
17	4	1012	CLA	C3D-C4D-CHA	-4.40	115.38	125.20
17	4	1014	CLA	C3D-C4D-CHA	-4.40	115.38	125.20
17	2	1022	CLA	C1C-NC-C4C	4.40	108.69	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	L	1503	CLA	C3D-C4D-CHA	-4.40	115.38	125.20
17	A	1110	CLA	C1B-NB-C4B	4.40	109.40	106.31
17	A	1129	CLA	C3D-C4D-CHA	-4.40	115.38	125.20
17	J	1101	CLA	C3D-C4D-CHA	-4.40	115.38	125.20
17	8	1013	CLA	C3D-C4D-CHA	-4.40	115.38	125.20
17	8	1033	CLA	C3D-C4D-CHA	-4.40	115.38	125.20
17	J	4008	CLA	C3D-C4D-CHA	-4.40	115.38	125.20
17	3	1032	CLA	C3D-C4D-CHA	-4.40	115.38	125.20
17	4	1011	CLA	C3D-C4D-CHA	-4.40	115.38	125.20
17	8	1015	CLA	C3D-C4D-CHA	-4.40	115.38	125.20
17	0	1026	CLA	C3D-C4D-CHA	-4.40	115.38	125.20
17	B	1240	CLA	C3D-C4D-CHA	-4.40	115.38	125.20
17	2	1013	CLA	C3D-C4D-CHA	-4.40	115.38	125.20
17	4	1016	CLA	C3D-C4D-CHA	-4.40	115.38	125.20
17	7	1011	CLA	C3D-C4D-CHA	-4.40	115.38	125.20
17	0	1023	CLA	C3D-C4D-CHA	-4.40	115.38	125.20
17	U	8004	CLA	C3D-C4D-CHA	-4.40	115.39	125.20
17	K	1403	CLA	C3D-C4D-CHA	-4.39	115.39	125.20
17	1	1011	CLA	C3D-C4D-CHA	-4.39	115.39	125.20
17	U	8005	CLA	C3D-C4D-CHA	-4.39	115.39	125.20
17	6	5503	CLA	C3D-C4D-CHA	-4.39	115.39	125.20
17	7	1025	CLA	C3D-C4D-CHA	-4.39	115.39	125.20
17	G	1701	CLA	C3D-C4D-CHA	-4.39	115.39	125.20
17	1	1022	CLA	C3D-C4D-CHA	-4.39	115.39	125.20
17	2	1033	CLA	C3D-C4D-CHA	-4.39	115.39	125.20
17	0	1011	CLA	C3D-C4D-CHA	-4.39	115.39	125.20
17	3	1015	CLA	C3D-C4D-CHA	-4.39	115.39	125.20
17	4	1015	CLA	C3D-C4D-CHA	-4.39	115.39	125.20
17	7	1015	CLA	C3D-C4D-CHA	-4.39	115.39	125.20
17	0	1022	CLA	C3D-C4D-CHA	-4.39	115.39	125.20
17	1	1013	CLA	C3D-C4D-CHA	-4.39	115.39	125.20
17	4	1033	CLA	C3D-C4D-CHA	-4.39	115.39	125.20
17	A	1125	CLA	C3D-C4D-CHA	-4.39	115.40	125.20
17	1	1023	CLA	C3D-C4D-CHA	-4.39	115.40	125.20
17	P	5129	CLA	C3D-C4D-CHA	-4.39	115.40	125.20
17	V	5701	CLA	C3D-C4D-CHA	-4.39	115.40	125.20
17	0	1033	CLA	C3D-C4D-CHA	-4.39	115.40	125.20
17	B	1204	CLA	C3D-C4D-CHA	-4.39	115.40	125.20
17	2	1014	CLA	C3D-C4D-CHA	-4.39	115.40	125.20
17	L	1502	CLA	C3D-C4D-CHA	-4.39	115.40	125.20
17	1	1017	CLA	C3D-C4D-CHA	-4.39	115.40	125.20
17	3	1041	CLA	C3D-C4D-CHA	-4.39	115.40	125.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	7	1023	CLA	C3D-C4D-CHA	-4.39	115.40	125.20
17	B	1212	CLA	C1C-NC-C4C	4.39	108.68	106.68
17	3	1011	CLA	C3D-C4D-CHA	-4.39	115.40	125.20
17	5	5403	CLA	C3D-C4D-CHA	-4.39	115.40	125.20
17	9	1041	CLA	C3D-C4D-CHA	-4.39	115.40	125.20
17	K	1404	CLA	C3D-C4D-CHA	-4.39	115.40	125.20
17	2	1012	CLA	C3D-C4D-CHA	-4.39	115.40	125.20
17	2	1015	CLA	C3D-C4D-CHA	-4.39	115.40	125.20
17	2	1026	CLA	C3D-C4D-CHA	-4.39	115.40	125.20
17	4	4002	CLA	C3D-C4D-CHA	-4.39	115.40	125.20
17	B	1231	CLA	C3D-C4D-CHA	-4.39	115.40	125.20
17	6	5504	CLA	C3D-C4D-CHA	-4.39	115.40	125.20
17	Q	5242	CLA	C3D-C4D-CHA	-4.39	115.41	125.20
17	0	1013	CLA	C3D-C4D-CHA	-4.39	115.41	125.20
17	1	1014	CLA	C3D-C4D-CHA	-4.38	115.41	125.20
17	7	1016	CLA	C3D-C4D-CHA	-4.38	115.41	125.20
17	1	1016	CLA	C3D-C4D-CHA	-4.38	115.41	125.20
17	1	1026	CLA	C3D-C4D-CHA	-4.38	115.41	125.20
17	0	1015	CLA	C3D-C4D-CHA	-4.38	115.41	125.20
17	L	1504	CLA	C3D-C4D-CHA	-4.38	115.41	125.20
17	1	1012	CLA	C3D-C4D-CHA	-4.38	115.41	125.20
17	2	1022	CLA	C3D-C4D-CHA	-4.38	115.41	125.20
17	0	1012	CLA	C3D-C4D-CHA	-4.38	115.41	125.20
17	A	1118	CLA	C3D-C4D-CHA	-4.38	115.41	125.20
17	Q	5231	CLA	C3D-C4D-CHA	-4.38	115.41	125.20
17	2	1017	CLA	C3D-C4D-CHA	-4.38	115.41	125.20
17	5	5404	CLA	C3D-C4D-CHA	-4.38	115.41	125.20
17	1	1015	CLA	C3D-C4D-CHA	-4.38	115.42	125.20
17	7	1012	CLA	C3D-C4D-CHA	-4.38	115.42	125.20
17	7	1013	CLA	C3D-C4D-CHA	-4.38	115.42	125.20
17	F	4004	CLA	C3D-C4D-CHA	-4.38	115.42	125.20
17	3	1017	CLA	C3D-C4D-CHA	-4.38	115.42	125.20
17	6	5502	CLA	C3D-C4D-CHA	-4.38	115.42	125.20
17	8	1014	CLA	C3D-C4D-CHA	-4.38	115.42	125.20
17	F	4005	CLA	C3D-C4D-CHA	-4.38	115.42	125.20
17	3	1033	CLA	C3D-C4D-CHA	-4.38	115.42	125.20
17	7	1026	CLA	C3D-C4D-CHA	-4.38	115.42	125.20
17	9	1032	CLA	C3D-C4D-CHA	-4.38	115.42	125.20
17	2	1016	CLA	C3D-C4D-CHA	-4.38	115.42	125.20
17	8	1017	CLA	C3D-C4D-CHA	-4.38	115.42	125.20
17	9	1025	CLA	C3D-C4D-CHA	-4.38	115.42	125.20
17	P	5125	CLA	C3D-C4D-CHA	-4.38	115.43	125.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	9	1033	CLA	C3D-C4D-CHA	-4.38	115.43	125.20
17	A	1127	CLA	C3D-C4D-CHA	-4.37	115.43	125.20
17	2	1031	CLA	C3D-C4D-CHA	-4.37	115.43	125.20
17	Q	5240	CLA	C3D-C4D-CHA	-4.37	115.43	125.20
17	9	1017	CLA	C3D-C4D-CHA	-4.37	115.43	125.20
17	B	1222	CLA	C3D-C4D-CHA	-4.37	115.43	125.20
17	4	1022	CLA	C3D-C4D-CHA	-4.37	115.43	125.20
17	P	5118	CLA	C3D-C4D-CHA	-4.37	115.43	125.20
17	P	5127	CLA	C3D-C4D-CHA	-4.37	115.43	125.20
17	B	1242	CLA	C3D-C4D-CHA	-4.37	115.43	125.20
17	3	1021	CLA	C3D-C4D-CHA	-4.37	115.43	125.20
17	P	5114	CLA	C3D-C4D-CHA	-4.37	115.43	125.20
17	9	1015	CLA	C3D-C4D-CHA	-4.37	115.43	125.20
17	2	1025	CLA	C3D-C4D-CHA	-4.37	115.44	125.20
17	7	1014	CLA	C3D-C4D-CHA	-4.37	115.44	125.20
17	7	1031	CLA	C3D-C4D-CHA	-4.37	115.44	125.20
17	8	1025	CLA	C3D-C4D-CHA	-4.37	115.44	125.20
17	4	1032	CLA	C3D-C4D-CHA	-4.37	115.44	125.20
17	8	1026	CLA	C3D-C4D-CHA	-4.37	115.44	125.20
17	0	1032	CLA	C3D-C4D-CHA	-4.37	115.44	125.20
17	Q	5219	CLA	C3D-C4D-CHA	-4.37	115.44	125.20
17	8	1012	CLA	C3D-C4D-CHA	-4.37	115.44	125.20
17	9	1021	CLA	C3D-C4D-CHA	-4.37	115.44	125.20
17	Z	5302	CLA	C4D-ND-C1D	4.37	109.38	106.31
17	B	1219	CLA	C3D-C4D-CHA	-4.37	115.44	125.20
17	8	1022	CLA	C3D-C4D-CHA	-4.37	115.44	125.20
17	A	1112	CLA	C3D-C4D-CHA	-4.37	115.44	125.20
17	P	5112	CLA	C3D-C4D-CHA	-4.37	115.44	125.20
17	1	1031	CLA	C3D-C4D-CHA	-4.37	115.45	125.20
17	8	1031	CLA	C3D-C4D-CHA	-4.37	115.45	125.20
17	Q	5214	CLA	C3D-C4D-CHA	-4.36	115.45	125.20
17	3	1025	CLA	C3D-C4D-CHA	-4.36	115.46	125.20
17	Q	5208	CLA	C3D-C4D-CHA	-4.36	115.46	125.20
17	0	1023	CLA	C1C-NC-C4C	4.36	108.67	106.68
17	A	1114	CLA	C3D-C4D-CHA	-4.36	115.47	125.20
17	8	1016	CLA	C3D-C4D-CHA	-4.36	115.47	125.20
17	B	1227	CLA	C3D-C4D-CHA	-4.36	115.47	125.20
17	B	1239	CLA	C3D-C4D-CHA	-4.36	115.47	125.20
17	Q	5239	CLA	C3D-C4D-CHA	-4.36	115.47	125.20
17	B	1208	CLA	C3D-C4D-CHA	-4.35	115.47	125.20
17	B	1214	CLA	C3D-C4D-CHA	-4.35	115.47	125.20
17	P	5111	CLA	C3D-C4D-CHA	-4.35	115.48	125.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	P	5139	CLA	C3D-C4D-CHA	-4.35	115.48	125.20
17	8	1022	CLA	C1C-NC-C4C	4.35	108.66	106.68
17	A	1139	CLA	C3D-C4D-CHA	-4.35	115.48	125.20
17	A	1107	CLA	C3D-C4D-CHA	-4.35	115.49	125.20
17	B	1220	CLA	C3D-C4D-CHA	-4.35	115.49	125.20
17	P	5107	CLA	C3D-C4D-CHA	-4.35	115.50	125.20
17	Q	5218	CLA	C1B-NB-C4B	4.35	109.36	106.31
17	P	5136	CLA	C3D-C4D-CHA	-4.34	115.50	125.20
17	P	5120	CLA	C3D-C4D-CHA	-4.34	115.50	125.20
17	B	1225	CLA	C3D-C4D-CHA	-4.34	115.50	125.20
17	Q	5227	CLA	C3D-C4D-CHA	-4.34	115.50	125.20
17	Q	5222	CLA	C3D-C4D-CHA	-4.34	115.50	125.20
17	Q	5220	CLA	C3D-C4D-CHA	-4.34	115.51	125.20
17	Q	5209	CLA	C3D-C4D-CHA	-4.34	115.52	125.20
17	B	1228	CLA	C3D-C4D-CHA	-4.34	115.52	125.20
17	P	5127	CLA	C1B-NB-C4B	4.33	109.35	106.31
17	Q	5228	CLA	C3D-C4D-CHA	-4.33	115.52	125.20
17	Q	5225	CLA	C3D-C4D-CHA	-4.33	115.53	125.20
17	A	1111	CLA	C3D-C4D-CHA	-4.33	115.53	125.20
17	Q	5223	CLA	C3D-C4D-CHA	-4.33	115.53	125.20
17	Q	5235	CLA	C3D-C4D-CHA	-4.33	115.54	125.20
17	B	1235	CLA	C3D-C4D-CHA	-4.33	115.54	125.20
17	P	5133	CLA	C3D-C4D-CHA	-4.33	115.54	125.20
17	A	1136	CLA	C3D-C4D-CHA	-4.32	115.54	125.20
17	A	1120	CLA	C3D-C4D-CHA	-4.32	115.55	125.20
17	Q	5207	CLA	C3D-C4D-CHA	-4.32	115.55	125.20
17	A	1402	CLA	C3D-C4D-CHA	-4.32	115.55	125.20
17	B	1209	CLA	C3D-C4D-CHA	-4.32	115.55	125.20
17	B	1223	CLA	C3D-C4D-CHA	-4.32	115.56	125.20
17	B	1207	CLA	C3D-C4D-CHA	-4.32	115.56	125.20
17	P	5103	CLA	C1C-NC-C4C	4.31	108.65	106.68
17	A	1133	CLA	C3D-C4D-CHA	-4.31	115.57	125.20
17	B	1218	CLA	C3D-C4D-CHA	-4.31	115.57	125.20
17	4	1023	CLA	C1C-NC-C4C	4.31	108.65	106.68
17	Q	5130	CLA	C1C-NC-C4C	4.31	108.65	106.68
17	A	1013	CLA	C3D-C4D-CHA	-4.31	115.58	125.20
17	A	1127	CLA	C1B-NB-C4B	4.31	109.33	106.31
17	P	5402	CLA	C3D-C4D-CHA	-4.31	115.58	125.20
17	A	1116	CLA	C3D-C4D-CHA	-4.31	115.58	125.20
17	B	1218	CLA	C1B-NB-C4B	4.31	109.33	106.31
17	P	5124	CLA	C3D-C4D-CHA	-4.31	115.58	125.20
17	Q	5224	CLA	C1B-NB-C4B	4.30	109.33	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	P	5135	CLA	C3D-C4D-CHA	-4.30	115.59	125.20
17	B	1224	CLA	C1B-NB-C4B	4.30	109.33	106.31
17	A	1124	CLA	C3D-C4D-CHA	-4.30	115.59	125.20
17	Q	5212	CLA	C3D-C4D-CHA	-4.30	115.60	125.20
17	B	1212	CLA	C3D-C4D-CHA	-4.30	115.60	125.20
17	Q	5218	CLA	C3D-C4D-CHA	-4.30	115.61	125.20
17	A	1135	CLA	C3D-C4D-CHA	-4.29	115.61	125.20
17	A	1103	CLA	C1C-NC-C4C	4.29	108.64	106.68
17	G	1233	CLA	C3D-C4D-CHA	-4.29	115.62	125.20
17	A	1109	CLA	C3D-C4D-CHA	-4.29	115.62	125.20
17	B	1022	CLA	C3D-C4D-CHA	-4.29	115.63	125.20
17	P	5116	CLA	C3D-C4D-CHA	-4.29	115.63	125.20
17	P	5901	CLA	C3D-C4D-CHA	-4.29	115.63	125.20
17	B	1217	CLA	C1B-NB-C4B	4.29	109.32	106.31
17	P	5013	CLA	C3D-C4D-CHA	-4.28	115.63	125.20
17	P	5106	CLA	C3D-C4D-CHA	-4.28	115.63	125.20
17	A	1138	CLA	C3D-C4D-CHA	-4.28	115.64	125.20
17	A	1901	CLA	C3D-C4D-CHA	-4.28	115.64	125.20
17	P	5138	CLA	C3D-C4D-CHA	-4.28	115.64	125.20
17	A	1106	CLA	C3D-C4D-CHA	-4.28	115.64	125.20
17	J	1302	CLA	C3D-C4D-CHA	-4.28	115.64	125.20
17	P	5133	CLA	C1B-NB-C4B	4.28	109.31	106.31
17	Q	5022	CLA	C3D-C4D-CHA	-4.28	115.65	125.20
17	Q	5217	CLA	C1B-NB-C4B	4.27	109.31	106.31
17	P	5109	CLA	C3D-C4D-CHA	-4.27	115.67	125.20
17	Q	5130	CLA	C3D-C4D-CHA	-4.27	115.67	125.20
17	Q	5217	CLA	C3D-C4D-CHA	-4.27	115.67	125.20
17	Z	5302	CLA	C3D-C4D-CHA	-4.27	115.67	125.20
17	V	5233	CLA	C3D-C4D-CHA	-4.26	115.68	125.20
17	B	1217	CLA	C3D-C4D-CHA	-4.26	115.69	125.20
17	A	1104	CLA	C3D-C4D-CHA	-4.25	115.70	125.20
17	B	1130	CLA	C3D-C4D-CHA	-4.25	115.72	125.20
17	Q	5216	CLA	C3D-C4D-CHA	-4.25	115.72	125.20
17	A	1117	CLA	C3D-C4D-CHA	-4.24	115.72	125.20
17	P	5117	CLA	C3D-C4D-CHA	-4.24	115.72	125.20
17	P	5110	CLA	C3D-C4D-CHA	-4.24	115.73	125.20
17	U	5301	CLA	C3D-C4D-CHA	-4.24	115.73	125.20
17	A	1134	CLA	C3D-C4D-CHA	-4.24	115.73	125.20
17	B	1204	CLA	C1B-NB-C4B	4.24	109.29	106.31
17	A	1133	CLA	C1B-NB-C4B	4.24	109.28	106.31
17	A	1110	CLA	C3D-C4D-CHA	-4.24	115.74	125.20
17	B	1216	CLA	C3D-C4D-CHA	-4.24	115.74	125.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	B	1130	CLA	C1C-NC-C4C	4.23	108.61	106.68
17	P	5104	CLA	C3D-C4D-CHA	-4.23	115.75	125.20
17	B	1226	CLA	C1C-NC-C4C	4.23	108.61	106.68
17	U	5301	CLA	C1C-NC-C4C	4.23	108.61	106.68
17	P	5107	CLA	C1B-NB-C4B	4.22	109.28	106.31
17	F	1301	CLA	C3D-C4D-CHA	-4.22	115.77	125.20
17	Q	5205	CLA	C1C-NC-C4C	4.22	108.61	106.68
17	Q	5204	CLA	C1B-NB-C4B	4.22	109.27	106.31
17	Q	5222	CLA	C1B-NB-C4B	4.22	109.27	106.31
17	A	1134	CLA	C1B-NB-C4B	4.22	109.27	106.31
17	P	5011	CLA	C1C-NC-C4C	4.22	108.60	106.68
17	B	1209	CLA	C1B-NB-C4B	4.22	109.27	106.31
17	A	1011	CLA	C1C-NC-C4C	4.22	108.60	106.68
17	P	5134	CLA	C3D-C4D-CHA	-4.21	115.79	125.20
17	F	1301	CLA	C1C-NC-C4C	4.21	108.60	106.68
17	A	1107	CLA	C1B-NB-C4B	4.21	109.26	106.31
17	Q	5206	CLA	C1C-NC-C4C	4.20	108.60	106.68
17	A	1113	CLA	C3D-C4D-CHA	-4.20	115.83	125.20
17	P	5113	CLA	C3D-C4D-CHA	-4.19	115.84	125.20
17	P	5134	CLA	C1B-NB-C4B	4.18	109.24	106.31
17	P	5140	CLA	C1B-NB-C4B	4.17	109.24	106.31
17	P	5127	CLA	C1C-NC-C4C	4.17	108.58	106.68
17	A	1127	CLA	C1C-NC-C4C	4.17	108.58	106.68
17	A	1129	CLA	C1B-NB-C4B	4.17	109.24	106.31
17	A	1140	CLA	C1B-NB-C4B	4.16	109.23	106.31
17	Q	5209	CLA	C1B-NB-C4B	4.16	109.23	106.31
17	P	5129	CLA	C1B-NB-C4B	4.15	109.22	106.31
17	B	1205	CLA	C1C-NC-C4C	4.15	108.57	106.68
17	B	1238	CLA	C1B-NB-C4B	4.14	109.22	106.31
17	B	1206	CLA	C1C-NC-C4C	4.13	108.56	106.68
17	B	1222	CLA	C1B-NB-C4B	4.12	109.20	106.31
17	P	5122	CLA	C1B-NB-C4B	4.11	109.19	106.31
17	Q	5226	CLA	C1C-NC-C4C	4.11	108.55	106.68
17	Q	5238	CLA	C1B-NB-C4B	4.10	109.19	106.31
17	B	1215	CLA	C1B-NB-C4B	4.07	109.17	106.31
17	A	1122	CLA	C1B-NB-C4B	4.06	109.16	106.31
17	G	1233	CLA	C1B-NB-C4B	4.06	109.16	106.31
17	Q	5215	CLA	C1B-NB-C4B	4.06	109.16	106.31
17	V	5233	CLA	C1B-NB-C4B	4.06	109.16	106.31
17	P	5119	CLA	C1B-NB-C4B	4.02	109.14	106.31
17	P	5104	CLA	C1C-NC-C4C	4.02	108.52	106.68
17	B	1227	CLA	C1B-NB-C4B	4.01	109.12	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	A	1119	CLA	C1B-NB-C4B	4.00	109.12	106.31
17	Q	5227	CLA	C1B-NB-C4B	3.99	109.11	106.31
17	K	1401	CLA	C1B-NB-C4B	3.99	109.11	106.31
17	5	5401	CLA	C1B-NB-C4B	3.96	109.09	106.31
17	B	1210	CLA	C1C-NC-C4C	3.93	108.47	106.68
17	A	1104	CLA	C1C-NC-C4C	3.93	108.47	106.68
17	B	1230	CLA	C1B-NB-C4B	3.92	109.06	106.31
17	P	5116	CLA	C1B-NB-C4B	3.92	109.06	106.31
17	Q	5206	CLA	C1B-NB-C4B	3.90	109.05	106.31
17	P	5901	CLA	C4D-ND-C1D	3.89	109.04	106.31
17	Q	5230	CLA	C1B-NB-C4B	3.89	109.04	106.31
17	Q	5210	CLA	C1C-NC-C4C	3.88	108.45	106.68
17	P	5120	CLA	C1B-NB-C4B	3.88	109.03	106.31
17	B	1206	CLA	C1B-NB-C4B	3.88	109.03	106.31
17	A	1901	CLA	C4D-ND-C1D	3.88	109.03	106.31
17	A	1102	CLA	C1B-NB-C4B	3.88	109.03	106.31
17	A	1123	CLA	C1C-NC-C4C	3.87	108.44	106.68
17	A	1116	CLA	C1B-NB-C4B	3.87	109.03	106.31
17	P	5114	CLA	C1B-NB-C4B	3.86	109.02	106.31
17	P	5123	CLA	C1C-NC-C4C	3.85	108.44	106.68
17	P	5402	CLA	C1C-NC-C4C	3.85	108.44	106.68
17	A	1120	CLA	C1B-NB-C4B	3.85	109.01	106.31
17	F	1301	CLA	C1B-NB-C4B	3.84	109.00	106.31
17	P	5102	CLA	C1B-NB-C4B	3.82	108.99	106.31
17	A	1114	CLA	C1B-NB-C4B	3.81	108.99	106.31
17	P	5011	CLA	C1B-NB-C4B	3.81	108.99	106.31
17	Q	5228	CLA	C1B-NB-C4B	3.81	108.99	106.31
17	U	5301	CLA	C1B-NB-C4B	3.81	108.99	106.31
17	A	1402	CLA	C1C-NC-C4C	3.79	108.41	106.68
17	B	1228	CLA	C1B-NB-C4B	3.78	108.97	106.31
17	Q	5203	CLA	C1C-NC-C4C	3.78	108.40	106.68
17	Q	5219	CLA	C4D-ND-C1D	3.78	108.96	106.31
17	A	1011	CLA	C1B-NB-C4B	3.77	108.96	106.31
17	B	1203	CLA	C1C-NC-C4C	3.75	108.39	106.68
17	B	1219	CLA	C4D-ND-C1D	3.72	108.92	106.31
17	B	1021	CLA	C1B-NB-C4B	3.71	108.92	106.31
17	Q	5232	CLA	C1B-NB-C4B	3.71	108.92	106.31
17	U	5229	CLA	C1B-NB-C4B	3.70	108.91	106.31
17	L	1503	CLA	C1B-NB-C4B	3.70	108.91	106.31
17	Q	5021	CLA	C1B-NB-C4B	3.70	108.91	106.31
17	A	1138	CLA	C1B-NB-C4B	3.69	108.90	106.31
17	B	1232	CLA	C1B-NB-C4B	3.69	108.90	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	Q	5219	CLA	C3C-C4C-NC	-3.69	106.70	109.92
17	Q	5023	CLA	C1B-NB-C4B	3.69	108.90	106.31
17	B	1023	CLA	C1B-NB-C4B	3.68	108.89	106.31
17	P	5137	CLA	C3C-C4C-NC	-3.68	106.71	109.92
17	B	1219	CLA	C3C-C4C-NC	-3.68	106.71	109.92
17	A	1137	CLA	C3C-C4C-NC	-3.67	106.72	109.92
17	A	1139	CLA	C1B-NB-C4B	3.67	108.89	106.31
17	P	5139	CLA	C1B-NB-C4B	3.67	108.88	106.31
17	F	1229	CLA	C1B-NB-C4B	3.66	108.88	106.31
17	P	5138	CLA	C1B-NB-C4B	3.65	108.88	106.31
17	6	5503	CLA	C1B-NB-C4B	3.64	108.87	106.31
17	A	1132	CLA	C1B-NB-C4B	3.64	108.86	106.31
17	Q	5220	CLA	C1B-NB-C4B	3.63	108.86	106.31
17	P	5117	CLA	C1B-NB-C4B	3.59	108.83	106.31
17	B	1237	CLA	C1B-NB-C4B	3.58	108.83	106.31
17	P	5132	CLA	C1B-NB-C4B	3.58	108.83	106.31
17	B	1220	CLA	C1B-NB-C4B	3.58	108.82	106.31
17	P	5128	CLA	C1B-NB-C4B	3.57	108.82	106.31
17	Q	5237	CLA	C1B-NB-C4B	3.55	108.80	106.31
17	A	1117	CLA	C1B-NB-C4B	3.54	108.80	106.31
17	A	1112	CLA	C1B-NB-C4B	3.54	108.80	106.31
17	B	1239	CLA	C1B-NB-C4B	3.54	108.80	106.31
17	6	5501	CLA	C1B-NB-C4B	3.53	108.79	106.31
17	P	5112	CLA	C1B-NB-C4B	3.52	108.78	106.31
17	A	1131	CLA	C1B-NB-C4B	3.51	108.78	106.31
17	Q	5239	CLA	C1B-NB-C4B	3.51	108.78	106.31
17	P	5131	CLA	C1B-NB-C4B	3.51	108.78	106.31
17	A	1128	CLA	C1B-NB-C4B	3.51	108.77	106.31
17	L	1501	CLA	C1B-NB-C4B	3.50	108.77	106.31
17	B	1213	CLA	C1B-NB-C4B	3.49	108.76	106.31
17	B	1207	CLA	C2A-C1A-CHA	3.49	128.58	122.63
17	B	1231	CLA	C1B-NB-C4B	3.49	108.76	106.31
17	Q	5207	CLA	C2A-C1A-CHA	3.48	128.58	122.63
17	Q	5213	CLA	C1B-NB-C4B	3.48	108.75	106.31
17	B	1216	CLA	C1B-NB-C4B	3.48	108.75	106.31
17	P	5113	CLA	C3C-C4C-NC	-3.46	106.90	109.92
17	Q	5216	CLA	C1B-NB-C4B	3.46	108.74	106.31
17	B	1201	CLA	C1B-NB-C4B	3.43	108.72	106.31
17	A	1113	CLA	C3C-C4C-NC	-3.42	106.93	109.92
17	A	1124	CLA	C1B-NB-C4B	3.42	108.71	106.31
17	A	1107	CLA	C2A-C1A-CHA	3.41	128.45	122.63
17	P	5107	CLA	C2A-C1A-CHA	3.41	128.44	122.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	P	5124	CLA	C1B-NB-C4B	3.40	108.70	106.31
17	Q	5231	CLA	C1B-NB-C4B	3.40	108.69	106.31
17	P	5126	CLA	C1B-NB-C4B	3.35	108.66	106.31
17	A	1109	CLA	C1B-NB-C4B	3.34	108.66	106.31
17	A	1135	CLA	C1C-NC-C4C	3.34	108.20	106.68
17	P	5106	CLA	C1B-NB-C4B	3.34	108.65	106.31
17	P	5135	CLA	C1C-NC-C4C	3.33	108.20	106.68
17	Q	5201	CLA	C1B-NB-C4B	3.33	108.65	106.31
17	A	1012	CLA	C2A-C1A-CHA	3.32	128.30	122.63
17	P	5012	CLA	C2A-C1A-CHA	3.32	128.30	122.63
17	A	1106	CLA	C1B-NB-C4B	3.31	108.64	106.31
17	A	1126	CLA	C1B-NB-C4B	3.31	108.63	106.31
17	B	1211	CLA	C1B-NB-C4B	3.30	108.63	106.31
17	Q	5211	CLA	C1B-NB-C4B	3.30	108.63	106.31
17	P	5113	CLA	C4D-ND-C1D	3.30	108.63	106.31
17	P	5109	CLA	C1B-NB-C4B	3.29	108.62	106.31
17	P	5104	CLA	C2A-C1A-CHA	3.24	128.17	122.63
17	A	1113	CLA	C4D-ND-C1D	3.24	108.58	106.31
17	A	1901	CLA	C3C-C4C-NC	-3.23	107.10	109.92
17	A	1104	CLA	C2A-C1A-CHA	3.23	128.14	122.63
17	P	5901	CLA	C3C-C4C-NC	-3.21	107.12	109.92
17	Q	5221	CLA	C2A-C1A-CHA	3.20	128.09	122.63
17	B	1223	CLA	C1C-NC-C4C	3.19	108.13	106.68
17	Q	5212	CLA	C1B-NB-C4B	3.18	108.54	106.31
17	B	1221	CLA	C2A-C1A-CHA	3.18	128.06	122.63
17	B	1235	CLA	C1B-NB-C4B	3.17	108.54	106.31
17	P	5115	CLA	C1B-NB-C4B	3.16	108.53	106.31
17	A	1115	CLA	C1B-NB-C4B	3.15	108.52	106.31
17	A	1901	CLA	C2A-C1A-CHA	3.15	128.00	122.63
17	P	5901	CLA	C2A-C1A-CHA	3.14	127.99	122.63
17	Q	5235	CLA	C1B-NB-C4B	3.13	108.51	106.31
17	Q	5223	CLA	C1C-NC-C4C	3.13	108.11	106.68
17	B	1212	CLA	C1B-NB-C4B	3.12	108.50	106.31
17	Z	5302	CLA	C3C-C4C-NC	-3.12	107.20	109.92
17	J	1302	CLA	C3C-C4C-NC	-3.12	107.20	109.92
17	P	5121	CLA	C1B-NB-C4B	3.11	108.49	106.31
17	Z	5302	CLA	C2A-C1A-CHA	3.10	127.92	122.63
17	U	5301	CLA	C2A-C1A-CHA	3.10	127.92	122.63
17	J	1302	CLA	C2A-C1A-CHA	3.09	127.91	122.63
17	A	1121	CLA	C1B-NB-C4B	3.09	108.48	106.31
17	F	1301	CLA	C2A-C1A-CHA	3.09	127.90	122.63
17	B	1208	CLA	C1B-NB-C4B	3.08	108.47	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	L	1502	CLA	C1B-NB-C4B	3.07	108.46	106.31
17	6	5502	CLA	C1B-NB-C4B	3.06	108.46	106.31
17	P	5118	CLA	C2A-C1A-CHA	3.06	127.86	122.63
17	Q	5218	CLA	C2A-C1A-CHA	3.06	127.85	122.63
17	A	1118	CLA	C2A-C1A-CHA	3.06	127.84	122.63
17	B	1218	CLA	C2A-C1A-CHA	3.06	127.84	122.63
17	Q	5208	CLA	C1B-NB-C4B	3.05	108.45	106.31
17	Q	5217	CLA	C2A-C1A-CHA	3.05	127.83	122.63
17	B	1217	CLA	C2A-C1A-CHA	3.04	127.82	122.63
17	B	1232	CLA	C2A-C1A-CHA	3.03	127.81	122.63
17	Q	5232	CLA	C2A-C1A-CHA	3.01	127.77	122.63
17	P	5105	CLA	C1B-NB-C4B	3.00	108.42	106.31
17	P	5135	CLA	C2A-C1A-CHA	2.98	127.72	122.63
17	A	1135	CLA	C2A-C1A-CHA	2.97	127.71	122.63
17	G	1233	CLA	C2A-C1A-CHA	2.97	127.70	122.63
17	P	5137	CLA	C4D-ND-C1D	2.97	108.40	106.31
17	V	5233	CLA	C2A-C1A-CHA	2.97	127.70	122.63
17	A	1137	CLA	C4D-ND-C1D	2.95	108.38	106.31
17	A	1105	CLA	C1B-NB-C4B	2.93	108.37	106.31
17	P	5136	CLA	C1B-NB-C4B	2.92	108.36	106.31
17	A	1111	CLA	C2A-C1A-CHA	2.91	127.60	122.63
17	Q	5214	CLA	C1B-NB-C4B	2.91	108.36	106.31
17	P	5111	CLA	C2A-C1A-CHA	2.90	127.58	122.63
17	P	5134	CLA	C2A-C1A-CHA	2.89	127.57	122.63
17	B	1210	CLA	C2A-C1A-CHA	2.89	127.56	122.63
17	A	1112	CLA	C2A-C1A-CHA	2.88	127.55	122.63
17	Q	5225	CLA	C1B-NB-C4B	2.88	108.33	106.31
17	A	1120	CLA	C2A-C1A-CHA	2.88	127.54	122.63
17	P	5120	CLA	C2A-C1A-CHA	2.88	127.54	122.63
17	Q	5210	CLA	C2A-C1A-CHA	2.88	127.54	122.63
17	B	1227	CLA	C3C-C4C-NC	-2.87	107.41	109.92
17	P	5112	CLA	C2A-C1A-CHA	2.87	127.53	122.63
17	A	1134	CLA	C2A-C1A-CHA	2.87	127.52	122.63
17	9	1015	CLA	C2A-C1A-CHA	2.86	127.52	122.63
17	Q	5227	CLA	C3C-C4C-NC	-2.86	107.42	109.92
17	A	1136	CLA	C1B-NB-C4B	2.86	108.32	106.31
17	P	5108	CLA	C3C-C4C-NC	-2.85	107.43	109.92
17	A	1123	CLA	C2A-C1A-CHA	2.85	127.50	122.63
17	A	1117	CLA	C2A-C1A-CHA	2.85	127.49	122.63
17	3	1015	CLA	C2A-C1A-CHA	2.85	127.49	122.63
17	P	5123	CLA	C2A-C1A-CHA	2.85	127.49	122.63
17	7	1011	CLA	C2A-C1A-CHA	2.84	127.48	122.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	B	1214	CLA	C1B-NB-C4B	2.84	108.31	106.31
17	B	1225	CLA	C1B-NB-C4B	2.84	108.31	106.31
17	A	1102	CLA	C2A-C1A-CHA	2.84	127.48	122.63
17	P	5102	CLA	C2A-C1A-CHA	2.84	127.48	122.63
17	A	1108	CLA	C3C-C4C-NC	-2.84	107.44	109.92
17	1	1011	CLA	C2A-C1A-CHA	2.84	127.47	122.63
17	9	1032	CLA	C2A-C1A-CHA	2.84	127.47	122.63
17	P	5113	CLA	C2A-C1A-CHA	2.83	127.47	122.63
17	A	1113	CLA	C2A-C1A-CHA	2.83	127.47	122.63
17	P	5117	CLA	C2A-C1A-CHA	2.83	127.46	122.63
17	5	5404	CLA	C2A-C1A-CHA	2.83	127.46	122.63
17	8	1014	CLA	C2A-C1A-CHA	2.83	127.46	122.63
17	8	1022	CLA	C2A-C1A-CHA	2.83	127.46	122.63
17	2	1014	CLA	C2A-C1A-CHA	2.82	127.45	122.63
17	9	1016	CLA	C2A-C1A-CHA	2.82	127.45	122.63
17	7	1013	CLA	C2A-C1A-CHA	2.82	127.45	122.63
17	3	1032	CLA	C2A-C1A-CHA	2.82	127.44	122.63
17	Q	5212	CLA	C2A-C1A-CHA	2.82	127.44	122.63
17	0	1023	CLA	C2A-C1A-CHA	2.82	127.44	122.63
17	A	1139	CLA	C2A-C1A-CHA	2.82	127.44	122.63
17	0	1013	CLA	C2A-C1A-CHA	2.82	127.44	122.63
17	4	1013	CLA	C2A-C1A-CHA	2.82	127.44	122.63
17	1	1015	CLA	C2A-C1A-CHA	2.81	127.43	122.63
17	3	1025	CLA	C2A-C1A-CHA	2.81	127.43	122.63
17	9	1012	CLA	C2A-C1A-CHA	2.81	127.43	122.63
17	3	1016	CLA	C2A-C1A-CHA	2.81	127.43	122.63
17	9	1033	CLA	C2A-C1A-CHA	2.81	127.43	122.63
17	3	1014	CLA	C2A-C1A-CHA	2.81	127.43	122.63
17	4	1023	CLA	C2A-C1A-CHA	2.81	127.43	122.63
17	U	8004	CLA	C2A-C1A-CHA	2.81	127.43	122.63
18	B	2002	PQN	C2-C3-C4	-2.81	119.57	123.25
17	2	1016	CLA	C2A-C1A-CHA	2.81	127.42	122.63
17	P	5139	CLA	C2A-C1A-CHA	2.81	127.42	122.63
18	Q	6002	PQN	C2-C3-C4	-2.81	119.58	123.25
17	0	1012	CLA	C2A-C1A-CHA	2.81	127.42	122.63
17	B	1214	CLA	C2A-C1A-CHA	2.81	127.42	122.63
17	9	1025	CLA	C2A-C1A-CHA	2.81	127.42	122.63
17	1	1013	CLA	C2A-C1A-CHA	2.81	127.42	122.63
17	3	1041	CLA	C2A-C1A-CHA	2.81	127.42	122.63
17	9	1021	CLA	C2A-C1A-CHA	2.81	127.42	122.63
17	0	1017	CLA	C2A-C1A-CHA	2.81	127.42	122.63
17	4	1032	CLA	C2A-C1A-CHA	2.81	127.42	122.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	P	5116	CLA	C2A-C1A-CHA	2.80	127.42	122.63
17	F	4006	CLA	C2A-C1A-CHA	2.80	127.42	122.63
17	7	1017	CLA	C2A-C1A-CHA	2.80	127.42	122.63
17	A	1114	CLA	C2A-C1A-CHA	2.80	127.42	122.63
17	U	8006	CLA	C2A-C1A-CHA	2.80	127.42	122.63
17	3	1033	CLA	C2A-C1A-CHA	2.80	127.41	122.63
17	P	8009	CLA	C2A-C1A-CHA	2.80	127.41	122.63
17	8	1016	CLA	C2A-C1A-CHA	2.80	127.41	122.63
17	7	1023	CLA	C2A-C1A-CHA	2.80	127.41	122.63
17	0	1011	CLA	C2A-C1A-CHA	2.80	127.41	122.63
17	1	1022	CLA	C2A-C1A-CHA	2.80	127.41	122.63
17	1	1023	CLA	C2A-C1A-CHA	2.80	127.41	122.63
17	8	1025	CLA	C2A-C1A-CHA	2.80	127.41	122.63
17	2	1022	CLA	C2A-C1A-CHA	2.80	127.41	122.63
17	0	1033	CLA	C2A-C1A-CHA	2.80	127.41	122.63
17	7	1015	CLA	C2A-C1A-CHA	2.80	127.41	122.63
17	8	1031	CLA	C2A-C1A-CHA	2.80	127.41	122.63
17	4	1033	CLA	C2A-C1A-CHA	2.80	127.40	122.63
17	A	1116	CLA	C2A-C1A-CHA	2.80	127.40	122.63
17	0	1026	CLA	C2A-C1A-CHA	2.80	127.40	122.63
17	U	8003	CLA	C2A-C1A-CHA	2.79	127.40	122.63
17	7	1022	CLA	C2A-C1A-CHA	2.79	127.40	122.63
17	K	1404	CLA	C2A-C1A-CHA	2.79	127.40	122.63
17	Z	5101	CLA	C2A-C1A-CHA	2.79	127.40	122.63
17	1	1026	CLA	C2A-C1A-CHA	2.79	127.40	122.63
17	1	1031	CLA	C2A-C1A-CHA	2.79	127.40	122.63
17	F	4003	CLA	C2A-C1A-CHA	2.79	127.40	122.63
17	3	1012	CLA	C2A-C1A-CHA	2.79	127.40	122.63
17	4	1021	CLA	C2A-C1A-CHA	2.79	127.40	122.63
17	5	5403	CLA	C2A-C1A-CHA	2.79	127.40	122.63
17	0	1022	CLA	C2A-C1A-CHA	2.79	127.39	122.63
17	2	1015	CLA	C2A-C1A-CHA	2.79	127.39	122.63
17	7	1031	CLA	C2A-C1A-CHA	2.79	127.39	122.63
17	A	4010	CLA	C2A-C1A-CHA	2.79	127.39	122.63
17	V	5701	CLA	C2A-C1A-CHA	2.79	127.39	122.63
17	0	1021	CLA	C2A-C1A-CHA	2.79	127.39	122.63
17	A	4009	CLA	C2A-C1A-CHA	2.79	127.39	122.63
17	B	1212	CLA	C2A-C1A-CHA	2.79	127.39	122.63
17	H	1801	CLA	C2A-C1A-CHA	2.79	127.39	122.63
17	2	1013	CLA	C2A-C1A-CHA	2.79	127.39	122.63
17	0	1014	CLA	C2A-C1A-CHA	2.79	127.39	122.63
17	8	8007	CLA	C2A-C1A-CHA	2.79	127.39	122.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	9	1041	CLA	C2A-C1A-CHA	2.79	127.39	122.63
17	Q	5214	CLA	C2A-C1A-CHA	2.79	127.39	122.63
17	1	1017	CLA	C2A-C1A-CHA	2.79	127.39	122.63
17	2	1012	CLA	C2A-C1A-CHA	2.79	127.39	122.63
17	4	1022	CLA	C2A-C1A-CHA	2.79	127.39	122.63
17	9	1017	CLA	C2A-C1A-CHA	2.79	127.39	122.63
17	0	1032	CLA	C2A-C1A-CHA	2.79	127.39	122.63
17	4	1011	CLA	C2A-C1A-CHA	2.79	127.39	122.63
17	8	1015	CLA	C2A-C1A-CHA	2.79	127.39	122.63
17	L	1504	CLA	C2A-C1A-CHA	2.79	127.39	122.63
17	1	1016	CLA	C2A-C1A-CHA	2.79	127.39	122.63
17	3	1021	CLA	C2A-C1A-CHA	2.79	127.39	122.63
17	1	1012	CLA	C2A-C1A-CHA	2.78	127.38	122.63
17	4	1026	CLA	C2A-C1A-CHA	2.78	127.38	122.63
17	2	4007	CLA	C2A-C1A-CHA	2.78	127.38	122.63
17	7	1016	CLA	C2A-C1A-CHA	2.78	127.38	122.63
17	J	1101	CLA	C2A-C1A-CHA	2.78	127.38	122.63
17	P	8010	CLA	C2A-C1A-CHA	2.78	127.38	122.63
17	8	1013	CLA	C2A-C1A-CHA	2.78	127.38	122.63
17	8	1017	CLA	C2A-C1A-CHA	2.78	127.38	122.63
17	0	8002	CLA	C2A-C1A-CHA	2.78	127.38	122.63
17	4	1014	CLA	C2A-C1A-CHA	2.78	127.38	122.63
17	P	5114	CLA	C2A-C1A-CHA	2.78	127.38	122.63
17	3	1017	CLA	C2A-C1A-CHA	2.78	127.38	122.63
17	F	4004	CLA	C2A-C1A-CHA	2.78	127.38	122.63
17	B	4001	CLA	C2A-C1A-CHA	2.78	127.37	122.63
17	2	1017	CLA	C2A-C1A-CHA	2.78	127.37	122.63
17	4	4002	CLA	C2A-C1A-CHA	2.78	127.37	122.63
17	P	5108	CLA	C2A-C1A-CHA	2.78	127.37	122.63
17	1	1014	CLA	C2A-C1A-CHA	2.78	127.37	122.63
17	4	1017	CLA	C2A-C1A-CHA	2.78	127.37	122.63
17	3	1026	CLA	C2A-C1A-CHA	2.78	127.37	122.63
17	4	1012	CLA	C2A-C1A-CHA	2.78	127.37	122.63
17	Q	8001	CLA	C2A-C1A-CHA	2.78	127.37	122.63
17	3	1011	CLA	C2A-C1A-CHA	2.78	127.37	122.63
17	P	5105	CLA	C2A-C1A-CHA	2.78	127.37	122.63
17	7	1026	CLA	C2A-C1A-CHA	2.78	127.37	122.63
17	9	1014	CLA	C2A-C1A-CHA	2.78	127.37	122.63
17	9	1011	CLA	C2A-C1A-CHA	2.78	127.37	122.63
17	2	1025	CLA	C2A-C1A-CHA	2.77	127.36	122.63
17	4	1016	CLA	C2A-C1A-CHA	2.77	127.36	122.63
17	8	1012	CLA	C2A-C1A-CHA	2.77	127.36	122.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	A	1105	CLA	C2A-C1A-CHA	2.77	127.36	122.63
17	2	1026	CLA	C2A-C1A-CHA	2.77	127.36	122.63
17	9	1031	CLA	C2A-C1A-CHA	2.77	127.36	122.63
17	6	5504	CLA	C2A-C1A-CHA	2.77	127.36	122.63
17	2	1031	CLA	C2A-C1A-CHA	2.77	127.36	122.63
17	B	1240	CLA	C2A-C1A-CHA	2.77	127.36	122.63
17	7	1014	CLA	C2A-C1A-CHA	2.77	127.36	122.63
17	8	1033	CLA	C2A-C1A-CHA	2.77	127.36	122.63
17	K	1403	CLA	C2A-C1A-CHA	2.77	127.36	122.63
17	Z	8008	CLA	C2A-C1A-CHA	2.77	127.36	122.63
17	8	1026	CLA	C2A-C1A-CHA	2.77	127.36	122.63
17	2	1023	CLA	C2A-C1A-CHA	2.77	127.36	122.63
17	1	1025	CLA	C2A-C1A-CHA	2.77	127.35	122.63
17	7	1021	CLA	C2A-C1A-CHA	2.76	127.35	122.63
17	J	4008	CLA	C2A-C1A-CHA	2.76	127.35	122.63
17	3	1022	CLA	C2A-C1A-CHA	2.76	127.35	122.63
17	2	1021	CLA	C2A-C1A-CHA	2.76	127.35	122.63
17	2	1033	CLA	C2A-C1A-CHA	2.76	127.35	122.63
17	A	1108	CLA	C2A-C1A-CHA	2.76	127.34	122.63
17	1	1021	CLA	C2A-C1A-CHA	2.76	127.34	122.63
17	7	1012	CLA	C2A-C1A-CHA	2.76	127.34	122.63
17	Q	5222	CLA	C2A-C1A-CHA	2.76	127.34	122.63
17	G	1701	CLA	C2A-C1A-CHA	2.76	127.34	122.63
17	W	5801	CLA	C2A-C1A-CHA	2.76	127.34	122.63
17	8	1023	CLA	C2A-C1A-CHA	2.76	127.34	122.63
17	B	1242	CLA	C2A-C1A-CHA	2.76	127.34	122.63
17	7	1025	CLA	C2A-C1A-CHA	2.76	127.33	122.63
17	9	1022	CLA	C2A-C1A-CHA	2.76	127.33	122.63
17	B	1241	CLA	C2A-C1A-CHA	2.75	127.33	122.63
17	4	1015	CLA	C2A-C1A-CHA	2.75	127.33	122.63
17	B	1222	CLA	C2A-C1A-CHA	2.75	127.33	122.63
17	2	1011	CLA	C2A-C1A-CHA	2.75	127.33	122.63
17	0	1016	CLA	C2A-C1A-CHA	2.75	127.33	122.63
17	3	1031	CLA	C2A-C1A-CHA	2.75	127.33	122.63
17	Q	5240	CLA	C2A-C1A-CHA	2.75	127.33	122.63
17	0	1015	CLA	C2A-C1A-CHA	2.75	127.33	122.63
17	9	1026	CLA	C2A-C1A-CHA	2.75	127.32	122.63
17	8	1021	CLA	C2A-C1A-CHA	2.74	127.31	122.63
17	F	4005	CLA	C2A-C1A-CHA	2.74	127.30	122.63
17	Q	5242	CLA	C2A-C1A-CHA	2.74	127.30	122.63
17	4	1031	CLA	C2A-C1A-CHA	2.74	127.30	122.63
17	0	1031	CLA	C2A-C1A-CHA	2.73	127.30	122.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	4	1025	CLA	C2A-C1A-CHA	2.73	127.30	122.63
17	0	1025	CLA	C2A-C1A-CHA	2.73	127.29	122.63
17	8	1011	CLA	C2A-C1A-CHA	2.73	127.29	122.63
18	P	6001	PQN	C2-C3-C4	-2.73	119.68	123.25
17	Q	5241	CLA	C2A-C1A-CHA	2.73	127.28	122.63
18	A	2001	PQN	C2-C3-C4	-2.72	119.69	123.25
17	U	8005	CLA	C2A-C1A-CHA	2.72	127.28	122.63
17	Q	5236	CLA	C1B-NB-C4B	2.71	108.21	106.31
17	P	5121	CLA	C2A-C1A-CHA	2.70	127.23	122.63
17	B	1236	CLA	C1B-NB-C4B	2.70	108.20	106.31
17	A	1125	CLA	C2A-C1A-CHA	2.69	127.23	122.63
17	P	5125	CLA	C2A-C1A-CHA	2.69	127.23	122.63
17	P	5402	CLA	C2A-C1A-CHA	2.69	127.22	122.63
17	A	1121	CLA	C2A-C1A-CHA	2.69	127.22	122.63
17	A	1402	CLA	C2A-C1A-CHA	2.68	127.21	122.63
17	6	5501	CLA	C2A-C1A-CHA	2.68	127.20	122.63
17	P	5126	CLA	C2A-C1A-CHA	2.68	127.20	122.63
17	A	1108	CLA	CHB-C1B-NB	2.67	127.94	124.08
17	Q	5207	CLA	C3D-C2D-C1D	-2.67	104.11	107.35
17	P	5108	CLA	CHB-C1B-NB	2.67	127.93	124.08
17	A	1126	CLA	C2A-C1A-CHA	2.66	127.18	122.63
17	J	1302	CLA	CHB-C1B-NB	2.66	127.92	124.08
17	L	1501	CLA	C2A-C1A-CHA	2.66	127.17	122.63
17	B	1207	CLA	C3D-C2D-C1D	-2.66	104.12	107.35
17	Q	5022	CLA	C2A-C1A-CHA	2.65	127.16	122.63
17	B	1130	CLA	C2A-C1A-CHA	2.65	127.16	122.63
17	B	1022	CLA	C2A-C1A-CHA	2.65	127.16	122.63
17	B	1223	CLA	C2A-C1A-CHA	2.65	127.15	122.63
17	Q	5130	CLA	C2A-C1A-CHA	2.65	127.15	122.63
17	Q	5208	CLA	C2A-C1A-CHA	2.64	127.14	122.63
17	Q	5225	CLA	C2A-C1A-CHA	2.64	127.14	122.63
17	Q	5216	CLA	C2A-C1A-CHA	2.64	127.13	122.63
17	B	1216	CLA	C2A-C1A-CHA	2.64	127.13	122.63
17	B	1220	CLA	C2A-C1A-CHA	2.63	127.12	122.63
17	B	1225	CLA	C2A-C1A-CHA	2.63	127.12	122.63
17	B	1208	CLA	C2A-C1A-CHA	2.63	127.12	122.63
17	Q	5223	CLA	C2A-C1A-CHA	2.63	127.12	122.63
17	Z	5302	CLA	CHB-C1B-NB	2.63	127.88	124.08
17	Q	5220	CLA	C2A-C1A-CHA	2.62	127.10	122.63
17	6	5502	CLA	C3C-C4C-NC	-2.62	107.64	109.92
17	P	5129	CLA	C2A-C1A-CHA	2.59	127.06	122.63
17	Q	5227	CLA	C2A-C1A-CHA	2.59	127.05	122.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	A	1110	CLA	C2A-C1A-CHA	2.59	127.05	122.63
17	P	5110	CLA	C2A-C1A-CHA	2.59	127.05	122.63
17	A	1129	CLA	C2A-C1A-CHA	2.59	127.04	122.63
17	P	5138	CLA	C2A-C1A-CHA	2.58	127.04	122.63
17	P	5901	CLA	CHB-C1B-NB	2.58	127.81	124.08
17	A	1138	CLA	C2A-C1A-CHA	2.58	127.04	122.63
17	L	1502	CLA	C3C-C4C-NC	-2.58	107.67	109.92
17	Q	5234	CLA	C2A-C1A-CHA	2.58	127.03	122.63
17	P	5013	CLA	C1B-NB-C4B	2.58	108.12	106.31
17	Q	5211	CLA	C2A-C1A-CHA	2.56	127.00	122.63
17	A	1901	CLA	CHB-C1B-NB	2.56	127.78	124.08
17	B	1234	CLA	C2A-C1A-CHA	2.55	126.99	122.63
17	A	1013	CLA	C1B-NB-C4B	2.55	108.10	106.31
17	P	5106	CLA	C2A-C1A-CHA	2.55	126.98	122.63
17	B	1227	CLA	C2A-C1A-CHA	2.55	126.98	122.63
17	A	1109	CLA	C2A-C1A-CHA	2.54	126.97	122.63
17	B	1211	CLA	C2A-C1A-CHA	2.54	126.96	122.63
17	P	5109	CLA	C2A-C1A-CHA	2.54	126.96	122.63
17	B	1213	CLA	C2A-C1A-CHA	2.54	126.96	122.63
17	5	5401	CLA	C2A-C1A-CHA	2.54	126.96	122.63
17	A	1106	CLA	C2A-C1A-CHA	2.53	126.96	122.63
17	K	1401	CLA	C2A-C1A-CHA	2.53	126.96	122.63
17	A	1127	CLA	C2A-C1A-CHA	2.53	126.95	122.63
17	Q	5238	CLA	C3C-C4C-NC	-2.52	107.72	109.92
17	B	1228	CLA	C2A-C1A-CHA	2.52	126.94	122.63
17	B	1206	CLA	C2A-C1A-CHA	2.52	126.93	122.63
17	A	1122	CLA	C2A-C1A-CHA	2.52	126.93	122.63
17	P	5122	CLA	C2A-C1A-CHA	2.52	126.92	122.63
17	P	5127	CLA	C2A-C1A-CHA	2.52	126.92	122.63
17	B	1231	CLA	C3C-C4C-NC	-2.51	107.73	109.92
17	Q	5213	CLA	C2A-C1A-CHA	2.51	126.92	122.63
17	Q	5206	CLA	C2A-C1A-CHA	2.51	126.92	122.63
17	P	5108	CLA	C4D-ND-C1D	2.50	108.06	106.31
17	Q	5228	CLA	C2A-C1A-CHA	2.49	126.89	122.63
17	B	1237	CLA	C3D-C2D-C1D	-2.49	104.32	107.35
17	Q	5237	CLA	C3D-C2D-C1D	-2.49	104.33	107.35
17	B	1204	CLA	C3C-C4C-NC	-2.49	107.75	109.92
17	B	1238	CLA	C3C-C4C-NC	-2.48	107.75	109.92
17	Q	5231	CLA	C3C-C4C-NC	-2.48	107.75	109.92
17	Q	5204	CLA	C3C-C4C-NC	-2.48	107.76	109.92
17	Q	5021	CLA	C2A-C1A-CHA	2.47	126.85	122.63
17	Q	5224	CLA	CHB-C1B-NB	2.47	127.65	124.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	B	1021	CLA	C2A-C1A-CHA	2.47	126.85	122.63
17	A	1108	CLA	C4D-ND-C1D	2.47	108.04	106.31
17	B	1235	CLA	C3C-C4C-NC	-2.47	107.77	109.92
17	A	1136	CLA	C3C-C4C-NC	-2.46	107.77	109.92
17	P	5136	CLA	C3C-C4C-NC	-2.45	107.78	109.92
17	B	1224	CLA	CHB-C1B-NB	2.45	127.61	124.08
17	Q	5235	CLA	C3C-C4C-NC	-2.44	107.79	109.92
17	B	1209	CLA	C2A-C1A-CHA	2.44	126.80	122.63
17	Q	5219	CLA	C2A-C1A-CHA	2.44	126.79	122.63
17	B	1219	CLA	C2A-C1A-CHA	2.43	126.78	122.63
17	P	5132	CLA	C3D-C2D-C1D	-2.43	104.40	107.35
17	Q	5209	CLA	C2A-C1A-CHA	2.43	126.77	122.63
17	P	5133	CLA	C3C-C4C-NC	-2.42	107.81	109.92
17	6	5501	CLA	CHB-C1B-NB	2.42	127.57	124.08
17	A	1137	CLA	C2A-C1A-CHA	2.41	126.74	122.63
17	P	5133	CLA	C2A-C1A-CHA	2.40	126.73	122.63
17	A	1133	CLA	C2A-C1A-CHA	2.40	126.73	122.63
17	A	1012	CLA	C3D-C2D-C1D	-2.40	104.43	107.35
17	B	1236	CLA	C2A-C1A-CHA	2.40	126.73	122.63
17	B	1221	CLA	CHB-C1B-NB	2.40	127.55	124.08
17	P	5012	CLA	C3D-C2D-C1D	-2.40	104.43	107.35
17	P	5110	CLA	C3C-C4C-NC	-2.40	107.83	109.92
17	Q	5221	CLA	CHB-C1B-NB	2.40	127.55	124.08
17	L	1501	CLA	C3D-C2D-C1D	-2.40	104.44	107.35
17	P	5137	CLA	C2A-C1A-CHA	2.40	126.72	122.63
17	B	1022	CLA	CHB-C1B-NB	2.40	127.54	124.08
17	B	1201	CLA	C2A-C1A-CHA	2.40	126.72	122.63
17	L	1501	CLA	CHB-C1B-NB	2.39	127.54	124.08
17	A	1132	CLA	C3D-C2D-C1D	-2.39	104.44	107.35
17	Q	5236	CLA	C2A-C1A-CHA	2.39	126.72	122.63
17	Q	5201	CLA	C2A-C1A-CHA	2.39	126.70	122.63
17	P	5113	CLA	CHB-C1B-NB	2.39	127.53	124.08
17	A	1133	CLA	C3C-C4C-NC	-2.38	107.84	109.92
17	6	5501	CLA	C3D-C2D-C1D	-2.38	104.45	107.35
17	P	5128	CLA	C2A-C1A-CHA	2.38	126.69	122.63
17	Q	5022	CLA	CHB-C1B-NB	2.38	127.52	124.08
17	Q	5215	CLA	C2A-C1A-CHA	2.38	126.69	122.63
17	A	1124	CLA	C3D-C2D-C1D	-2.38	104.46	107.35
17	A	1110	CLA	C3C-C4C-NC	-2.37	107.85	109.92
17	B	1201	CLA	C3D-C2D-C1D	-2.37	104.47	107.35
17	B	1228	CLA	C3D-C2D-C1D	-2.37	104.47	107.35
17	A	1128	CLA	C2A-C1A-CHA	2.37	126.68	122.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	B	1215	CLA	C2A-C1A-CHA	2.37	126.68	122.63
17	Q	5201	CLA	C3D-C2D-C1D	-2.37	104.47	107.35
17	P	5125	CLA	C3D-C2D-C1D	-2.37	104.47	107.35
17	P	5107	CLA	CHB-C1B-NB	2.37	127.50	124.08
17	A	1113	CLA	CHB-C1B-NB	2.36	127.50	124.08
17	P	5111	CLA	C3D-C2D-C1D	-2.36	104.48	107.35
17	A	1107	CLA	CHB-C1B-NB	2.36	127.49	124.08
17	P	5124	CLA	C3D-C2D-C1D	-2.36	104.49	107.35
17	Q	5228	CLA	C3D-C2D-C1D	-2.35	104.49	107.35
17	A	1125	CLA	C3D-C2D-C1D	-2.34	104.50	107.35
17	A	1111	CLA	C3D-C2D-C1D	-2.34	104.50	107.35
17	A	1131	CLA	C3C-C4C-NC	-2.34	107.88	109.92
17	P	5131	CLA	C3C-C4C-NC	-2.33	107.89	109.92
17	Q	5206	CLA	CHB-C1B-NB	2.33	127.44	124.08
17	B	1206	CLA	CHB-C1B-NB	2.32	127.43	124.08
17	B	1210	CLA	C3D-C2D-C1D	-2.32	104.53	107.35
17	Q	5223	CLA	C3D-C2D-C1D	-2.31	104.54	107.35
17	P	5137	CLA	CHB-C1B-NB	2.31	127.42	124.08
17	Q	5023	CLA	CHB-C1B-NB	2.31	127.42	124.08
17	Q	5237	CLA	C3C-C4C-NC	-2.31	107.91	109.92
17	P	5013	CLA	C3D-C2D-C1D	-2.31	104.55	107.35
17	P	5013	CLA	C2A-C1A-CHA	2.31	126.57	122.63
17	B	1023	CLA	CHB-C1B-NB	2.30	127.41	124.08
17	B	1237	CLA	C3C-C4C-NC	-2.30	107.91	109.92
17	Q	5023	CLA	C3C-C4C-NC	-2.30	107.91	109.92
17	Q	5230	CLA	C3D-C2D-C1D	-2.30	104.56	107.35
17	A	1123	CLA	CHB-C1B-NB	2.29	127.39	124.08
17	A	1137	CLA	CHB-C1B-NB	2.29	127.39	124.08
17	Q	5226	CLA	C2A-C1A-CHA	2.29	126.54	122.63
17	Q	5238	CLA	C3D-C2D-C1D	-2.29	104.57	107.35
17	Q	5210	CLA	C3D-C2D-C1D	-2.29	104.57	107.35
17	B	1238	CLA	C3D-C2D-C1D	-2.29	104.57	107.35
17	P	5126	CLA	C3D-C2D-C1D	-2.28	104.58	107.35
17	A	1013	CLA	C2A-C1A-CHA	2.28	126.52	122.63
17	P	5128	CLA	CHB-C1B-NB	2.28	127.37	124.08
17	Q	5210	CLA	CHB-C1B-NB	2.28	127.37	124.08
17	B	1210	CLA	CHB-C1B-NB	2.27	127.37	124.08
17	B	1219	CLA	CHB-C1B-NB	2.27	127.37	124.08
17	P	5106	CLA	C3D-C2D-C1D	-2.27	104.59	107.35
17	B	1226	CLA	C2A-C1A-CHA	2.27	126.51	122.63
17	P	5123	CLA	CHB-C1B-NB	2.27	127.36	124.08
17	A	1126	CLA	C3D-C2D-C1D	-2.27	104.59	107.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	Q	5212	CLA	C3D-C2D-C1D	-2.27	104.59	107.35
17	6	5503	CLA	C3D-C2D-C1D	-2.27	104.59	107.35
17	A	1013	CLA	C3D-C2D-C1D	-2.27	104.60	107.35
17	B	1212	CLA	C3D-C2D-C1D	-2.26	104.60	107.35
17	P	5112	CLA	C3C-C4C-NC	-2.26	107.94	109.92
17	B	1223	CLA	C3D-C2D-C1D	-2.26	104.60	107.35
17	B	1230	CLA	C3D-C2D-C1D	-2.26	104.60	107.35
17	B	1224	CLA	C2A-C1A-CHA	2.26	126.49	122.63
17	A	1128	CLA	CHB-C1B-NB	2.26	127.34	124.08
17	Q	5219	CLA	CHB-C1B-NB	2.26	127.34	124.08
17	Q	5232	CLA	CHB-C1B-NB	2.26	127.34	124.08
17	B	1232	CLA	CHB-C1B-NB	2.25	127.33	124.08
17	B	1023	CLA	C3C-C4C-NC	-2.25	107.96	109.92
17	Q	5228	CLA	CHB-C1B-NB	2.25	127.33	124.08
17	A	1106	CLA	C3D-C2D-C1D	-2.25	104.62	107.35
17	L	1503	CLA	C3D-C2D-C1D	-2.25	104.62	107.35
17	B	1202	CLA	C1C-NC-C4C	2.25	107.70	106.68
17	Q	5215	CLA	C3C-C4C-NC	-2.25	107.96	109.92
17	A	1131	CLA	C2A-C1A-CHA	2.24	126.46	122.63
17	Q	5224	CLA	C2A-C1A-CHA	2.24	126.46	122.63
17	A	1012	CLA	CHB-C1B-NB	2.24	127.32	124.08
17	P	5129	CLA	C3D-C2D-C1D	-2.24	104.63	107.35
17	P	5131	CLA	C2A-C1A-CHA	2.24	126.45	122.63
17	B	1220	CLA	C3C-C4C-NC	-2.23	107.97	109.92
17	A	1129	CLA	C3D-C2D-C1D	-2.23	104.64	107.35
17	B	1215	CLA	C3C-C4C-NC	-2.23	107.97	109.92
17	P	5012	CLA	CHB-C1B-NB	2.23	127.30	124.08
17	A	1140	CLA	C2A-C1A-CHA	2.23	126.43	122.63
17	A	1112	CLA	C3C-C4C-NC	-2.23	107.98	109.92
17	B	1228	CLA	CHB-C1B-NB	2.23	127.30	124.08
17	B	1130	CLA	C3D-C2D-C1D	-2.23	104.64	107.35
17	Q	5203	CLA	C3D-C2D-C1D	-2.23	104.64	107.35
17	Q	5202	CLA	C1C-NC-C4C	2.22	107.69	106.68
17	Q	5220	CLA	C3C-C4C-NC	-2.22	107.98	109.92
17	Q	5228	CLA	C3C-C4C-NC	-2.22	107.98	109.92
17	B	1202	CLA	C3D-C2D-C1D	-2.22	104.65	107.35
17	P	5140	CLA	C2A-C1A-CHA	2.22	126.42	122.63
17	6	5502	CLA	C3D-C2D-C1D	-2.22	104.66	107.35
17	B	1228	CLA	C3C-C4C-NC	-2.21	107.99	109.92
17	P	5138	CLA	C3C-C4C-NC	-2.21	107.99	109.92
17	A	1116	CLA	C3C-C4C-NC	-2.21	107.99	109.92
17	Q	5202	CLA	C3D-C2D-C1D	-2.21	104.67	107.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	P	5103	CLA	C3C-C4C-NC	-2.20	108.00	109.92
17	Q	5235	CLA	C2A-C1A-CHA	2.20	126.38	122.63
17	B	1203	CLA	C3D-C2D-C1D	-2.20	104.68	107.35
17	P	5116	CLA	C3C-C4C-NC	-2.19	108.01	109.92
17	P	5134	CLA	C3D-C2D-C1D	-2.19	104.69	107.35
17	A	1117	CLA	C3C-C4C-NC	-2.19	108.01	109.92
17	A	1122	CLA	C3C-C4C-NC	-2.19	108.01	109.92
17	Q	5130	CLA	C3D-C2D-C1D	-2.19	104.69	107.35
17	B	1235	CLA	C2A-C1A-CHA	2.19	126.36	122.63
17	B	1209	CLA	C3C-C4C-NC	-2.18	108.02	109.92
17	L	1502	CLA	C3D-C2D-C1D	-2.18	104.70	107.35
17	A	1108	CLA	CHC-C1C-NC	2.18	127.54	124.33
17	B	1203	CLA	C2A-C1A-CHA	2.18	126.36	122.63
17	Q	5204	CLA	C3D-C2D-C1D	-2.18	104.70	107.35
17	A	1119	CLA	C3C-C4C-NC	-2.18	108.02	109.92
17	Q	5203	CLA	C2A-C1A-CHA	2.17	126.34	122.63
17	P	5108	CLA	CHC-C1C-NC	2.17	127.53	124.33
17	B	1218	CLA	C3D-C2D-C1D	-2.17	104.71	107.35
17	P	5118	CLA	C3D-C2D-C1D	-2.17	104.71	107.35
17	P	5122	CLA	C3C-C4C-NC	-2.17	108.03	109.92
17	A	1138	CLA	C3C-C4C-NC	-2.17	108.03	109.92
17	A	1134	CLA	C3D-C2D-C1D	-2.17	104.71	107.35
17	U	5229	CLA	C3D-C2D-C1D	-2.17	104.72	107.35
17	B	1204	CLA	C3D-C2D-C1D	-2.16	104.72	107.35
17	Q	5218	CLA	CHB-C1B-NB	2.16	127.20	124.08
17	Q	5209	CLA	C3C-C4C-NC	-2.16	108.03	109.92
17	P	5119	CLA	C3C-C4C-NC	-2.16	108.04	109.92
17	4	1025	CLA	CHB-C1B-NB	2.16	127.20	124.08
17	A	1103	CLA	C3C-C4C-NC	-2.15	108.04	109.92
17	P	5119	CLA	C2A-C1A-CHA	2.15	126.30	122.63
17	Q	5218	CLA	C3D-C2D-C1D	-2.15	104.73	107.35
17	Q	5225	CLA	CHB-C1B-NB	2.15	127.19	124.08
17	9	1014	CLA	CHB-C1B-NB	2.15	127.19	124.08
17	A	1132	CLA	CHB-C1B-NB	2.15	127.19	124.08
17	B	1214	CLA	C3C-C4C-NC	-2.15	108.05	109.92
17	A	1118	CLA	C3D-C2D-C1D	-2.15	104.74	107.35
17	8	8007	CLA	CHB-C1B-NB	2.15	127.18	124.08
17	0	1025	CLA	CHB-C1B-NB	2.14	127.18	124.08
17	B	1218	CLA	CHB-C1B-NB	2.14	127.18	124.08
17	F	1229	CLA	C3D-C2D-C1D	-2.14	104.74	107.35
17	P	5104	CLA	C3C-C4C-NC	-2.14	108.05	109.92
17	9	1017	CLA	CHB-C1B-NB	2.14	127.18	124.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	P	5117	CLA	C3C-C4C-NC	-2.14	108.05	109.92
17	4	1012	CLA	CHB-C1B-NB	2.14	127.17	124.08
17	Q	5241	CLA	CHB-C1B-NB	2.14	127.17	124.08
17	9	1012	CLA	CHB-C1B-NB	2.14	127.17	124.08
17	F	4003	CLA	CHB-C1B-NB	2.13	127.17	124.08
17	9	1033	CLA	CHB-C1B-NB	2.13	127.17	124.08
17	A	1105	CLA	C3D-C2D-C1D	-2.13	104.76	107.35
17	A	1119	CLA	C2A-C1A-CHA	2.13	126.27	122.63
17	2	4007	CLA	CHB-C1B-NB	2.13	127.15	124.08
17	3	1014	CLA	CHB-C1B-NB	2.13	127.15	124.08
17	0	1031	CLA	CHB-C1B-NB	2.13	127.15	124.08
17	P	5105	CLA	C3D-C2D-C1D	-2.13	104.77	107.35
17	P	5901	CLA	C3D-C2D-C1D	-2.13	104.77	107.35
17	F	1229	CLA	C3C-C4C-NC	-2.13	108.07	109.92
17	A	1119	CLA	CHB-C1B-NB	2.12	127.15	124.08
17	7	1013	CLA	CHB-C1B-NB	2.12	127.15	124.08
17	A	1901	CLA	C3D-C2D-C1D	-2.12	104.77	107.35
17	1	1014	CLA	CHB-C1B-NB	2.12	127.15	124.08
17	P	5119	CLA	CHB-C1B-NB	2.12	127.15	124.08
17	3	1017	CLA	CHB-C1B-NB	2.12	127.15	124.08
17	Q	8001	CLA	CHB-C1B-NB	2.12	127.15	124.08
17	K	1404	CLA	CHB-C1B-NB	2.12	127.15	124.08
17	B	1218	CLA	C3C-C4C-NC	-2.12	108.07	109.92
17	Q	5214	CLA	C3C-C4C-NC	-2.12	108.07	109.92
17	3	1033	CLA	CHB-C1B-NB	2.12	127.15	124.08
17	5	5403	CLA	CHB-C1B-NB	2.12	127.14	124.08
17	A	1135	CLA	C3D-C2D-C1D	-2.12	104.77	107.35
17	7	1014	CLA	CHB-C1B-NB	2.12	127.14	124.08
17	0	1022	CLA	CHB-C1B-NB	2.12	127.14	124.08
17	A	1103	CLA	C3D-C2D-C1D	-2.12	104.78	107.35
17	Q	5227	CLA	C3D-C2D-C1D	-2.12	104.78	107.35
17	P	5132	CLA	CHB-C1B-NB	2.12	127.14	124.08
17	7	1011	CLA	CHB-C1B-NB	2.12	127.14	124.08
17	P	8010	CLA	CHB-C1B-NB	2.12	127.14	124.08
17	5	5404	CLA	CHB-C1B-NB	2.12	127.14	124.08
17	A	1111	CLA	C3C-C4C-NC	-2.12	108.07	109.92
17	K	1403	CLA	CHB-C1B-NB	2.12	127.14	124.08
17	Q	5201	CLA	C3C-C4C-NC	-2.11	108.08	109.92
17	B	1225	CLA	CHB-C1B-NB	2.11	127.14	124.08
17	U	8003	CLA	CHB-C1B-NB	2.11	127.14	124.08
17	A	1117	CLA	CHB-C1B-NB	2.11	127.13	124.08
17	A	1131	CLA	C3D-C2D-C1D	-2.11	104.78	107.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	P	5113	CLA	C3D-C2D-C1D	-2.11	104.78	107.35
17	P	5135	CLA	C3D-C2D-C1D	-2.11	104.78	107.35
17	A	4009	CLA	CHB-C1B-NB	2.11	127.13	124.08
17	B	4001	CLA	CHB-C1B-NB	2.11	127.13	124.08
17	7	1025	CLA	CHB-C1B-NB	2.11	127.13	124.08
17	0	1015	CLA	CHB-C1B-NB	2.11	127.13	124.08
17	A	1113	CLA	C3D-C2D-C1D	-2.11	104.78	107.35
17	3	1012	CLA	CHB-C1B-NB	2.11	127.13	124.08
17	Q	5238	CLA	CHB-C1B-NB	2.11	127.13	124.08
17	P	5103	CLA	C3D-C2D-C1D	-2.11	104.79	107.35
17	P	5131	CLA	C3D-C2D-C1D	-2.11	104.79	107.35
17	8	1026	CLA	CHB-C1B-NB	2.11	127.12	124.08
17	P	5117	CLA	CHB-C1B-NB	2.11	127.12	124.08
17	8	1033	CLA	CHB-C1B-NB	2.11	127.12	124.08
17	P	5102	CLA	C3C-C4C-NC	-2.11	108.08	109.92
17	K	1401	CLA	C3D-C2D-C1D	-2.11	104.79	107.35
17	W	5801	CLA	CHB-C1B-NB	2.11	127.12	124.08
17	4	1031	CLA	CHB-C1B-NB	2.10	127.12	124.08
17	A	1901	CLA	CHD-C4C-NC	2.10	127.44	124.24
17	P	5125	CLA	CHB-C1B-NB	2.10	127.12	124.08
17	2	1026	CLA	CHB-C1B-NB	2.10	127.12	124.08
17	7	1015	CLA	CHB-C1B-NB	2.10	127.12	124.08
17	0	1026	CLA	CHB-C1B-NB	2.10	127.12	124.08
17	A	1103	CLA	C2A-C1A-CHA	2.10	126.22	122.63
17	B	1227	CLA	C3D-C2D-C1D	-2.10	104.79	107.35
17	0	1012	CLA	CHB-C1B-NB	2.10	127.12	124.08
17	0	1014	CLA	CHB-C1B-NB	2.10	127.12	124.08
17	B	1241	CLA	CHB-C1B-NB	2.10	127.12	124.08
17	A	4010	CLA	CHB-C1B-NB	2.10	127.12	124.08
17	B	1238	CLA	CHB-C1B-NB	2.10	127.12	124.08
17	1	1011	CLA	CHB-C1B-NB	2.10	127.12	124.08
17	4	1022	CLA	CHB-C1B-NB	2.10	127.11	124.08
17	4	1026	CLA	CHB-C1B-NB	2.10	127.11	124.08
17	A	1120	CLA	C3D-C2D-C1D	-2.10	104.80	107.35
17	P	5120	CLA	C3D-C2D-C1D	-2.10	104.80	107.35
17	Q	5239	CLA	C3D-C2D-C1D	-2.10	104.80	107.35
17	4	1033	CLA	CHB-C1B-NB	2.10	127.11	124.08
17	V	5701	CLA	CHB-C1B-NB	2.10	127.11	124.08
17	A	1104	CLA	C3C-C4C-NC	-2.10	108.09	109.92
17	4	4002	CLA	CHB-C1B-NB	2.10	127.11	124.08
17	0	1033	CLA	CHB-C1B-NB	2.10	127.11	124.08
17	F	4006	CLA	CHB-C1B-NB	2.10	127.11	124.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	L	1504	CLA	CHB-C1B-NB	2.10	127.11	124.08
17	1	1013	CLA	CHB-C1B-NB	2.10	127.11	124.08
17	2	1033	CLA	CHB-C1B-NB	2.10	127.11	124.08
17	8	1017	CLA	CHB-C1B-NB	2.10	127.11	124.08
17	A	1115	CLA	C3D-C2D-C1D	-2.09	104.80	107.35
17	1	1025	CLA	CHB-C1B-NB	2.09	127.11	124.08
17	P	8009	CLA	CHB-C1B-NB	2.09	127.11	124.08
17	9	1026	CLA	CHB-C1B-NB	2.09	127.11	124.08
17	4	1014	CLA	CHB-C1B-NB	2.09	127.10	124.08
17	0	1013	CLA	CHB-C1B-NB	2.09	127.10	124.08
17	Q	5218	CLA	C3C-C4C-NC	-2.09	108.09	109.92
17	B	1216	CLA	CHB-C1B-NB	2.09	127.10	124.08
17	Z	8008	CLA	CHB-C1B-NB	2.09	127.10	124.08
17	4	1015	CLA	CHB-C1B-NB	2.09	127.10	124.08
17	8	1012	CLA	CHB-C1B-NB	2.09	127.10	124.08
17	B	1201	CLA	C3C-C4C-NC	-2.09	108.10	109.92
17	U	5229	CLA	C3C-C4C-NC	-2.09	108.10	109.92
17	K	1401	CLA	CHB-C1B-NB	2.09	127.10	124.08
17	A	1102	CLA	C3C-C4C-NC	-2.09	108.10	109.92
17	P	5103	CLA	C2A-C1A-CHA	2.09	126.20	122.63
17	7	1026	CLA	CHB-C1B-NB	2.09	127.10	124.08
17	P	5111	CLA	C3C-C4C-NC	-2.09	108.10	109.92
17	Q	5217	CLA	C3C-C4C-NC	-2.09	108.10	109.92
17	A	1117	CLA	C3D-C2D-C1D	-2.09	104.81	107.35
17	B	1240	CLA	CHB-C1B-NB	2.09	127.10	124.08
17	3	1032	CLA	CHB-C1B-NB	2.09	127.10	124.08
17	P	5107	CLA	C3D-C2D-C1D	-2.09	104.81	107.35
17	1	1023	CLA	CHB-C1B-NB	2.09	127.09	124.08
17	2	1017	CLA	CHB-C1B-NB	2.09	127.09	124.08
17	4	1013	CLA	CHB-C1B-NB	2.09	127.09	124.08
17	P	5112	CLA	CHB-C1B-NB	2.08	127.09	124.08
17	A	1138	CLA	C3D-C2D-C1D	-2.08	104.82	107.35
17	J	4008	CLA	CHB-C1B-NB	2.08	127.09	124.08
17	1	1026	CLA	CHB-C1B-NB	2.08	127.09	124.08
17	9	1032	CLA	CHB-C1B-NB	2.08	127.09	124.08
17	4	1017	CLA	CHB-C1B-NB	2.08	127.09	124.08
17	Q	5216	CLA	CHB-C1B-NB	2.08	127.09	124.08
17	P	5118	CLA	C3C-C4C-NC	-2.08	108.10	109.92
17	P	5115	CLA	C2A-C1A-CHA	2.08	126.18	122.63
17	P	5110	CLA	CHB-C1B-NB	2.08	127.09	124.08
17	0	1016	CLA	CHB-C1B-NB	2.08	127.09	124.08
17	A	1107	CLA	C3D-C2D-C1D	-2.08	104.82	107.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	A	1115	CLA	C2A-C1A-CHA	2.08	126.18	122.63
17	B	1239	CLA	C3D-C2D-C1D	-2.08	104.82	107.35
17	A	1125	CLA	CHB-C1B-NB	2.08	127.08	124.08
17	4	1016	CLA	CHB-C1B-NB	2.08	127.08	124.08
17	G	1701	CLA	CHB-C1B-NB	2.08	127.08	124.08
17	J	1101	CLA	CHB-C1B-NB	2.08	127.08	124.08
17	Q	5213	CLA	CHB-C1B-NB	2.08	127.08	124.08
17	8	1022	CLA	CHB-C1B-NB	2.08	127.08	124.08
17	L	1502	CLA	CHB-C1B-NB	2.08	127.08	124.08
17	0	8002	CLA	CHB-C1B-NB	2.08	127.08	124.08
17	P	5117	CLA	C3D-C2D-C1D	-2.08	104.83	107.35
17	2	1012	CLA	CHB-C1B-NB	2.08	127.08	124.08
17	2	1022	CLA	CHB-C1B-NB	2.08	127.08	124.08
17	4	1023	CLA	CHB-C1B-NB	2.08	127.08	124.08
17	7	1023	CLA	CHB-C1B-NB	2.08	127.08	124.08
17	U	8006	CLA	CHB-C1B-NB	2.08	127.08	124.08
17	8	1015	CLA	CHB-C1B-NB	2.08	127.08	124.08
17	P	5129	CLA	C3C-C4C-NC	-2.07	108.11	109.92
17	1	1017	CLA	CHB-C1B-NB	2.07	127.08	124.08
17	0	1021	CLA	CHB-C1B-NB	2.07	127.08	124.08
17	Q	5208	CLA	C3D-C2D-C1D	-2.07	104.83	107.35
17	5	5401	CLA	C3D-C2D-C1D	-2.07	104.83	107.35
17	1	1015	CLA	CHB-C1B-NB	2.07	127.08	124.08
17	6	5504	CLA	CHB-C1B-NB	2.07	127.08	124.08
17	7	1016	CLA	CHB-C1B-NB	2.07	127.08	124.08
17	F	4004	CLA	CHB-C1B-NB	2.07	127.08	124.08
17	B	1224	CLA	C3D-C2D-C1D	-2.07	104.83	107.35
17	B	1242	CLA	CHB-C1B-NB	2.07	127.07	124.08
17	3	1011	CLA	CHB-C1B-NB	2.07	127.07	124.08
17	P	5138	CLA	C3D-C2D-C1D	-2.07	104.83	107.35
17	9	1011	CLA	CHB-C1B-NB	2.07	127.07	124.08
17	B	1213	CLA	CHB-C1B-NB	2.07	127.07	124.08
17	H	1801	CLA	CHB-C1B-NB	2.07	127.07	124.08
17	3	1026	CLA	CHB-C1B-NB	2.07	127.07	124.08
17	6	5502	CLA	CHB-C1B-NB	2.07	127.07	124.08
17	A	1115	CLA	CHB-C1B-NB	2.07	127.07	124.08
17	7	1031	CLA	CHB-C1B-NB	2.07	127.07	124.08
17	P	5115	CLA	C3D-C2D-C1D	-2.07	104.83	107.35
17	Q	5224	CLA	C3D-C2D-C1D	-2.07	104.83	107.35
17	7	1012	CLA	CHB-C1B-NB	2.07	127.07	124.08
17	2	1015	CLA	CHB-C1B-NB	2.07	127.07	124.08
17	7	1022	CLA	CHB-C1B-NB	2.07	127.07	124.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	9	1022	CLA	CHB-C1B-NB	2.07	127.07	124.08
17	0	1023	CLA	CHB-C1B-NB	2.07	127.07	124.08
17	Q	5240	CLA	CHB-C1B-NB	2.07	127.06	124.08
17	B	1205	CLA	C1B-NB-C4B	2.07	107.76	106.31
17	9	1031	CLA	CHB-C1B-NB	2.06	127.06	124.08
17	Q	5205	CLA	C2A-C1A-CHA	2.06	126.16	122.63
17	0	1017	CLA	CHB-C1B-NB	2.06	127.06	124.08
17	1	1031	CLA	CHB-C1B-NB	2.06	127.06	124.08
17	U	8004	CLA	CHB-C1B-NB	2.06	127.06	124.08
17	5	5401	CLA	CHB-C1B-NB	2.06	127.06	124.08
17	3	1022	CLA	CHB-C1B-NB	2.06	127.06	124.08
17	P	5901	CLA	CHD-C4C-NC	2.06	127.37	124.24
17	A	1112	CLA	CHB-C1B-NB	2.06	127.06	124.08
17	4	1021	CLA	CHB-C1B-NB	2.06	127.06	124.08
17	1	1022	CLA	CHB-C1B-NB	2.06	127.06	124.08
17	P	5115	CLA	CHB-C1B-NB	2.06	127.06	124.08
17	8	1021	CLA	CHB-C1B-NB	2.06	127.06	124.08
17	Q	5236	CLA	C3D-C2D-C1D	-2.06	104.84	107.35
17	1	1016	CLA	CHB-C1B-NB	2.06	127.06	124.08
17	Q	5242	CLA	CHB-C1B-NB	2.06	127.06	124.08
17	7	1021	CLA	CHB-C1B-NB	2.06	127.06	124.08
17	9	1041	CLA	CHB-C1B-NB	2.06	127.06	124.08
17	A	1113	CLA	CHC-C1C-NC	2.06	127.36	124.33
17	P	5114	CLA	CHB-C1B-NB	2.06	127.06	124.08
17	P	5113	CLA	CHC-C1C-NC	2.06	127.36	124.33
17	B	1236	CLA	C3D-C2D-C1D	-2.06	104.85	107.35
17	A	1118	CLA	C3C-C4C-NC	-2.06	108.12	109.92
17	2	1011	CLA	CHB-C1B-NB	2.06	127.05	124.08
17	3	1041	CLA	CHB-C1B-NB	2.06	127.05	124.08
17	7	1017	CLA	CHB-C1B-NB	2.06	127.05	124.08
17	8	1013	CLA	CHB-C1B-NB	2.06	127.05	124.08
17	3	1015	CLA	CHB-C1B-NB	2.06	127.05	124.08
17	Q	5225	CLA	C3D-C2D-C1D	-2.06	104.85	107.35
17	8	1014	CLA	C3D-C2D-C1D	-2.06	104.85	107.35
17	3	1021	CLA	CHB-C1B-NB	2.05	127.05	124.08
17	1	1021	CLA	CHB-C1B-NB	2.05	127.05	124.08
17	Q	5204	CLA	CHD-C1D-ND	-2.05	121.95	124.84
17	Q	5230	CLA	C2A-C1A-CHA	2.05	126.13	122.63
18	B	2002	PQN	C5-C4-C3	2.05	120.68	116.55
17	A	1129	CLA	C3C-C4C-NC	-2.05	108.13	109.92
17	B	1217	CLA	C3C-C4C-NC	-2.05	108.13	109.92
18	Q	6002	PQN	C5-C4-C3	2.05	120.68	116.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	8	1011	CLA	CHB-C1B-NB	2.05	127.04	124.08
17	A	1124	CLA	C2A-C1A-CHA	2.05	126.13	122.63
17	B	1205	CLA	C2A-C1A-CHA	2.05	126.13	122.63
17	Z	5101	CLA	CHB-C1B-NB	2.05	127.04	124.08
17	A	1140	CLA	C3D-C2D-C1D	-2.05	104.86	107.35
17	0	1011	CLA	CHB-C1B-NB	2.05	127.04	124.08
17	A	1114	CLA	CHB-C1B-NB	2.05	127.04	124.08
17	B	1230	CLA	C2A-C1A-CHA	2.05	126.12	122.63
17	2	1016	CLA	CHB-C1B-NB	2.05	127.04	124.08
17	Q	5227	CLA	CHB-C1B-NB	2.05	127.04	124.08
17	P	5128	CLA	C3D-C2D-C1D	-2.05	104.86	107.35
17	Q	5023	CLA	C3D-C2D-C1D	-2.05	104.86	107.35
17	2	1031	CLA	CHB-C1B-NB	2.05	127.04	124.08
17	4	1011	CLA	CHB-C1B-NB	2.04	127.03	124.08
17	3	1031	CLA	CHB-C1B-NB	2.04	127.03	124.08
17	B	1208	CLA	C3D-C2D-C1D	-2.04	104.86	107.35
17	P	5124	CLA	C2A-C1A-CHA	2.04	126.12	122.63
17	2	1021	CLA	CHB-C1B-NB	2.04	127.03	124.08
17	8	1023	CLA	CHB-C1B-NB	2.04	127.03	124.08
17	B	1023	CLA	C3D-C2D-C1D	-2.04	104.87	107.35
17	A	1110	CLA	CHB-C1B-NB	2.04	127.03	124.08
17	2	1013	CLA	CHB-C1B-NB	2.04	127.03	124.08
17	9	1015	CLA	CHB-C1B-NB	2.04	127.03	124.08
17	A	1136	CLA	CHD-C1D-ND	-2.04	121.96	124.84
17	B	1204	CLA	CHD-C1D-ND	-2.04	121.96	124.84
17	B	1023	CLA	C2A-C1A-CHA	2.04	126.11	122.63
17	9	1025	CLA	CHB-C1B-NB	2.04	127.03	124.08
17	2	1023	CLA	CHB-C1B-NB	2.04	127.03	124.08
17	3	1025	CLA	CHB-C1B-NB	2.04	127.03	124.08
17	B	1227	CLA	CHB-C1B-NB	2.04	127.03	124.08
17	1	1012	CLA	CHB-C1B-NB	2.04	127.02	124.08
17	B	1225	CLA	C3D-C2D-C1D	-2.04	104.87	107.35
17	B	1226	CLA	C3D-C2D-C1D	-2.04	104.87	107.35
17	8	1025	CLA	CHB-C1B-NB	2.04	127.02	124.08
17	P	5140	CLA	C3D-C2D-C1D	-2.03	104.88	107.35
17	Q	5213	CLA	C3C-C4C-NC	-2.03	108.15	109.92
17	8	1016	CLA	CHB-C1B-NB	2.03	127.02	124.08
17	Q	5226	CLA	C3D-C2D-C1D	-2.03	104.88	107.35
17	2	1014	CLA	CHB-C1B-NB	2.03	127.02	124.08
17	A	1129	CLA	CHB-C1B-NB	2.03	127.02	124.08
17	A	1013	CLA	C3C-C4C-NC	-2.03	108.15	109.92
17	Q	5023	CLA	C2A-C1A-CHA	2.03	126.09	122.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	2	1025	CLA	CHB-C1B-NB	2.03	127.01	124.08
17	P	5109	CLA	C3D-C2D-C1D	-2.03	104.89	107.35
17	2	1014	CLA	C3D-C2D-C1D	-2.03	104.89	107.35
17	P	5136	CLA	C3D-C2D-C1D	-2.02	104.89	107.35
17	8	1031	CLA	CHB-C1B-NB	2.02	127.01	124.08
17	P	5134	CLA	CHD-C1D-ND	-2.02	121.99	124.84
17	4	1032	CLA	CHB-C1B-NB	2.02	127.00	124.08
17	A	1134	CLA	CHD-C1D-ND	-2.02	121.99	124.84
17	9	1021	CLA	C3D-C2D-C1D	-2.02	104.89	107.35
17	B	1231	CLA	C2A-C1A-CHA	2.02	126.08	122.63
17	Q	5022	CLA	C3D-C2D-C1D	-2.02	104.89	107.35
17	B	1223	CLA	CHB-C1B-NB	2.02	127.00	124.08
17	Q	5226	CLA	CHB-C1B-NB	2.02	127.00	124.08
17	P	5123	CLA	C3D-C2D-C1D	-2.02	104.89	107.35
17	9	1021	CLA	CHB-C1B-NB	2.02	127.00	124.08
17	A	1128	CLA	C3D-C2D-C1D	-2.02	104.90	107.35
17	Q	5205	CLA	C1B-NB-C4B	2.02	107.73	106.31
17	A	1136	CLA	C3D-C2D-C1D	-2.02	104.90	107.35
17	F	4005	CLA	CHB-C1B-NB	2.01	126.99	124.08
17	B	1213	CLA	C3C-C4C-NC	-2.01	108.16	109.92
17	P	5129	CLA	CHB-C1B-NB	2.01	126.99	124.08
17	0	8002	CLA	C3D-C2D-C1D	-2.01	104.90	107.35
17	Q	5231	CLA	C2A-C1A-CHA	2.01	126.07	122.63
17	U	8005	CLA	CHB-C1B-NB	2.01	126.99	124.08
17	0	1032	CLA	CHB-C1B-NB	2.01	126.99	124.08
17	9	1016	CLA	C3D-C2D-C1D	-2.01	104.90	107.35
17	A	1109	CLA	C3D-C2D-C1D	-2.01	104.90	107.35
17	Q	5223	CLA	CHB-C1B-NB	2.01	126.99	124.08
17	B	1022	CLA	C3C-C4C-NC	-2.01	108.17	109.92
17	P	5133	CLA	C3D-C2D-C1D	-2.01	104.91	107.35
17	P	5136	CLA	CHD-C1D-ND	-2.01	122.01	124.84
17	P	5013	CLA	C3C-C4C-NC	-2.01	108.17	109.92
17	8	1015	CLA	C3D-C2D-C1D	-2.01	104.91	107.35
17	B	1226	CLA	CHB-C1B-NB	2.01	126.98	124.08
17	3	1016	CLA	CHB-C1B-NB	2.01	126.98	124.08
17	A	1123	CLA	C3D-C2D-C1D	-2.00	104.91	107.35
17	A	1013	CLA	CHD-C1D-ND	-2.00	122.02	124.84
17	9	1016	CLA	CHB-C1B-NB	2.00	126.97	124.08
17	A	1133	CLA	C3D-C2D-C1D	-2.00	104.92	107.35
17	0	1023	CLA	C3D-C2D-C1D	-2.00	104.92	107.35
17	P	5118	CLA	CHD-C1D-ND	-2.00	122.02	124.84
17	0	1016	CLA	C3D-C2D-C1D	-2.00	104.92	107.35

All (332) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
17	A	1011	CLA	ND
17	A	1012	CLA	ND
17	A	1013	CLA	ND
17	A	1102	CLA	ND
17	A	1103	CLA	ND
17	A	1104	CLA	ND
17	A	1105	CLA	ND
17	A	1106	CLA	ND
17	A	1107	CLA	ND
17	A	1108	CLA	ND
17	A	1109	CLA	ND
17	A	1110	CLA	ND
17	A	1111	CLA	ND
17	A	1112	CLA	ND
17	A	1113	CLA	ND
17	A	1114	CLA	ND
17	A	1115	CLA	ND
17	A	1116	CLA	ND
17	A	1117	CLA	ND
17	A	1118	CLA	ND
17	A	1119	CLA	ND
17	A	1120	CLA	ND
17	A	1121	CLA	ND
17	A	1122	CLA	ND
17	A	1123	CLA	ND
17	A	1124	CLA	ND
17	A	1125	CLA	ND
17	A	1126	CLA	ND
17	A	1127	CLA	ND
17	A	1128	CLA	ND
17	A	1129	CLA	ND
17	A	1131	CLA	ND
17	A	1132	CLA	ND
17	A	1133	CLA	ND
17	A	1134	CLA	ND
17	A	1135	CLA	ND
17	A	1136	CLA	ND
17	A	1137	CLA	ND
17	A	1138	CLA	ND
17	A	1139	CLA	ND
17	A	1140	CLA	ND
17	A	1402	CLA	ND

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Mol	Chain	Res	Type	Atom
17	A	1901	CLA	ND
17	A	4009	CLA	ND
17	A	4010	CLA	ND
17	B	1021	CLA	ND
17	B	1022	CLA	ND
17	B	1023	CLA	ND
17	B	1130	CLA	ND
17	B	1201	CLA	ND
17	B	1202	CLA	ND
17	B	1203	CLA	ND
17	B	1204	CLA	ND
17	B	1205	CLA	ND
17	B	1206	CLA	ND
17	B	1207	CLA	ND
17	B	1208	CLA	ND
17	B	1209	CLA	ND
17	B	1210	CLA	ND
17	B	1211	CLA	ND
17	B	1212	CLA	ND
17	B	1213	CLA	ND
17	B	1214	CLA	ND
17	B	1215	CLA	ND
17	B	1216	CLA	ND
17	B	1217	CLA	ND
17	B	1218	CLA	ND
17	B	1219	CLA	ND
17	B	1220	CLA	ND
17	B	1221	CLA	ND
17	B	1222	CLA	ND
17	B	1223	CLA	ND
17	B	1224	CLA	ND
17	B	1225	CLA	ND
17	B	1226	CLA	ND
17	B	1227	CLA	ND
17	B	1228	CLA	ND
17	B	1230	CLA	ND
17	B	1231	CLA	ND
17	B	1232	CLA	ND
17	B	1234	CLA	ND
17	B	1235	CLA	ND
17	B	1236	CLA	ND
17	B	1237	CLA	ND

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Mol	Chain	Res	Type	Atom
17	B	1238	CLA	ND
17	B	1239	CLA	ND
17	B	1240	CLA	ND
17	B	1241	CLA	ND
17	B	1242	CLA	ND
17	B	4001	CLA	ND
17	F	1229	CLA	ND
17	F	1301	CLA	ND
17	F	4003	CLA	ND
17	F	4004	CLA	ND
17	F	4005	CLA	ND
17	F	4006	CLA	ND
17	G	1233	CLA	ND
17	G	1701	CLA	ND
17	H	1801	CLA	ND
17	J	1101	CLA	ND
17	J	1302	CLA	ND
17	J	4008	CLA	ND
17	K	1401	CLA	ND
17	K	1403	CLA	ND
17	K	1404	CLA	ND
17	L	1501	CLA	ND
17	L	1503	CLA	ND
17	L	1504	CLA	ND
17	1	1011	CLA	ND
17	1	1012	CLA	ND
17	1	1013	CLA	ND
17	1	1014	CLA	ND
17	1	1015	CLA	ND
17	1	1016	CLA	ND
17	1	1017	CLA	ND
17	1	1021	CLA	ND
17	1	1022	CLA	ND
17	1	1023	CLA	ND
17	1	1025	CLA	ND
17	1	1026	CLA	ND
17	1	1031	CLA	ND
17	2	4007	CLA	ND
17	2	1011	CLA	ND
17	2	1012	CLA	ND
17	2	1013	CLA	ND
17	2	1014	CLA	ND

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Mol	Chain	Res	Type	Atom
17	2	1015	CLA	ND
17	2	1016	CLA	ND
17	2	1017	CLA	ND
17	2	1021	CLA	ND
17	2	1022	CLA	ND
17	2	1023	CLA	ND
17	2	1025	CLA	ND
17	2	1026	CLA	ND
17	2	1031	CLA	ND
17	2	1033	CLA	ND
17	3	1011	CLA	ND
17	3	1012	CLA	ND
17	3	1014	CLA	ND
17	3	1015	CLA	ND
17	3	1016	CLA	ND
17	3	1017	CLA	ND
17	3	1021	CLA	ND
17	3	1022	CLA	ND
17	3	1025	CLA	ND
17	3	1026	CLA	ND
17	3	1031	CLA	ND
17	3	1032	CLA	ND
17	3	1033	CLA	ND
17	3	1041	CLA	ND
17	4	4002	CLA	ND
17	4	1011	CLA	ND
17	4	1012	CLA	ND
17	4	1013	CLA	ND
17	4	1014	CLA	ND
17	4	1015	CLA	ND
17	4	1016	CLA	ND
17	4	1017	CLA	ND
17	4	1021	CLA	ND
17	4	1022	CLA	ND
17	4	1023	CLA	ND
17	4	1025	CLA	ND
17	4	1026	CLA	ND
17	4	1031	CLA	ND
17	4	1032	CLA	ND
17	4	1033	CLA	ND
17	P	5011	CLA	ND
17	P	5012	CLA	ND

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Mol	Chain	Res	Type	Atom
17	P	5013	CLA	ND
17	P	5102	CLA	ND
17	P	5103	CLA	ND
17	P	5104	CLA	ND
17	P	5105	CLA	ND
17	P	5106	CLA	ND
17	P	5107	CLA	ND
17	P	5108	CLA	ND
17	P	5109	CLA	ND
17	P	5110	CLA	ND
17	P	5111	CLA	ND
17	P	5112	CLA	ND
17	P	5113	CLA	ND
17	P	5114	CLA	ND
17	P	5115	CLA	ND
17	P	5116	CLA	ND
17	P	5117	CLA	ND
17	P	5118	CLA	ND
17	P	5119	CLA	ND
17	P	5120	CLA	ND
17	P	5121	CLA	ND
17	P	5122	CLA	ND
17	P	5123	CLA	ND
17	P	5124	CLA	ND
17	P	5125	CLA	ND
17	P	5126	CLA	ND
17	P	5127	CLA	ND
17	P	5128	CLA	ND
17	P	5129	CLA	ND
17	P	5131	CLA	ND
17	P	5132	CLA	ND
17	P	5133	CLA	ND
17	P	5134	CLA	ND
17	P	5135	CLA	ND
17	P	5136	CLA	ND
17	P	5137	CLA	ND
17	P	5138	CLA	ND
17	P	5139	CLA	ND
17	P	5140	CLA	ND
17	P	5402	CLA	ND
17	P	5901	CLA	ND
17	P	8009	CLA	ND

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Mol	Chain	Res	Type	Atom
17	P	8010	CLA	ND
17	Q	5021	CLA	ND
17	Q	5022	CLA	ND
17	Q	5023	CLA	ND
17	Q	5130	CLA	ND
17	Q	5201	CLA	ND
17	Q	5202	CLA	ND
17	Q	5203	CLA	ND
17	Q	5204	CLA	ND
17	Q	5205	CLA	ND
17	Q	5206	CLA	ND
17	Q	5207	CLA	ND
17	Q	5208	CLA	ND
17	Q	5209	CLA	ND
17	Q	5210	CLA	ND
17	Q	5211	CLA	ND
17	Q	5212	CLA	ND
17	Q	5213	CLA	ND
17	Q	5214	CLA	ND
17	Q	5215	CLA	ND
17	Q	5216	CLA	ND
17	Q	5217	CLA	ND
17	Q	5218	CLA	ND
17	Q	5219	CLA	ND
17	Q	5220	CLA	ND
17	Q	5221	CLA	ND
17	Q	5222	CLA	ND
17	Q	5223	CLA	ND
17	Q	5224	CLA	ND
17	Q	5225	CLA	ND
17	Q	5226	CLA	ND
17	Q	5227	CLA	ND
17	Q	5228	CLA	ND
17	Q	5230	CLA	ND
17	Q	5231	CLA	ND
17	Q	5232	CLA	ND
17	Q	5234	CLA	ND
17	Q	5235	CLA	ND
17	Q	5236	CLA	ND
17	Q	5237	CLA	ND
17	Q	5238	CLA	ND
17	Q	5239	CLA	ND

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Mol	Chain	Res	Type	Atom
17	Q	5240	CLA	ND
17	Q	5241	CLA	ND
17	Q	5242	CLA	ND
17	Q	8001	CLA	ND
17	U	5229	CLA	ND
17	U	5301	CLA	ND
17	U	8003	CLA	ND
17	U	8004	CLA	ND
17	U	8005	CLA	ND
17	U	8006	CLA	ND
17	V	5233	CLA	ND
17	V	5701	CLA	ND
17	W	5801	CLA	ND
17	Z	5101	CLA	ND
17	Z	5302	CLA	ND
17	Z	8008	CLA	ND
17	5	5401	CLA	ND
17	5	5403	CLA	ND
17	5	5404	CLA	ND
17	6	5501	CLA	ND
17	6	5503	CLA	ND
17	6	5504	CLA	ND
17	7	1011	CLA	ND
17	7	1012	CLA	ND
17	7	1013	CLA	ND
17	7	1014	CLA	ND
17	7	1015	CLA	ND
17	7	1016	CLA	ND
17	7	1017	CLA	ND
17	7	1021	CLA	ND
17	7	1022	CLA	ND
17	7	1023	CLA	ND
17	7	1025	CLA	ND
17	7	1026	CLA	ND
17	7	1031	CLA	ND
17	8	8007	CLA	ND
17	8	1011	CLA	ND
17	8	1012	CLA	ND
17	8	1013	CLA	ND
17	8	1014	CLA	ND
17	8	1015	CLA	ND
17	8	1016	CLA	ND

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Mol	Chain	Res	Type	Atom
17	8	1017	CLA	ND
17	8	1021	CLA	ND
17	8	1022	CLA	ND
17	8	1023	CLA	ND
17	8	1025	CLA	ND
17	8	1026	CLA	ND
17	8	1031	CLA	ND
17	8	1033	CLA	ND
17	9	1011	CLA	ND
17	9	1012	CLA	ND
17	9	1014	CLA	ND
17	9	1015	CLA	ND
17	9	1016	CLA	ND
17	9	1017	CLA	ND
17	9	1021	CLA	ND
17	9	1022	CLA	ND
17	9	1025	CLA	ND
17	9	1026	CLA	ND
17	9	1031	CLA	ND
17	9	1032	CLA	ND
17	9	1033	CLA	ND
17	9	1041	CLA	ND
17	0	8002	CLA	ND
17	0	1011	CLA	ND
17	0	1012	CLA	ND
17	0	1013	CLA	ND
17	0	1014	CLA	ND
17	0	1015	CLA	ND
17	0	1016	CLA	ND
17	0	1017	CLA	ND
17	0	1021	CLA	ND
17	0	1022	CLA	ND
17	0	1023	CLA	ND
17	0	1025	CLA	ND
17	0	1026	CLA	ND
17	0	1031	CLA	ND
17	0	1032	CLA	ND
17	0	1033	CLA	ND

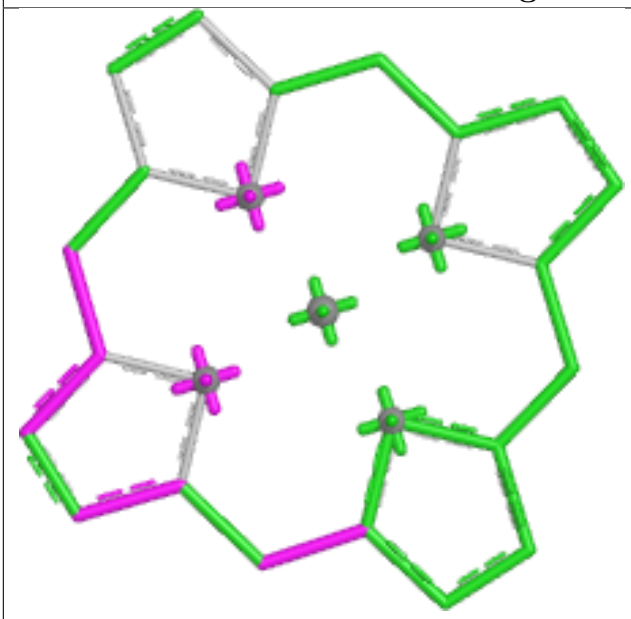
There are no torsion outliers.

There are no ring outliers.

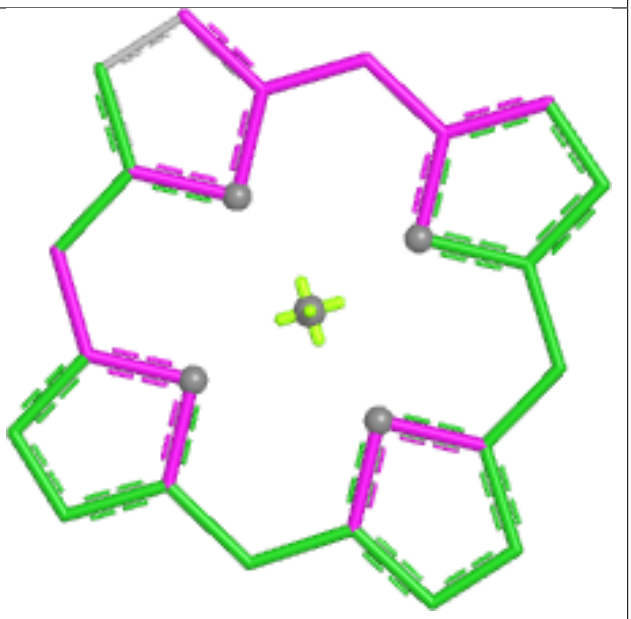
No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

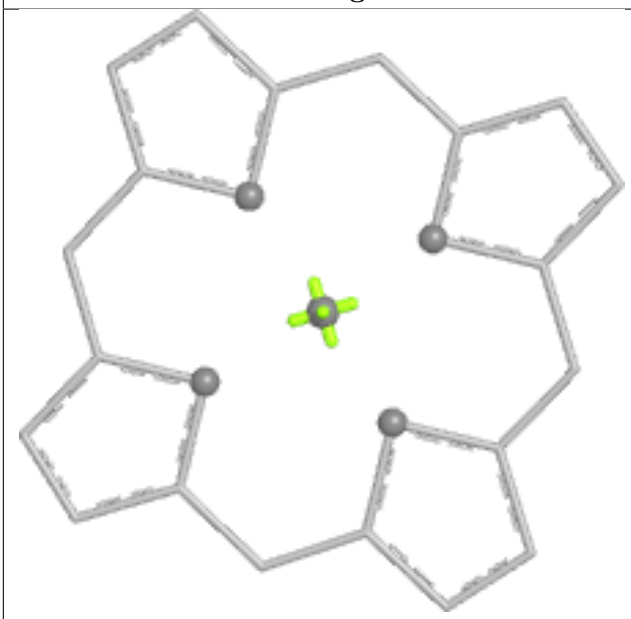
Ligand CLA 9 1033



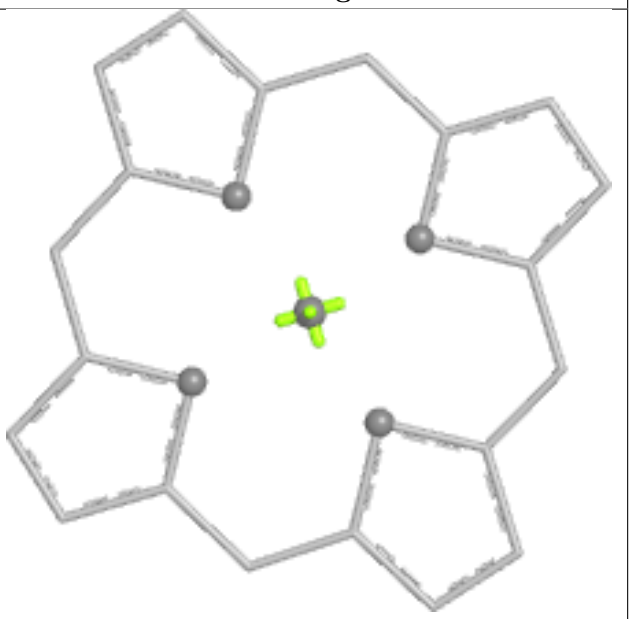
Bond lengths



Bond angles

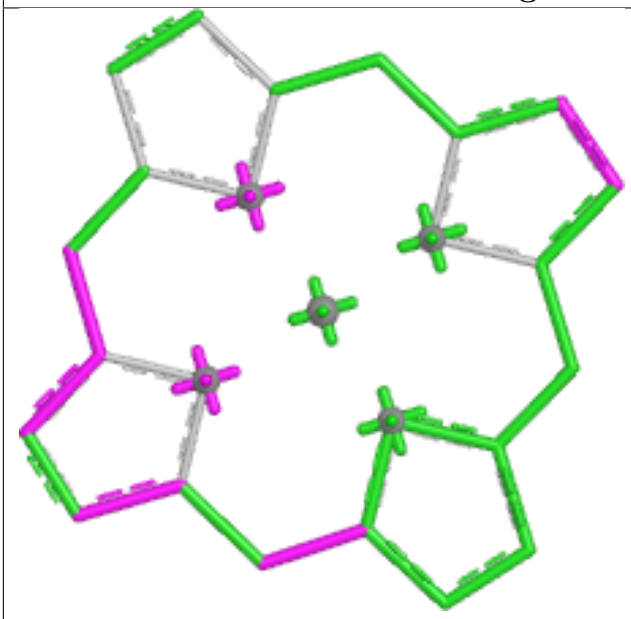


Torsions

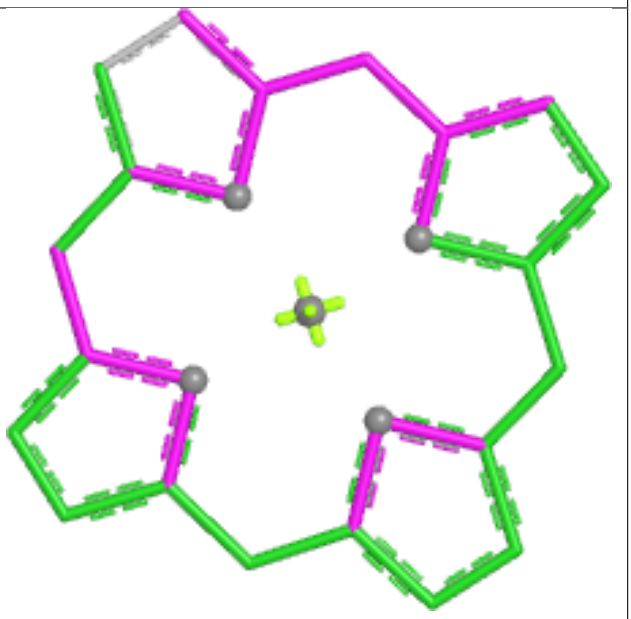


Rings

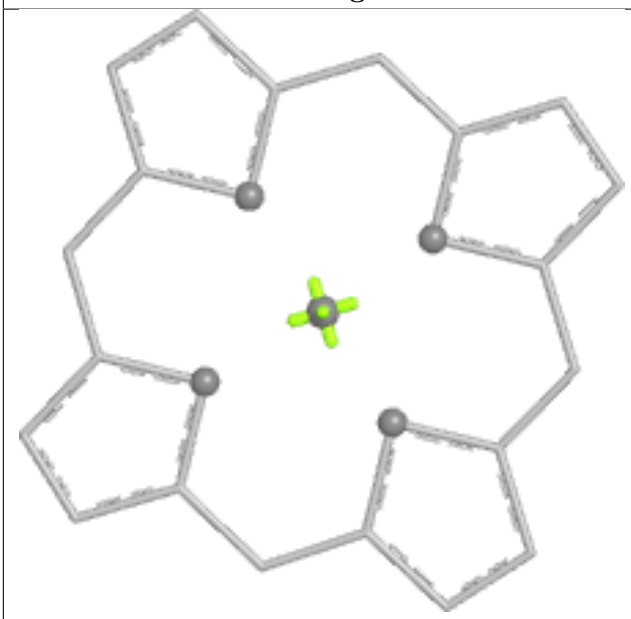
Ligand CLA 4 1031



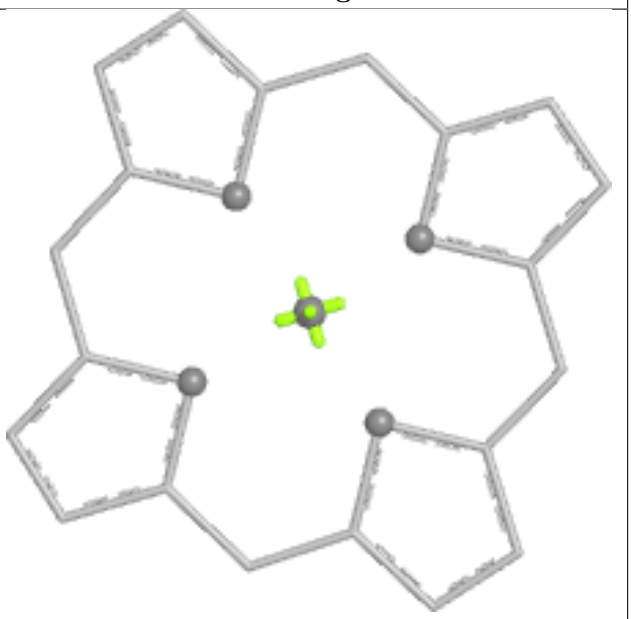
Bond lengths



Bond angles

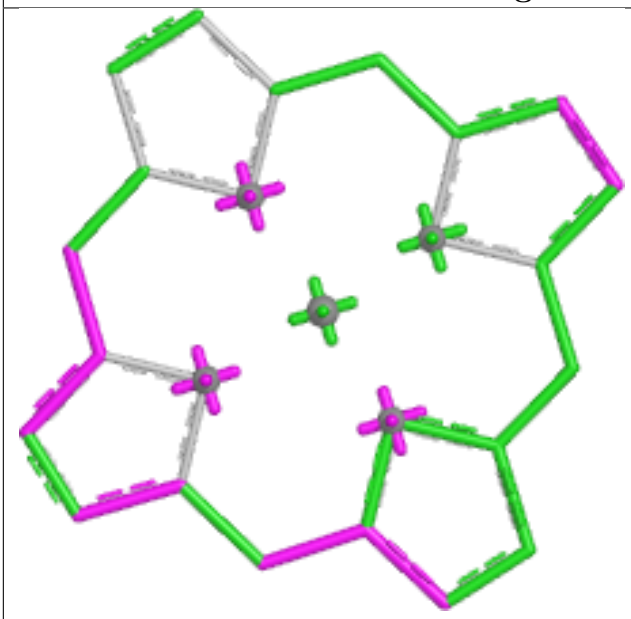


Torsions

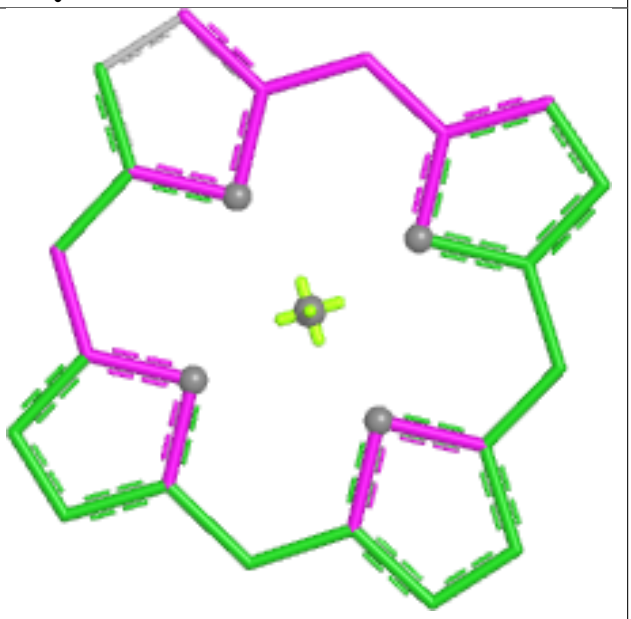


Rings

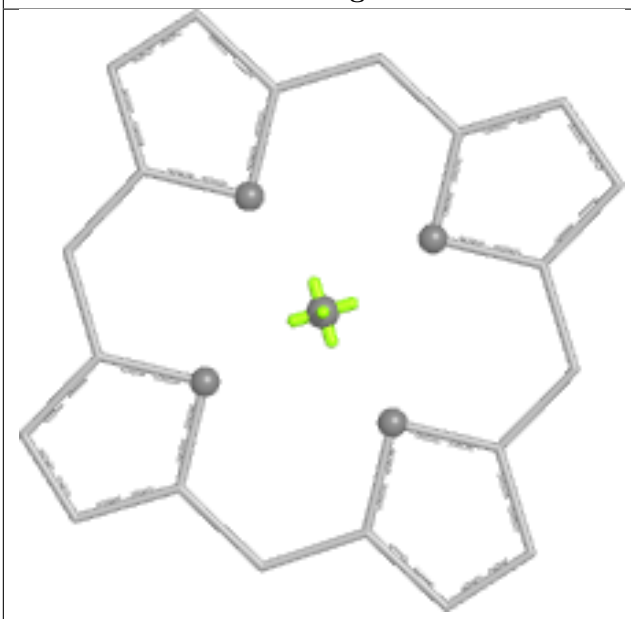
Ligand CLA Q 5221



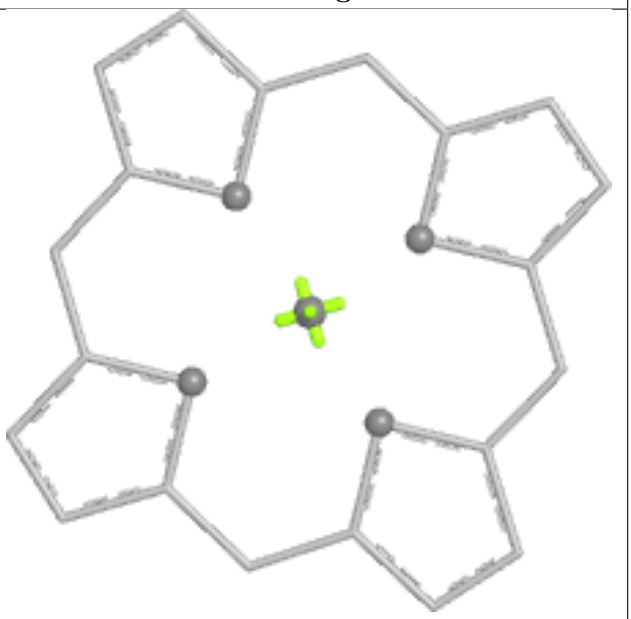
Bond lengths



Bond angles

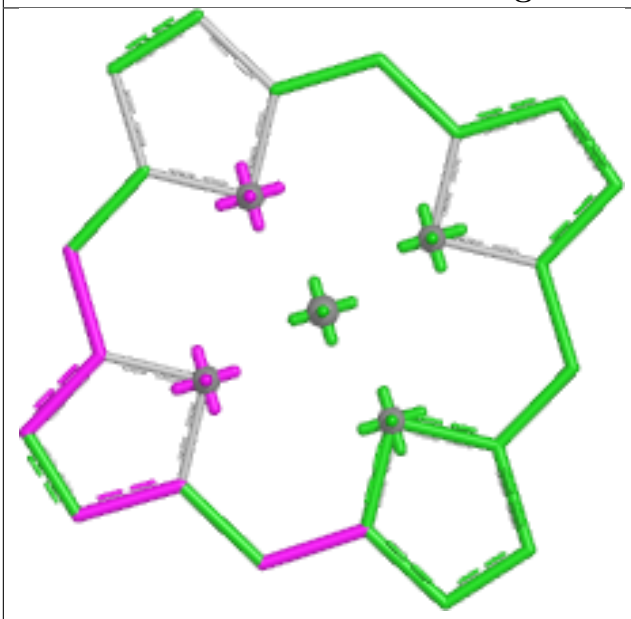


Torsions

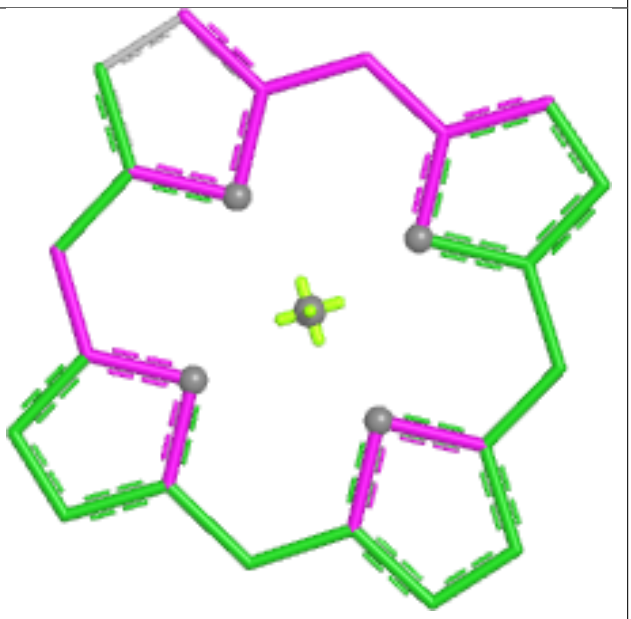


Rings

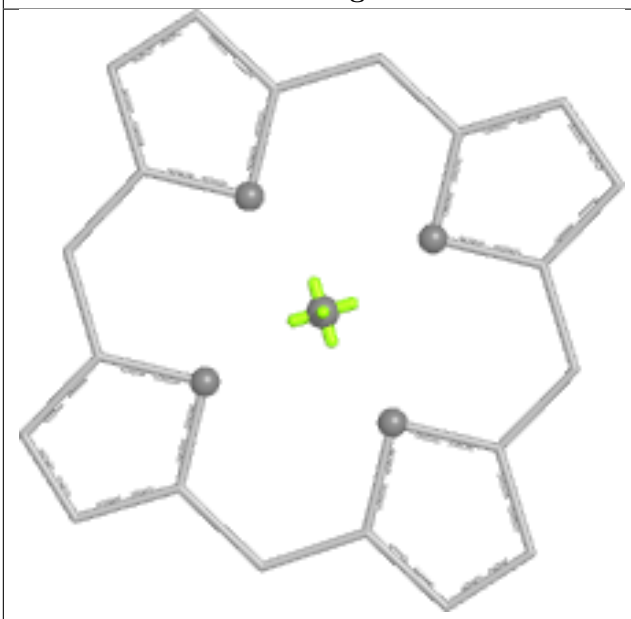
Ligand CLA V 5701



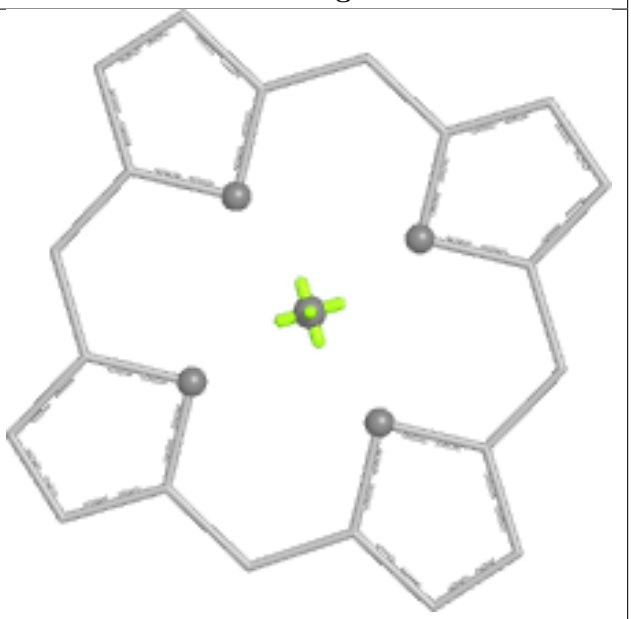
Bond lengths



Bond angles

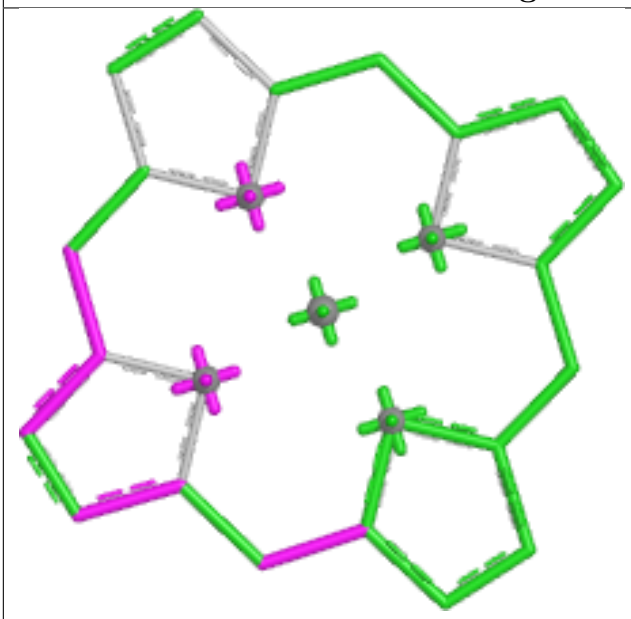


Torsions

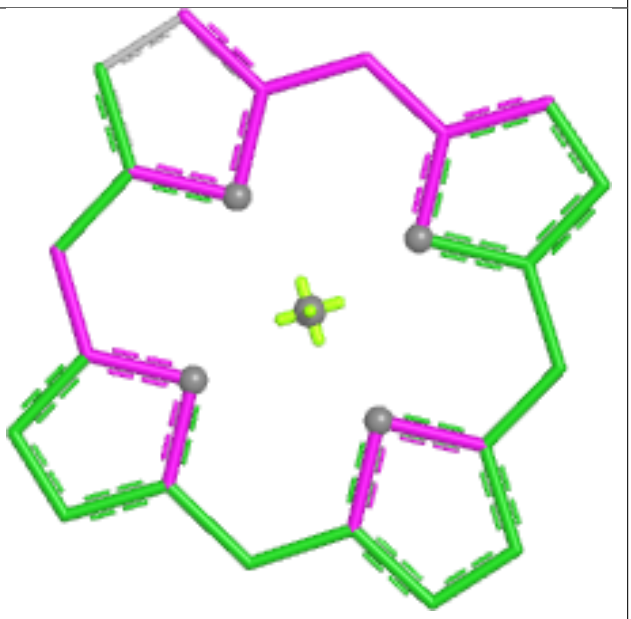


Rings

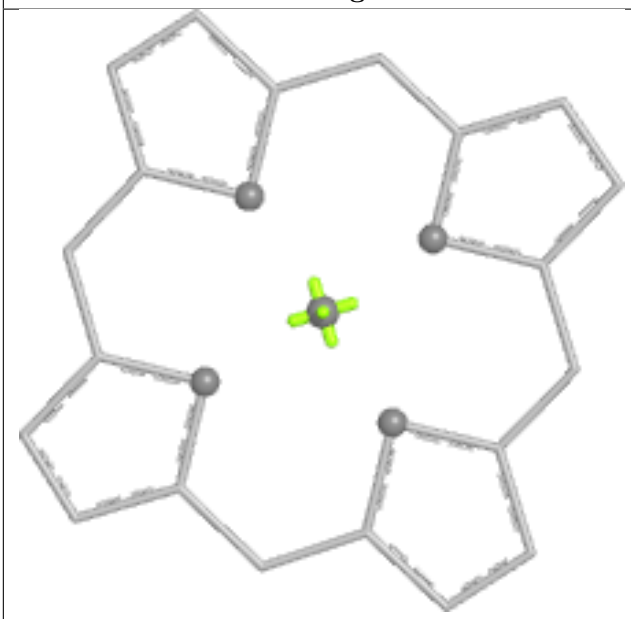
Ligand CLA 3 1022



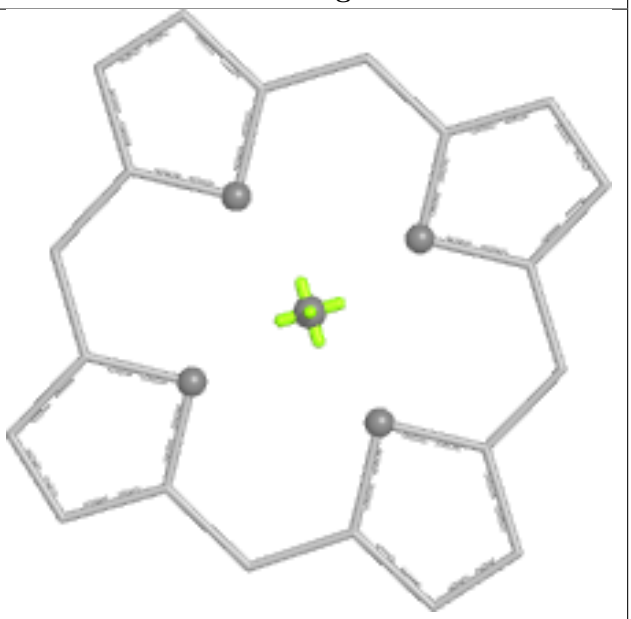
Bond lengths



Bond angles

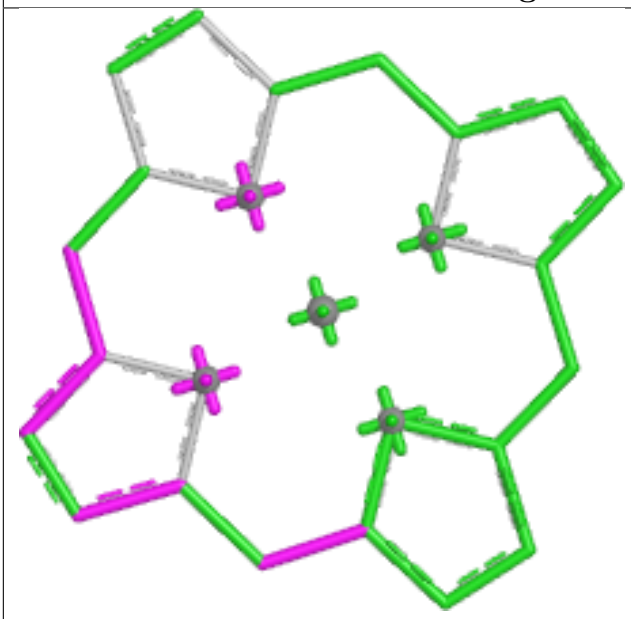


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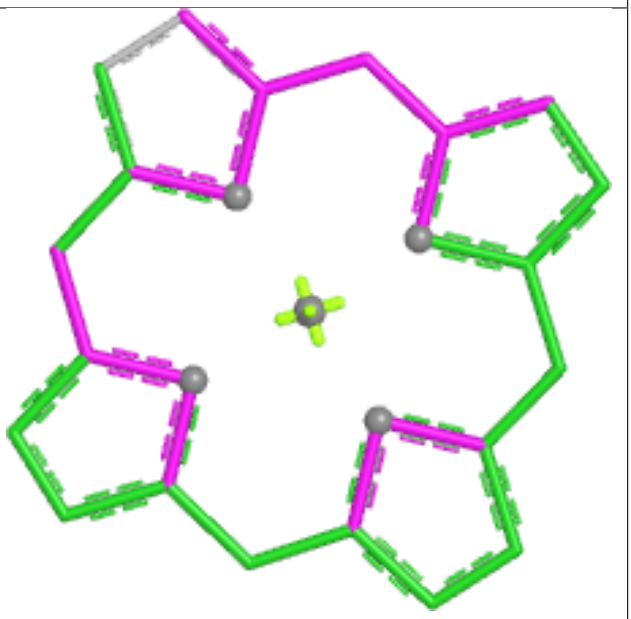


Rings

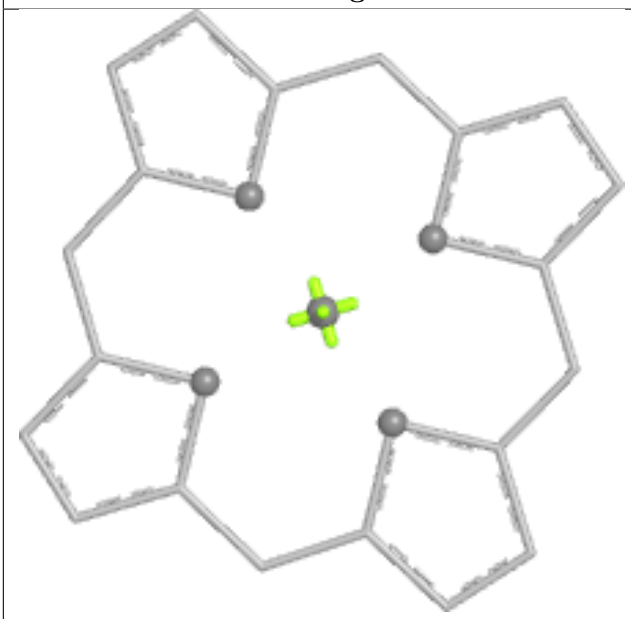
Ligand CLA J 1101



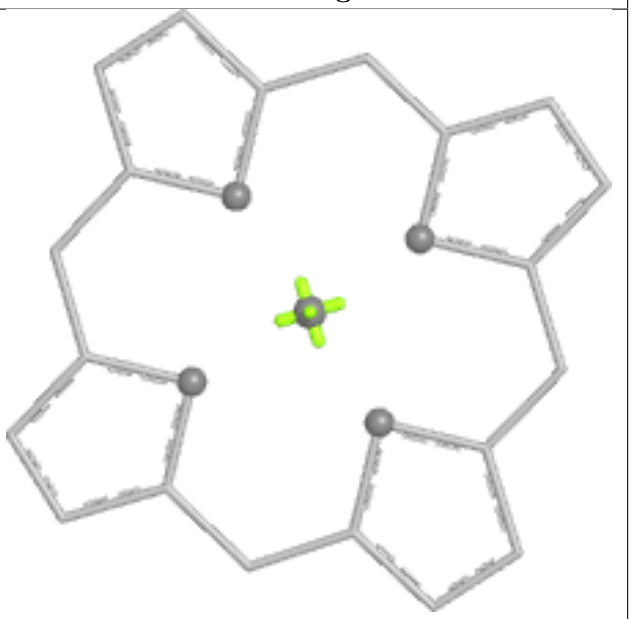
Bond lengths



Bond angles

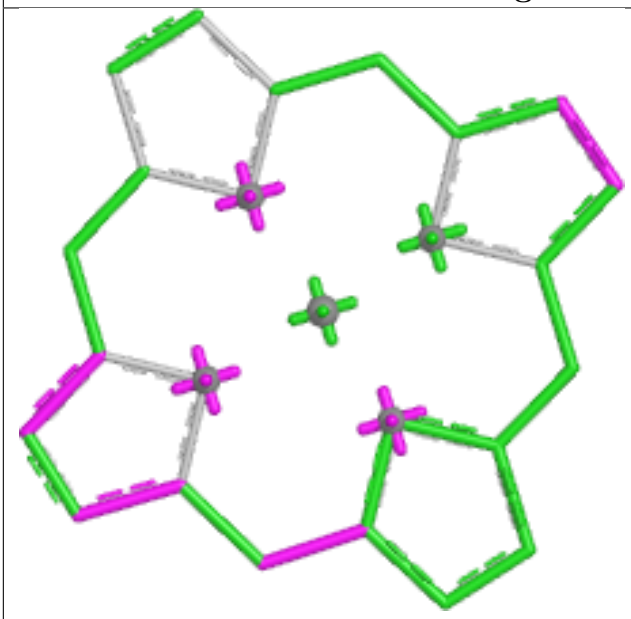


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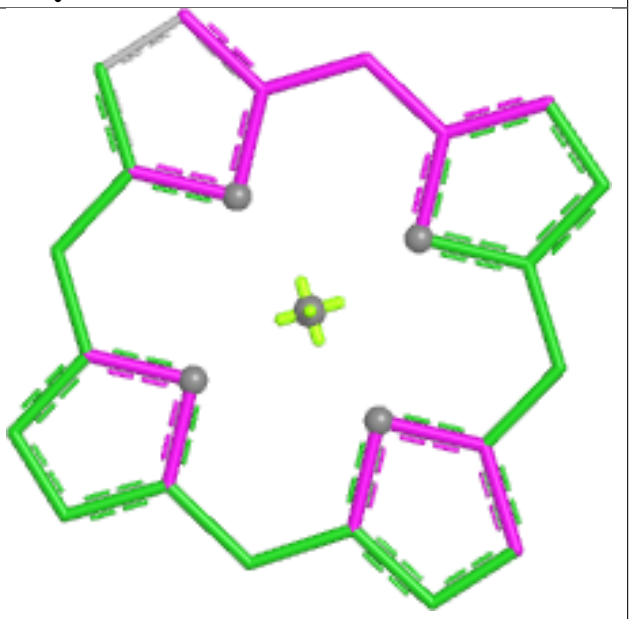


Rings

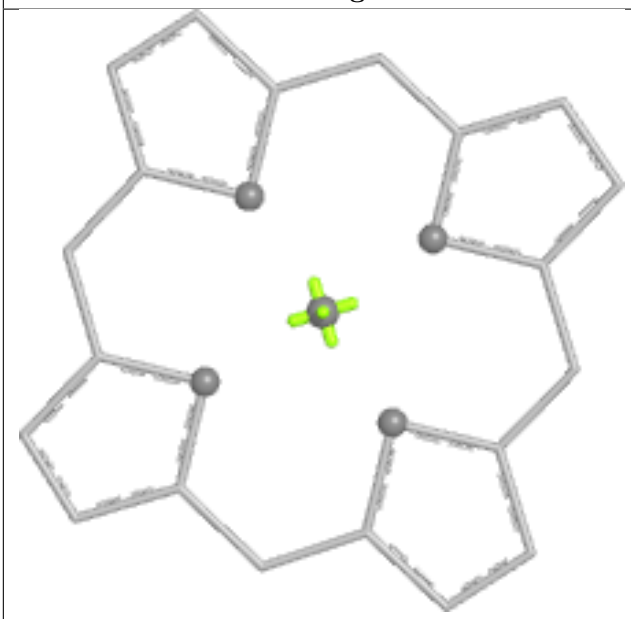
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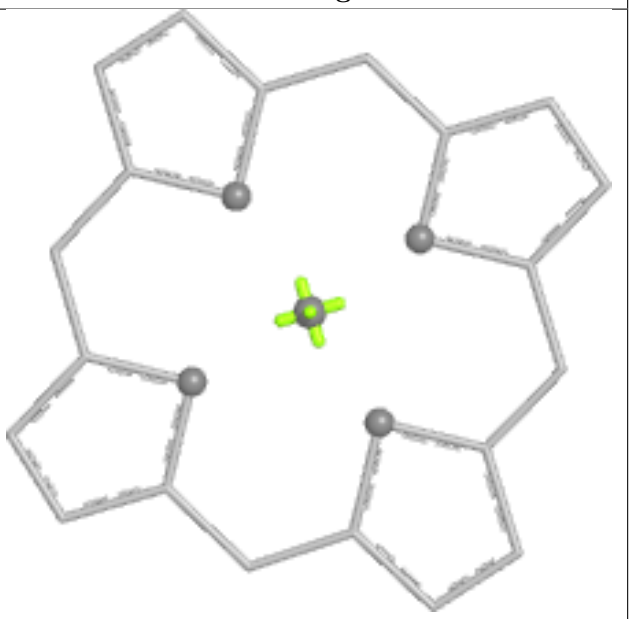
Bond lengths



Bond angles

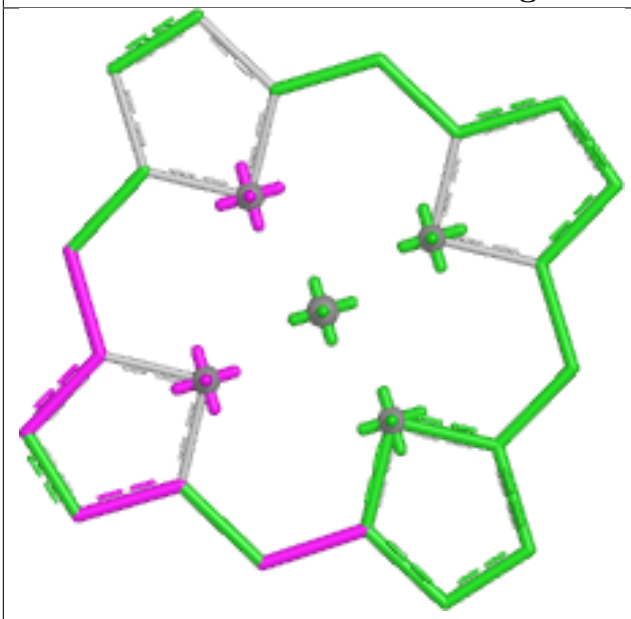


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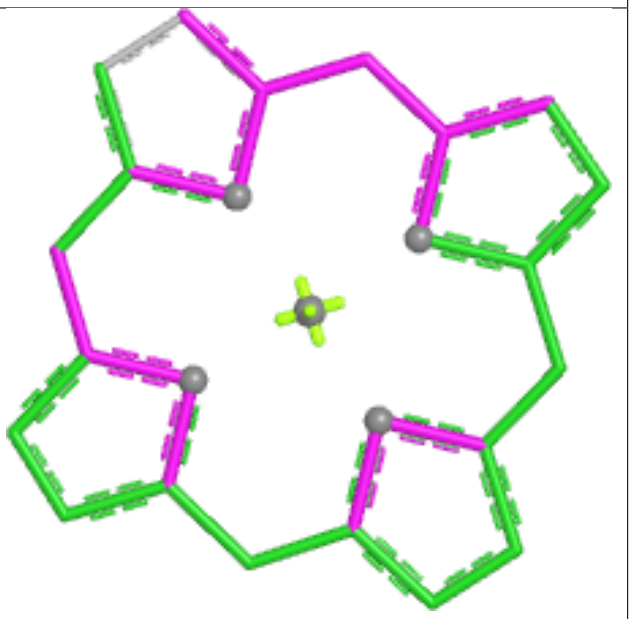


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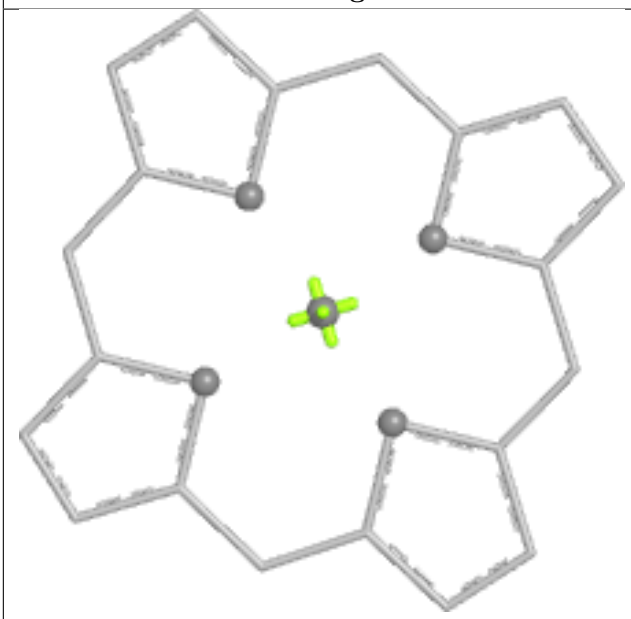
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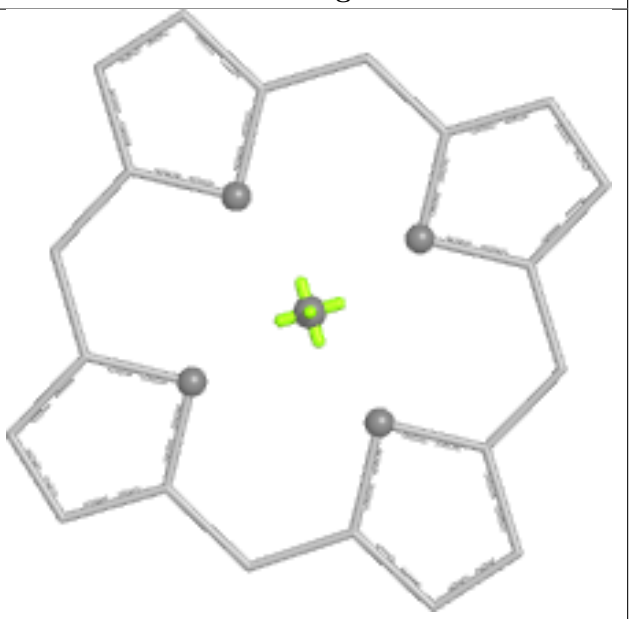
Bond lengths



Bond angles

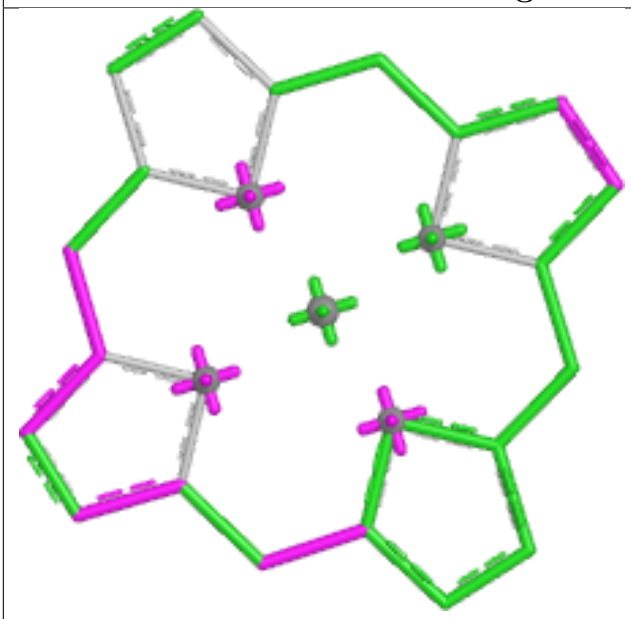


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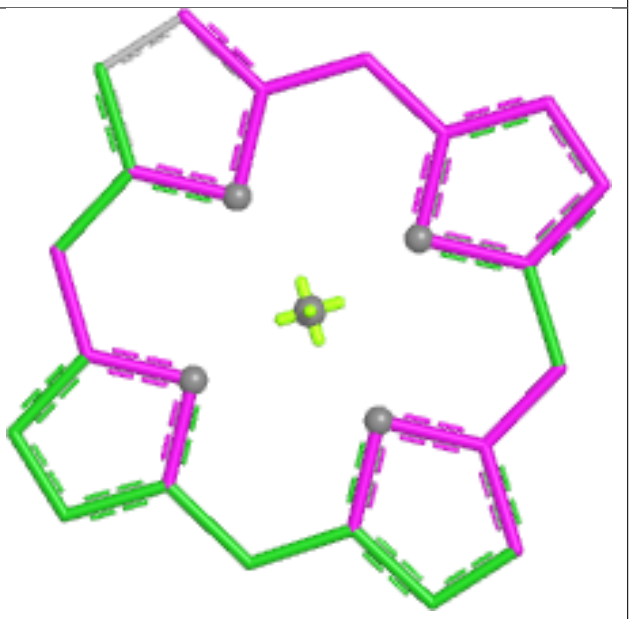


Rings

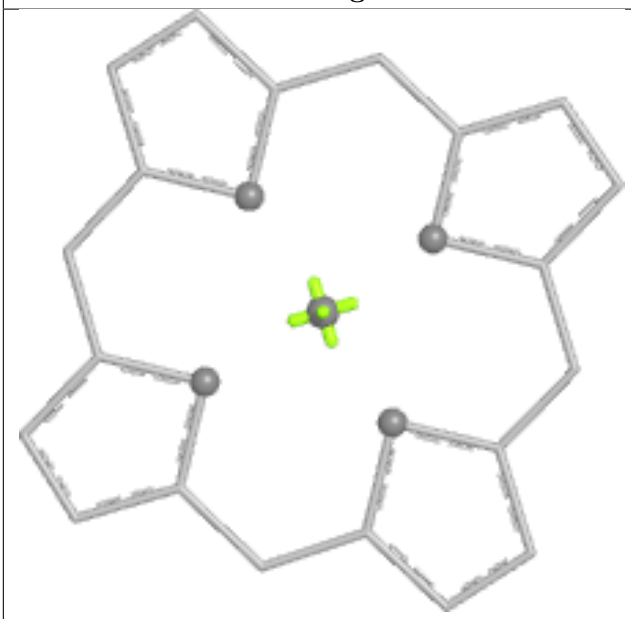
Ligand CLA P 5901



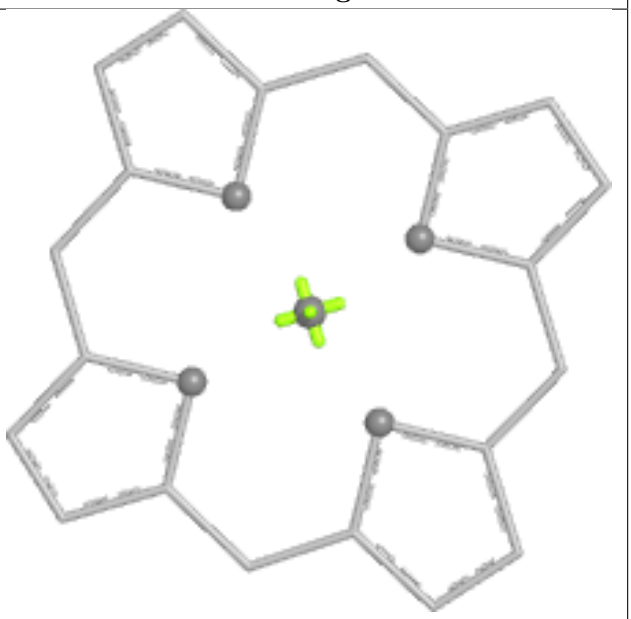
Bond lengths



Bond angles

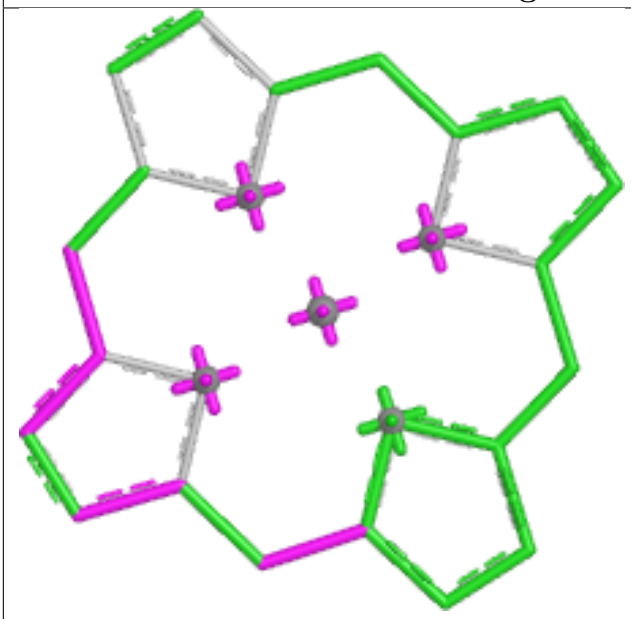


Torsions

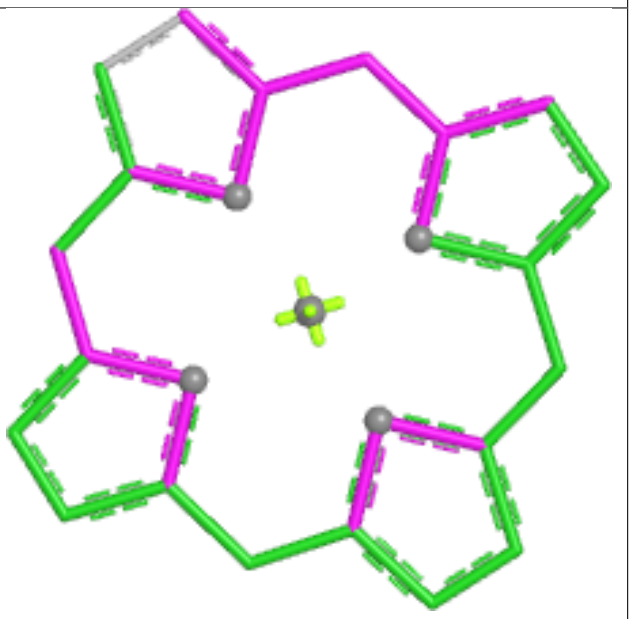


Rings

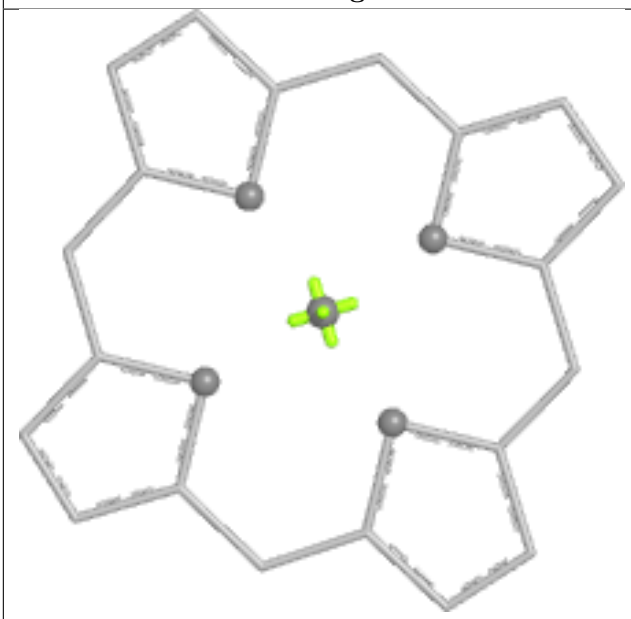
Ligand CLA 7 1021



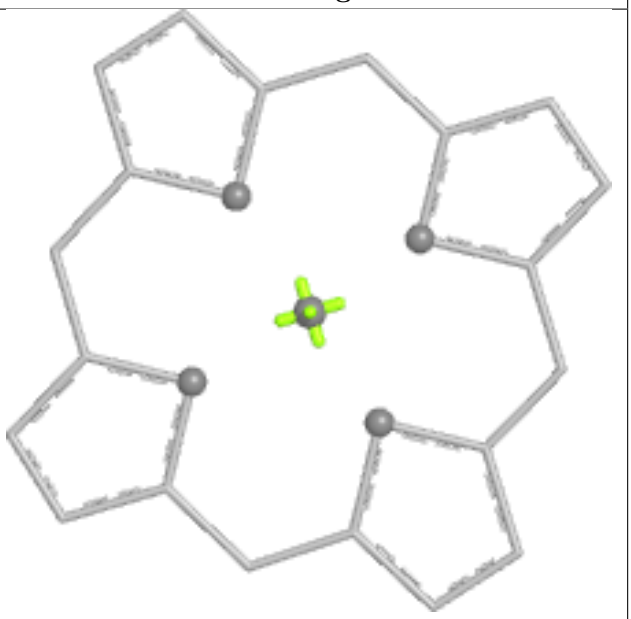
Bond lengths



Bond angles

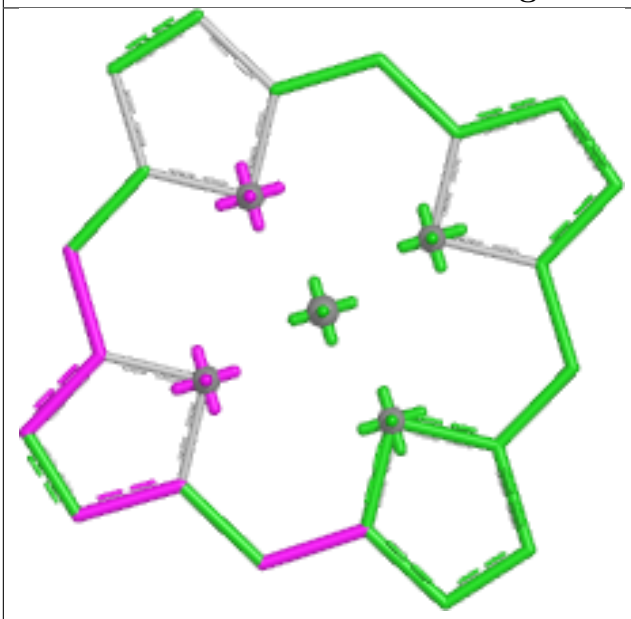


Torsions

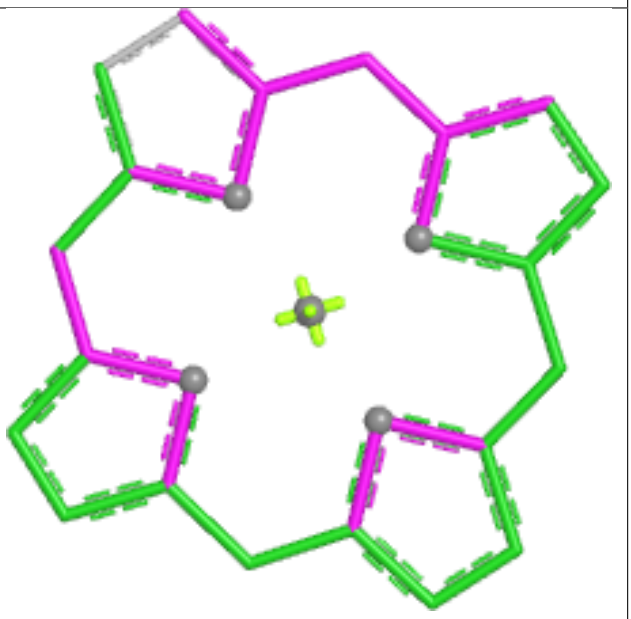


Rings

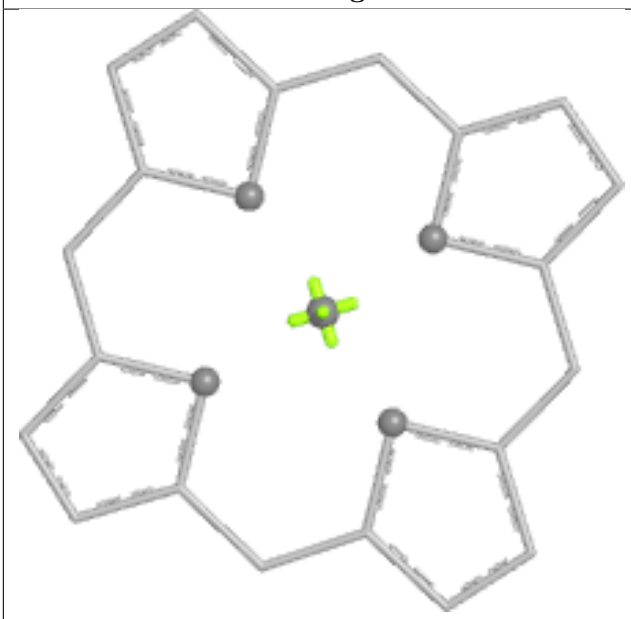
Ligand CLA 4 1023



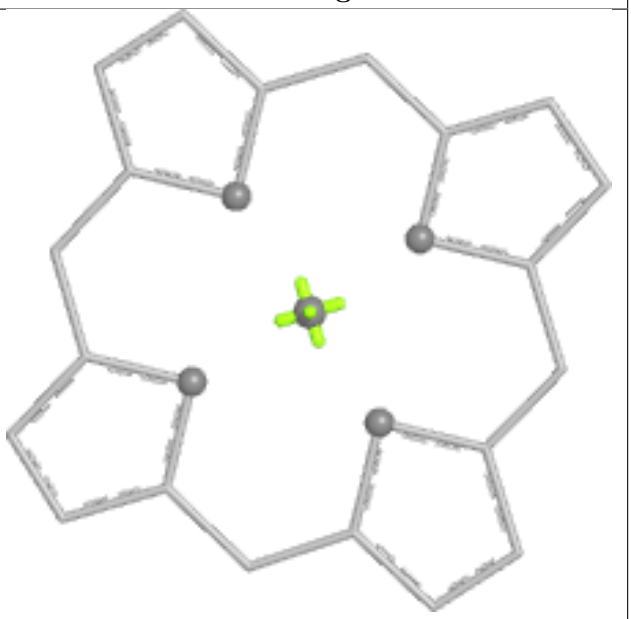
Bond lengths



Bond angles

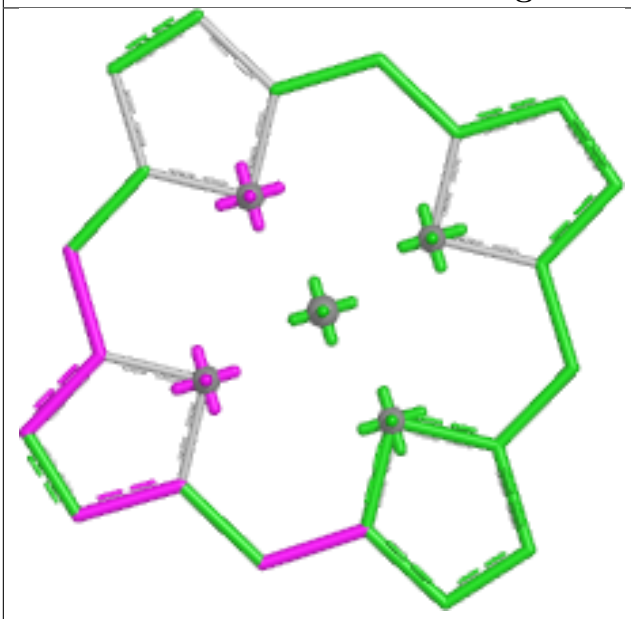


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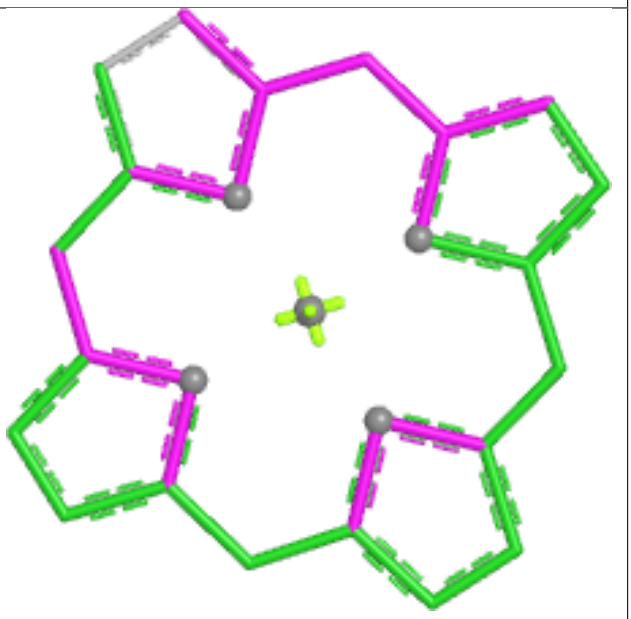


Rings

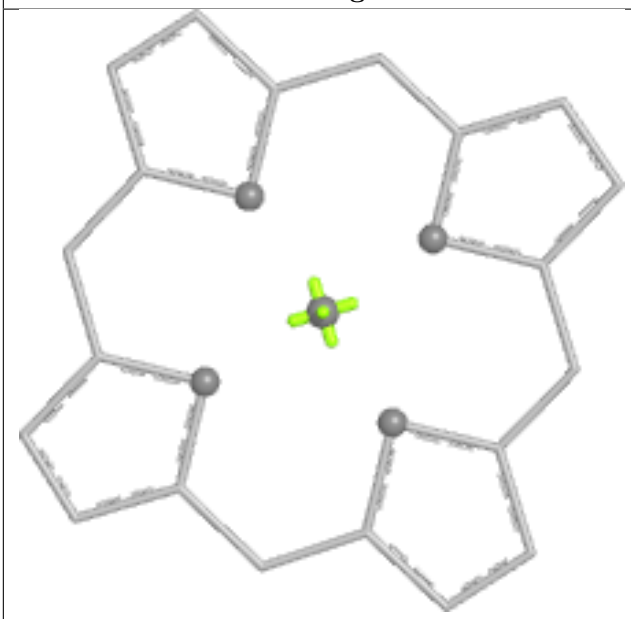
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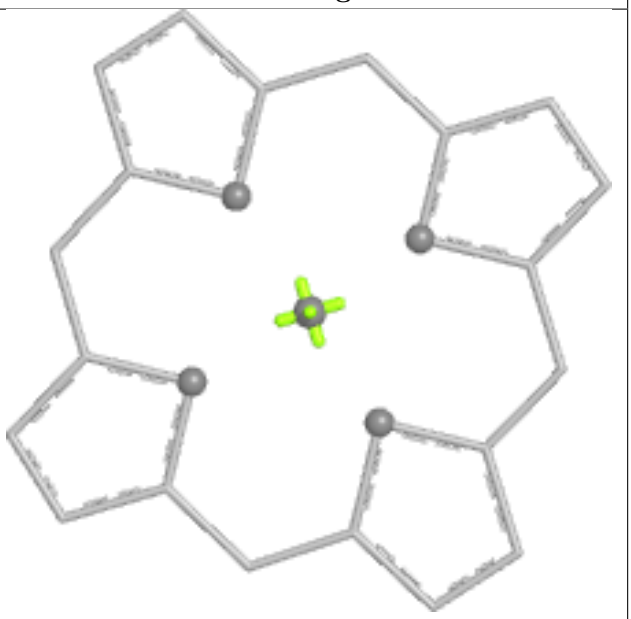
Bond lengths



Bond angles

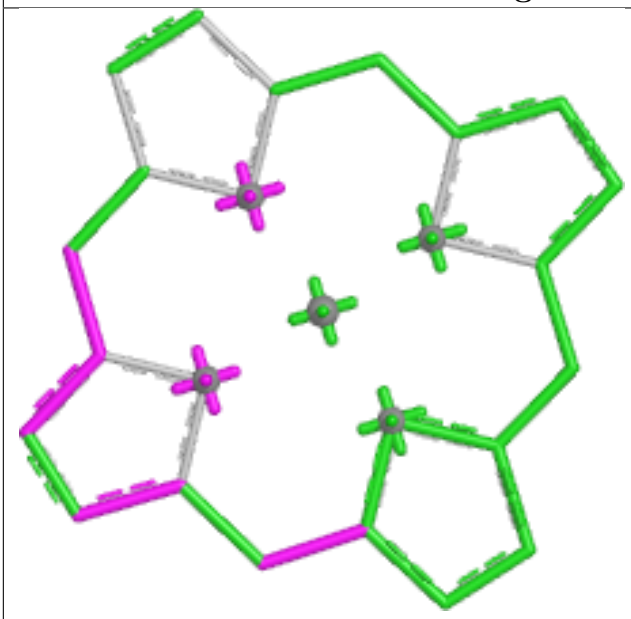


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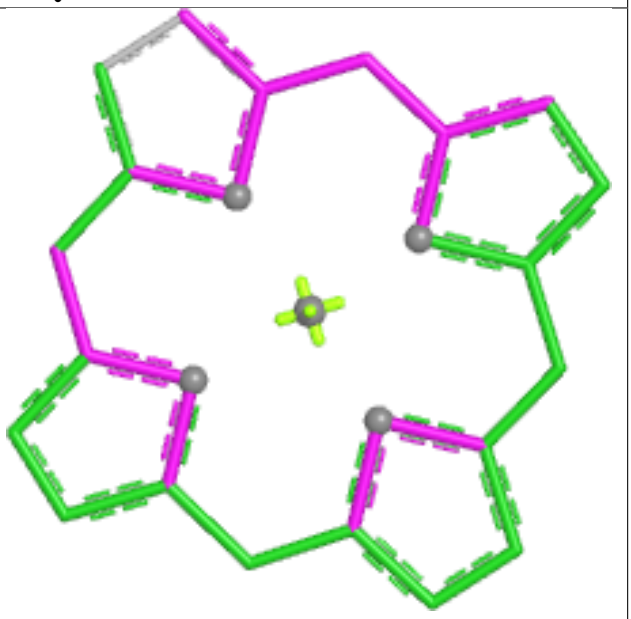


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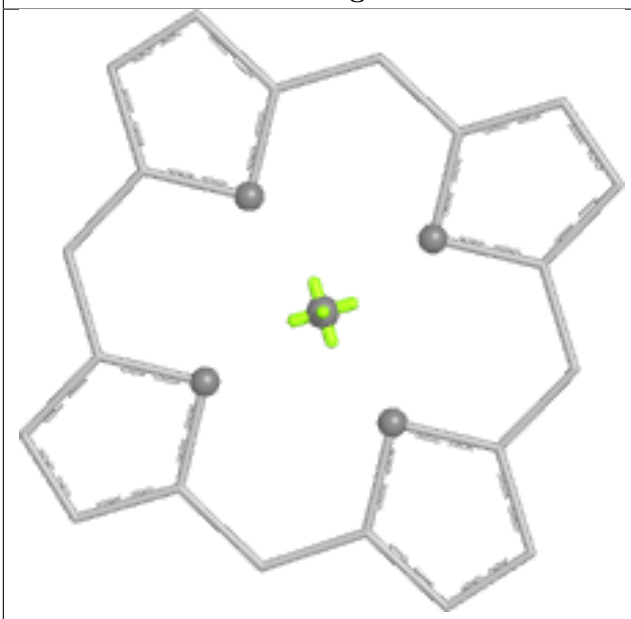
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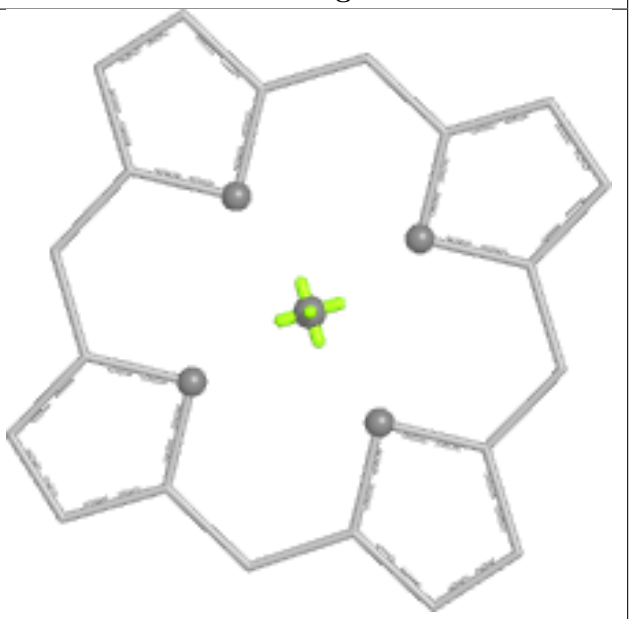
Bond lengths



Bond angles

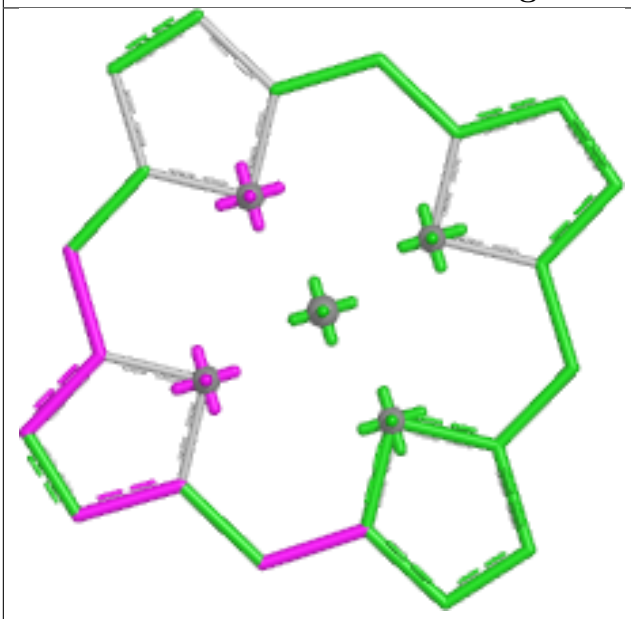


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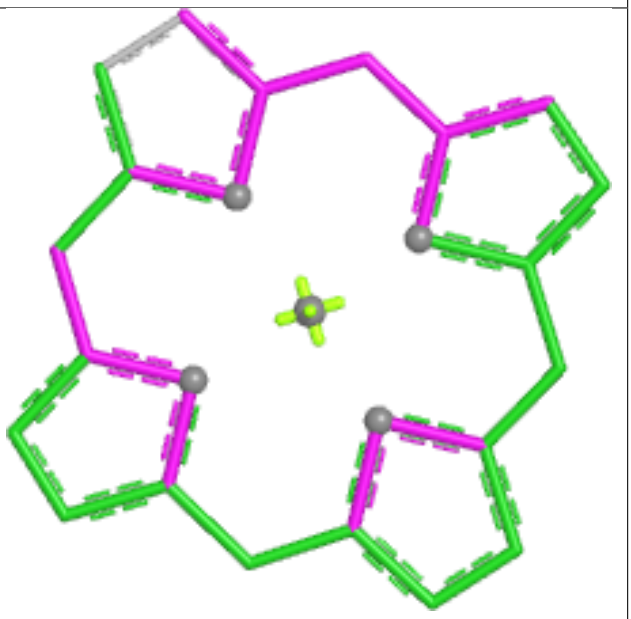


Rings

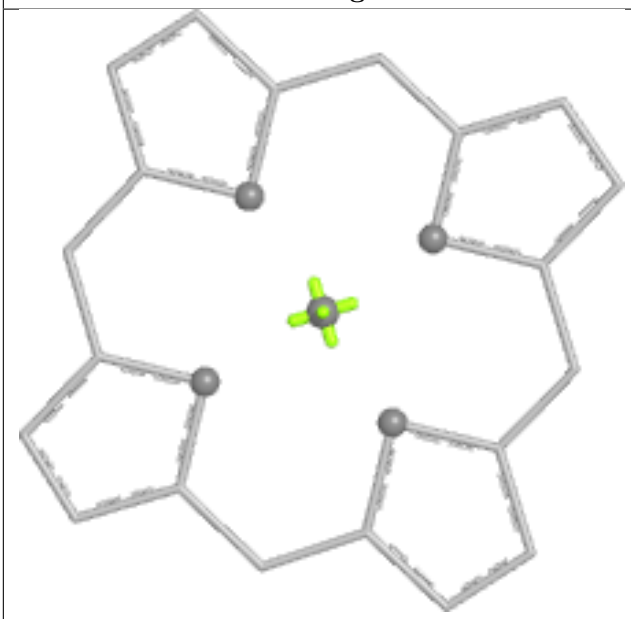
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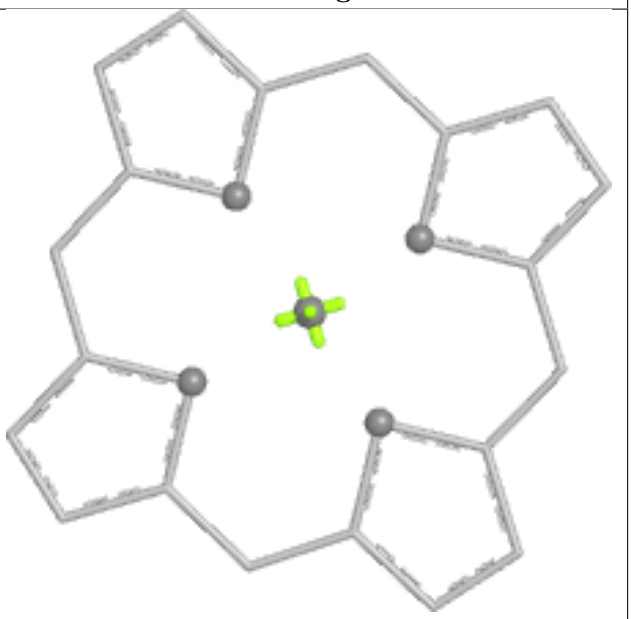
Bond lengths



Bond angles

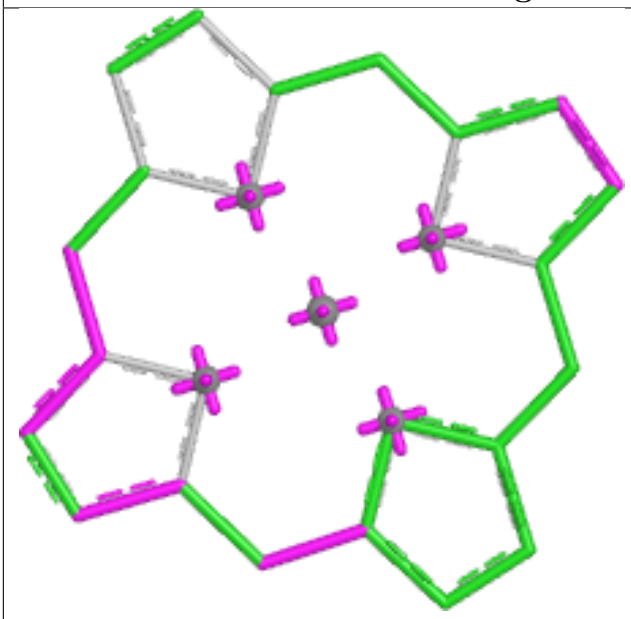


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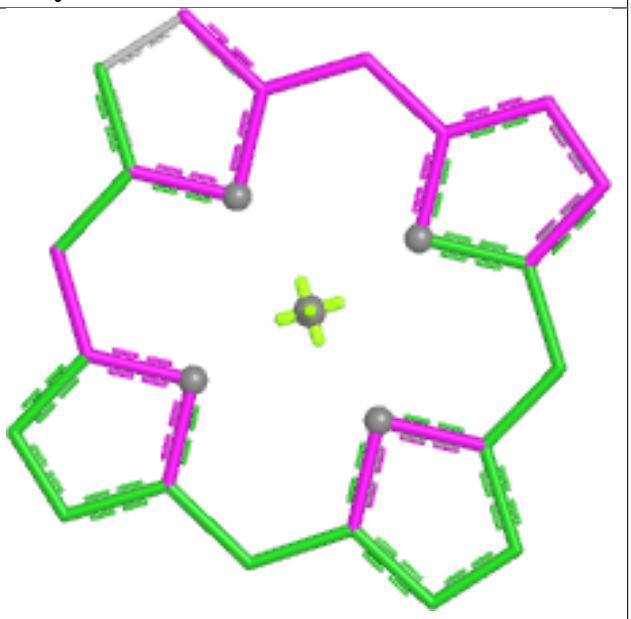


Rings

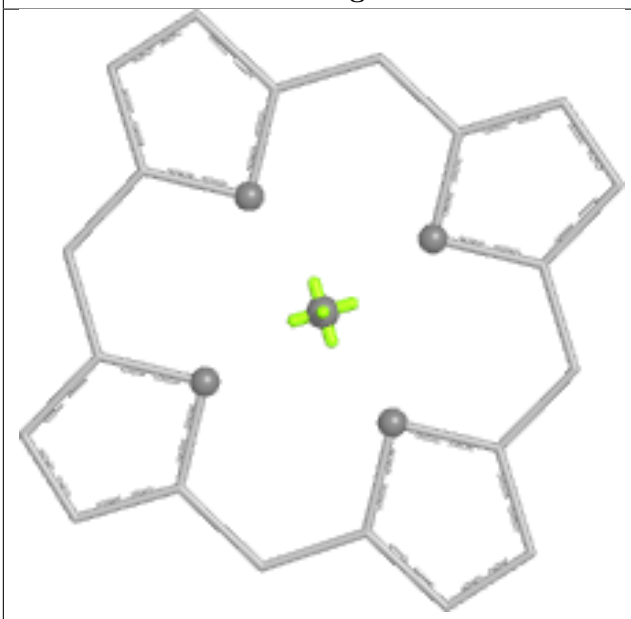
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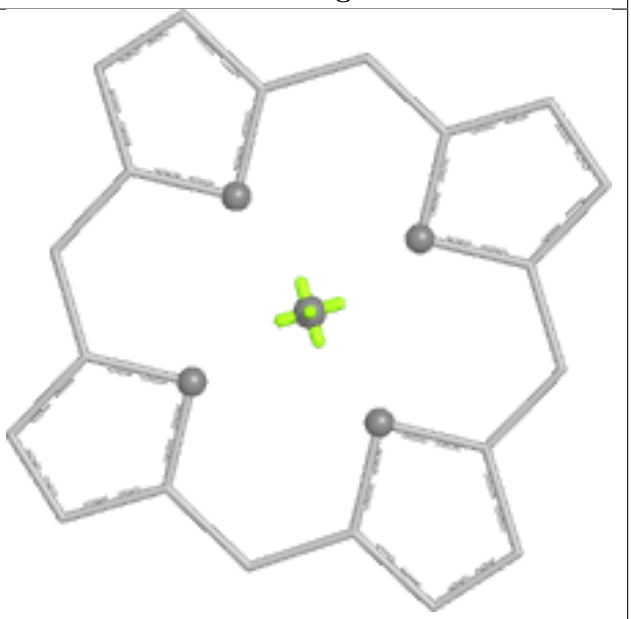
Bond lengths



Bond angles

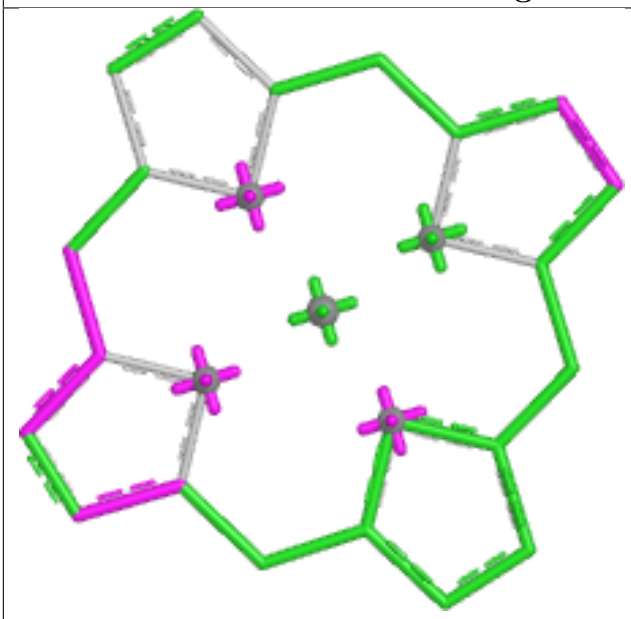


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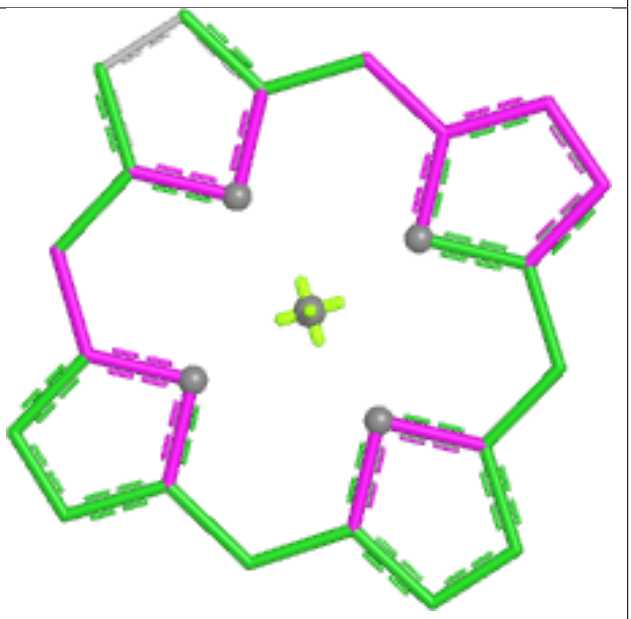


Rings

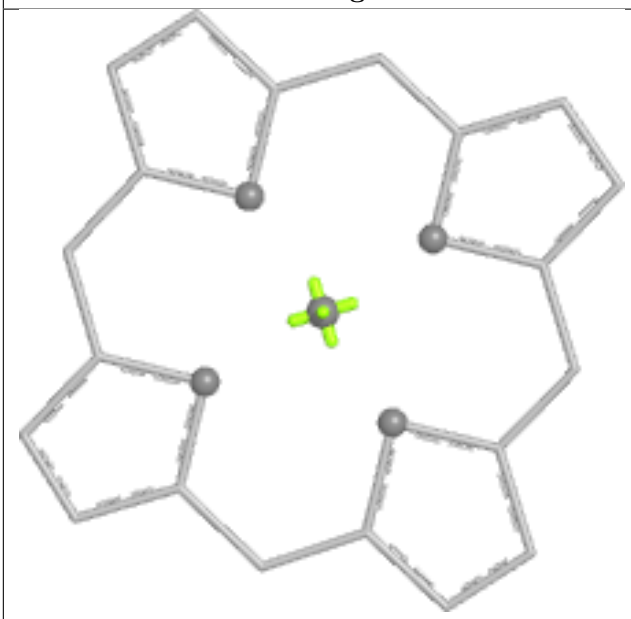
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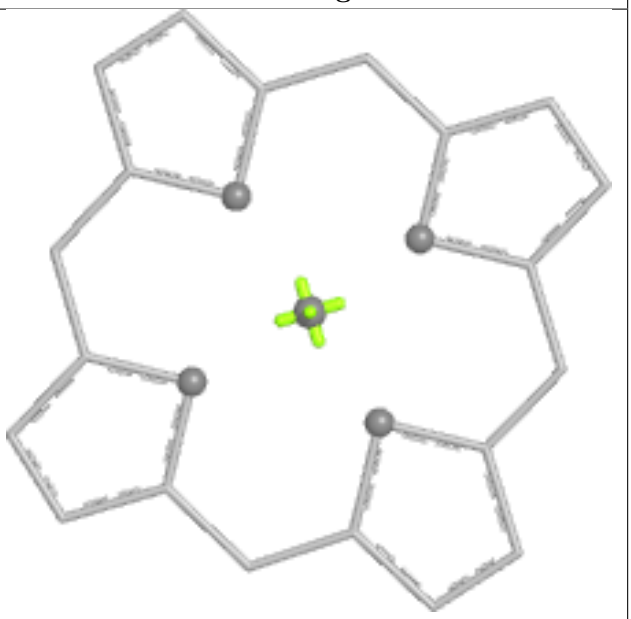
Bond lengths



Bond angles

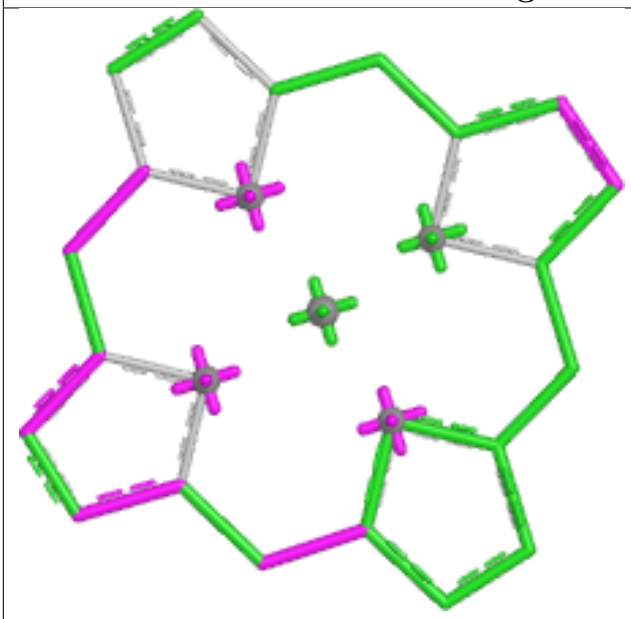


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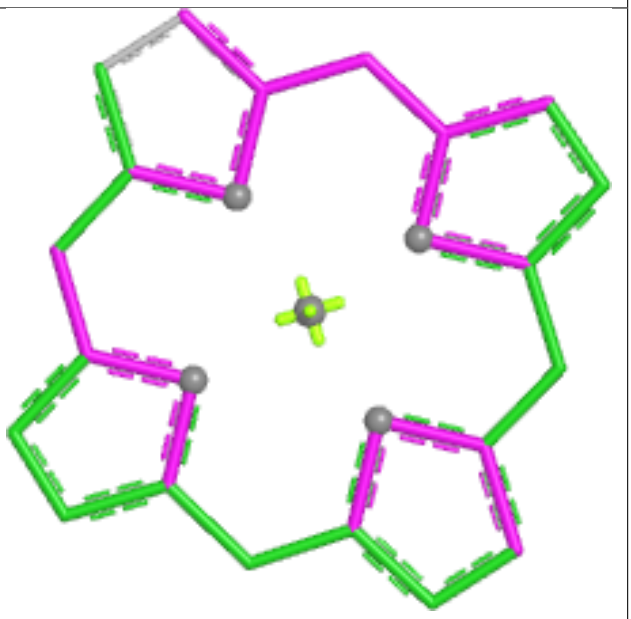


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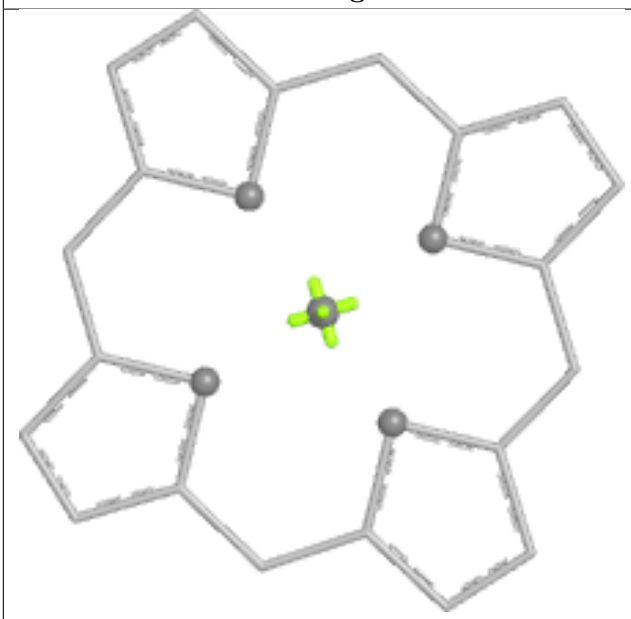
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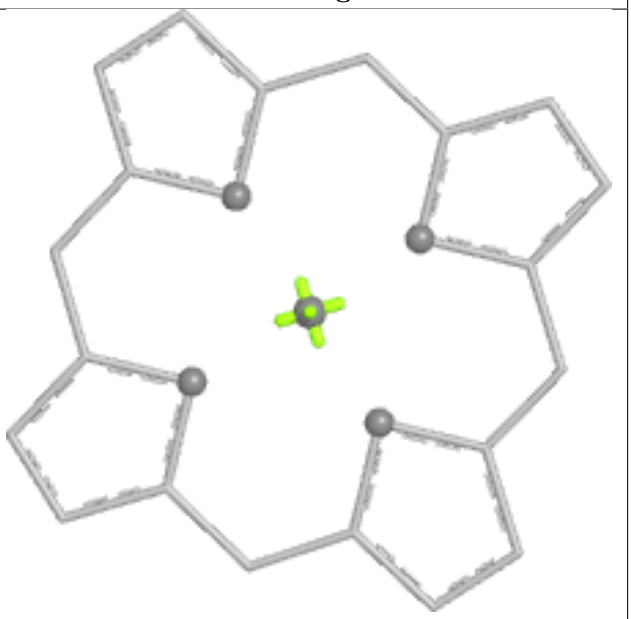
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Bond angles

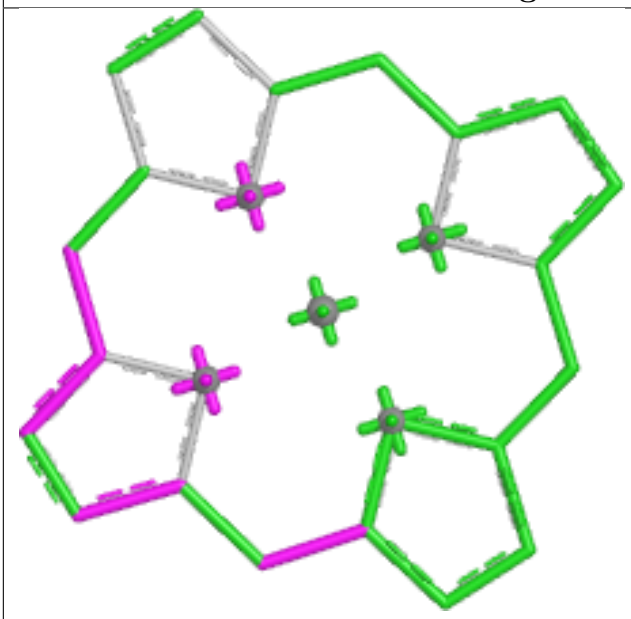


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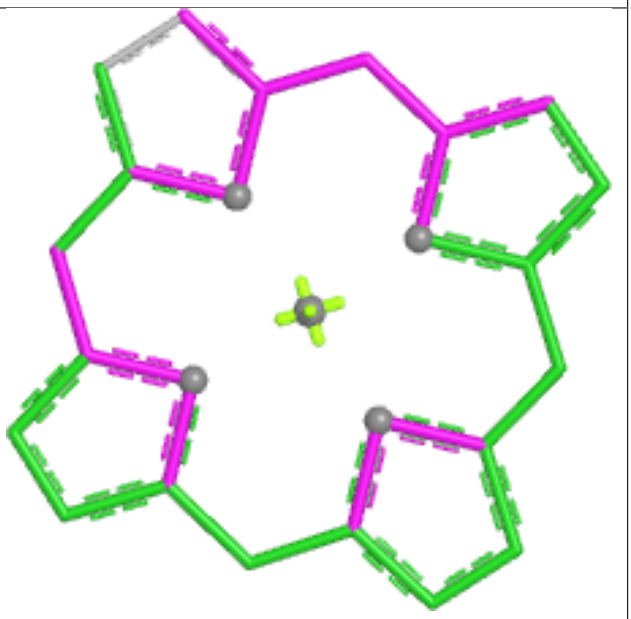


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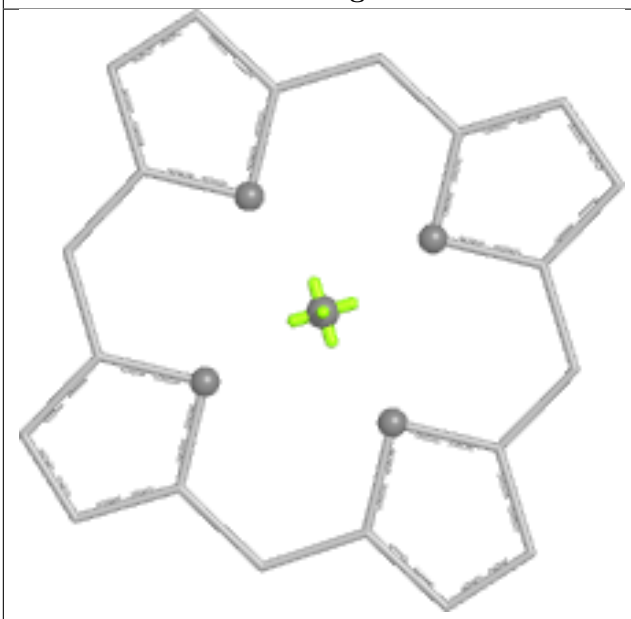
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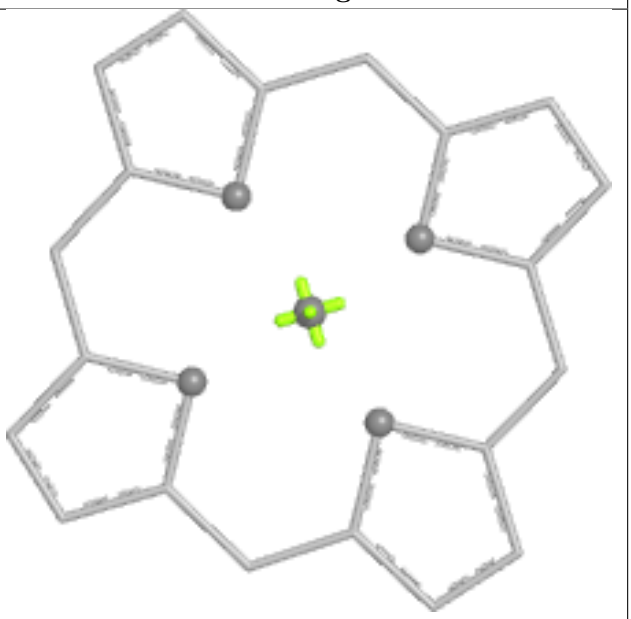
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Bond angles

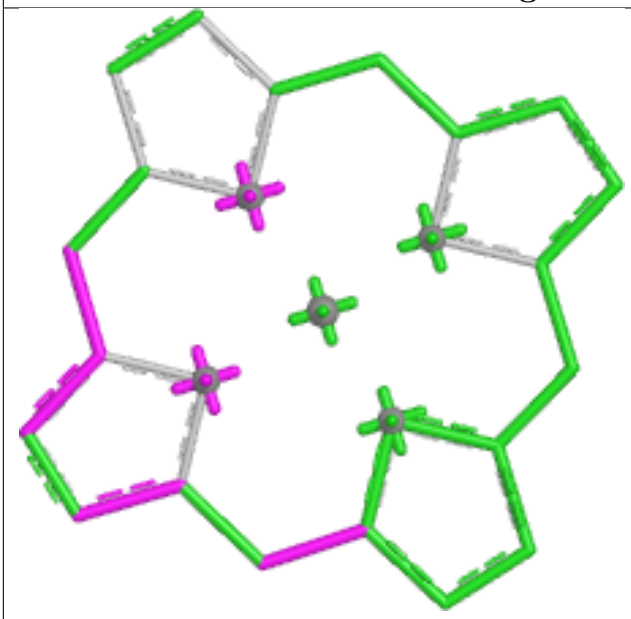


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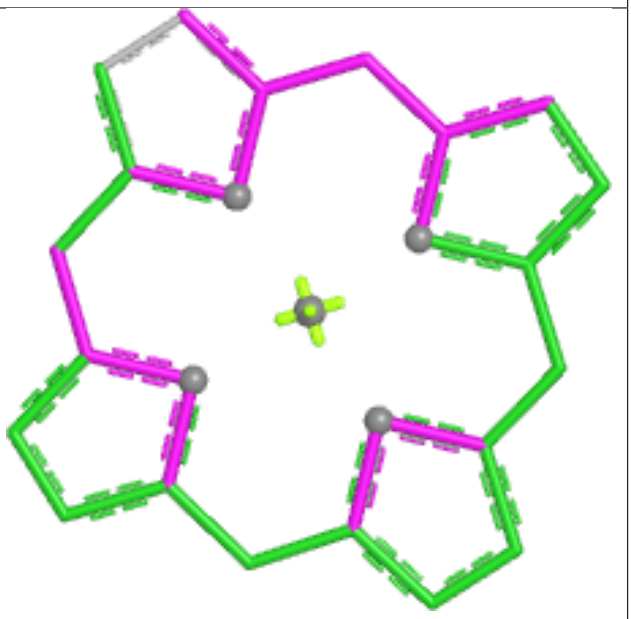


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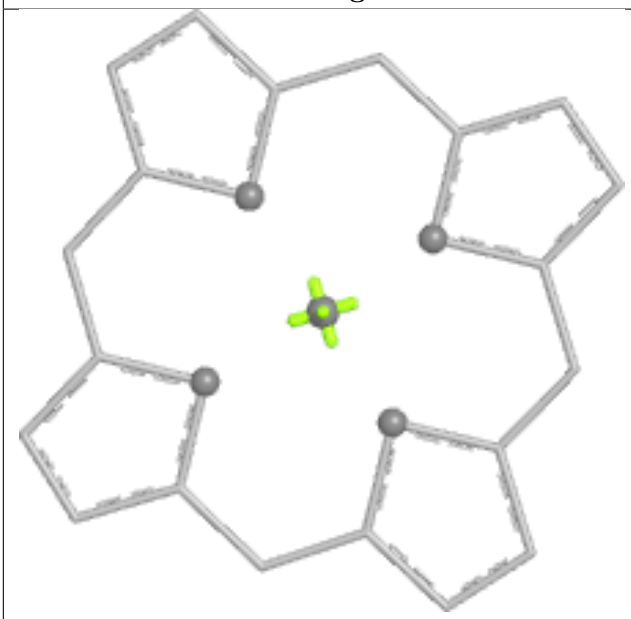
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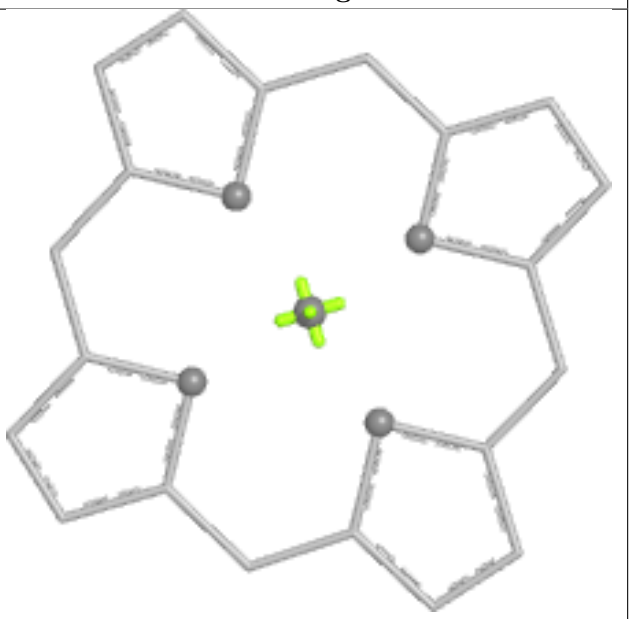
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Bond angles

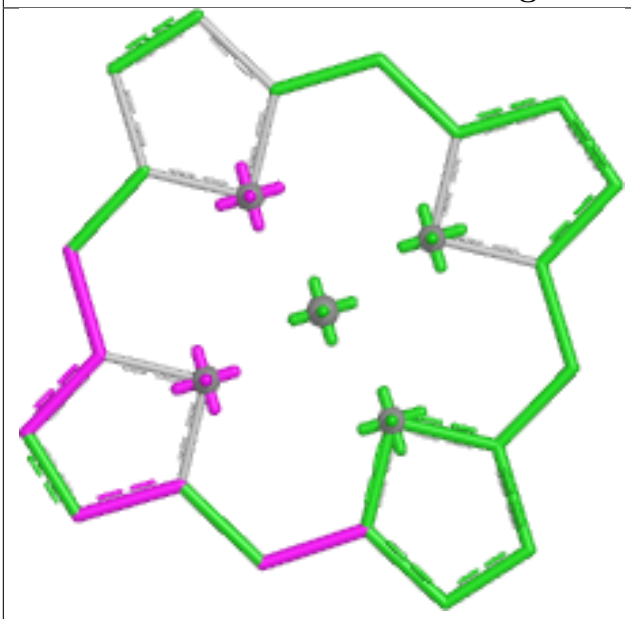


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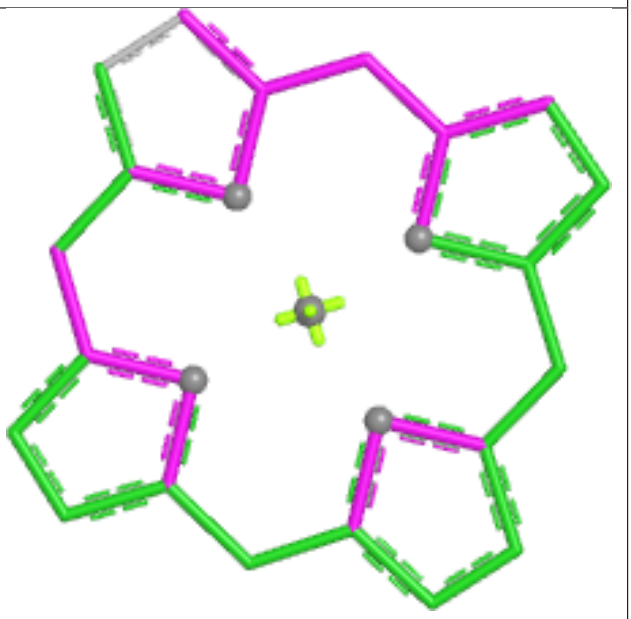


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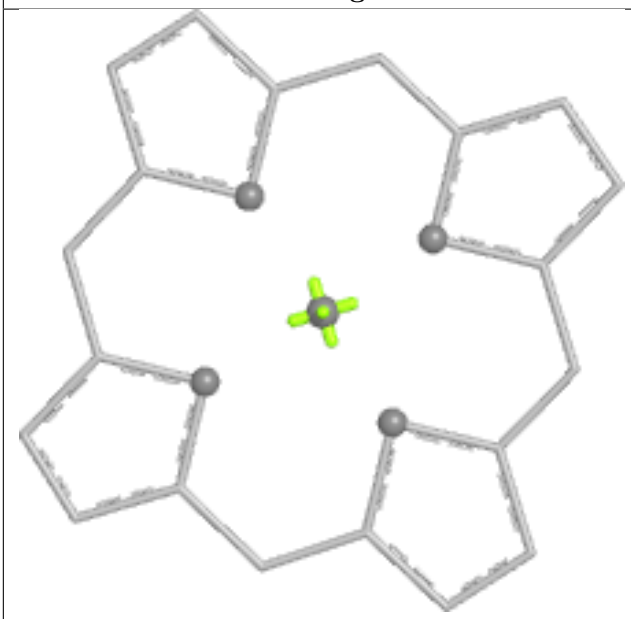
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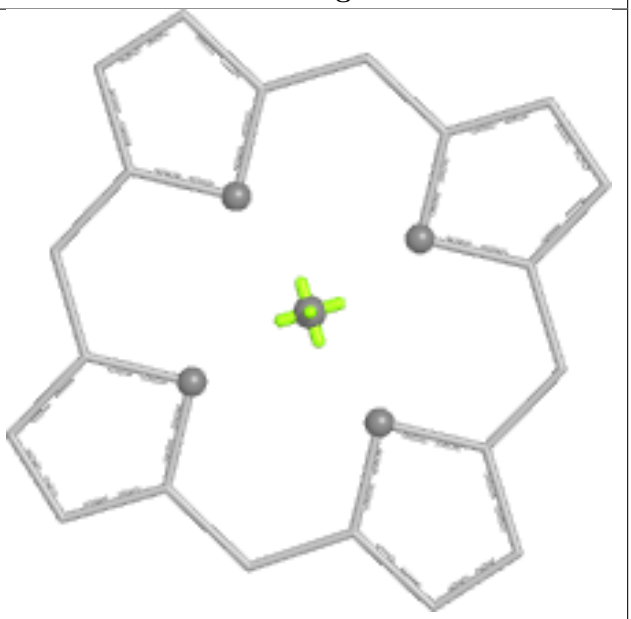
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Bond angles

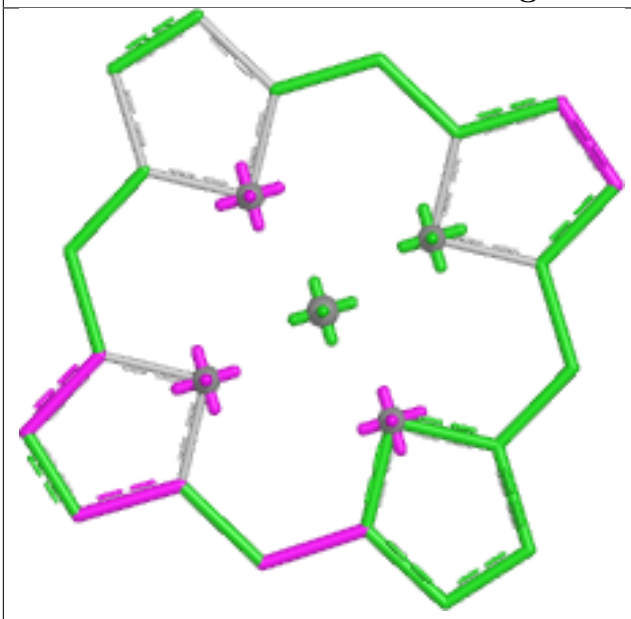


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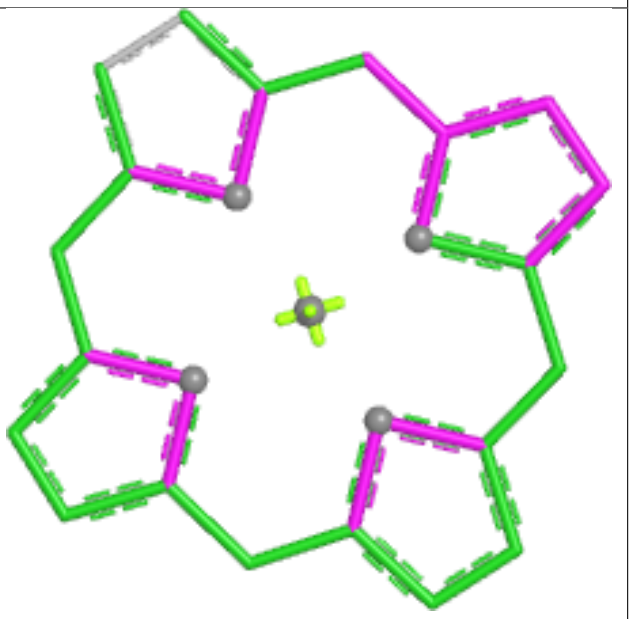


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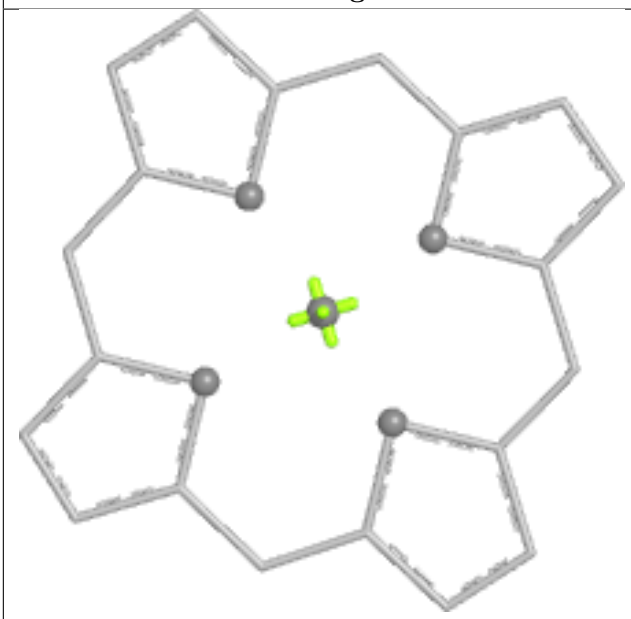
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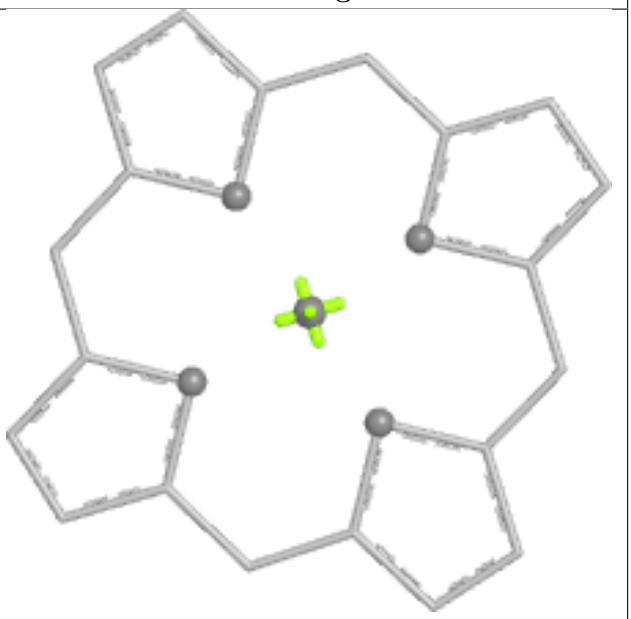
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Bond angles

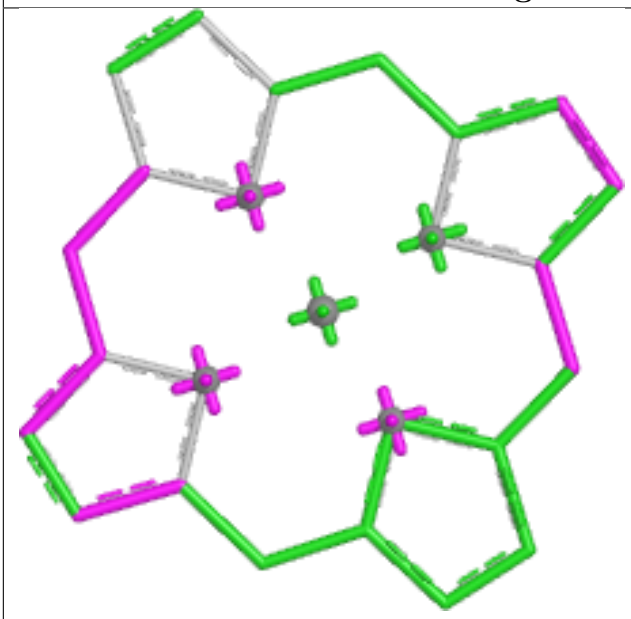


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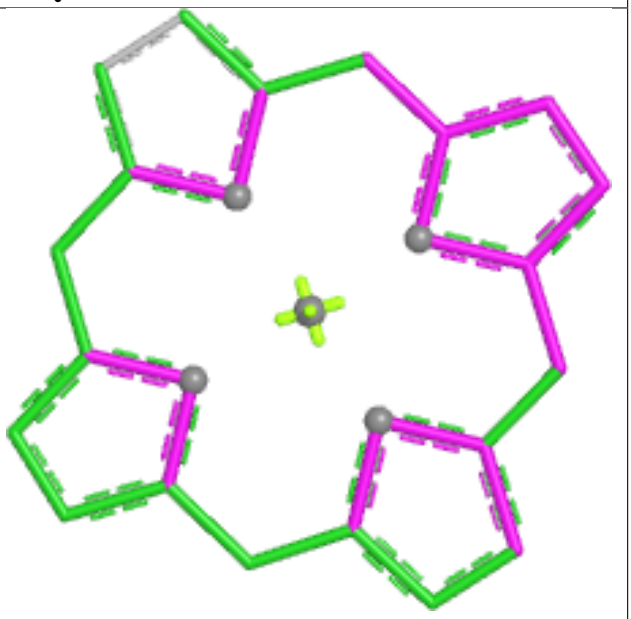


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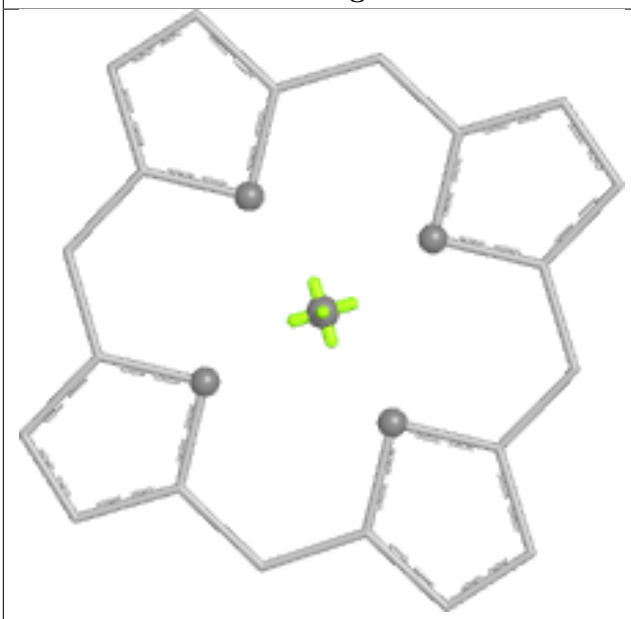
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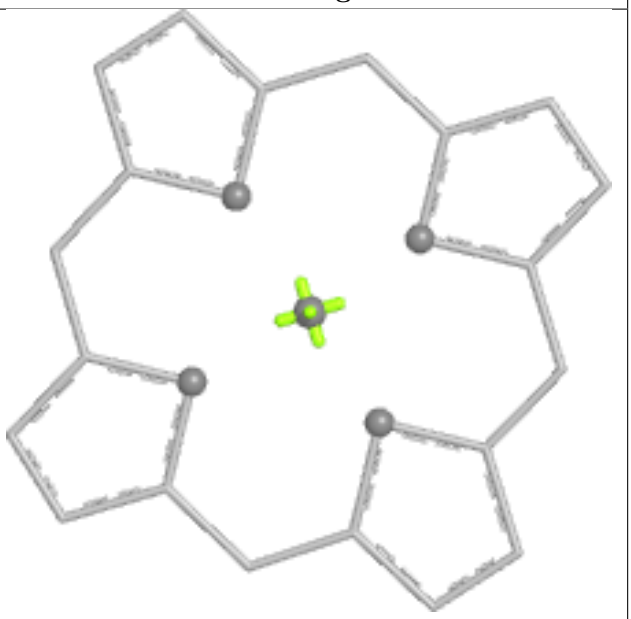
Bond lengths



Bond angles

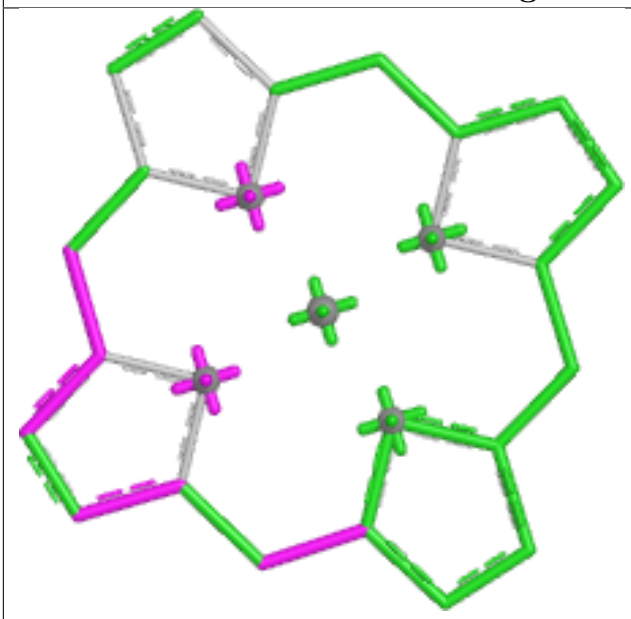


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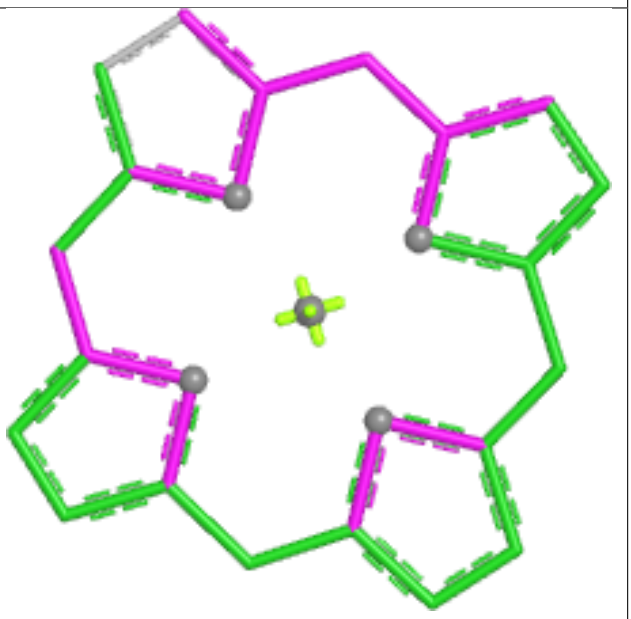


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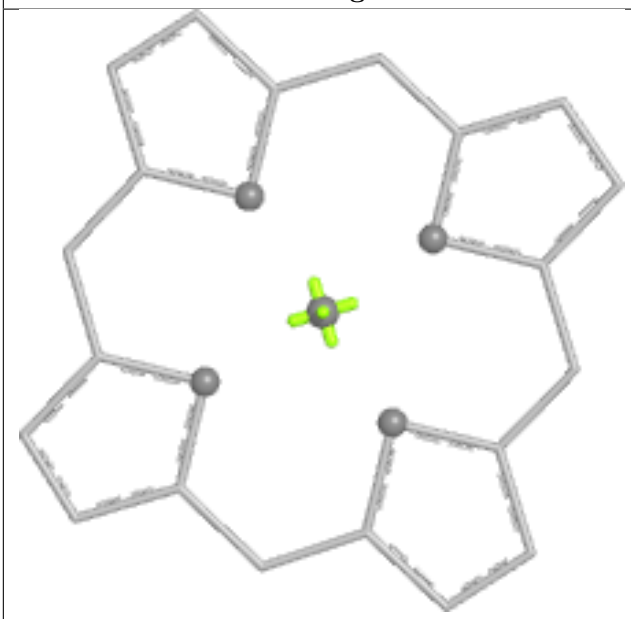
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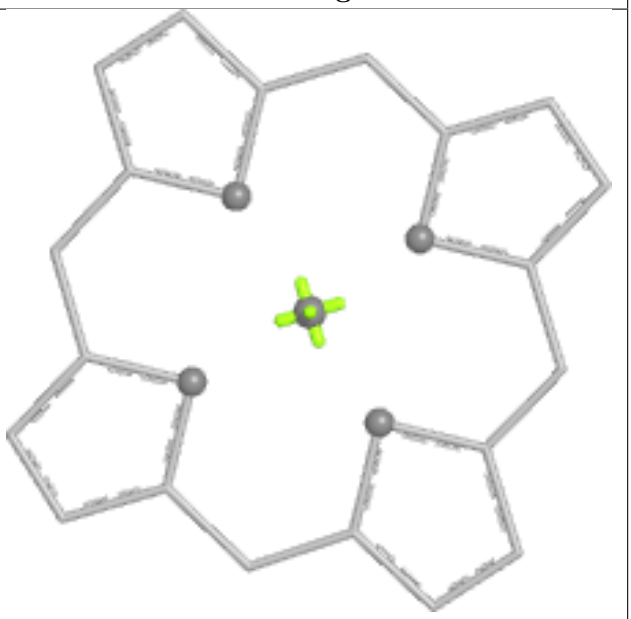
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Bond angles

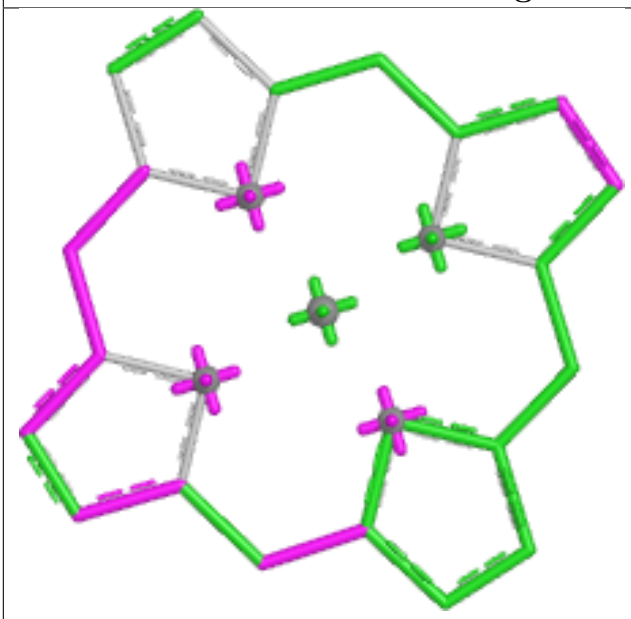


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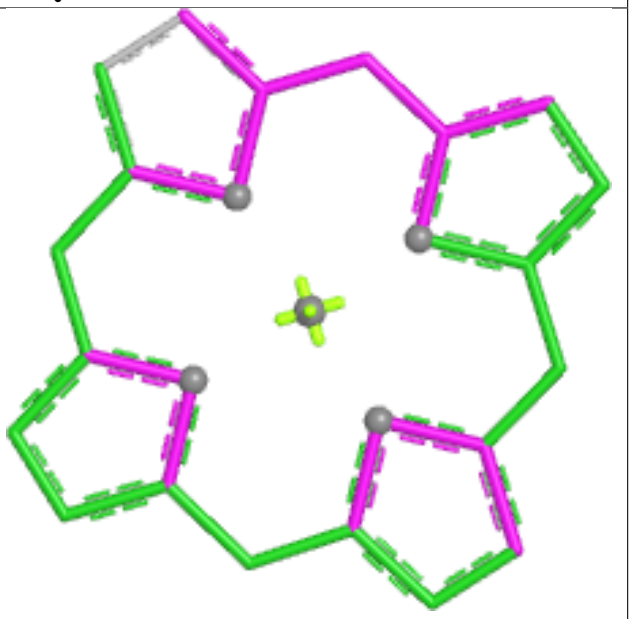


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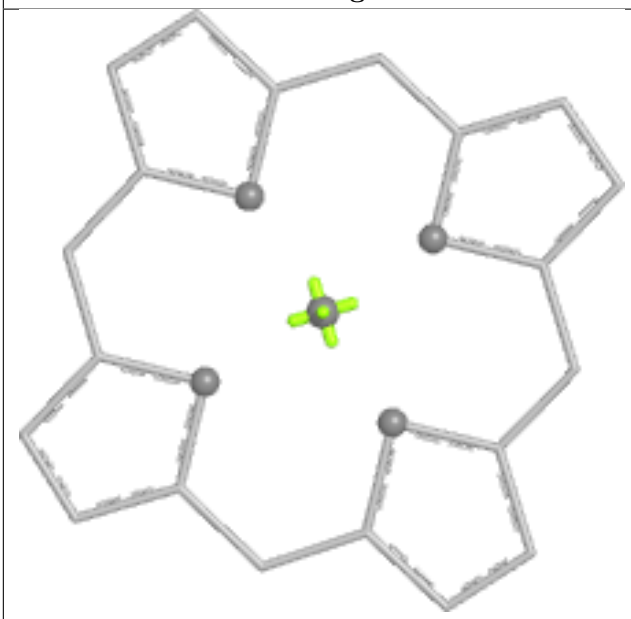
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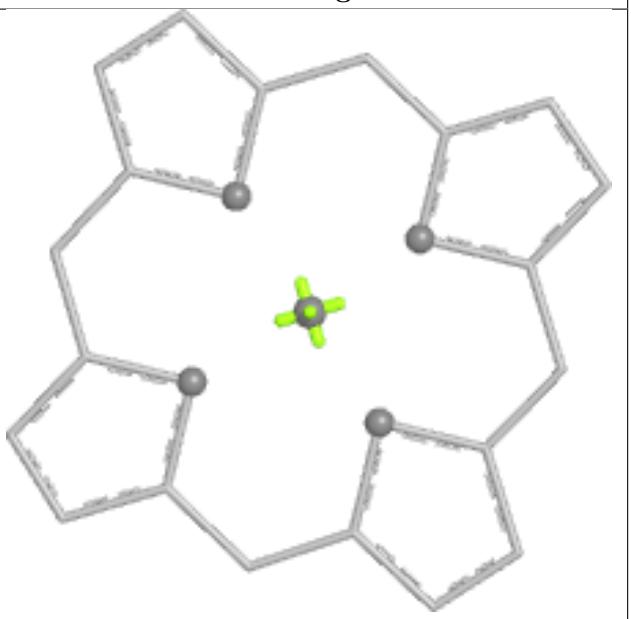
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Bond angles

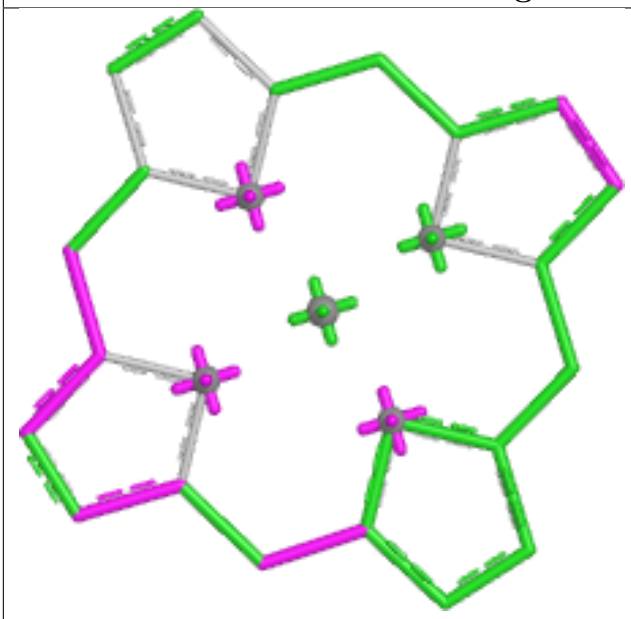


Torsions

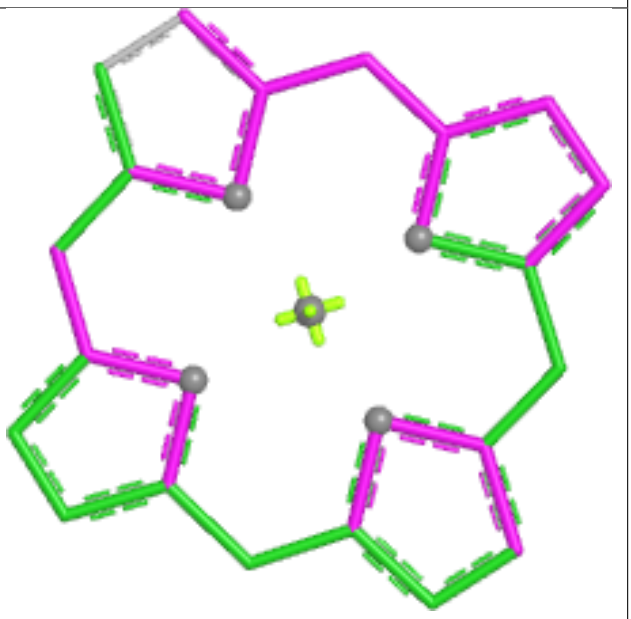


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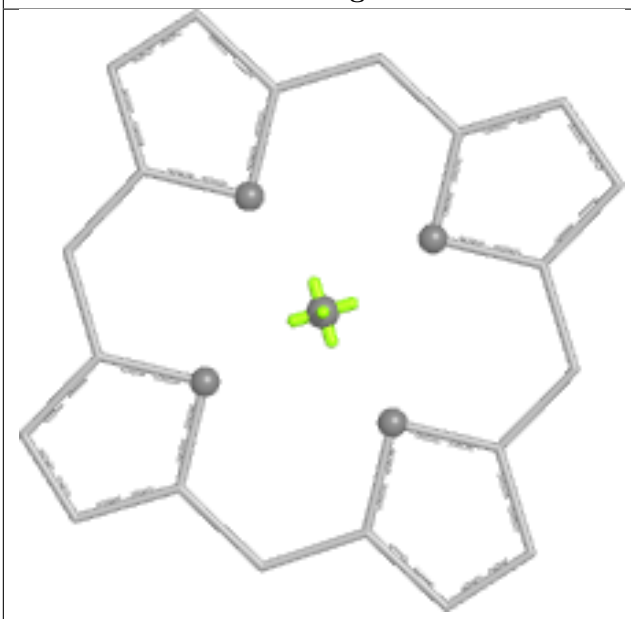
Ligand CLA A 1129



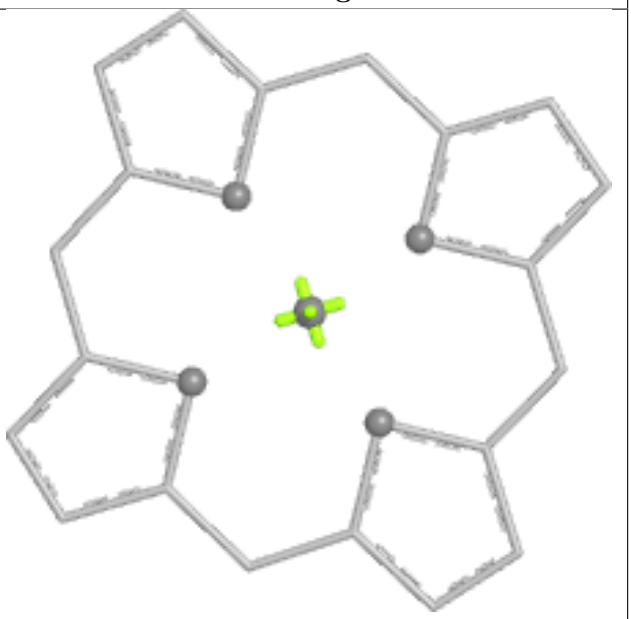
Bond lengths



Bond angles

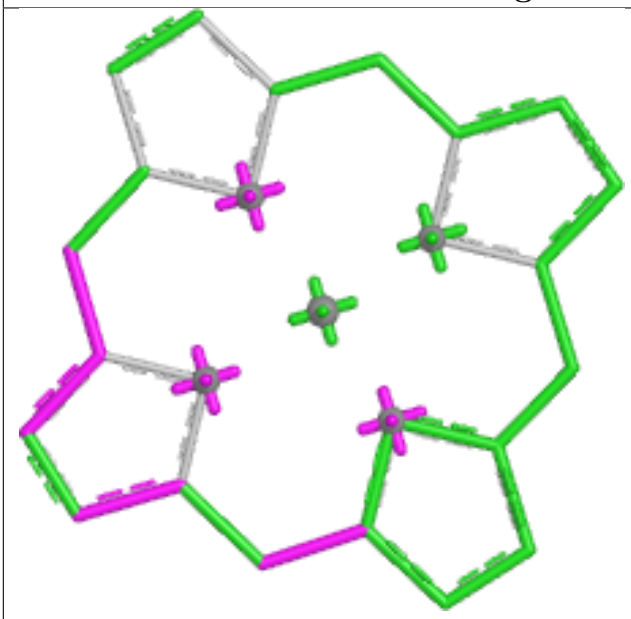


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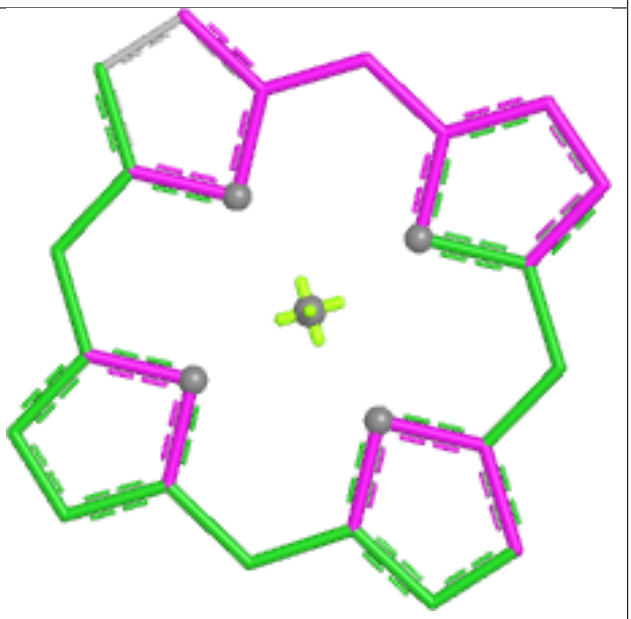


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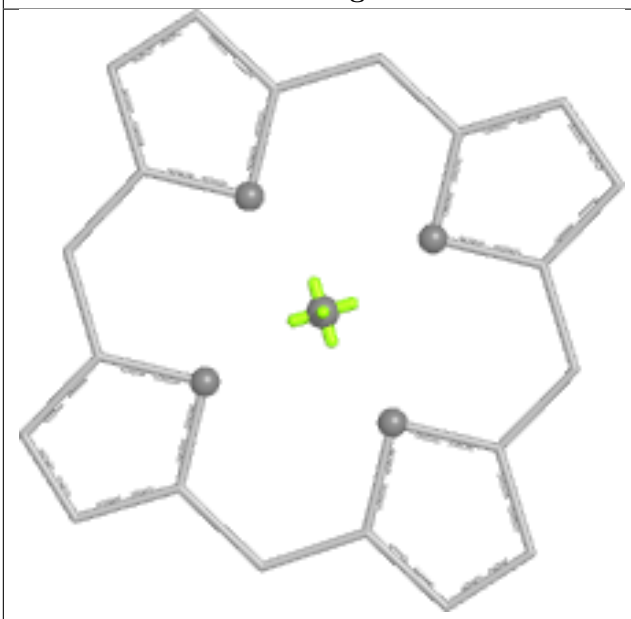
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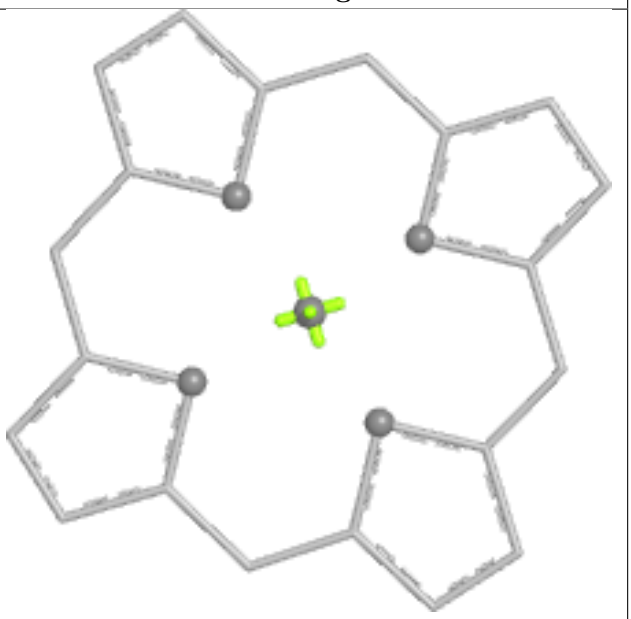
Bond lengths



Bond angles

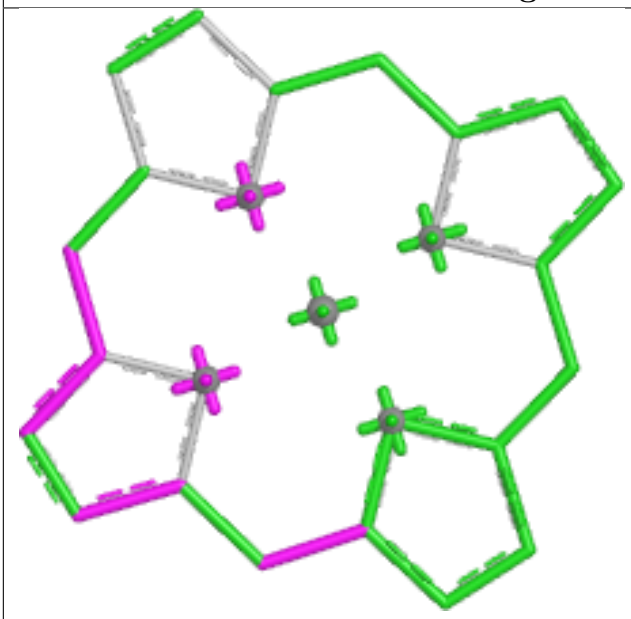


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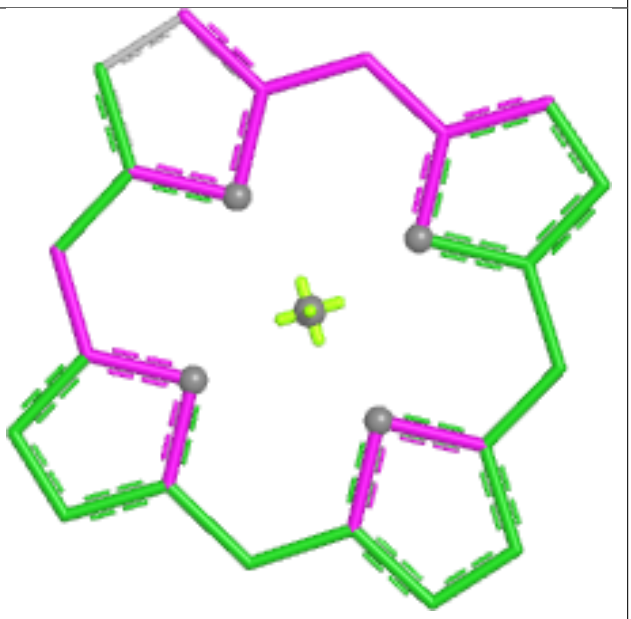


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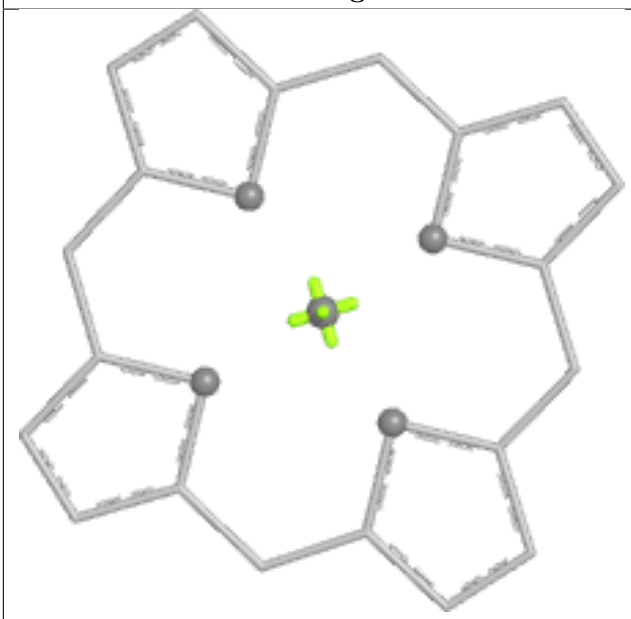
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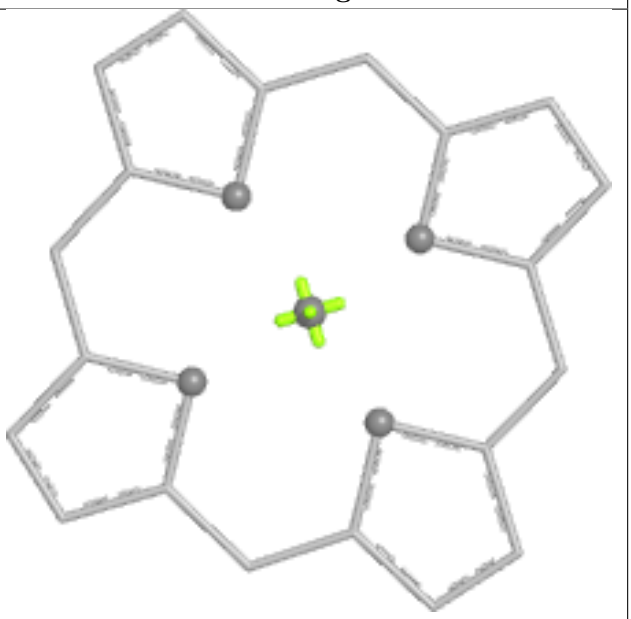
Bond lengths



Bond angles

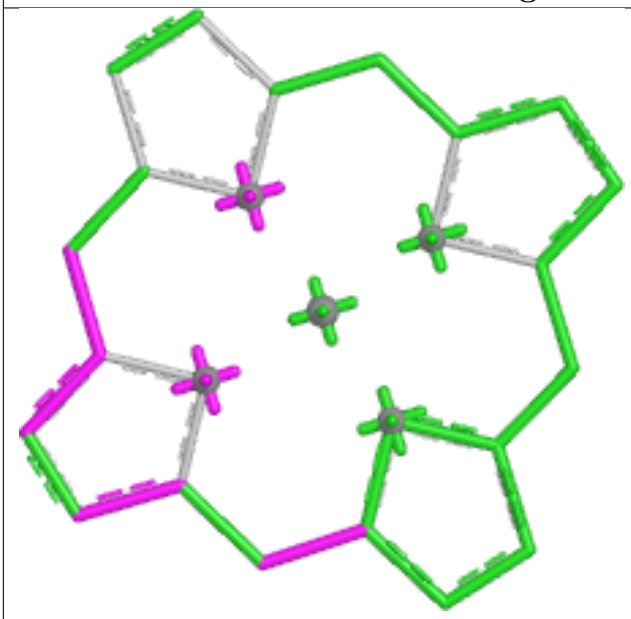


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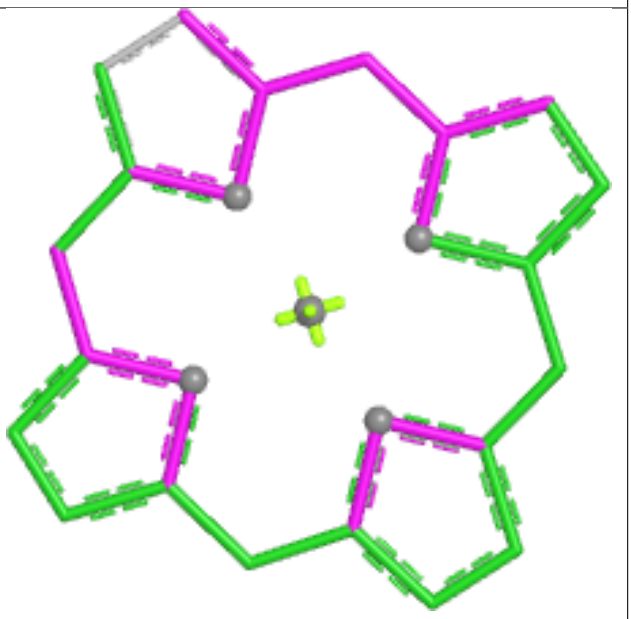


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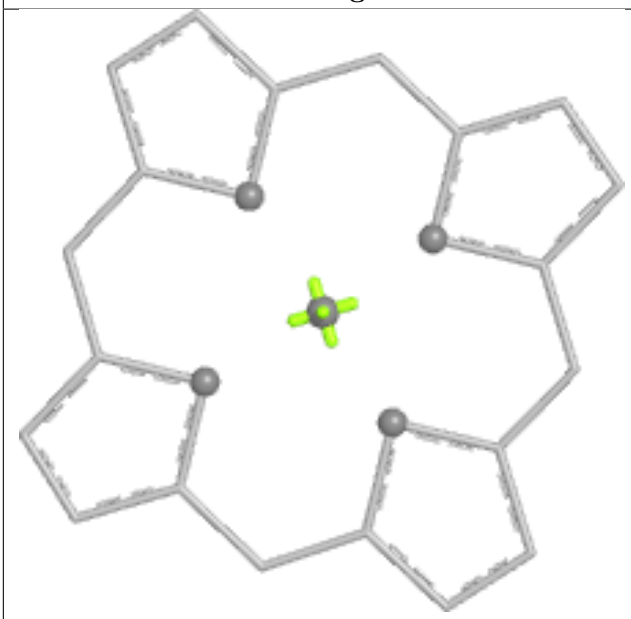
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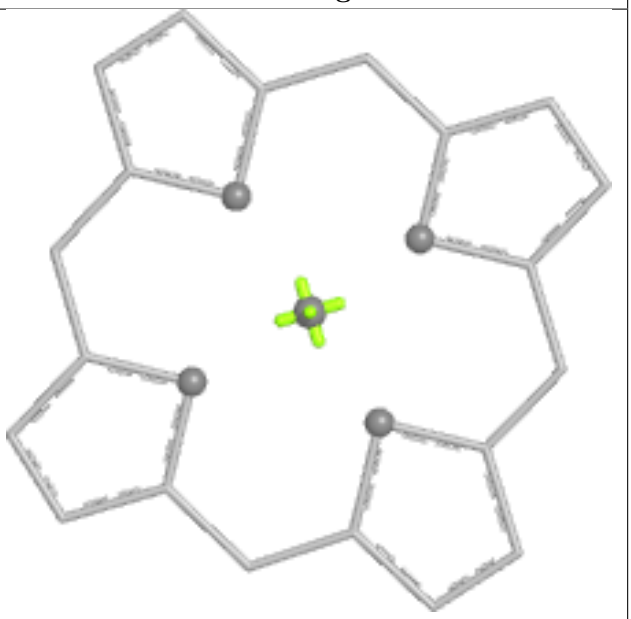
Bond lengths



Bond angles

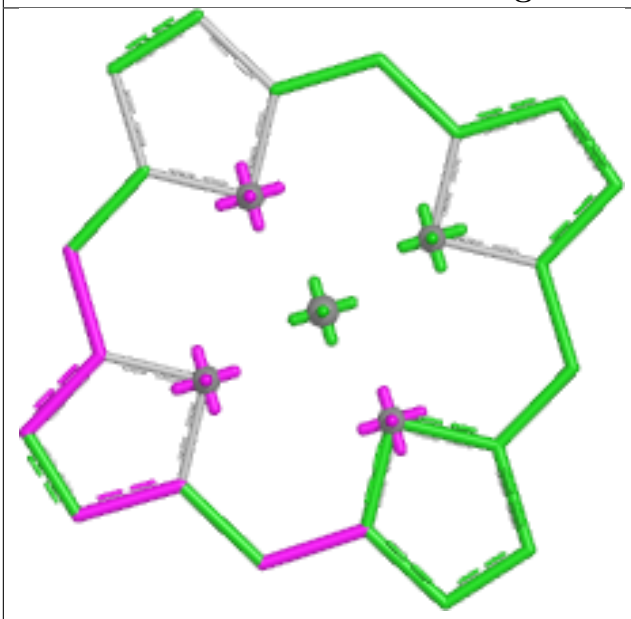


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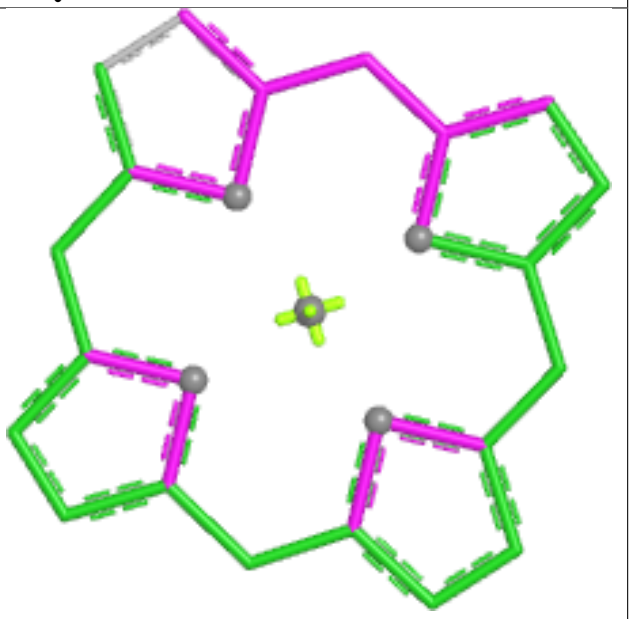


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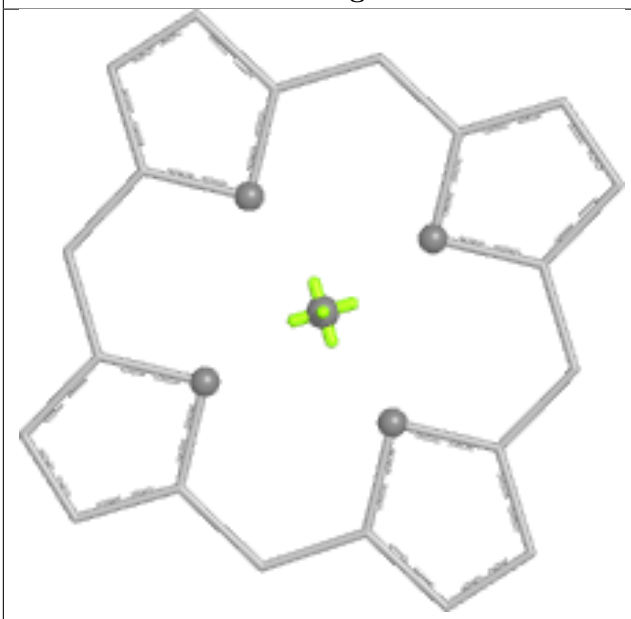
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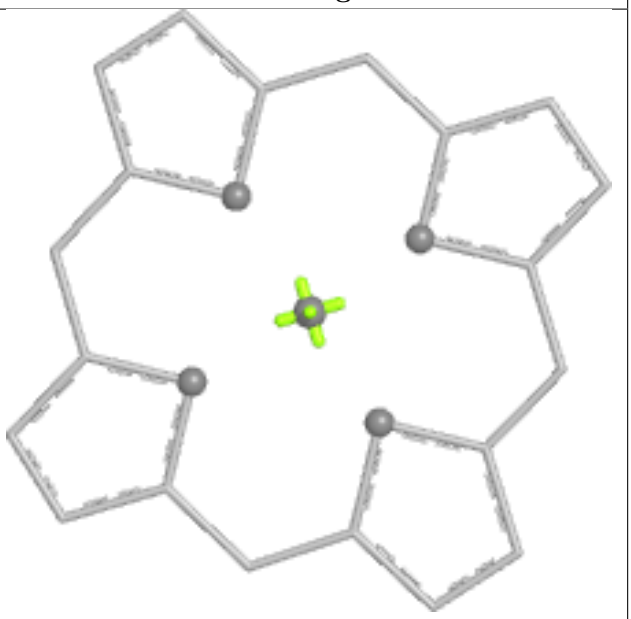
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Bond angles

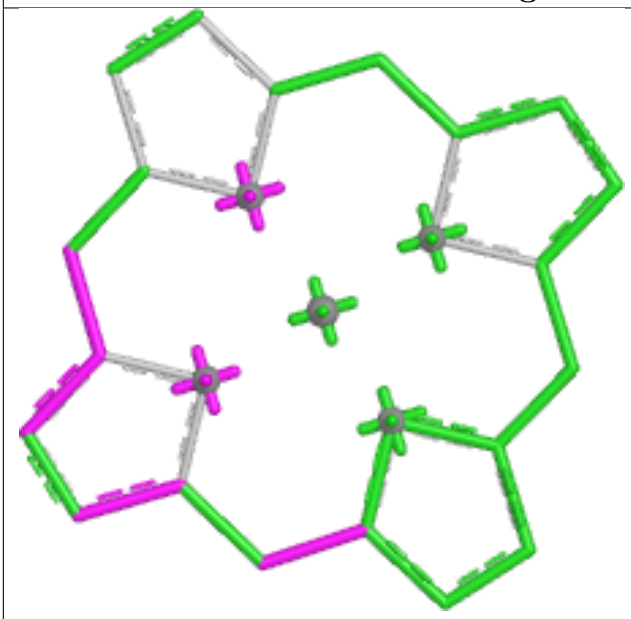


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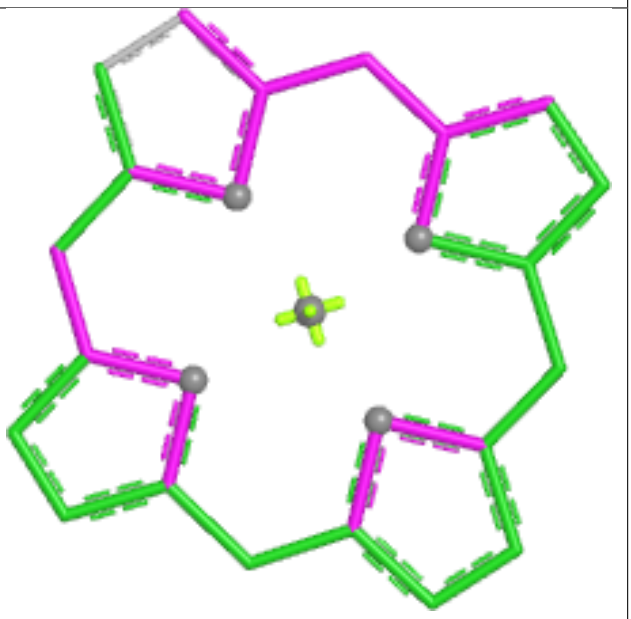


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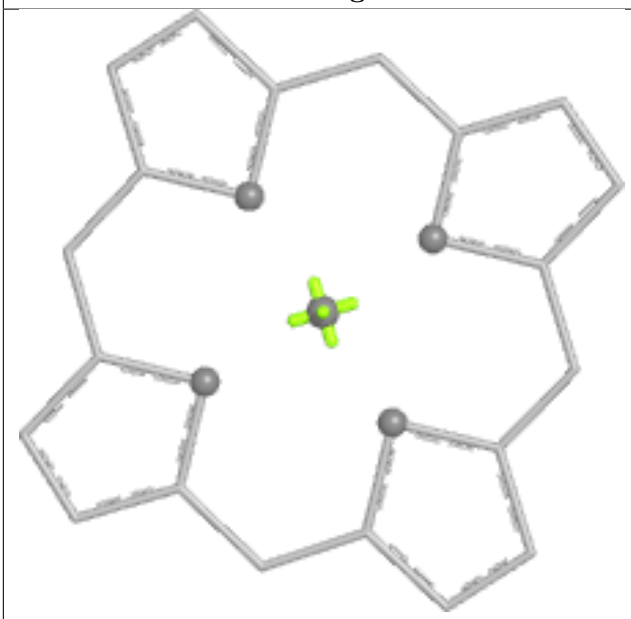
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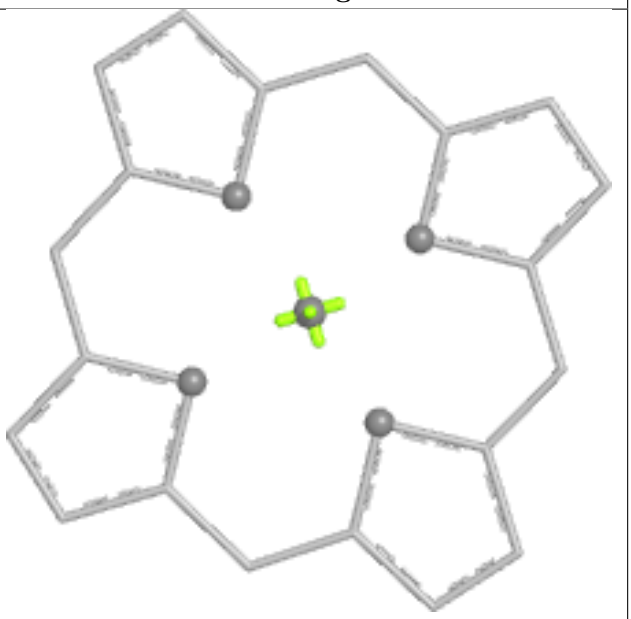
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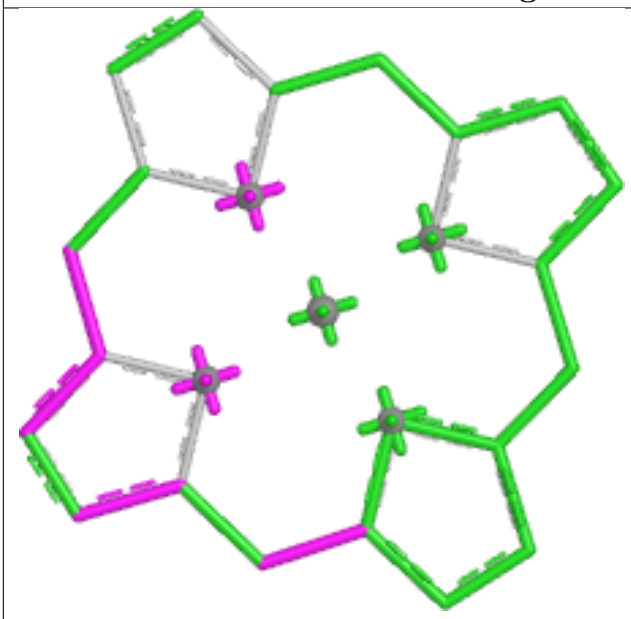


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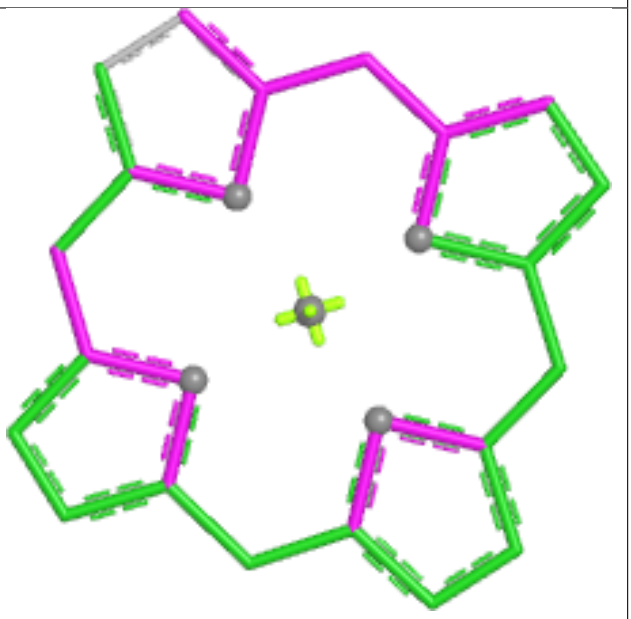


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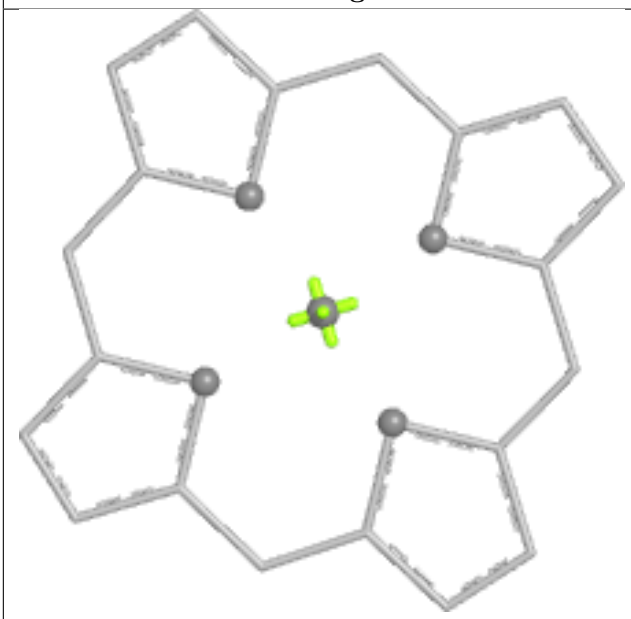
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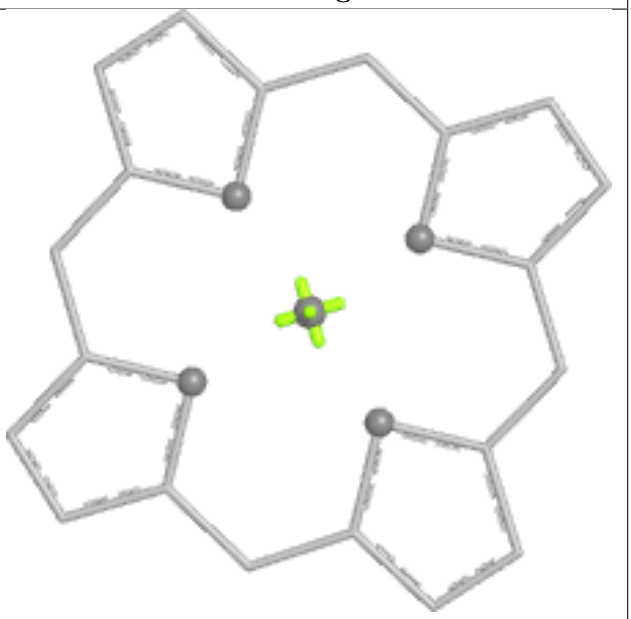
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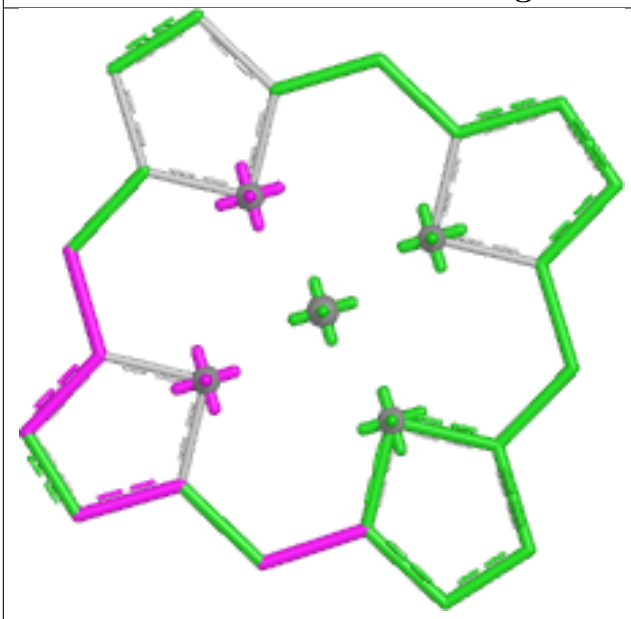


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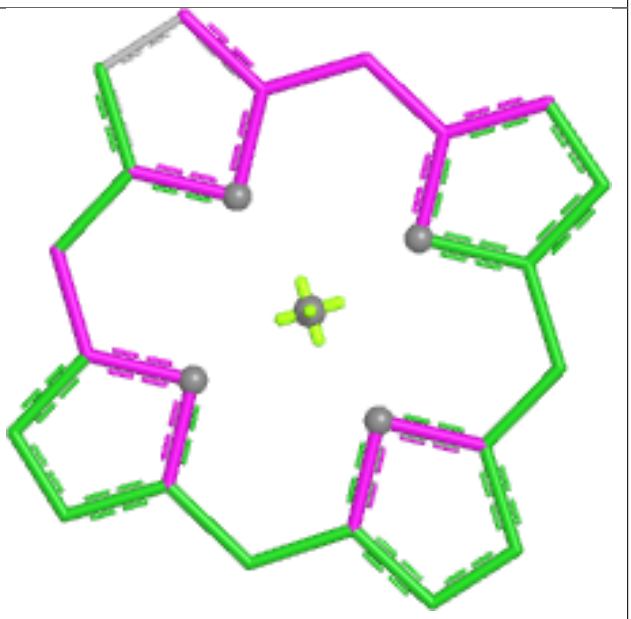


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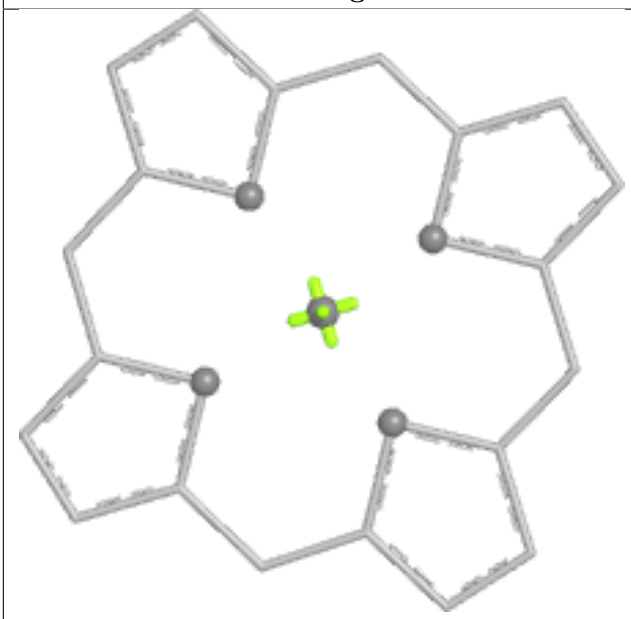
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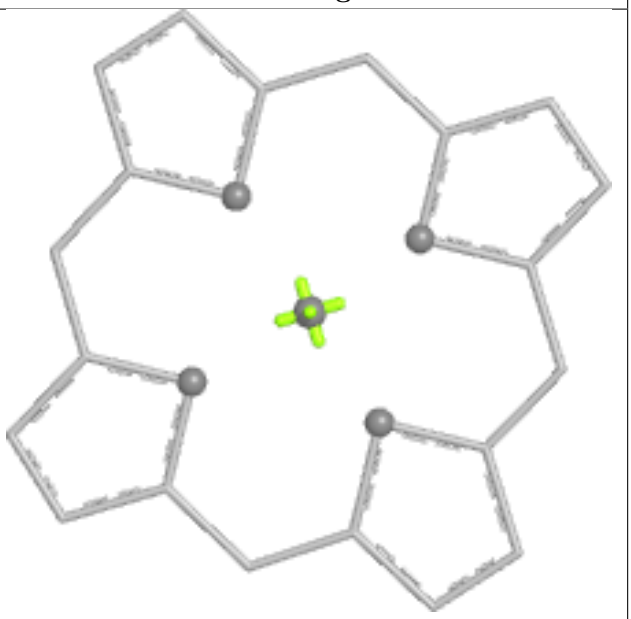
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Bond angles

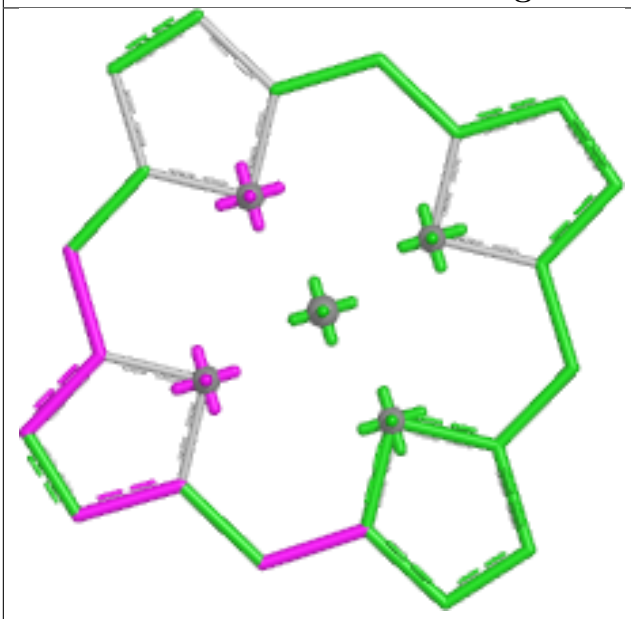


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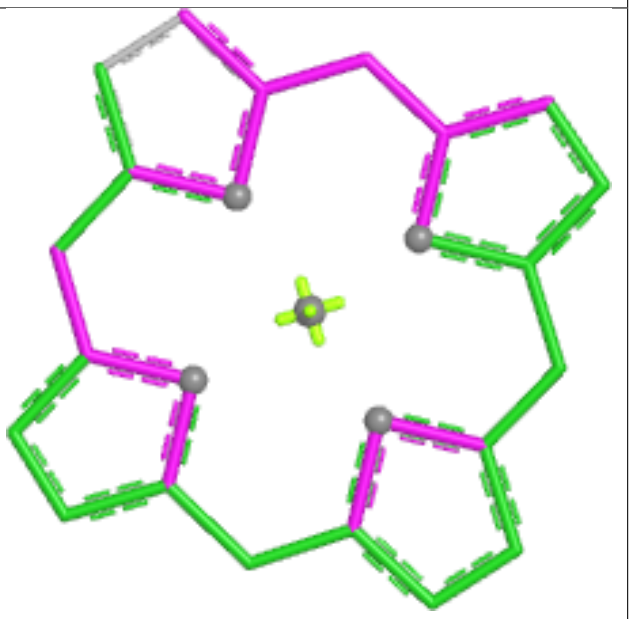


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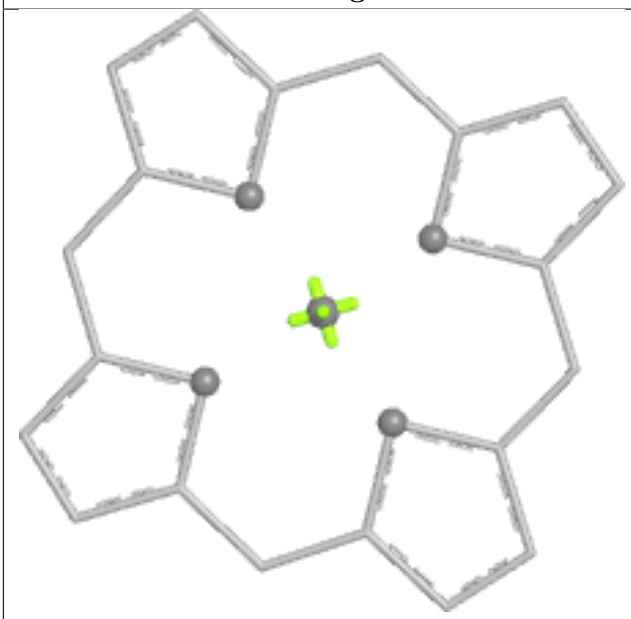
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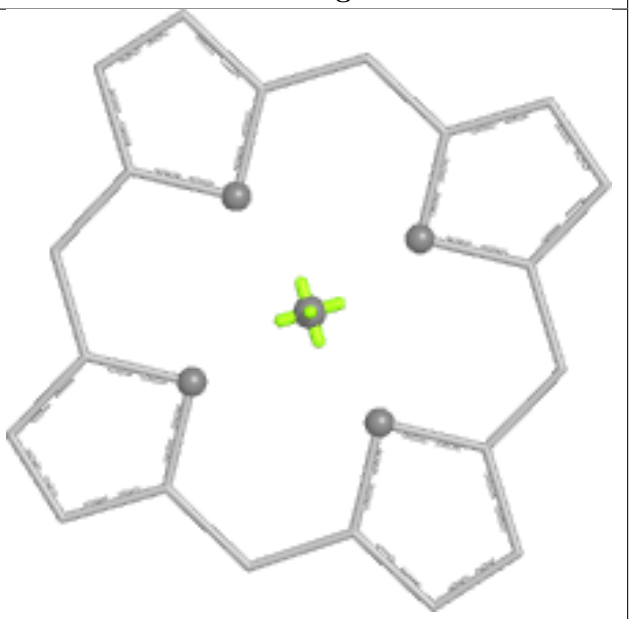
Bond lengths



Bond angles

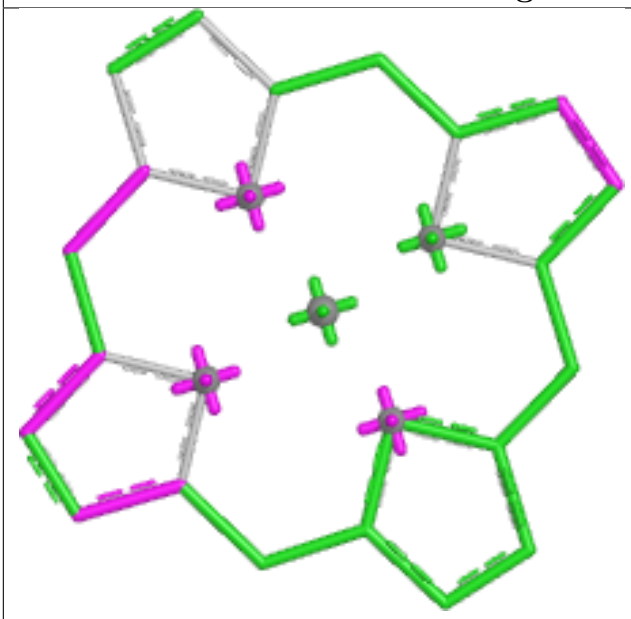


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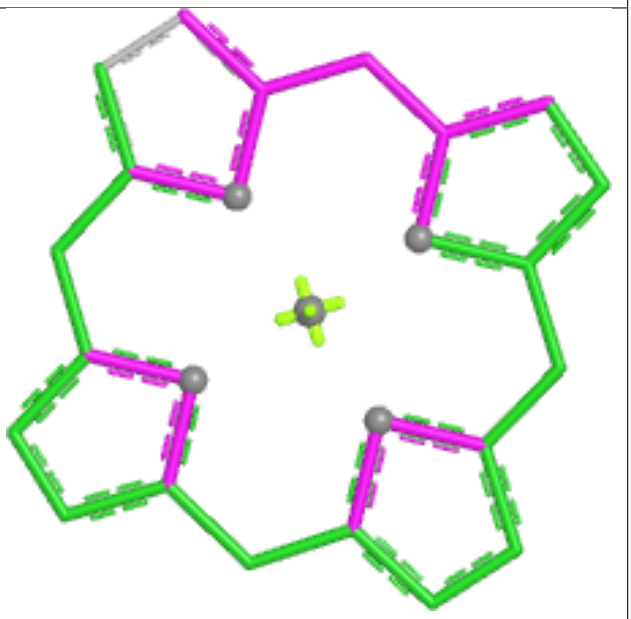


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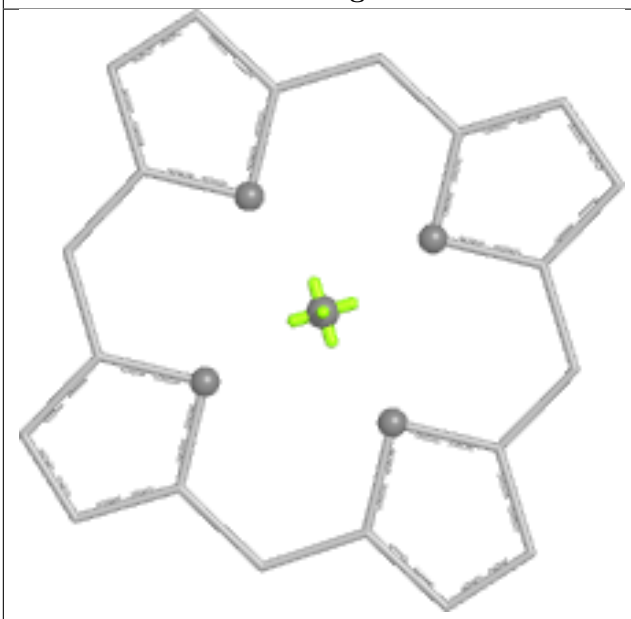
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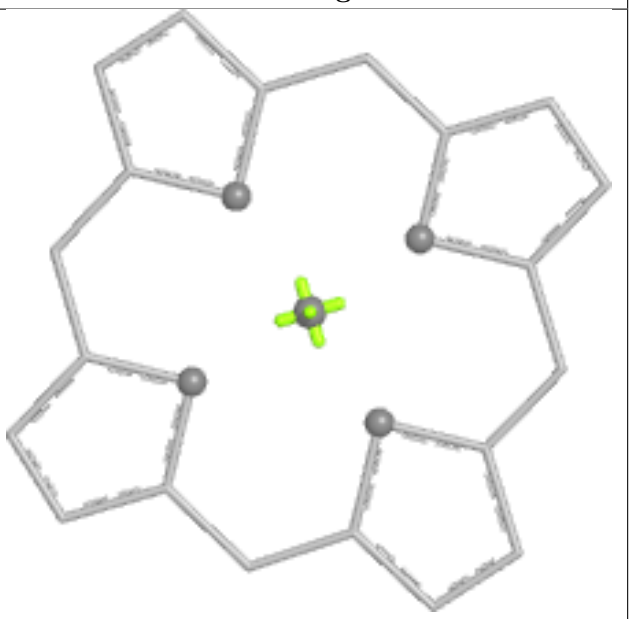
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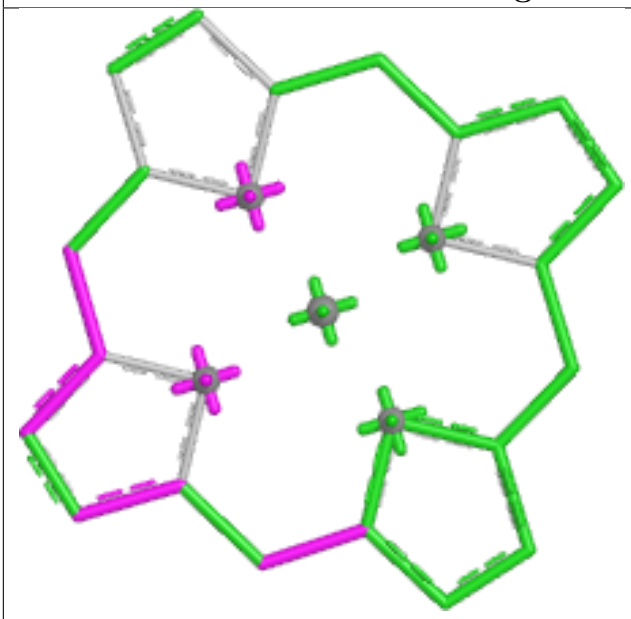


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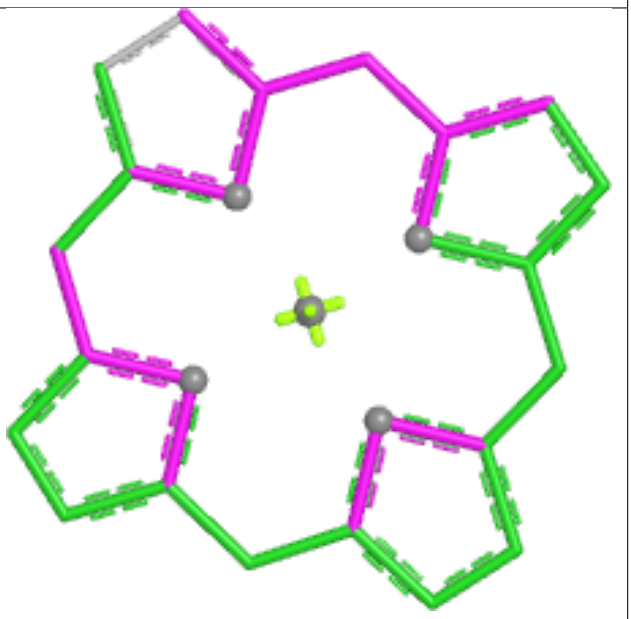


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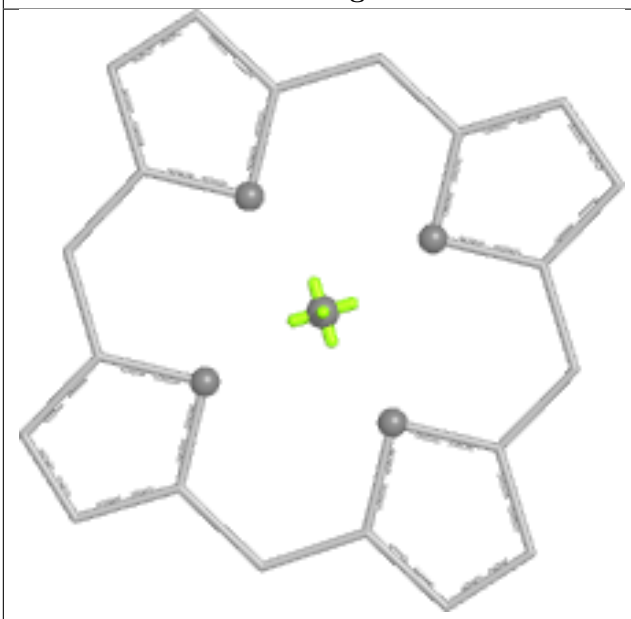
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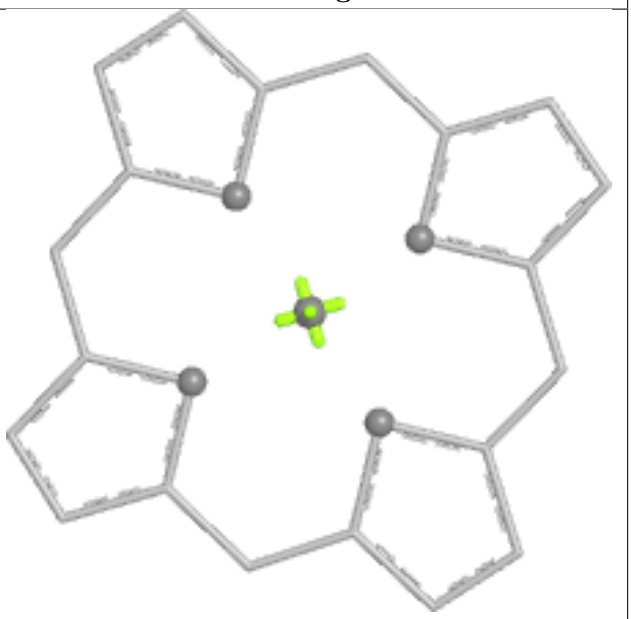
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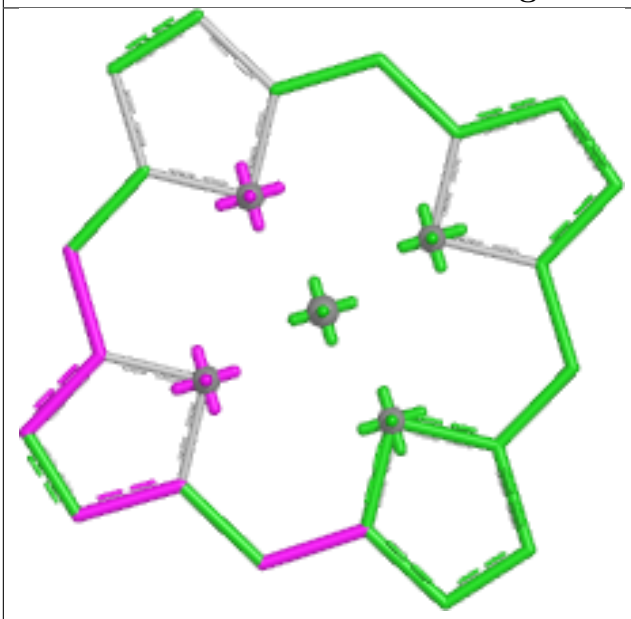


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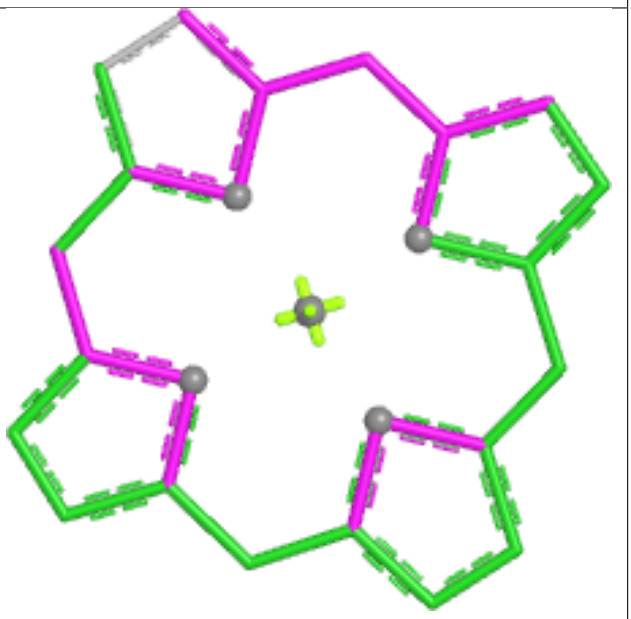


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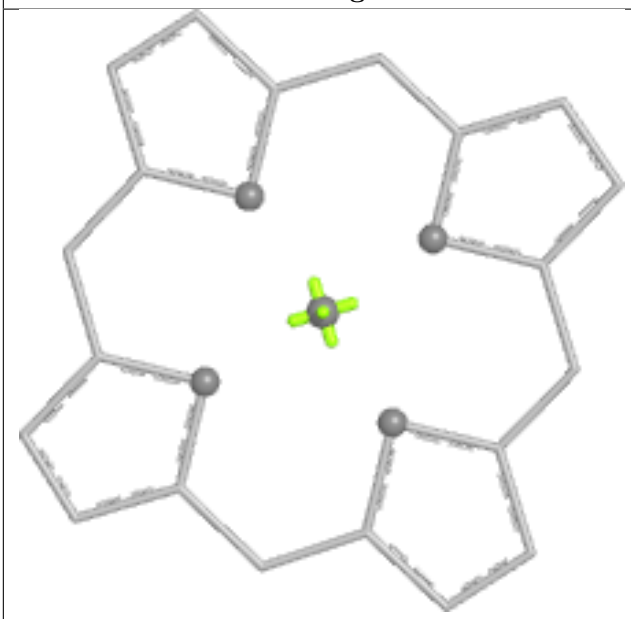
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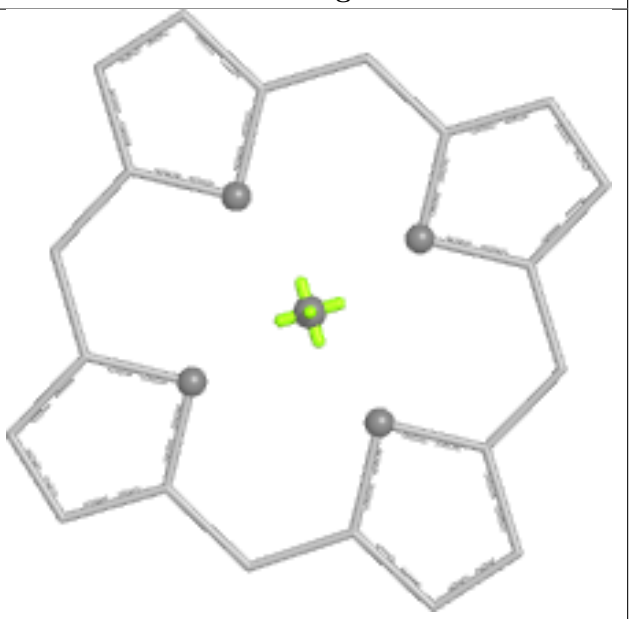
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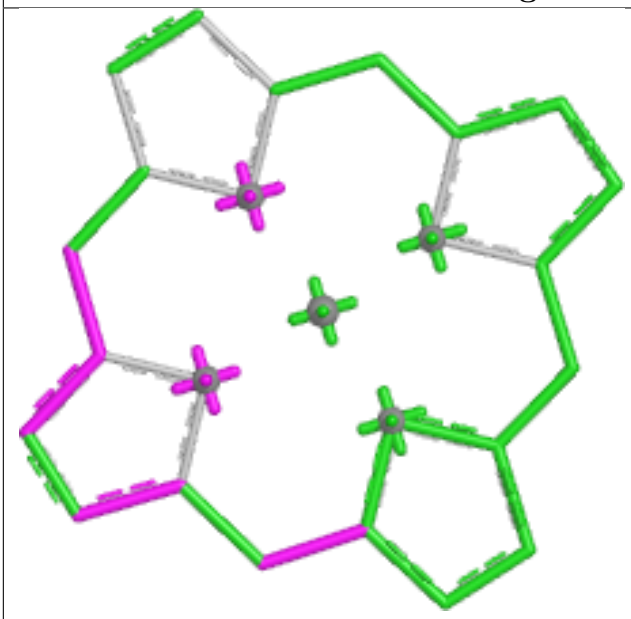


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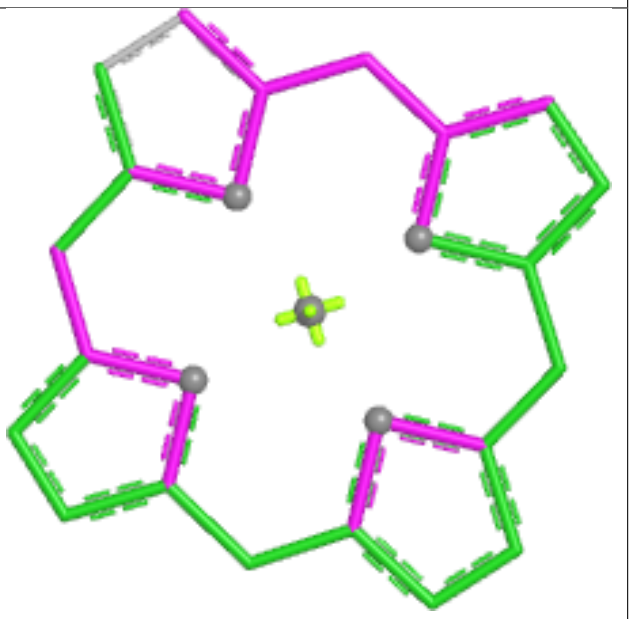


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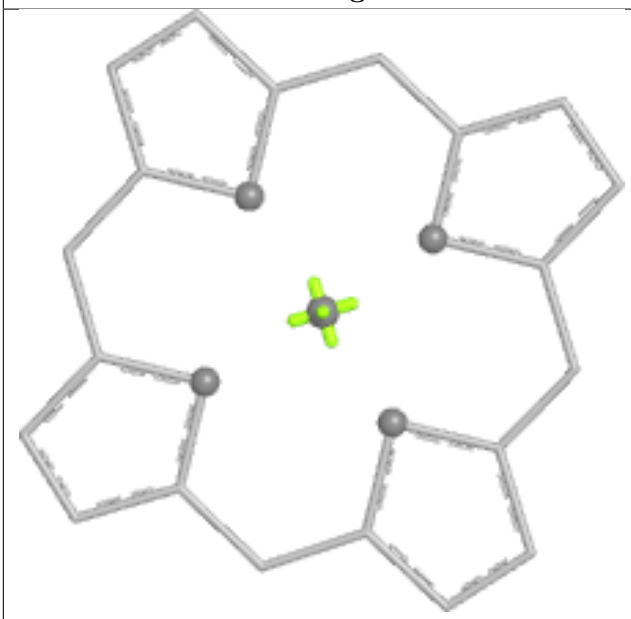
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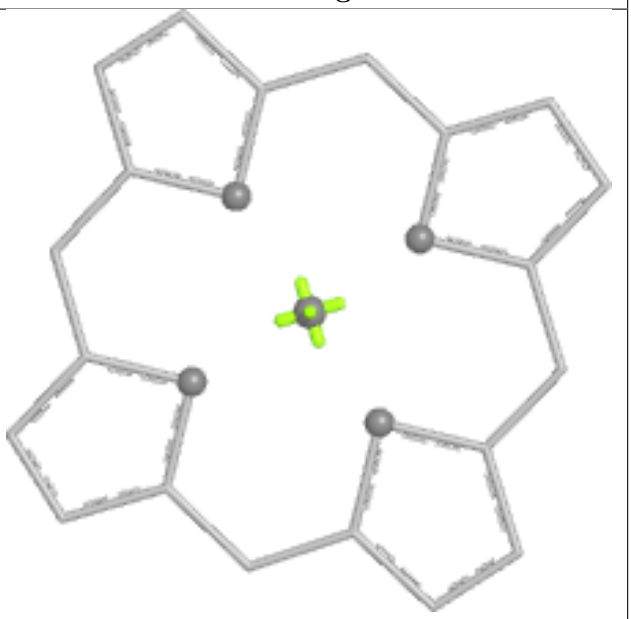
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Bond angles

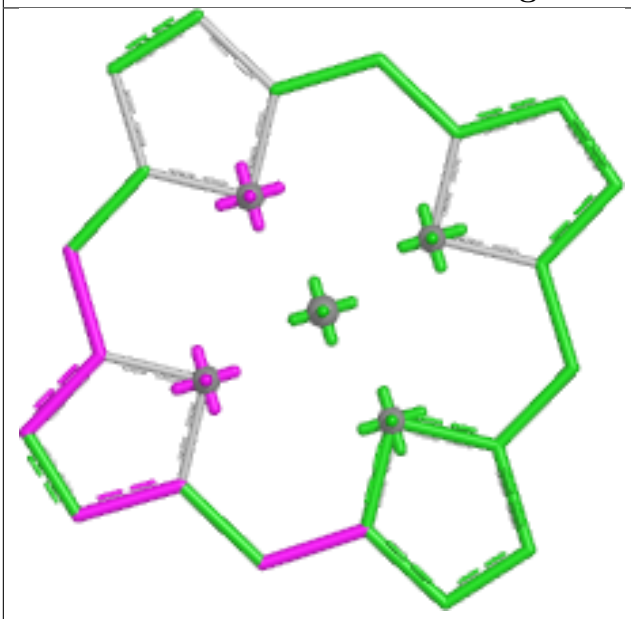


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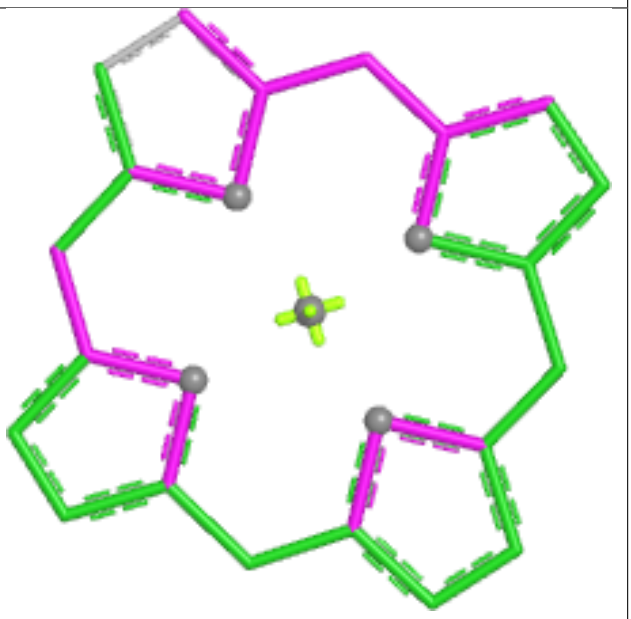


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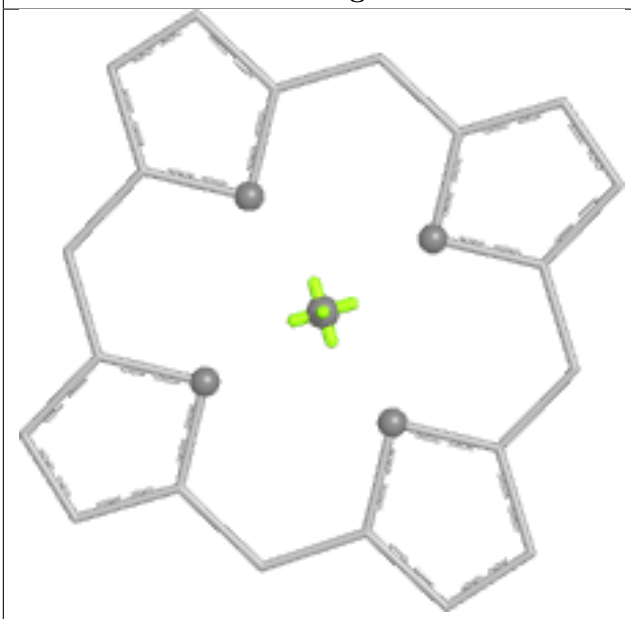
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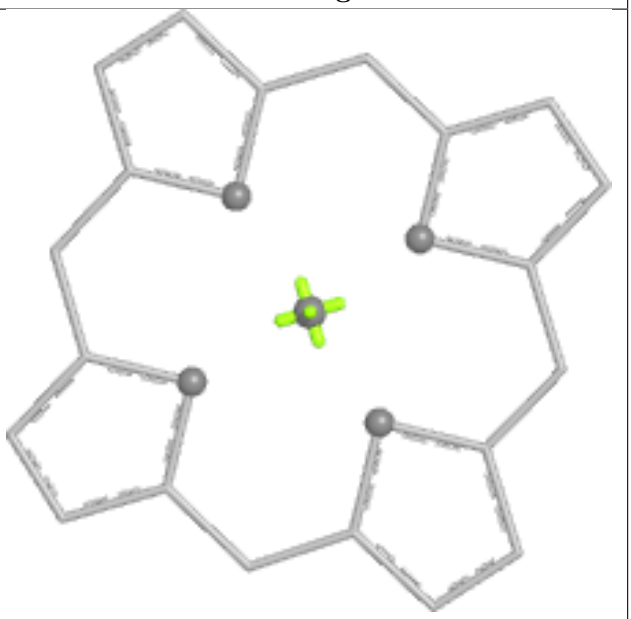
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Bond angles

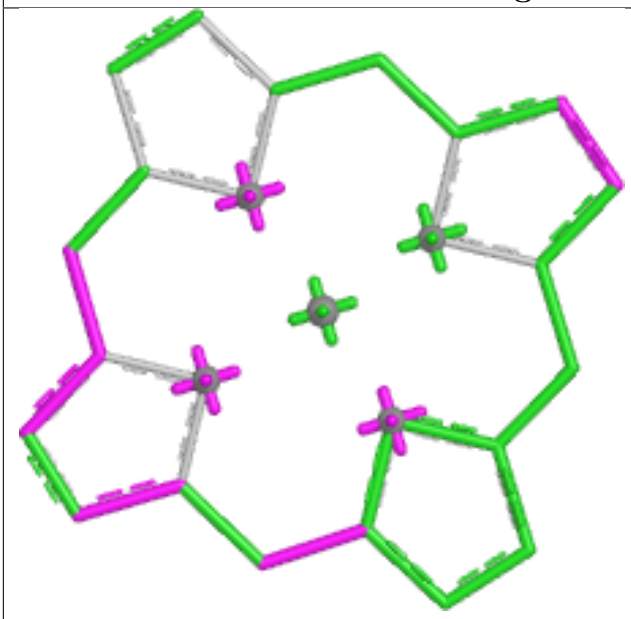


Torsions

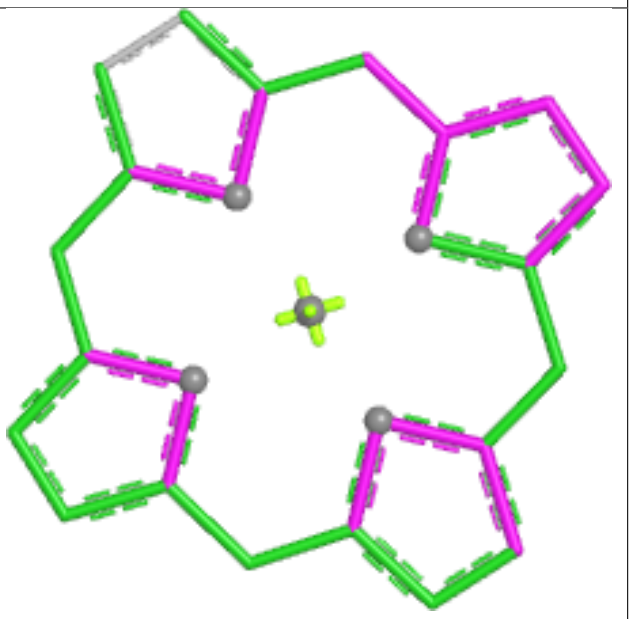


Rings

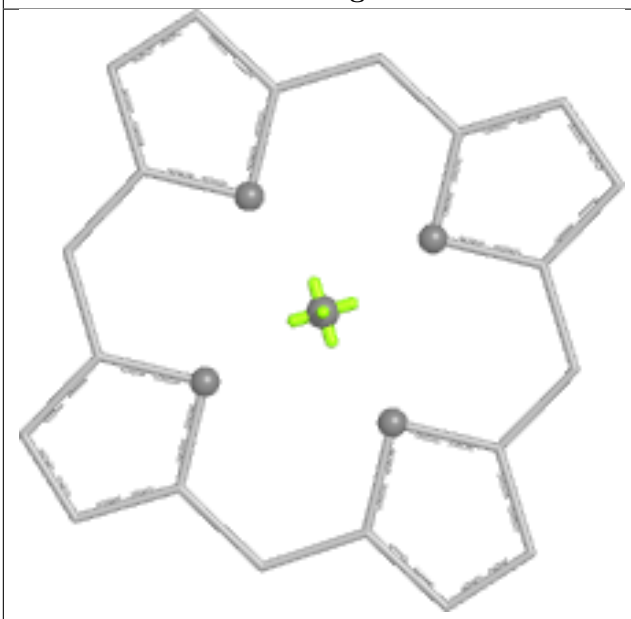
Ligand CLA U 5229



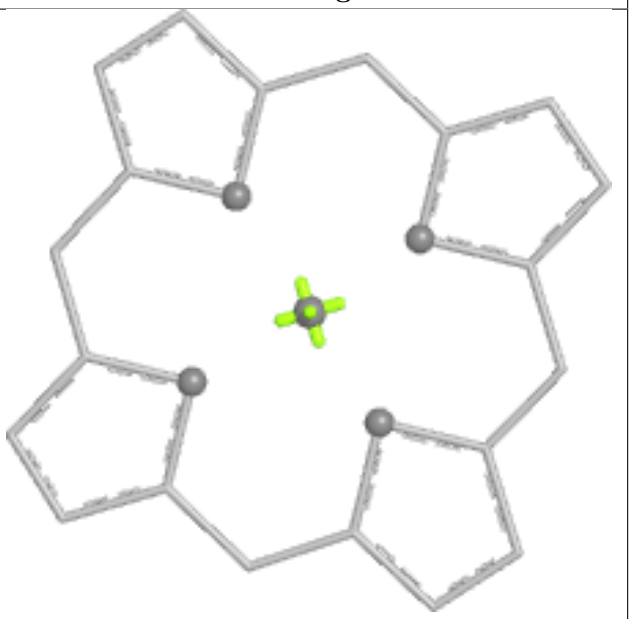
Bond lengths



Bond angles

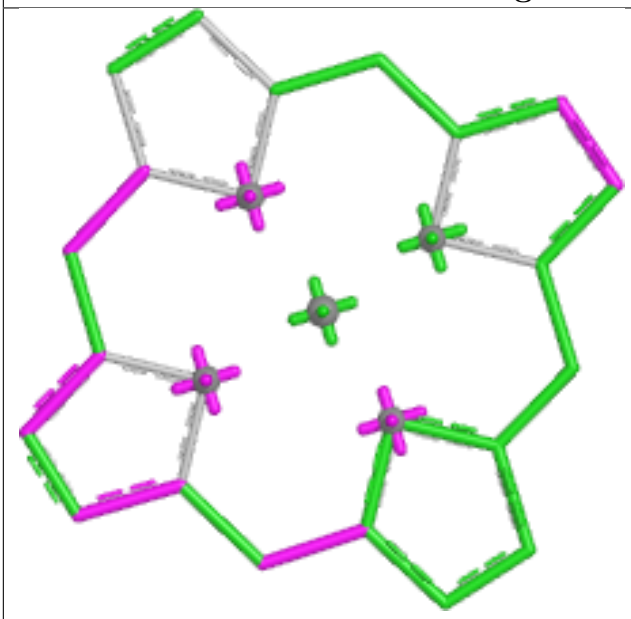


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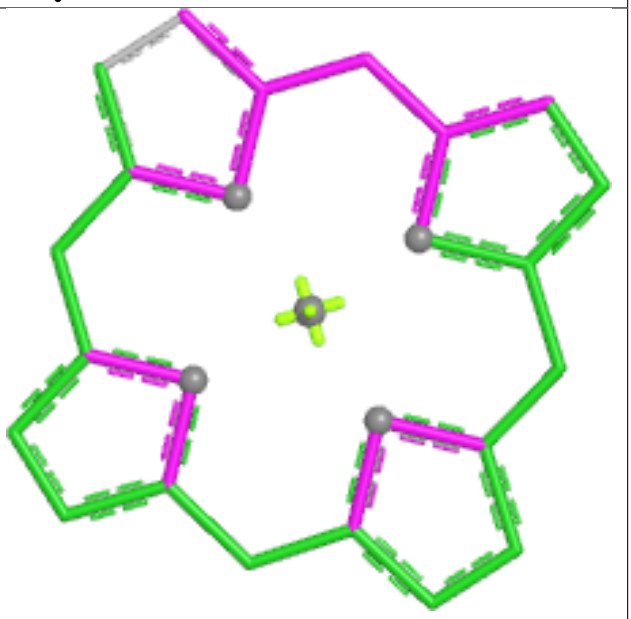


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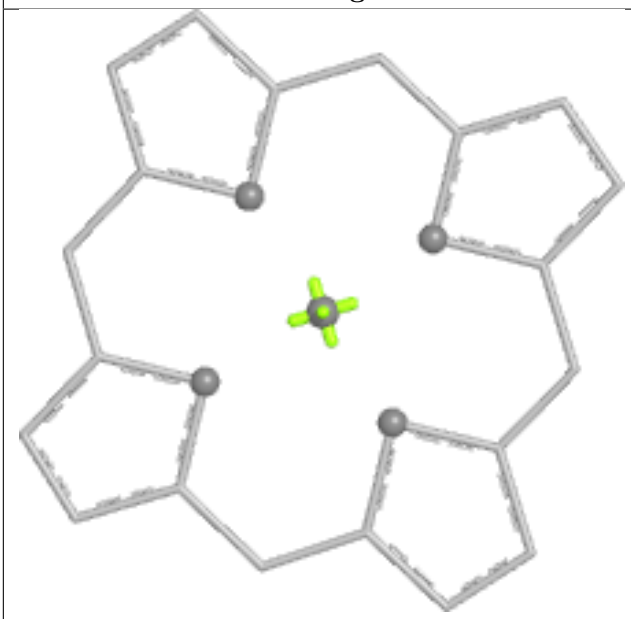
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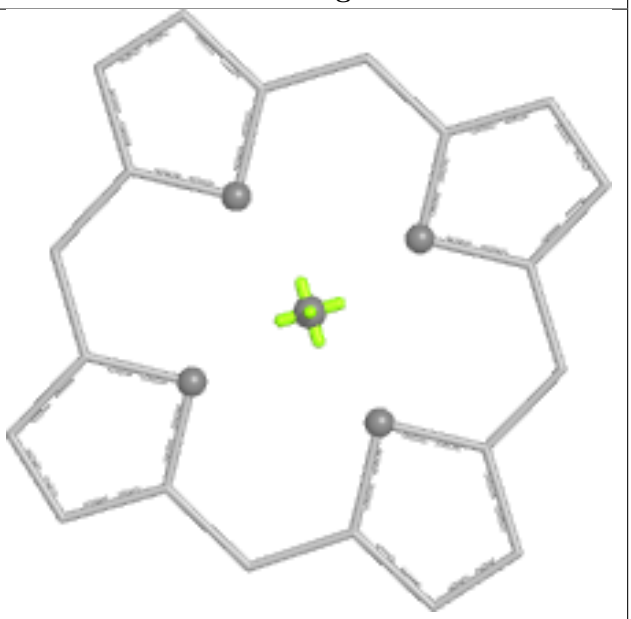
Bond lengths



Bond angles

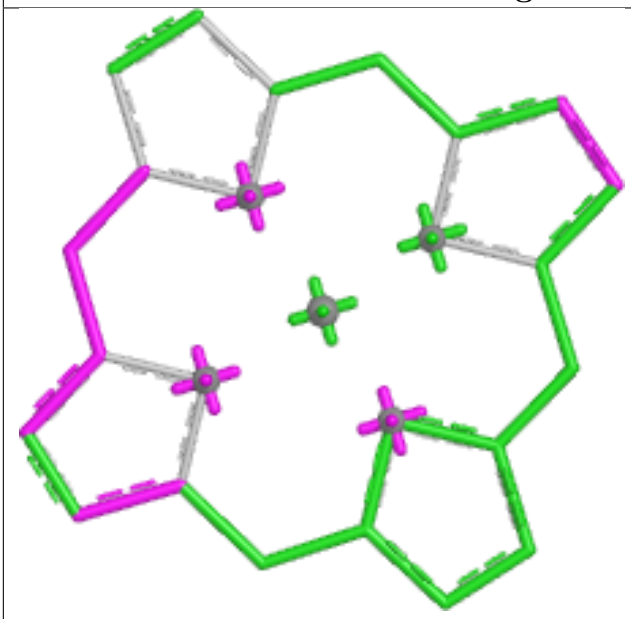


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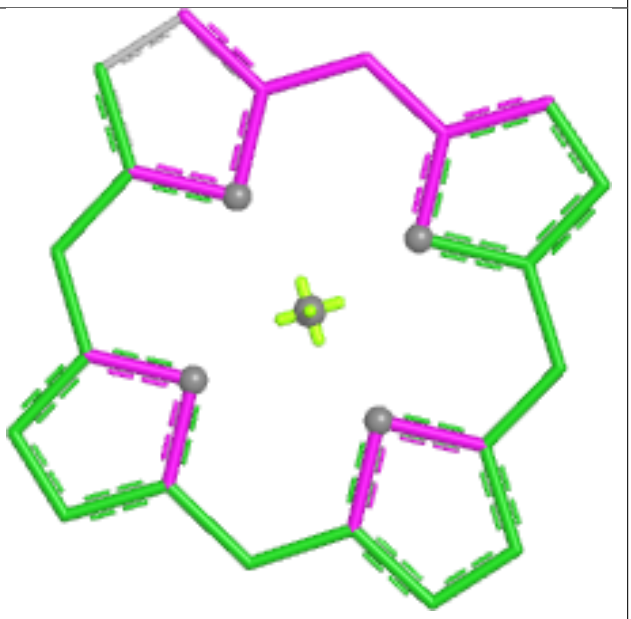


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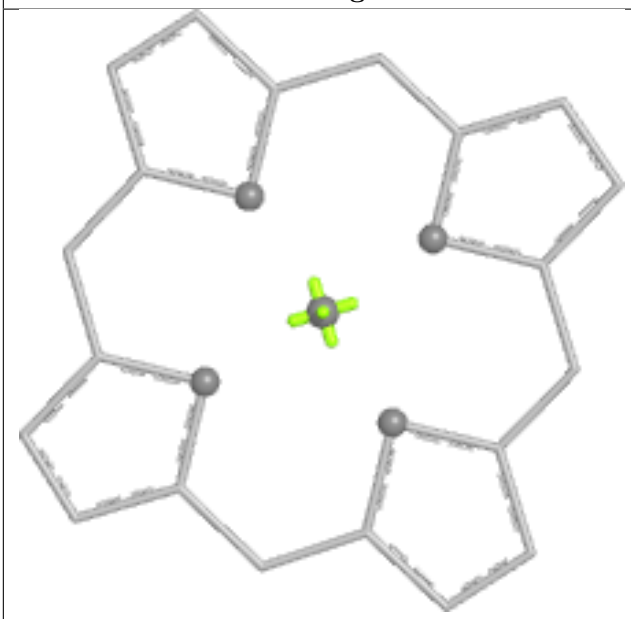
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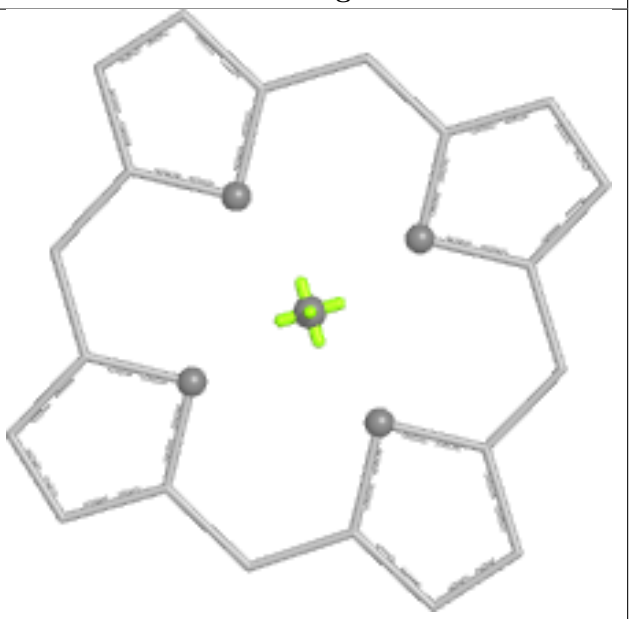
Bond lengths



Bond angles

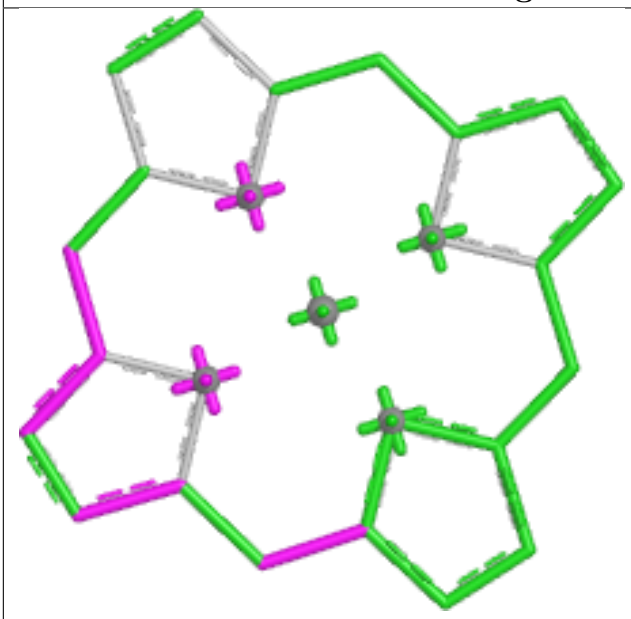


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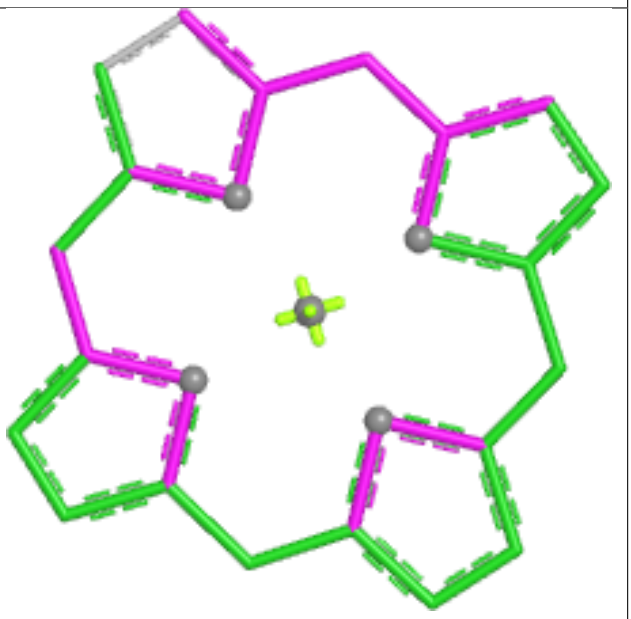


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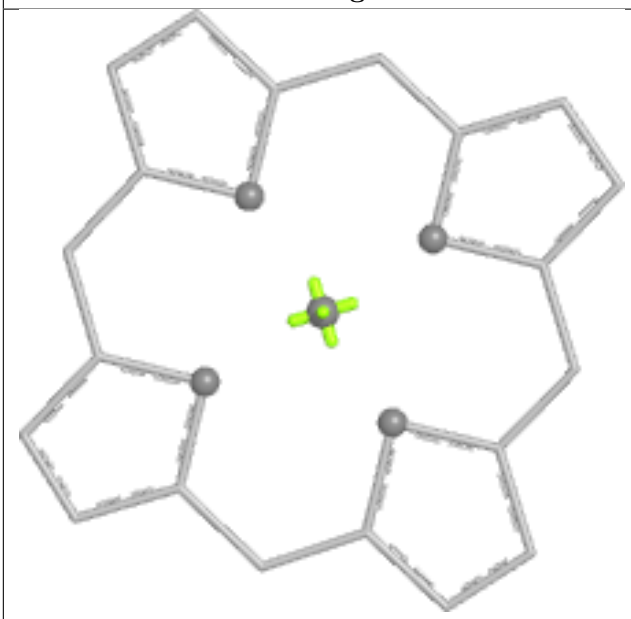
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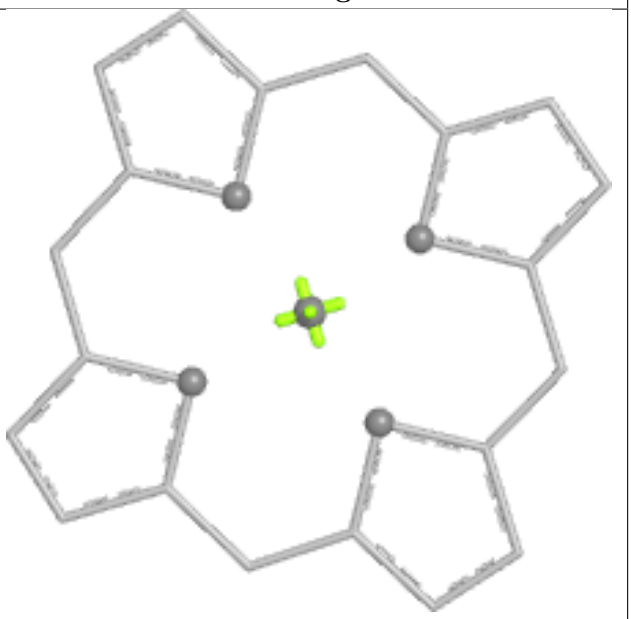
Bond lengths



Bond angles

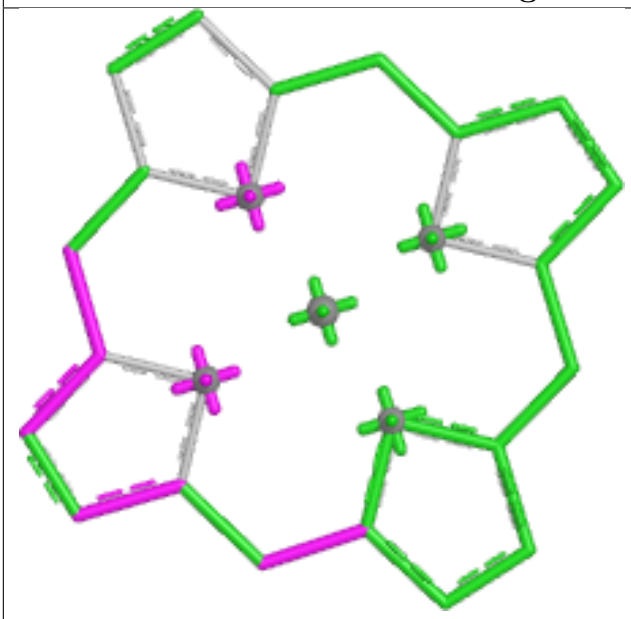


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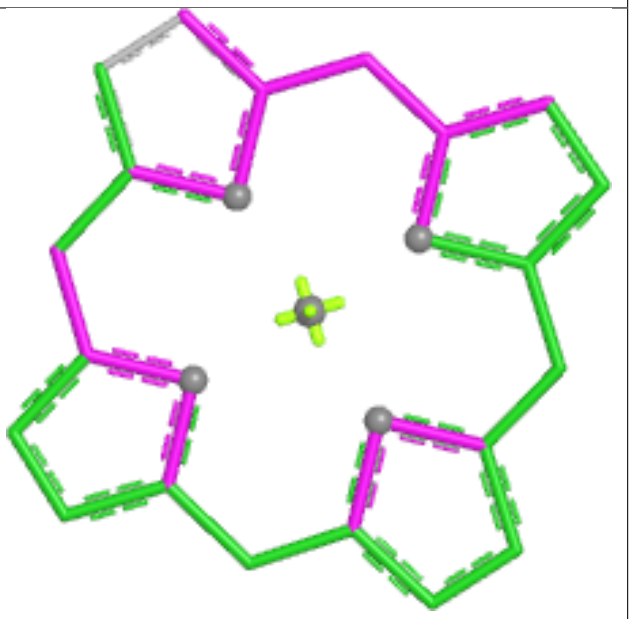


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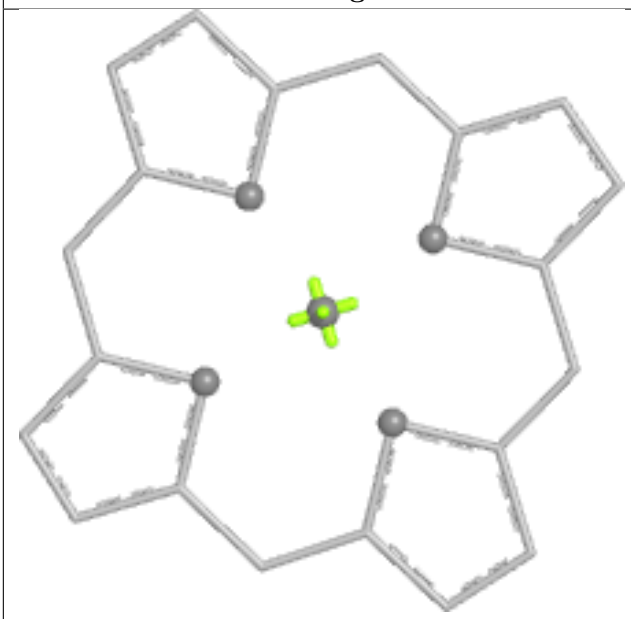
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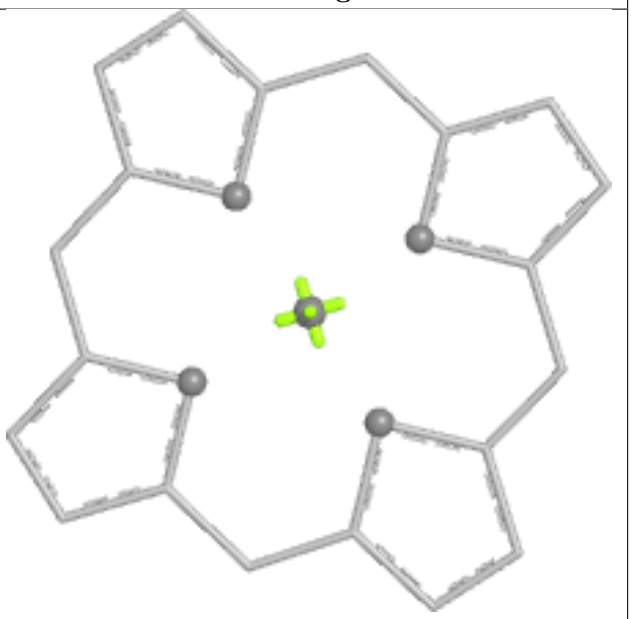
Bond lengths



Bond angles

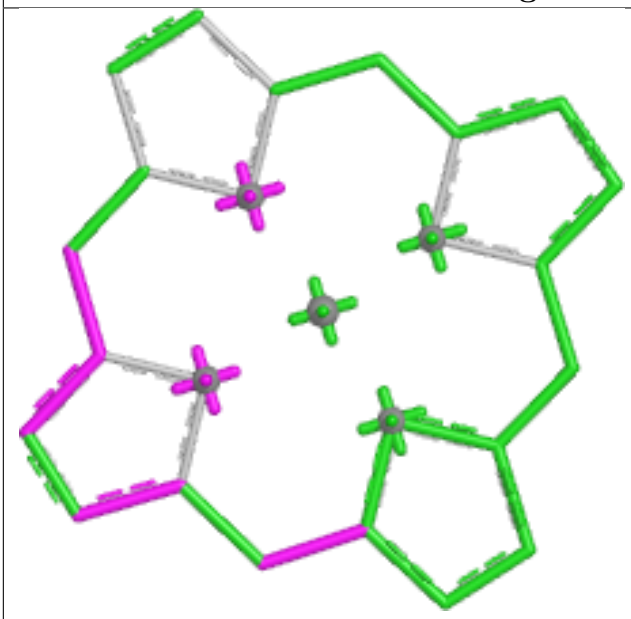


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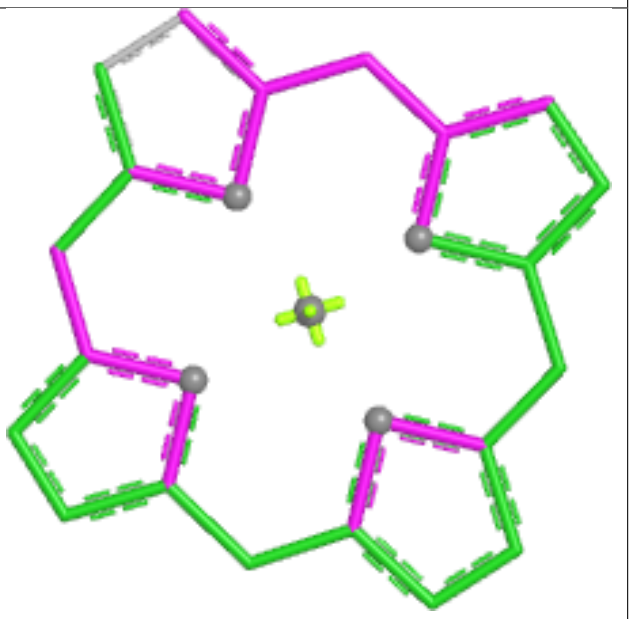


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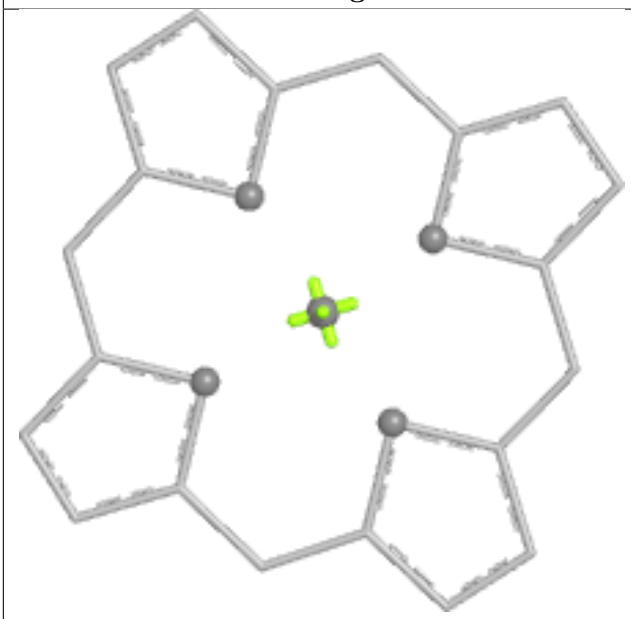
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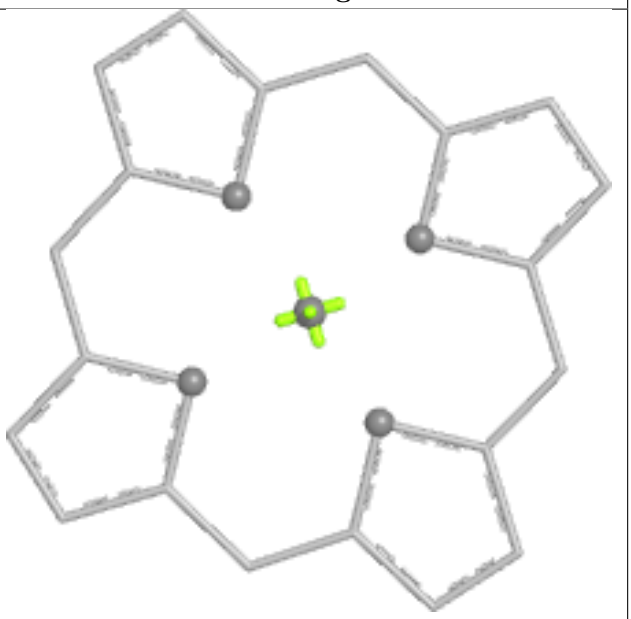
Bond lengths



Bond angles

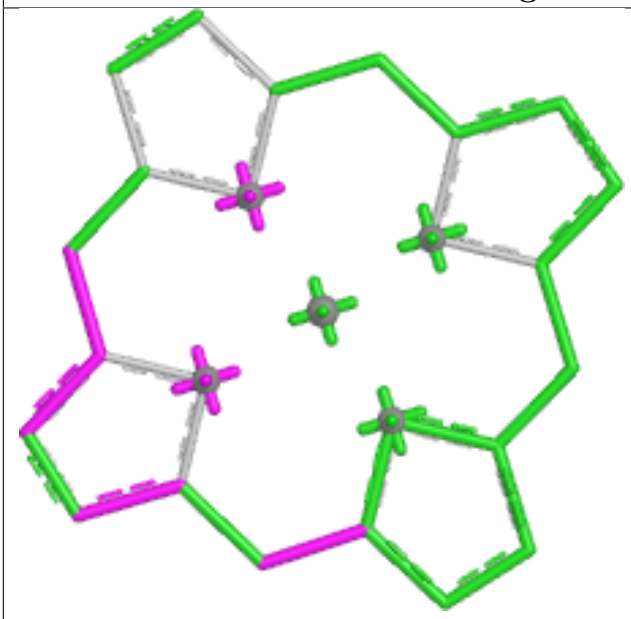


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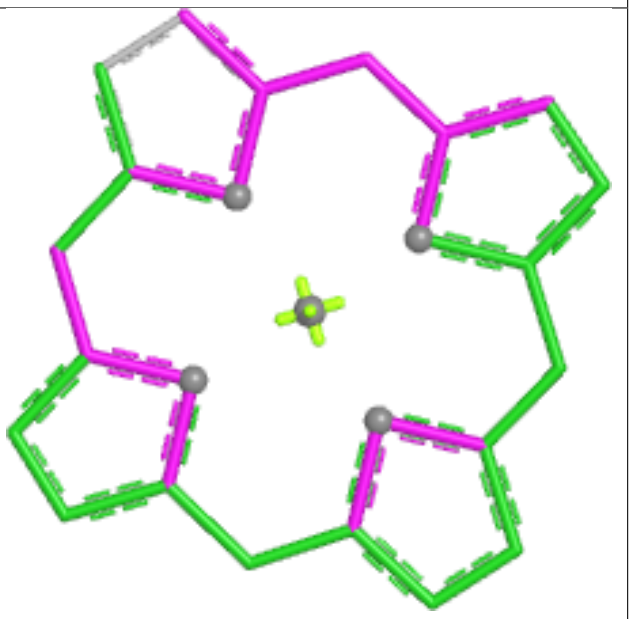


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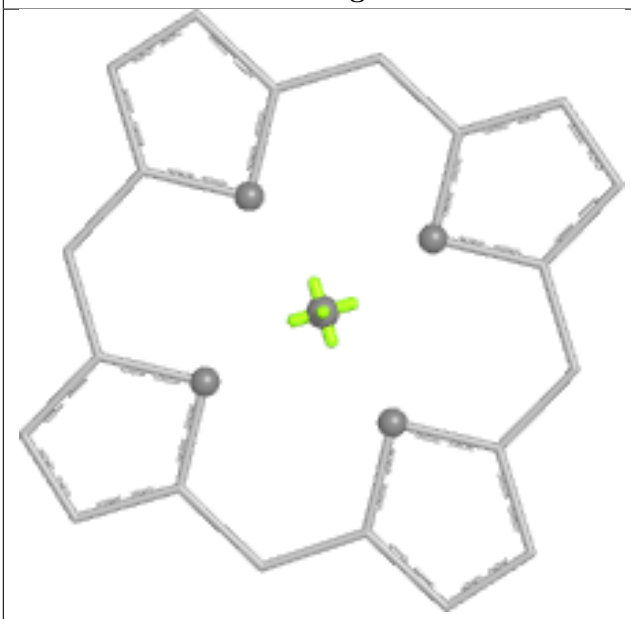
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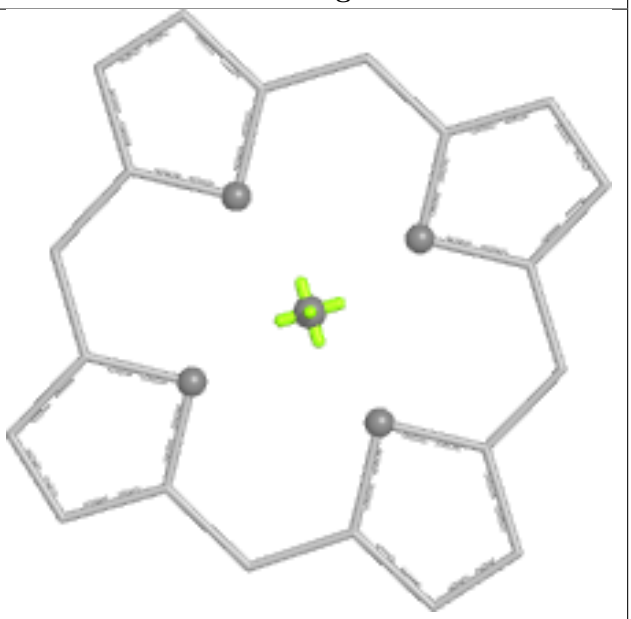
Bond lengths



Bond angles

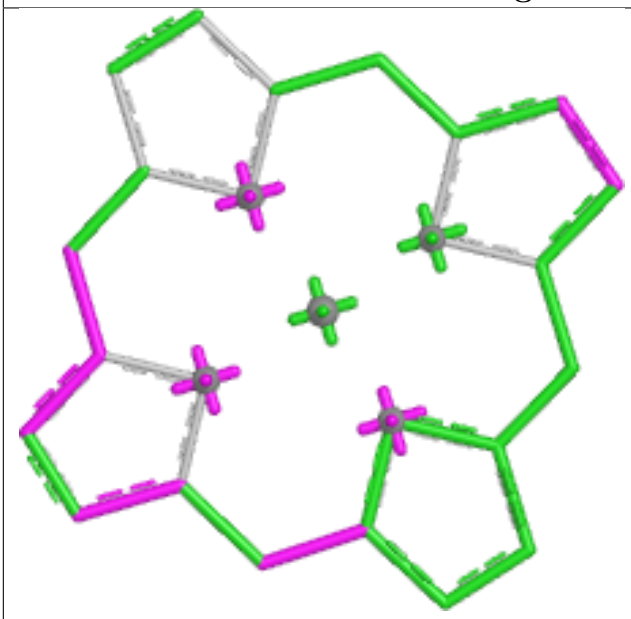


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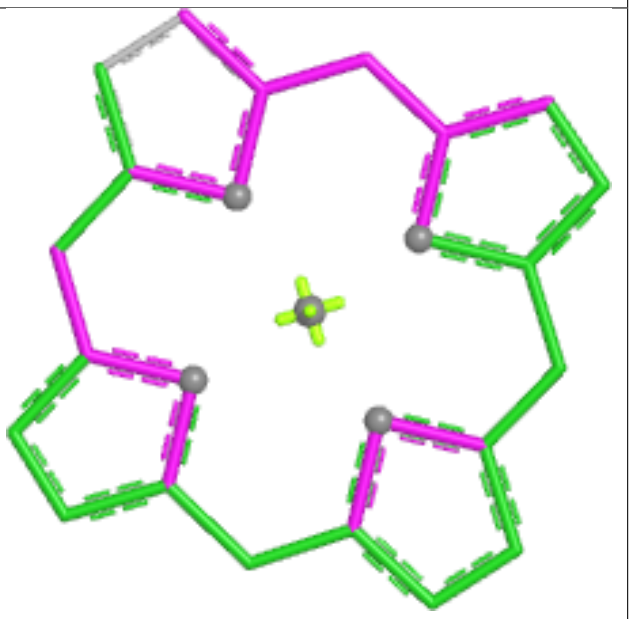


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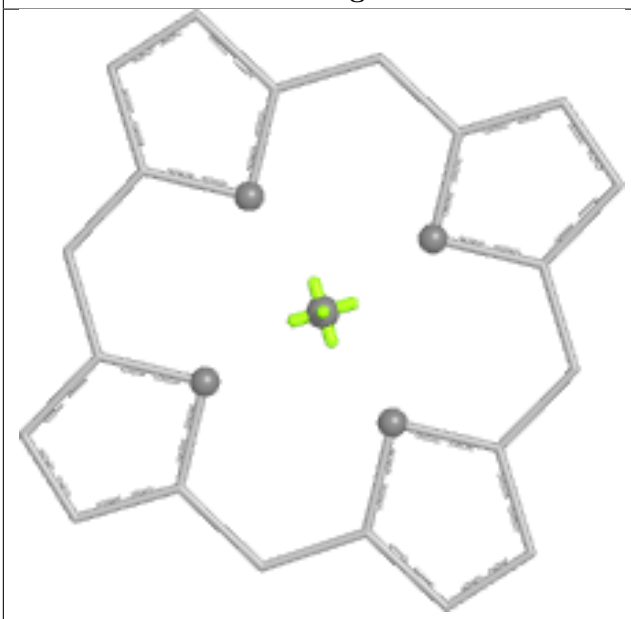
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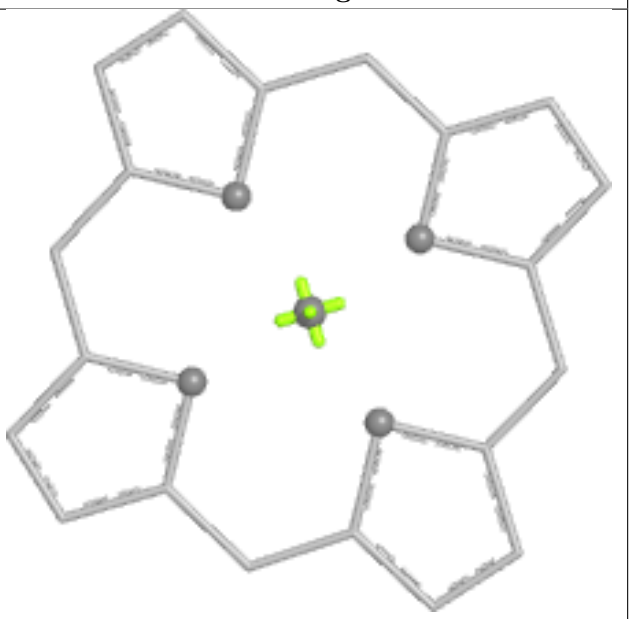
Bond lengths



Bond angles

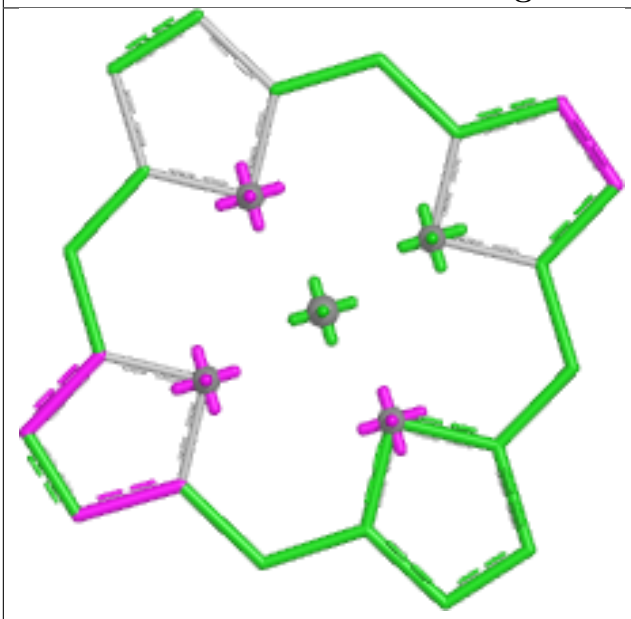


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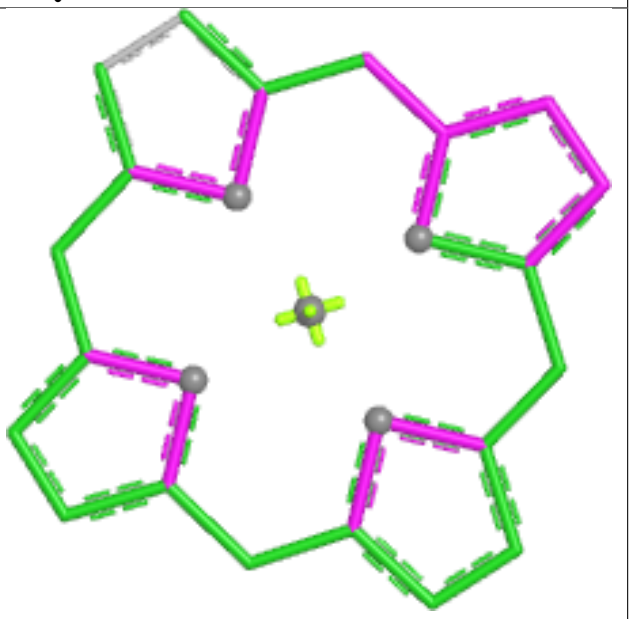


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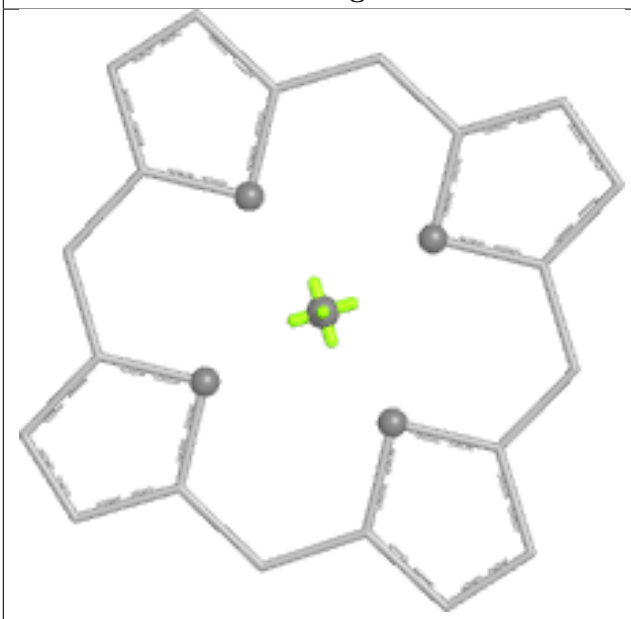
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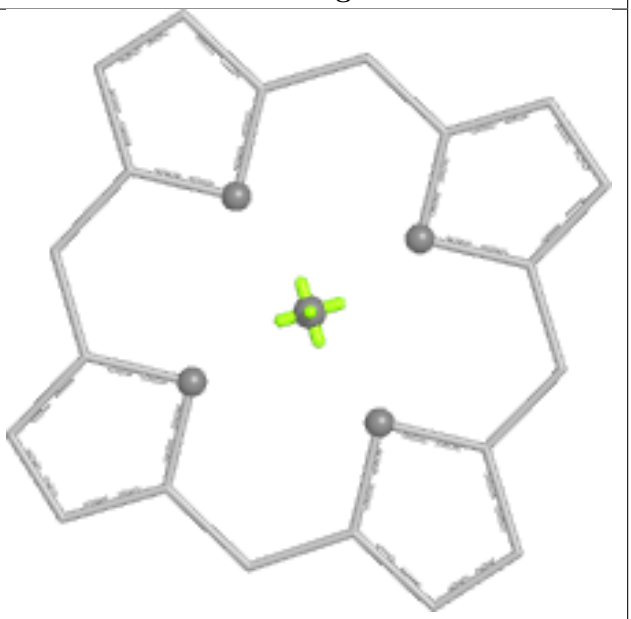
Bond lengths



Bond angles

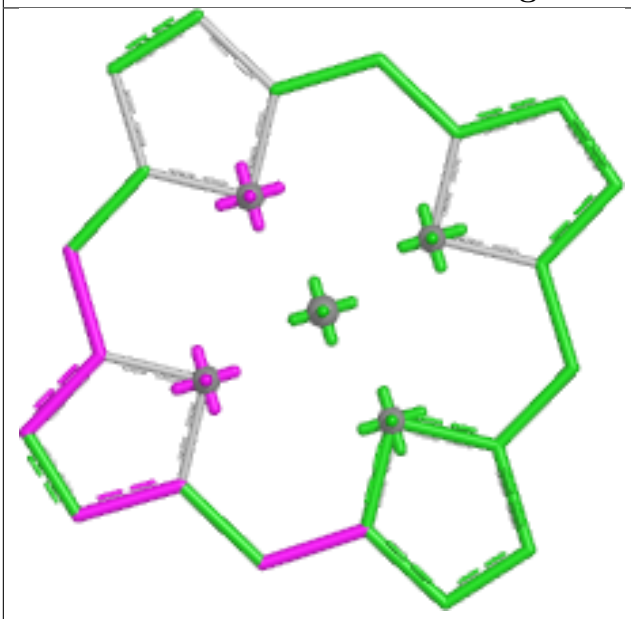


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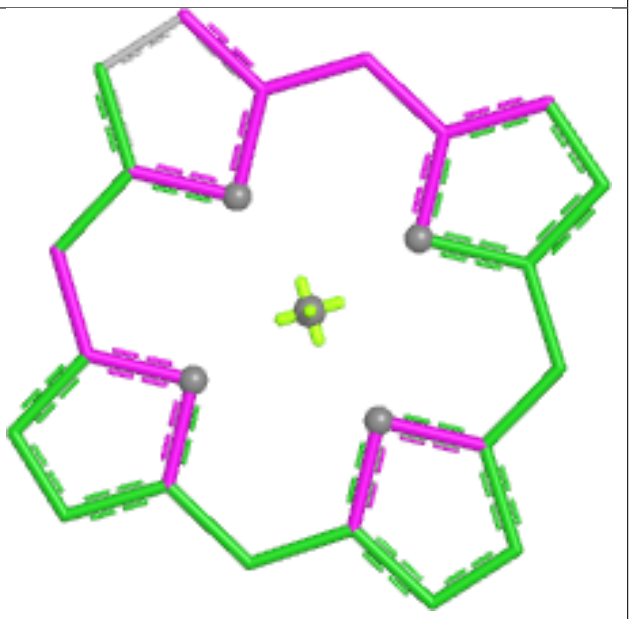


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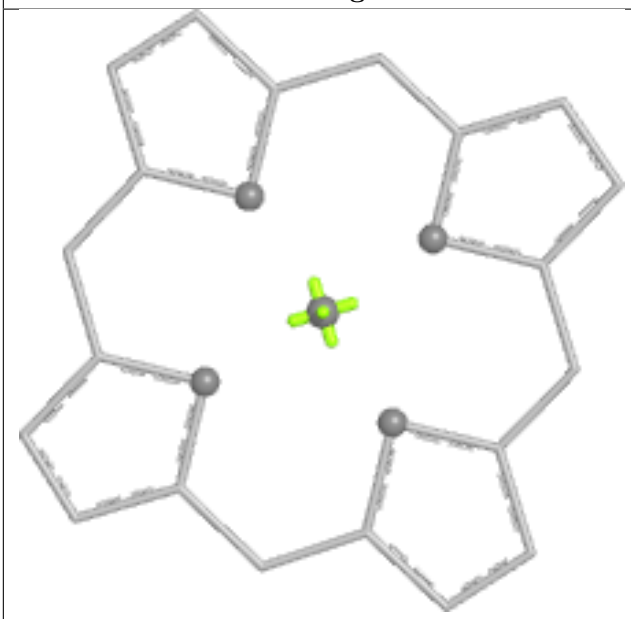
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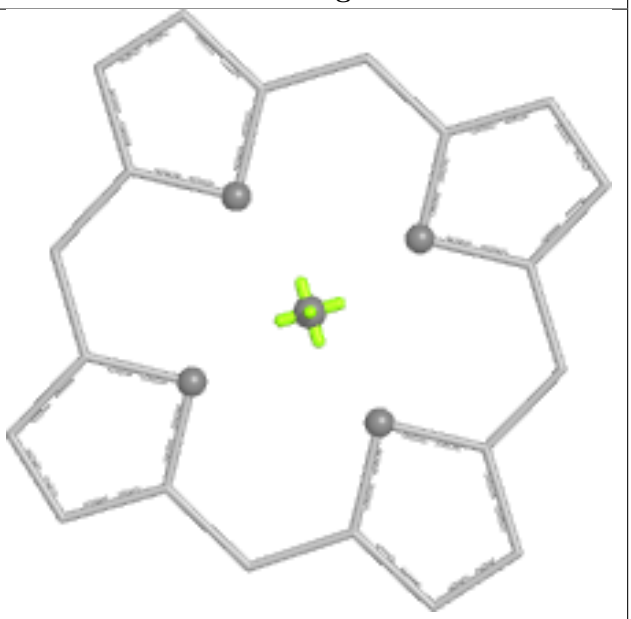
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Bond angles

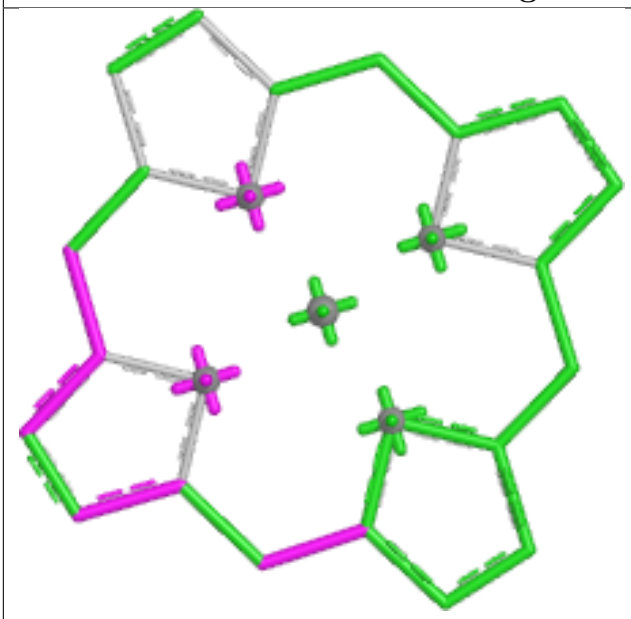


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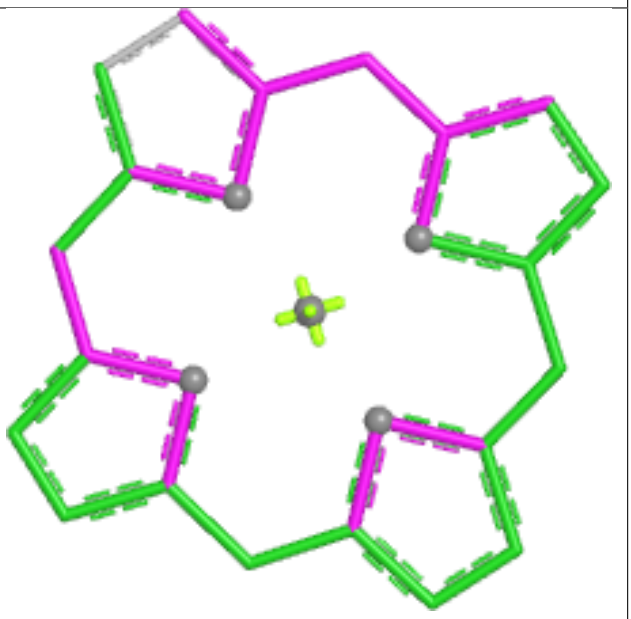


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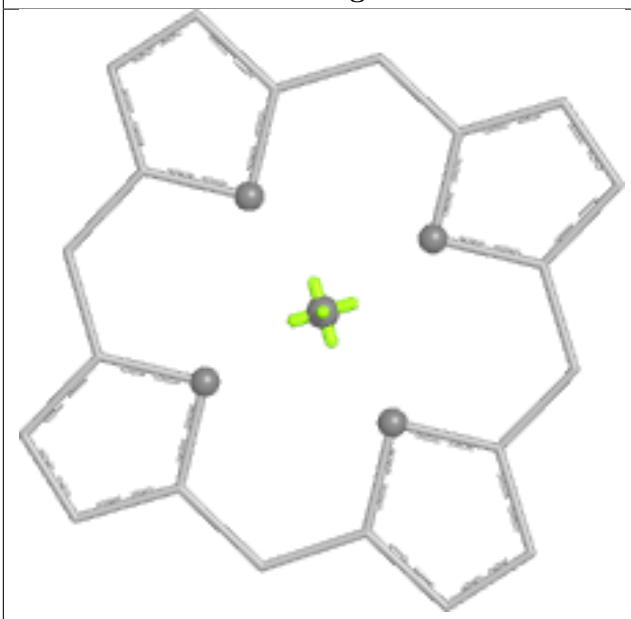
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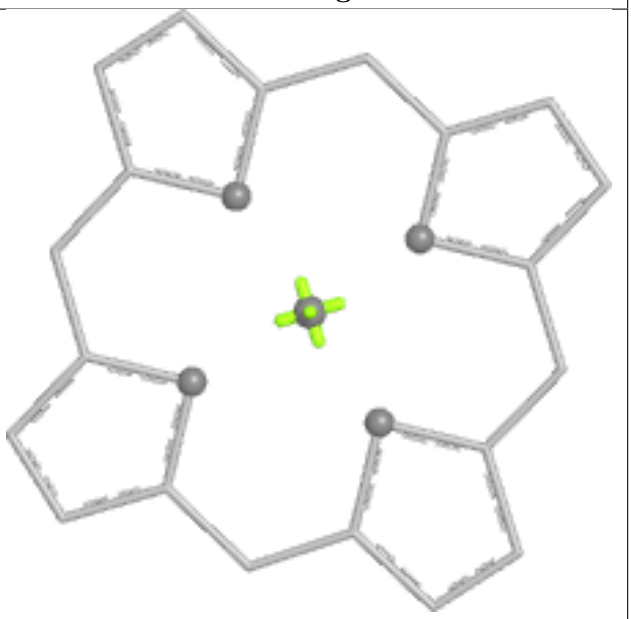
Bond lengths



Bond angles

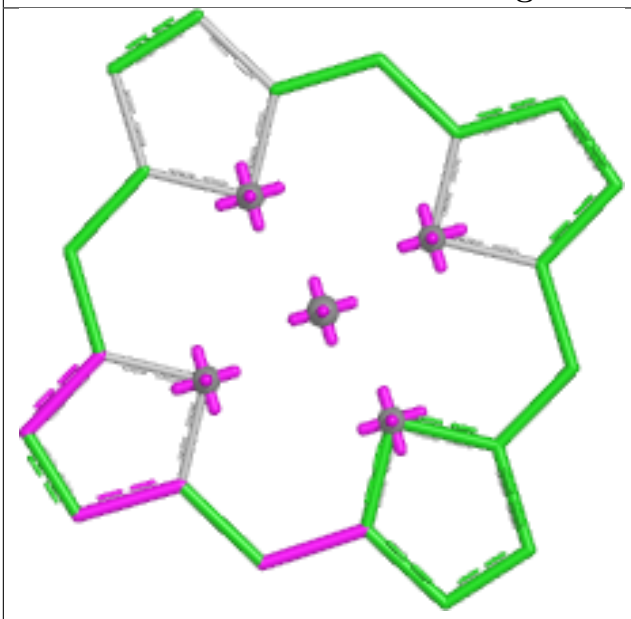


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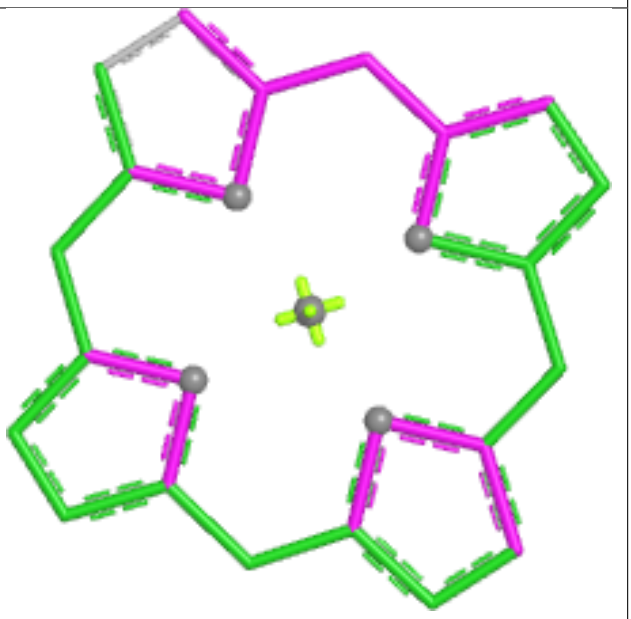


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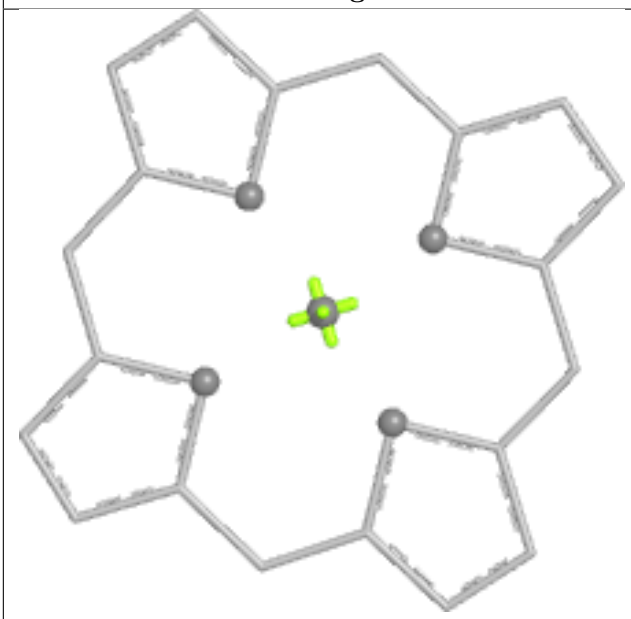
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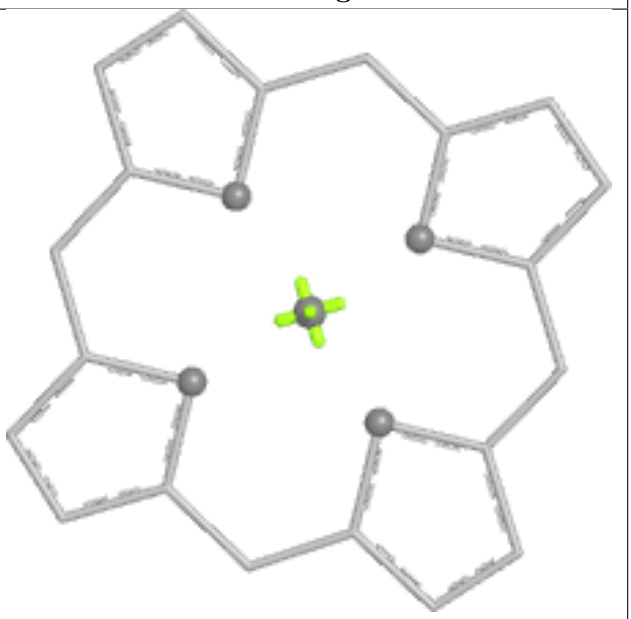
Bond lengths



Bond angles

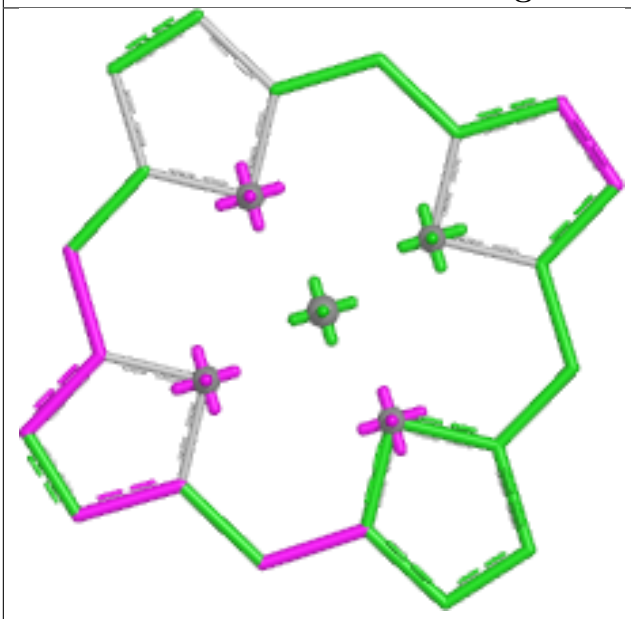


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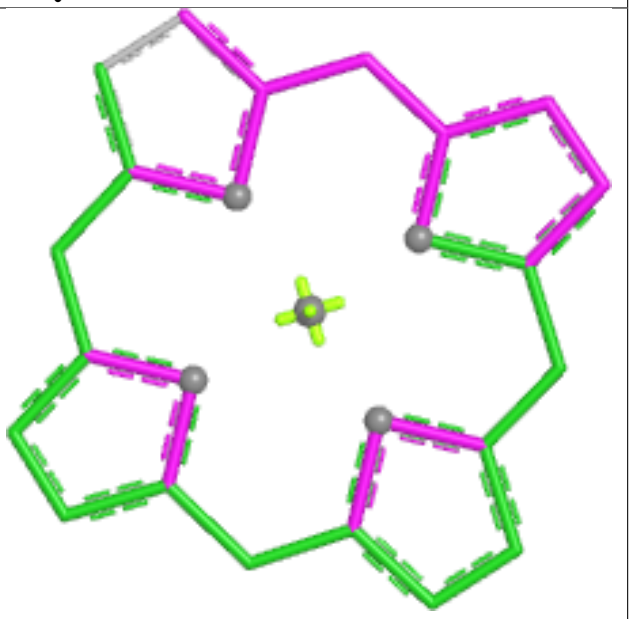


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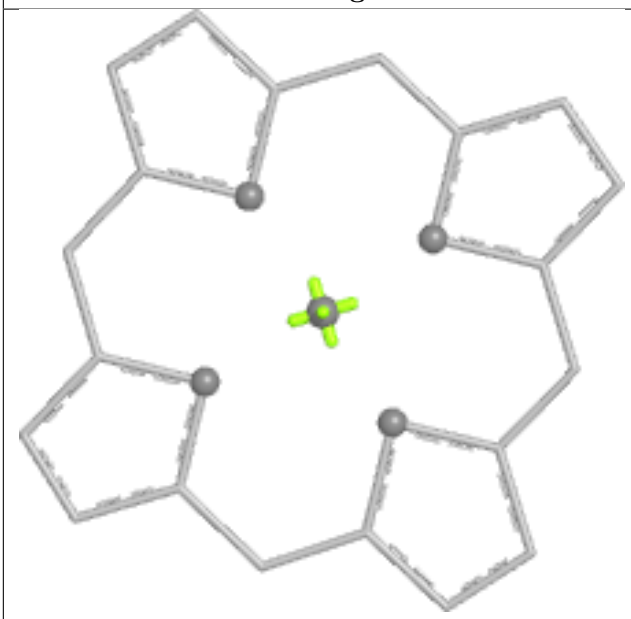
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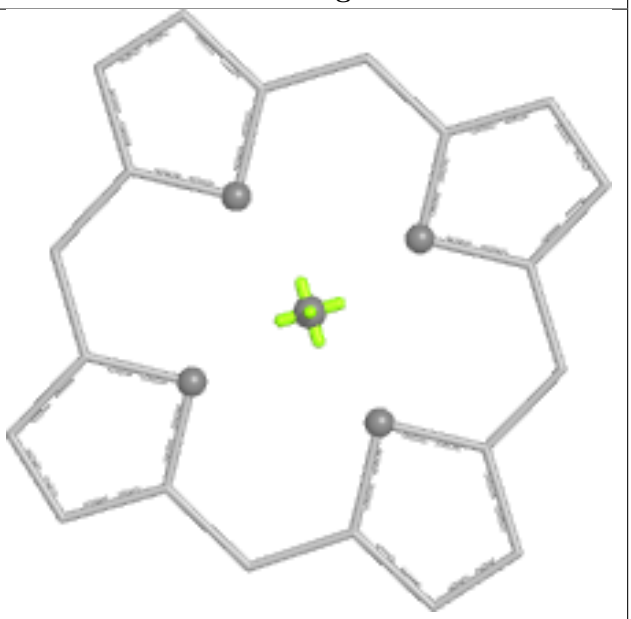
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Bond angles

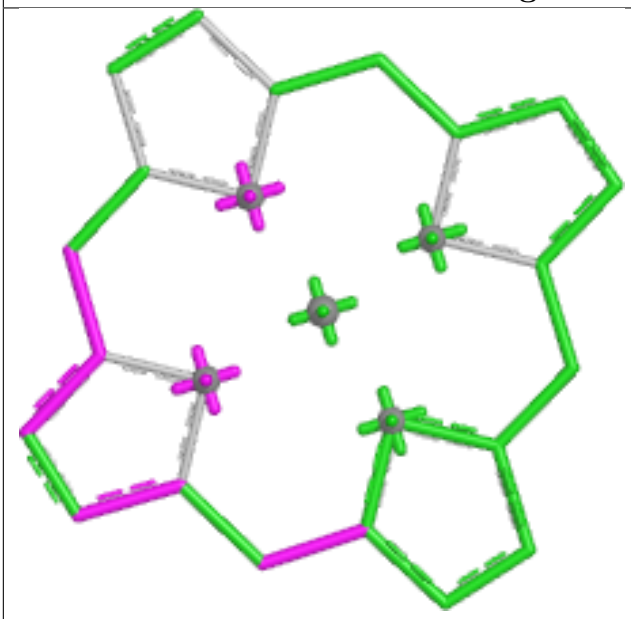


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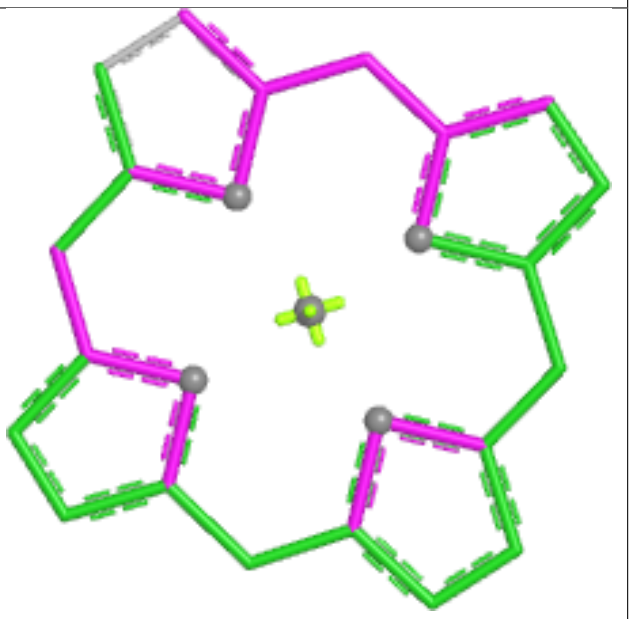


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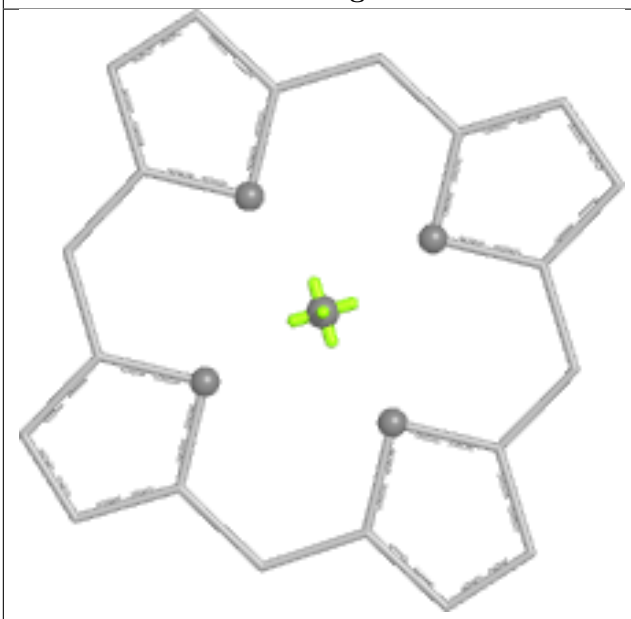
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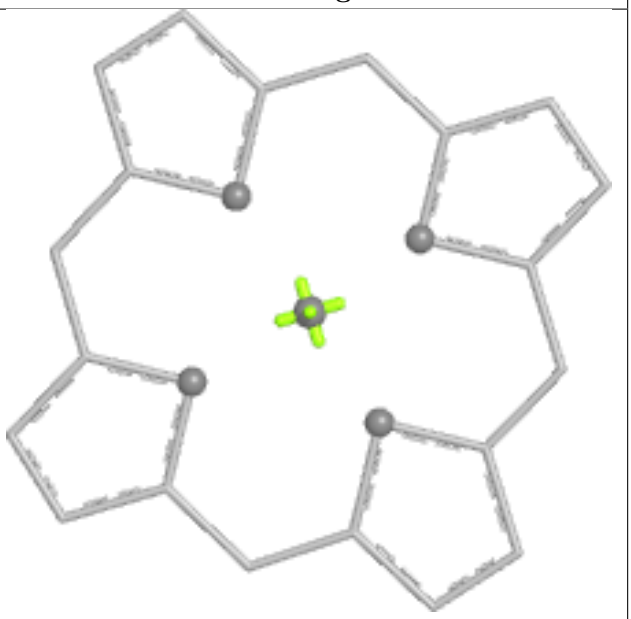
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Bond angles

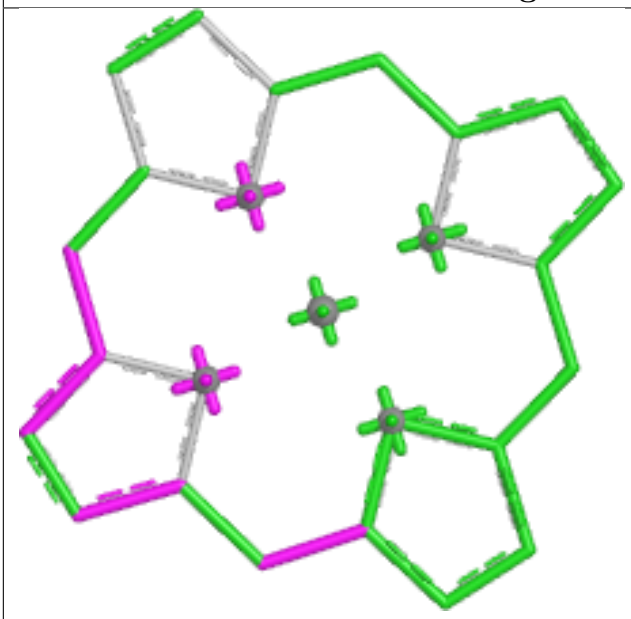


Torsions

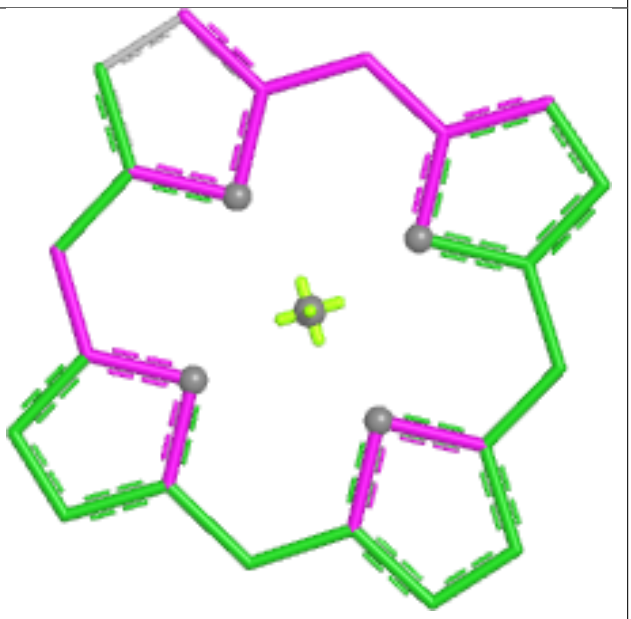


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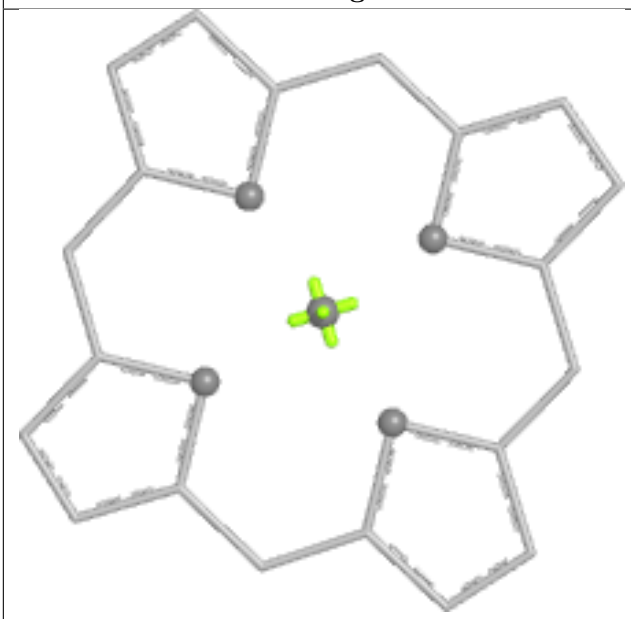
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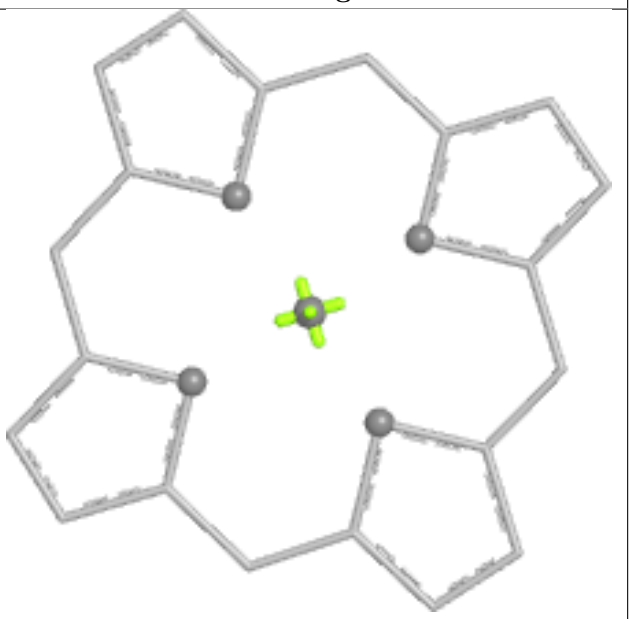
Bond lengths



Bond angles

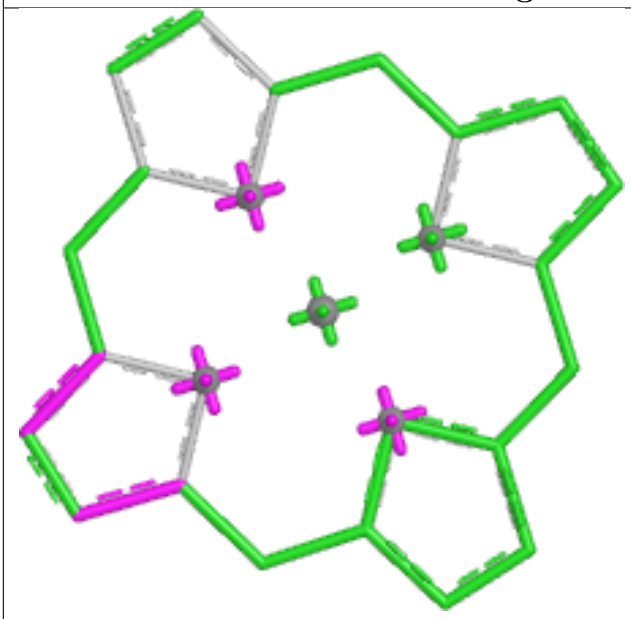


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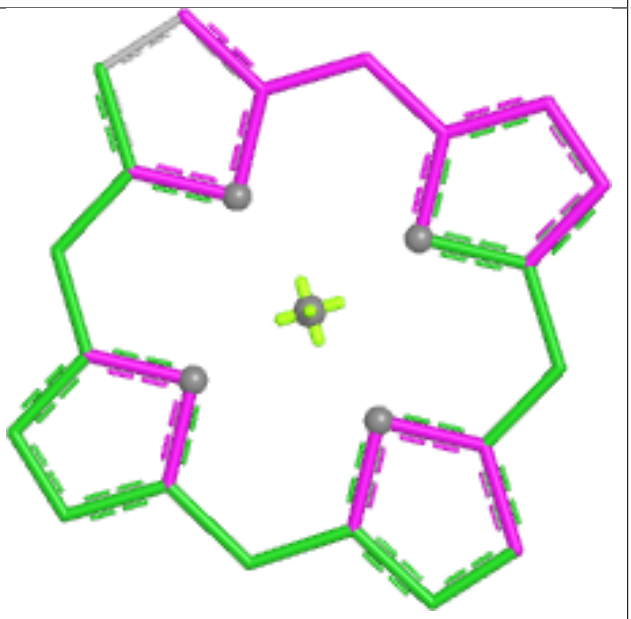


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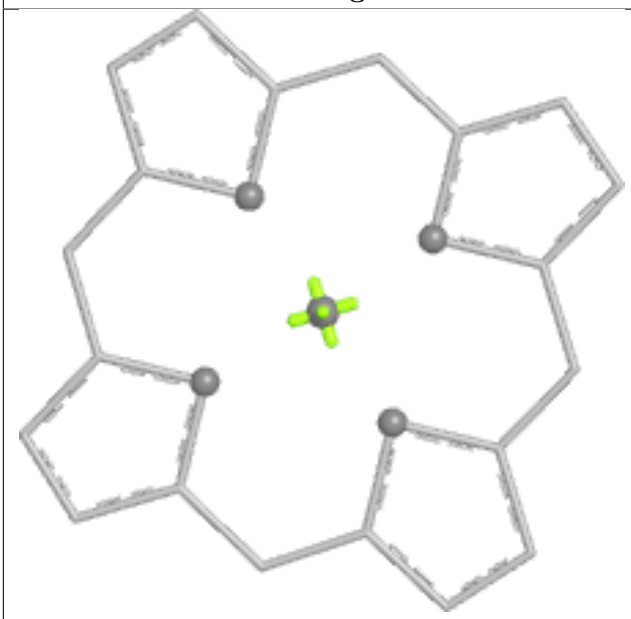
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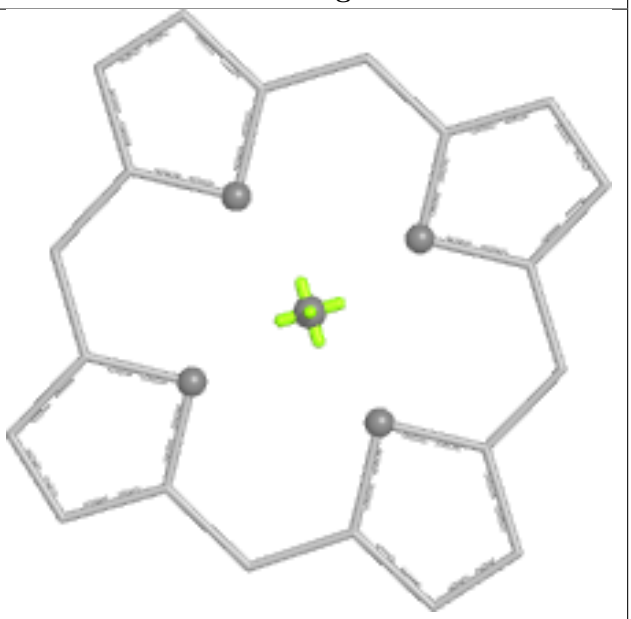
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Bond angles

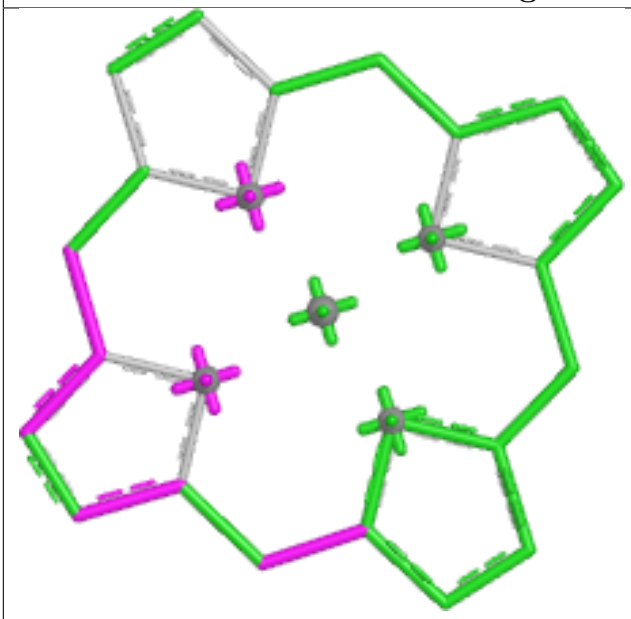


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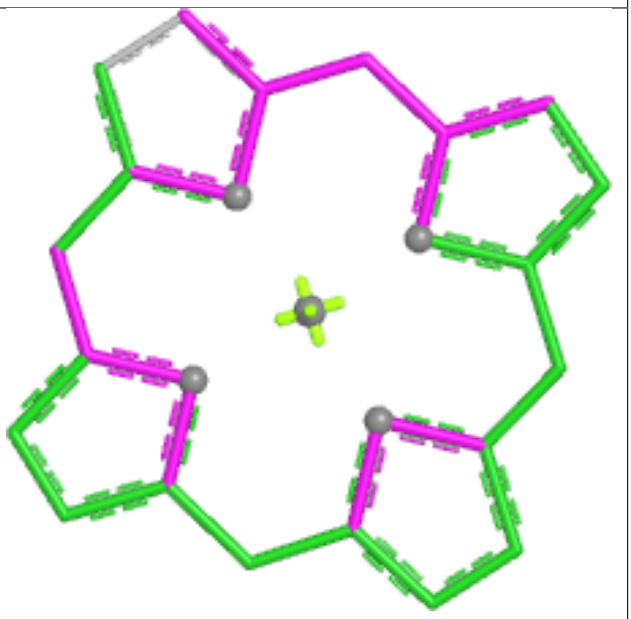


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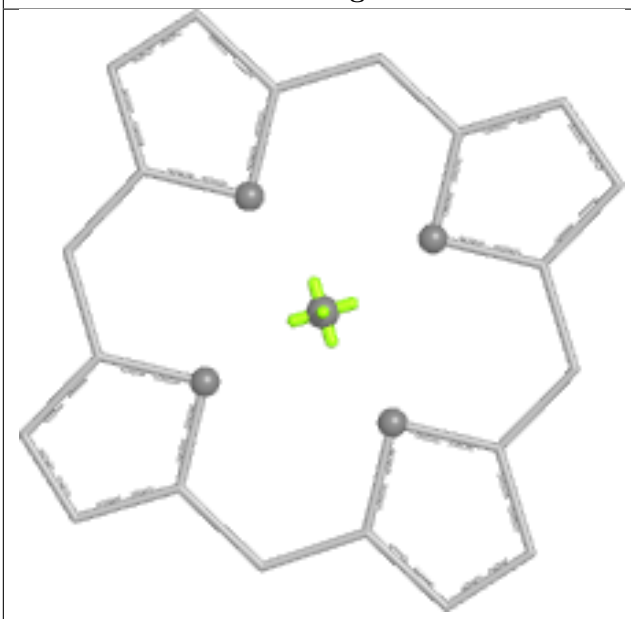
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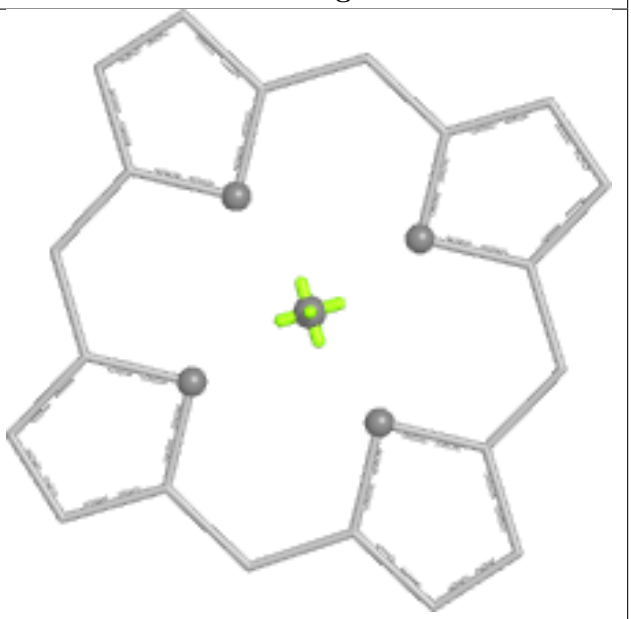
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Bond angles

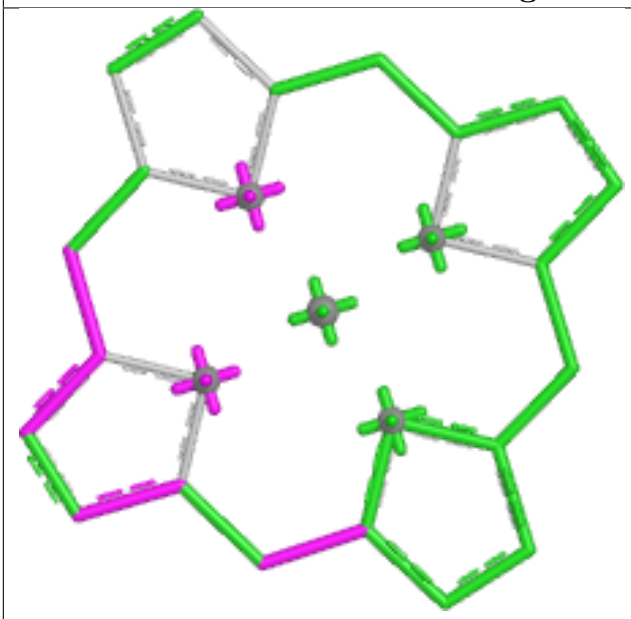


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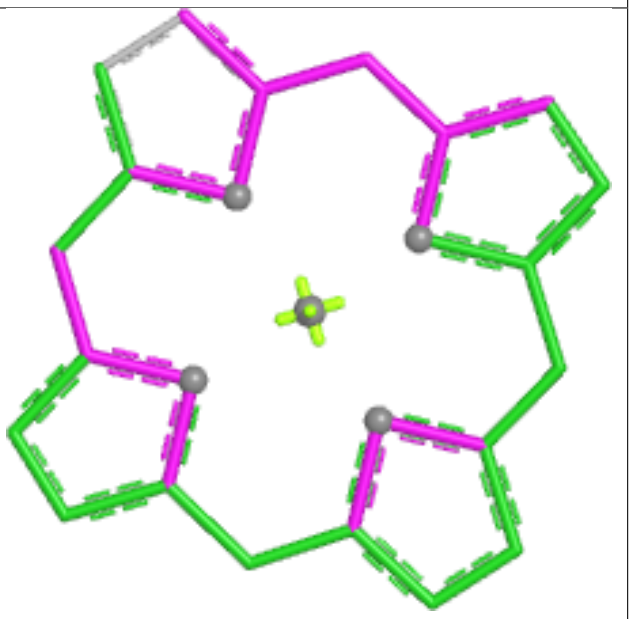


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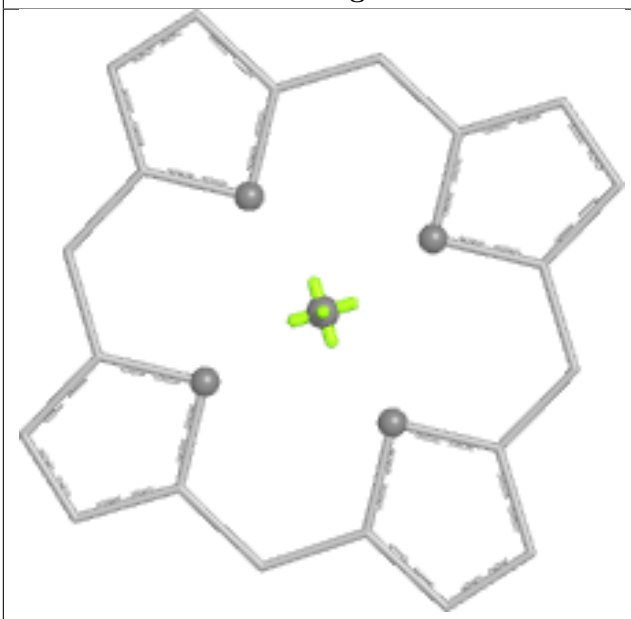
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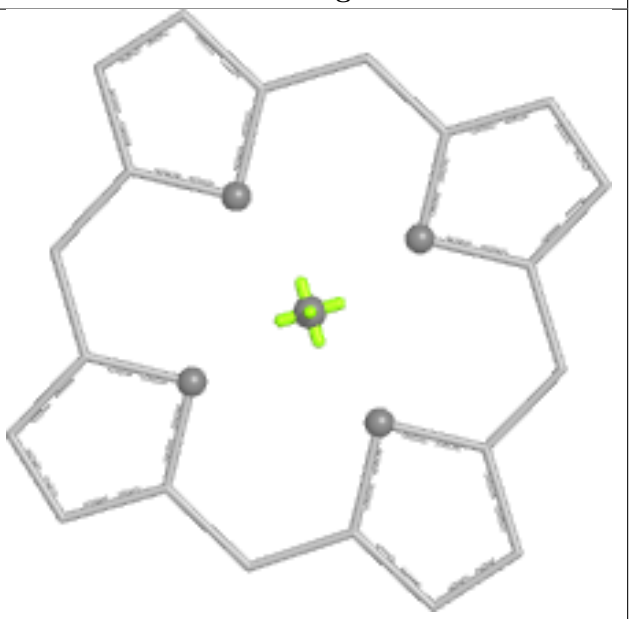
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Bond angles

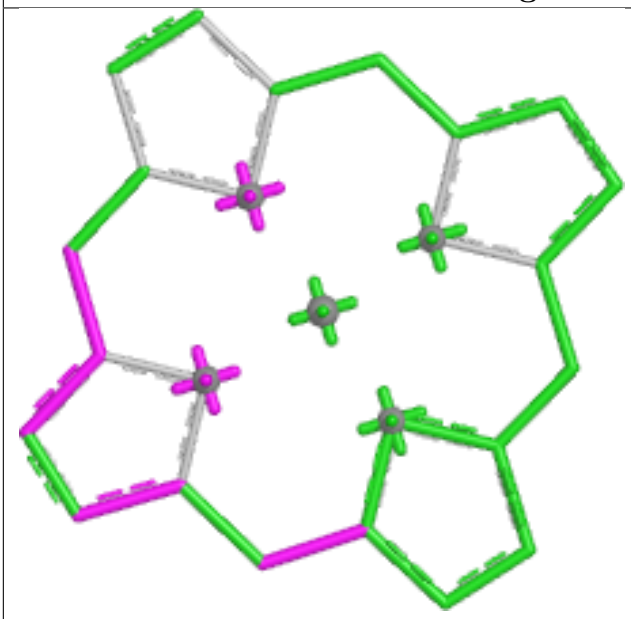


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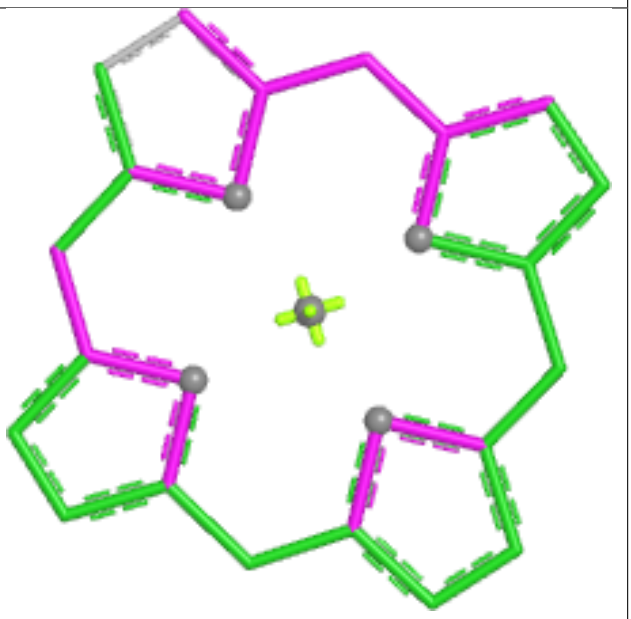


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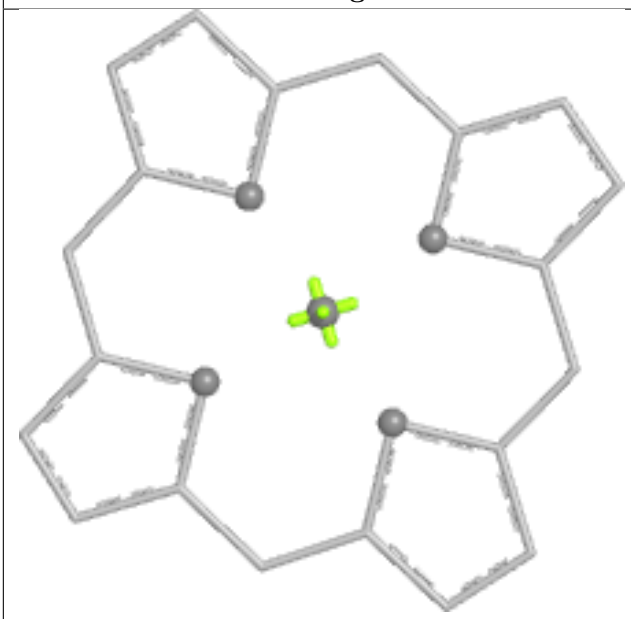
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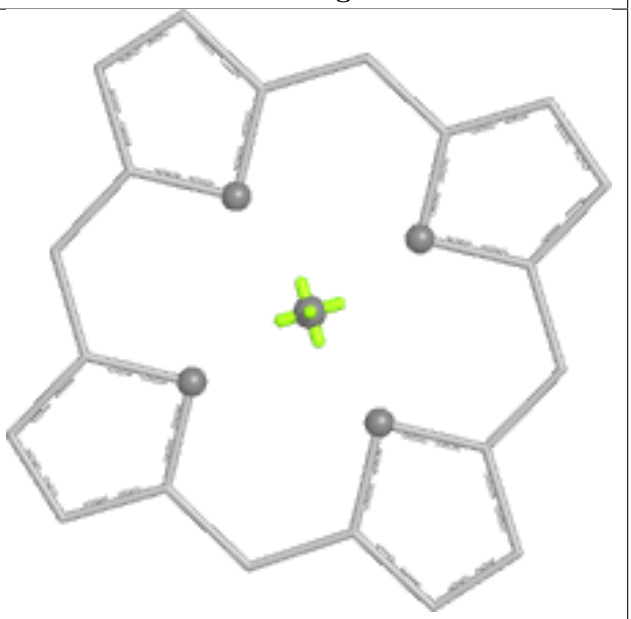
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Bond angles

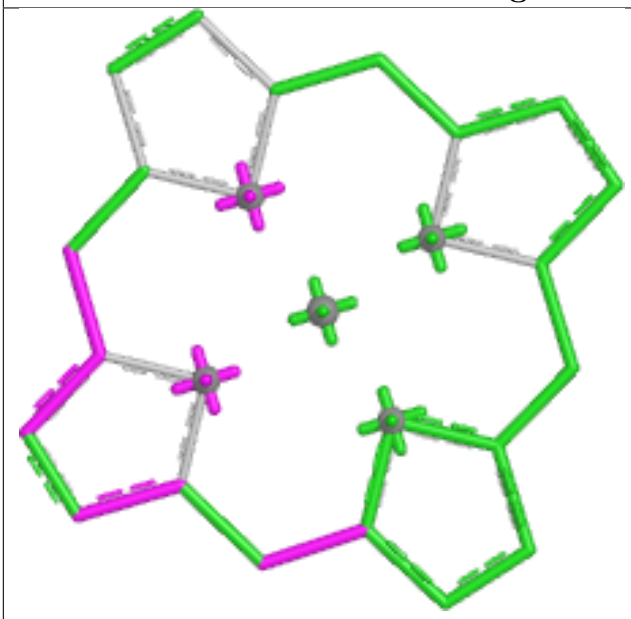


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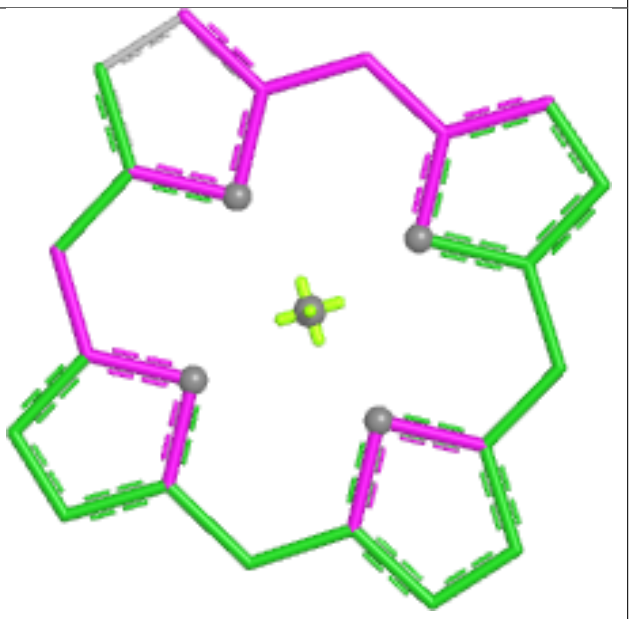


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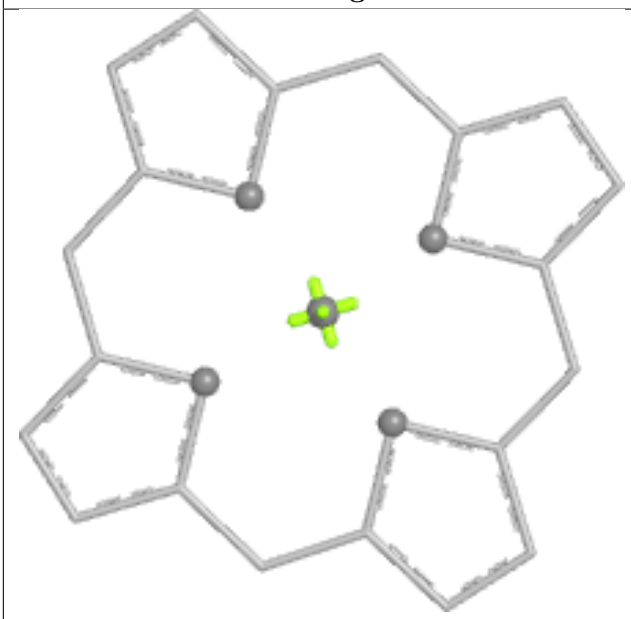
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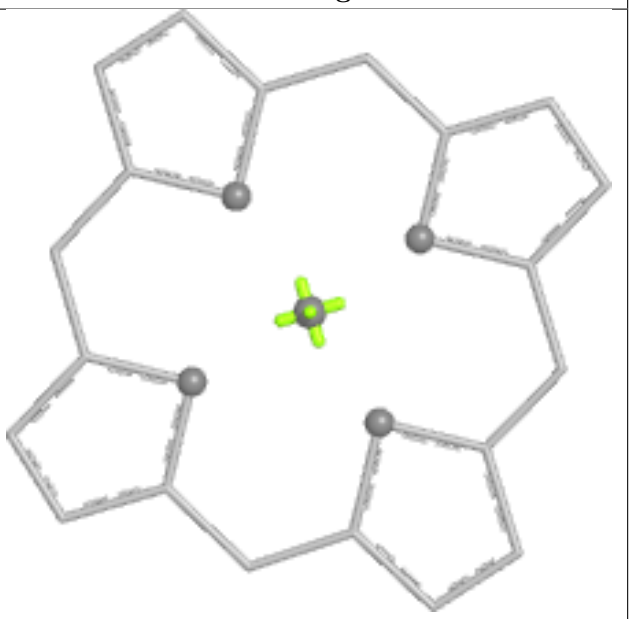
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Bond angles

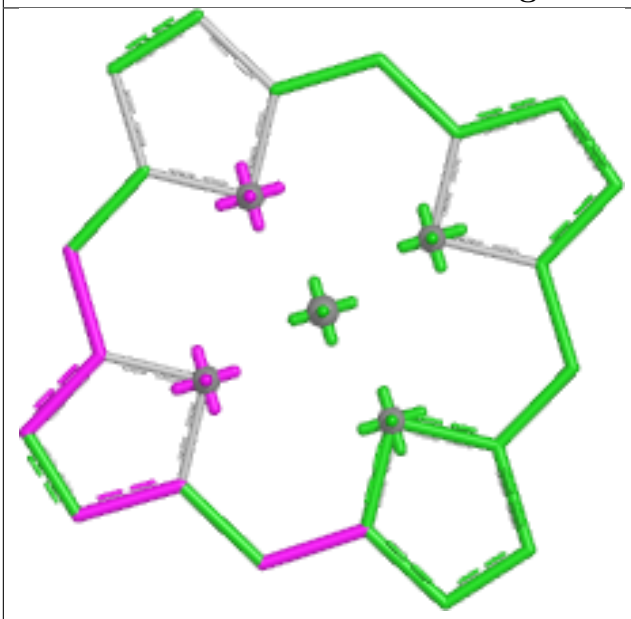


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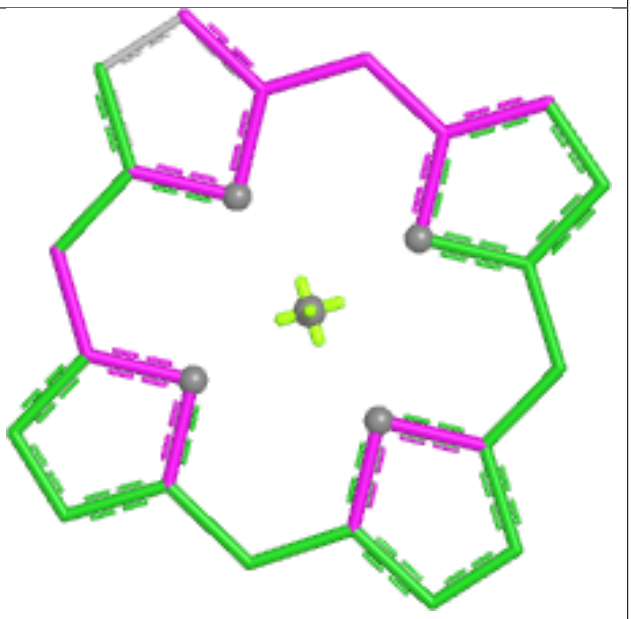


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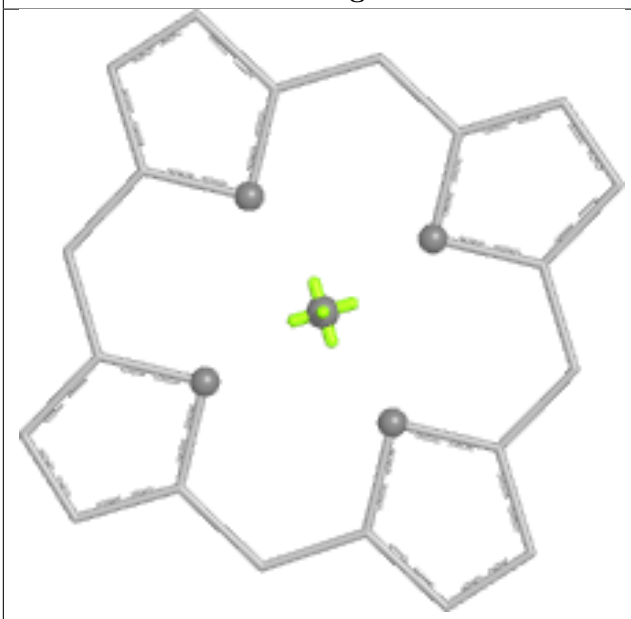
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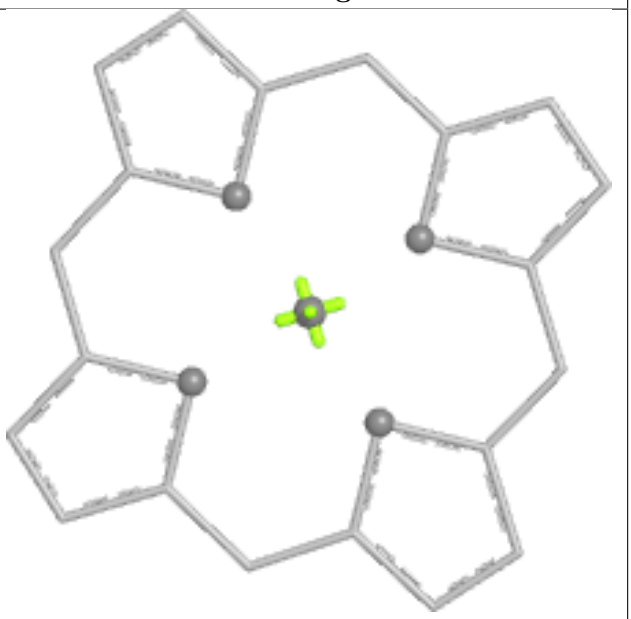
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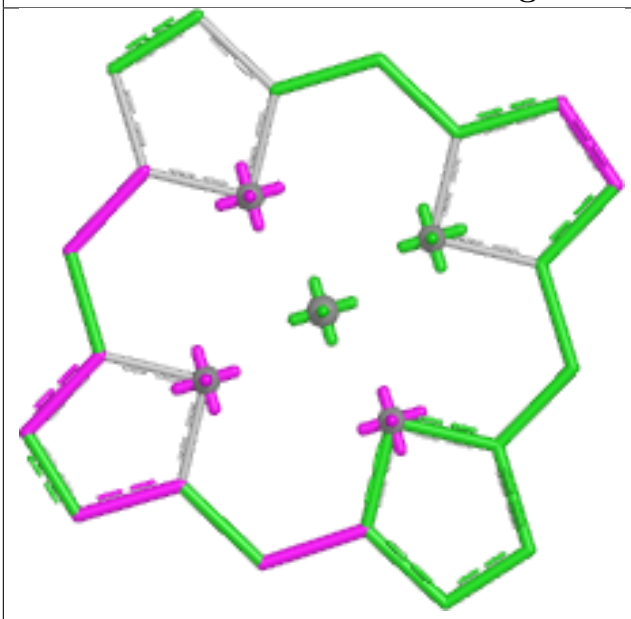


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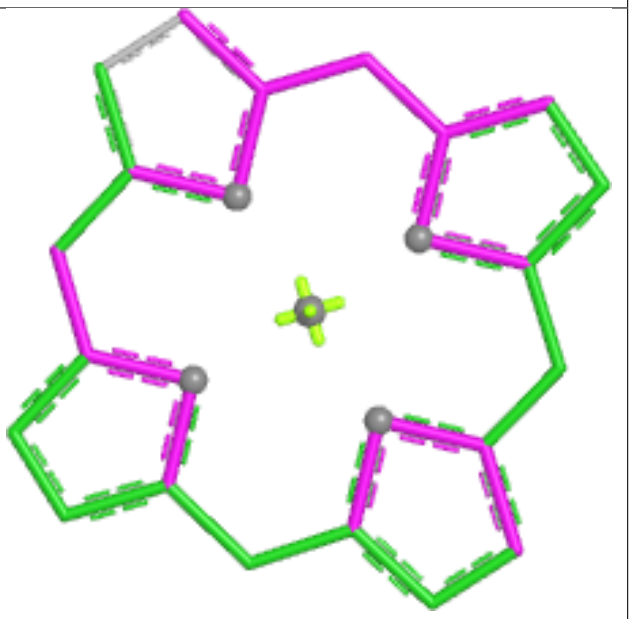


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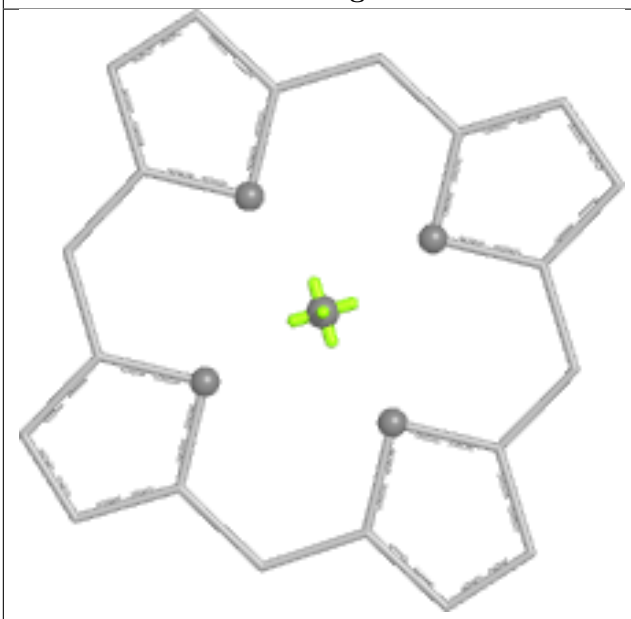
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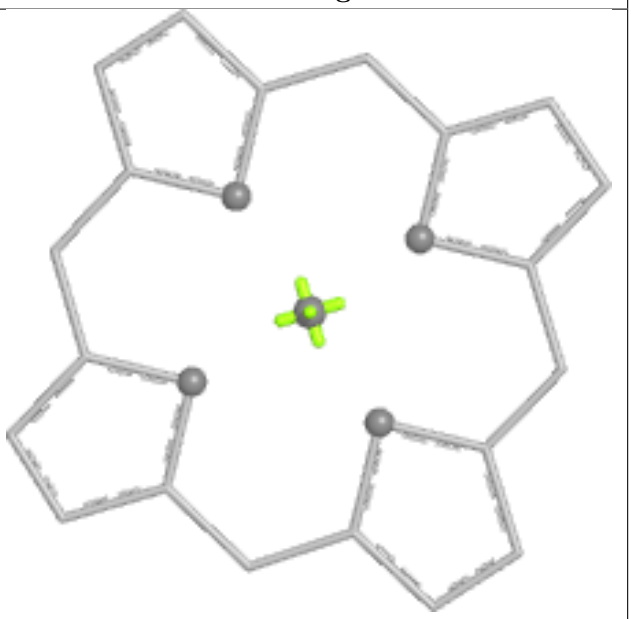
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Bond angles

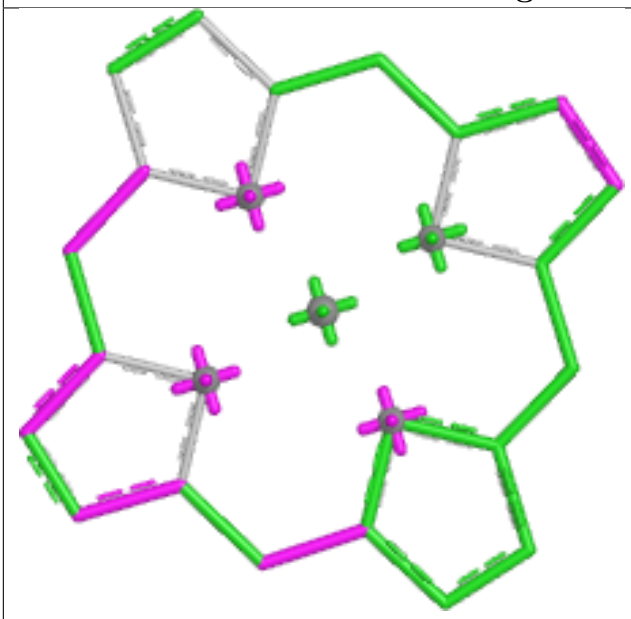


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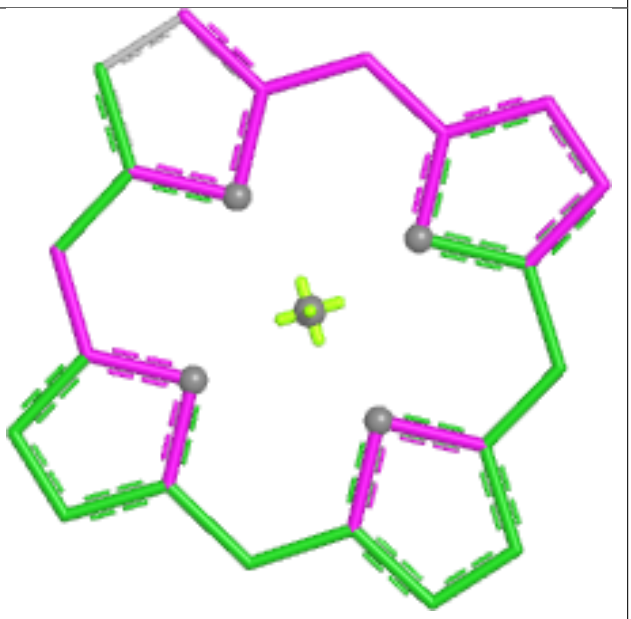


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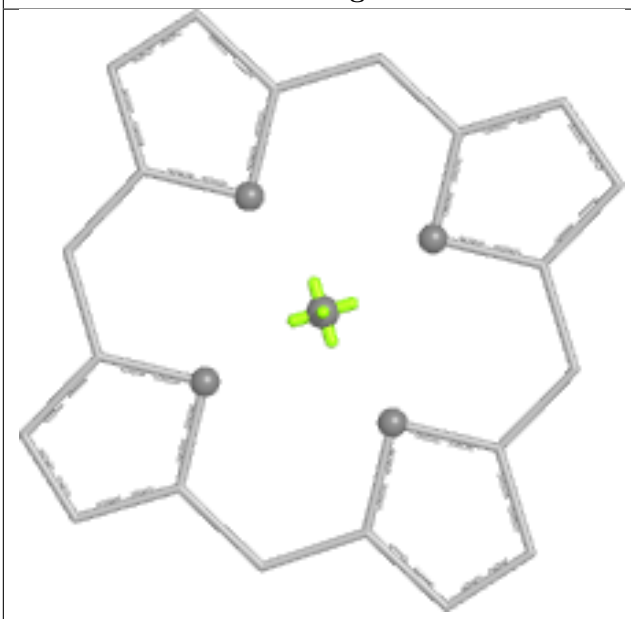
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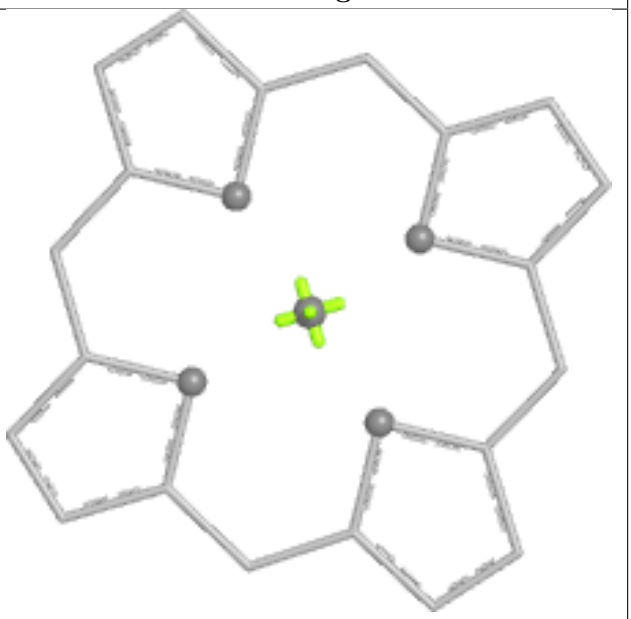
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Bond angles

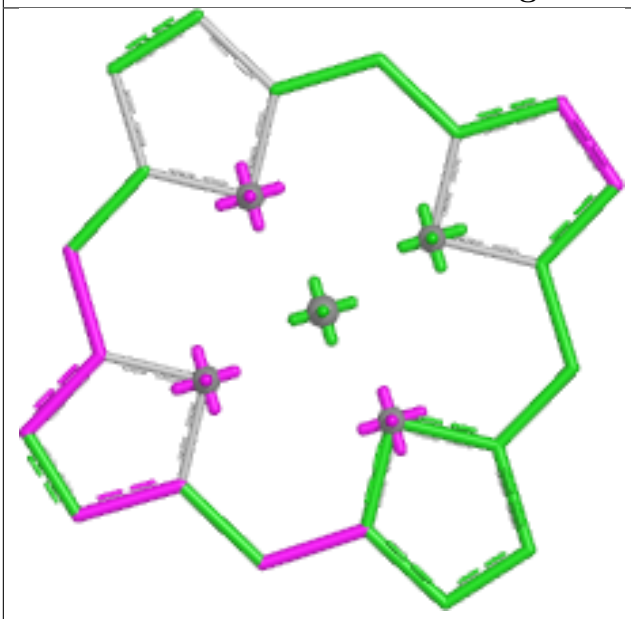


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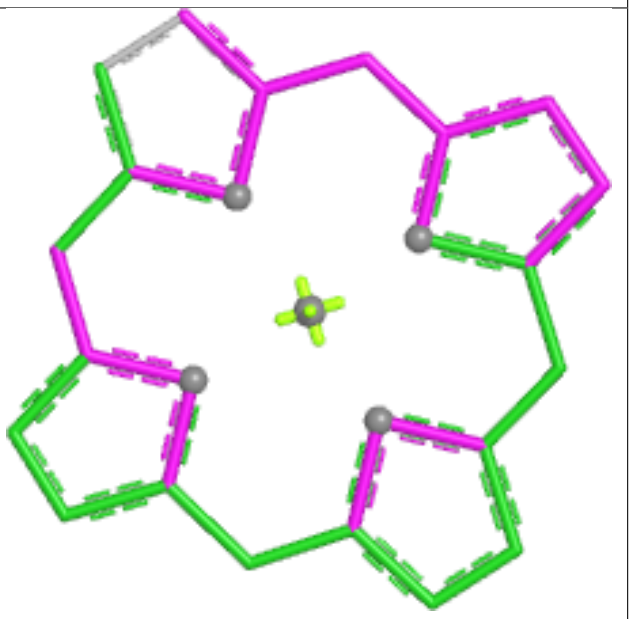


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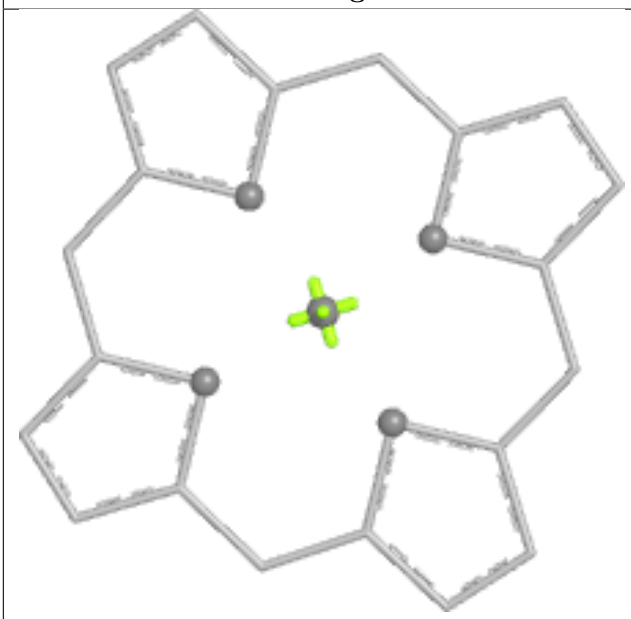
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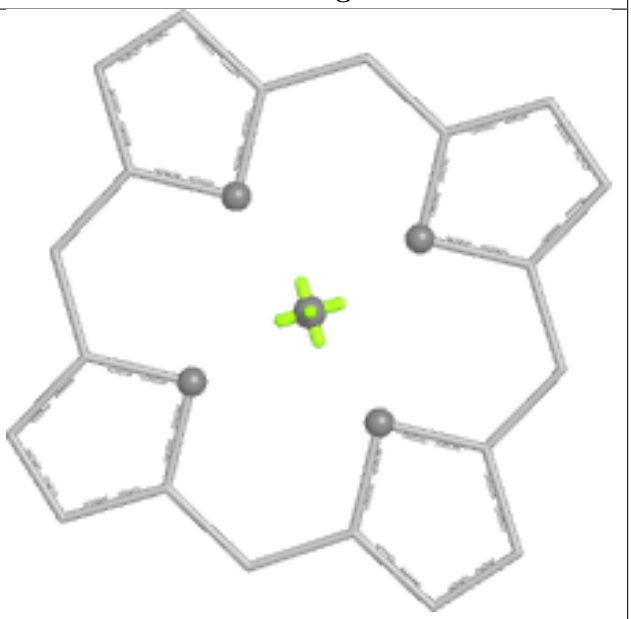
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Bond angles

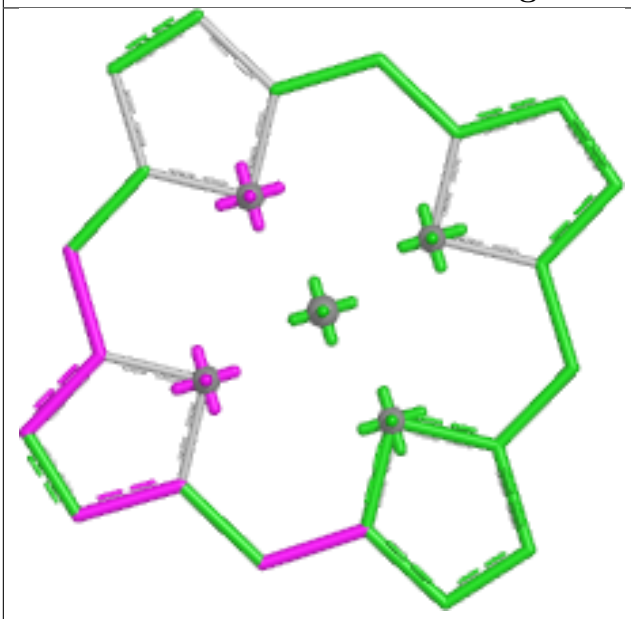


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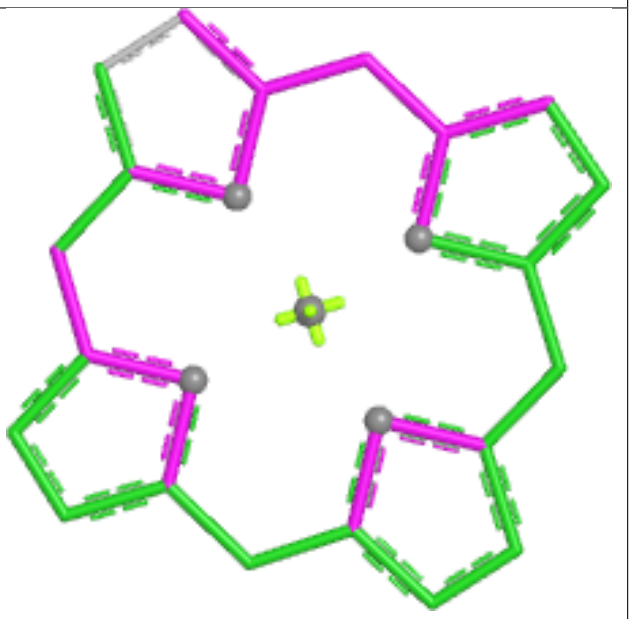


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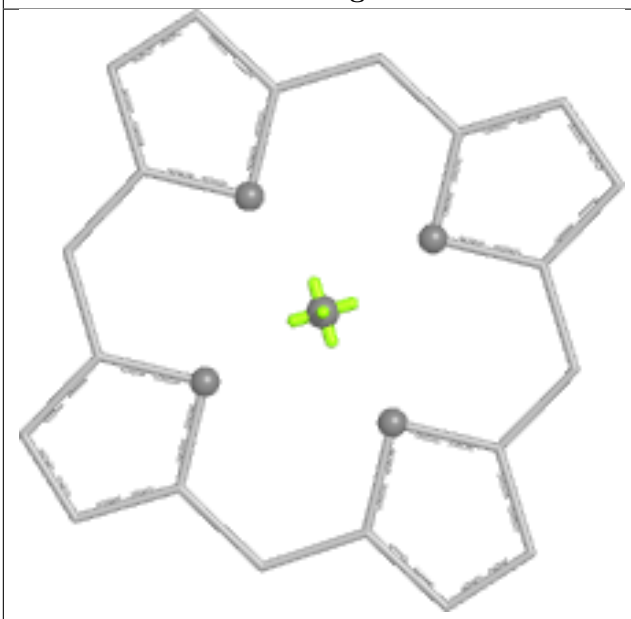
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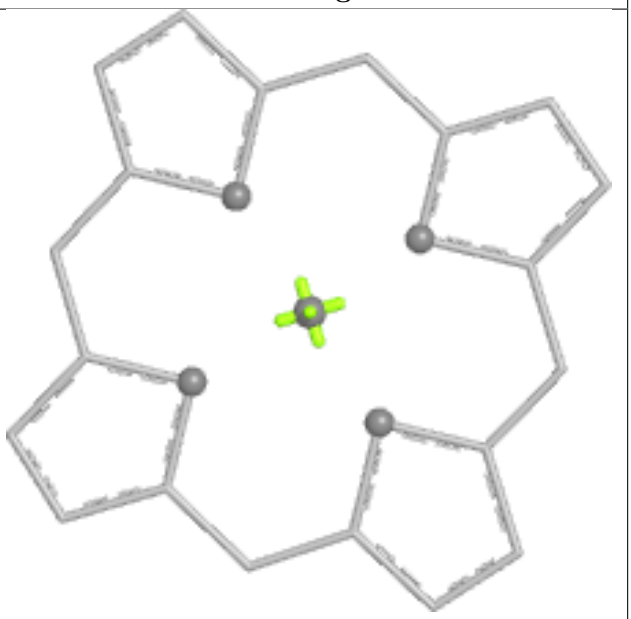
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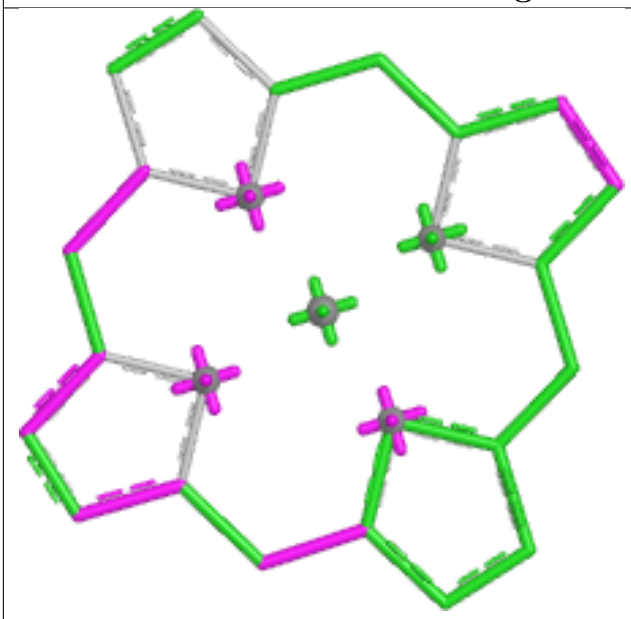


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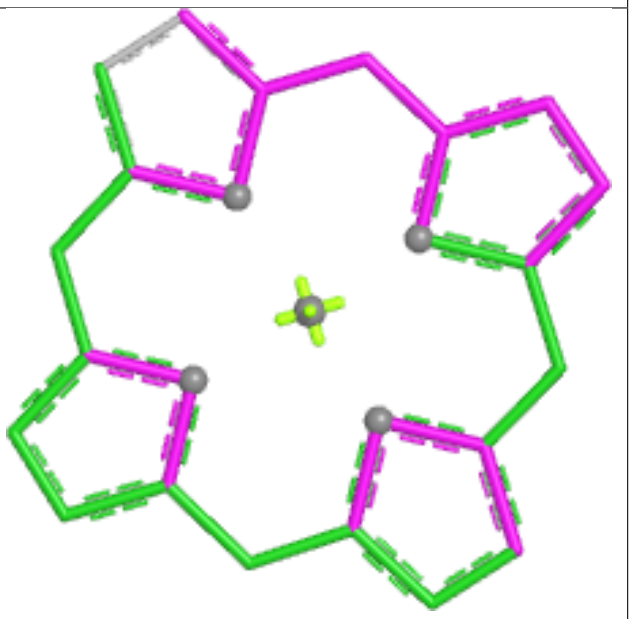


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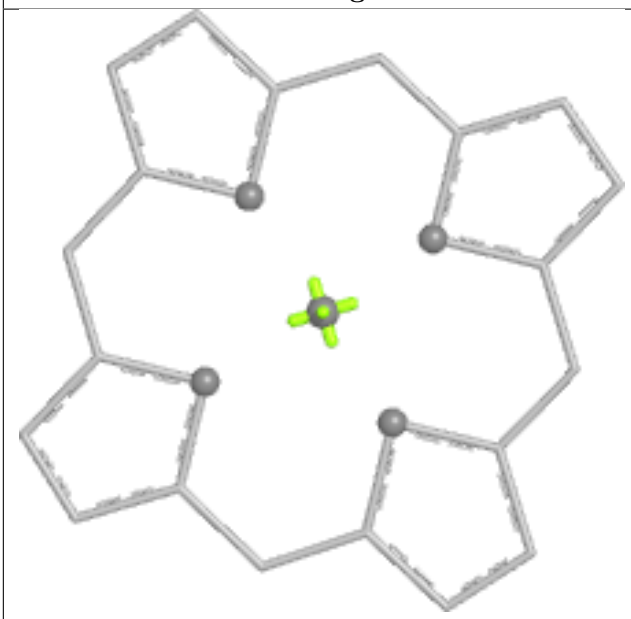
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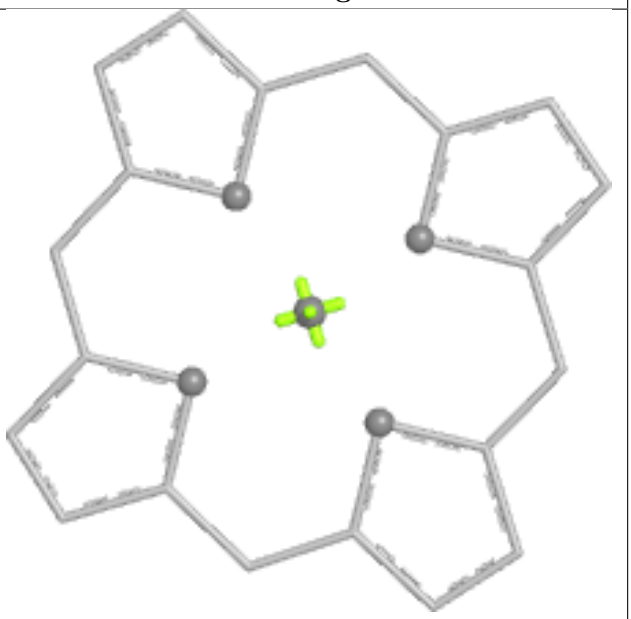
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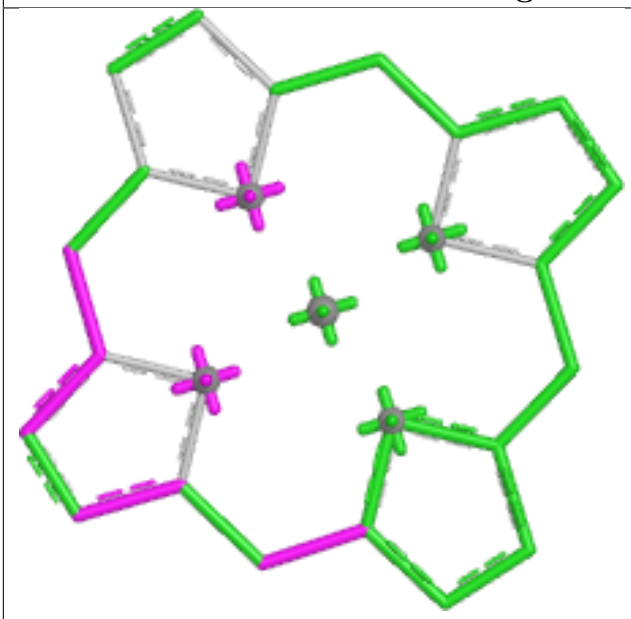


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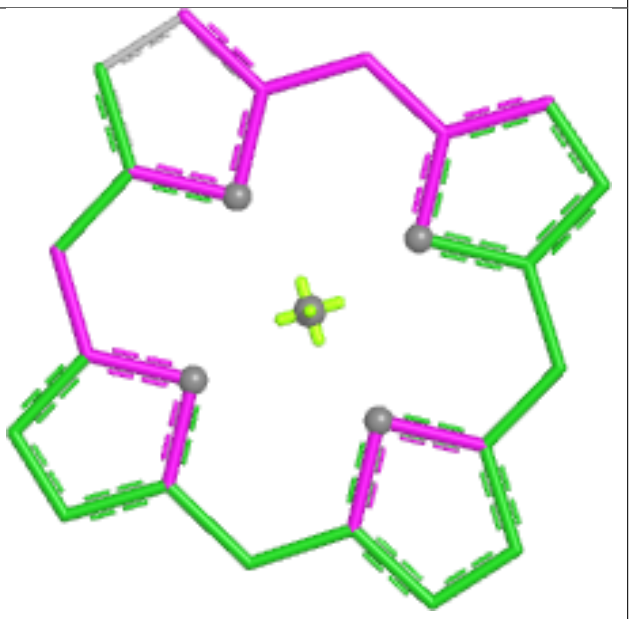


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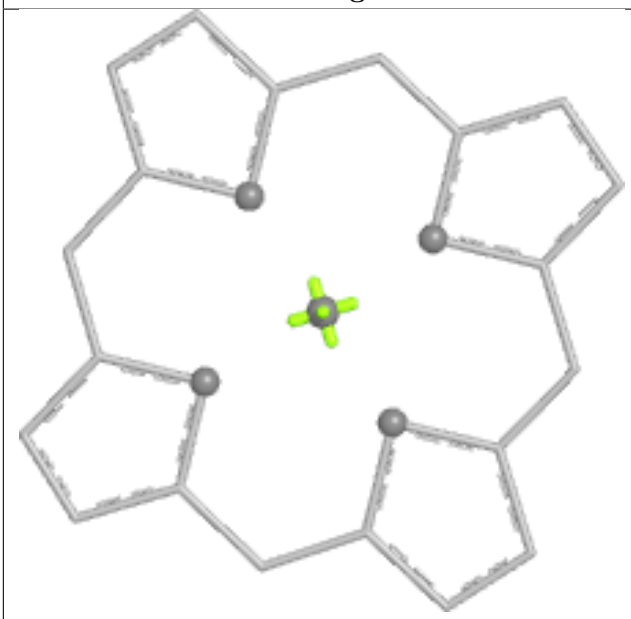
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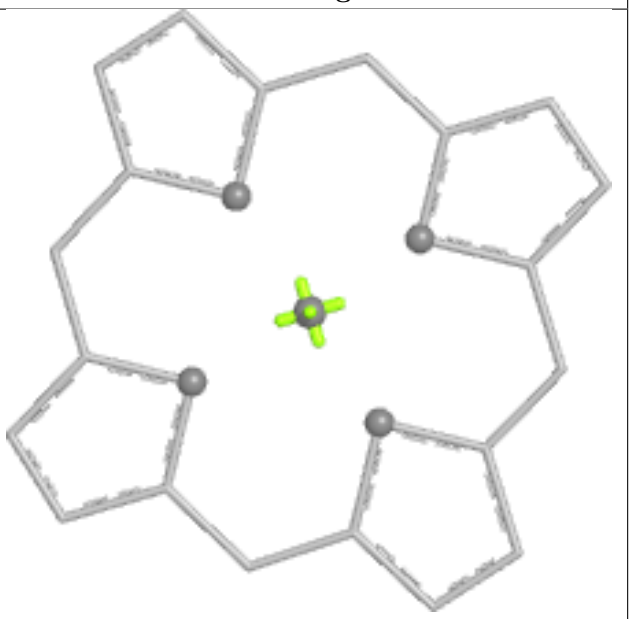
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Bond angles

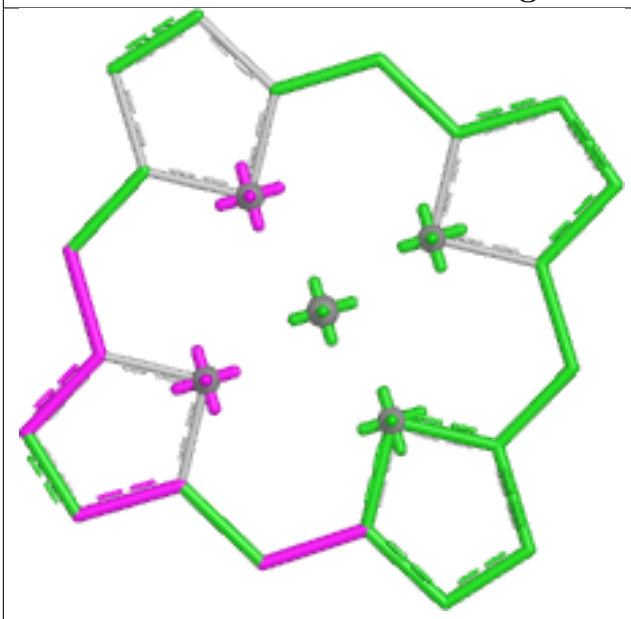


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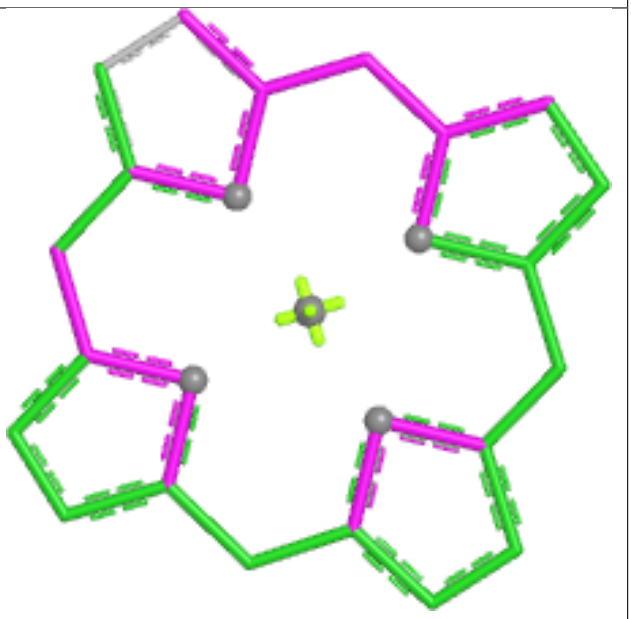


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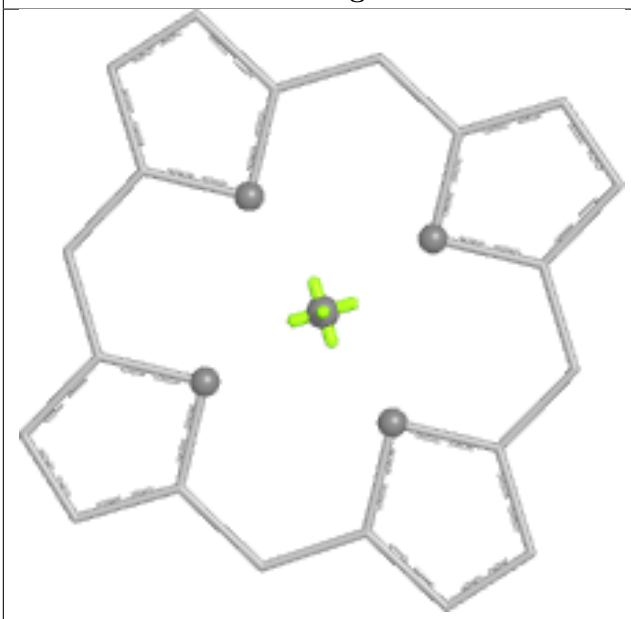
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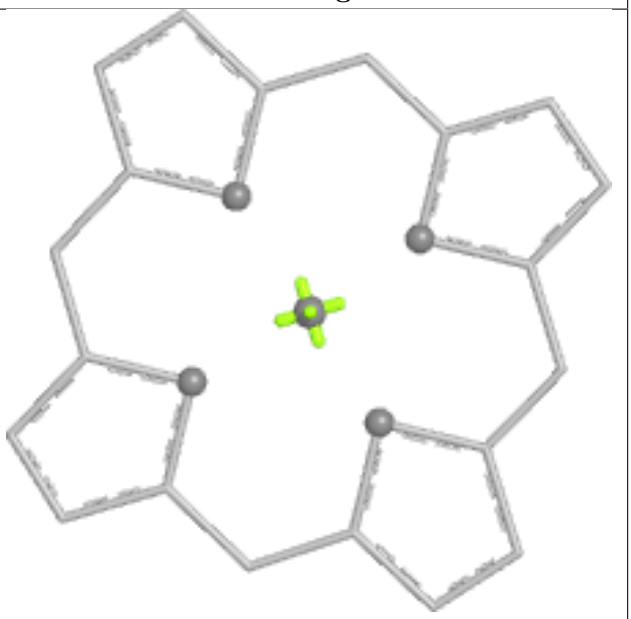
Bond lengths



Bond angles

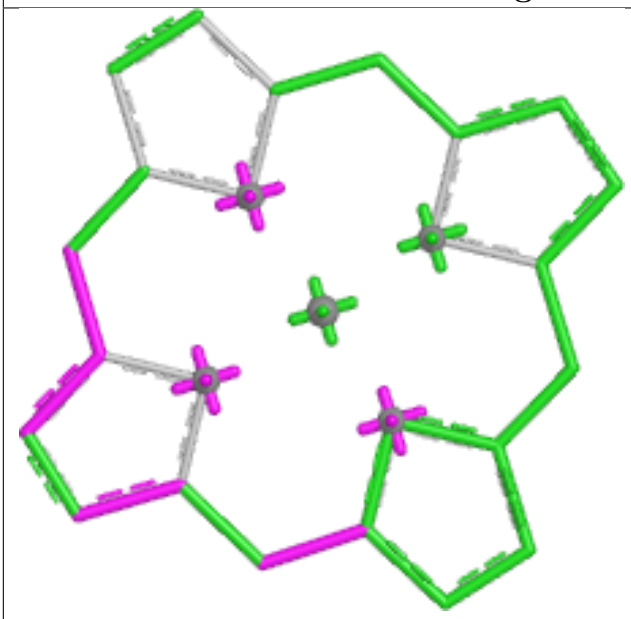


Torsions

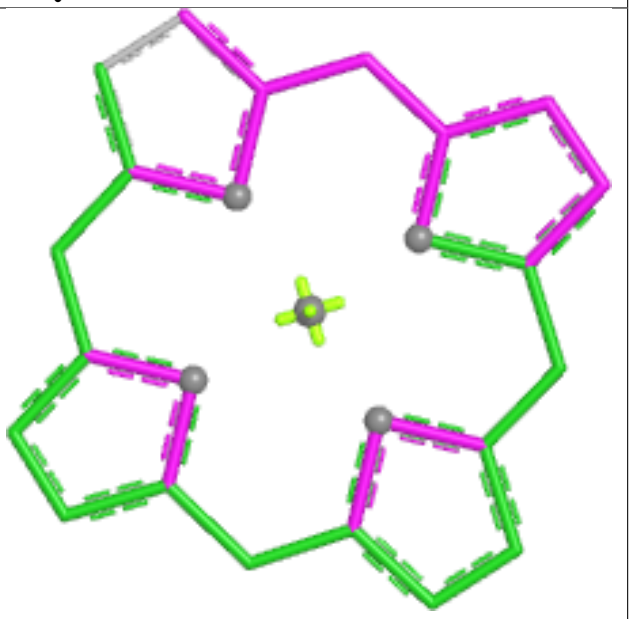


Rings

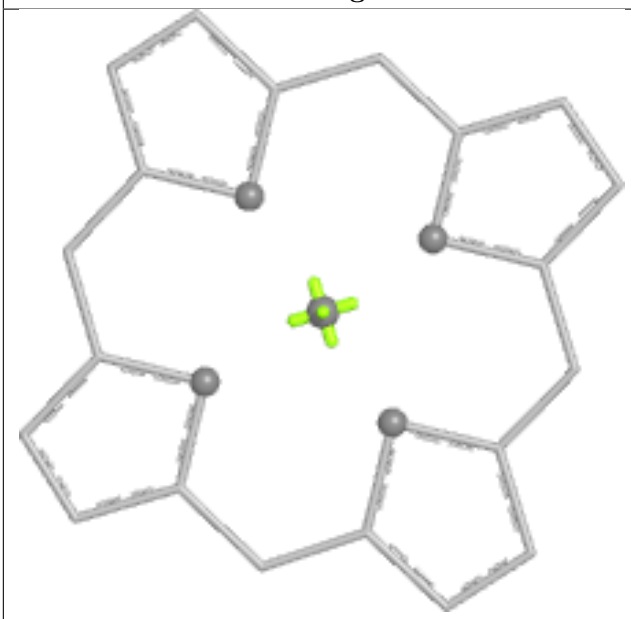
Ligand CLA Q 5236



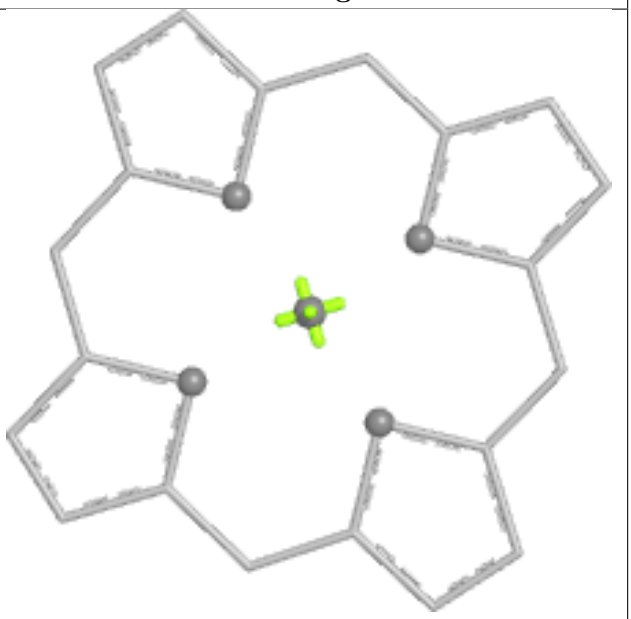
Bond lengths



Bond angles

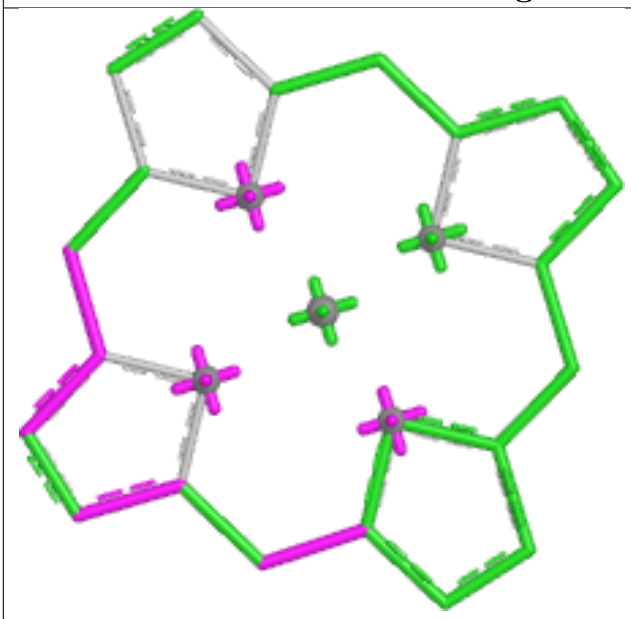


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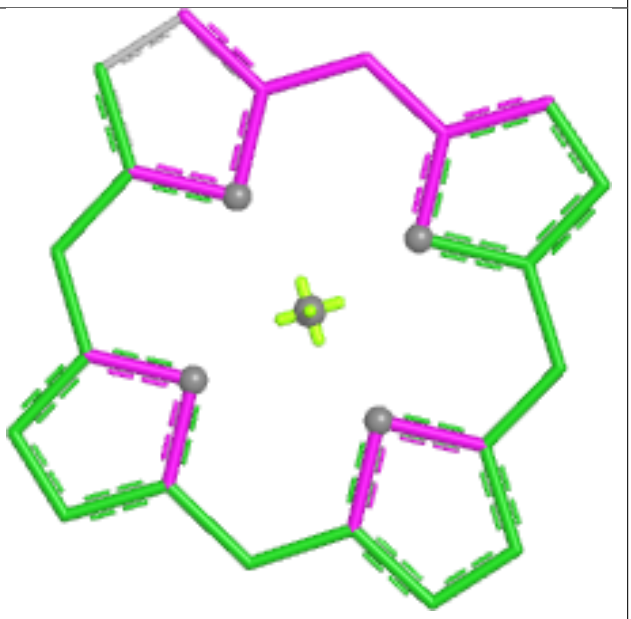


Rings

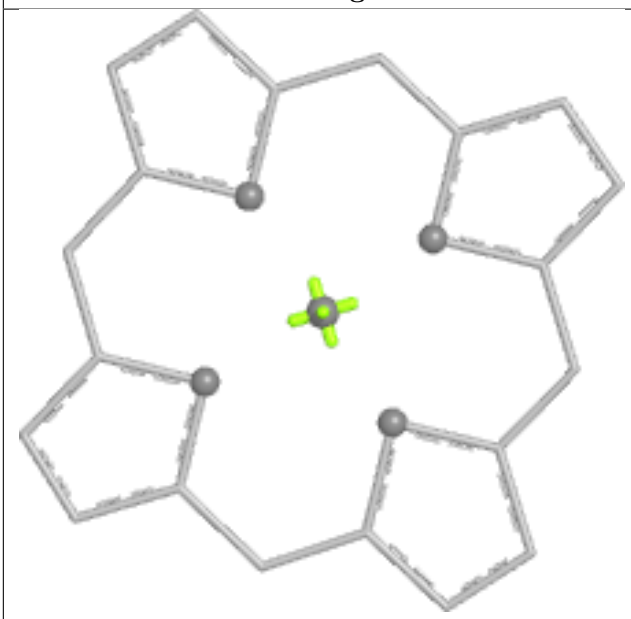
Ligand CLA B 1211



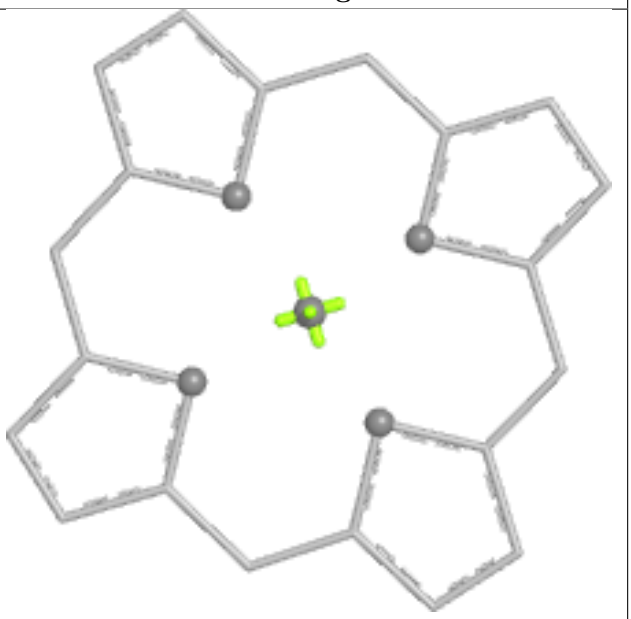
Bond lengths



Bond angles

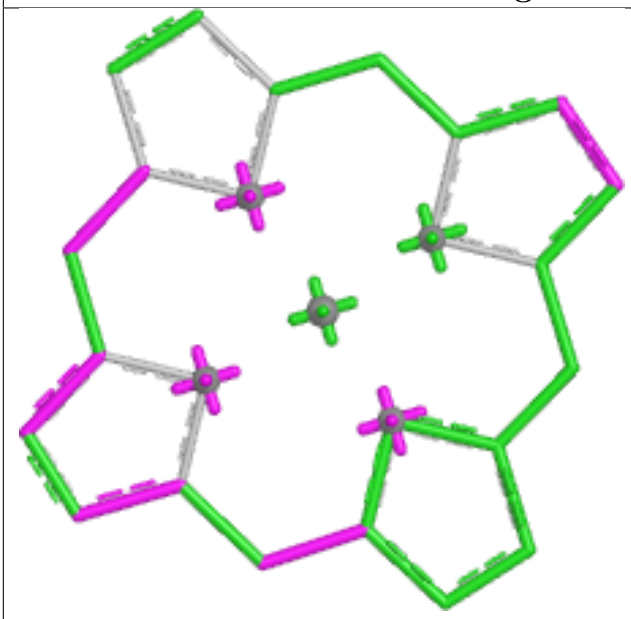


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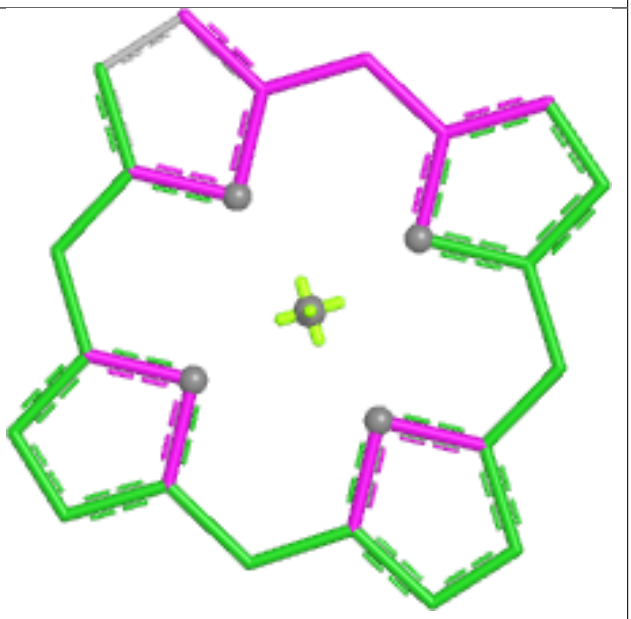


Rings

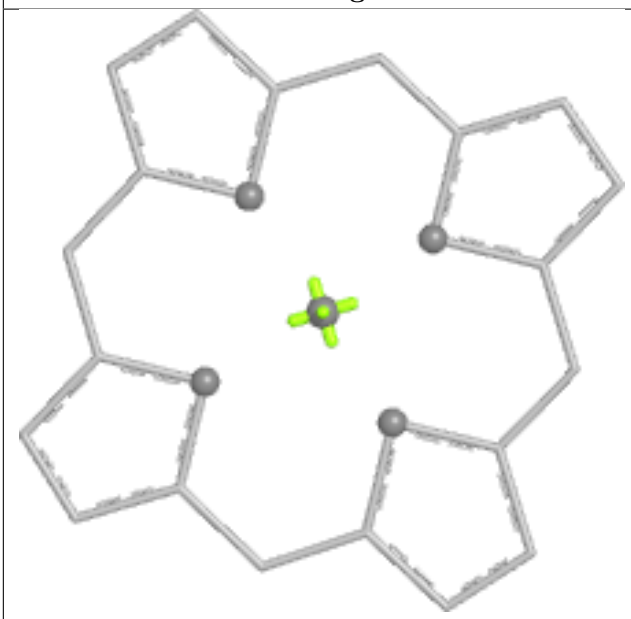
Ligand CLA V 5233



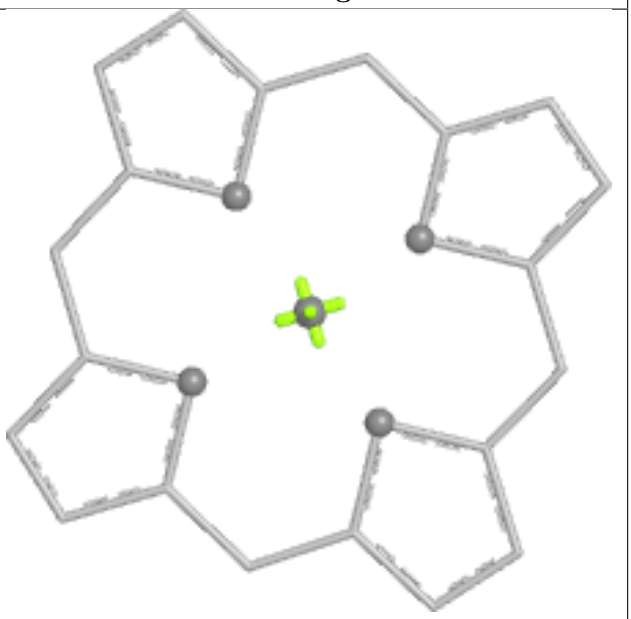
Bond lengths



Bond angles

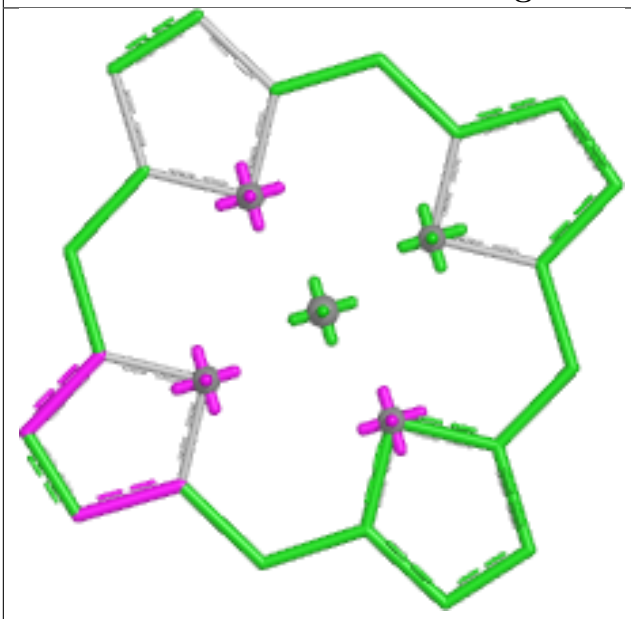


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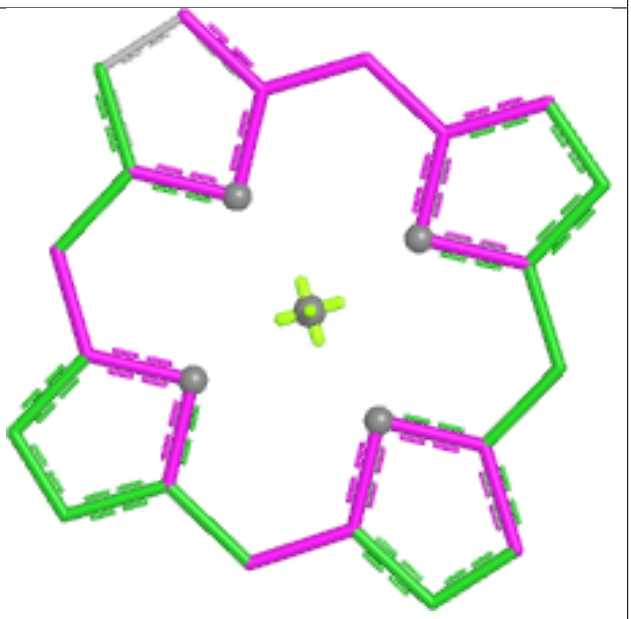


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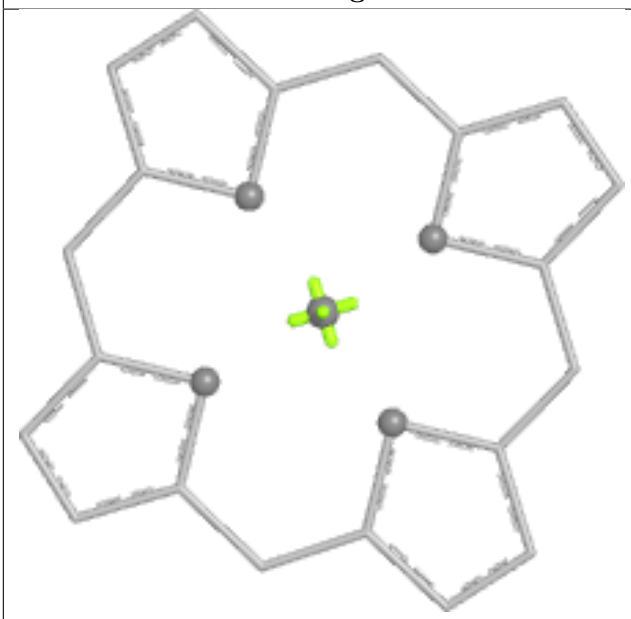
Ligand CLA A 1108



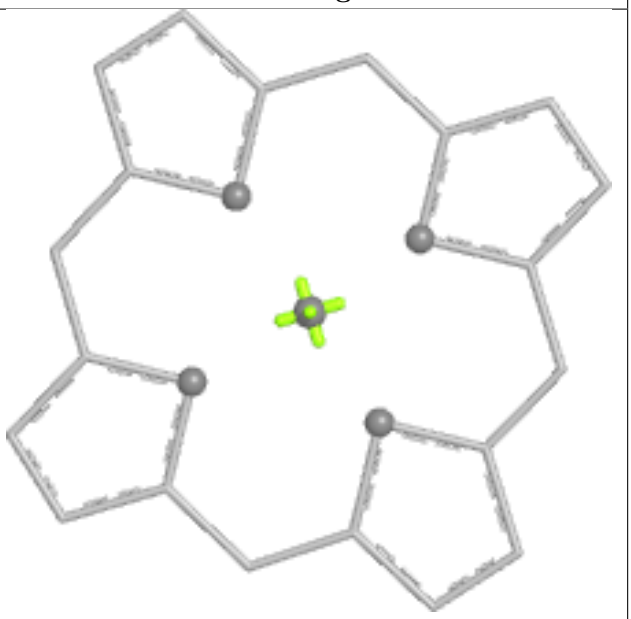
Bond lengths



Bond angles

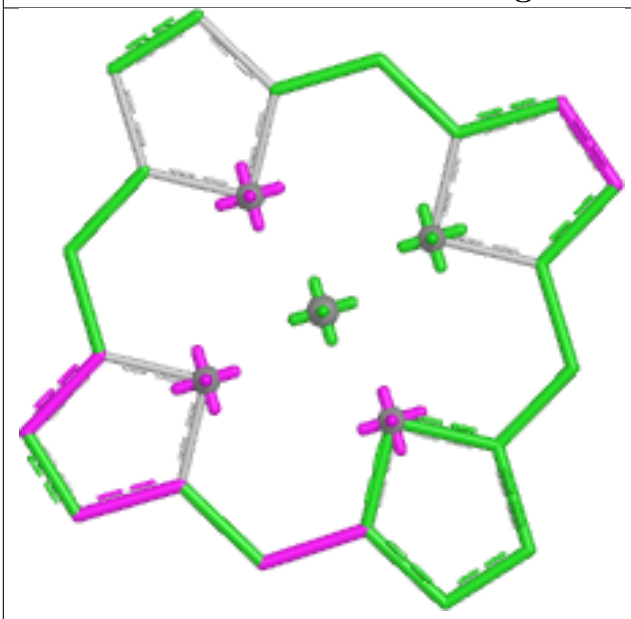


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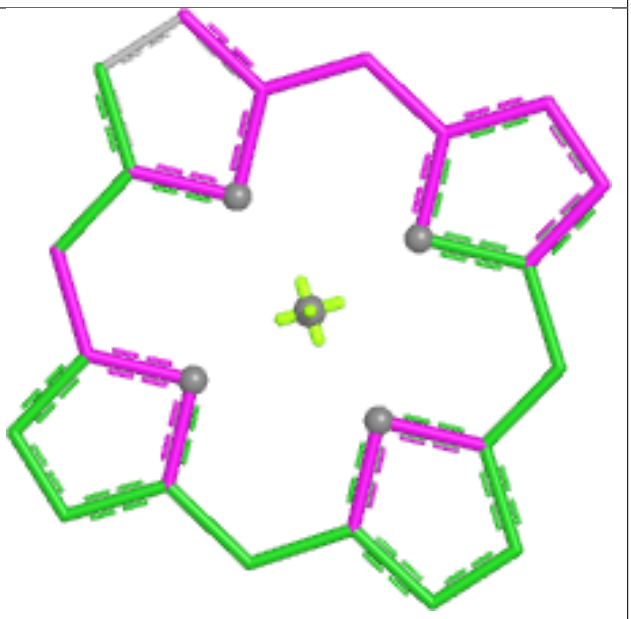


Rings

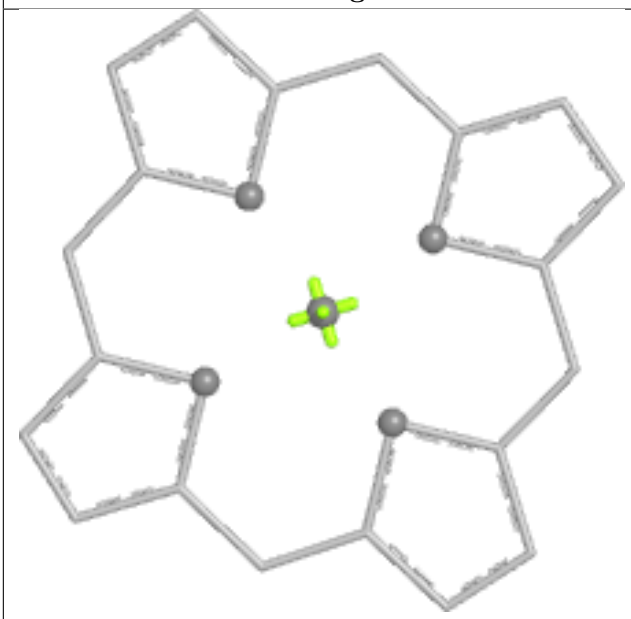
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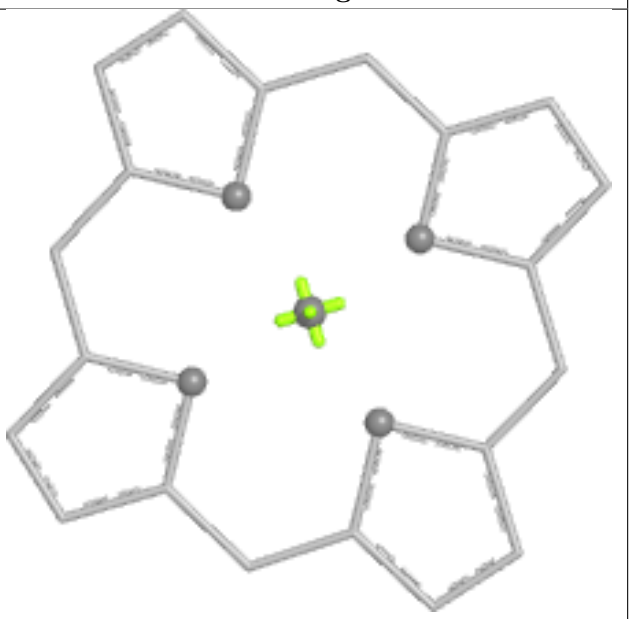
Bond lengths



Bond angles

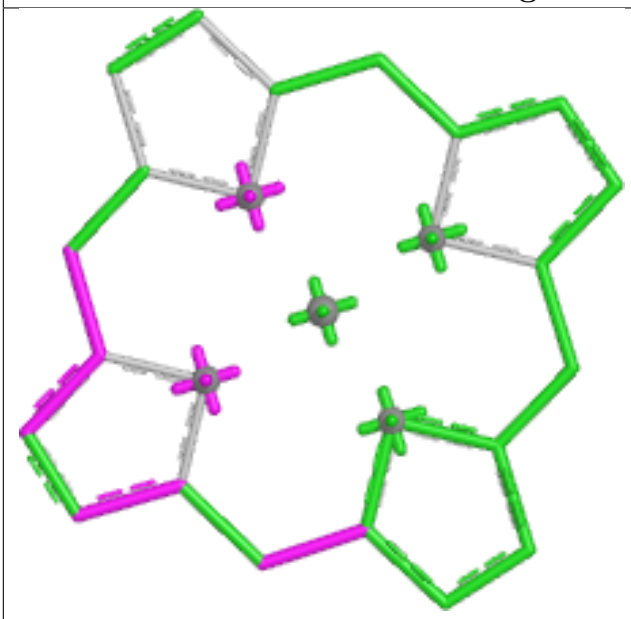


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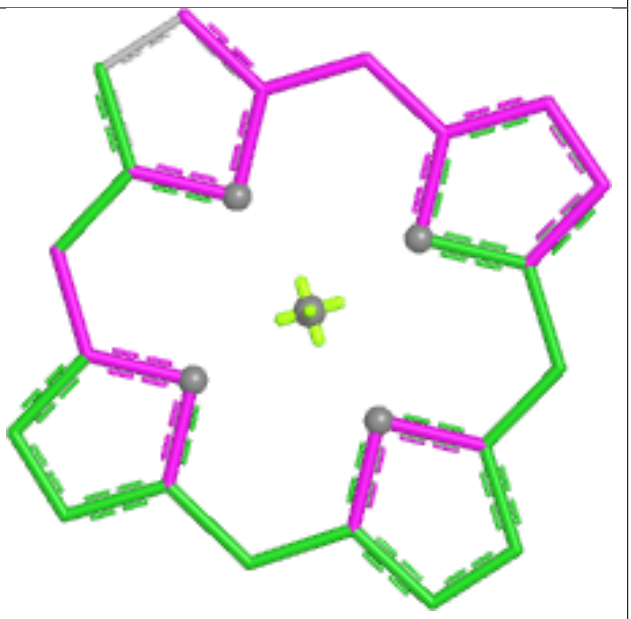


Rings

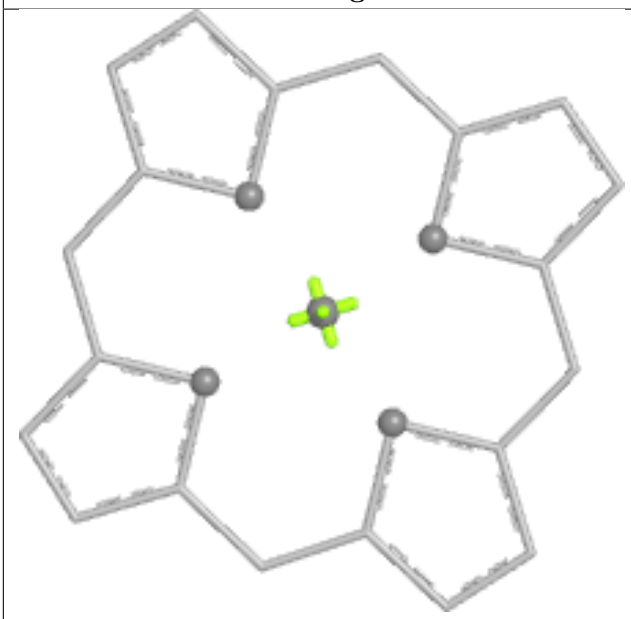
Ligand CLA 9 1021



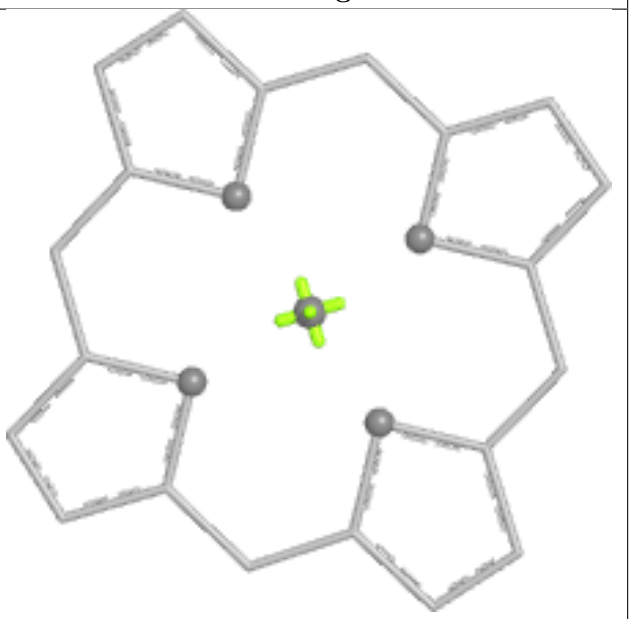
Bond lengths



Bond angles

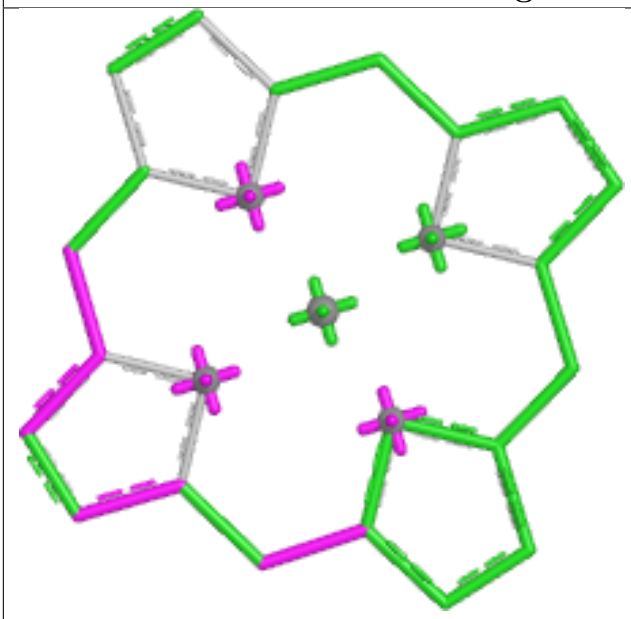


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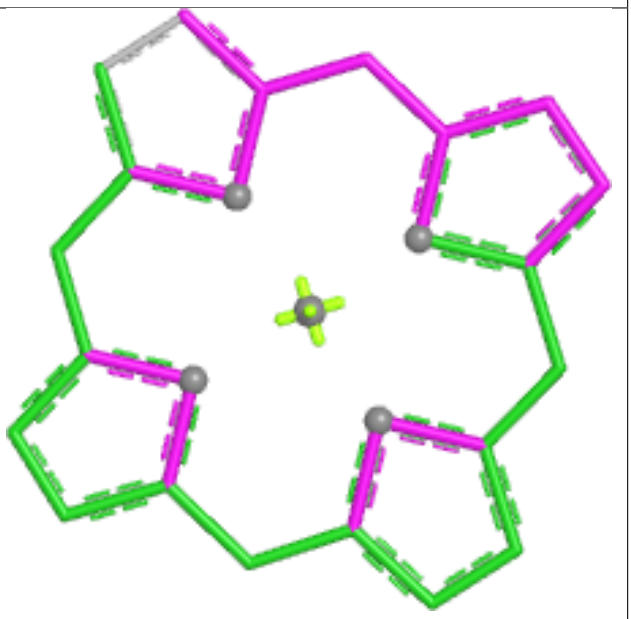


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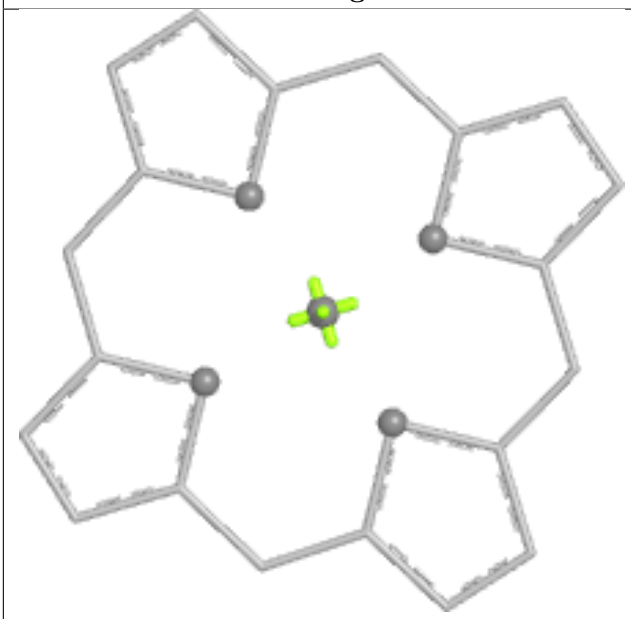
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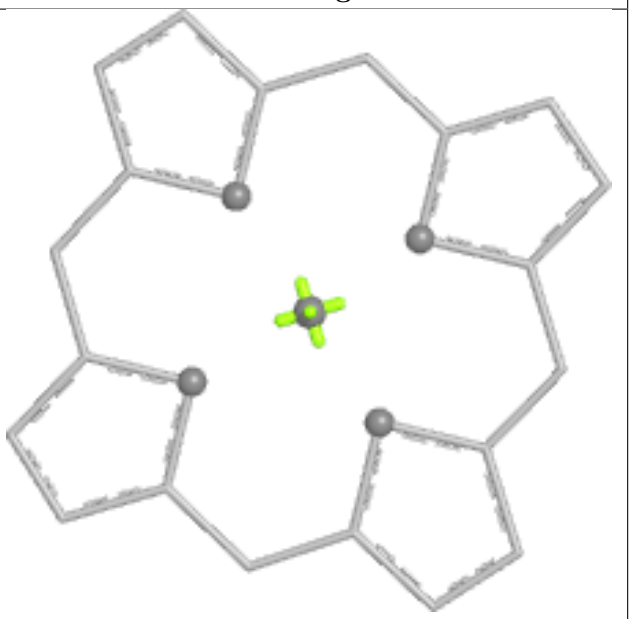
Bond lengths



Bond angles

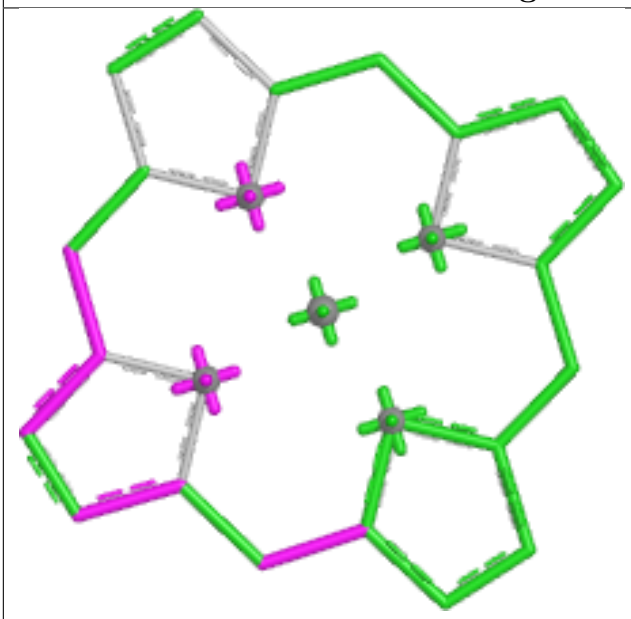


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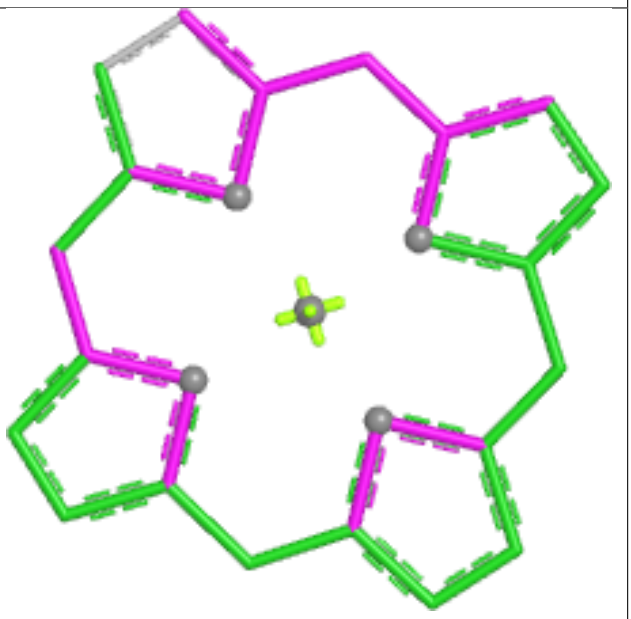


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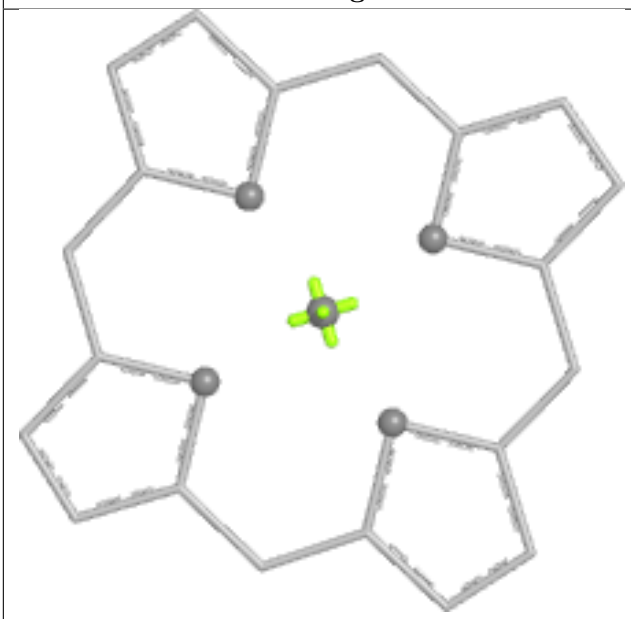
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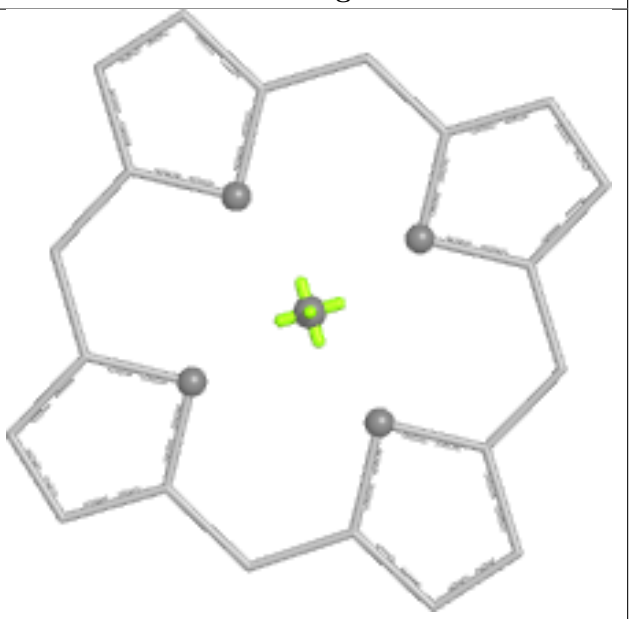
Bond lengths



Bond angles

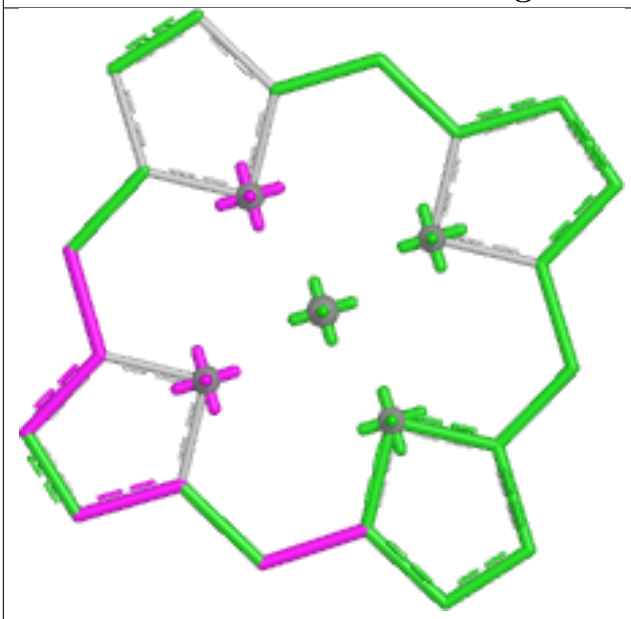


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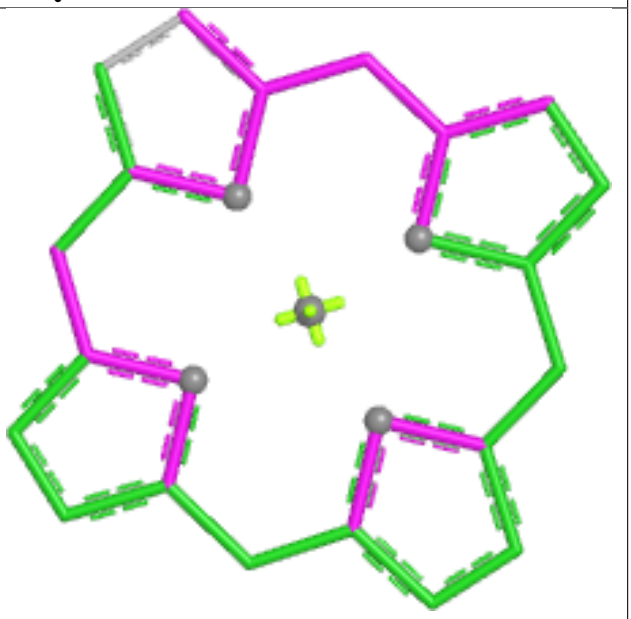


Rings

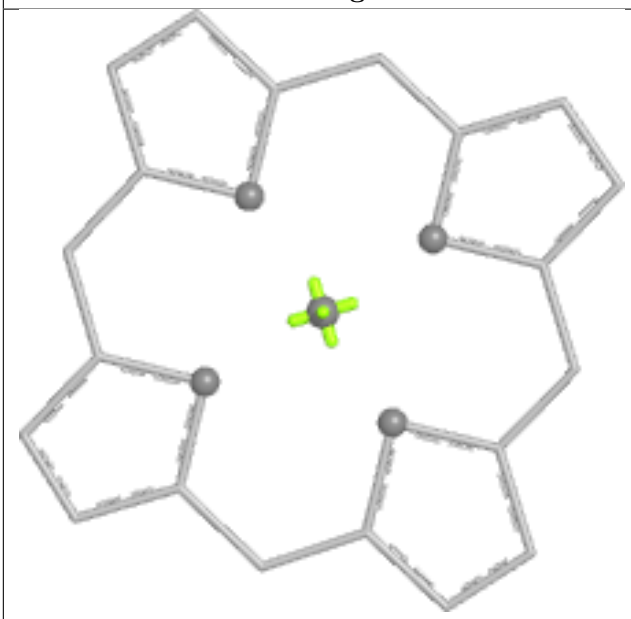
Ligand CLA Q 8001



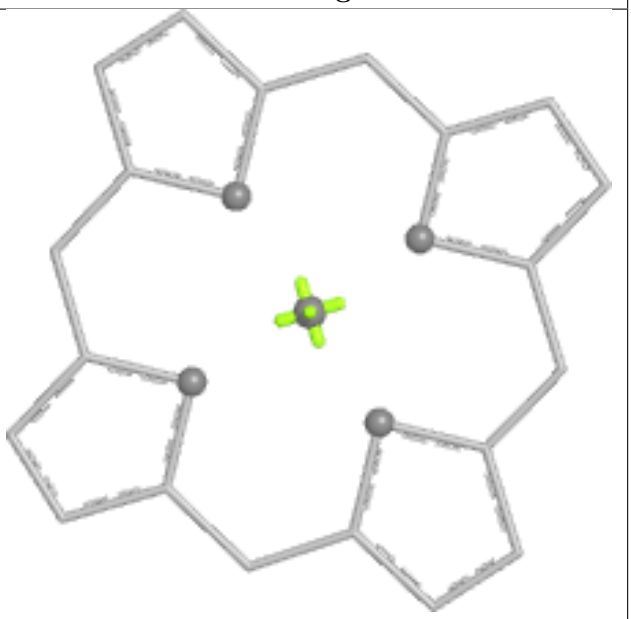
Bond lengths



Bond angles

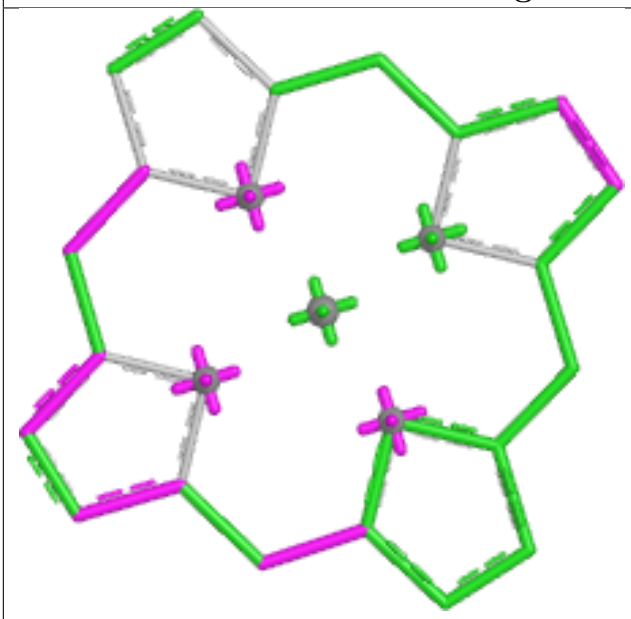


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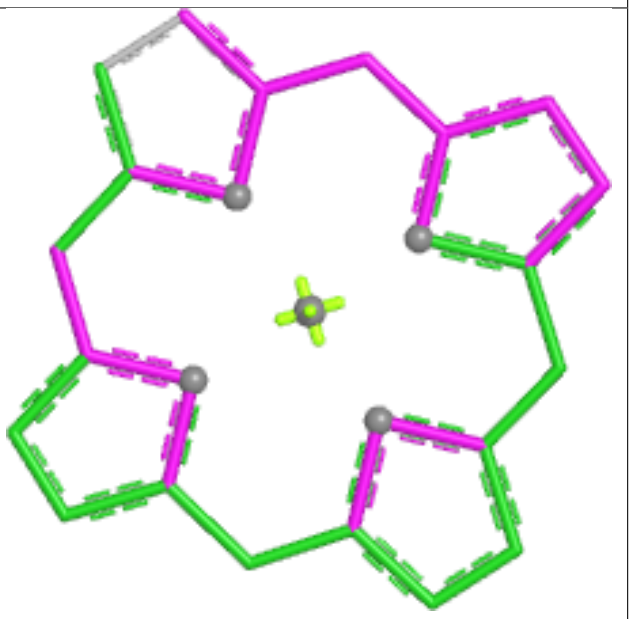


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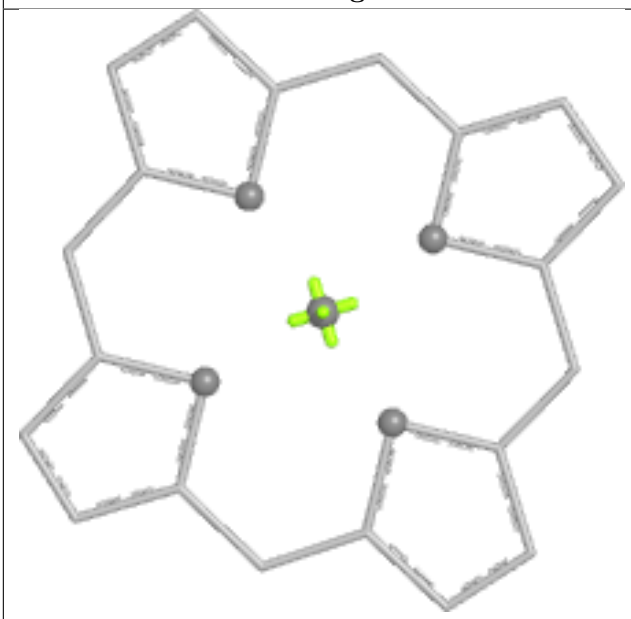
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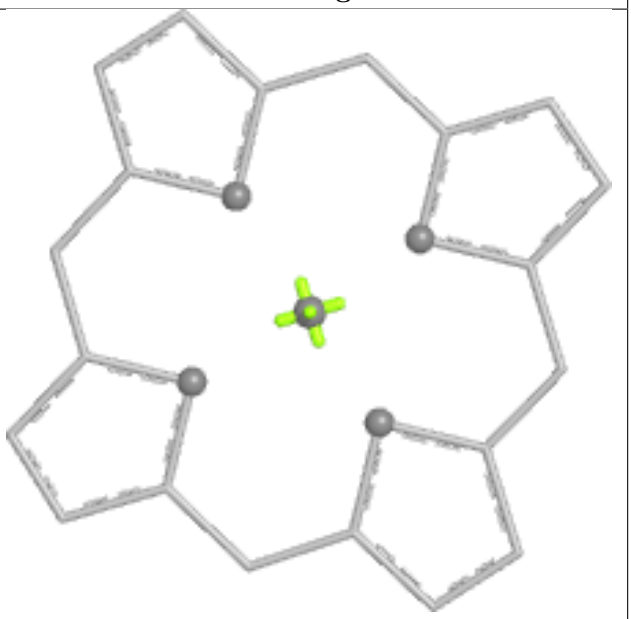
Bond lengths



Bond angles

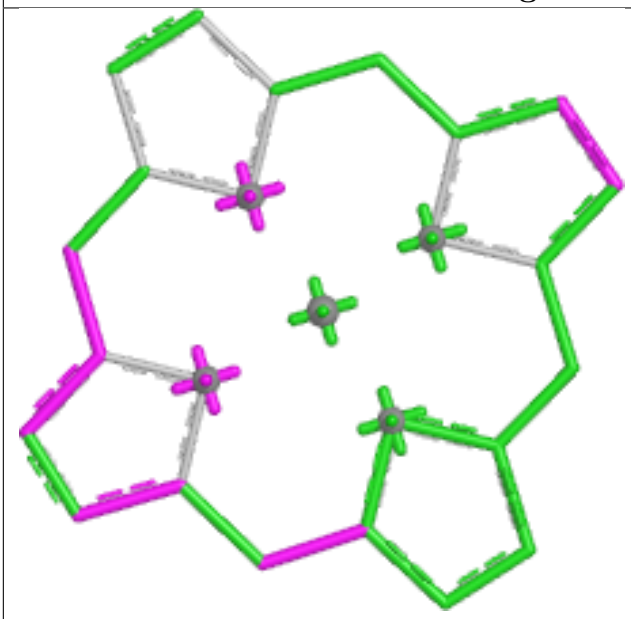


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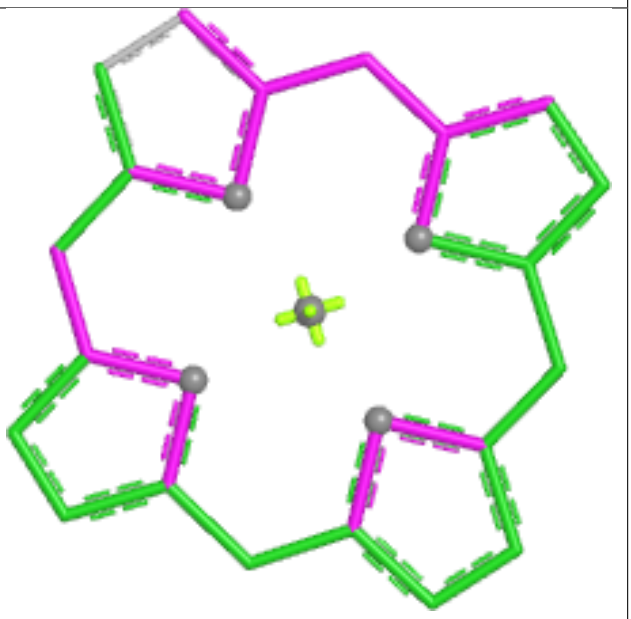


Rings

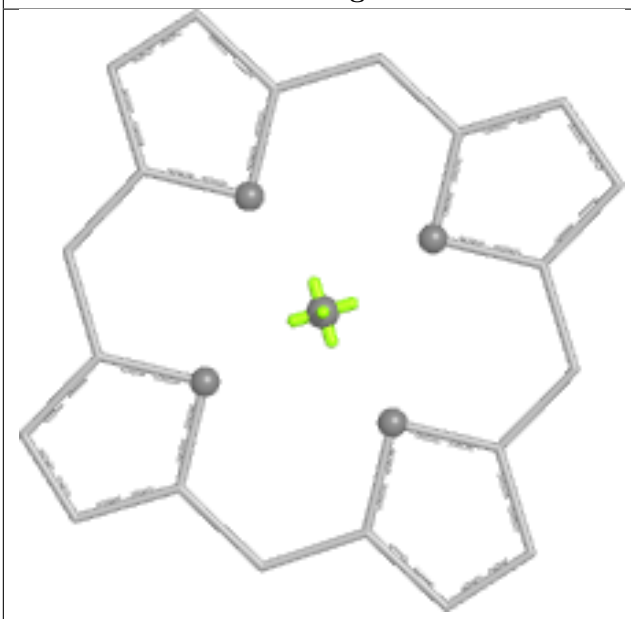
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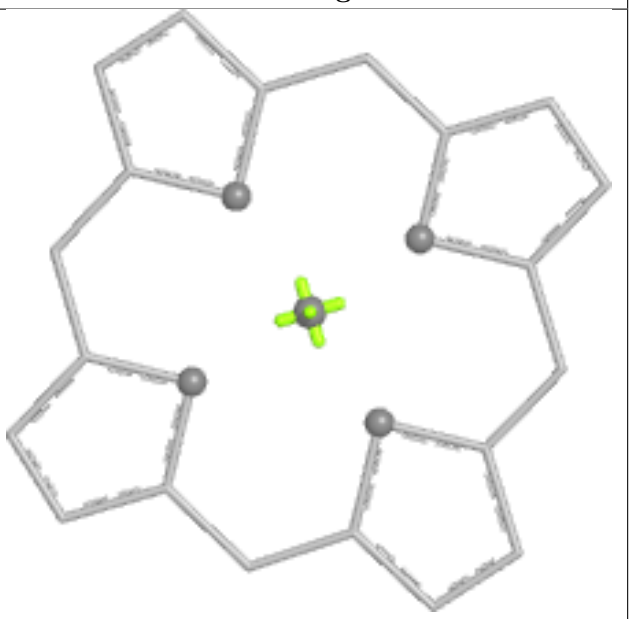
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Bond angles

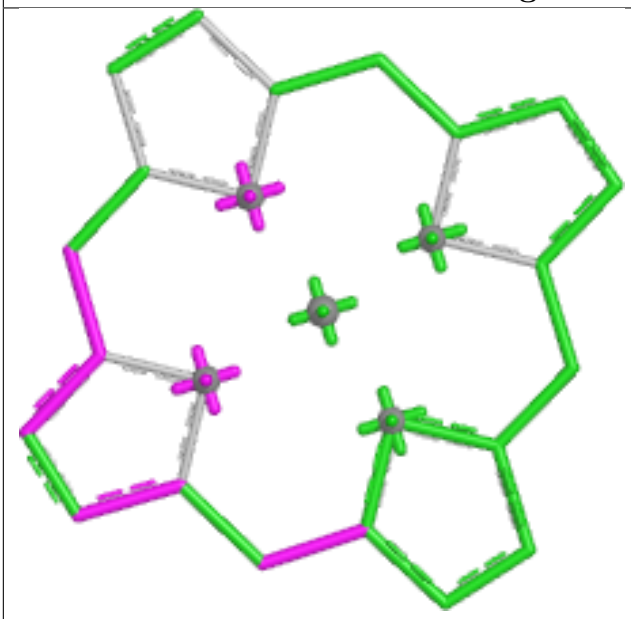


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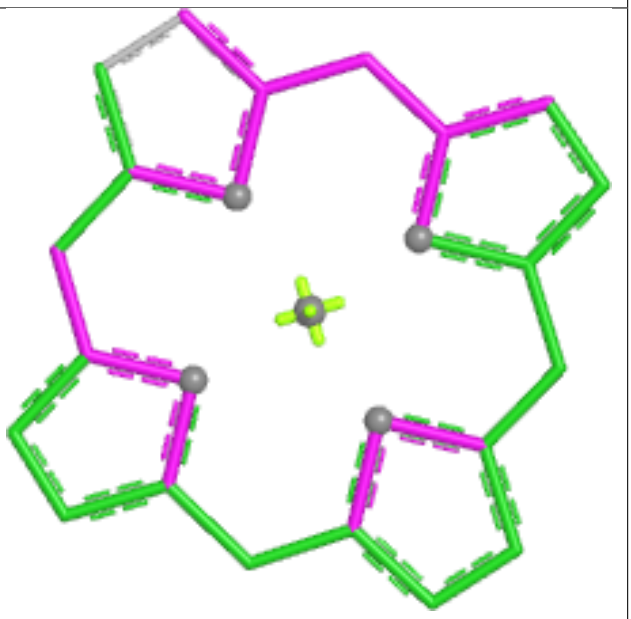


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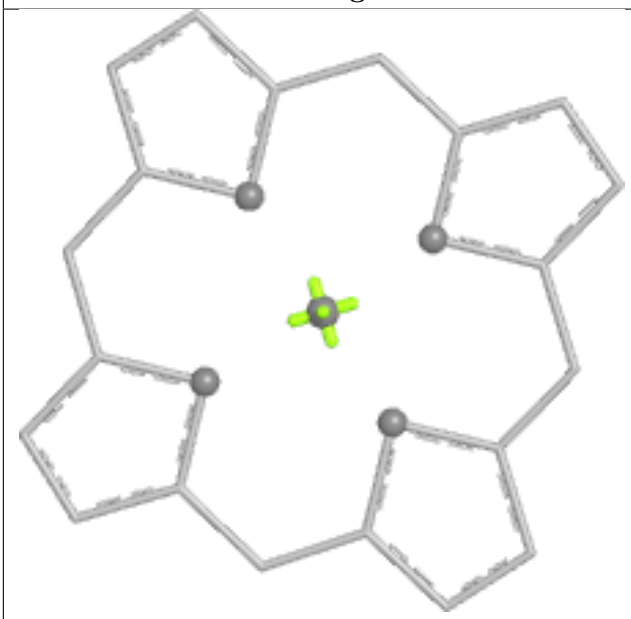
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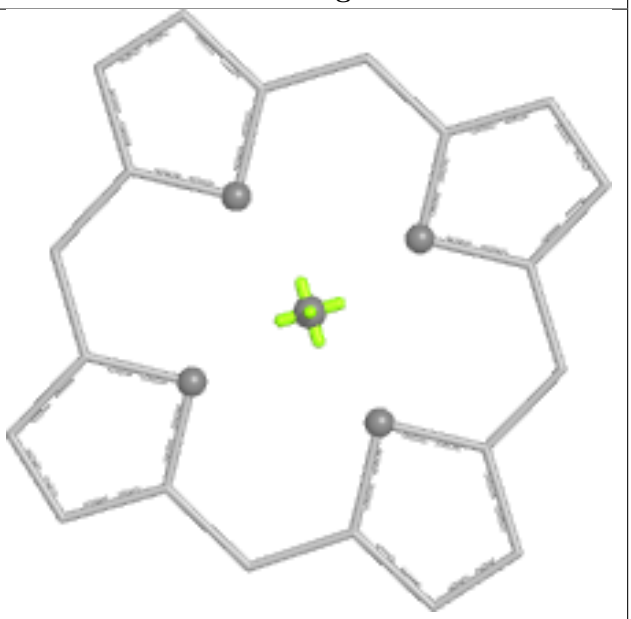
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Bond angles

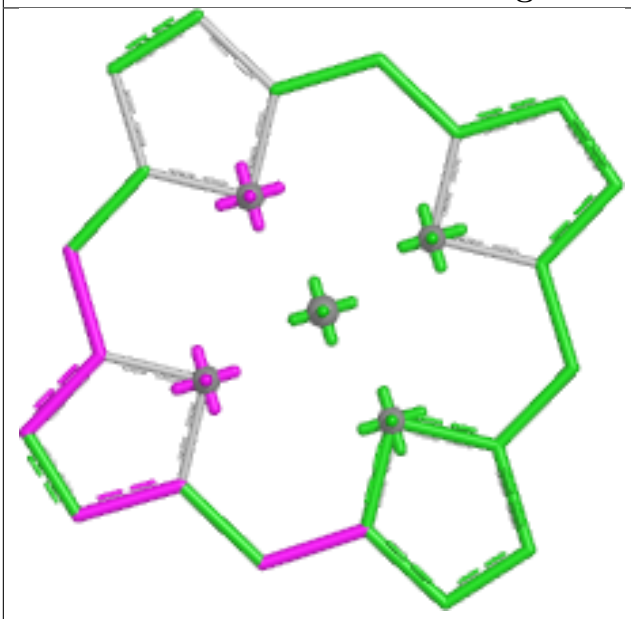


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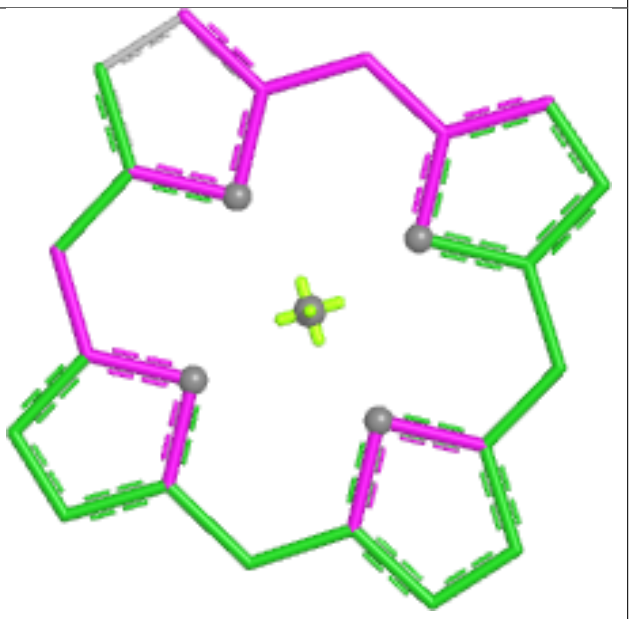


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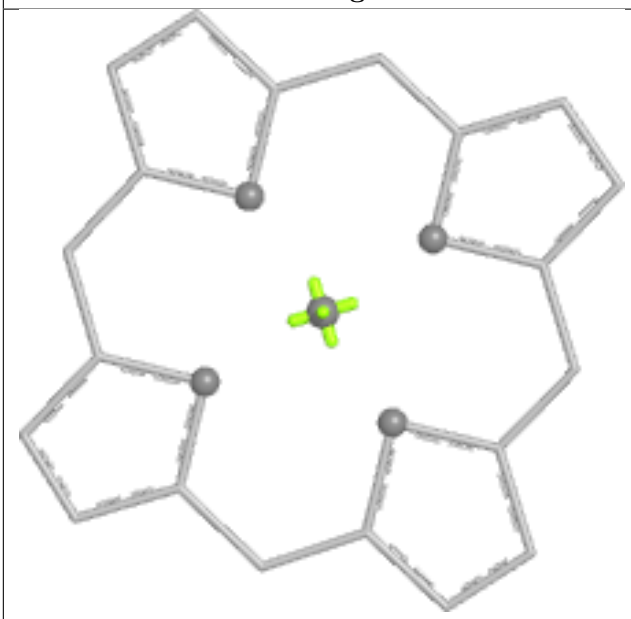
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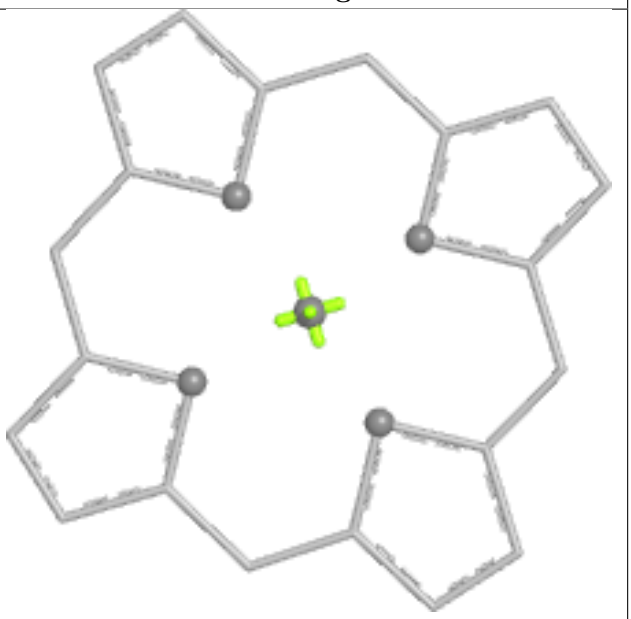
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Bond angles

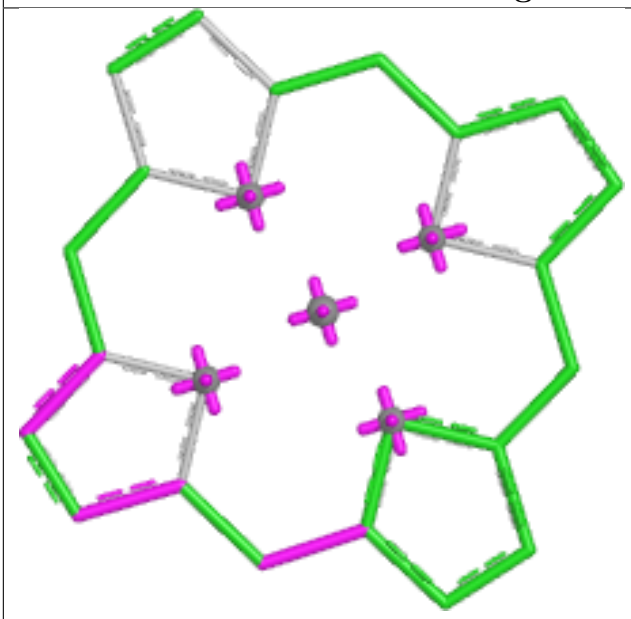


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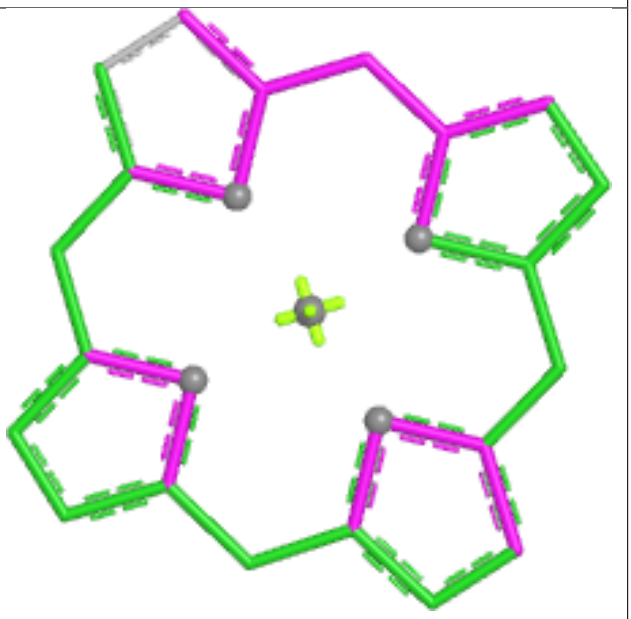


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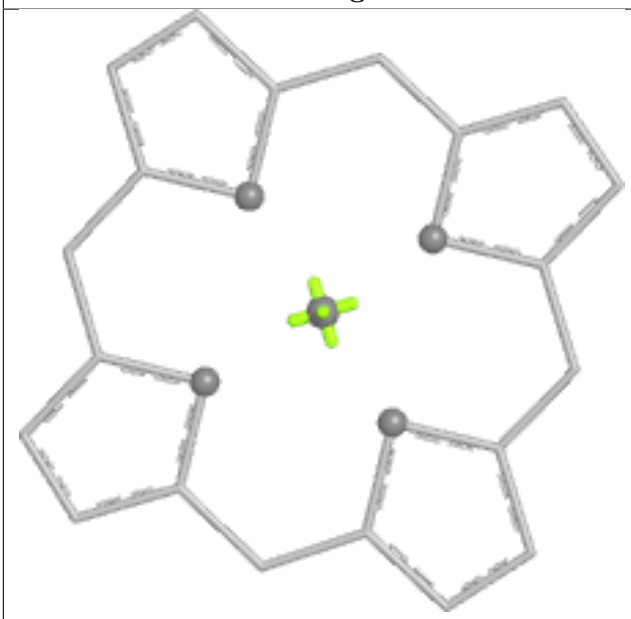
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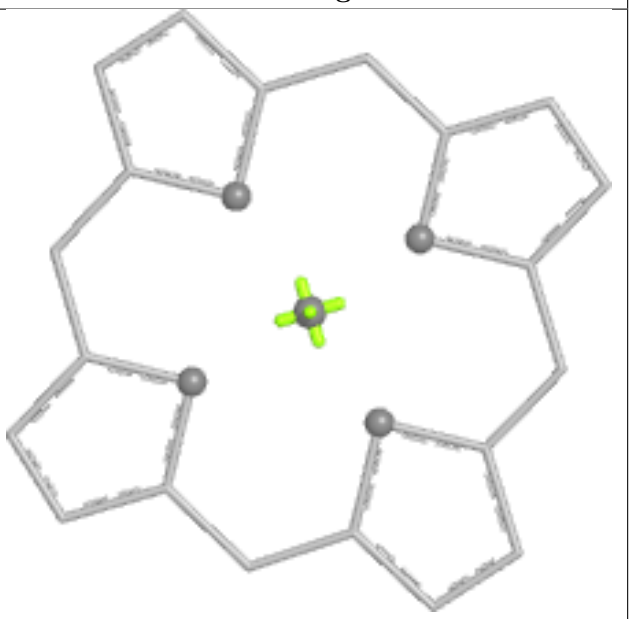
Bond lengths



Bond angles

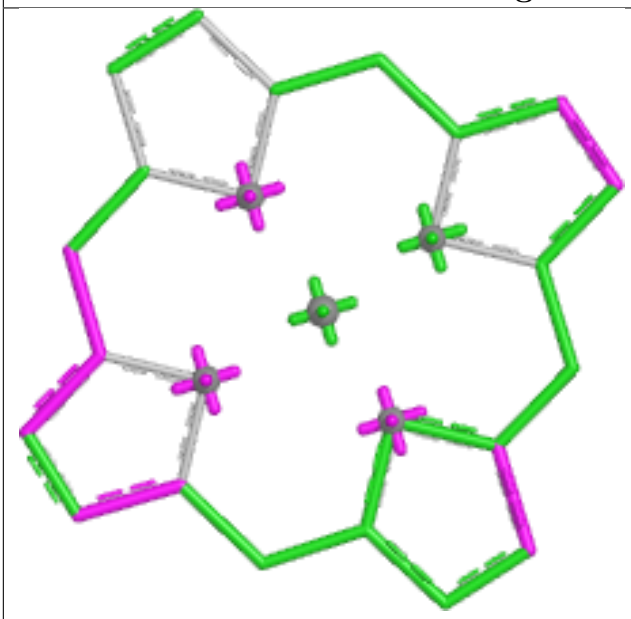


Torsions

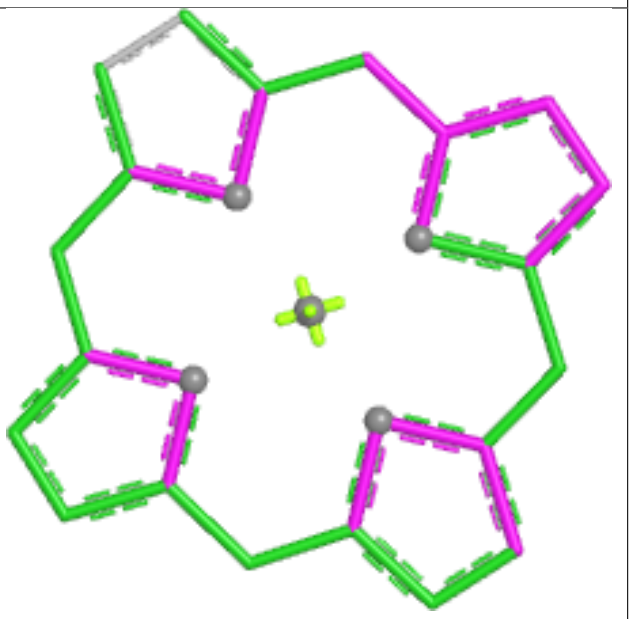


Rings

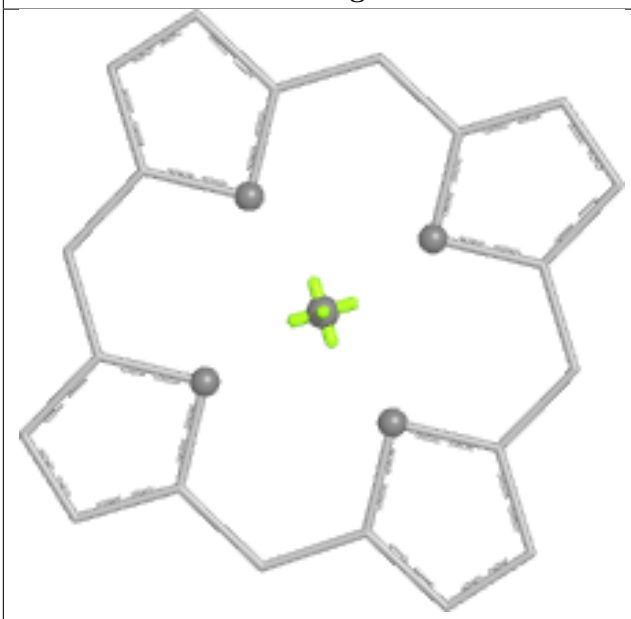
Ligand CLA B 1237



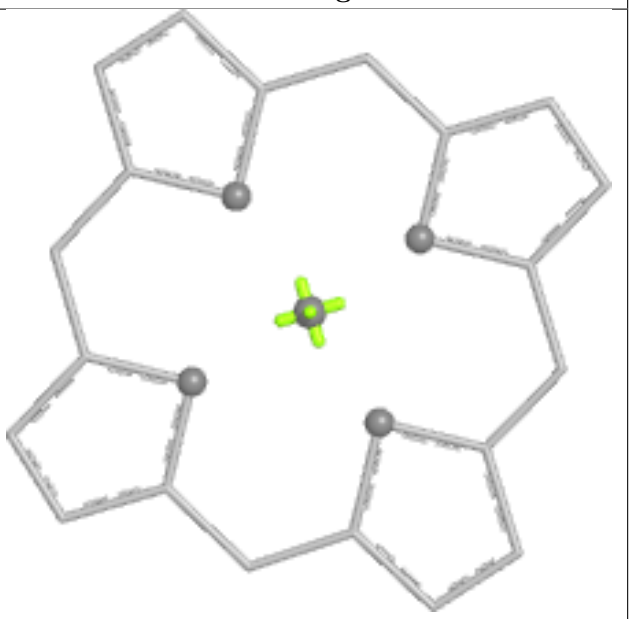
Bond lengths



Bond angles

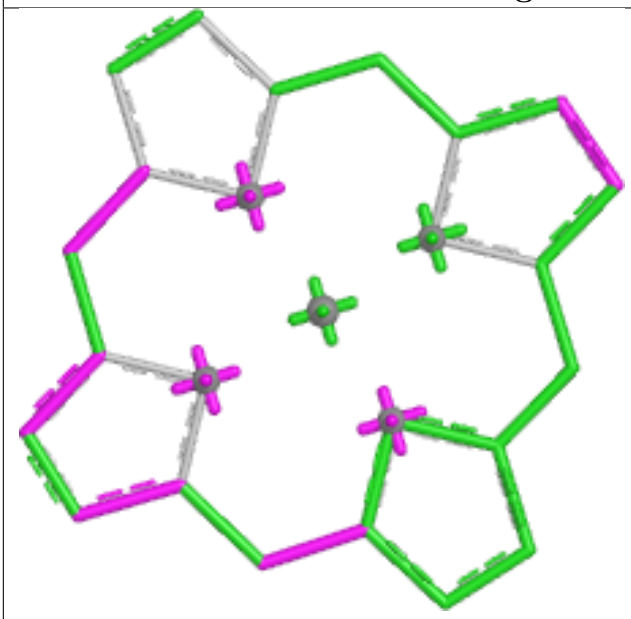


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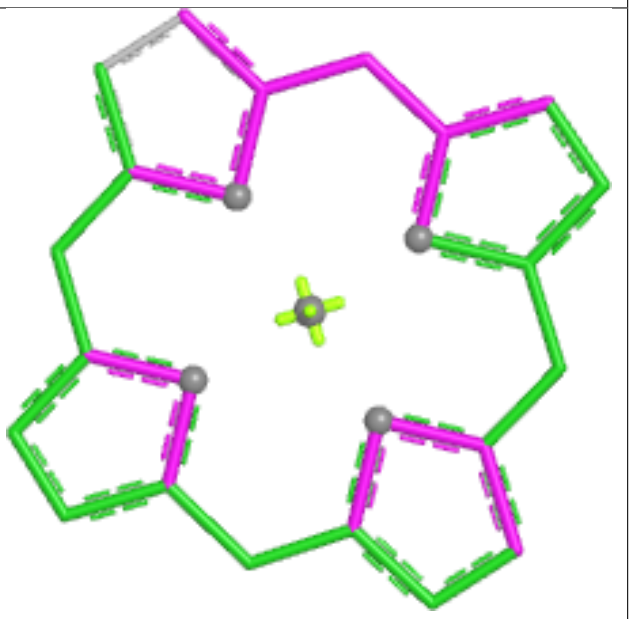


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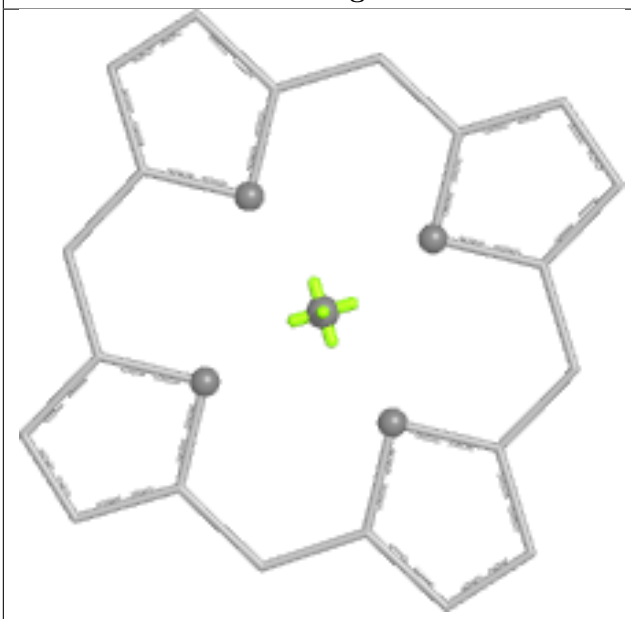
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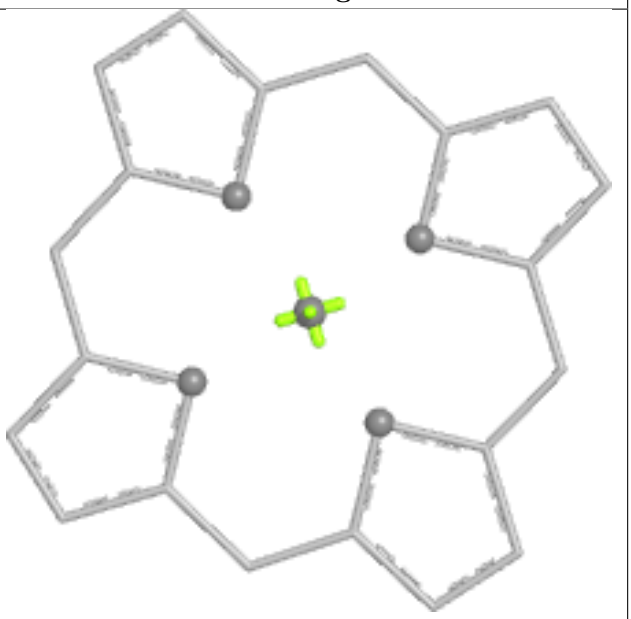
Bond lengths



Bond angles

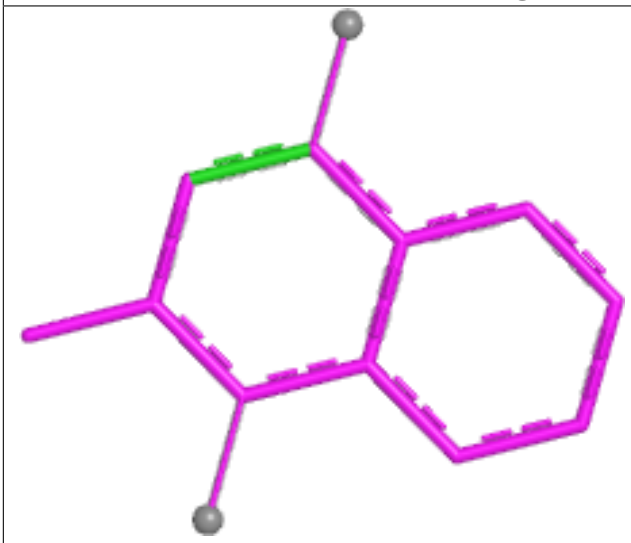


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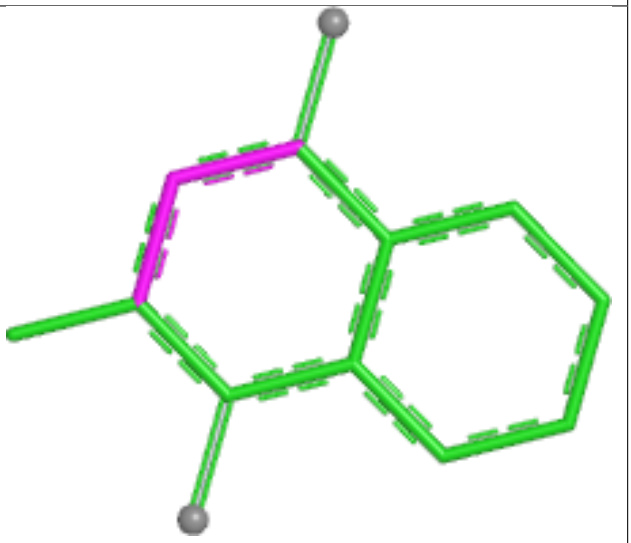


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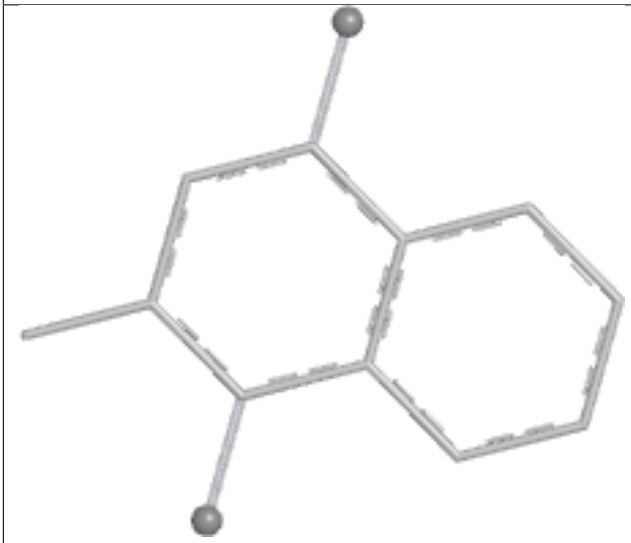
Ligand PQN P 6001



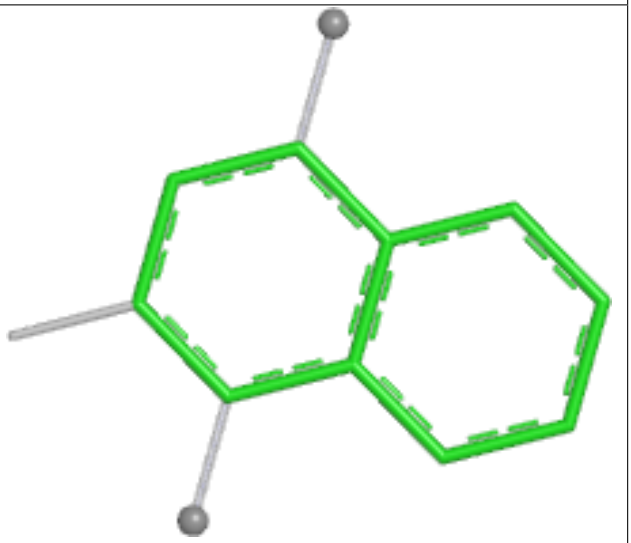
Bond lengths



Bond angles

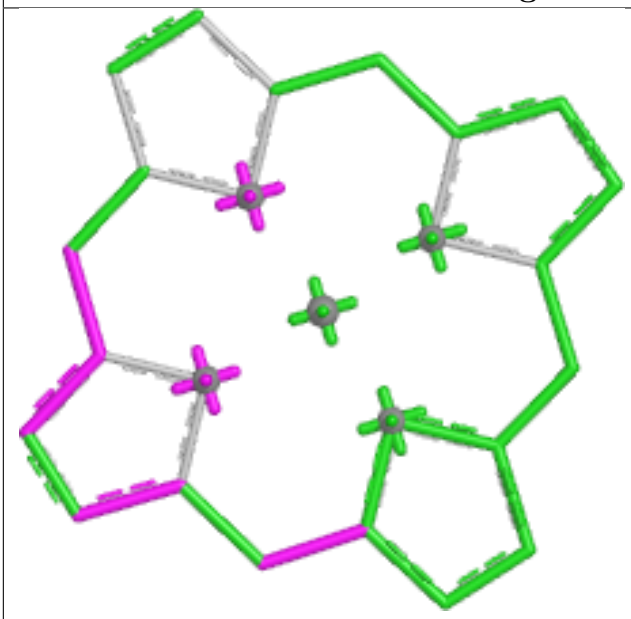


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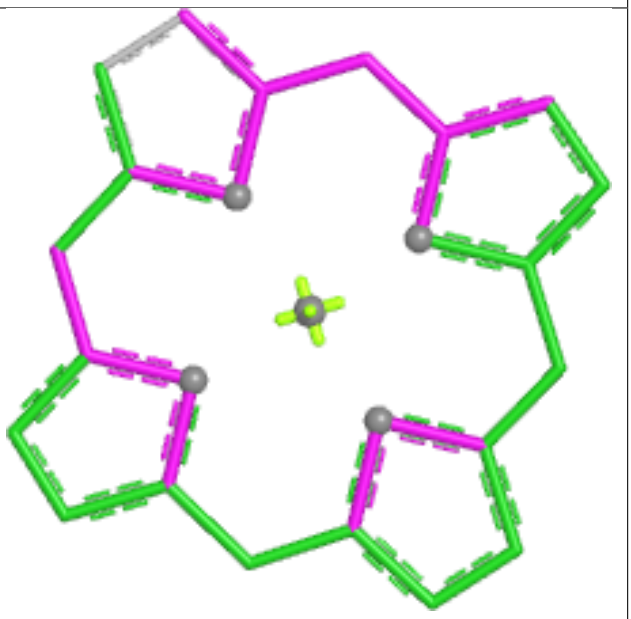


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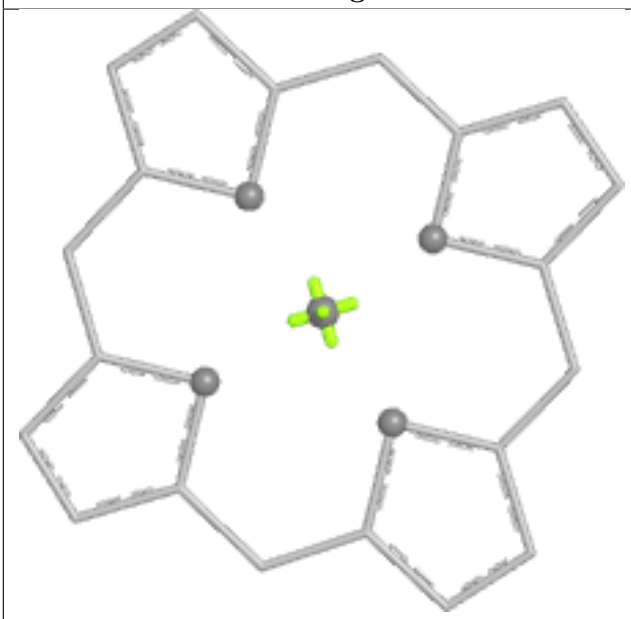
Ligand CLA 4 1017



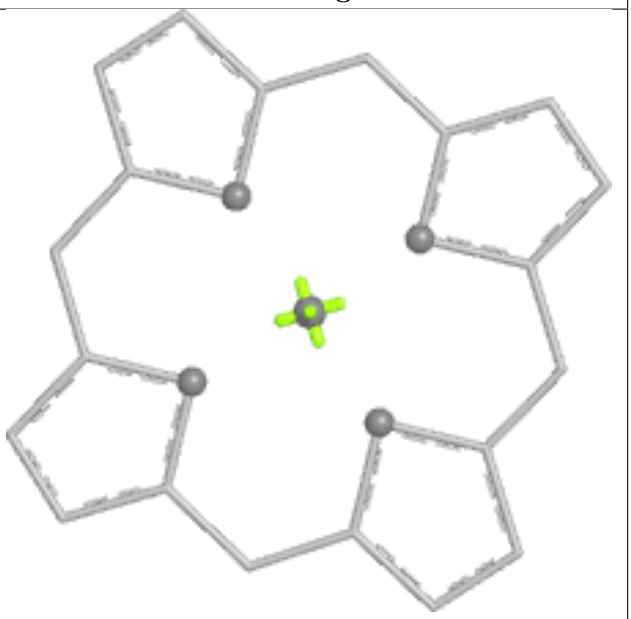
Bond lengths



Bond angles

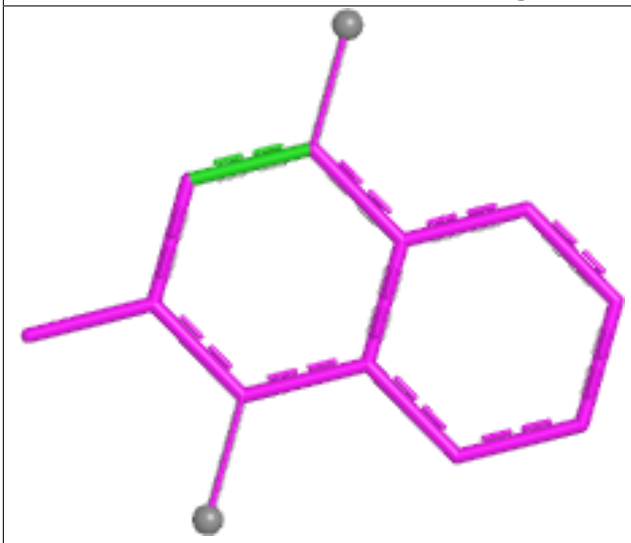


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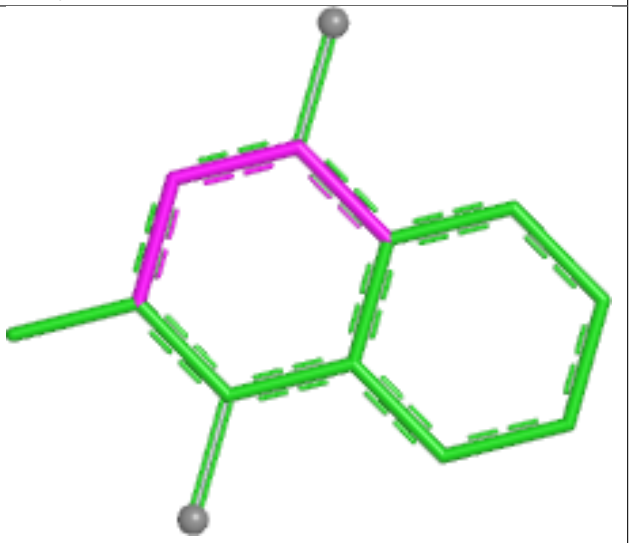


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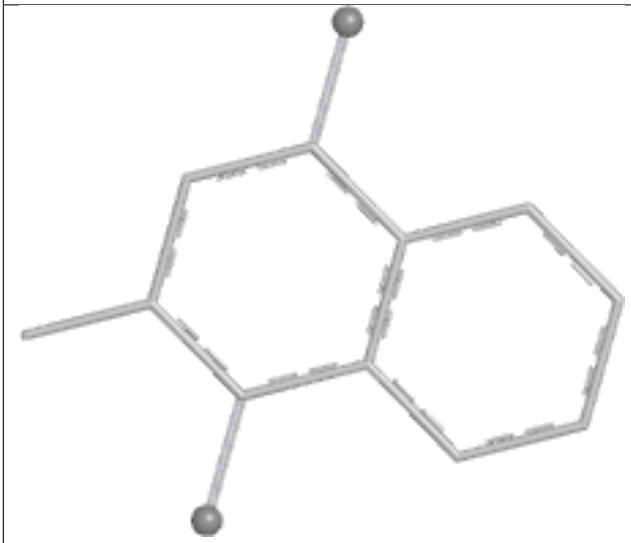
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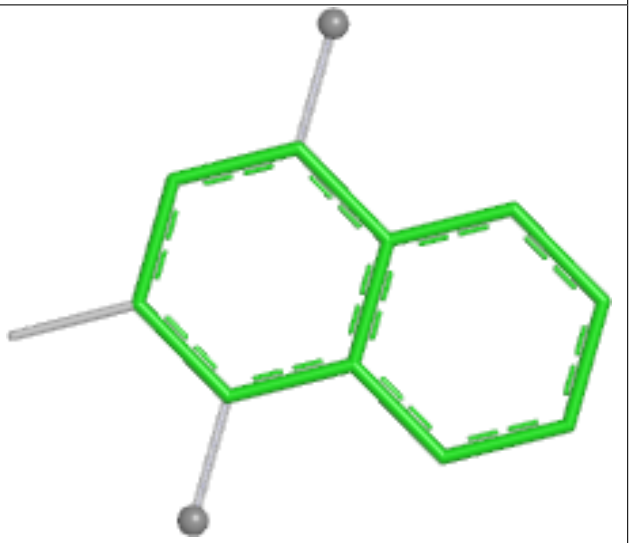
Bond lengths



Bond angles

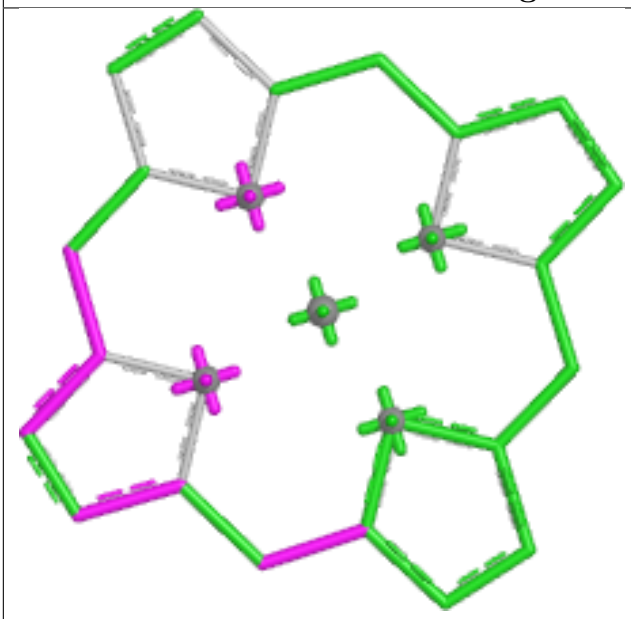


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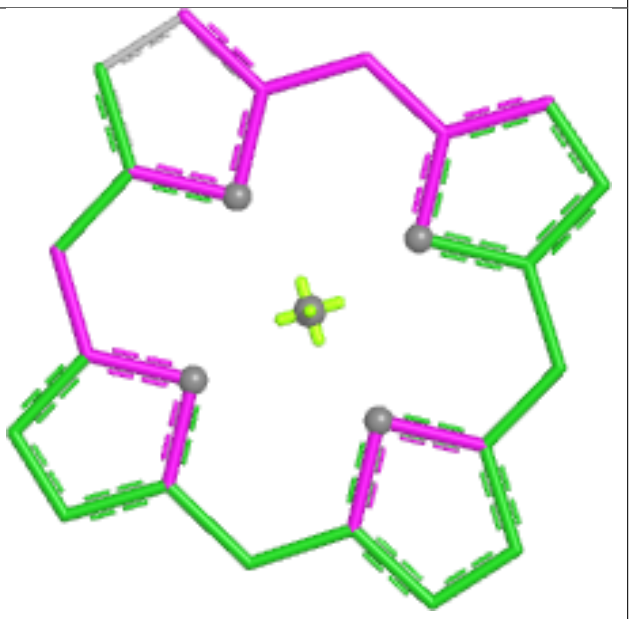


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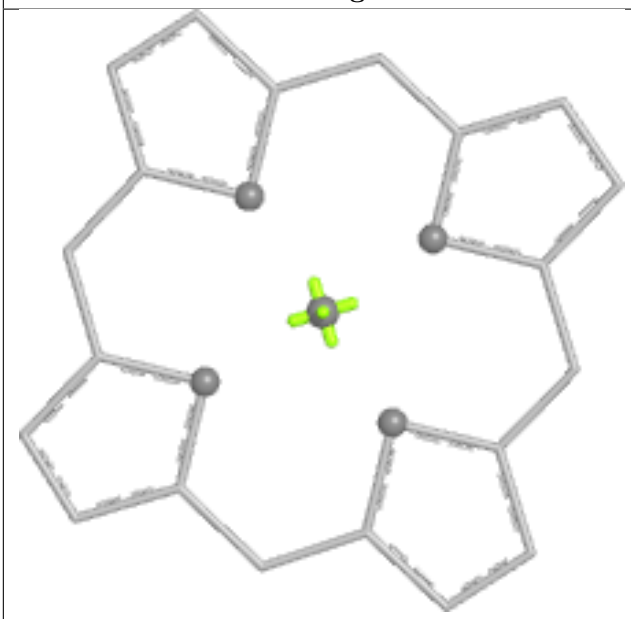
Ligand CLA 2 1033



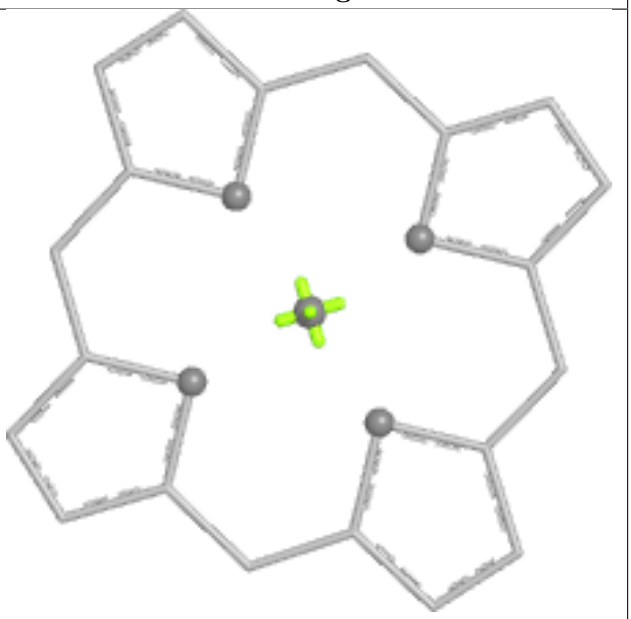
Bond lengths



Bond angles

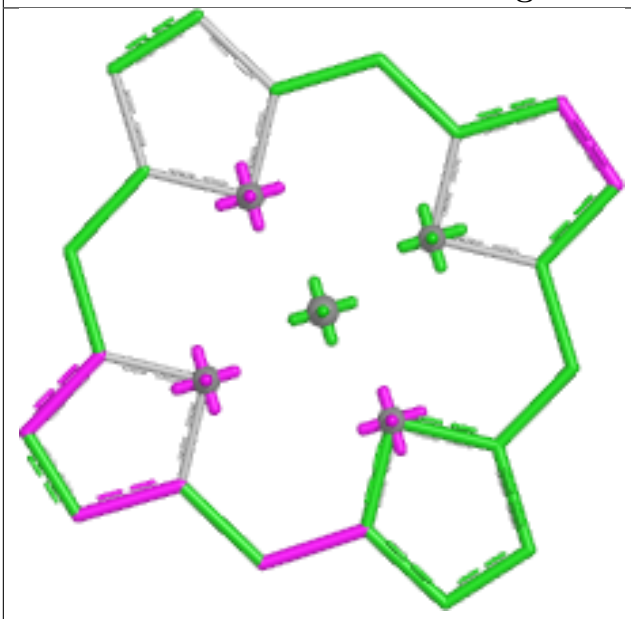


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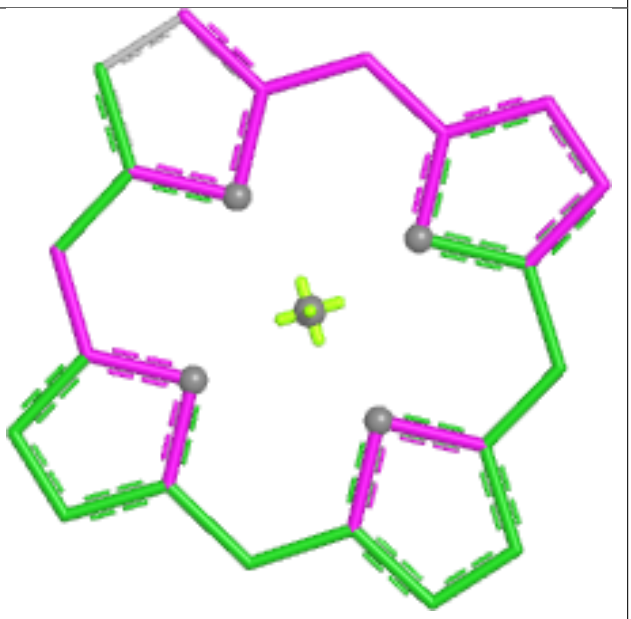


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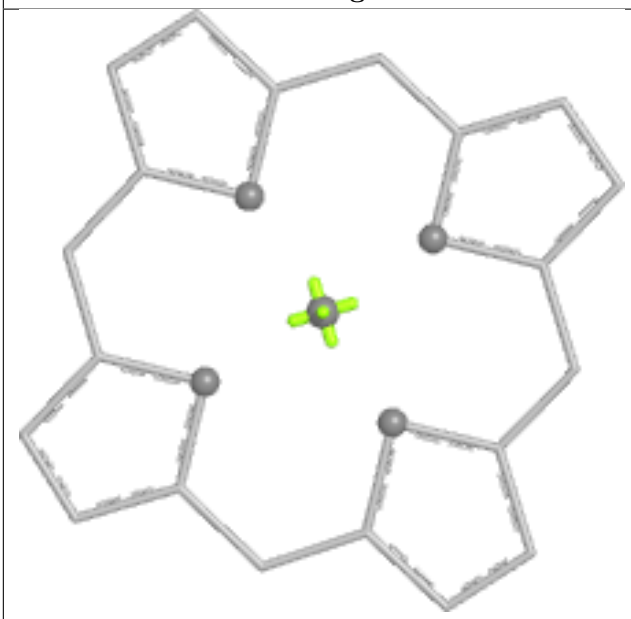
Ligand CLA P 5123



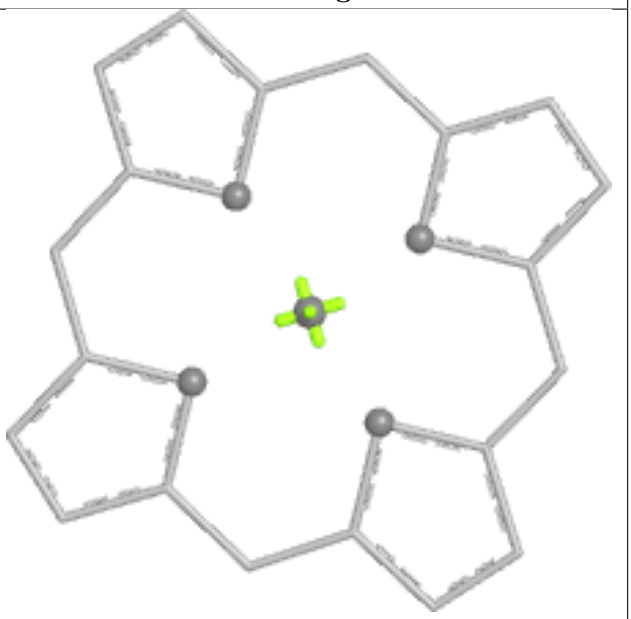
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Bond angles

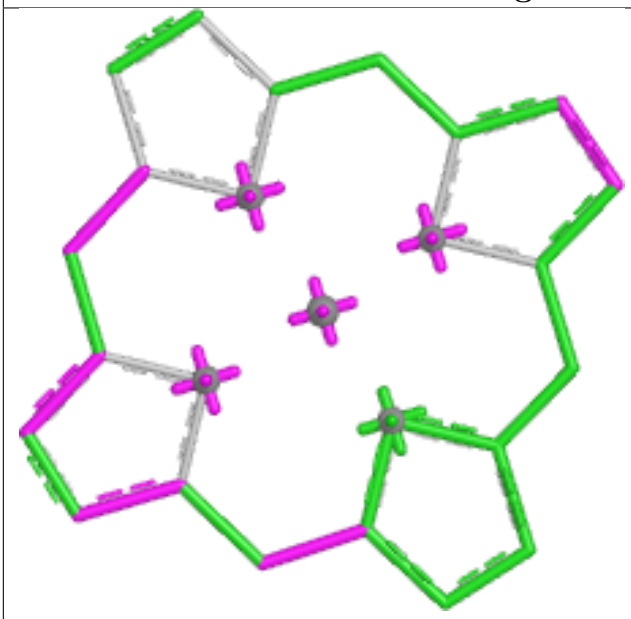


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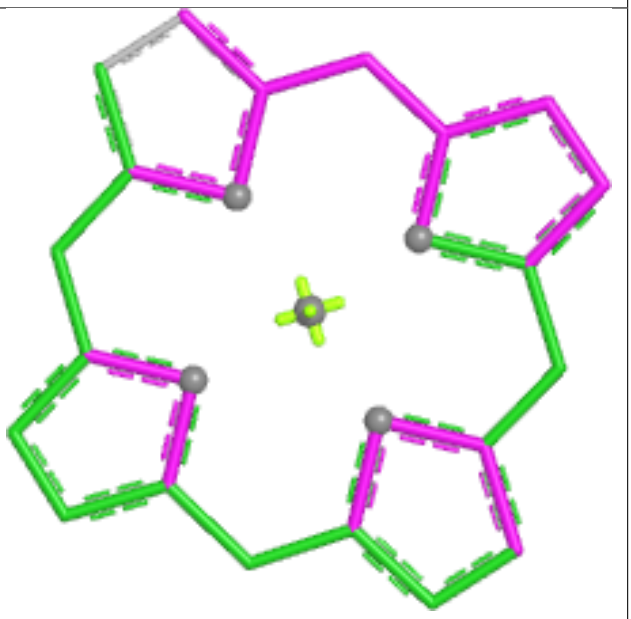


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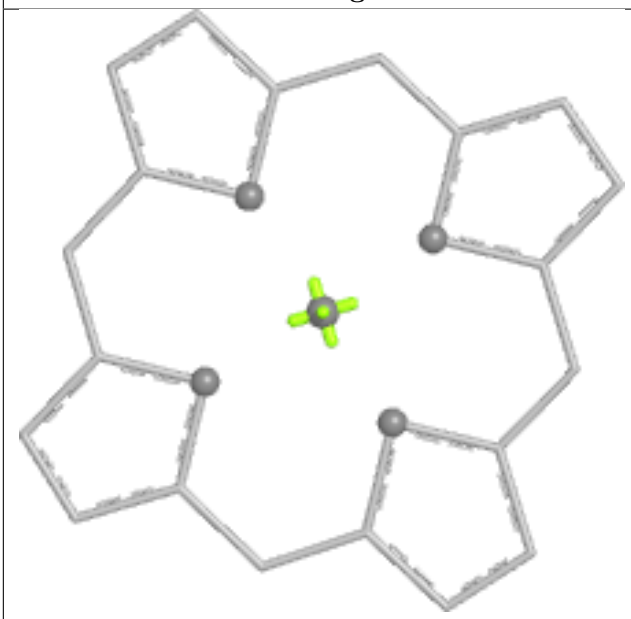
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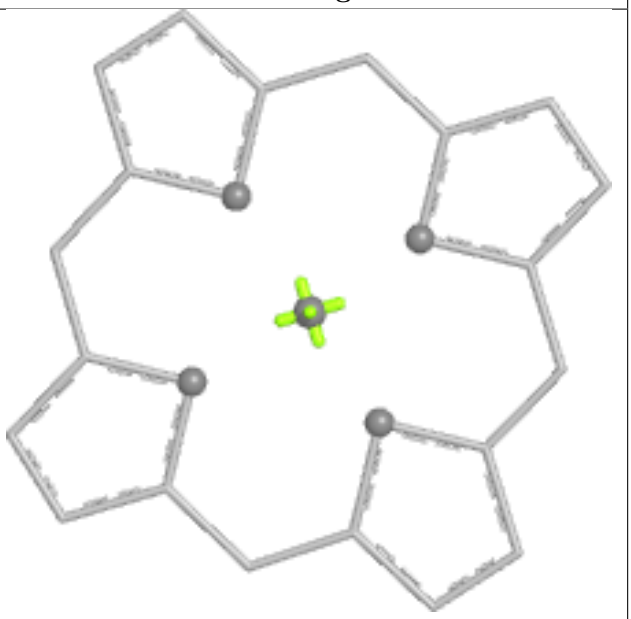
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Bond angles

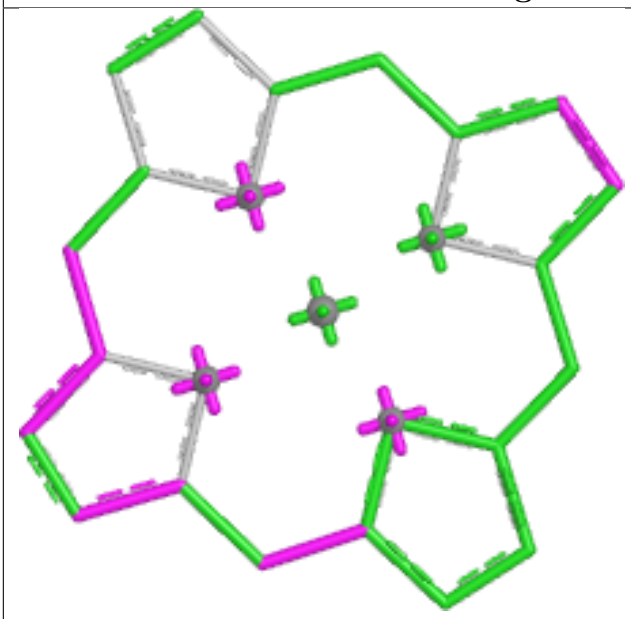


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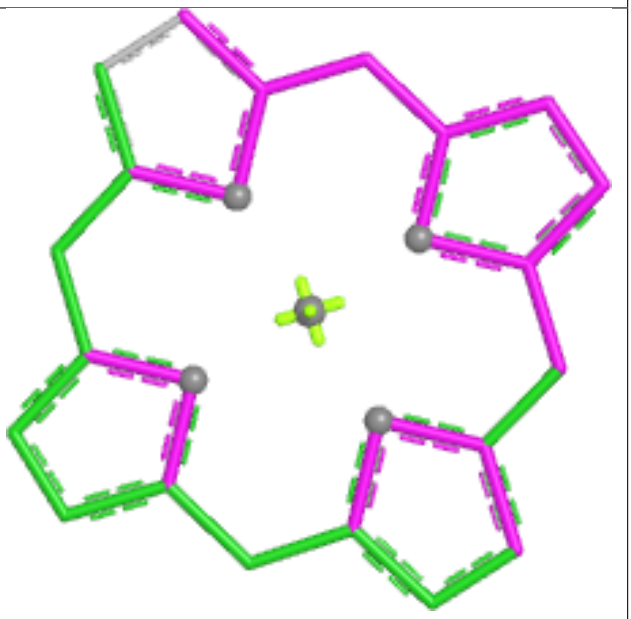


Rings

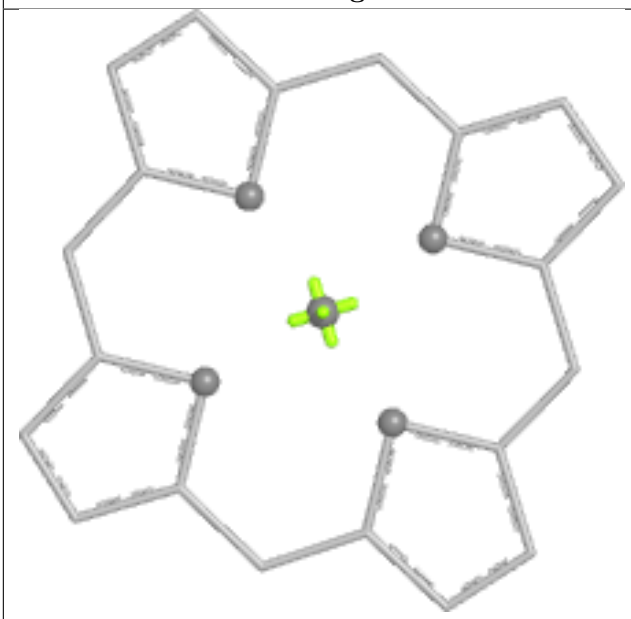
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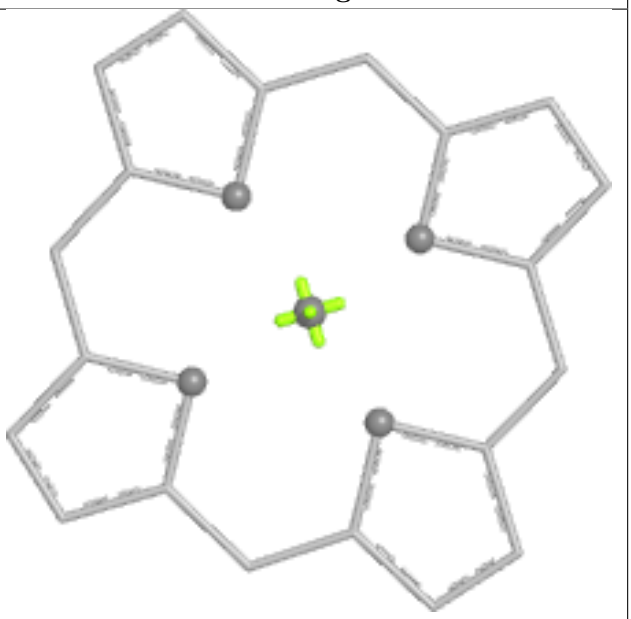
Bond lengths



Bond angles

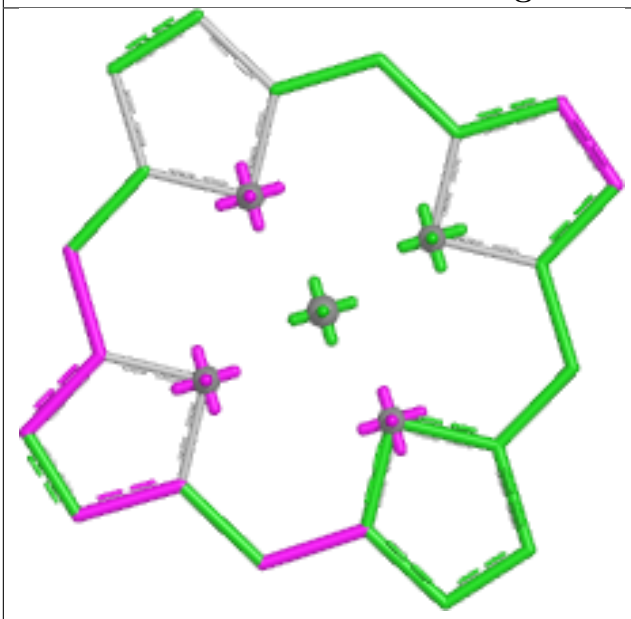


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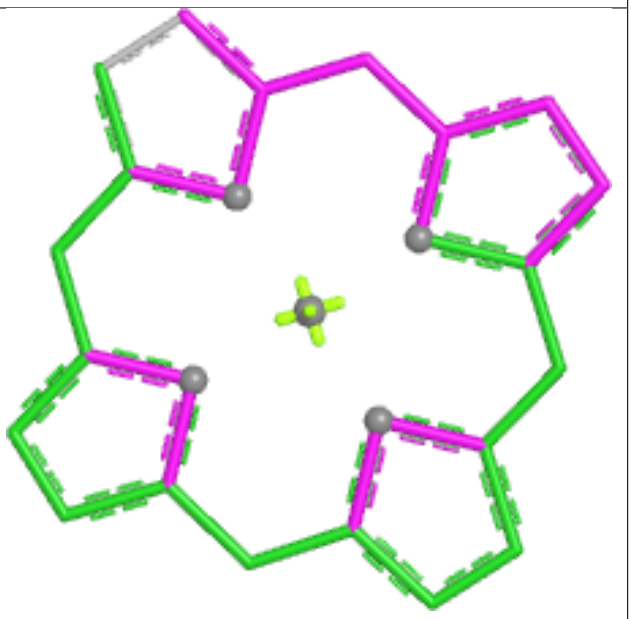


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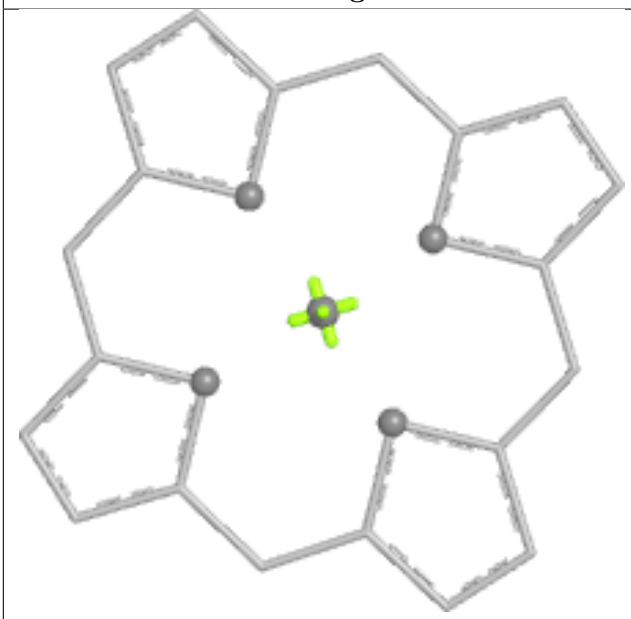
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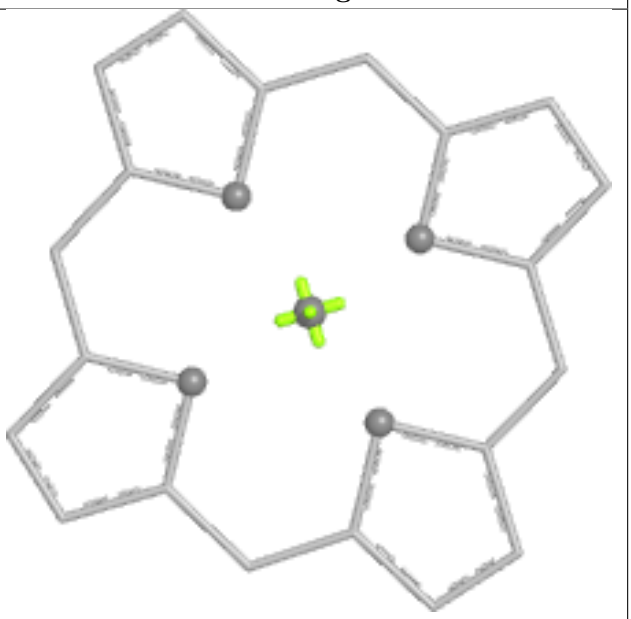
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Bond angles

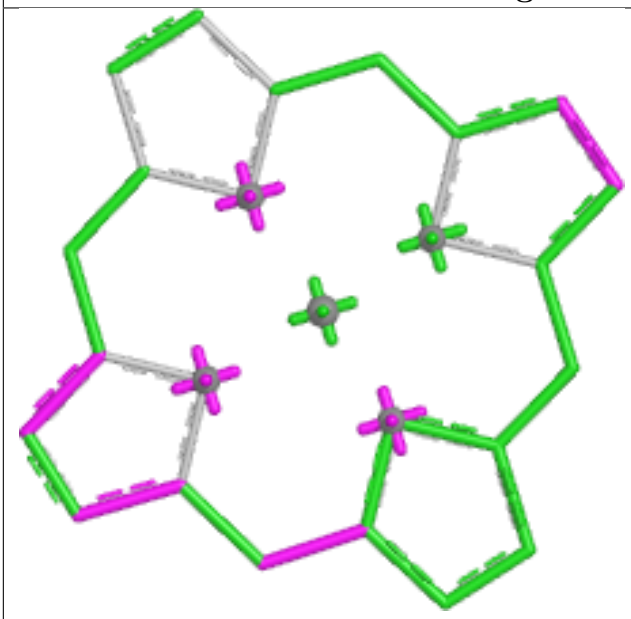


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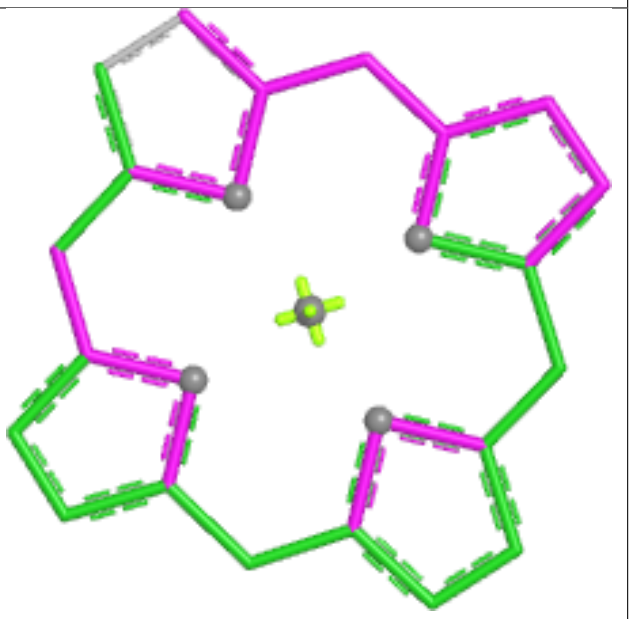


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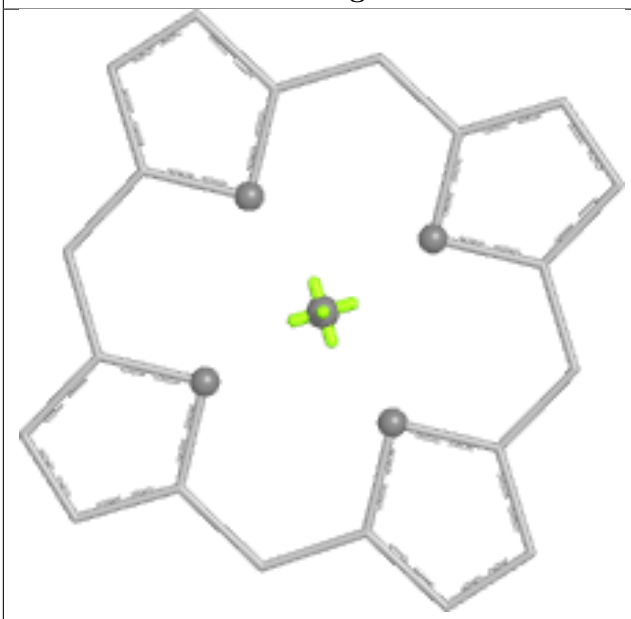
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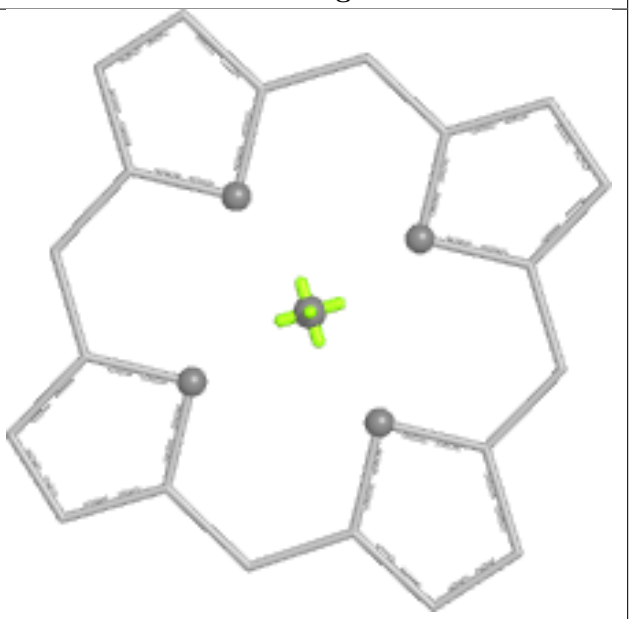
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Bond angles

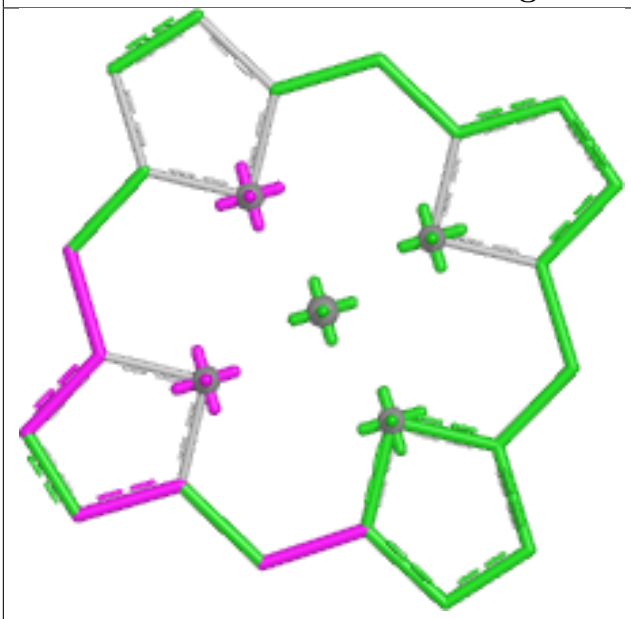


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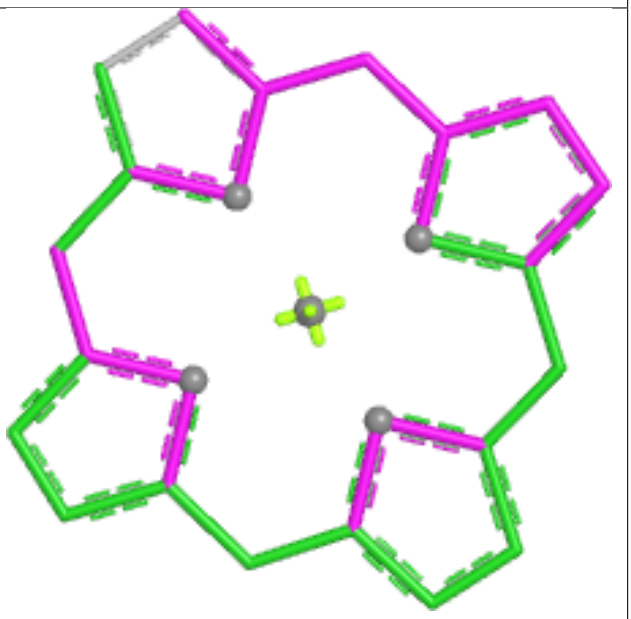


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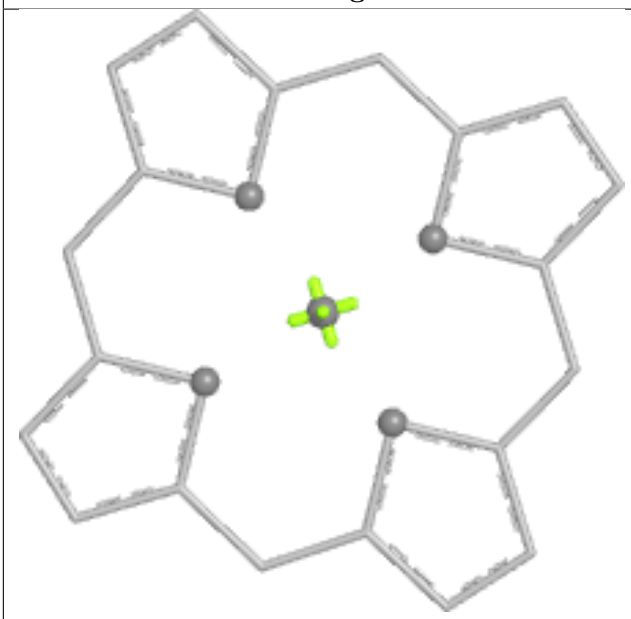
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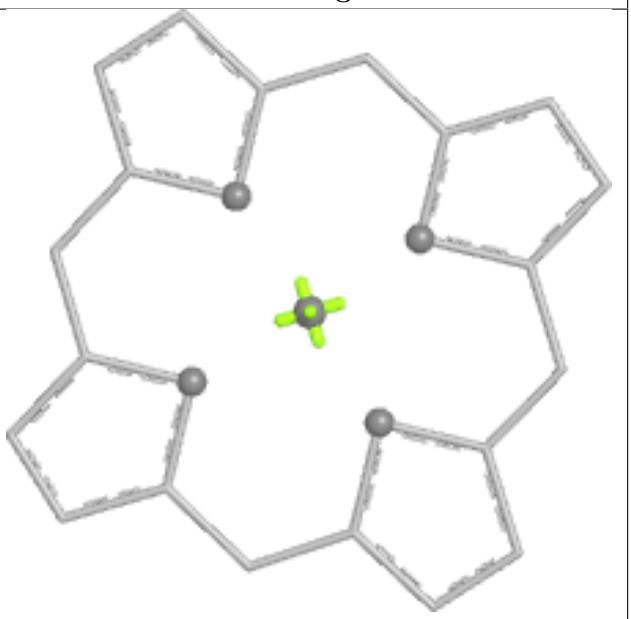
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Bond angles

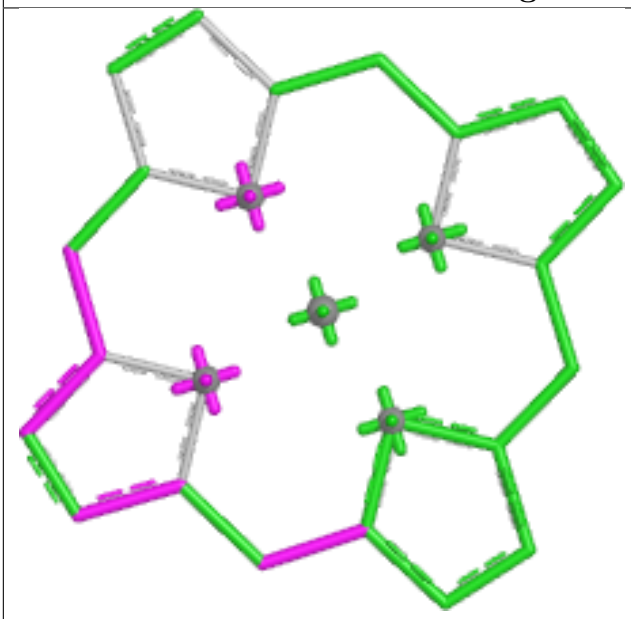


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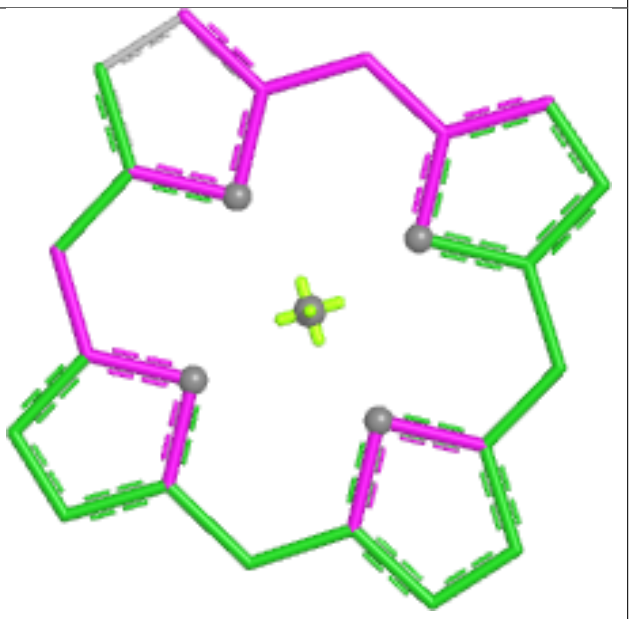


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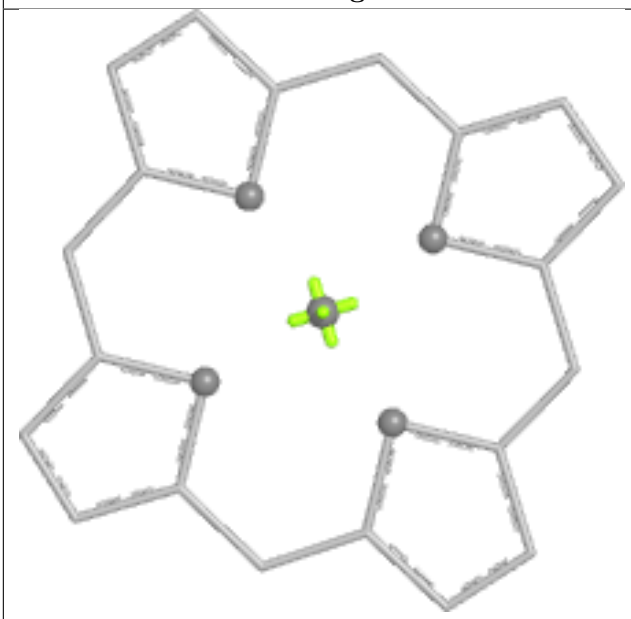
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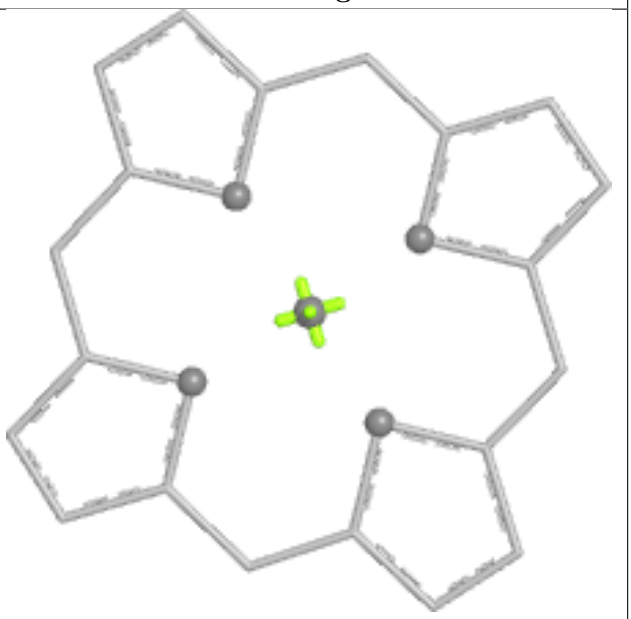
Bond lengths



Bond angles

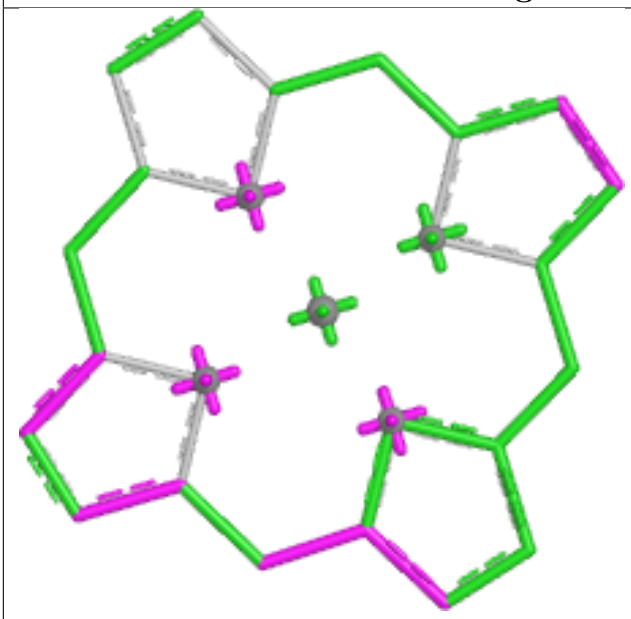


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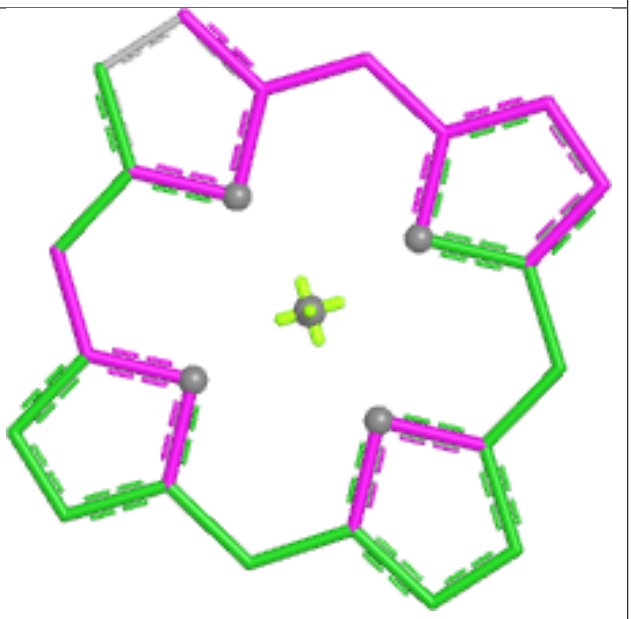


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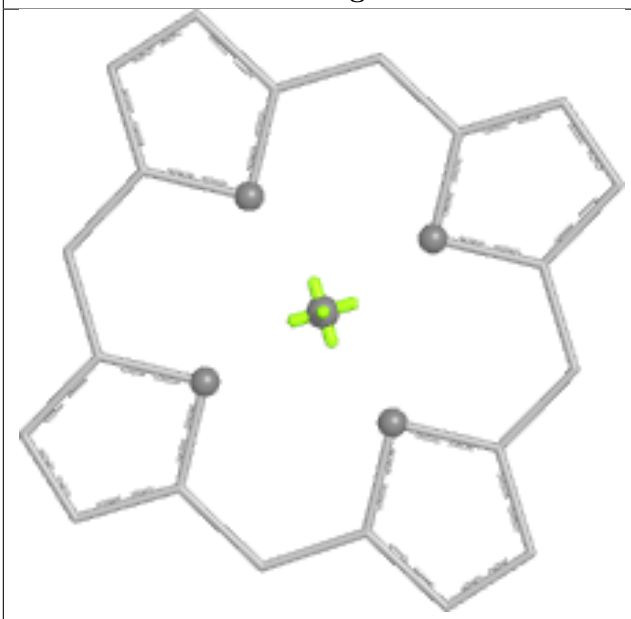
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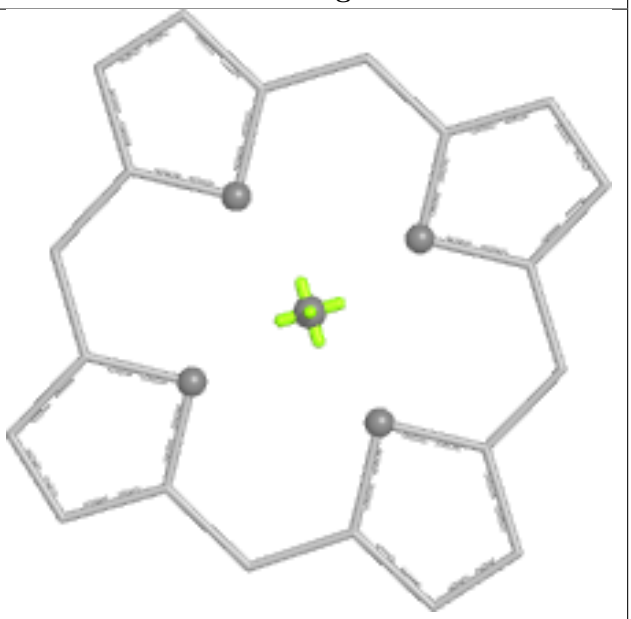
Bond lengths



Bond angles

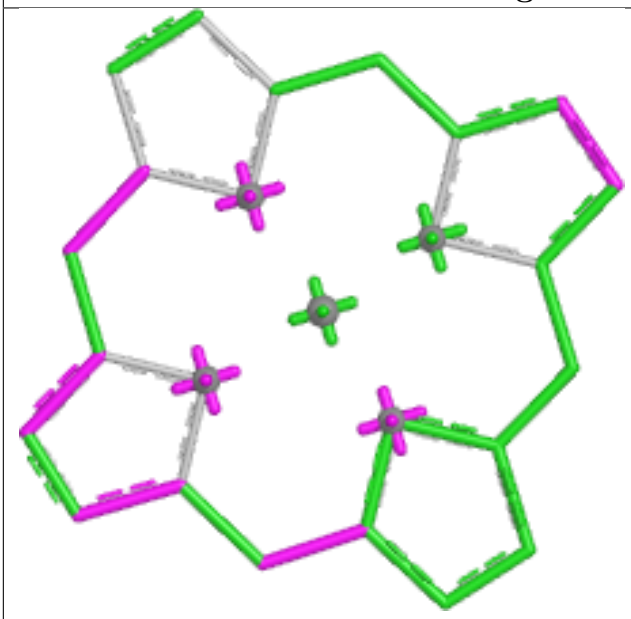


Torsions

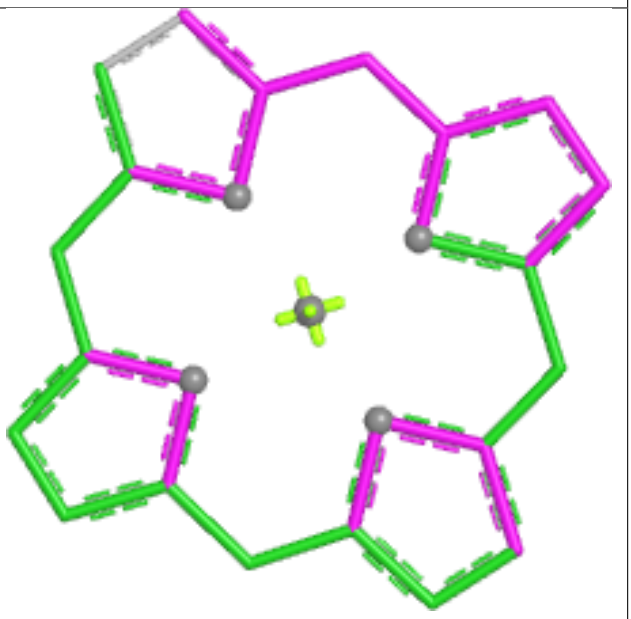


Rings

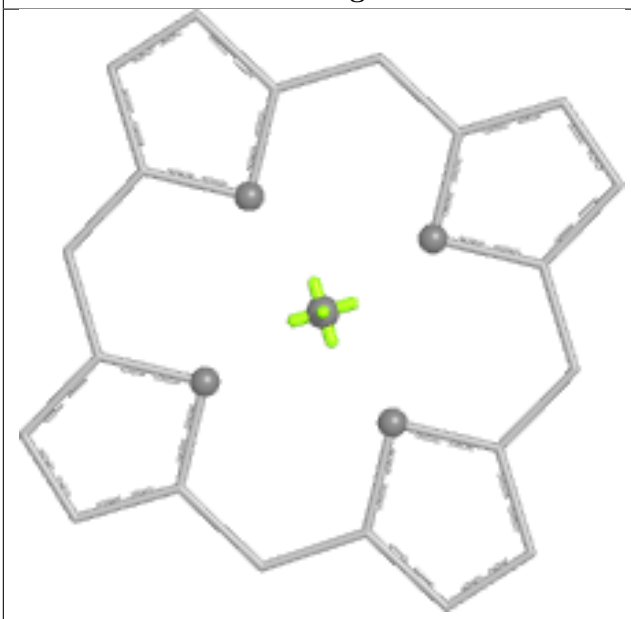
Ligand CLA P 5133



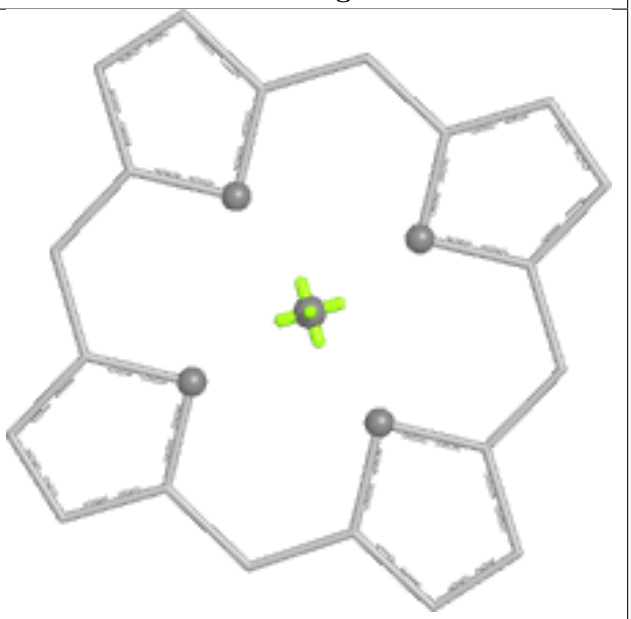
Bond lengths



Bond angles

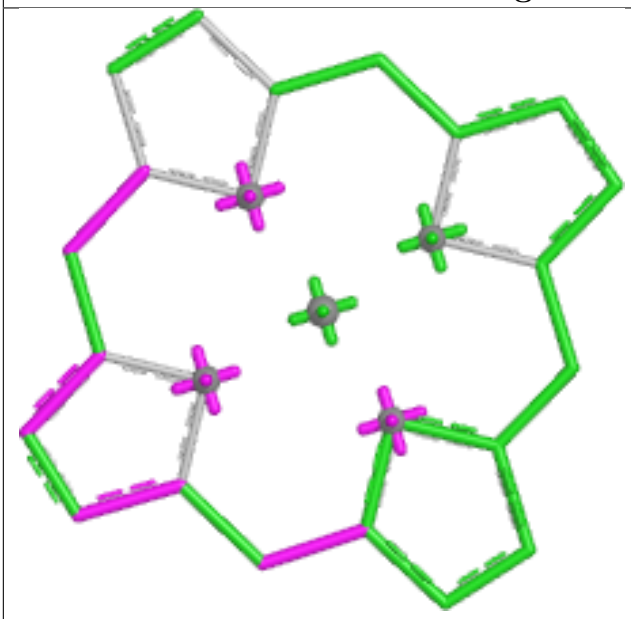


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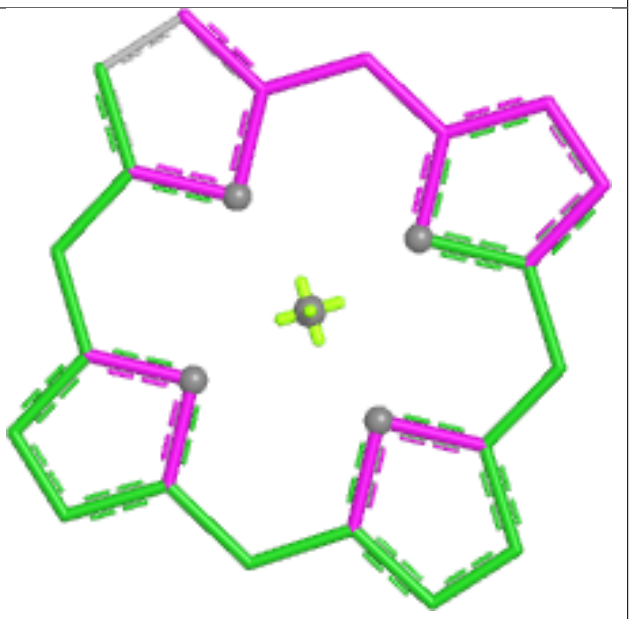


Rings

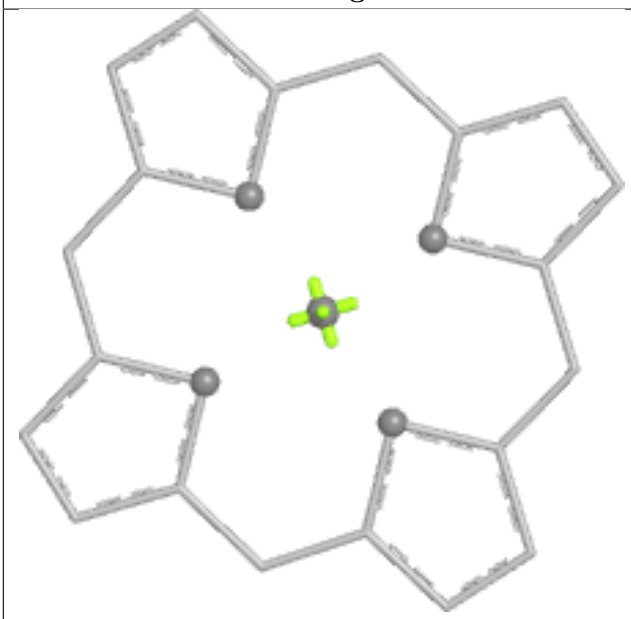
Ligand CLA A 1105



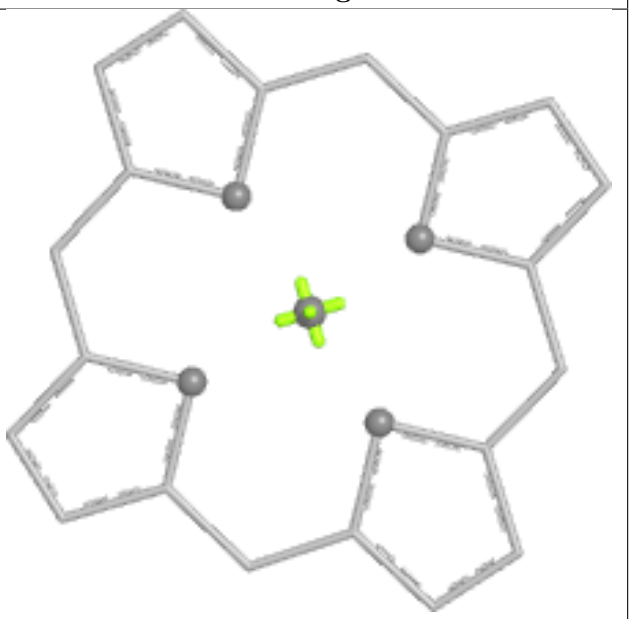
Bond lengths



Bond angles

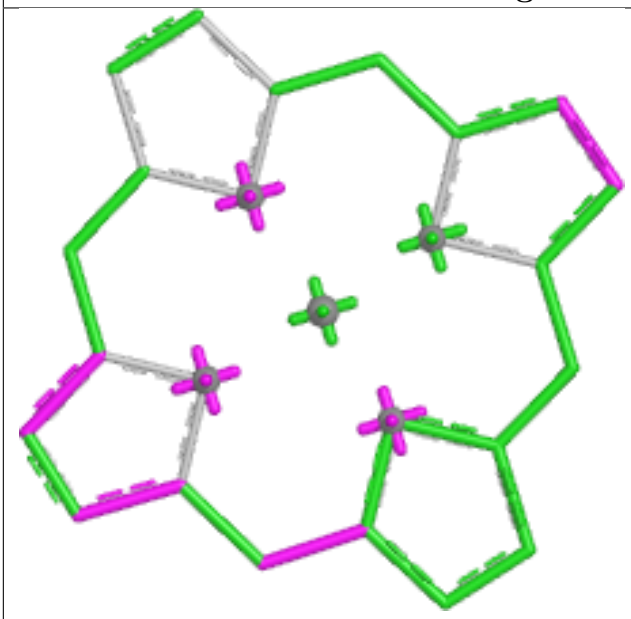


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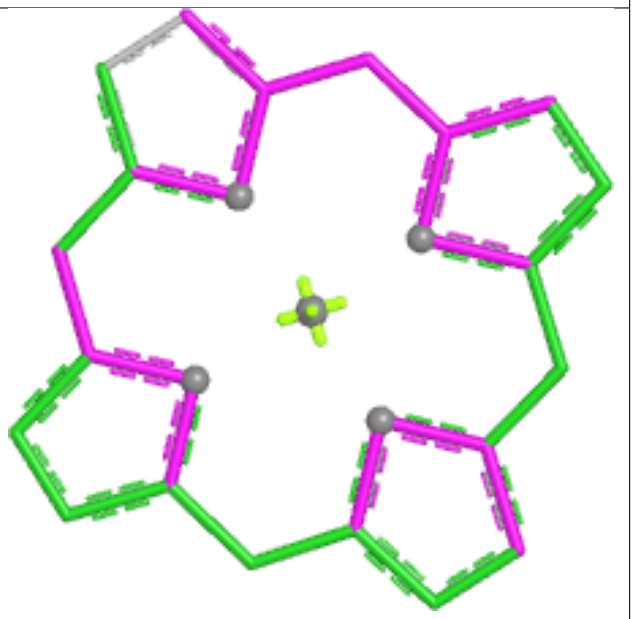


Rings

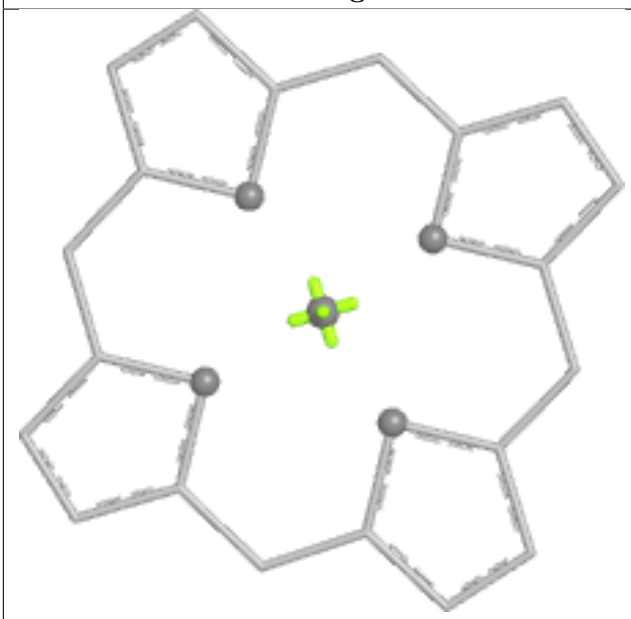
Ligand CLA P 5137



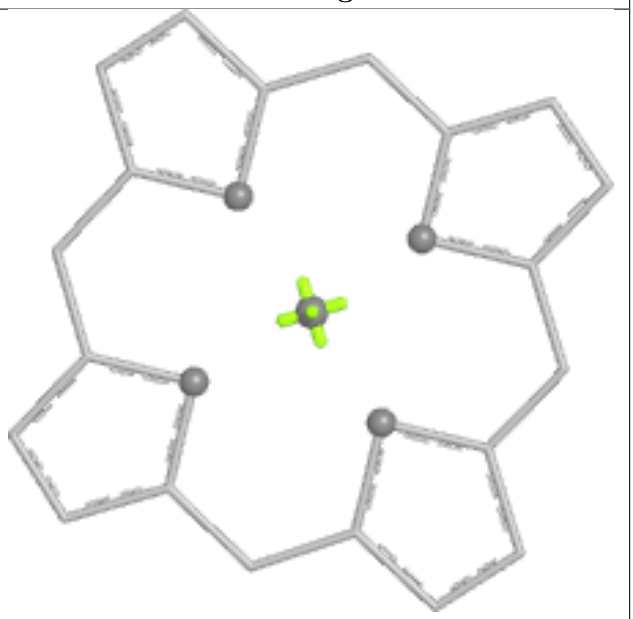
Bond lengths



Bond angles

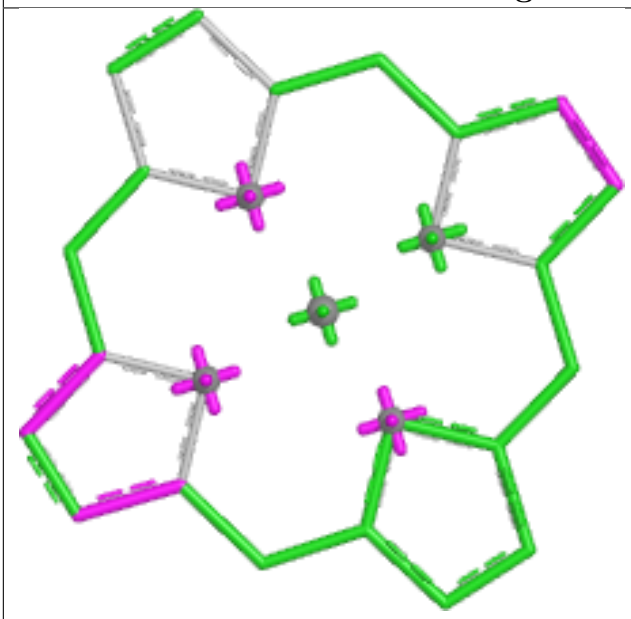


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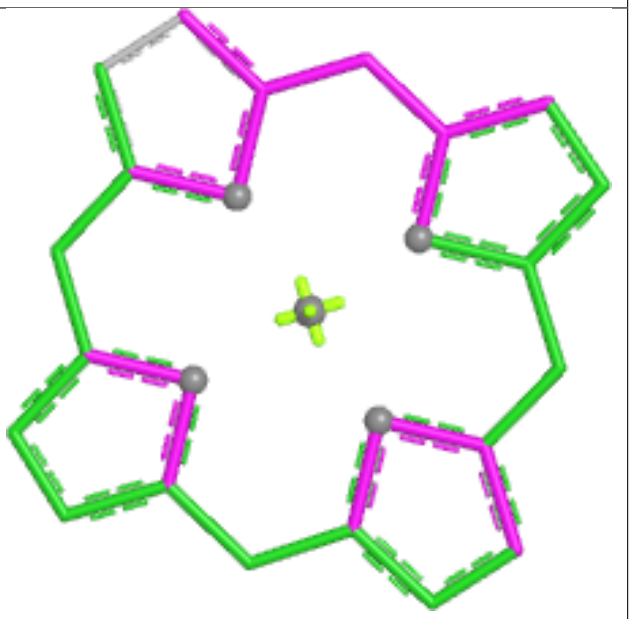


Rings

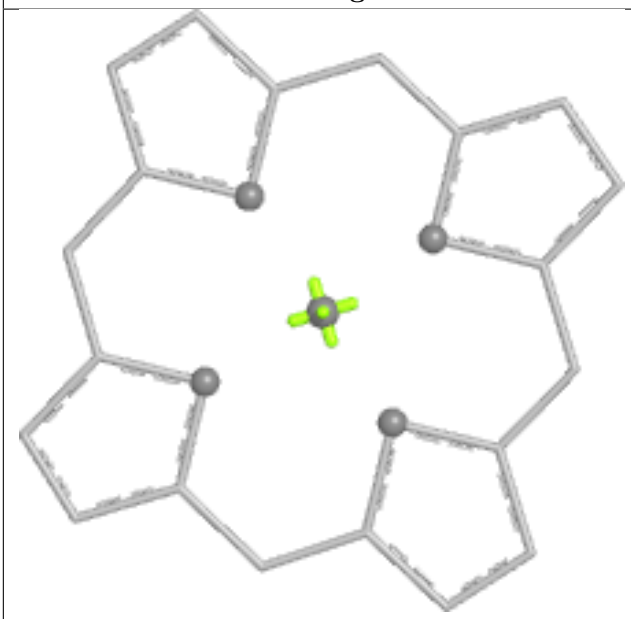
Ligand CLA B 1215



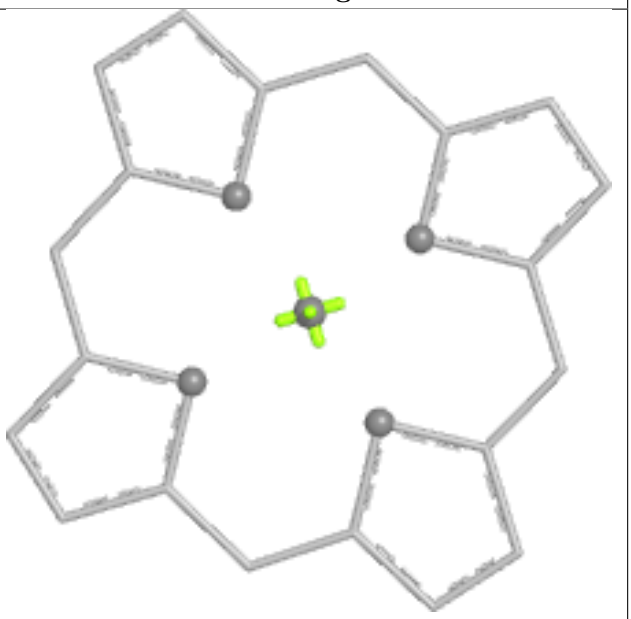
Bond lengths



Bond angles

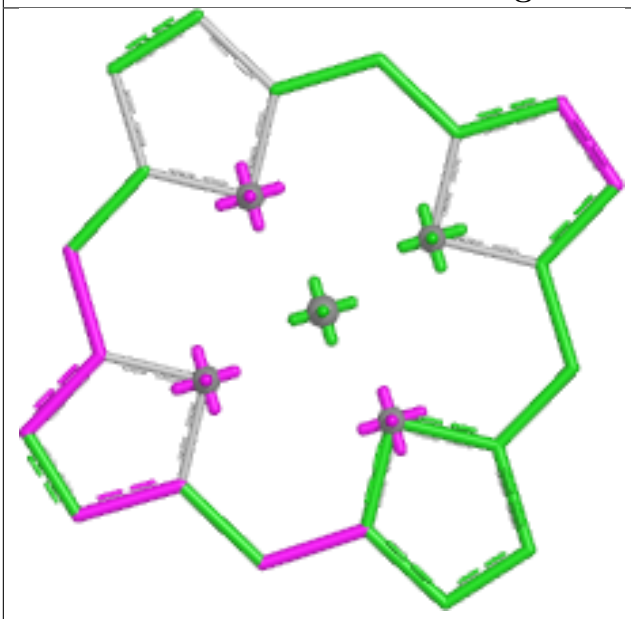


Torsions

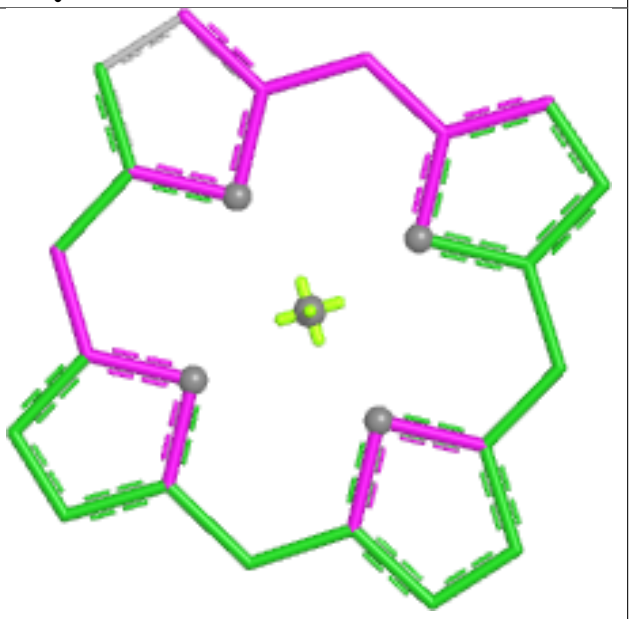


Rings

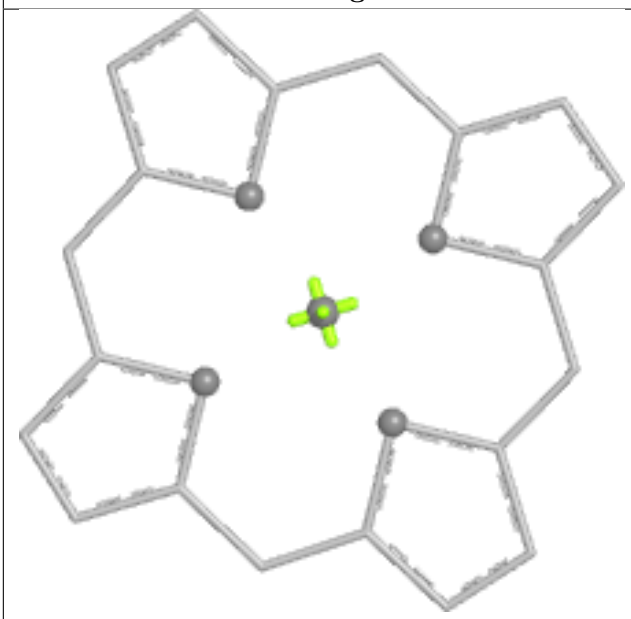
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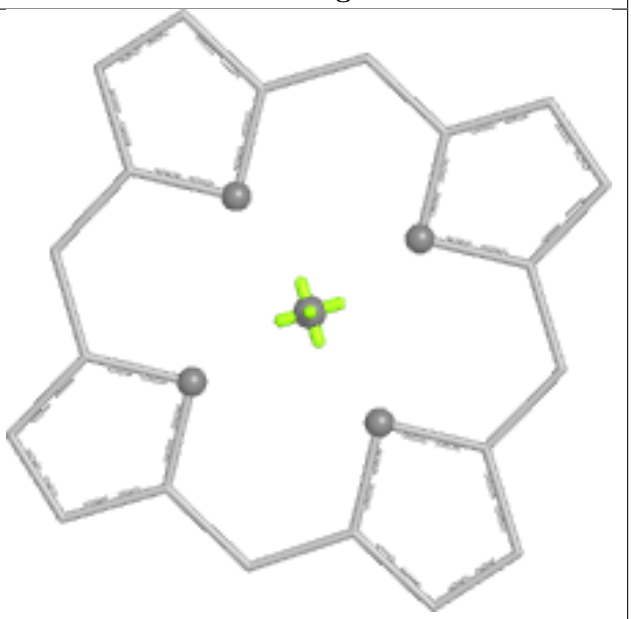
Bond lengths



Bond angles

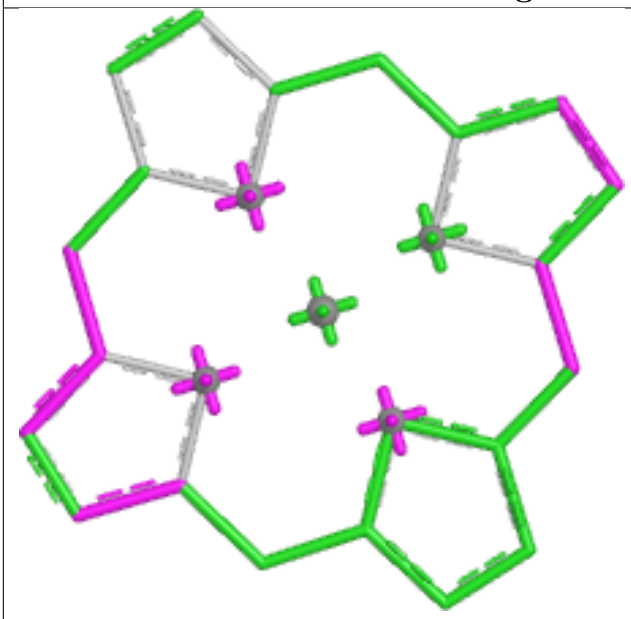


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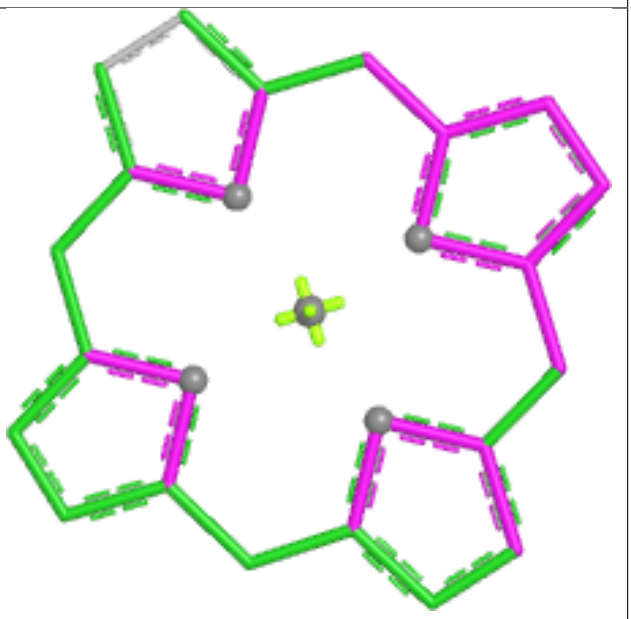


Rings

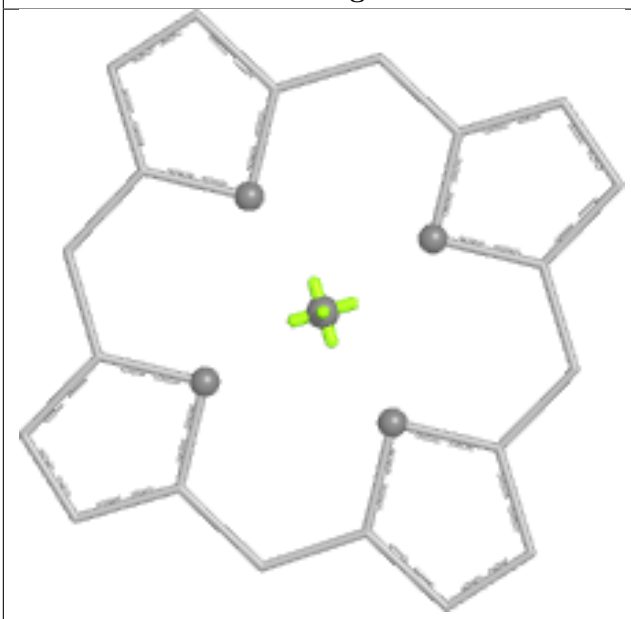
Ligand CLA B 1204



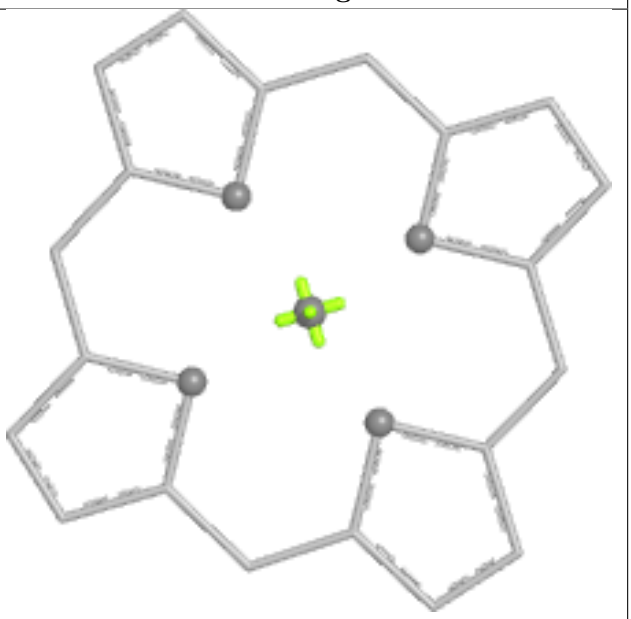
Bond lengths



Bond angles

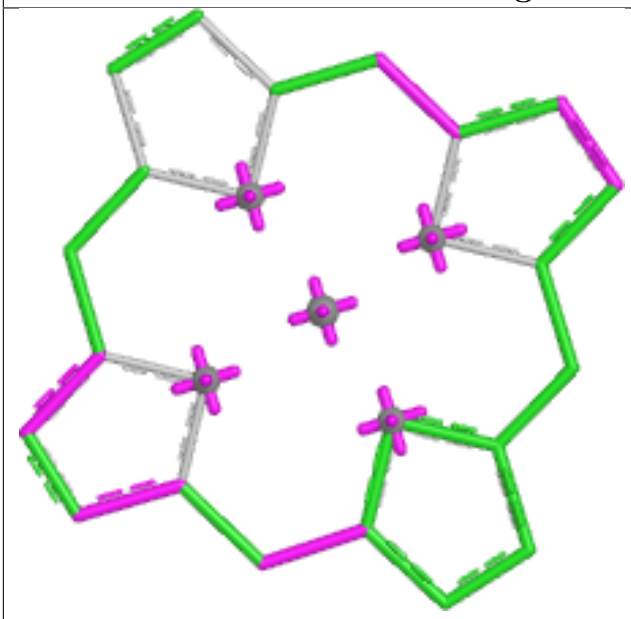


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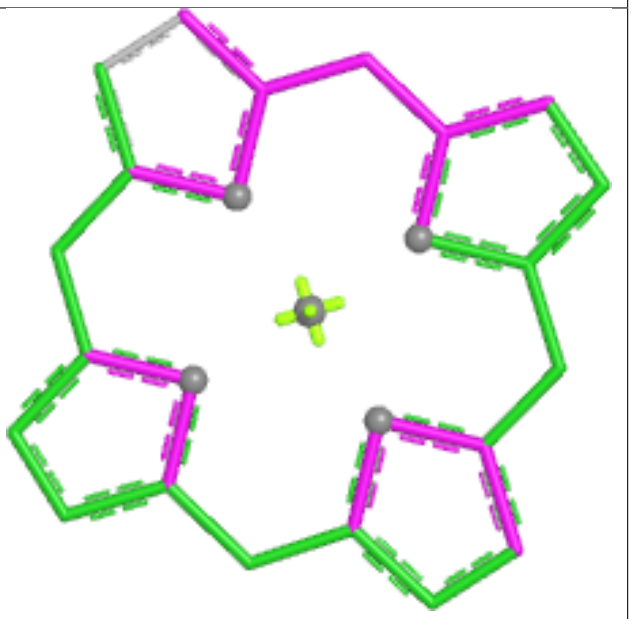


Rings

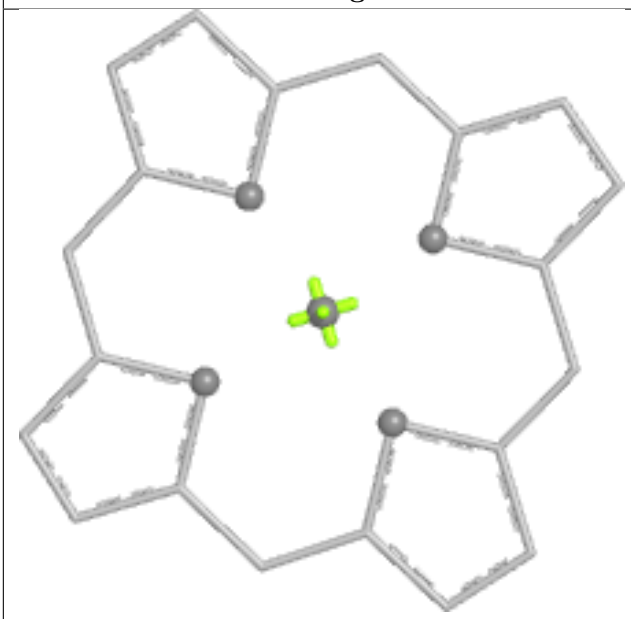
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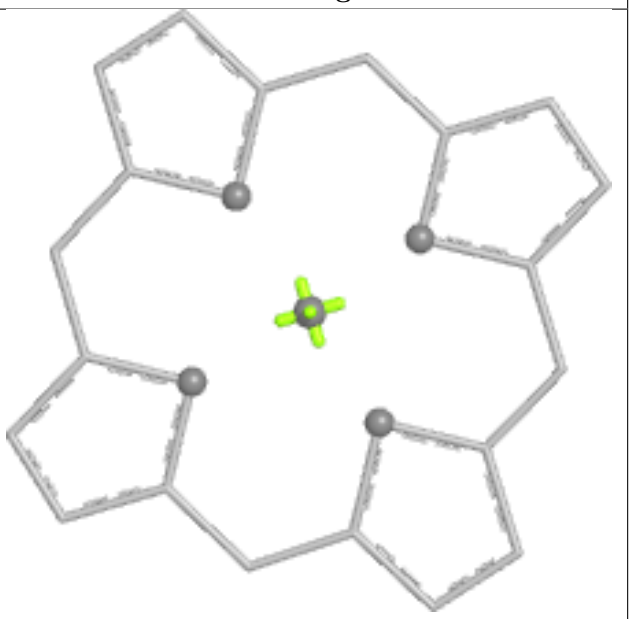
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Bond angles

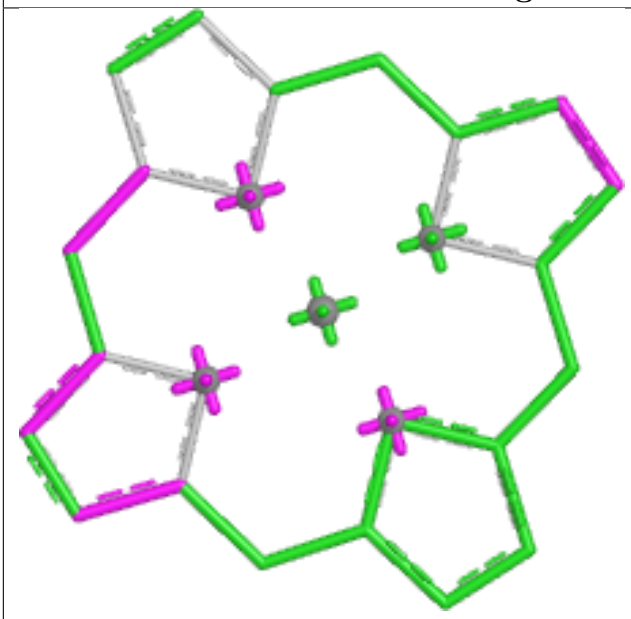


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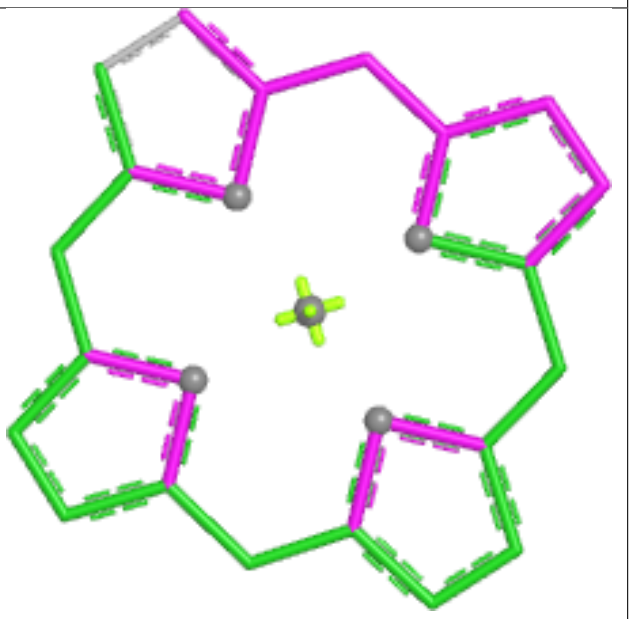


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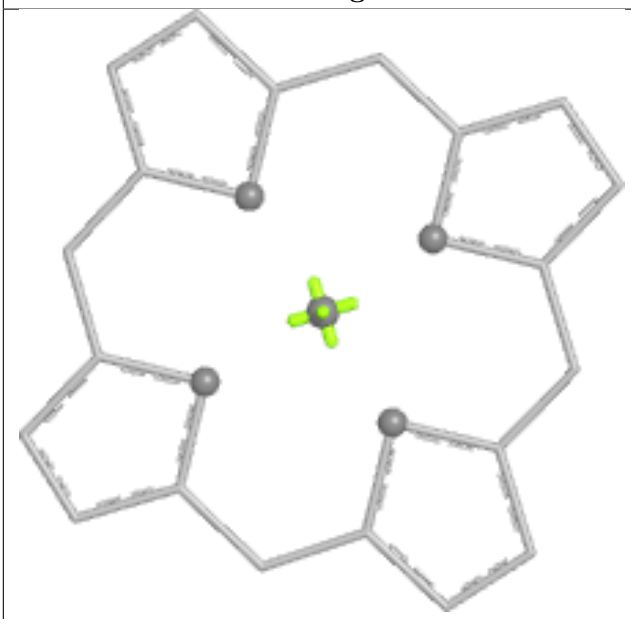
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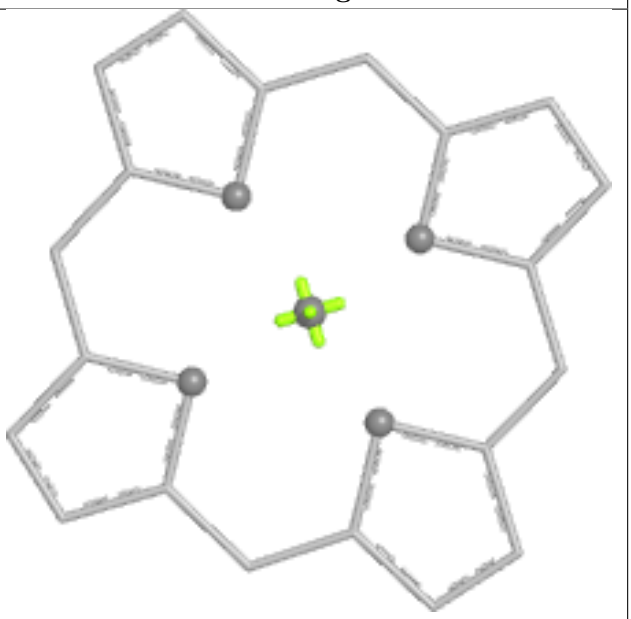
Bond lengths



Bond angles

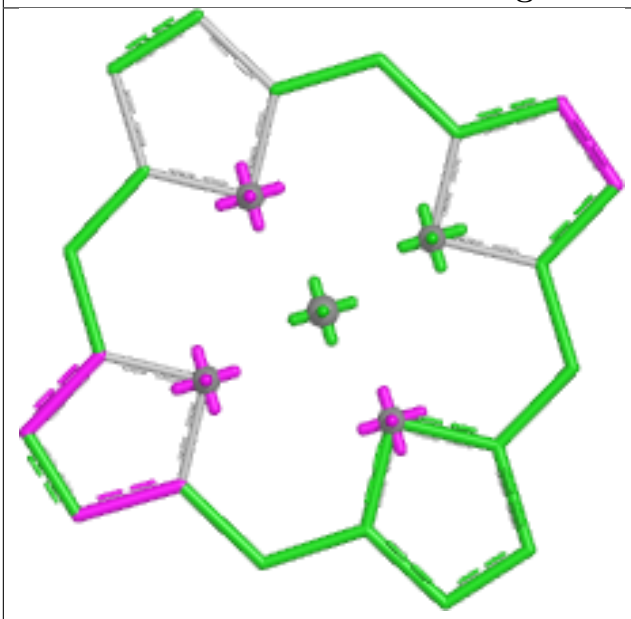


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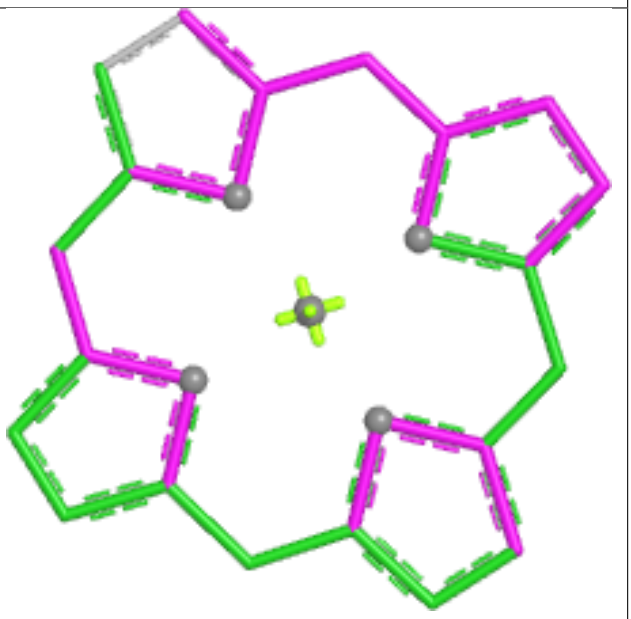


Rings

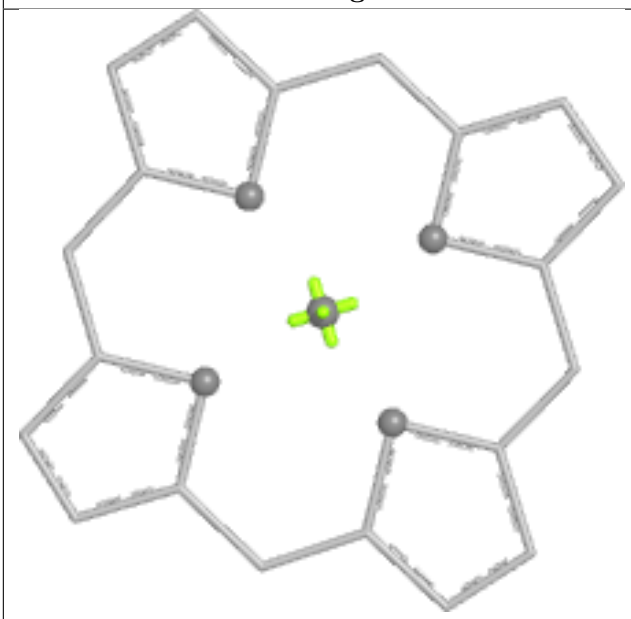
Ligand CLA P 5117



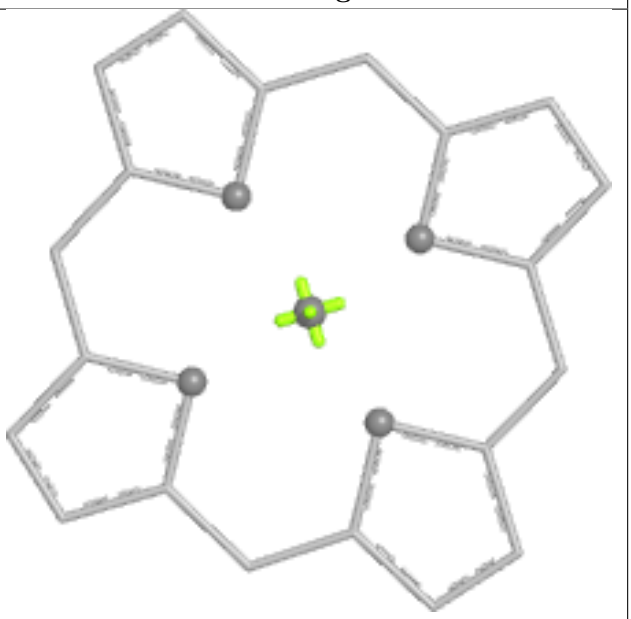
Bond lengths



Bond angles

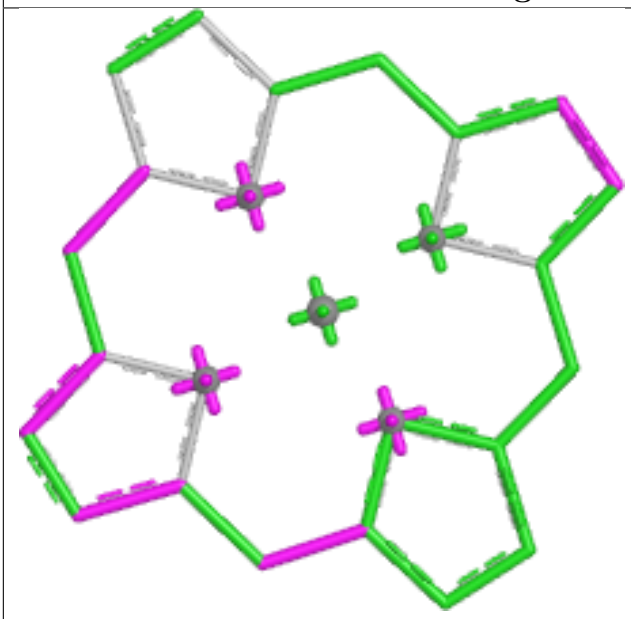


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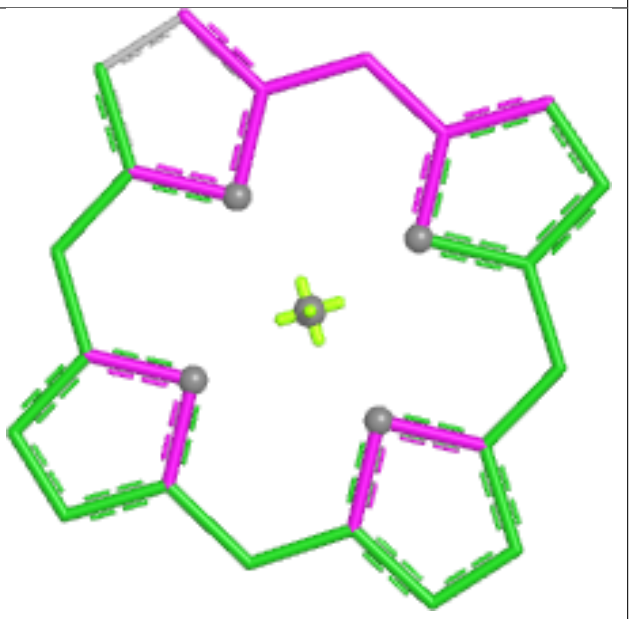


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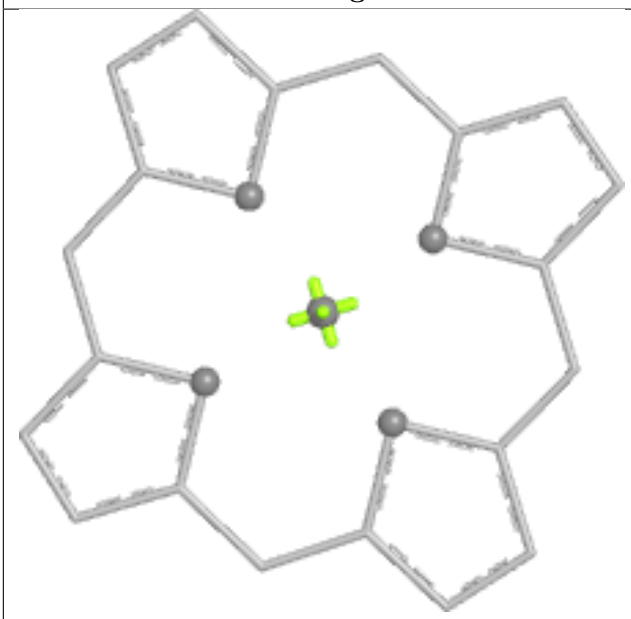
Ligand CLA G 1233



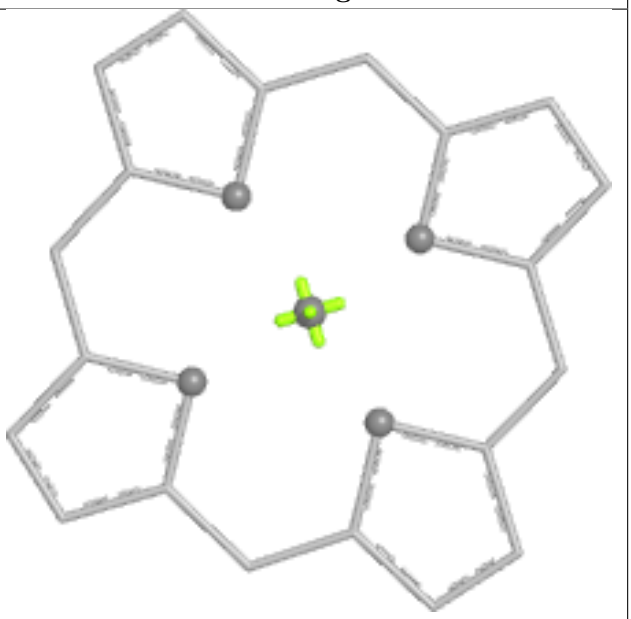
Bond lengths



Bond angles

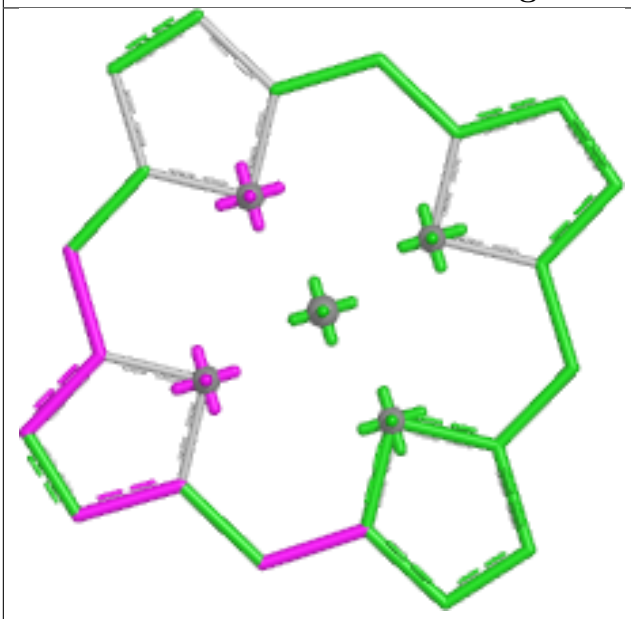


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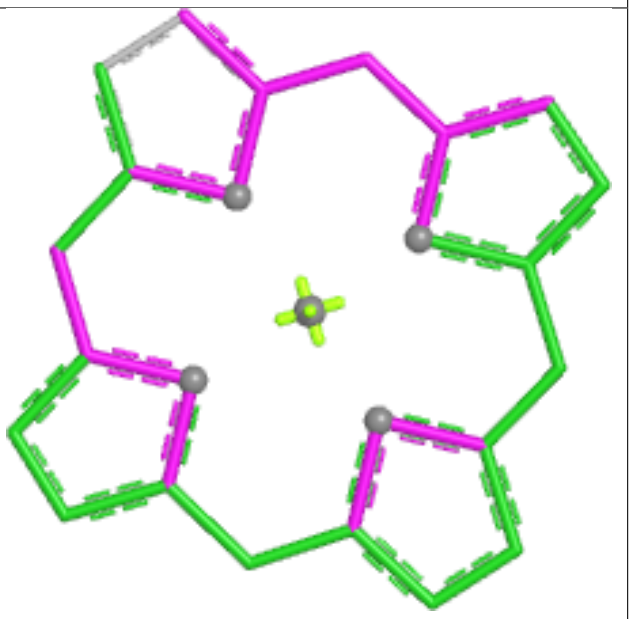


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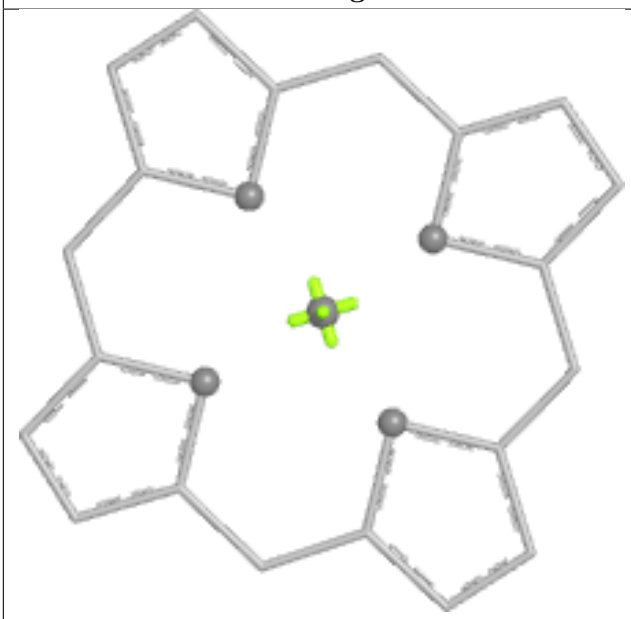
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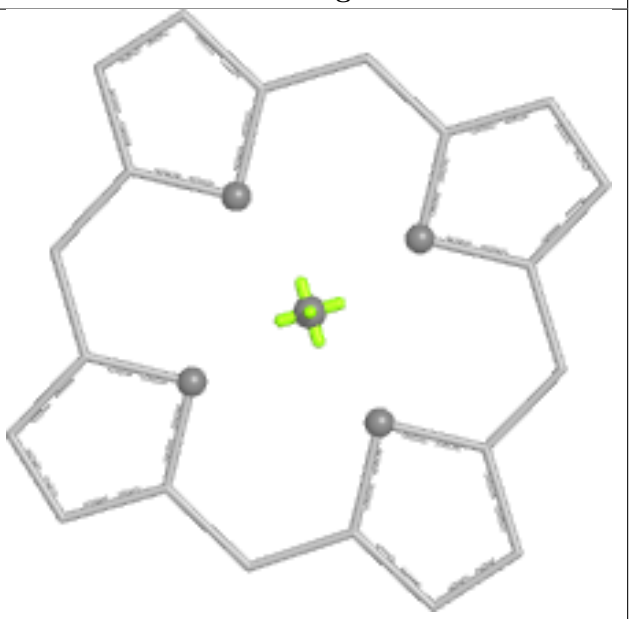
Bond lengths



Bond angles

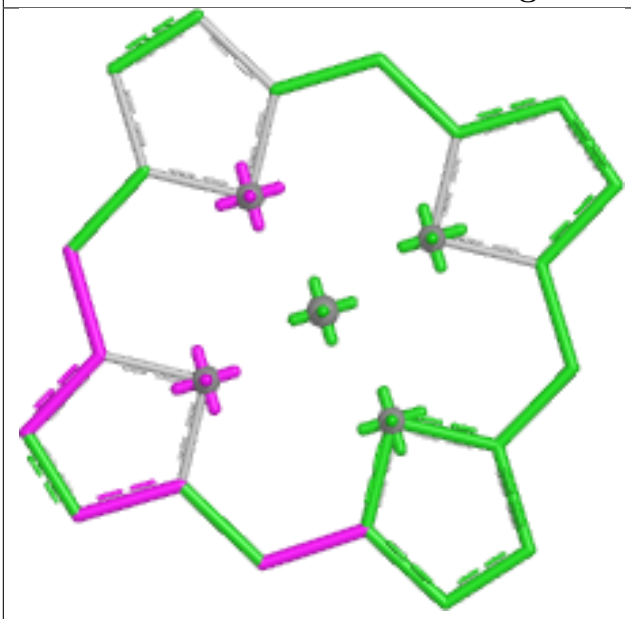


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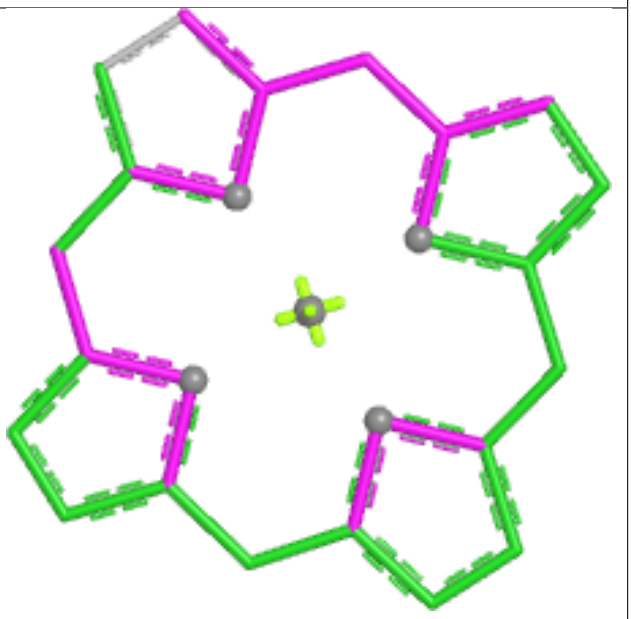


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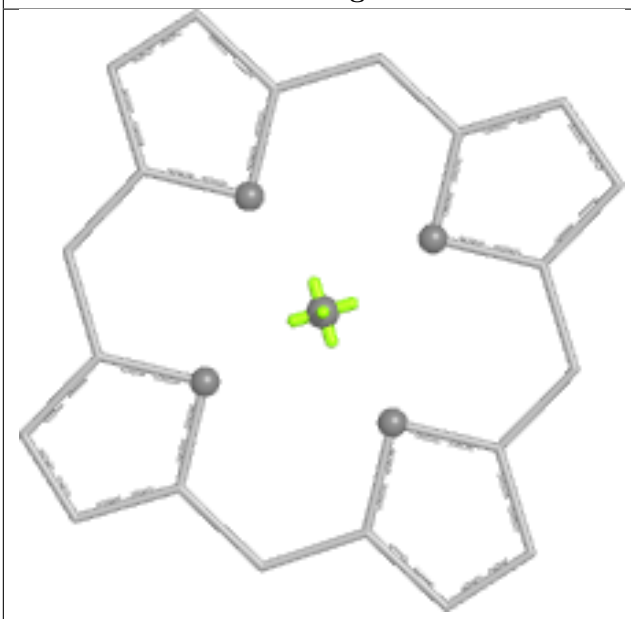
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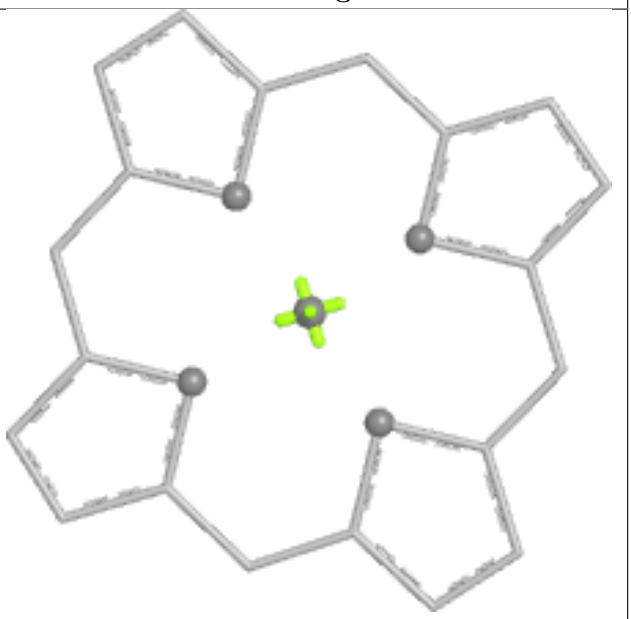
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Bond angles

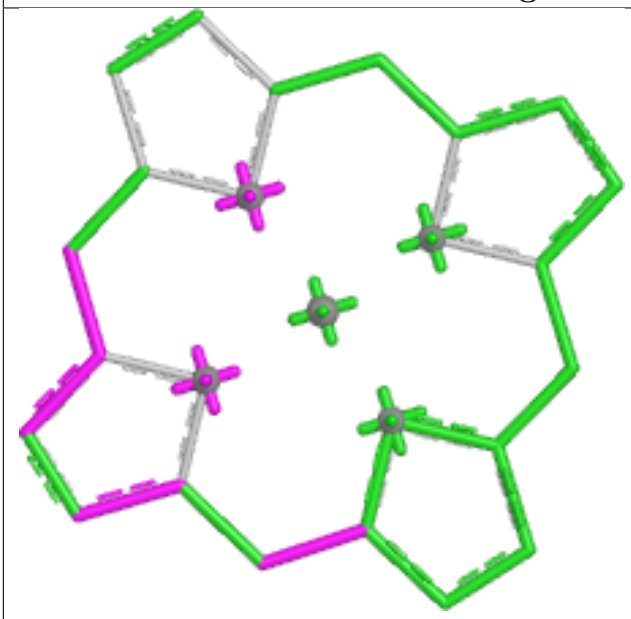


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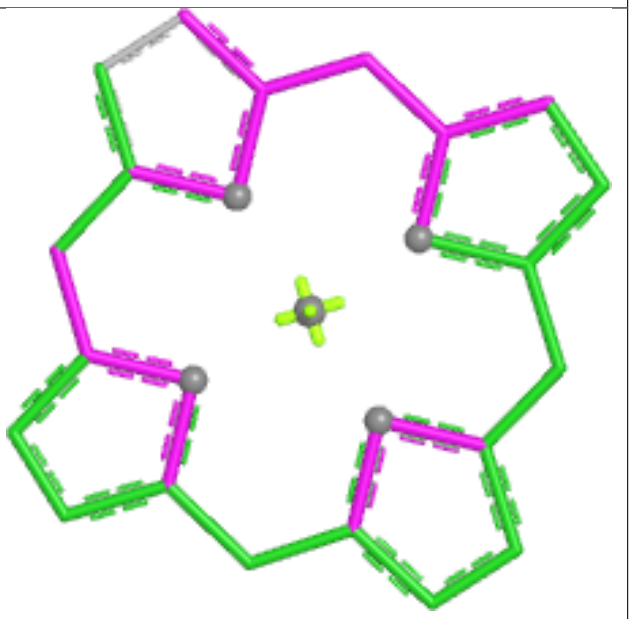


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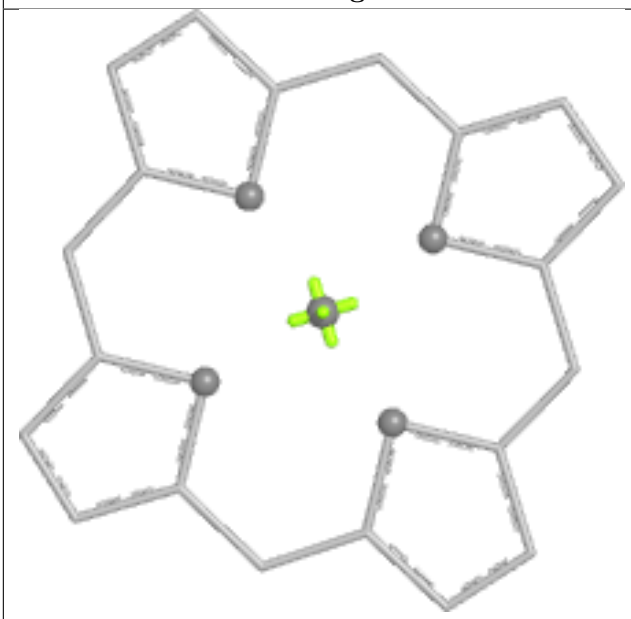
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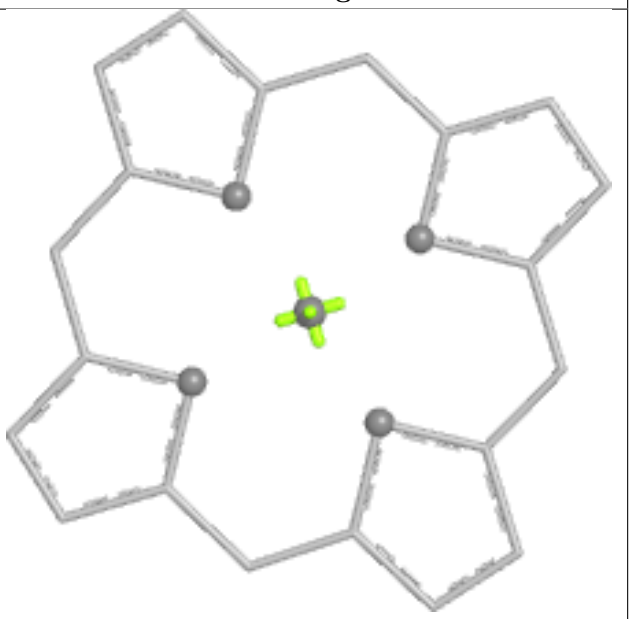
Bond lengths



Bond angles

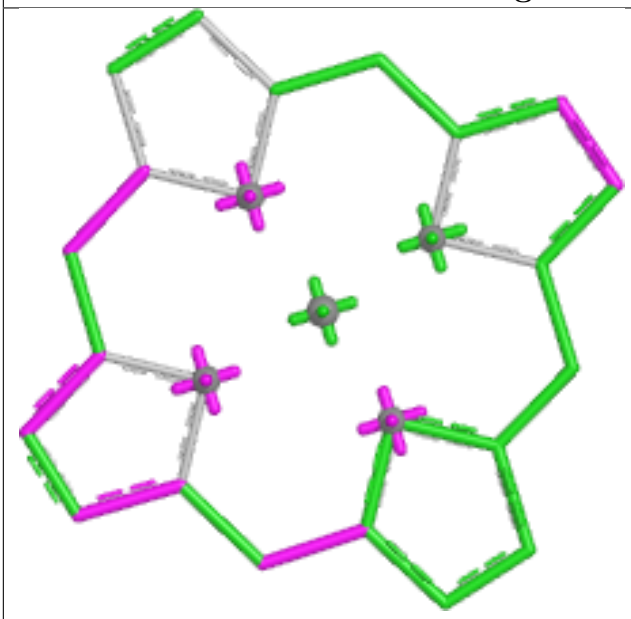


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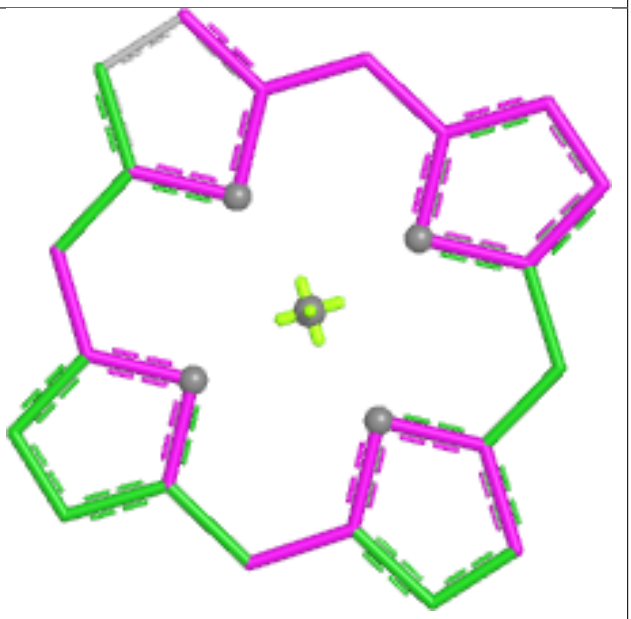


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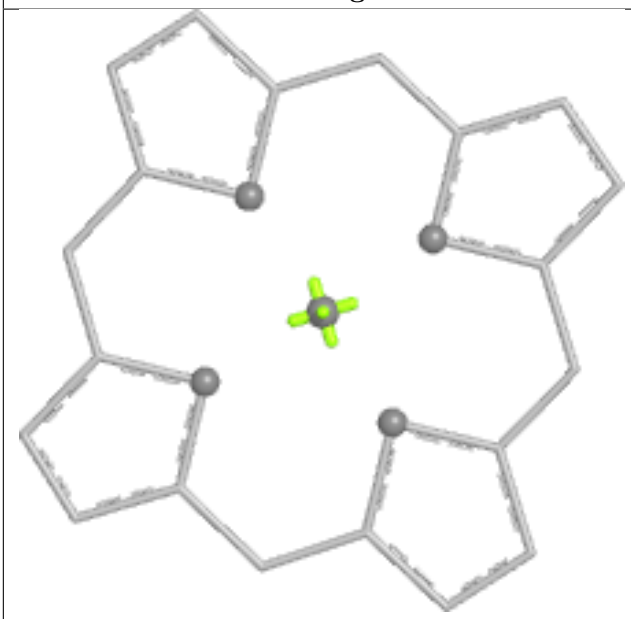
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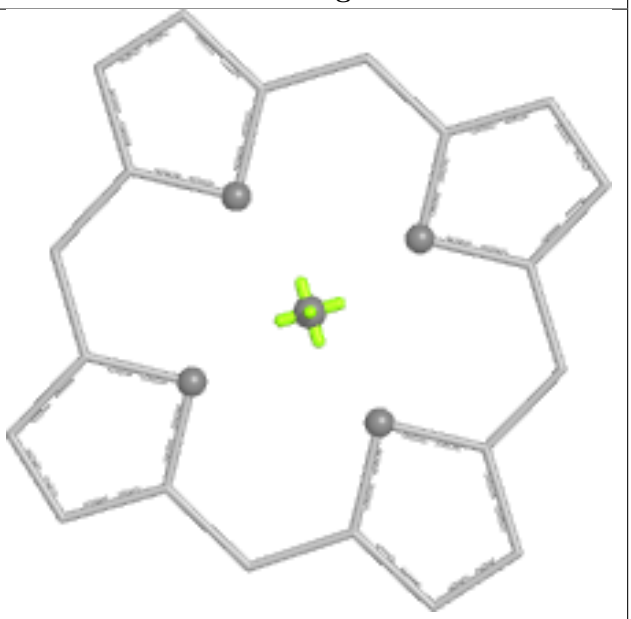
Bond lengths



Bond angles

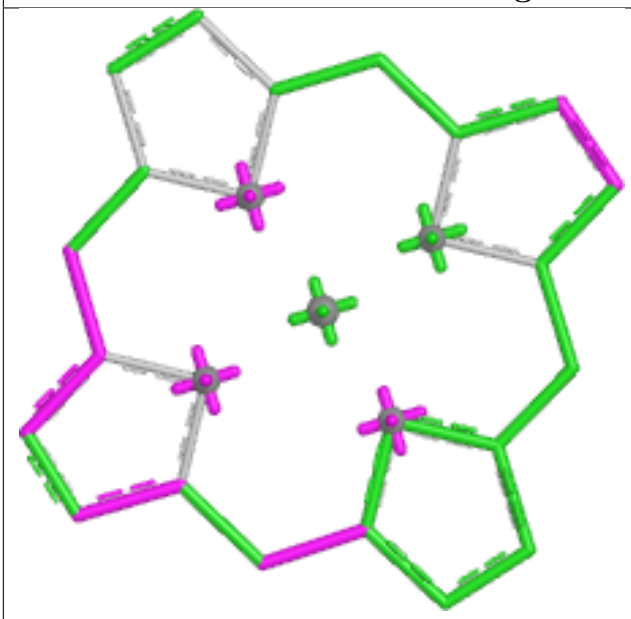


Torsions

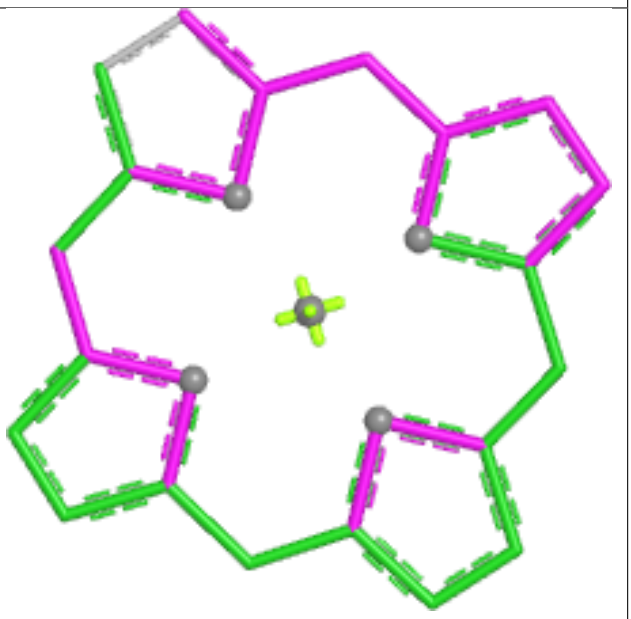


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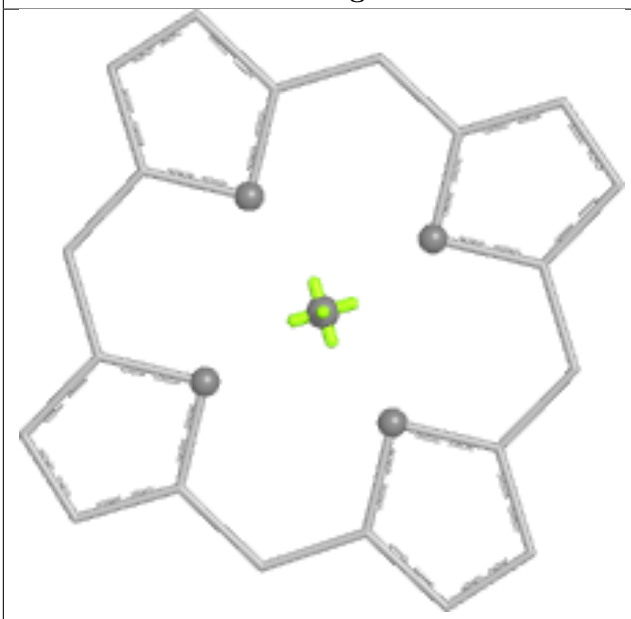
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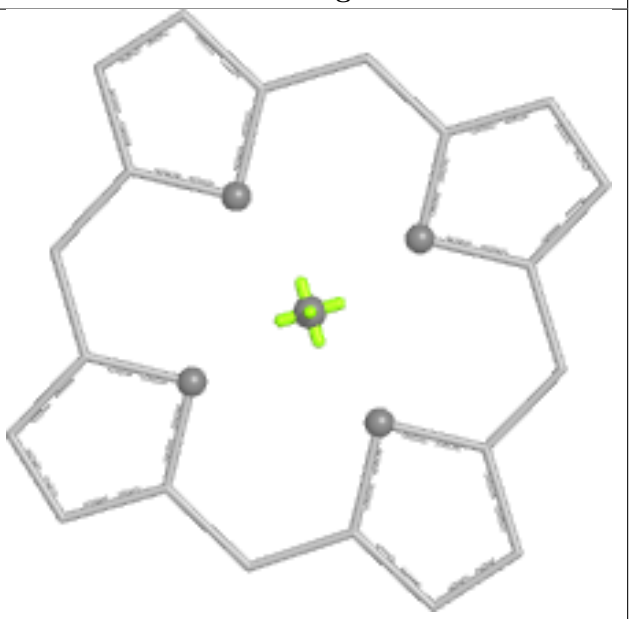
Bond lengths



Bond angles

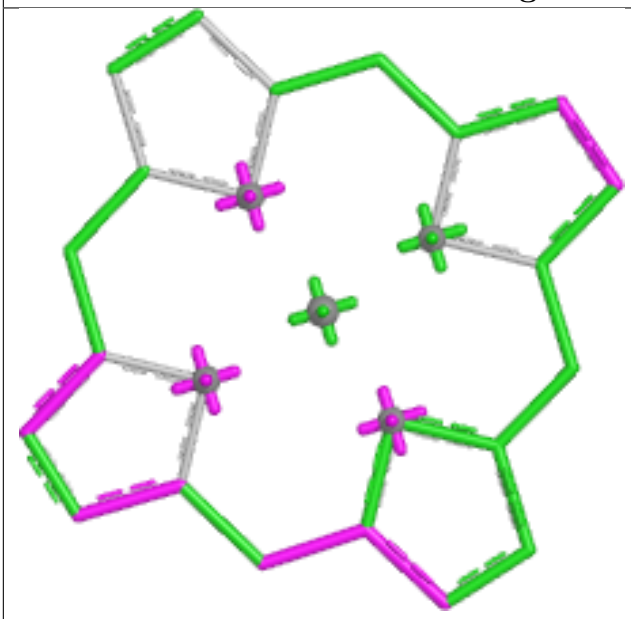


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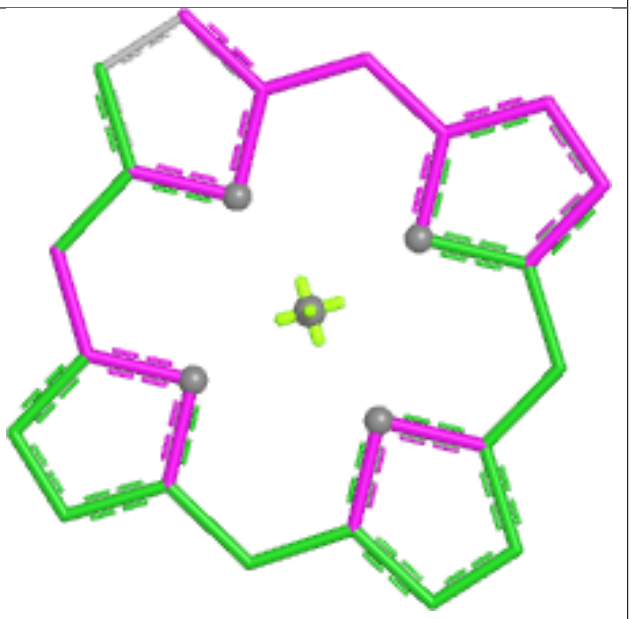


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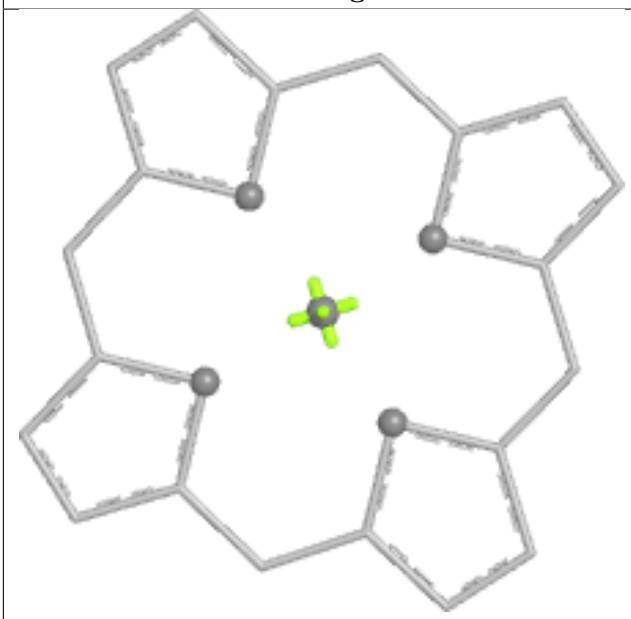
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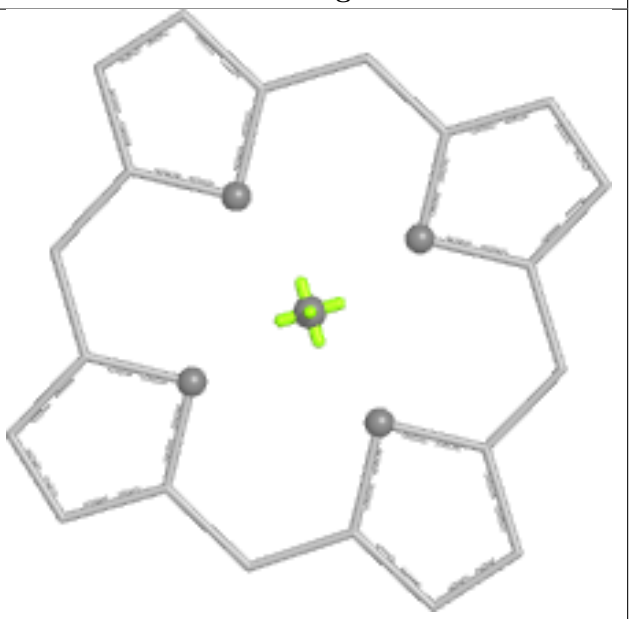
Bond lengths



Bond angles

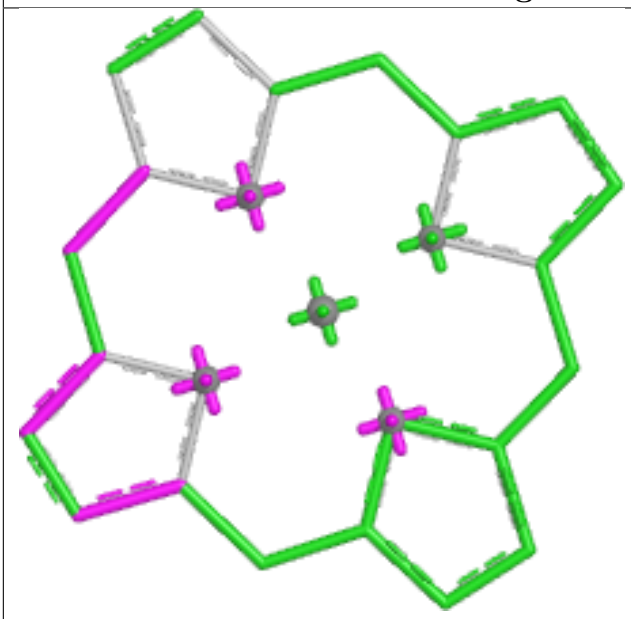


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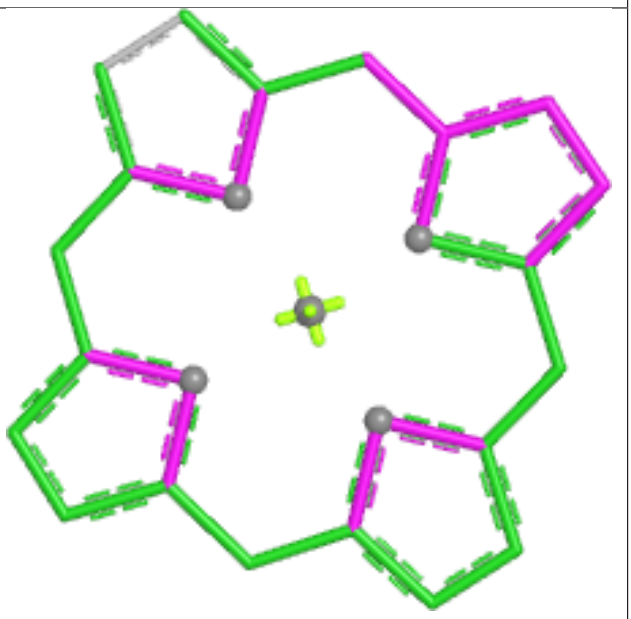


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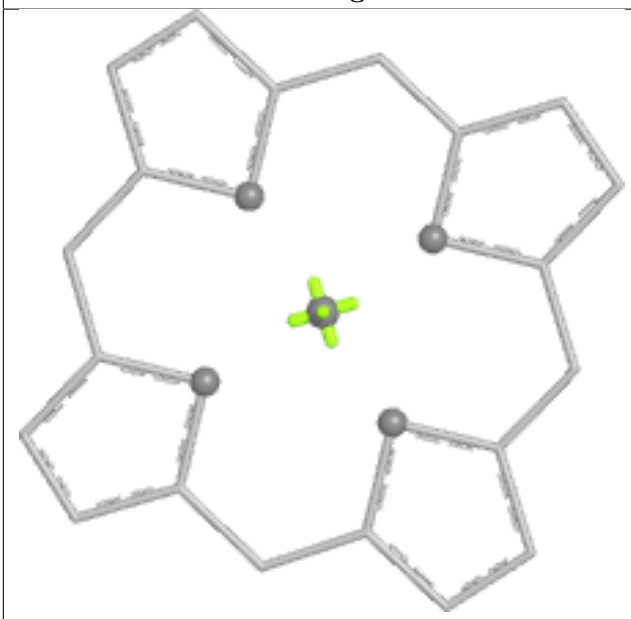
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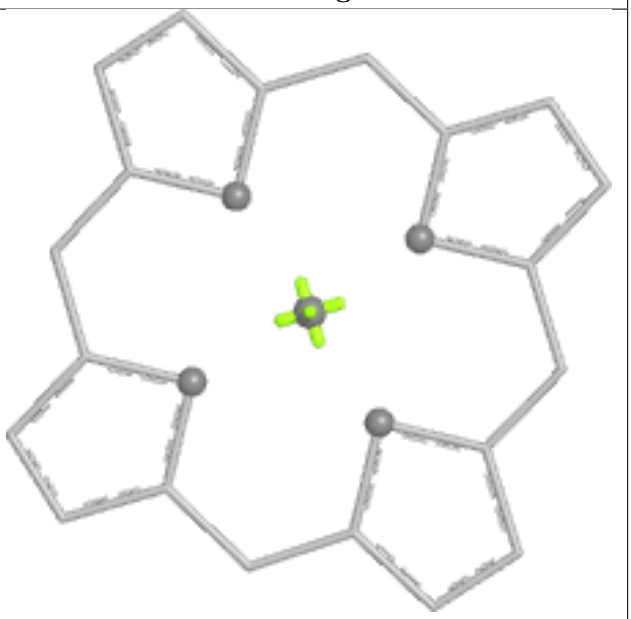
Bond lengths



Bond angles

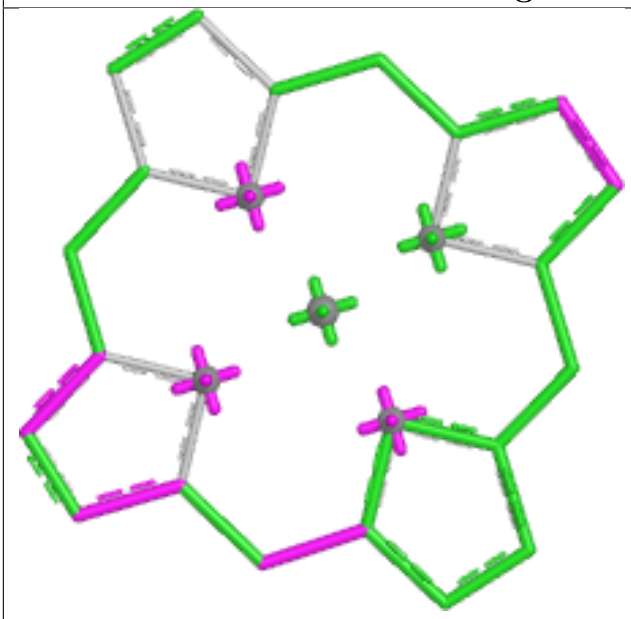


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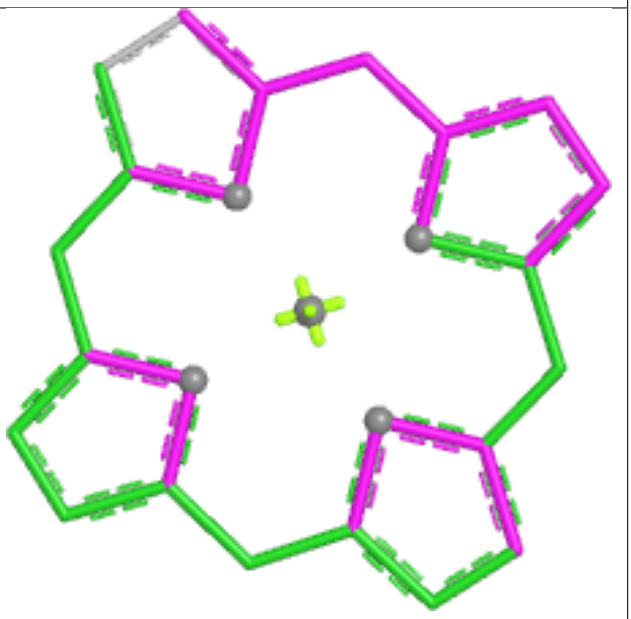


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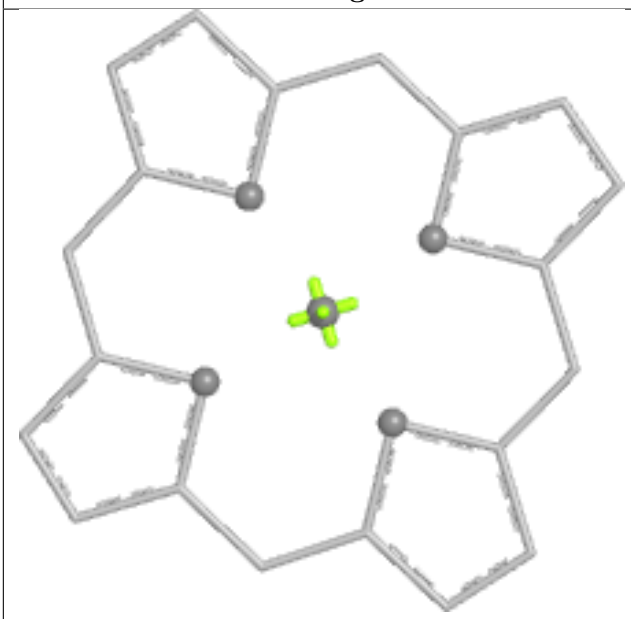
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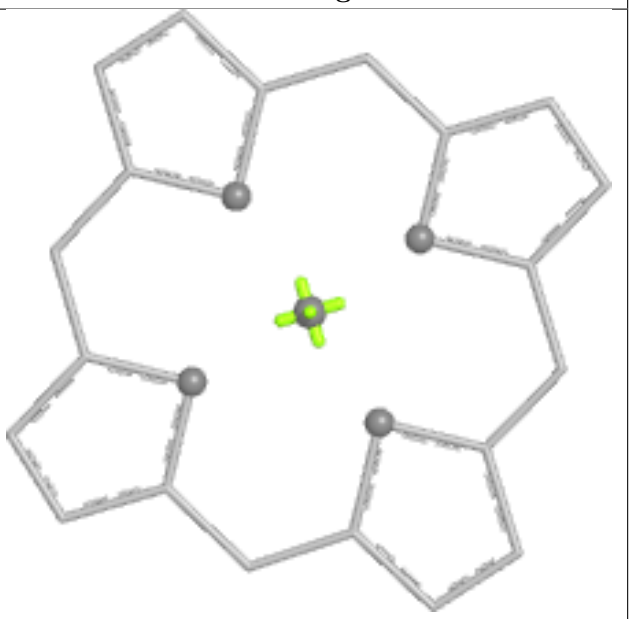
Bond lengths



Bond angles

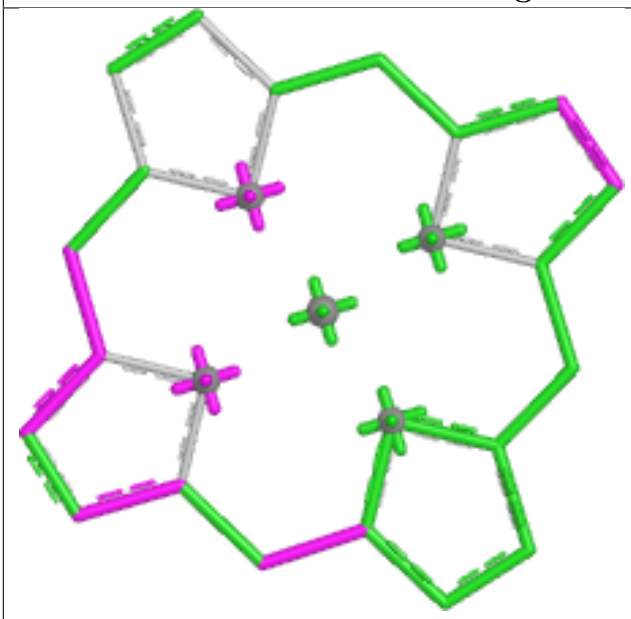


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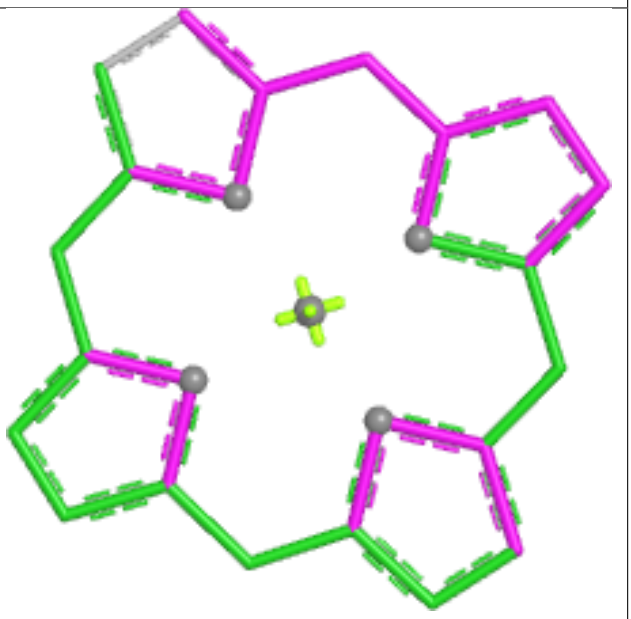


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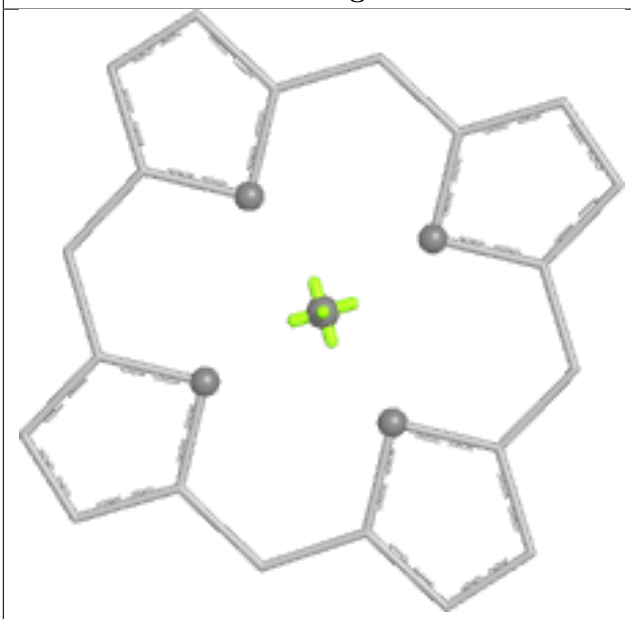
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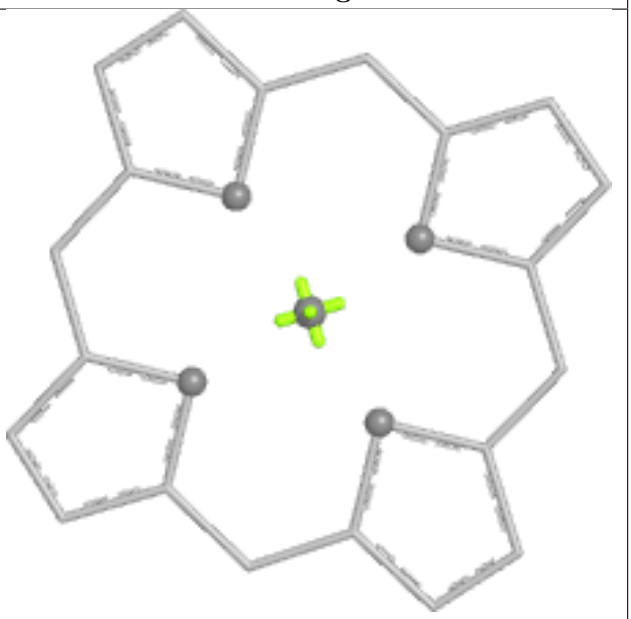
Bond lengths



Bond angles

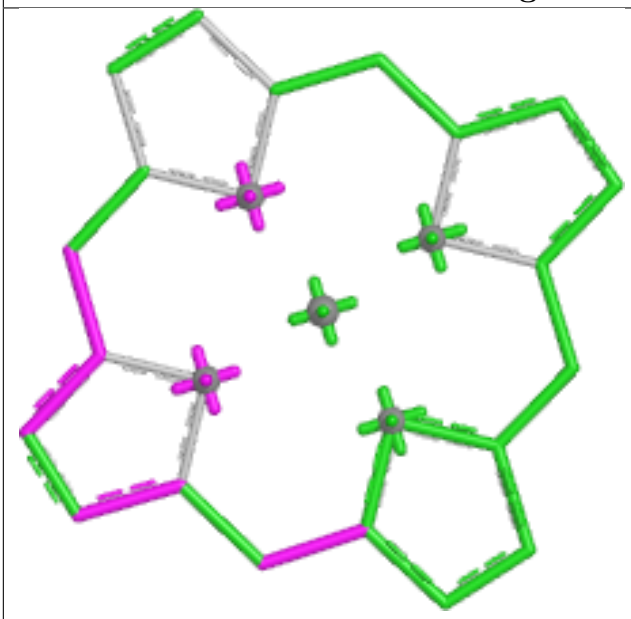


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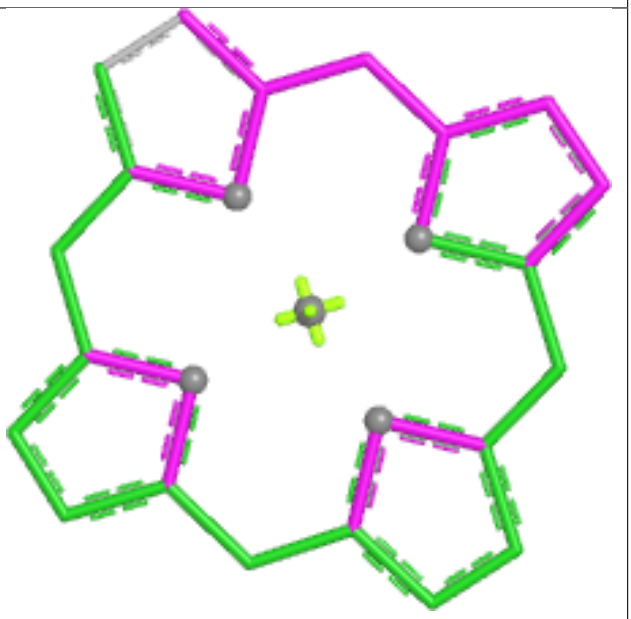


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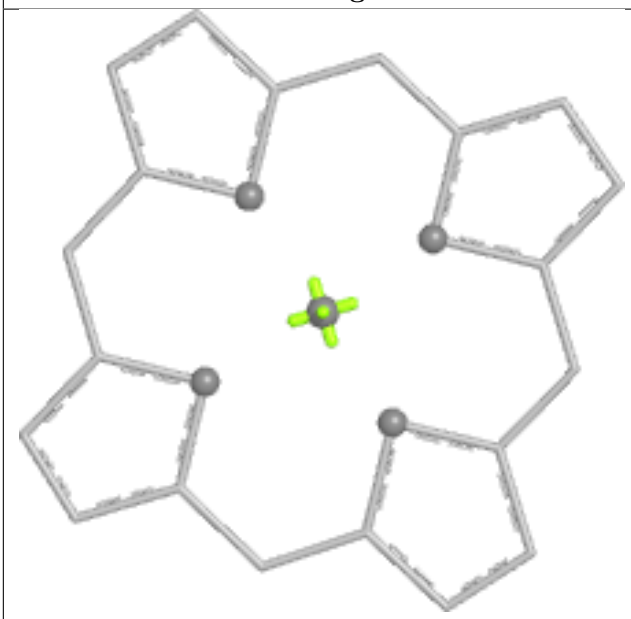
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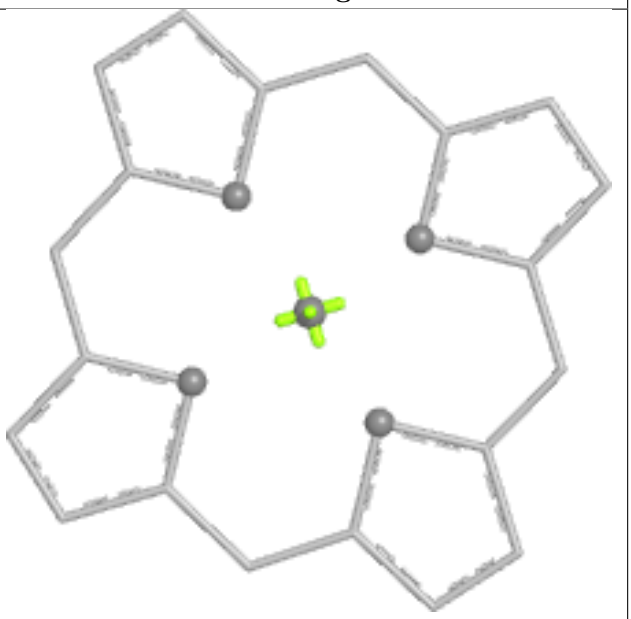
Bond lengths



Bond angles

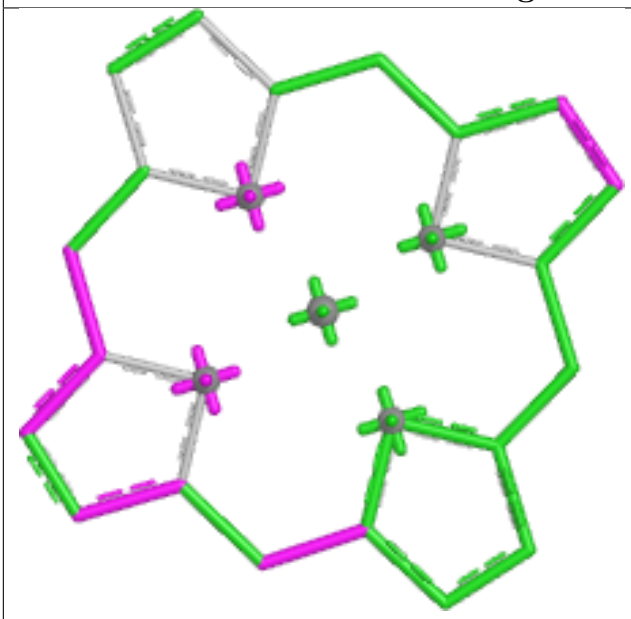


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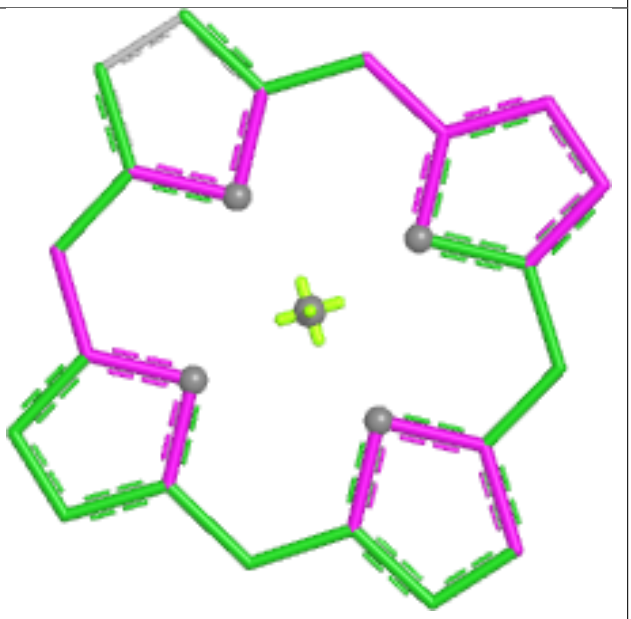


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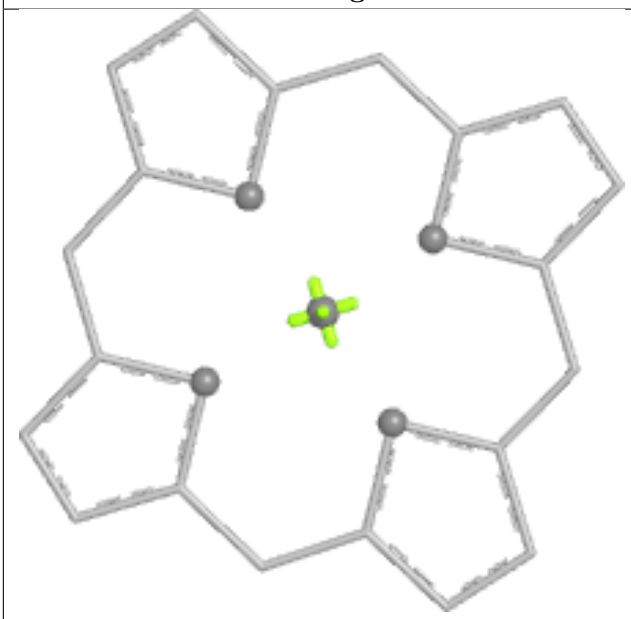
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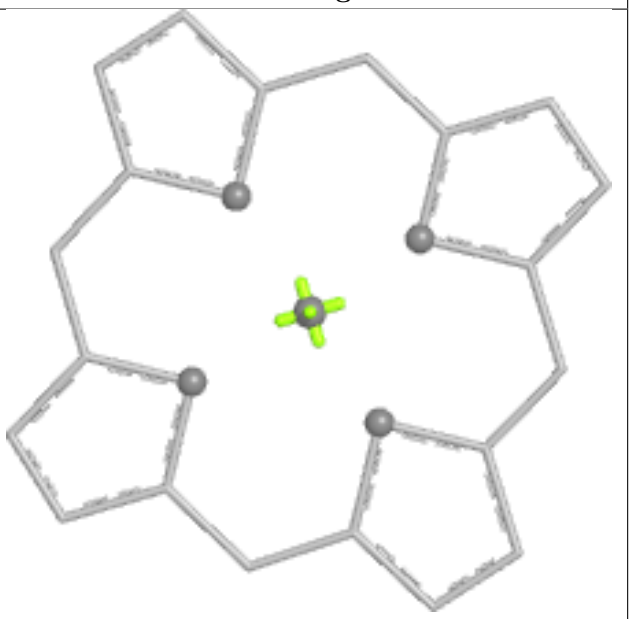
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Bond angles

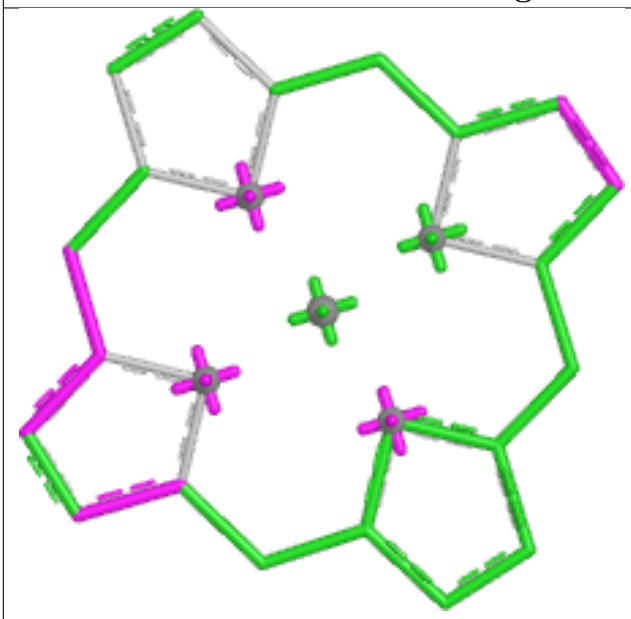


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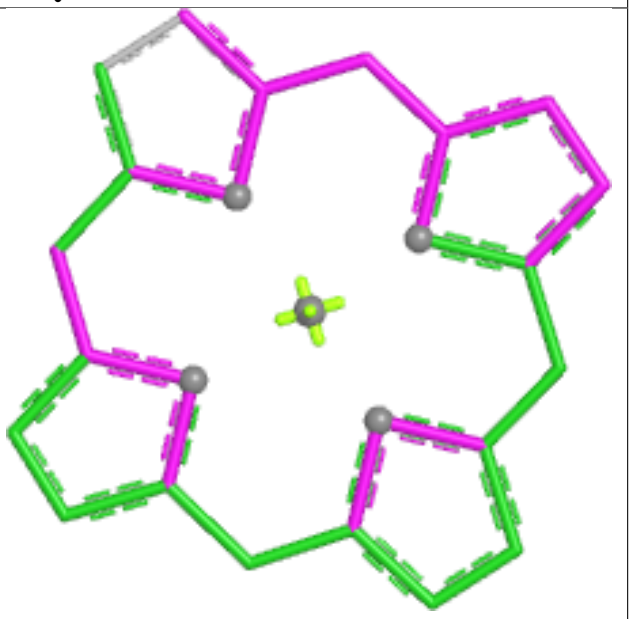


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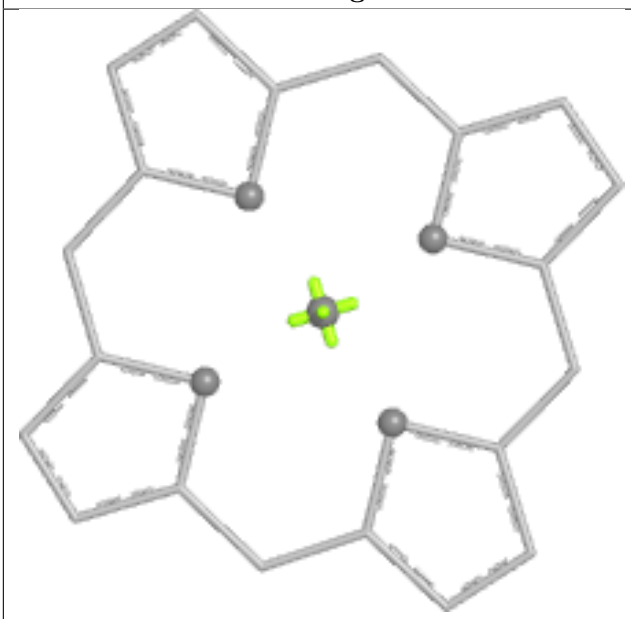
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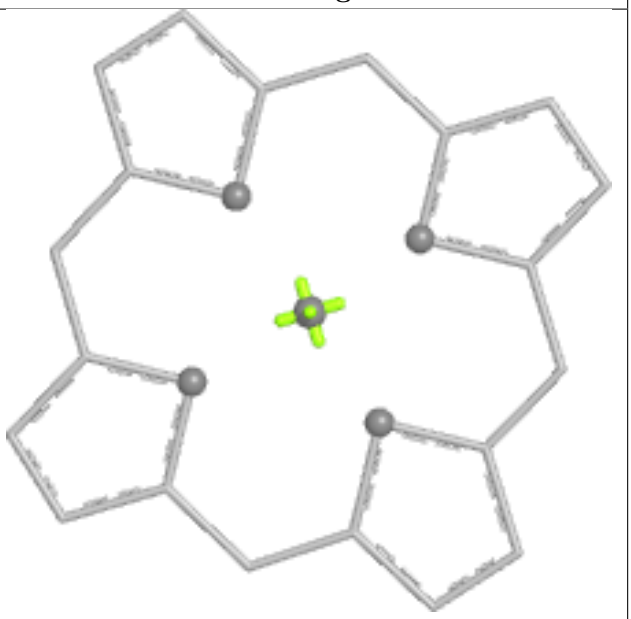
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Bond angles

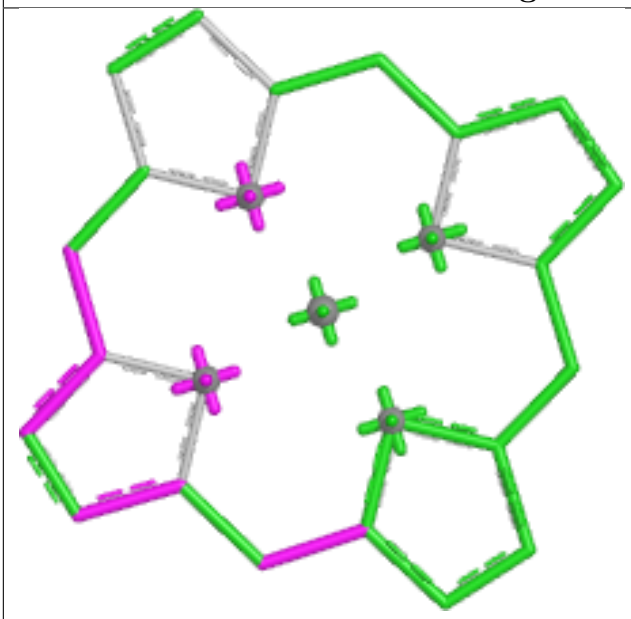


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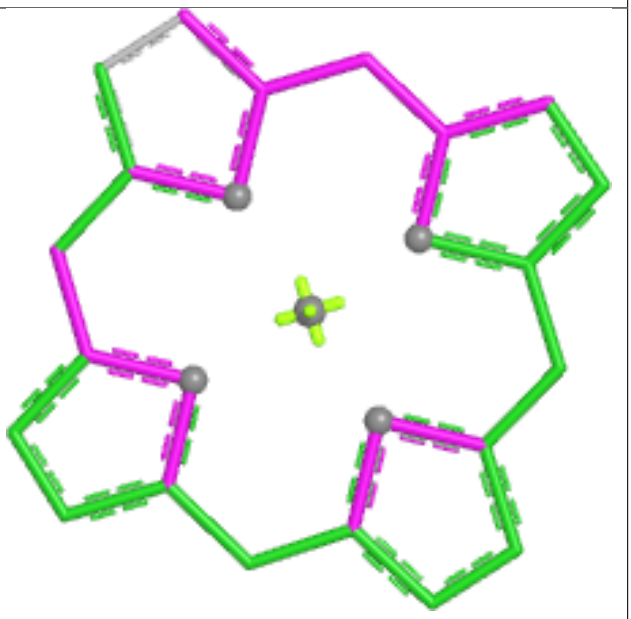


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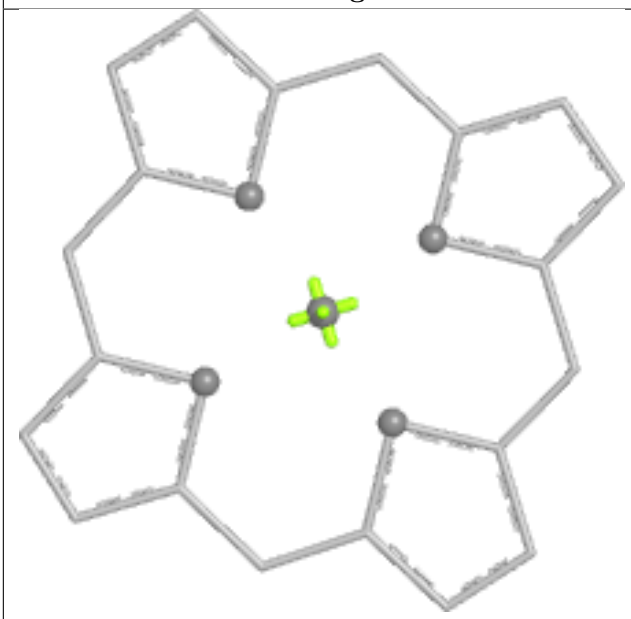
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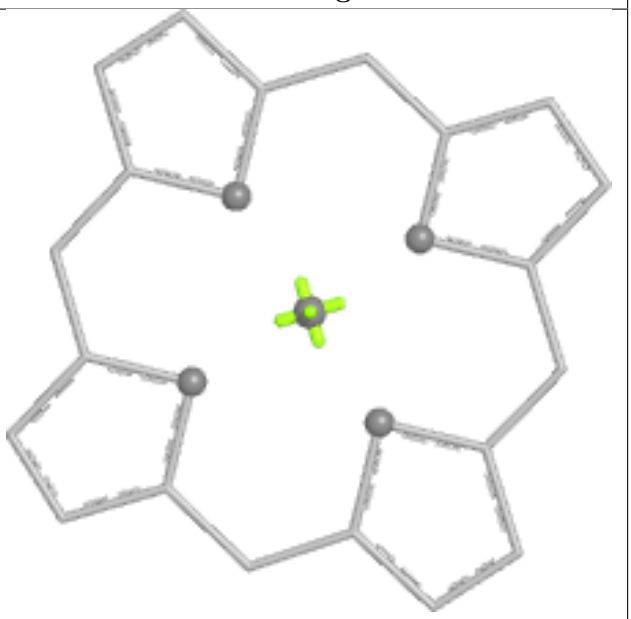
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Bond angles

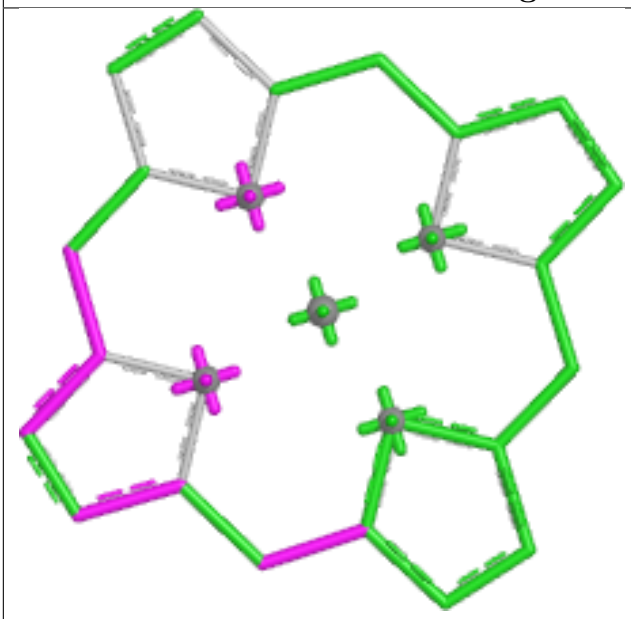


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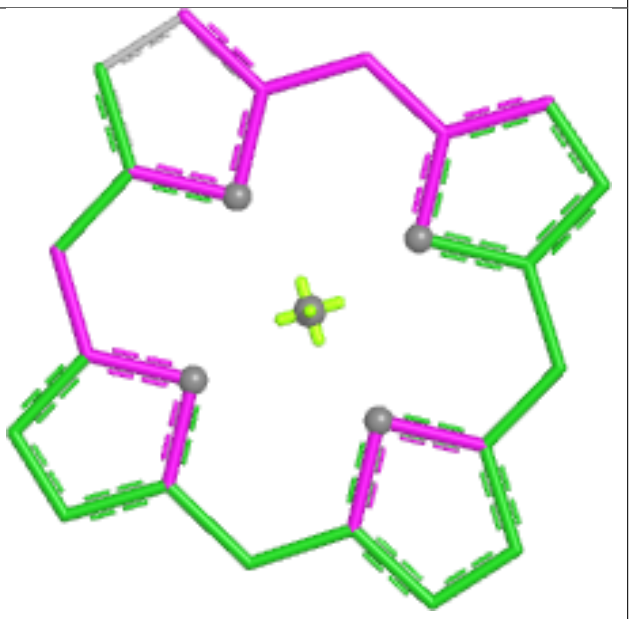


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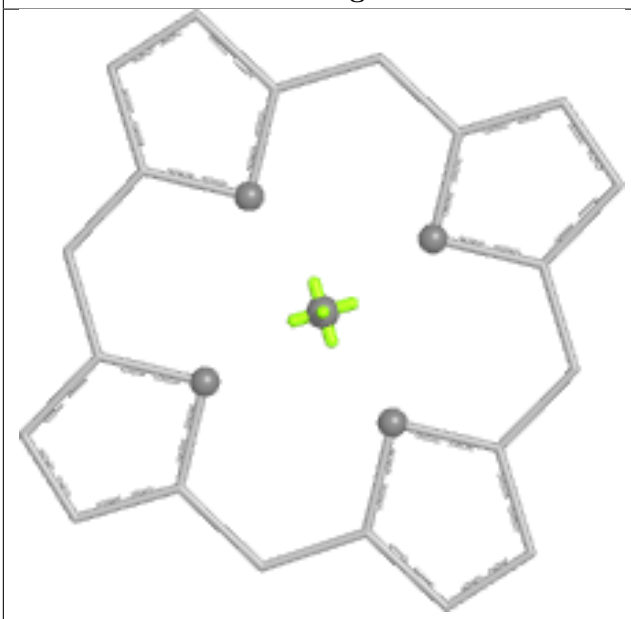
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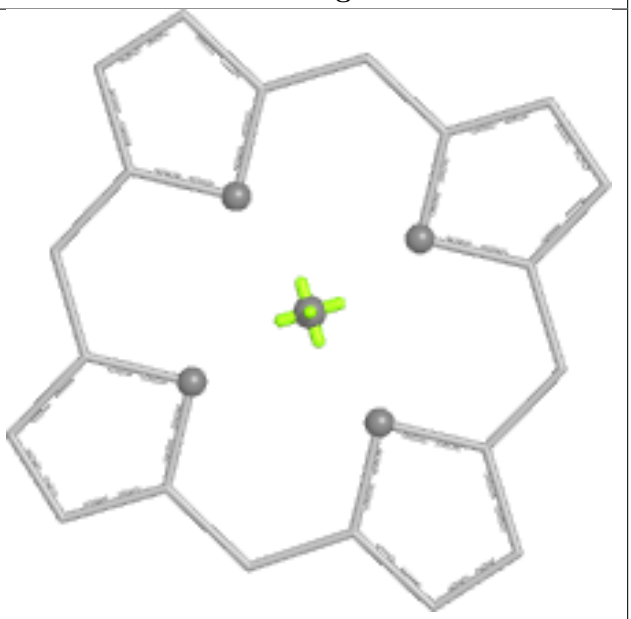
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Bond angles

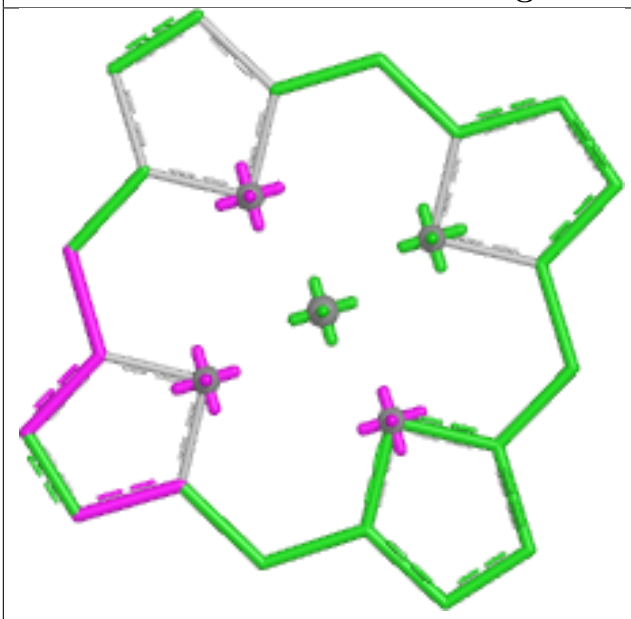


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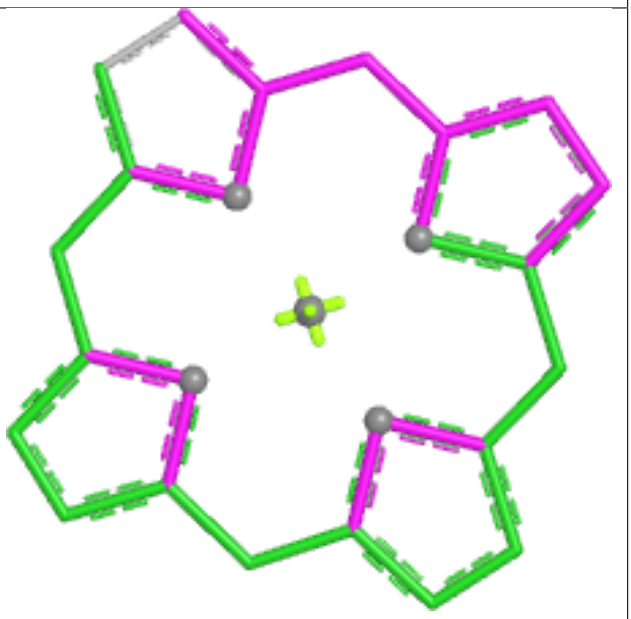


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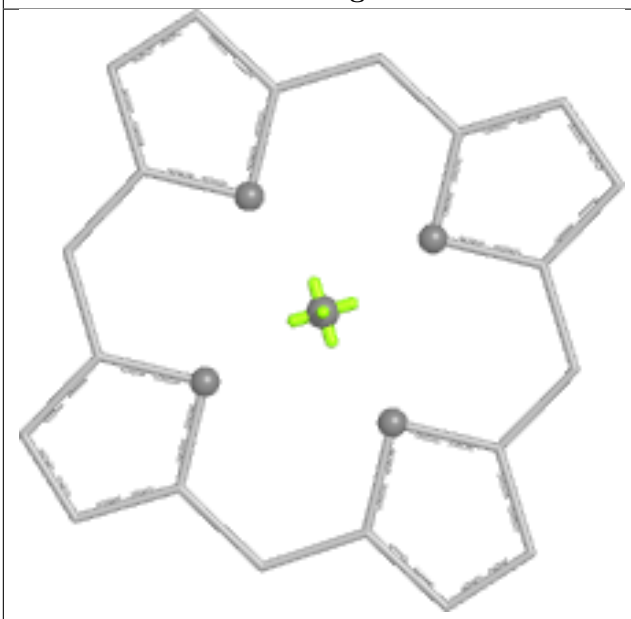
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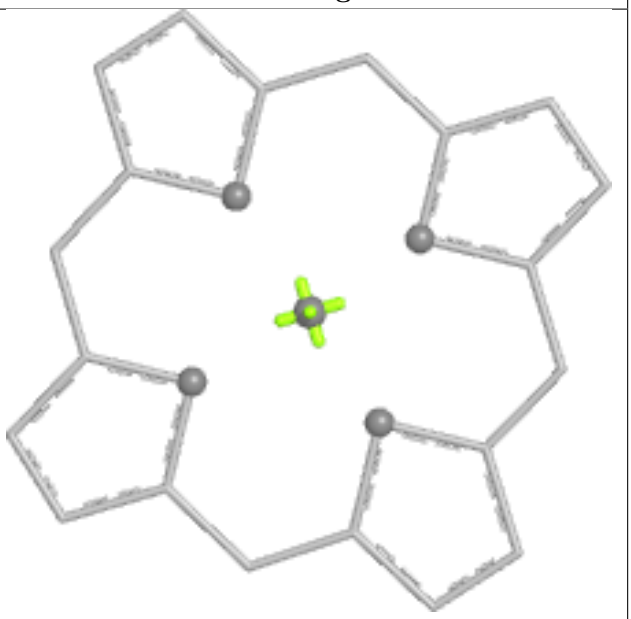
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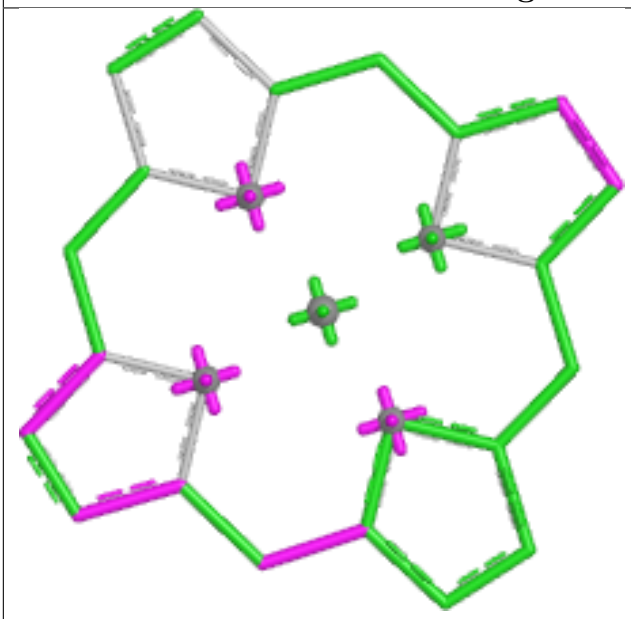


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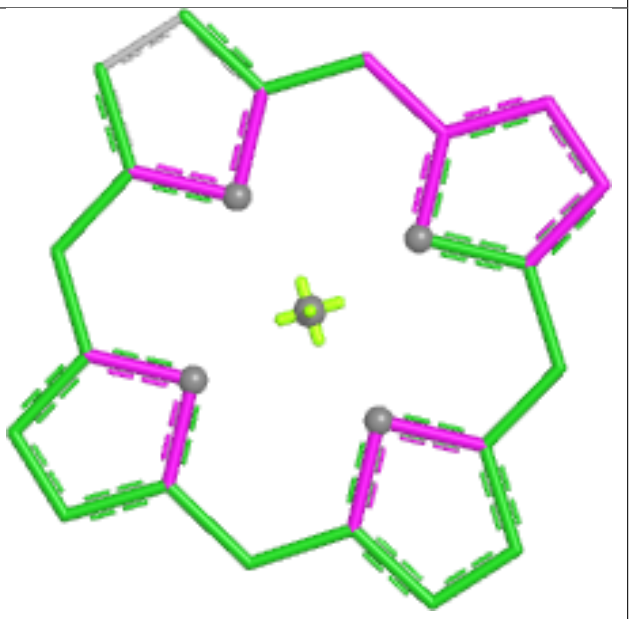


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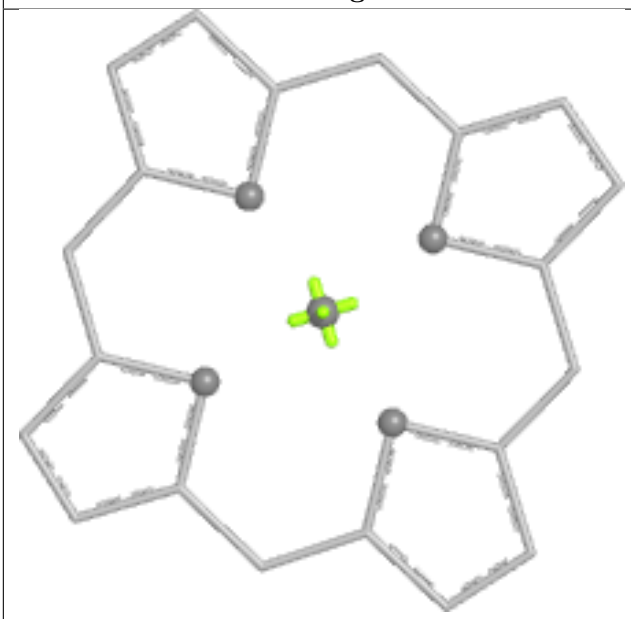
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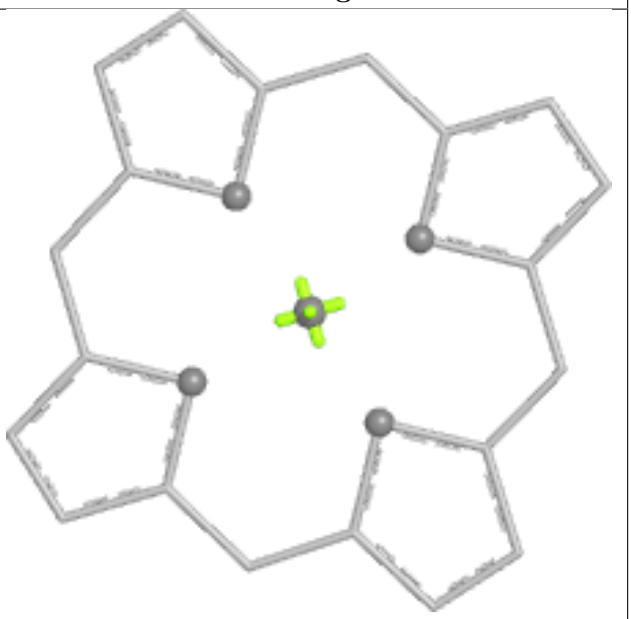
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Bond angles

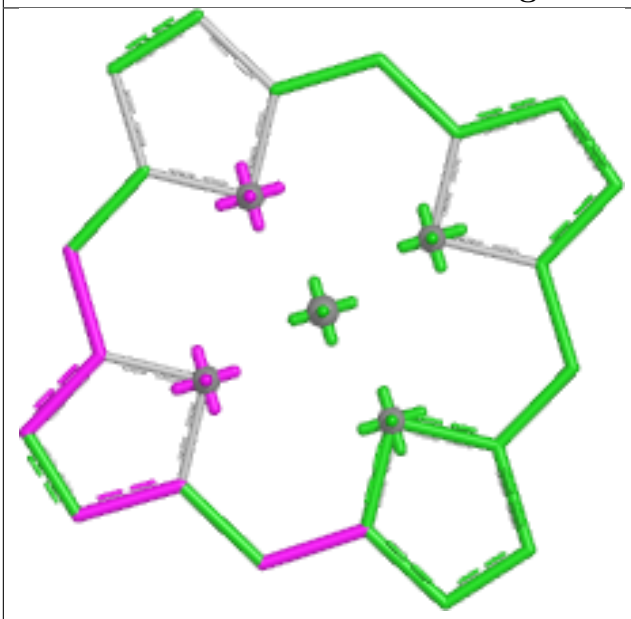


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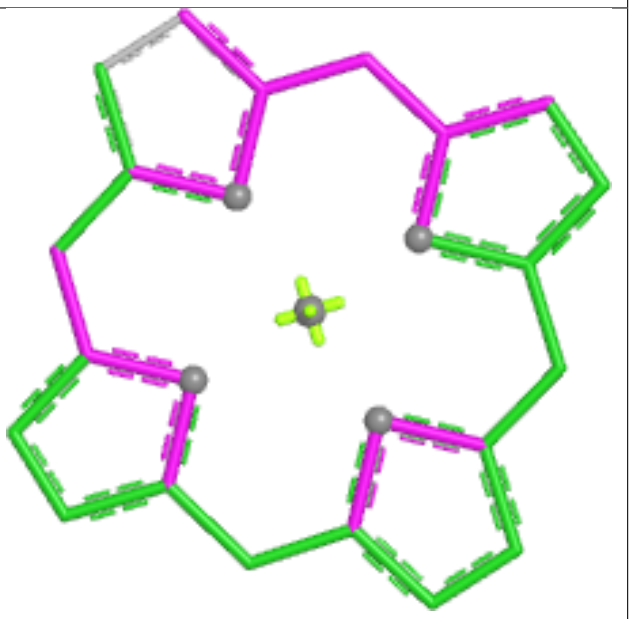


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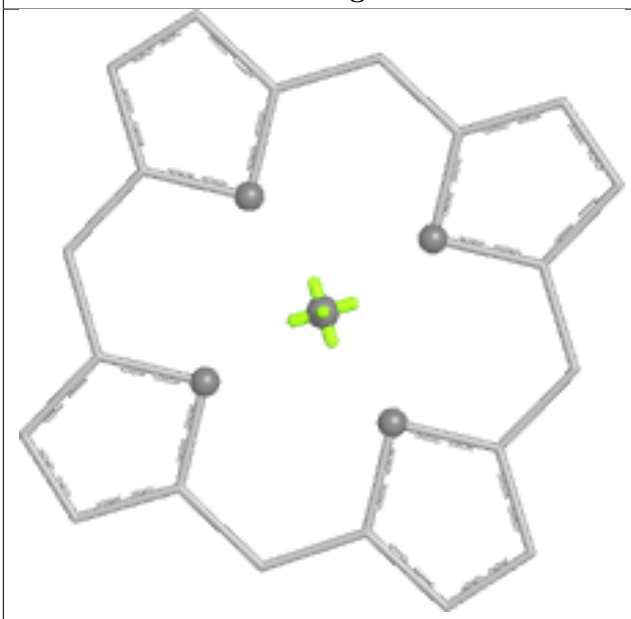
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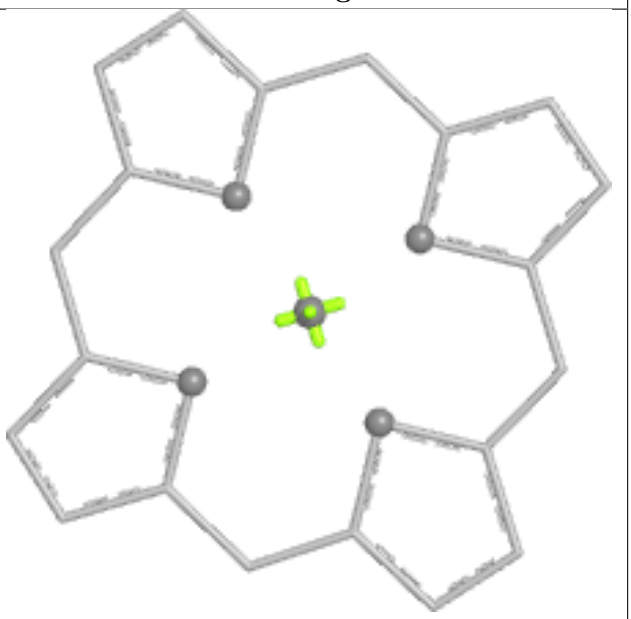
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Bond angles

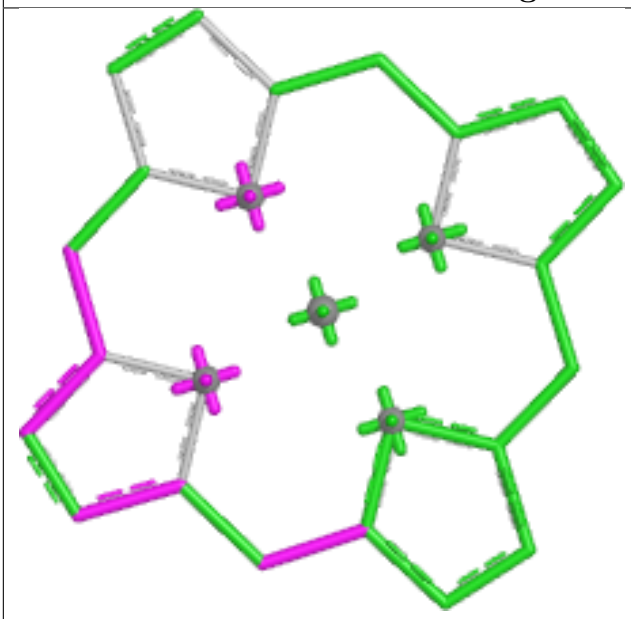


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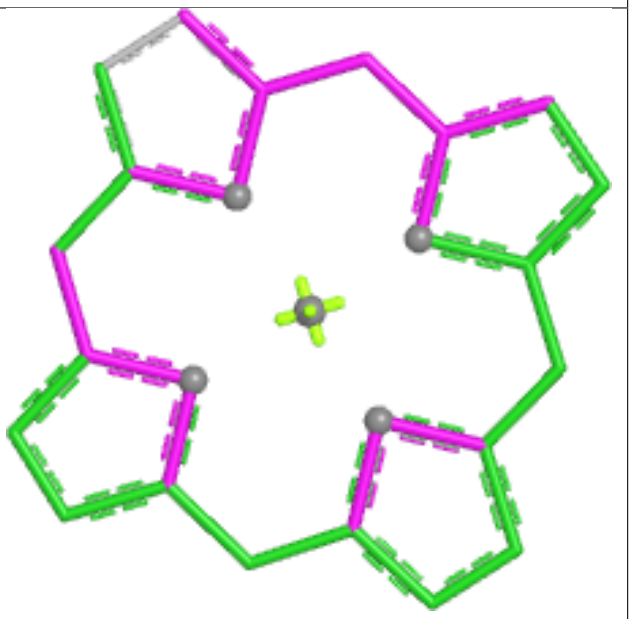


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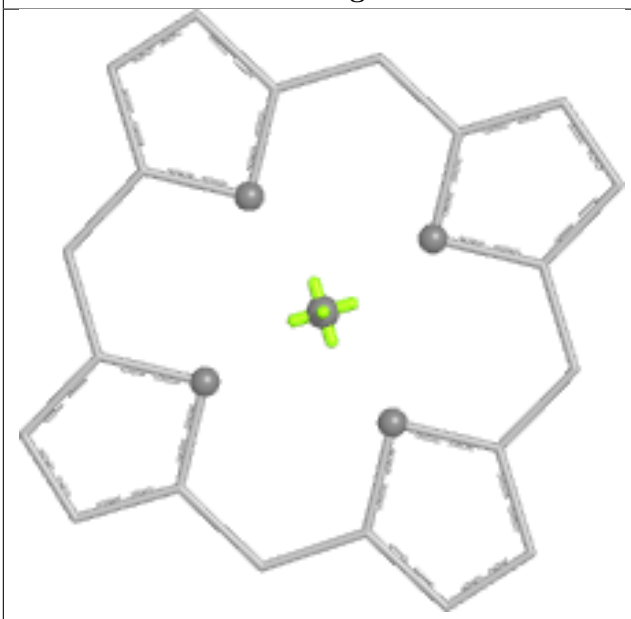
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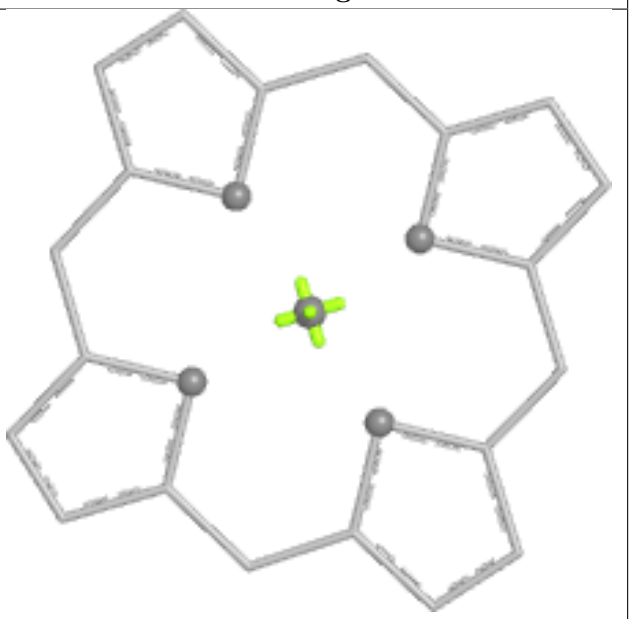
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Bond angles

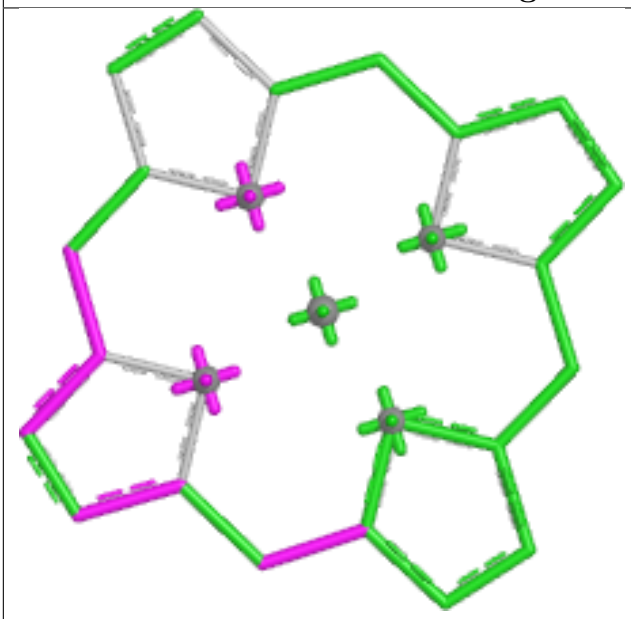


Torsions

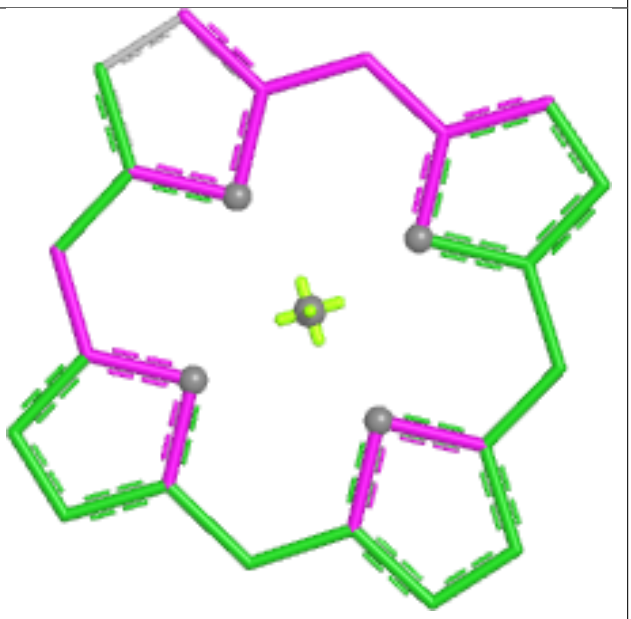


Rings

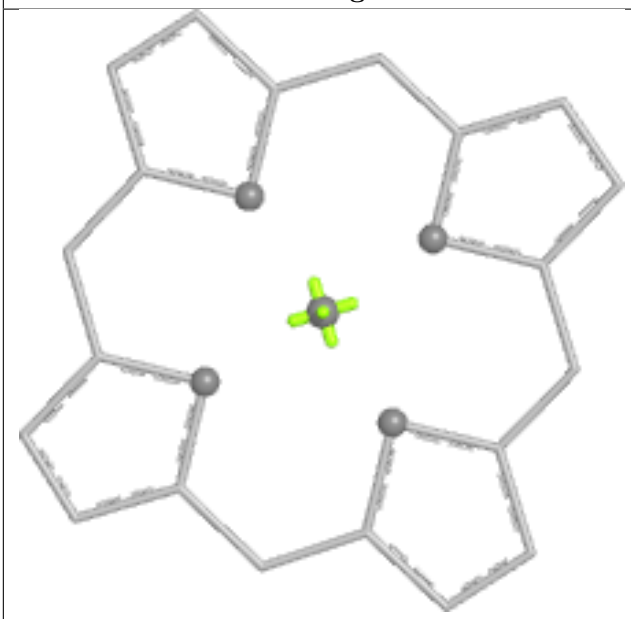
Ligand CLA 4 1021



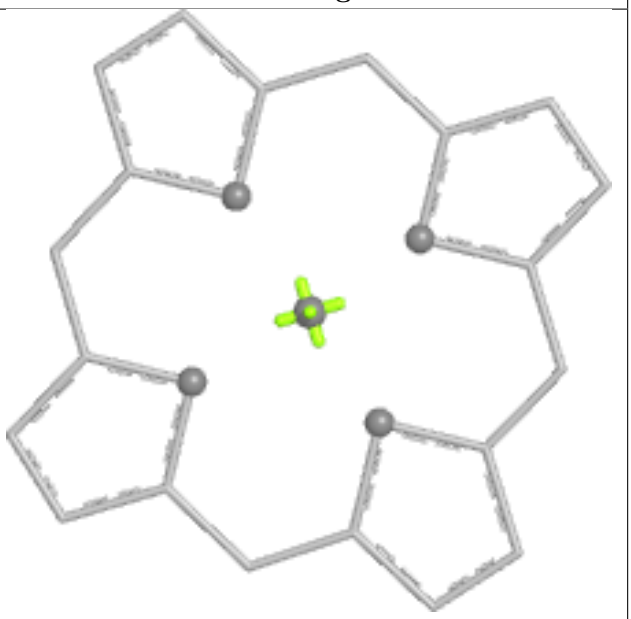
Bond lengths



Bond angles

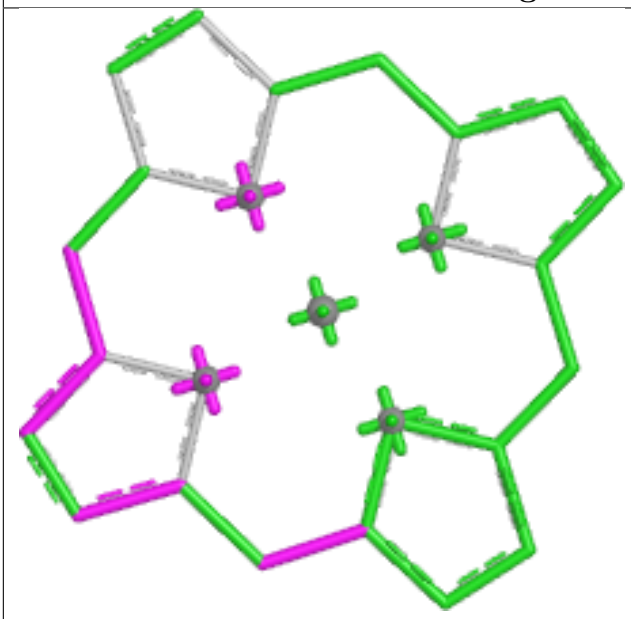


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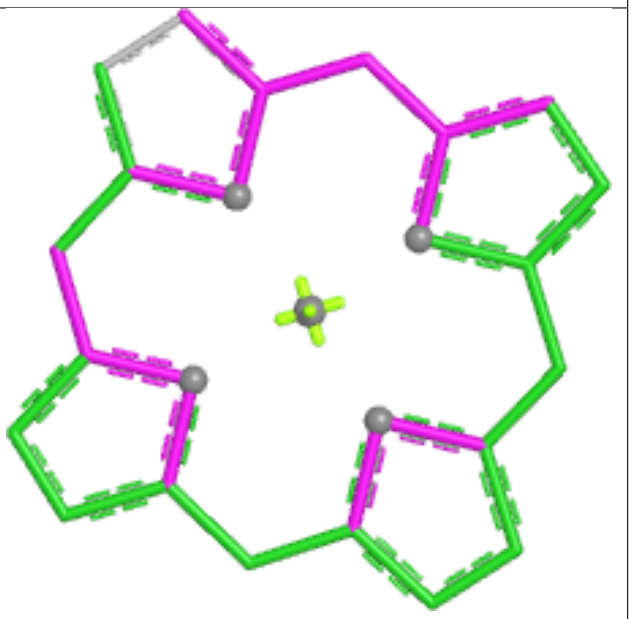


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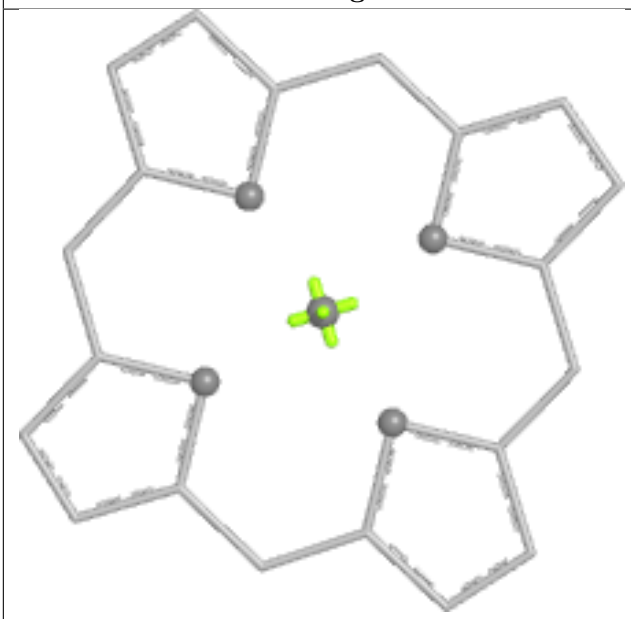
Ligand CLA 9 1014



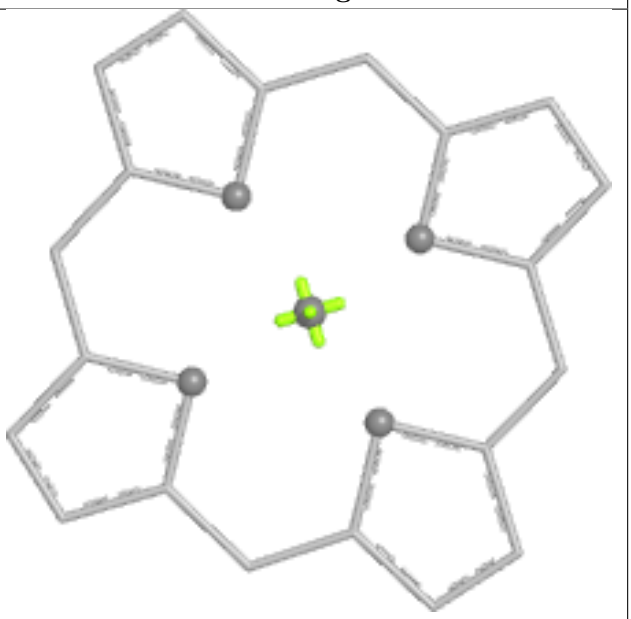
Bond lengths



Bond angles

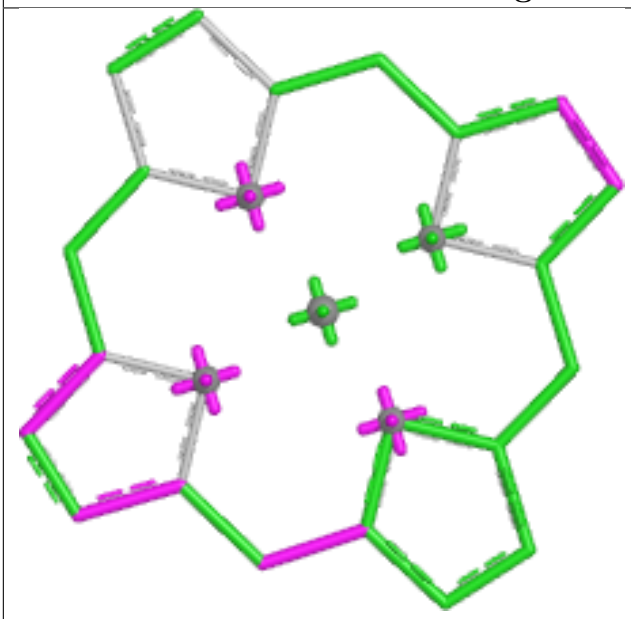


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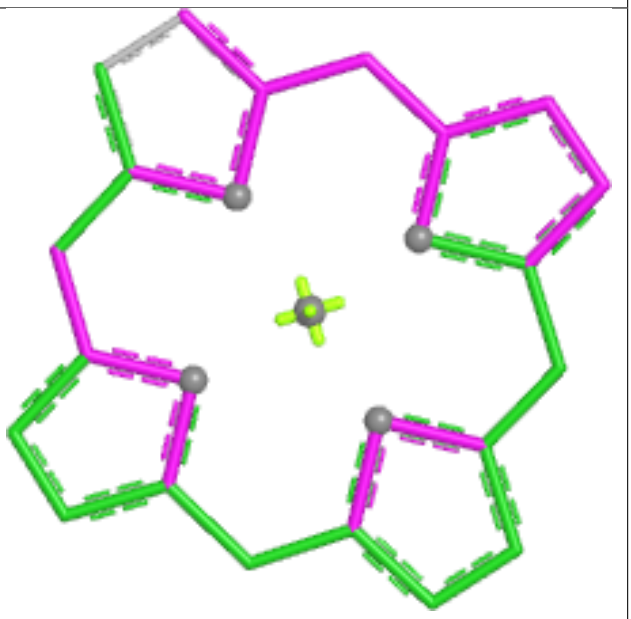


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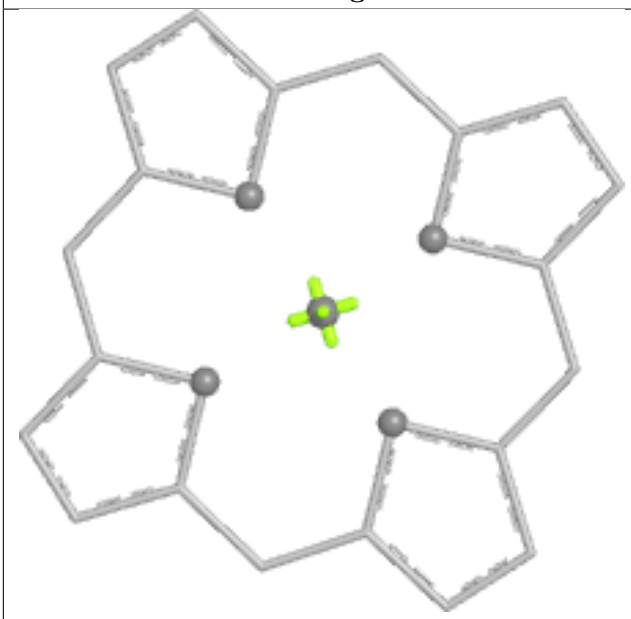
Ligand CLA A 1123



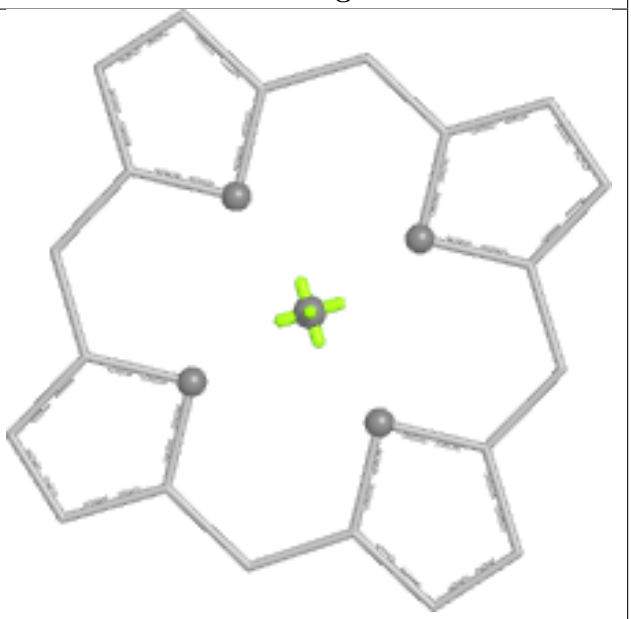
Bond lengths



Bond angles

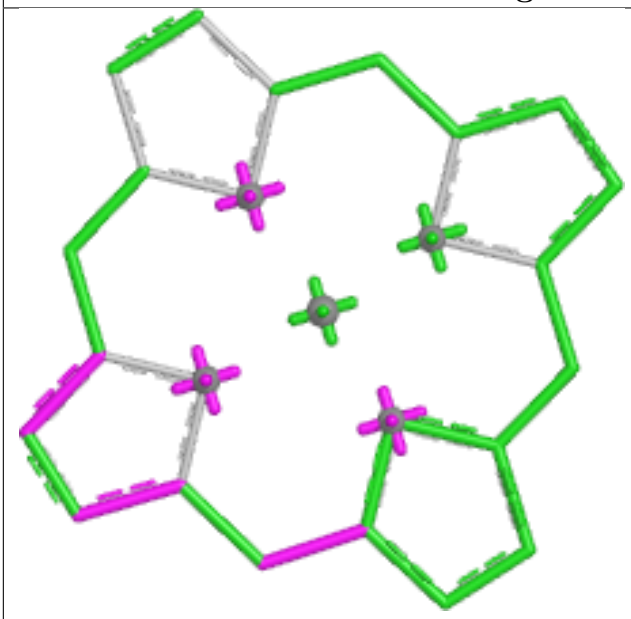


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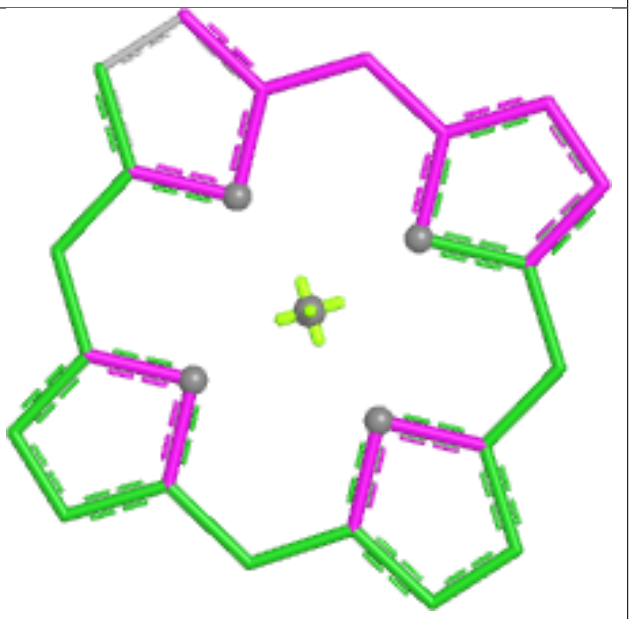


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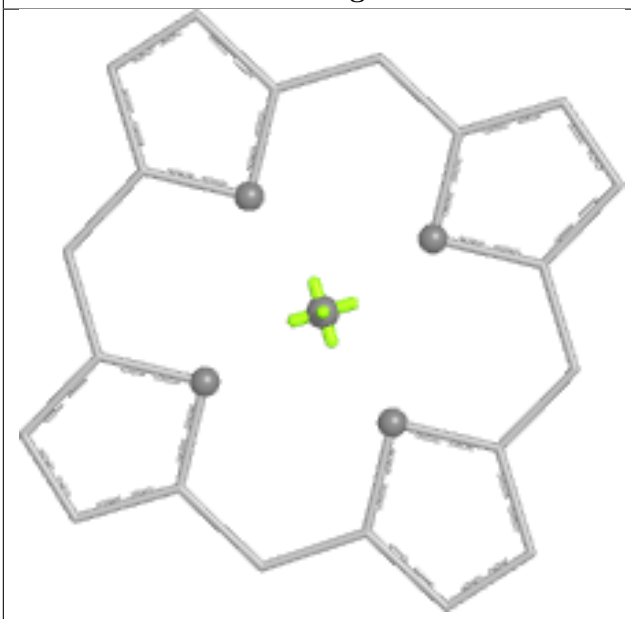
Ligand CLA P 5140



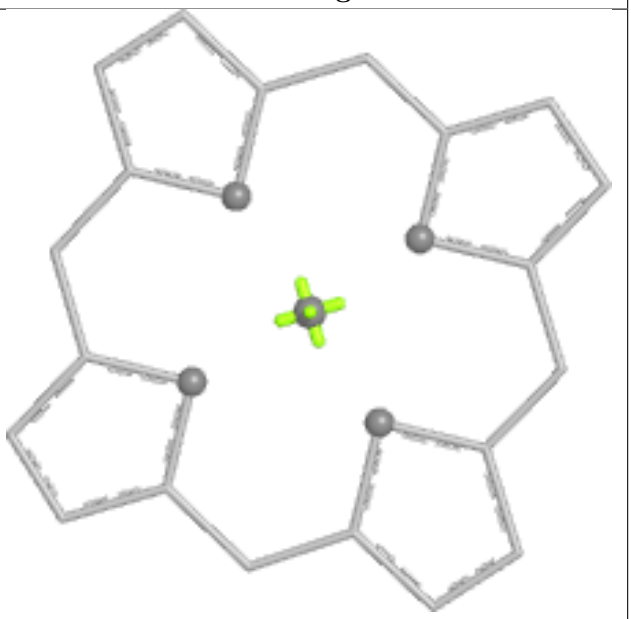
Bond lengths



Bond angles

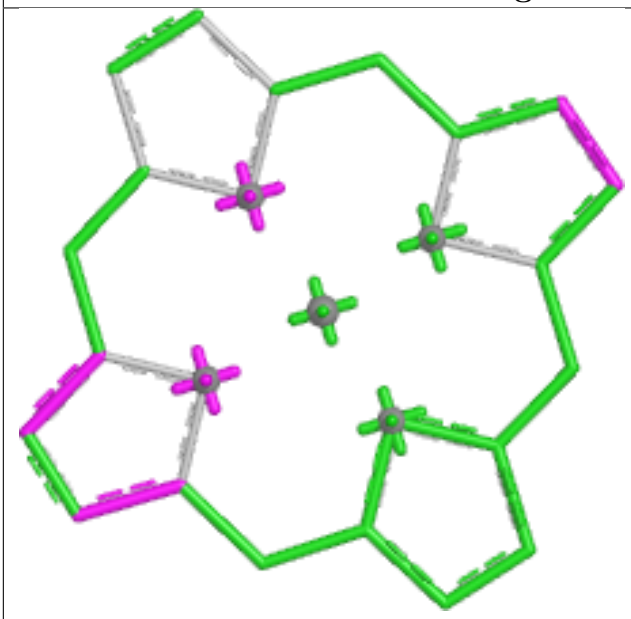


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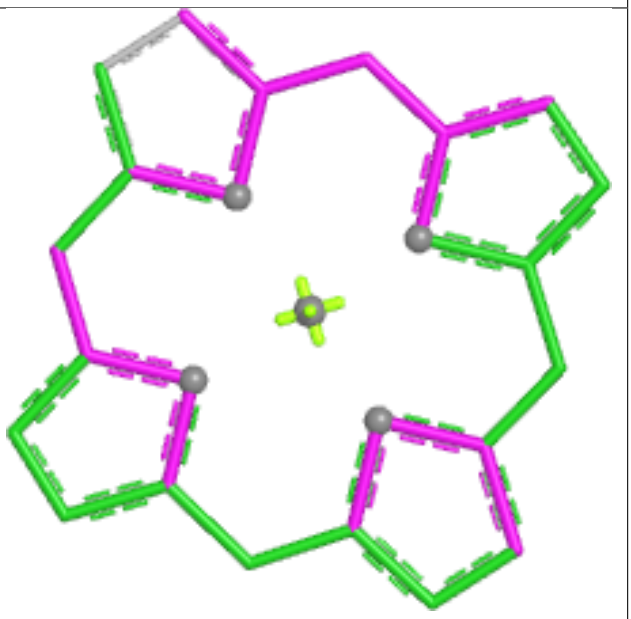


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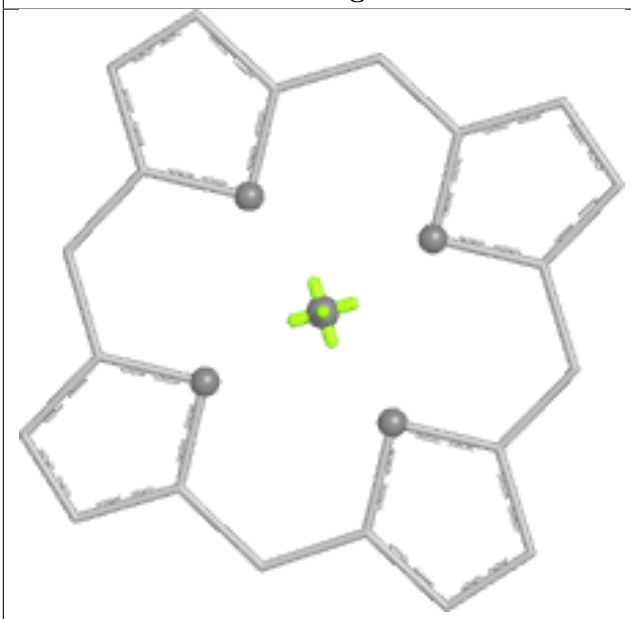
Ligand CLA A 1110



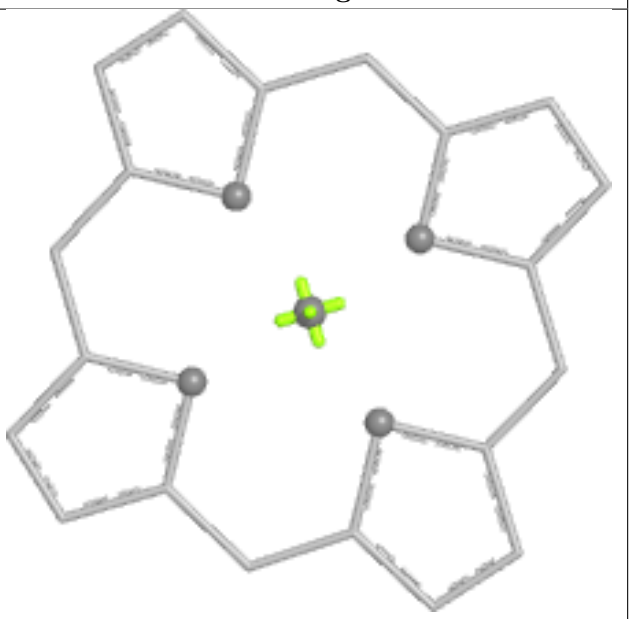
Bond lengths



Bond angles

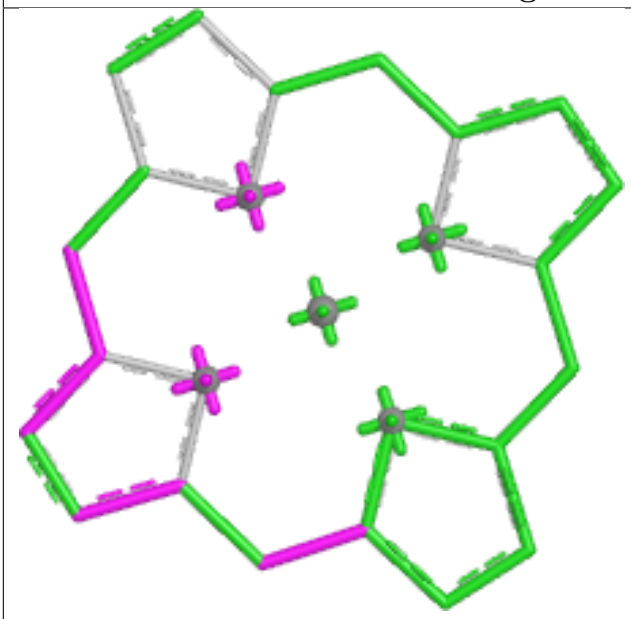


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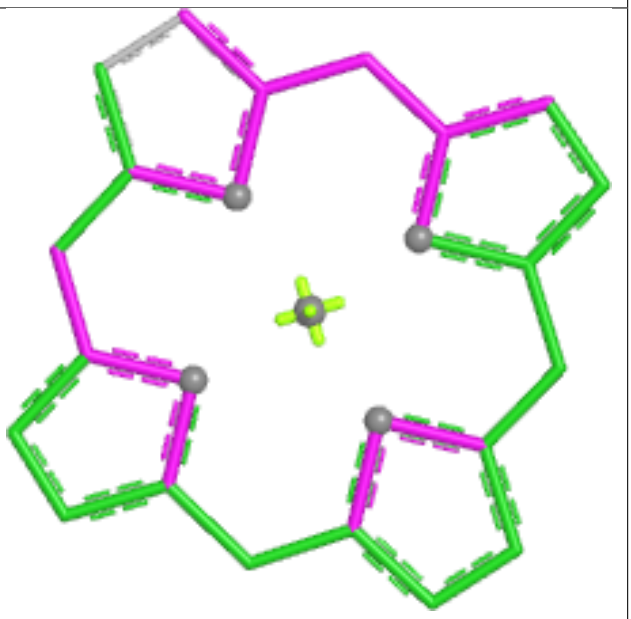


Rings

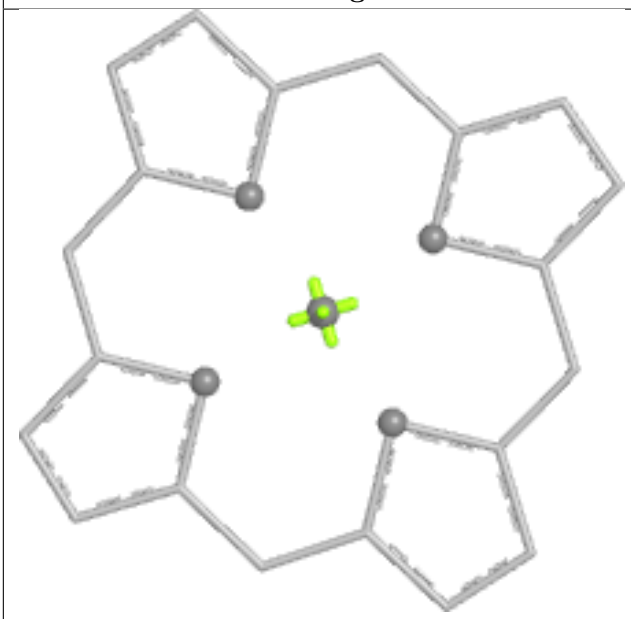
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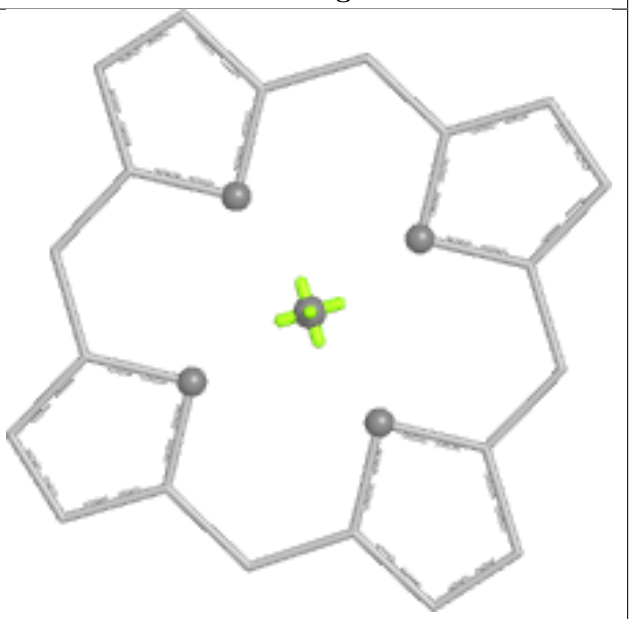
Bond lengths



Bond angles

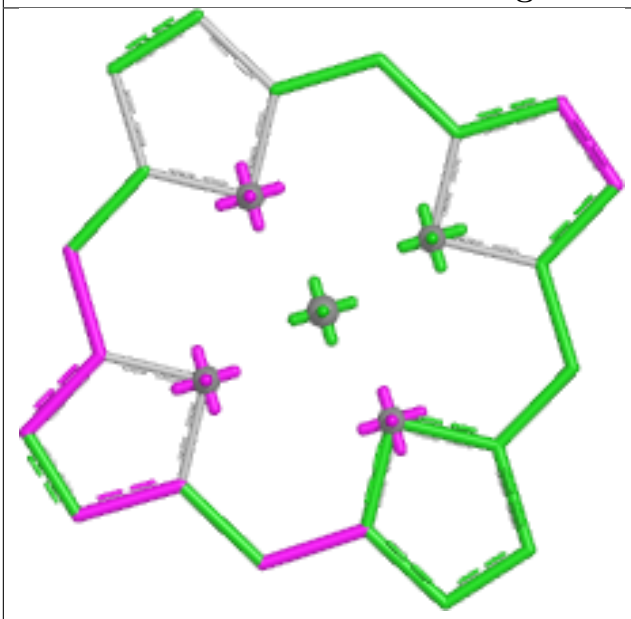


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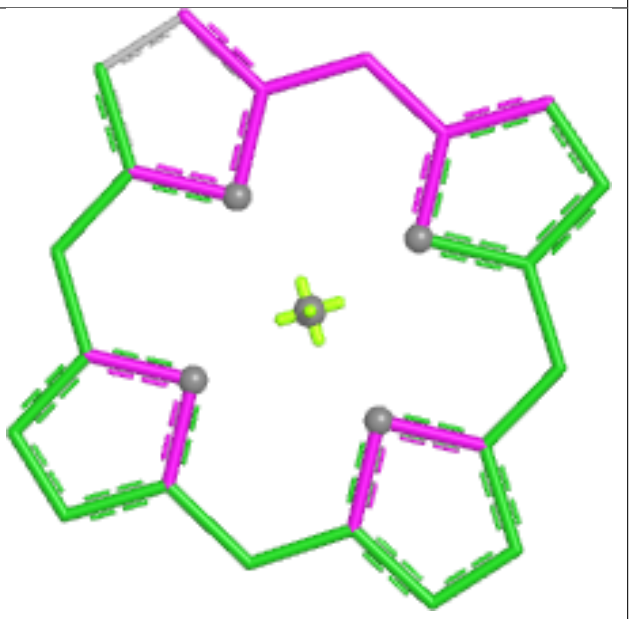


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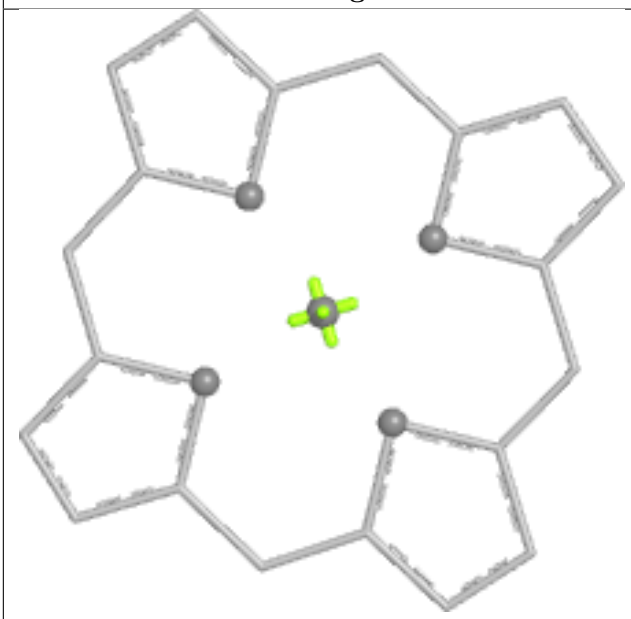
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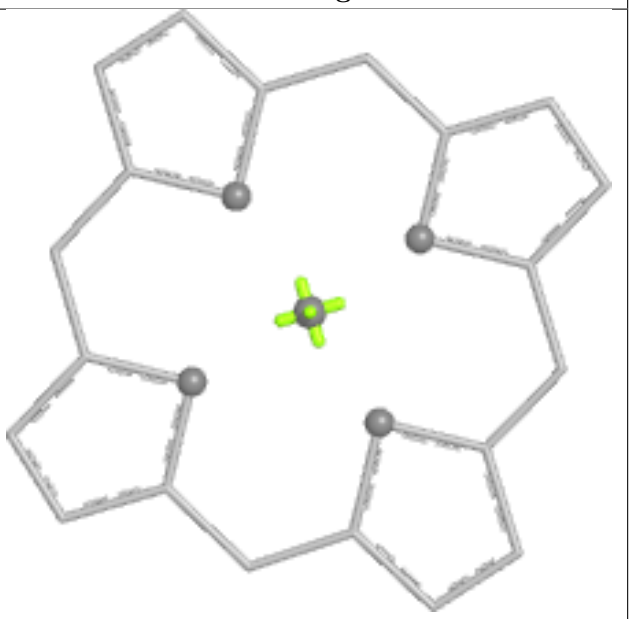
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Bond angles

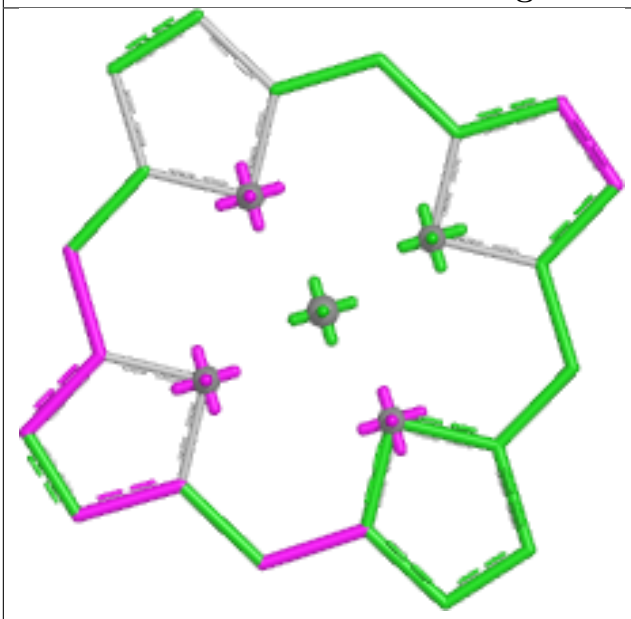


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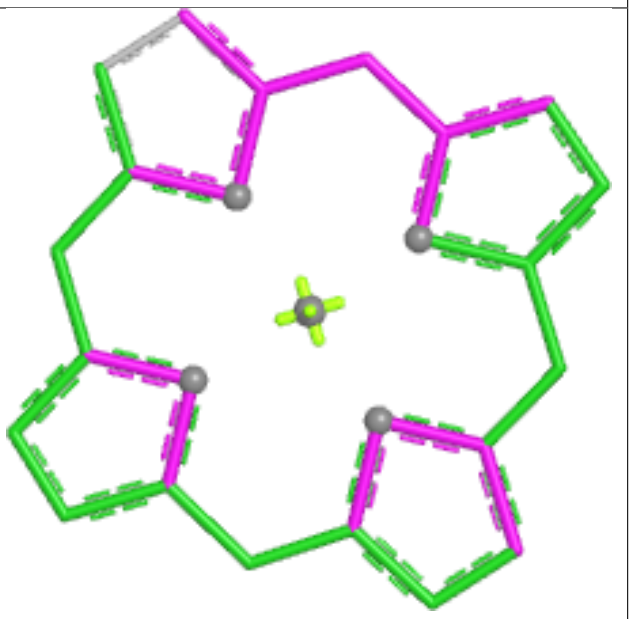


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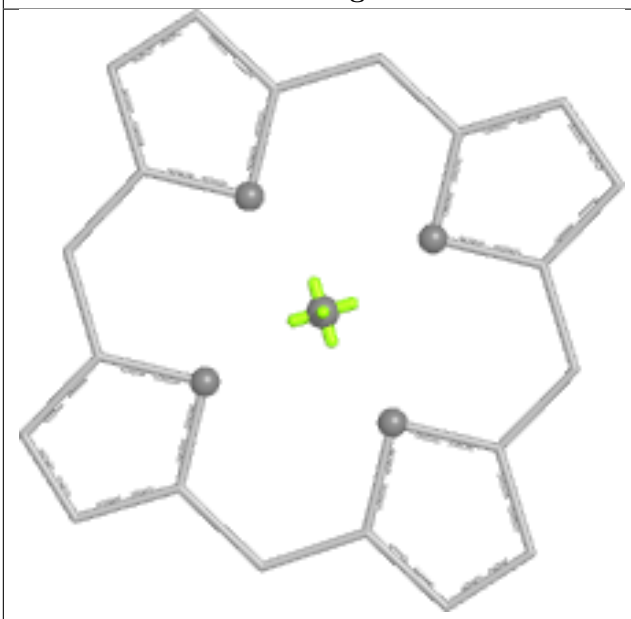
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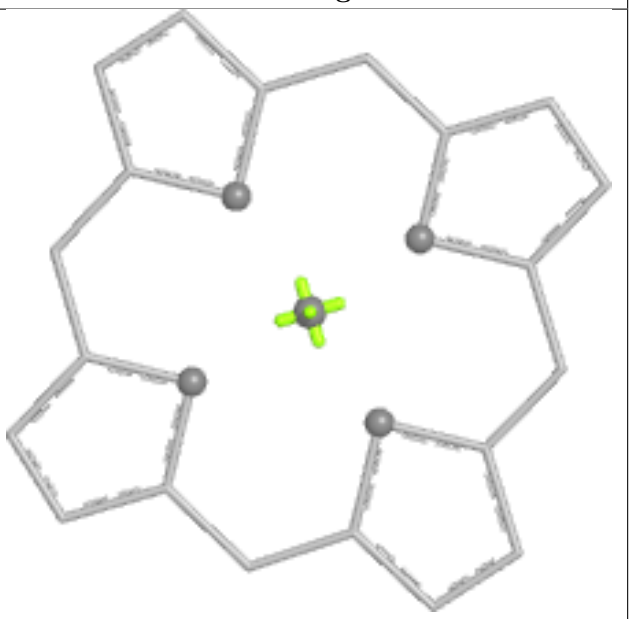
Bond lengths



Bond angles

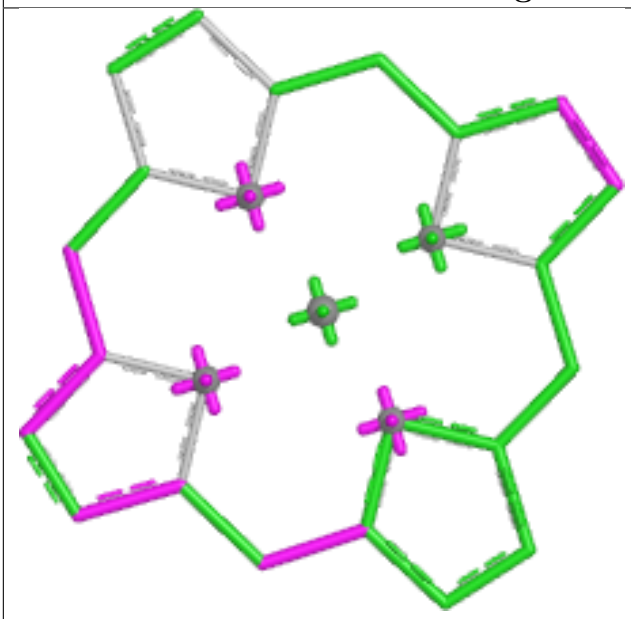


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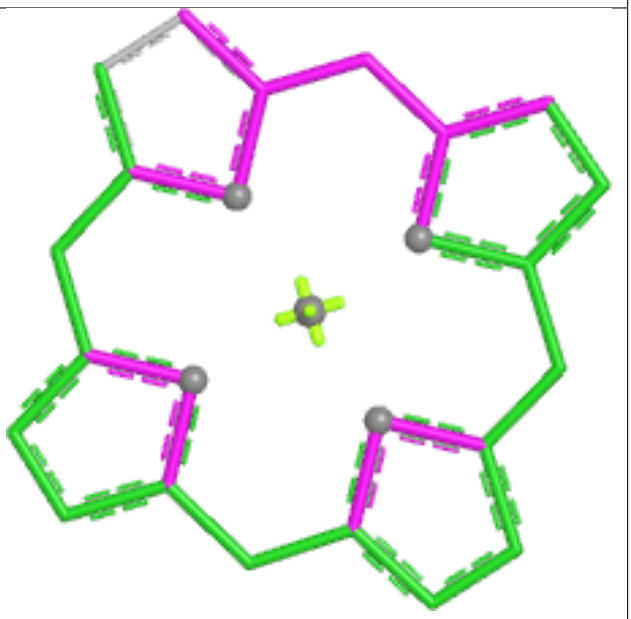


Rings

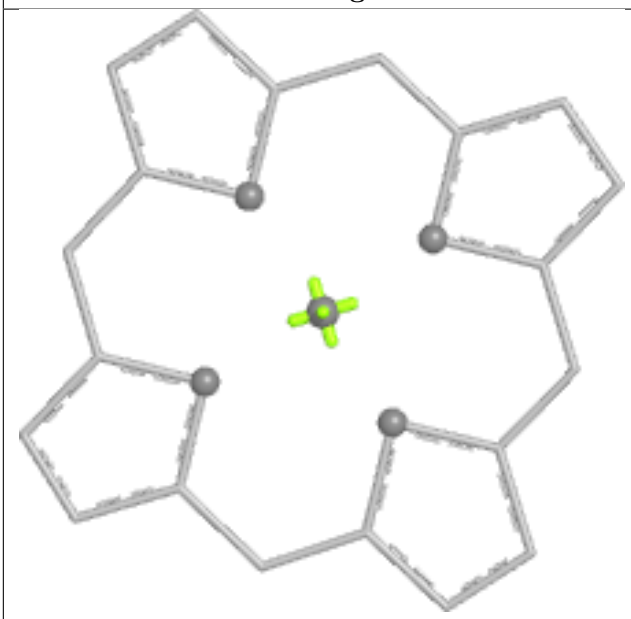
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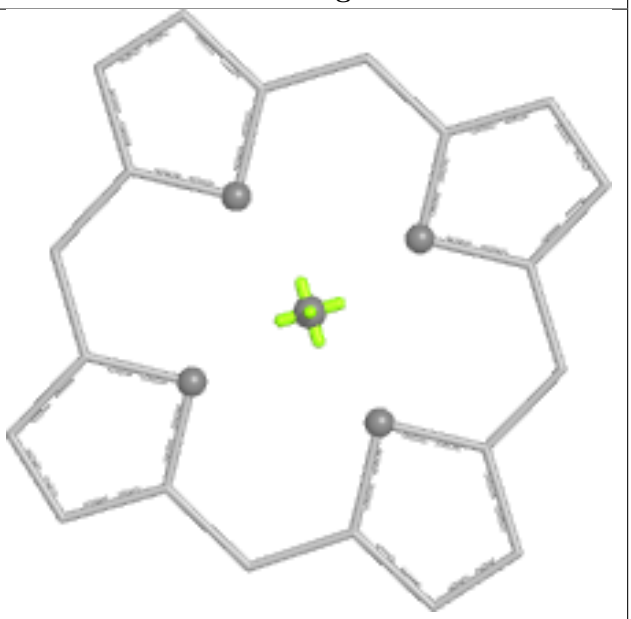
Bond lengths



Bond angles

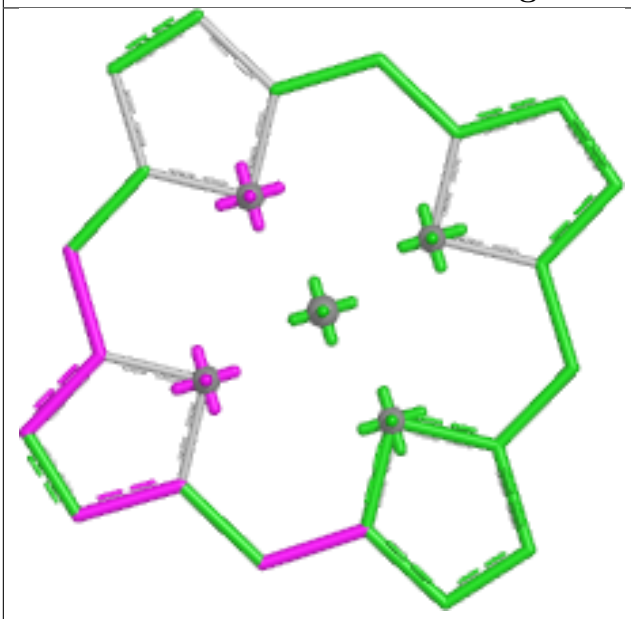


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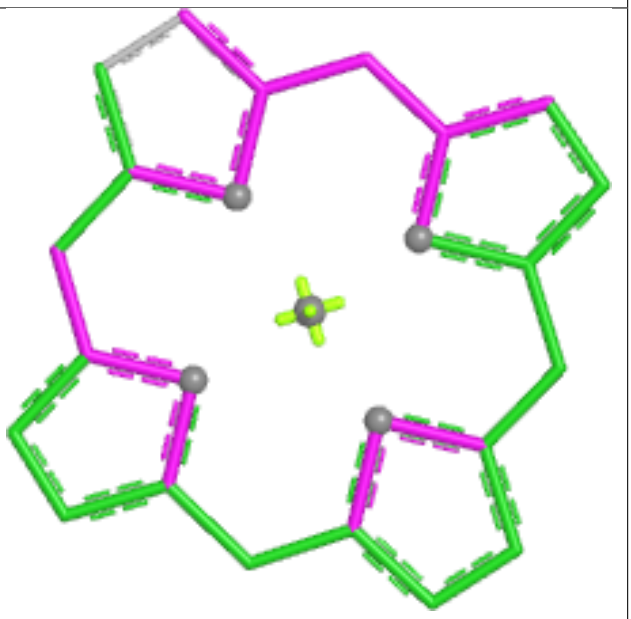


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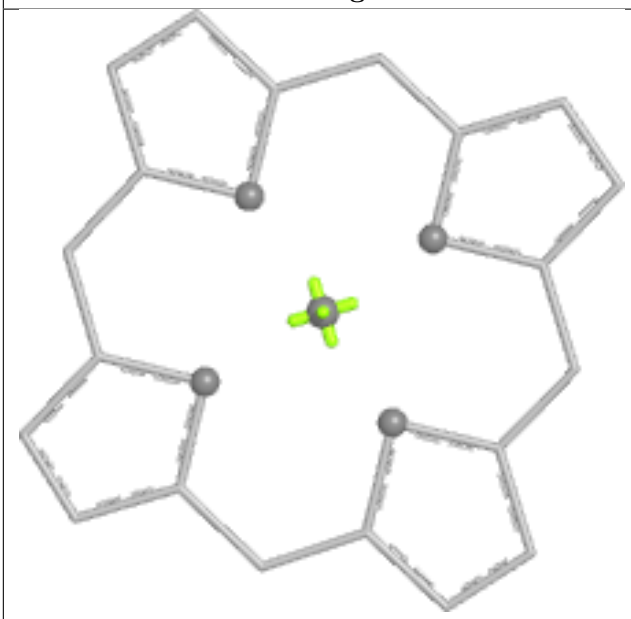
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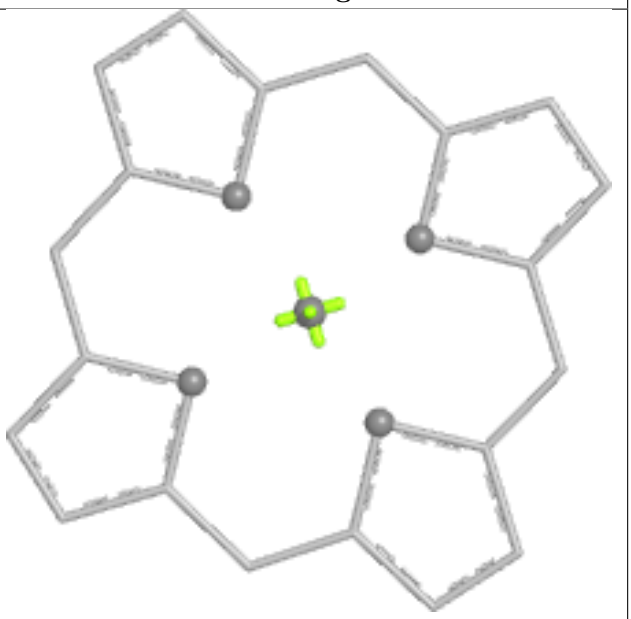
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Bond angles

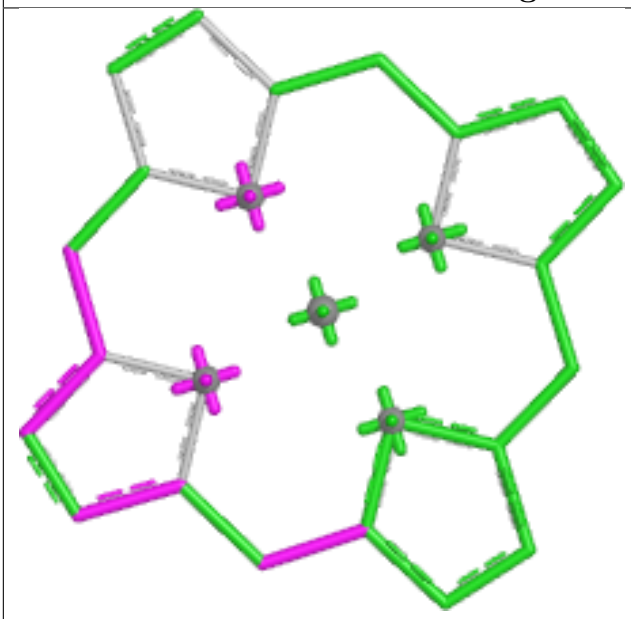


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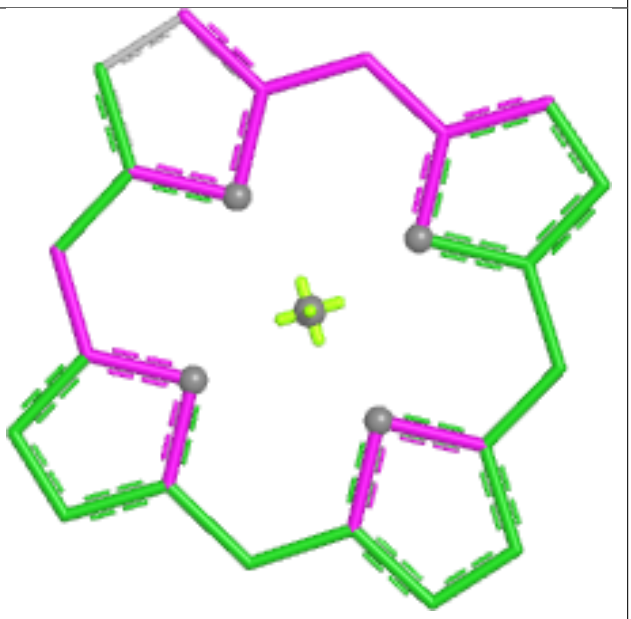


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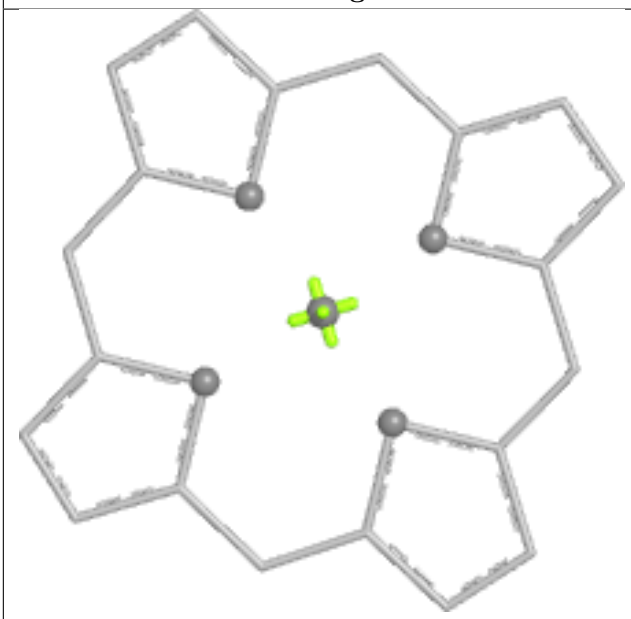
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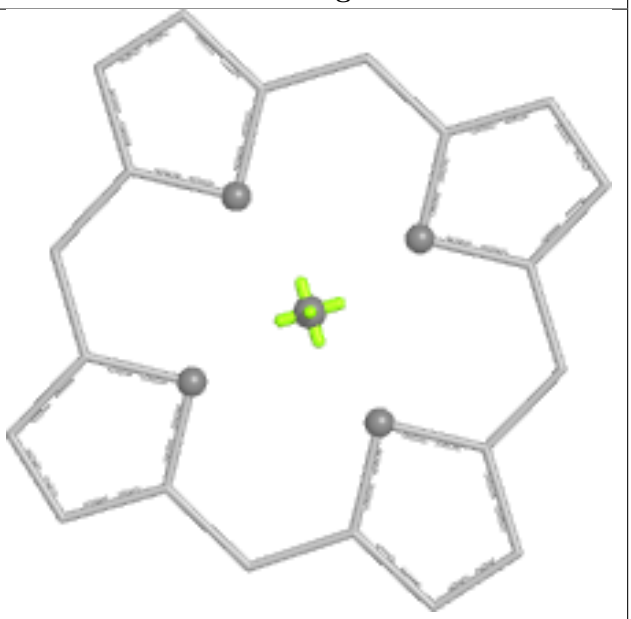
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Bond angles

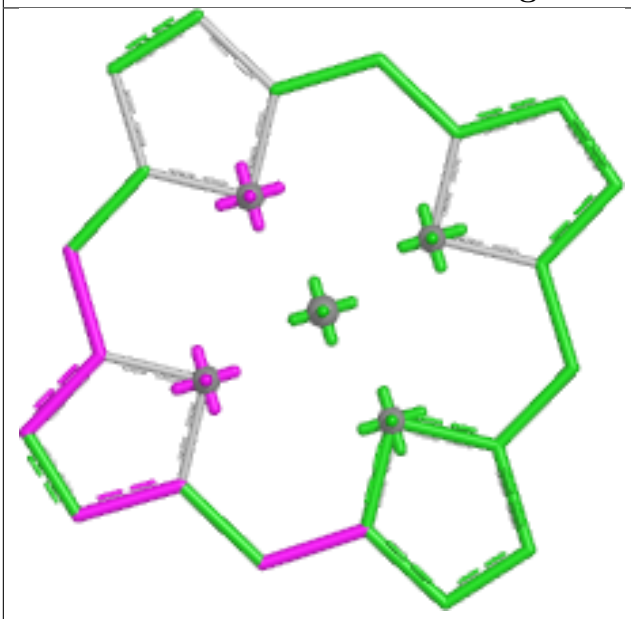


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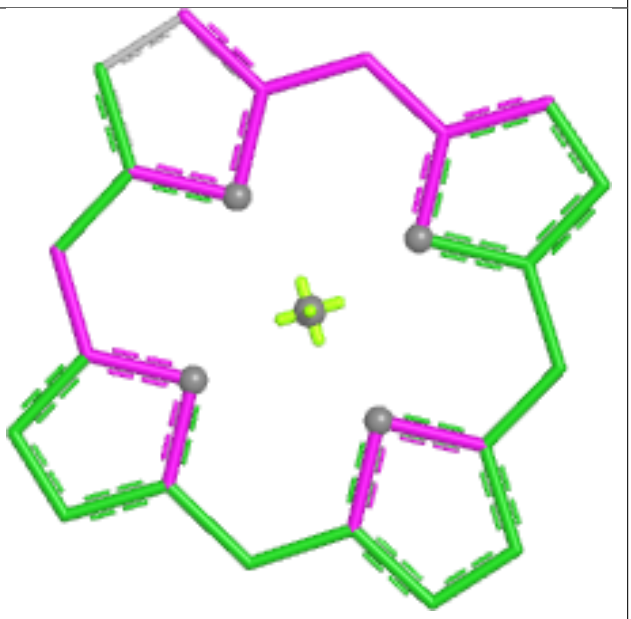


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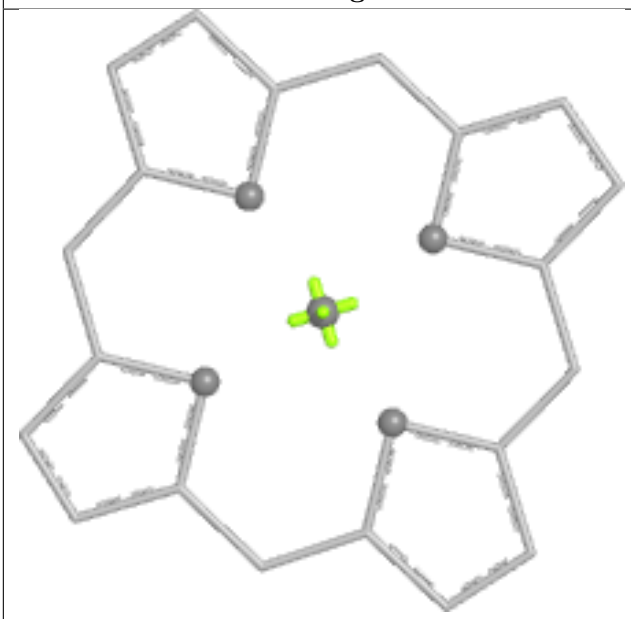
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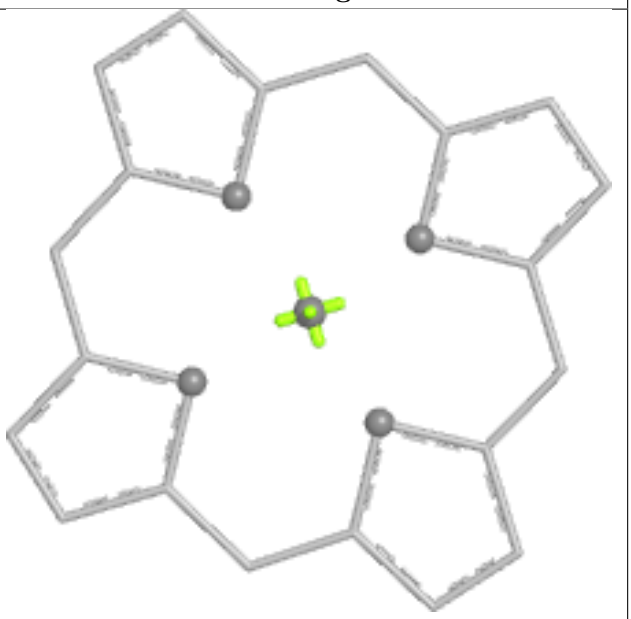
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Bond angles

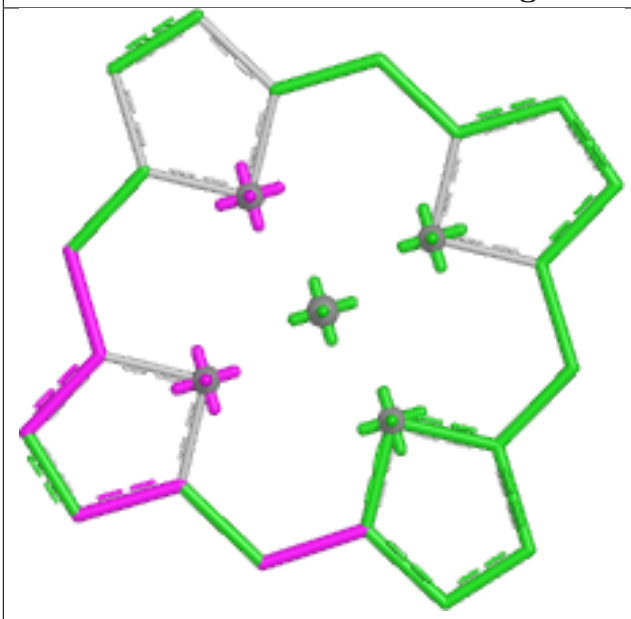


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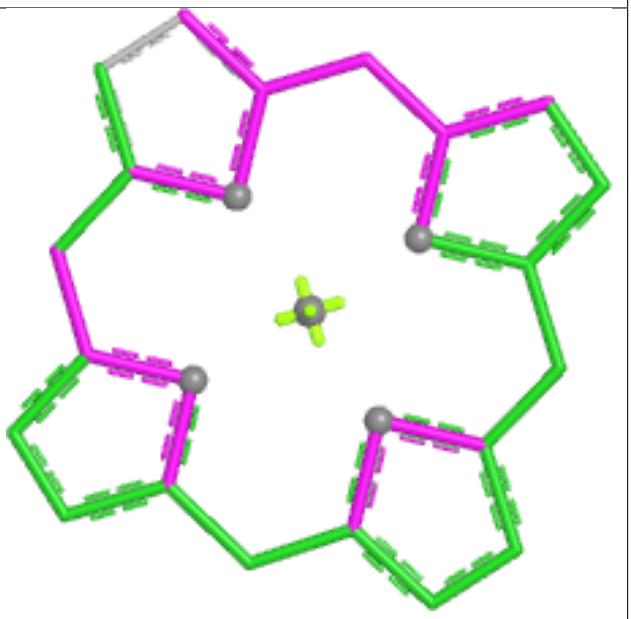


Rings

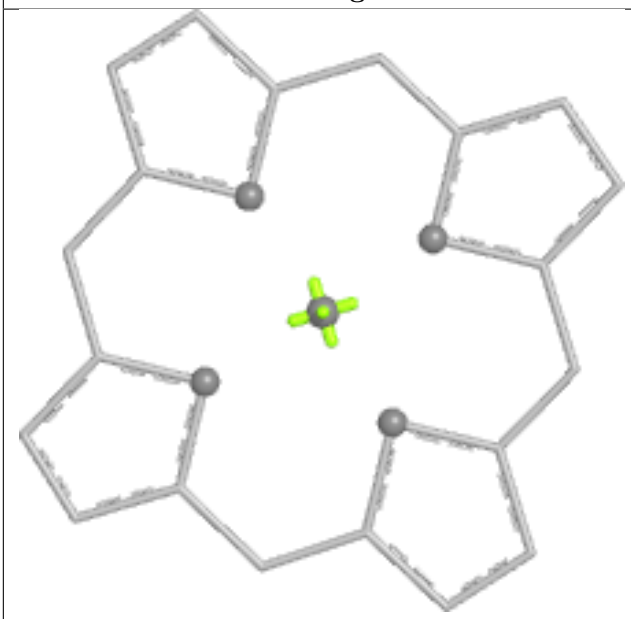
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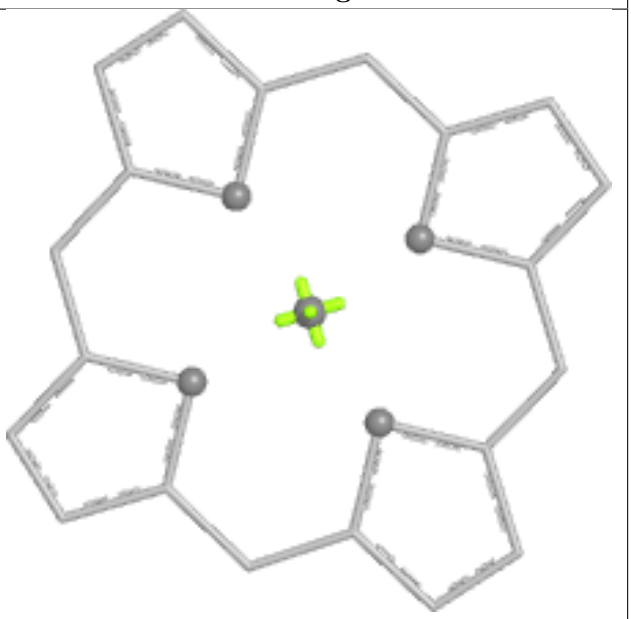
Bond lengths



Bond angles

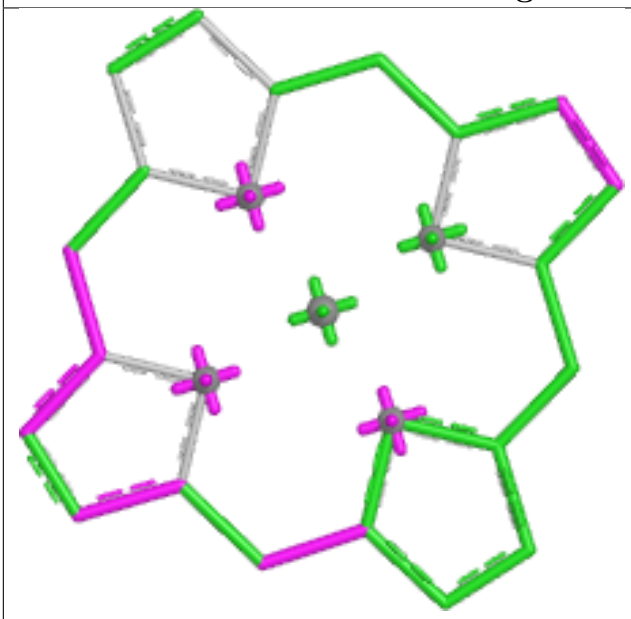


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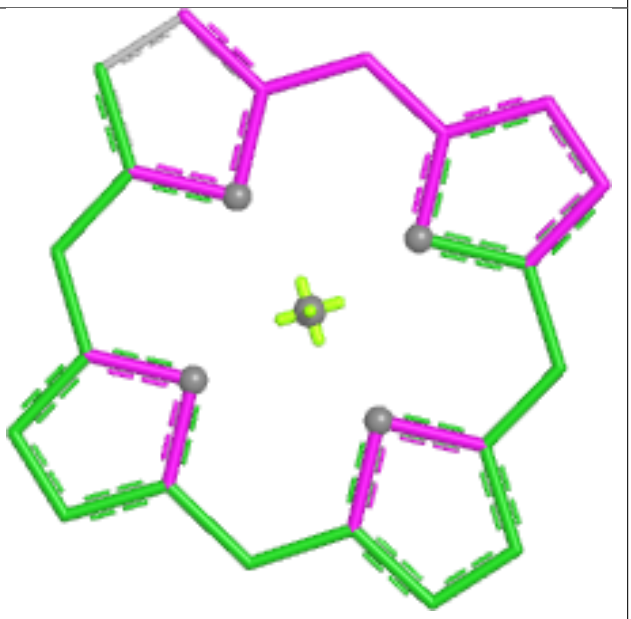


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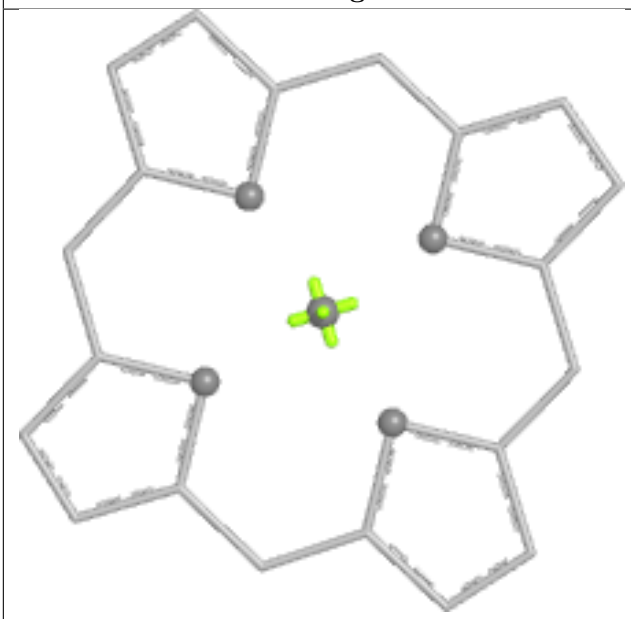
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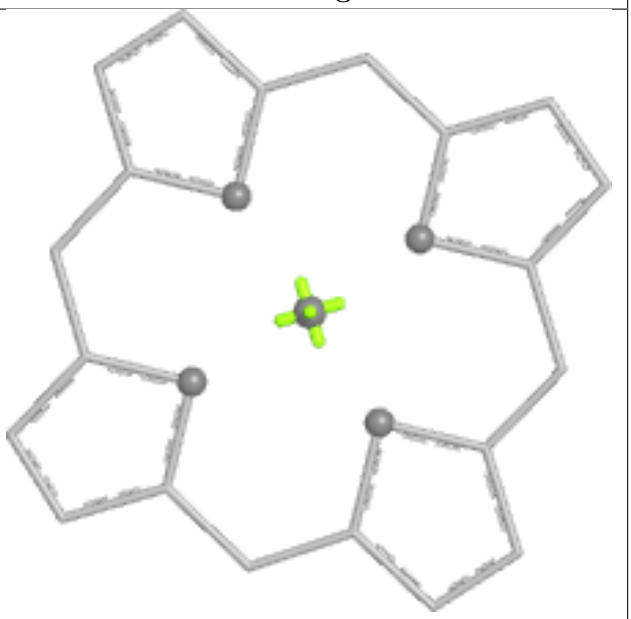
Bond lengths



Bond angles

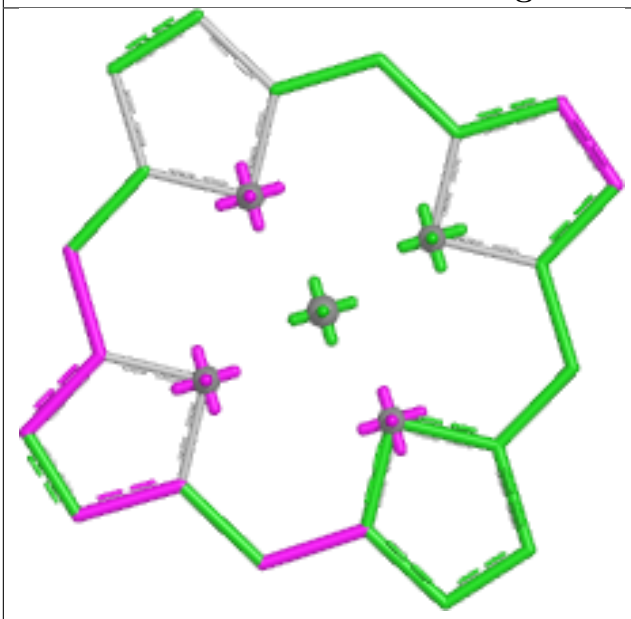


Torsions

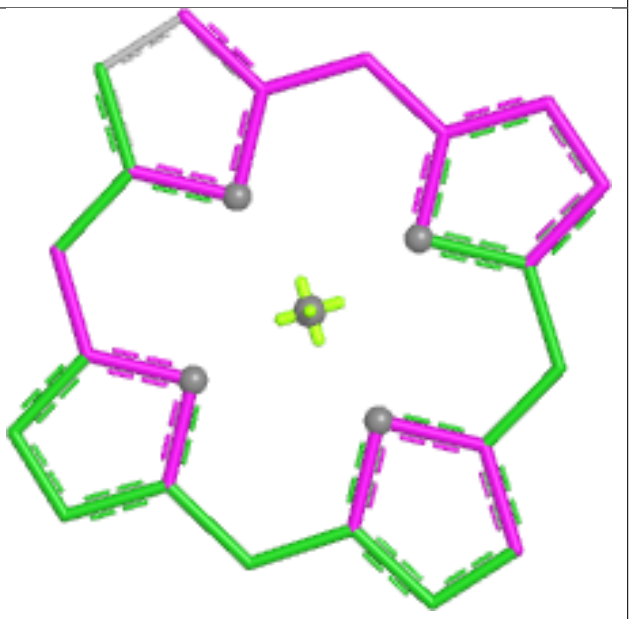


Rings

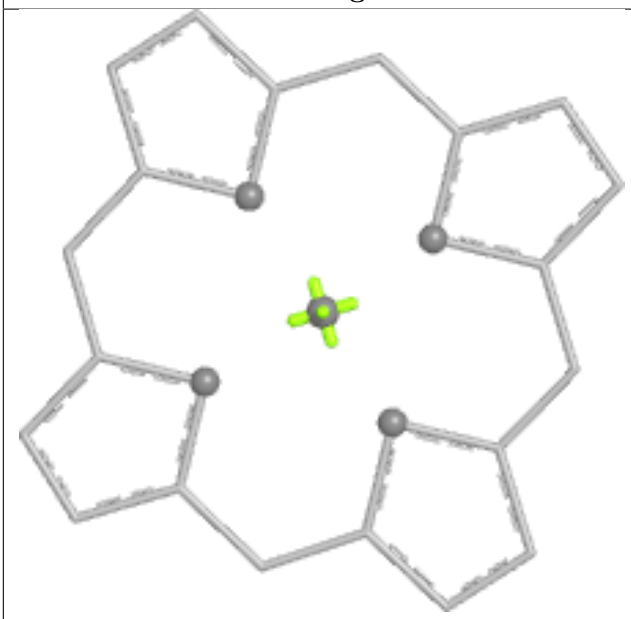
Ligand CLA B 1228



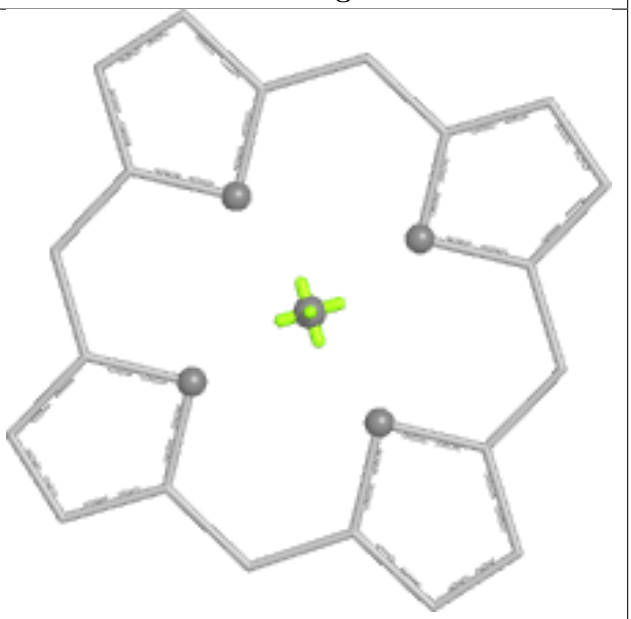
Bond lengths



Bond angles

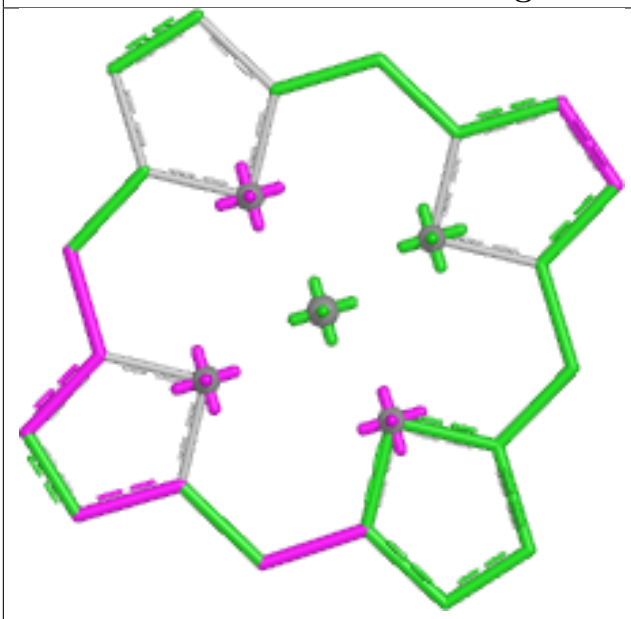


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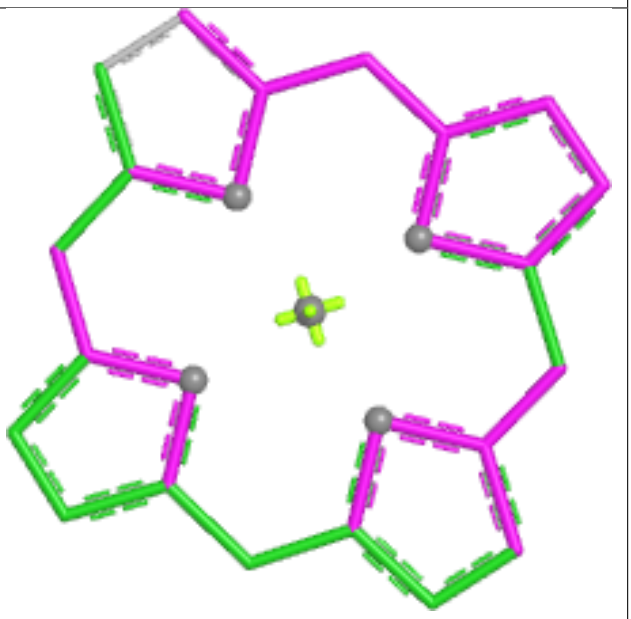


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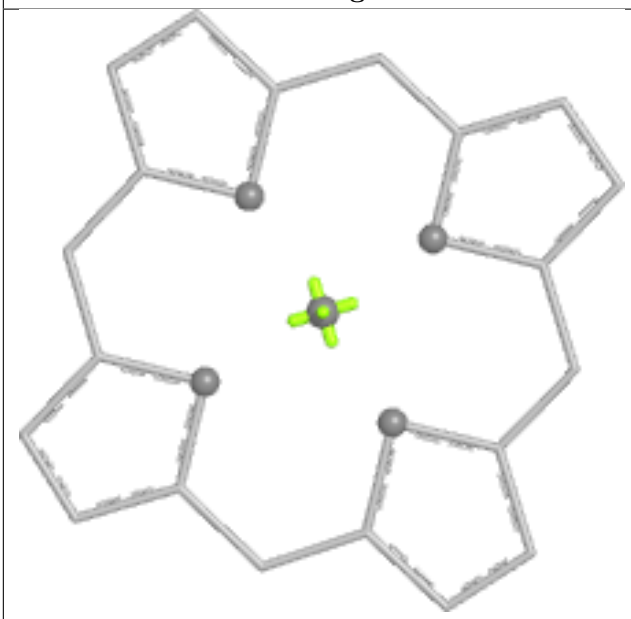
Ligand CLA A 1901



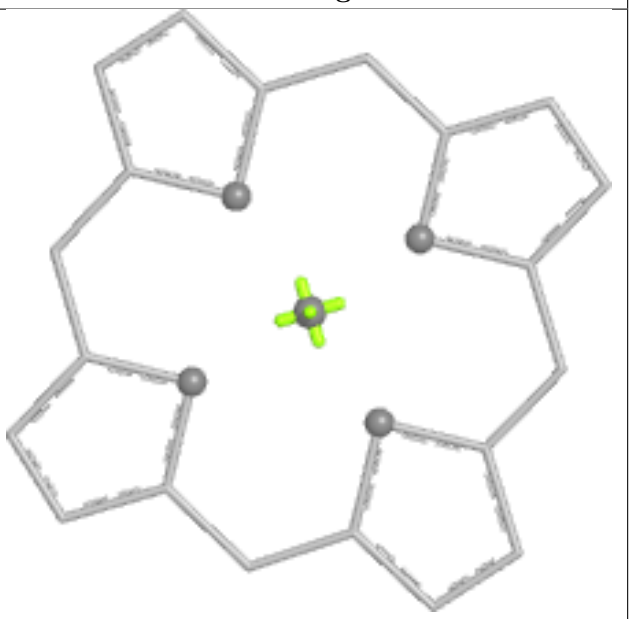
Bond lengths



Bond angles

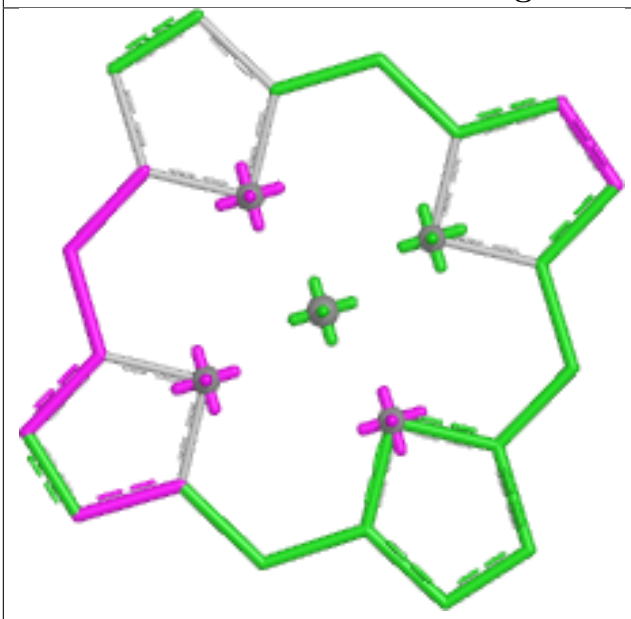


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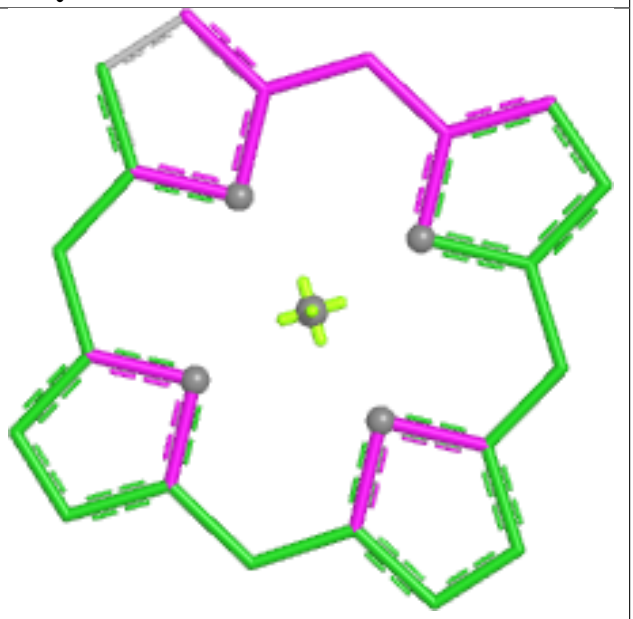


Rings

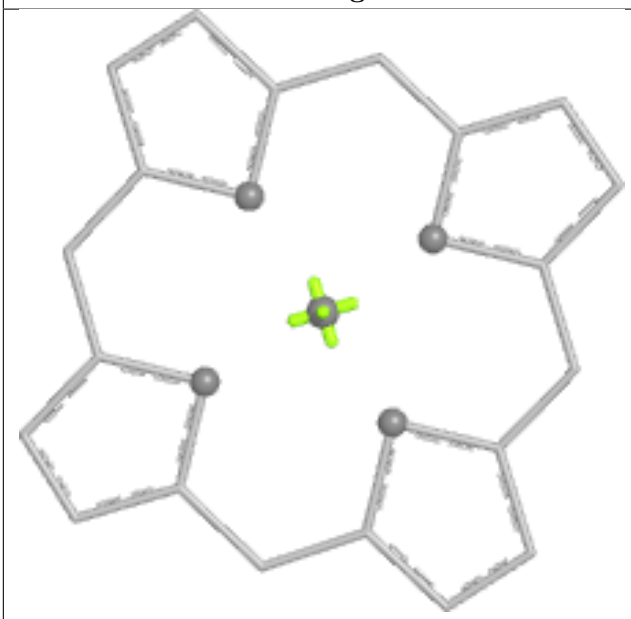
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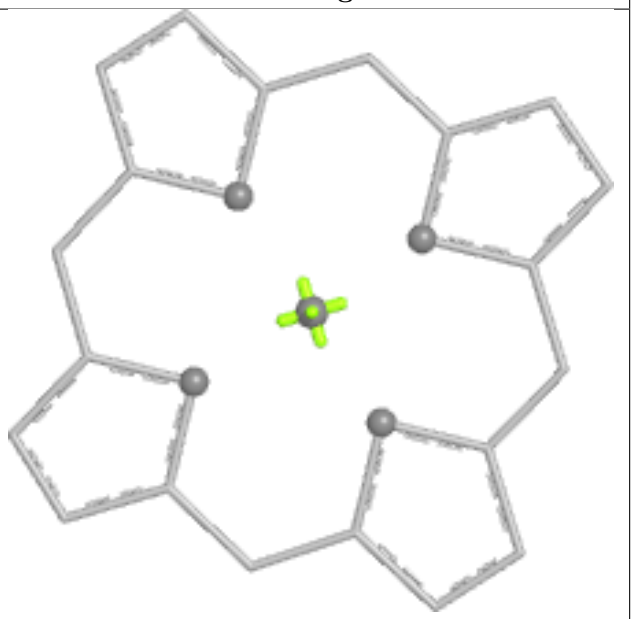
Bond lengths



Bond angles

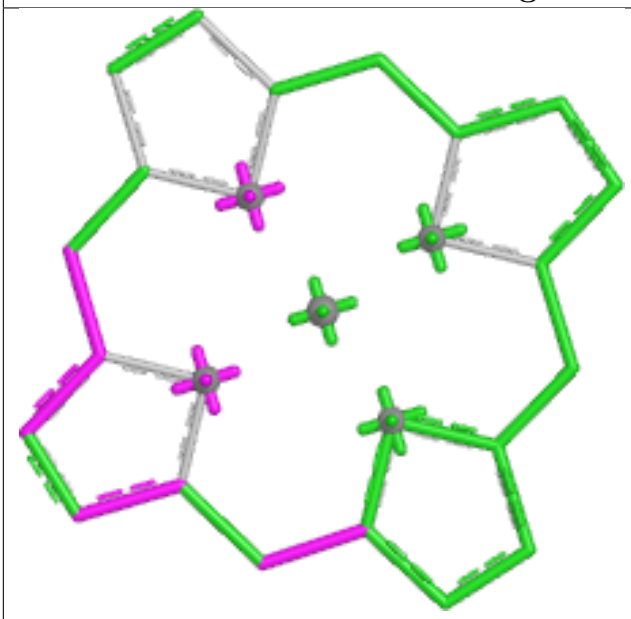


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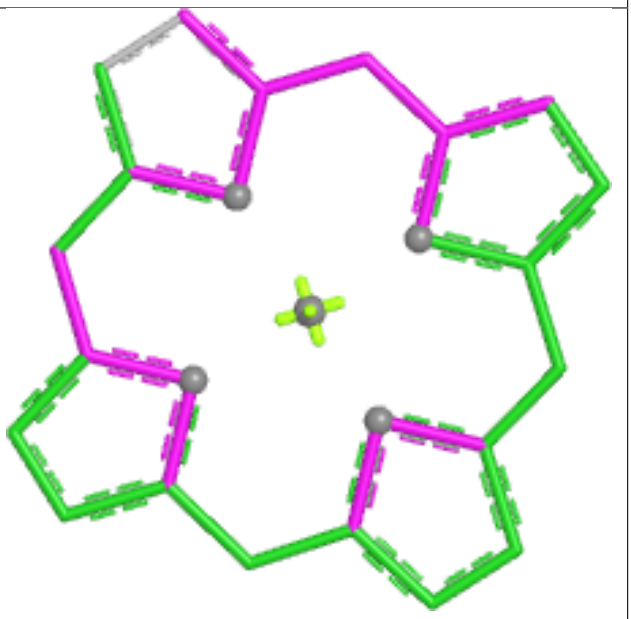


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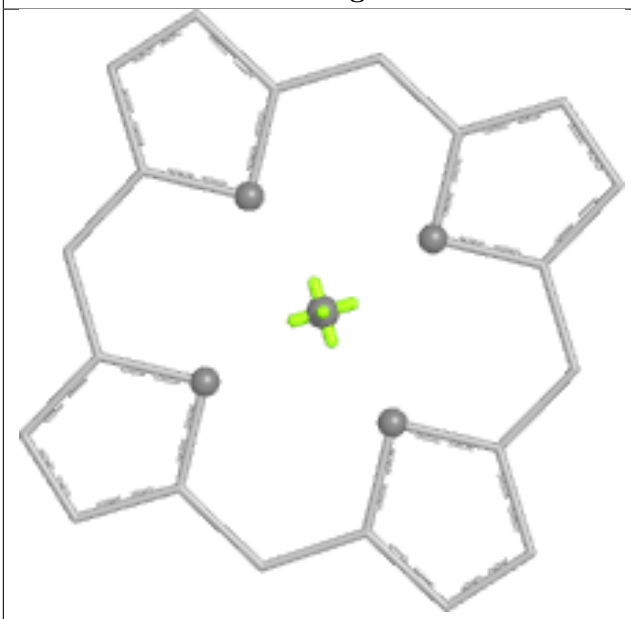
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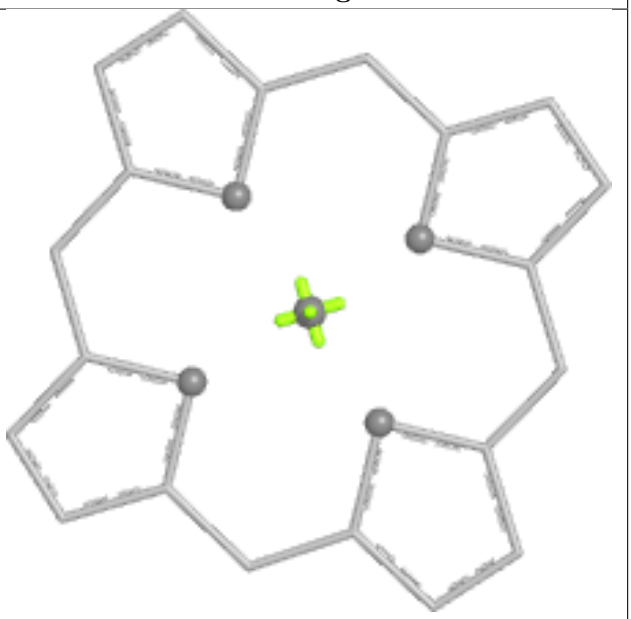
Bond lengths



Bond angles

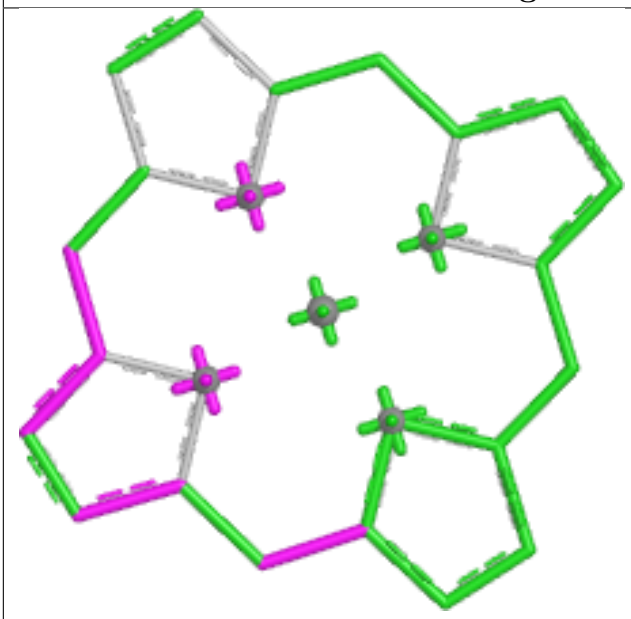


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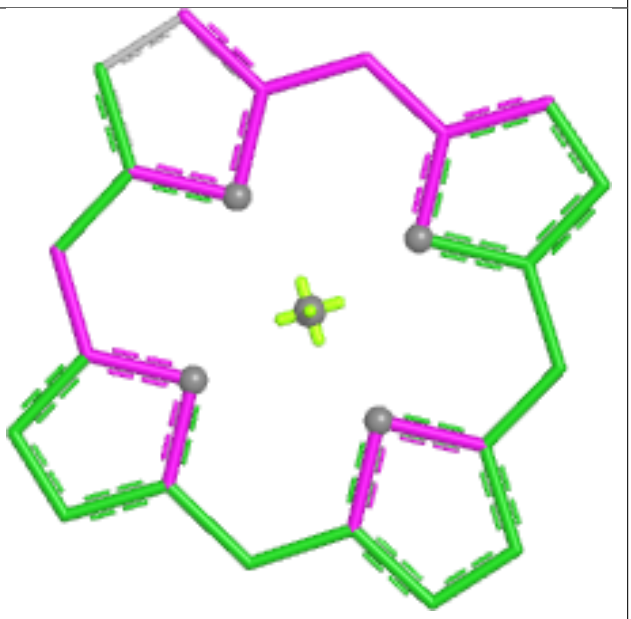


Rings

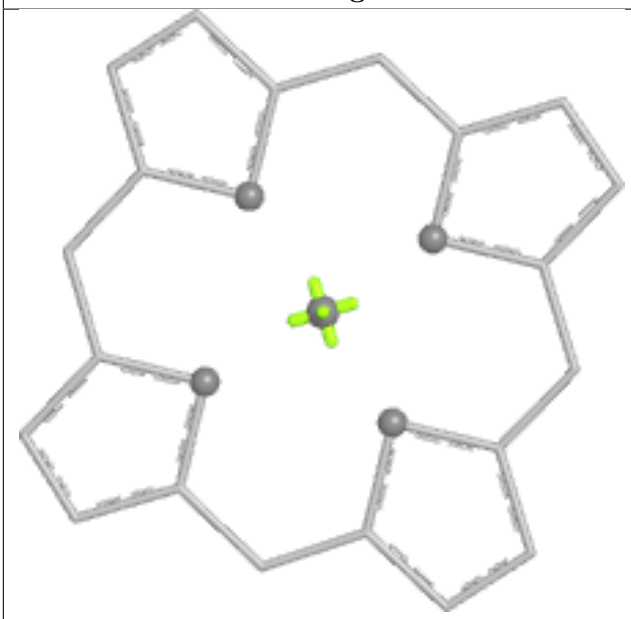
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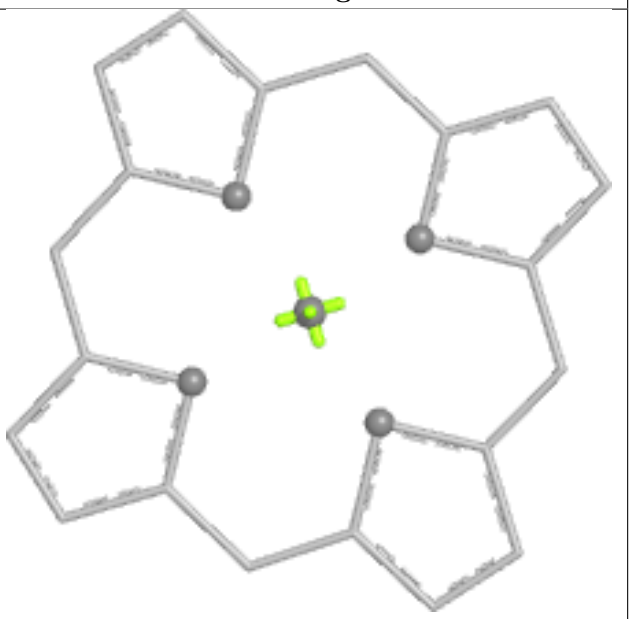
Bond lengths



Bond angles

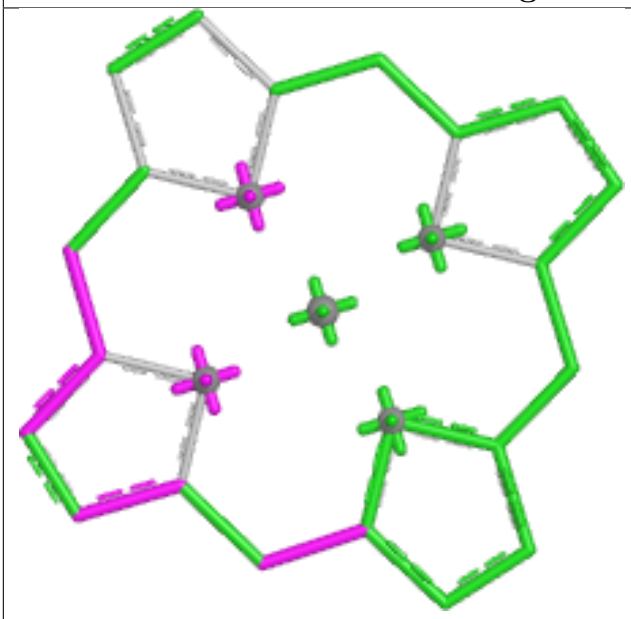


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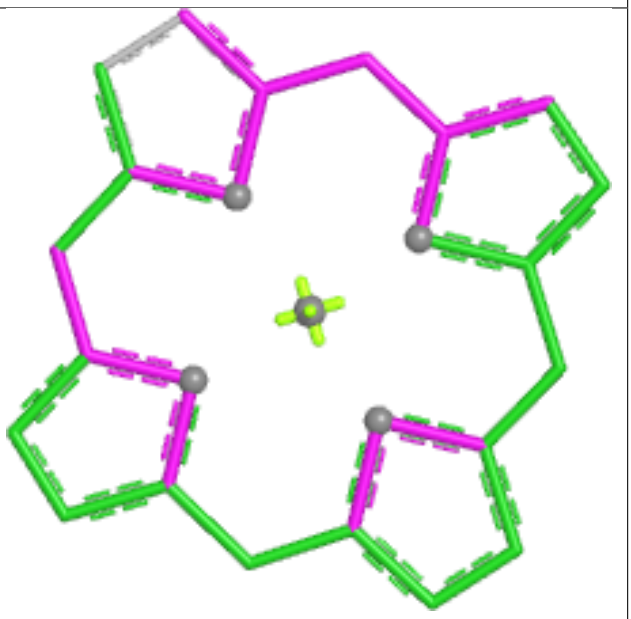


Rings

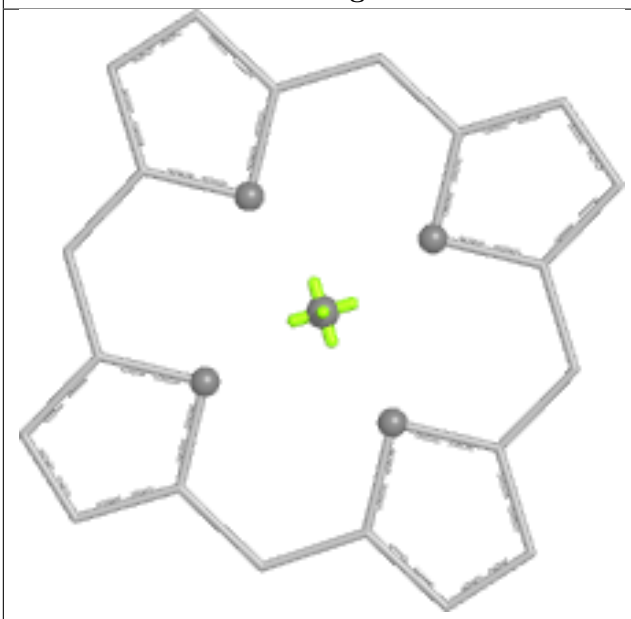
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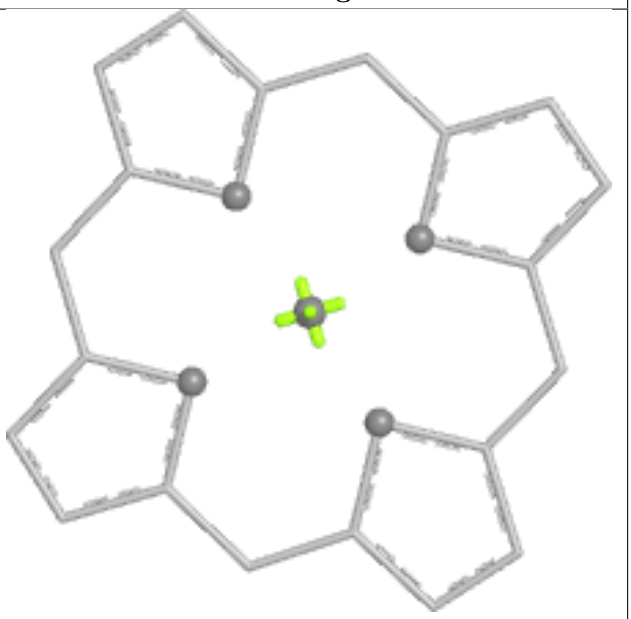
Bond lengths



Bond angles

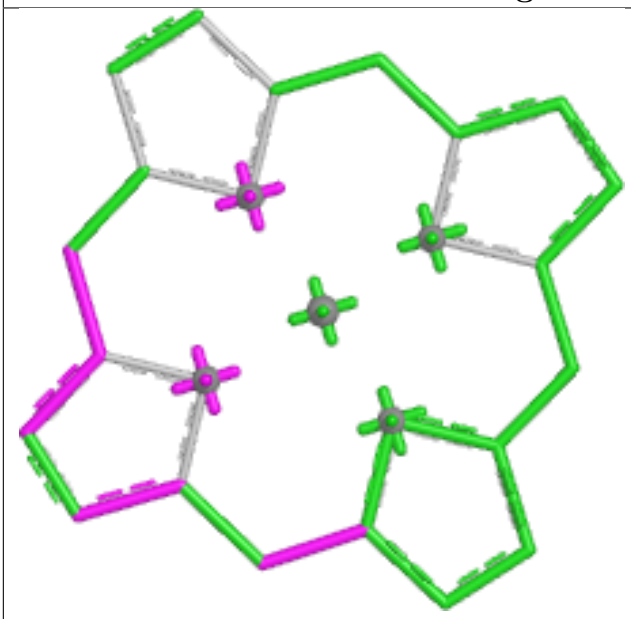


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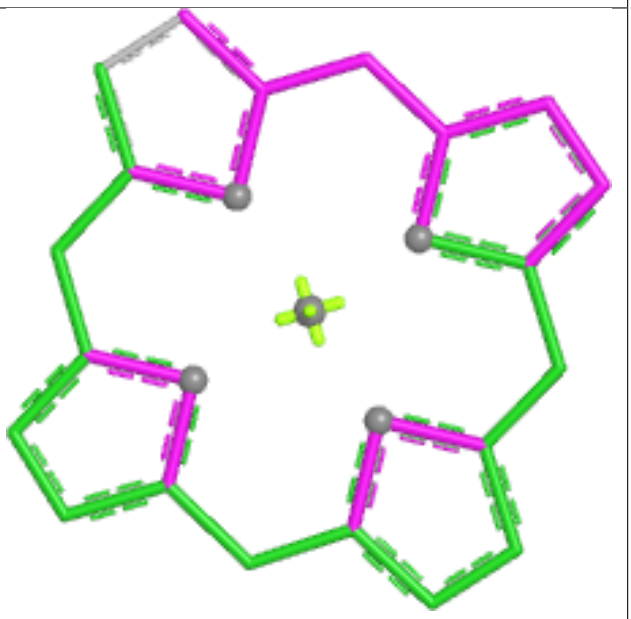


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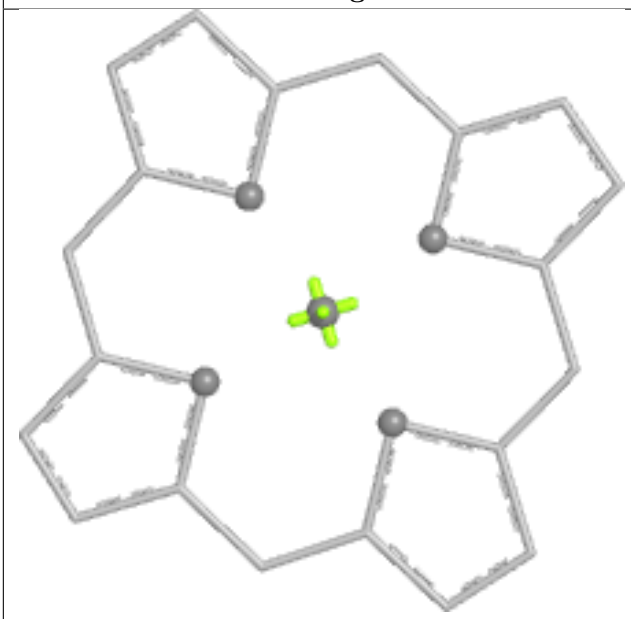
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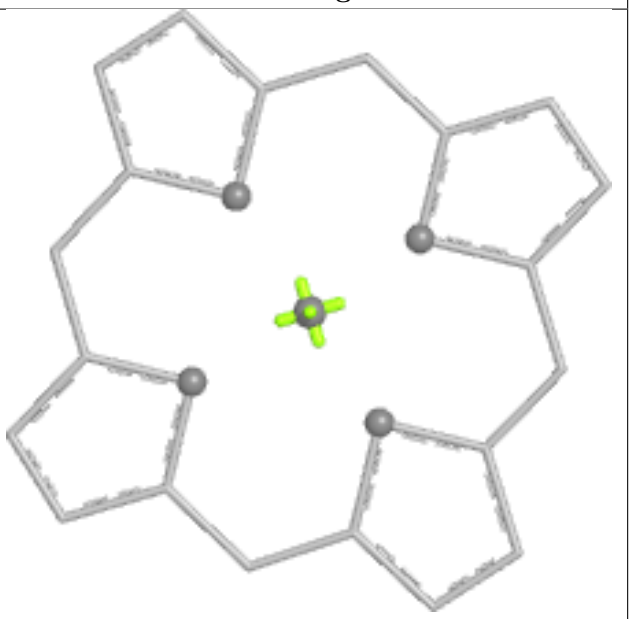
Bond lengths



Bond angles

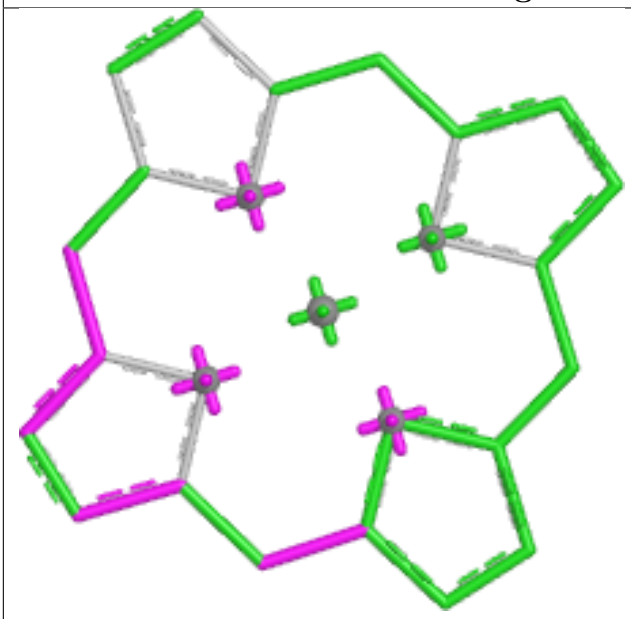


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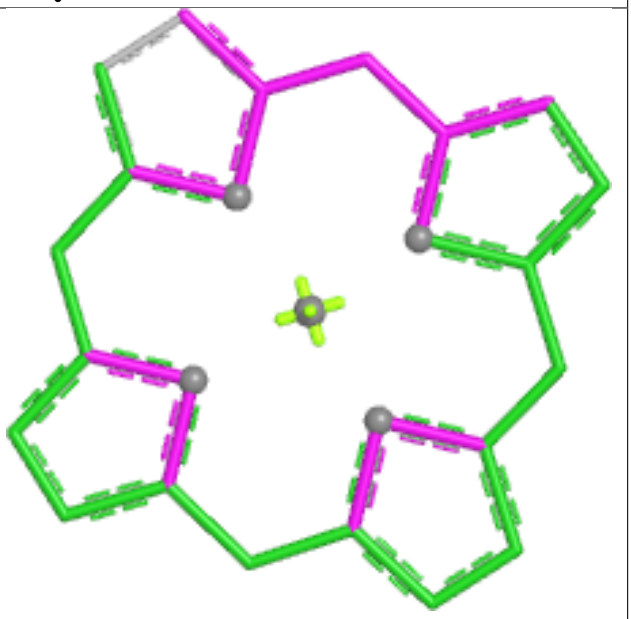


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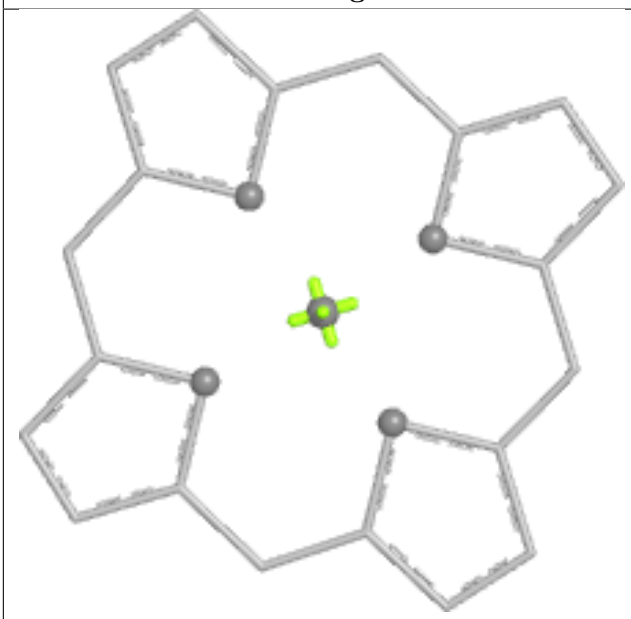
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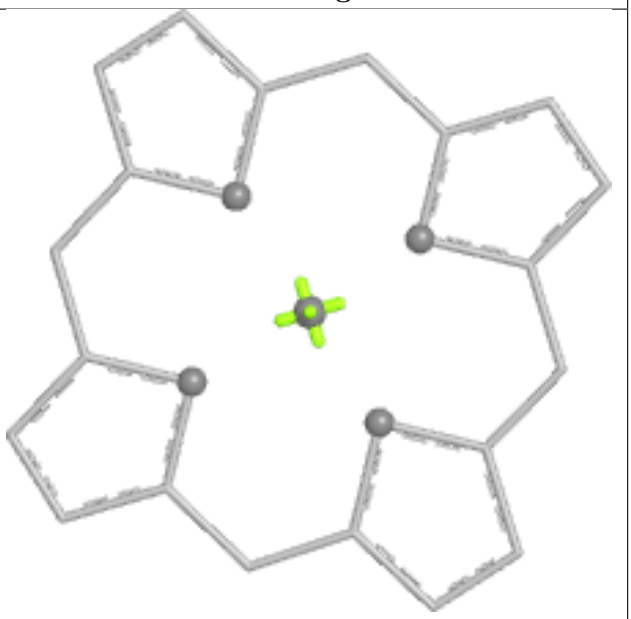
Bond lengths



Bond angles

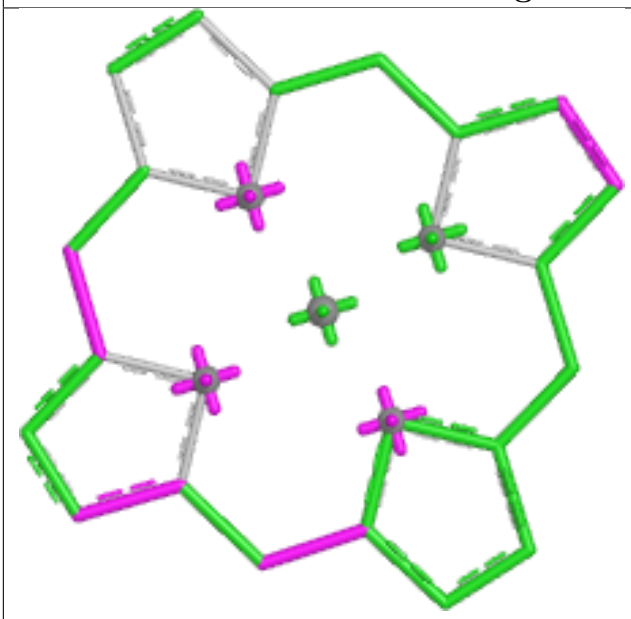


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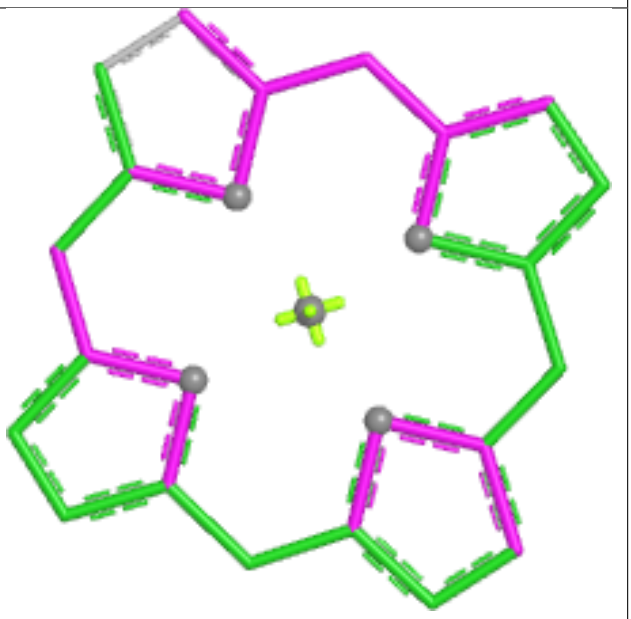


Rings

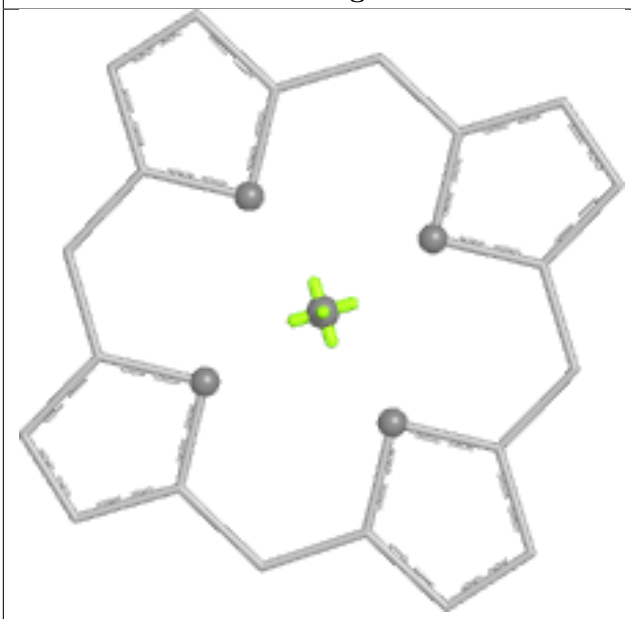
Ligand CLA A 1119



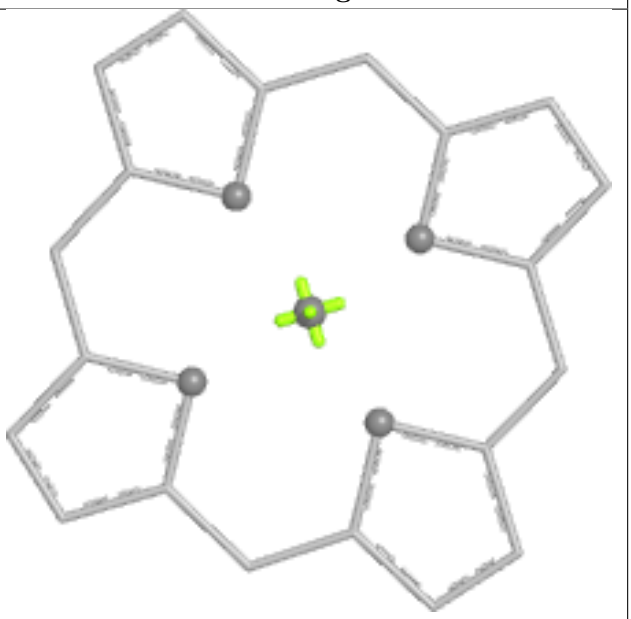
Bond lengths



Bond angles

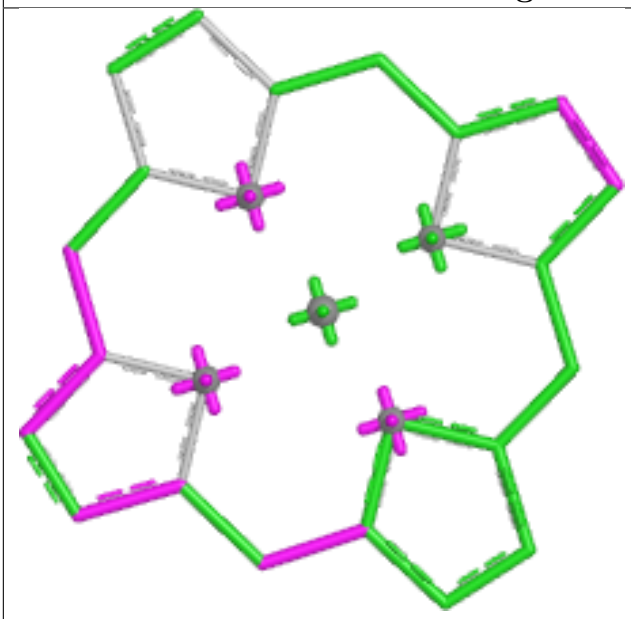


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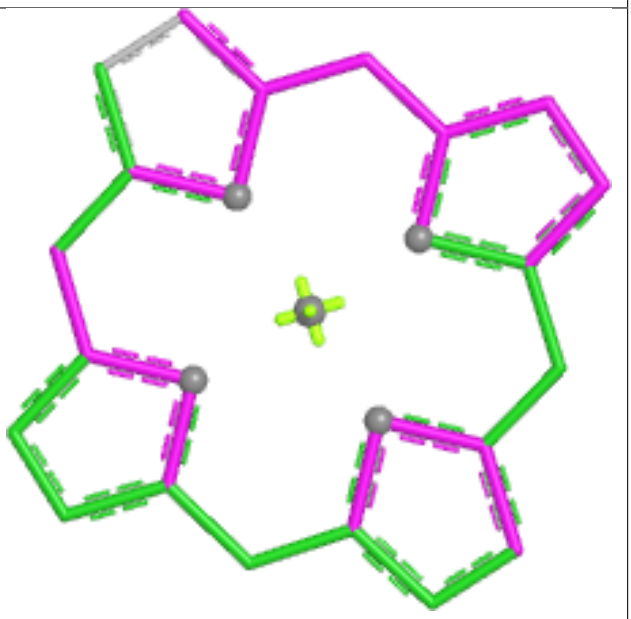


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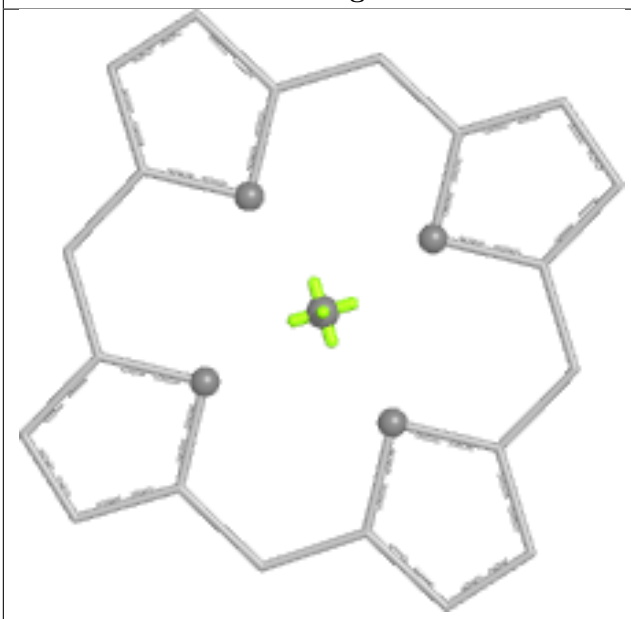
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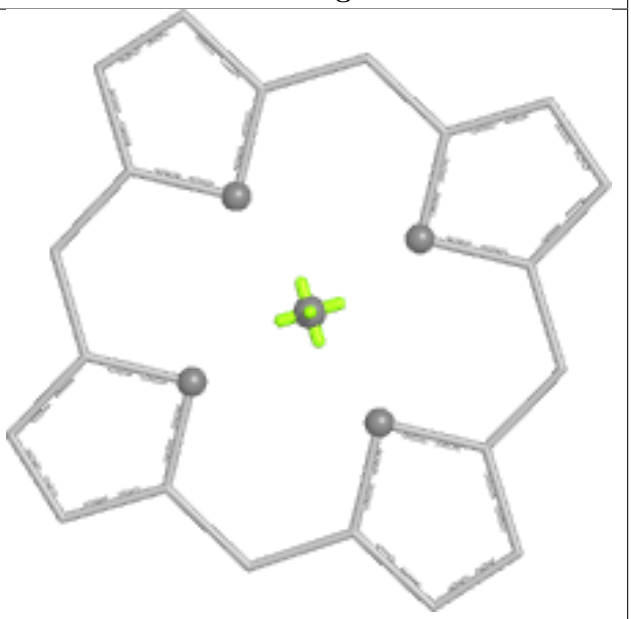
Bond lengths



Bond angles

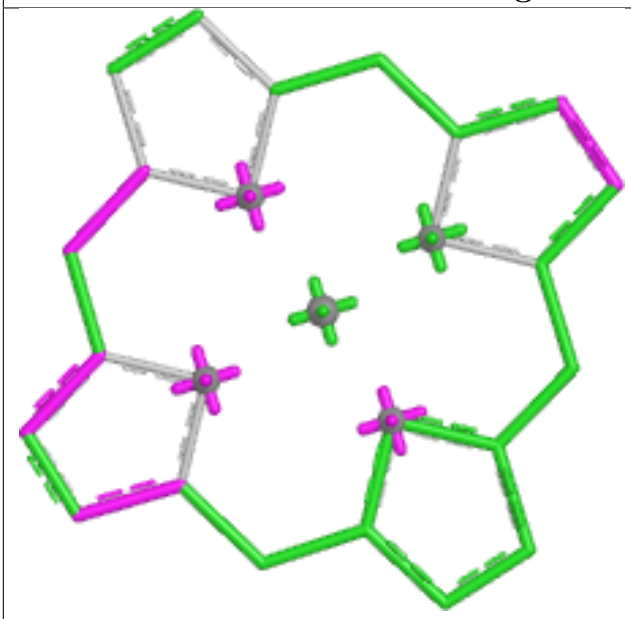


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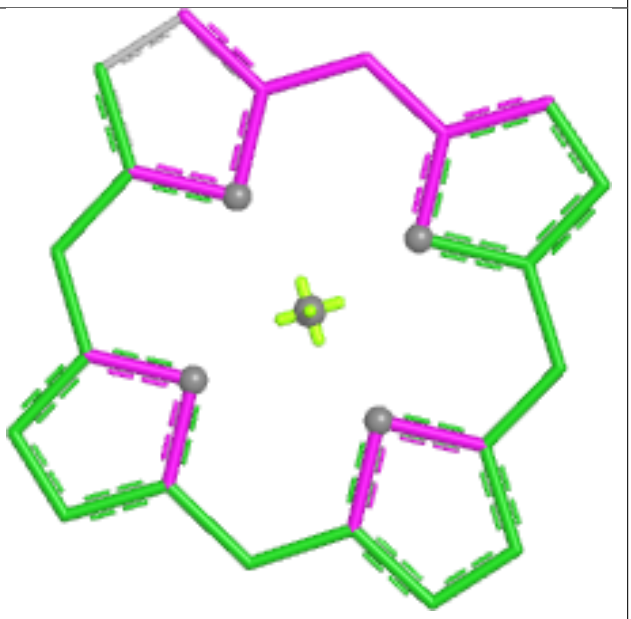


Rings

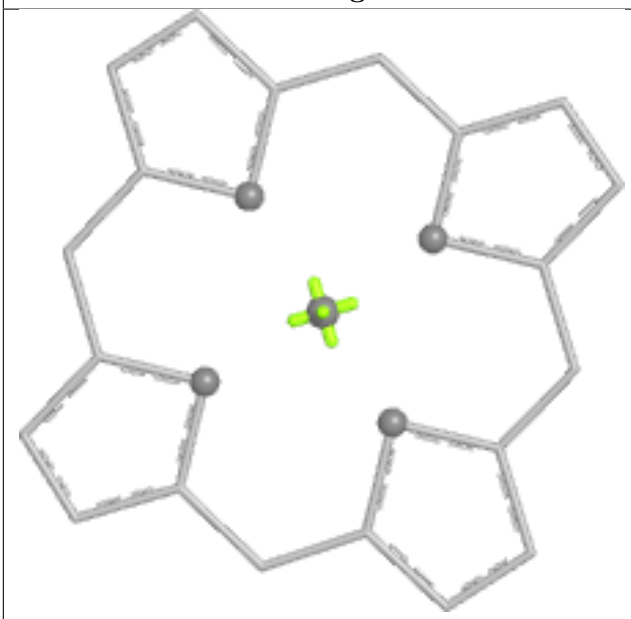
Ligand CLA A 1402



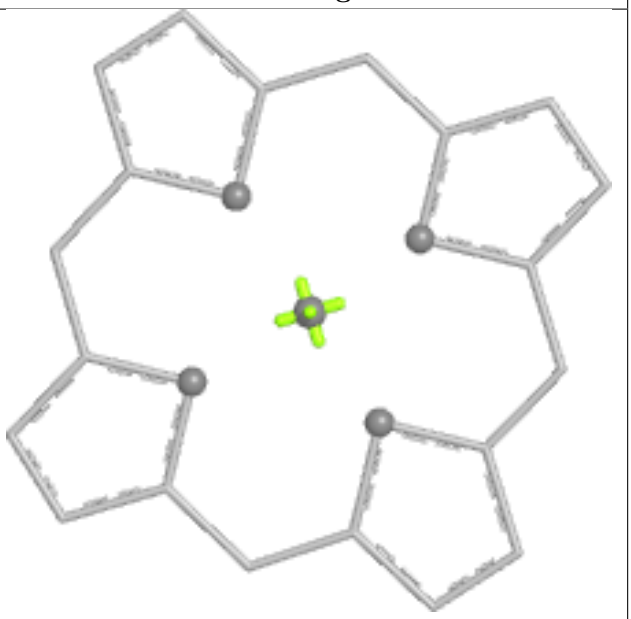
Bond lengths



Bond angles

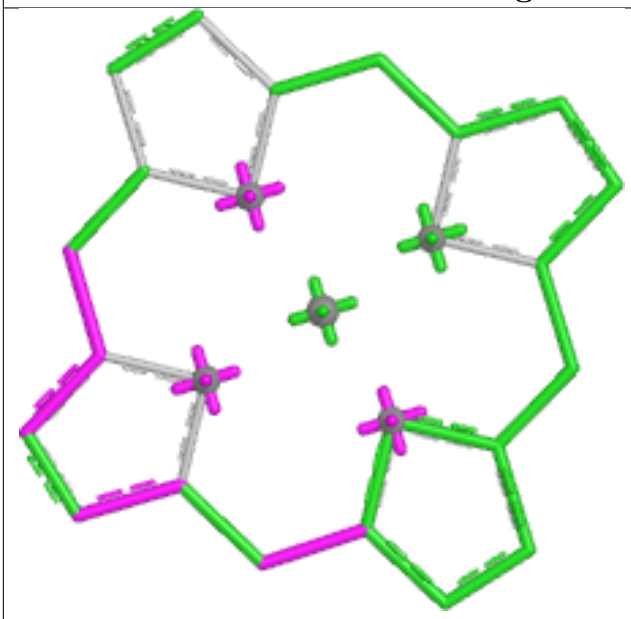


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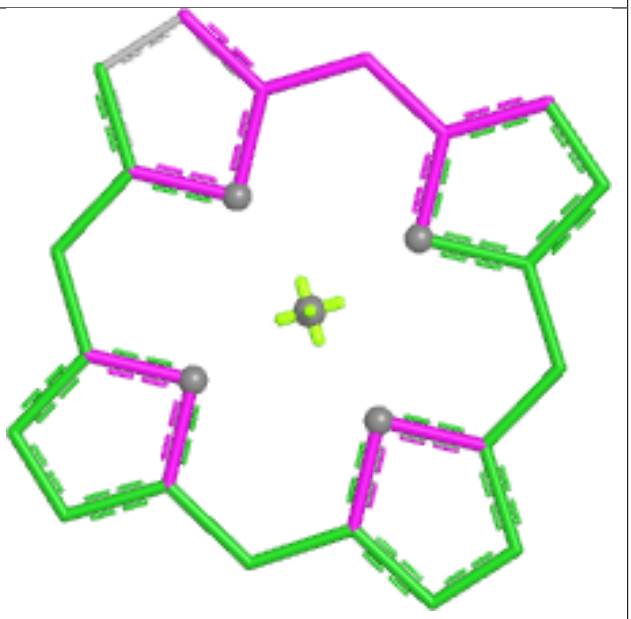


Rings

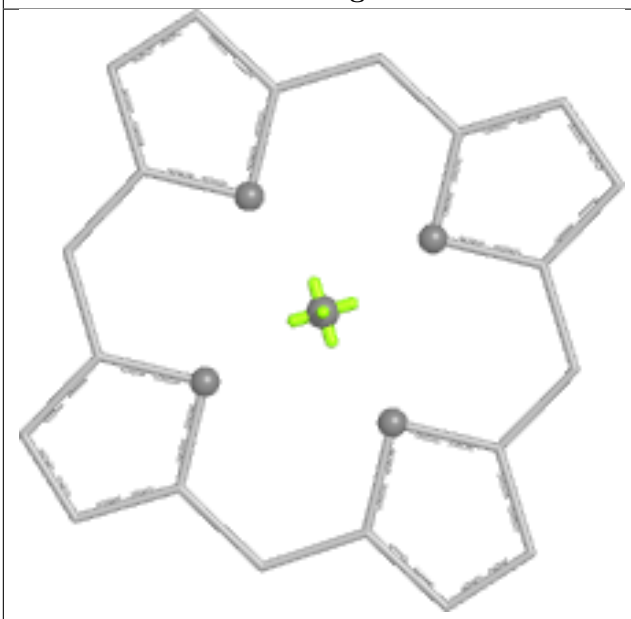
Ligand CLA B 1205



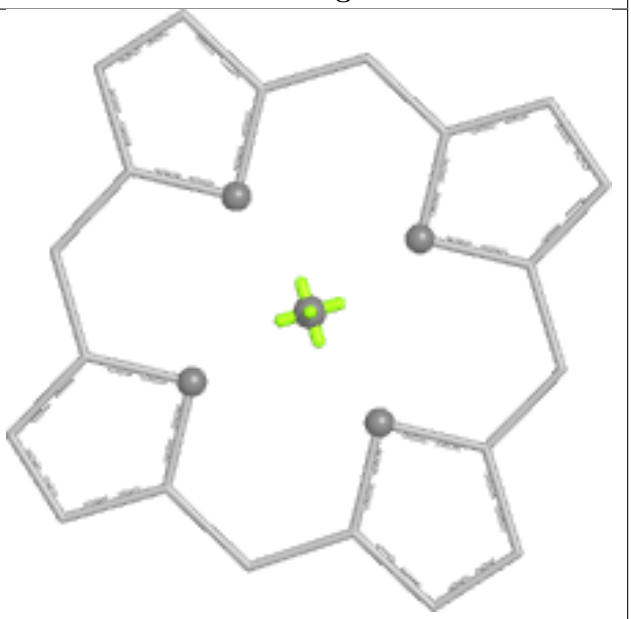
Bond lengths



Bond angles

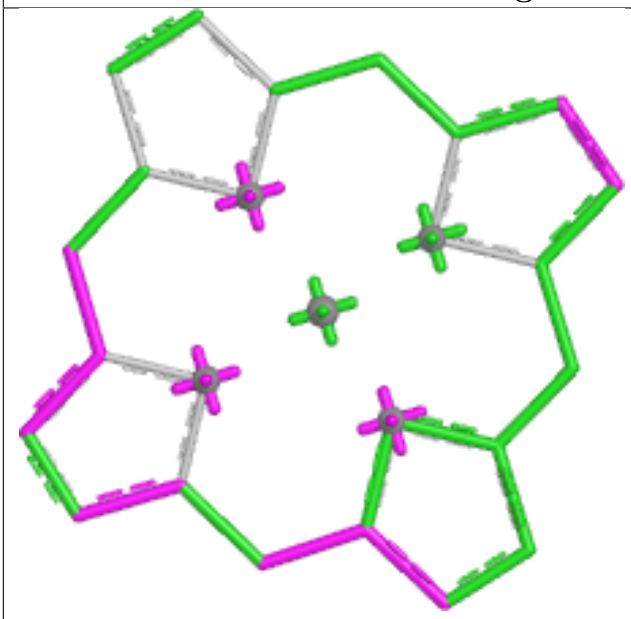


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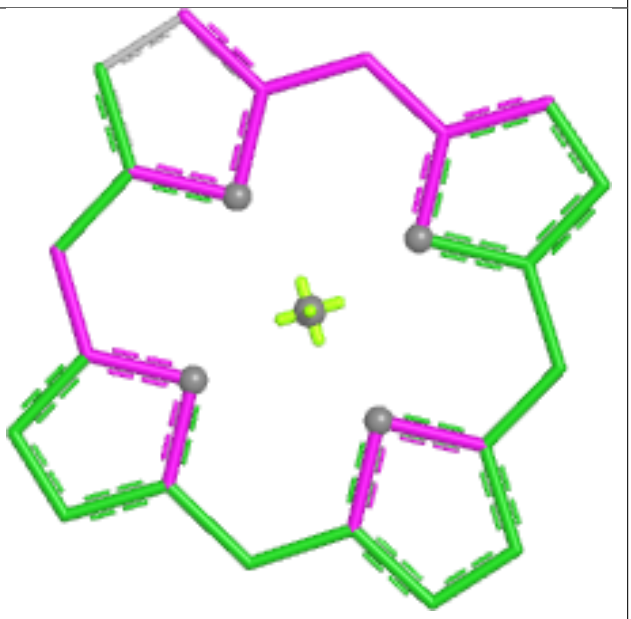


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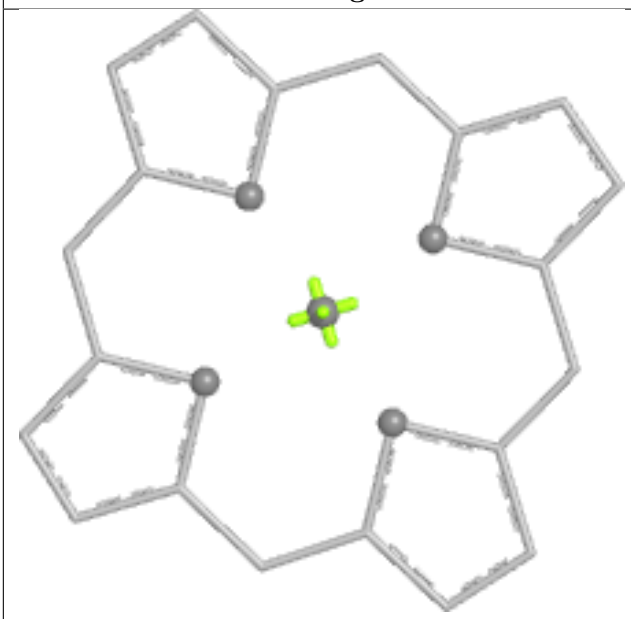
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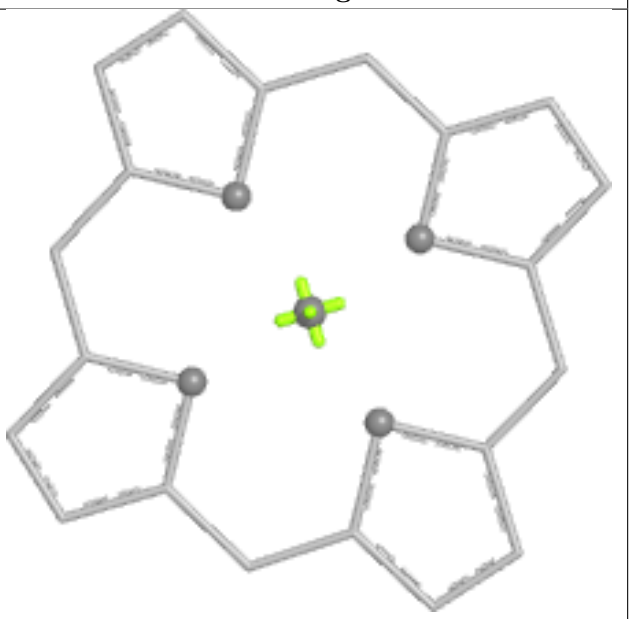
Bond lengths



Bond angles

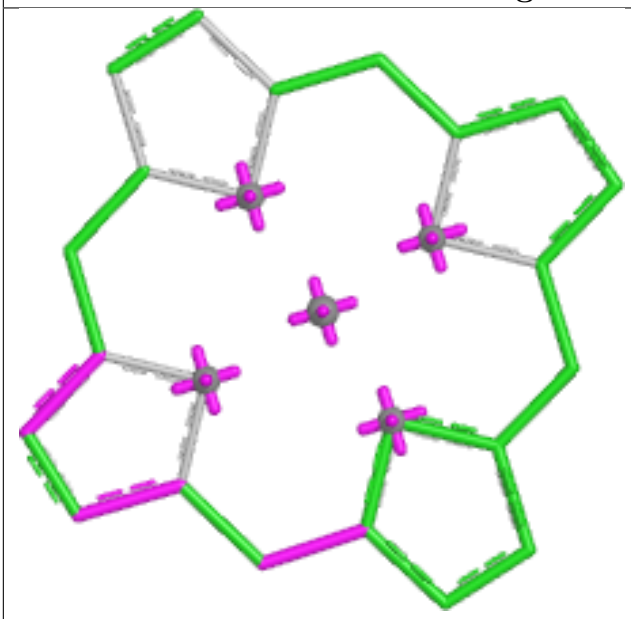


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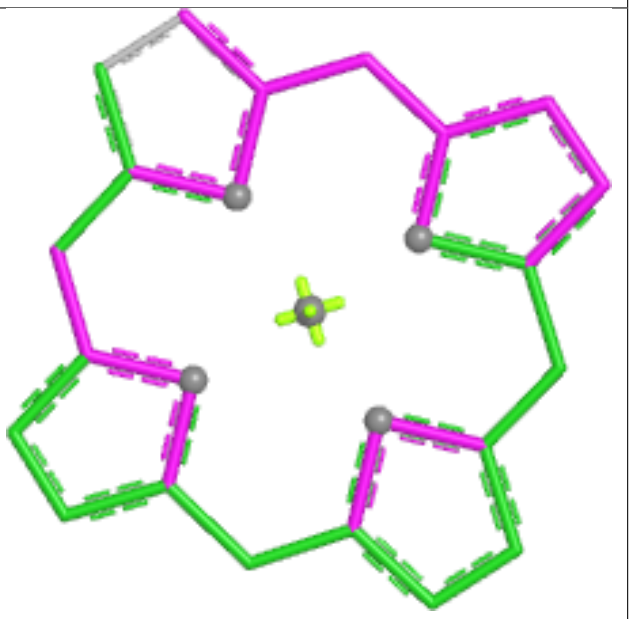


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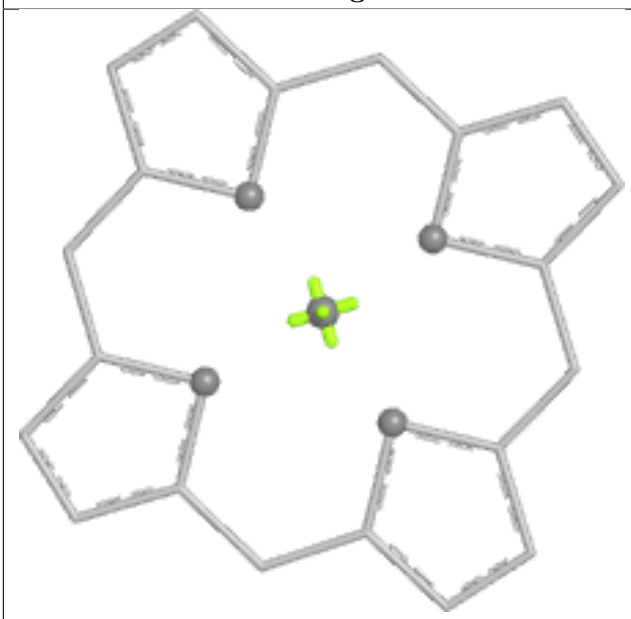
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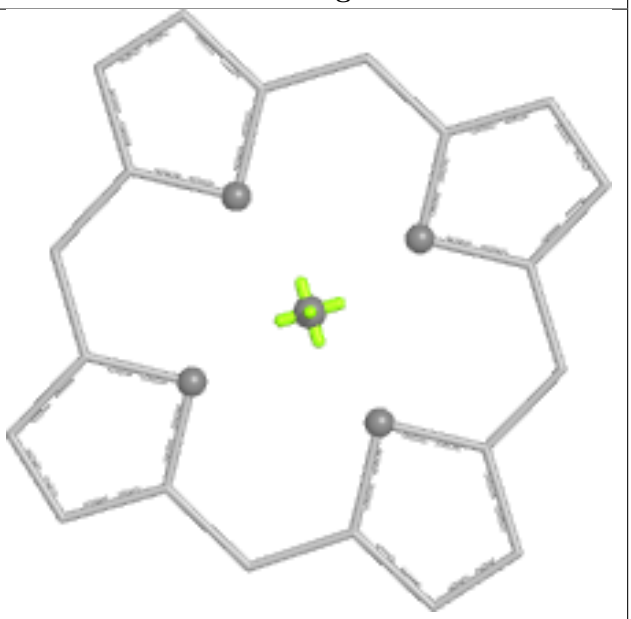
Bond lengths



Bond angles

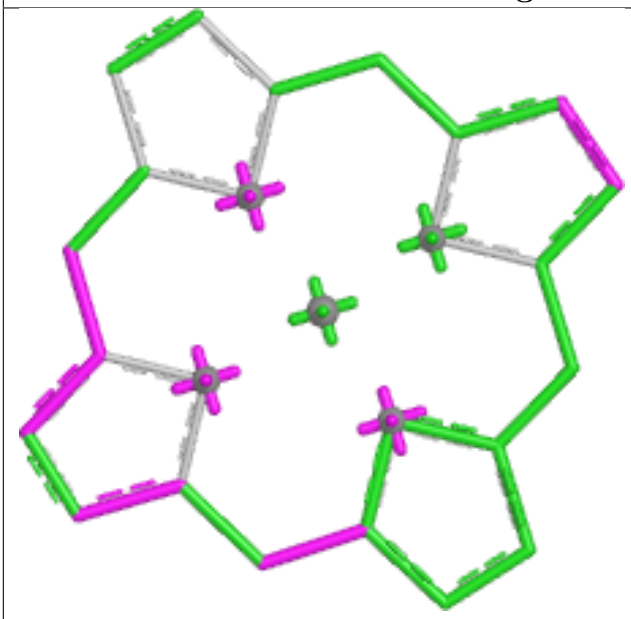


Torsions

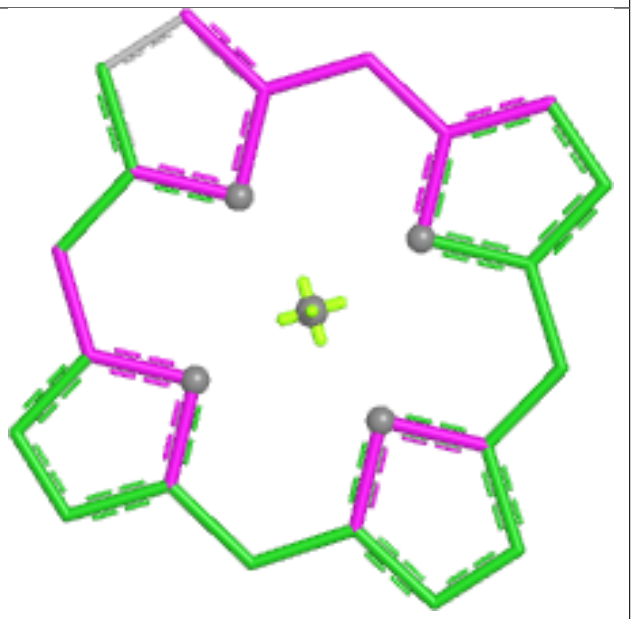


Rings

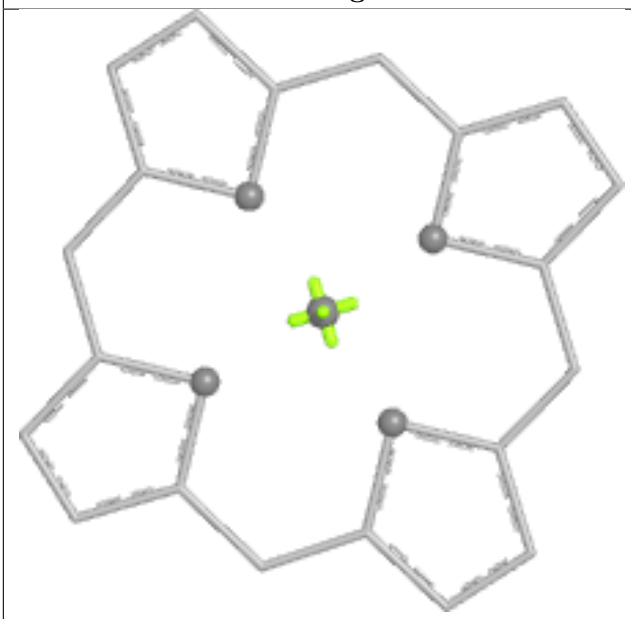
Ligand CLA P 5114



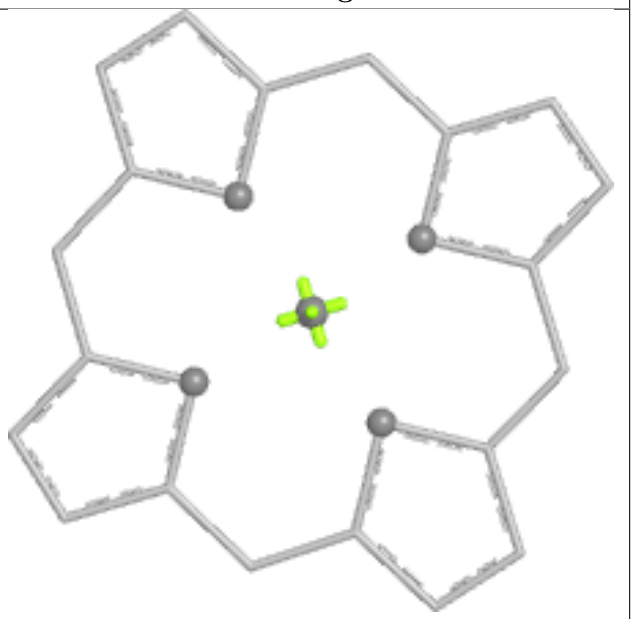
Bond lengths



Bond angles

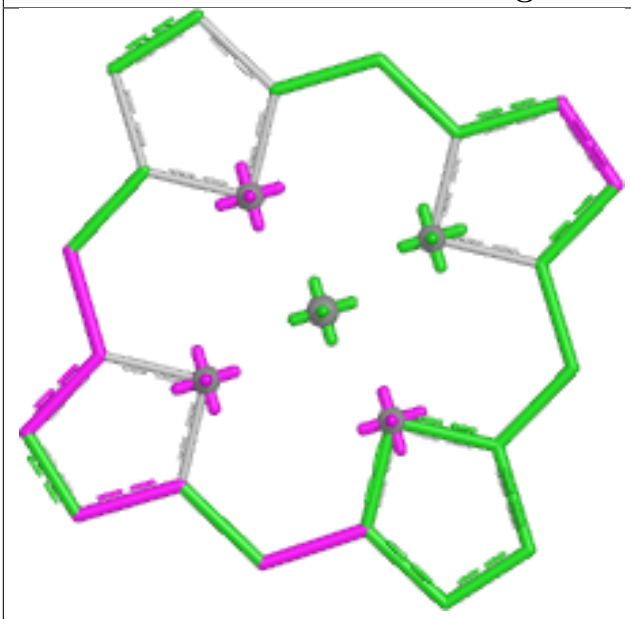


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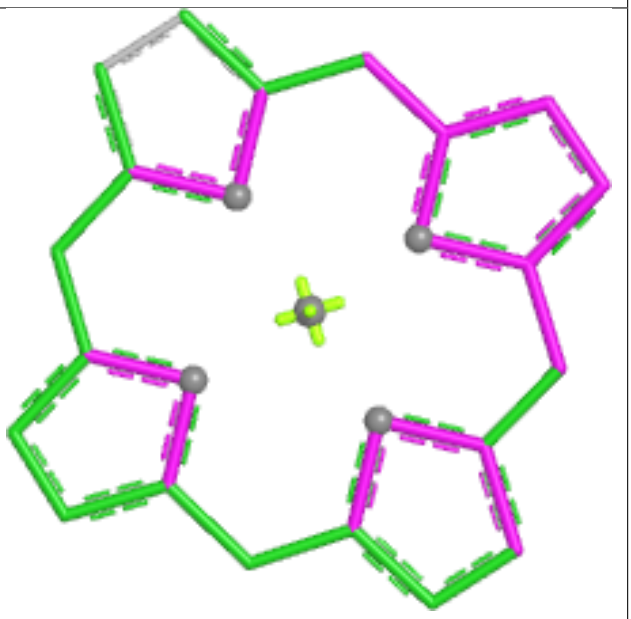


Rings

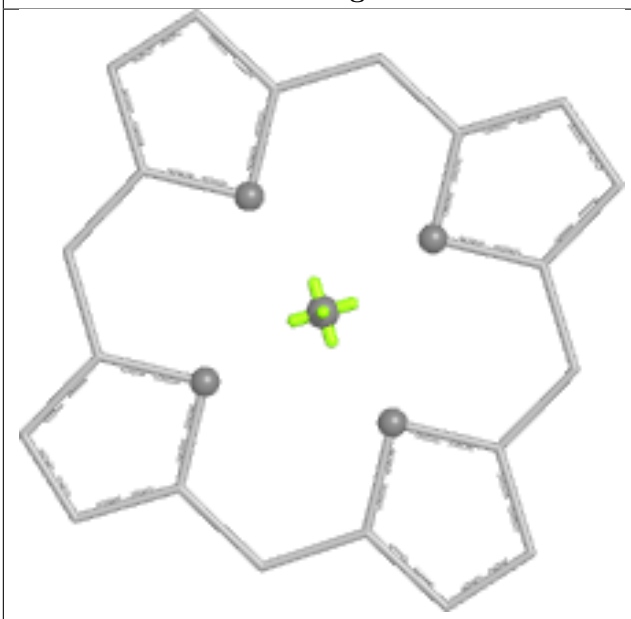
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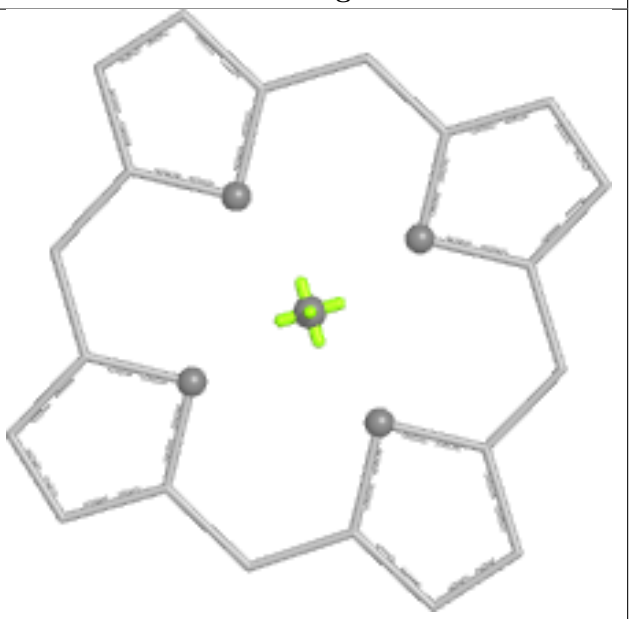
Bond lengths



Bond angles

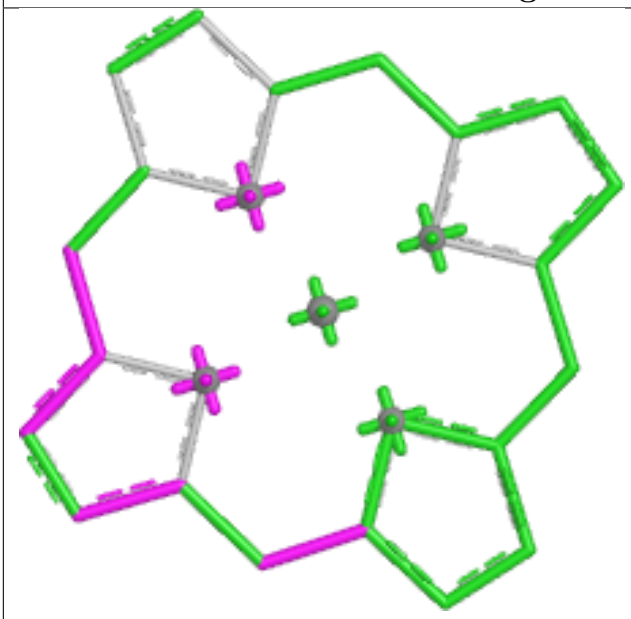


Torsions

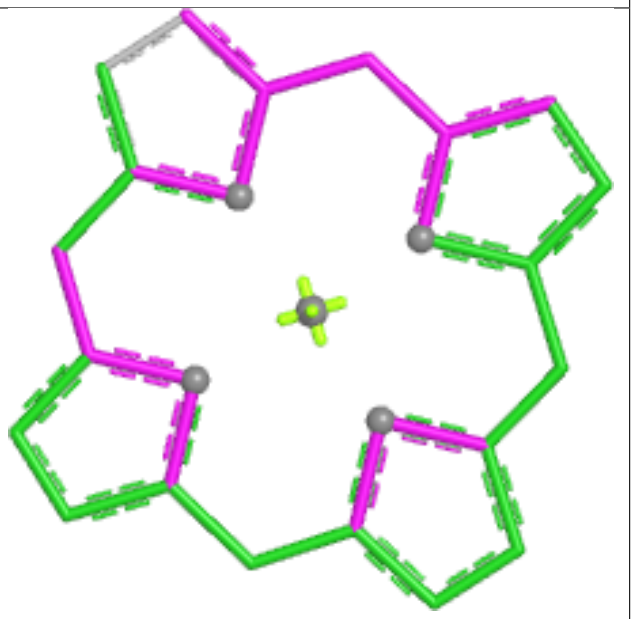


Rings

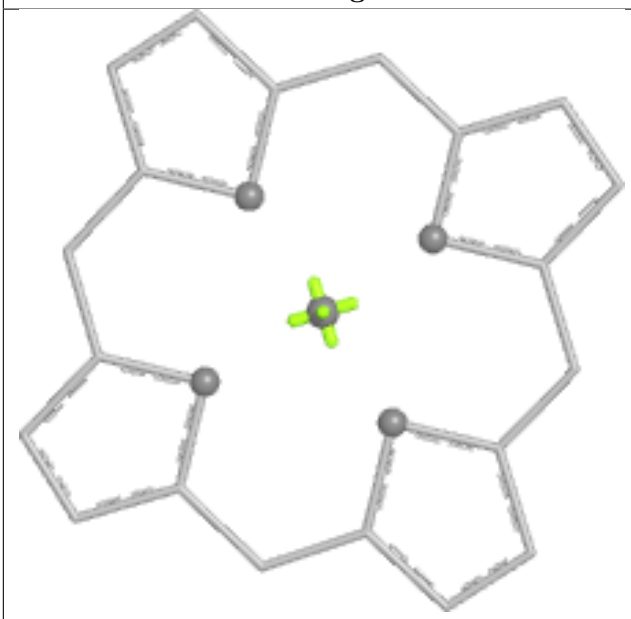
Ligand CLA 2 1011



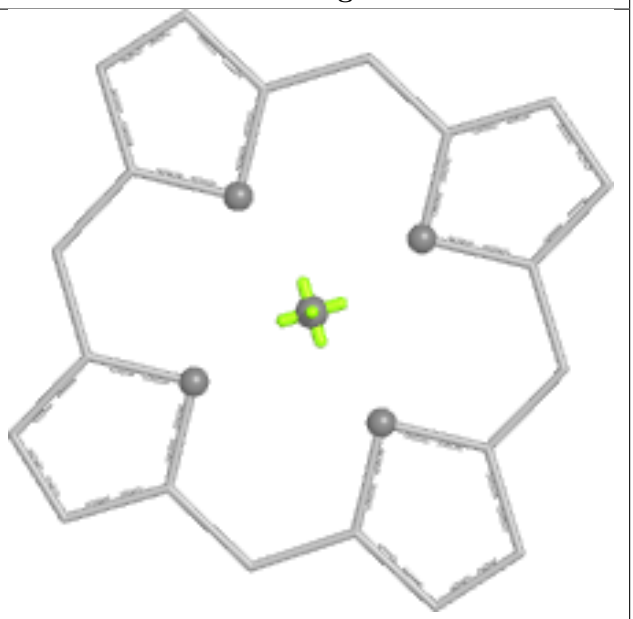
Bond lengths



Bond angles

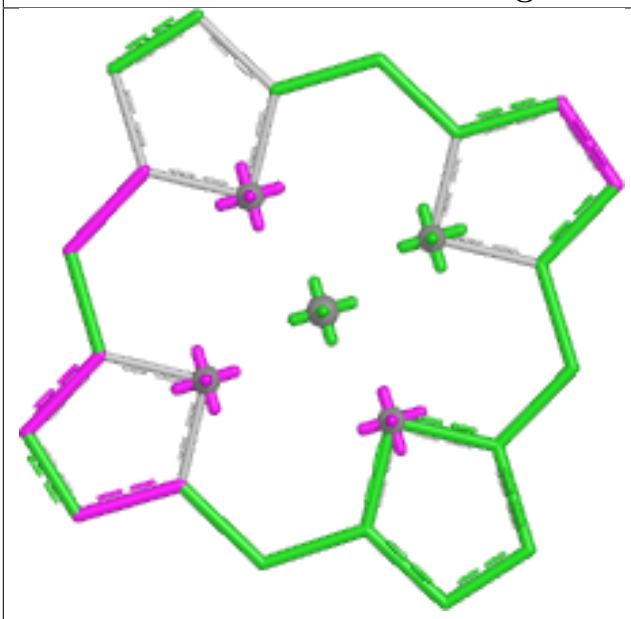


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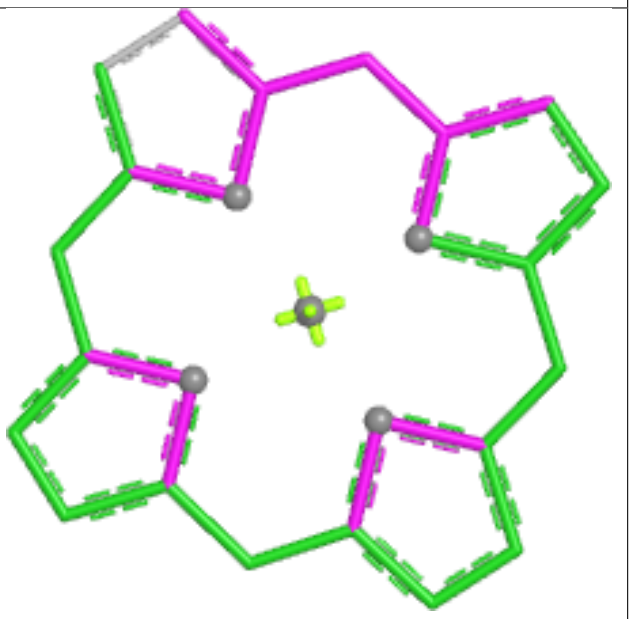


Rings

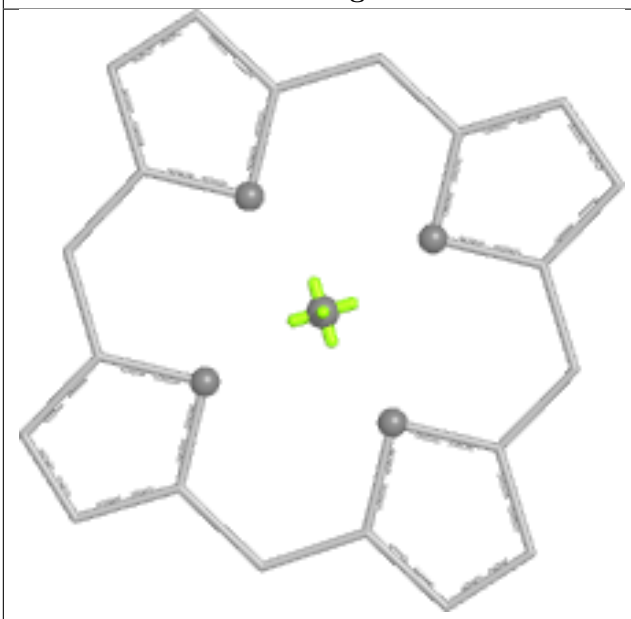
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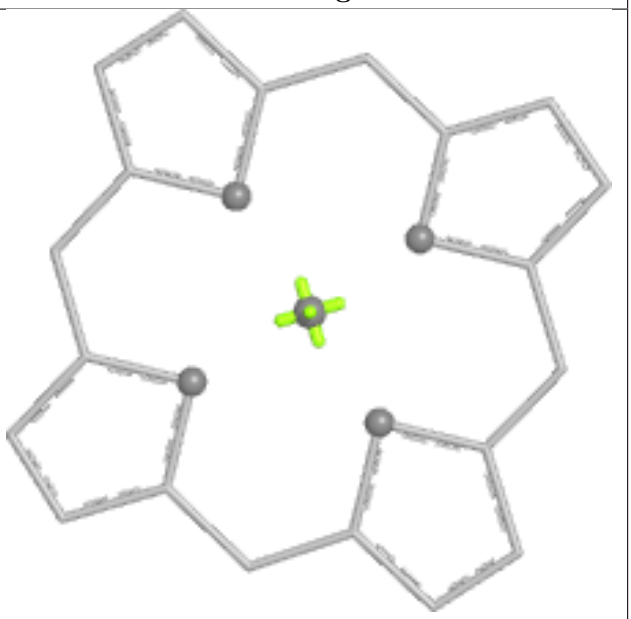
Bond lengths



Bond angles

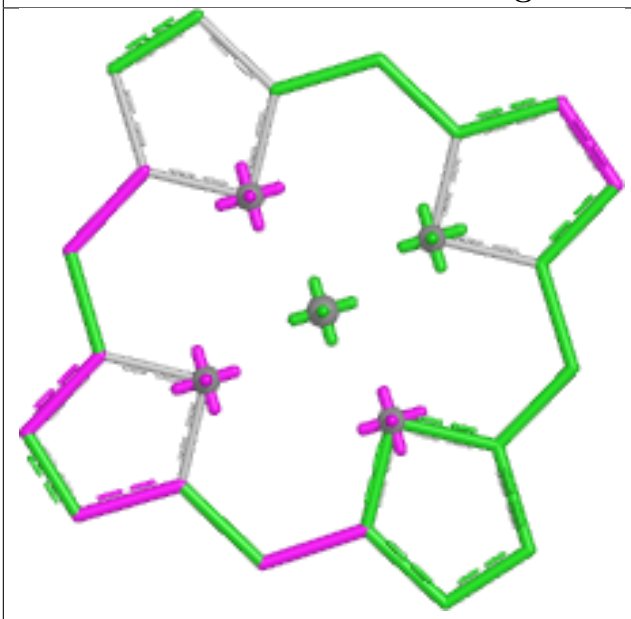


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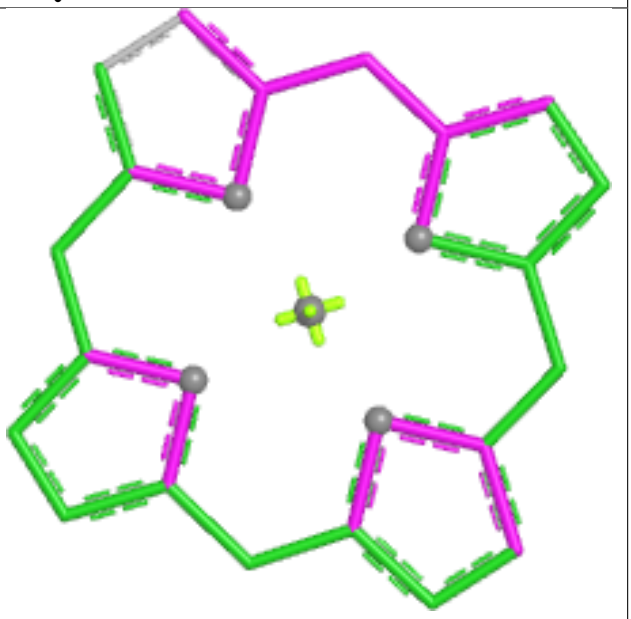


Rings

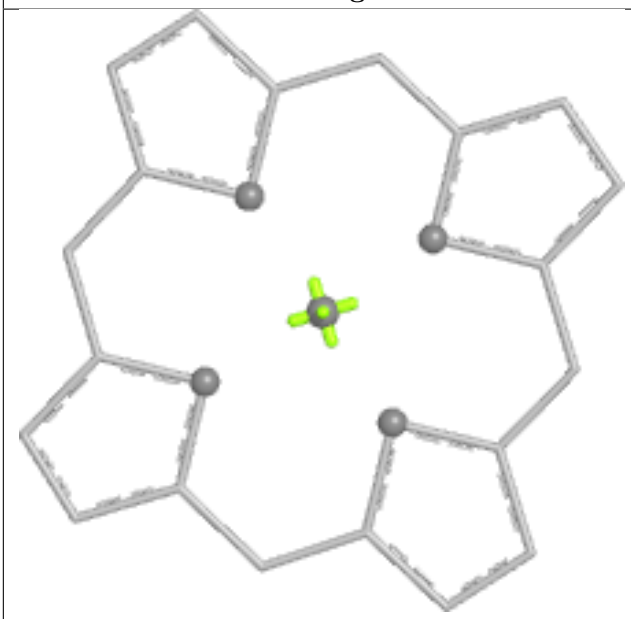
Ligand CLA Q 5217



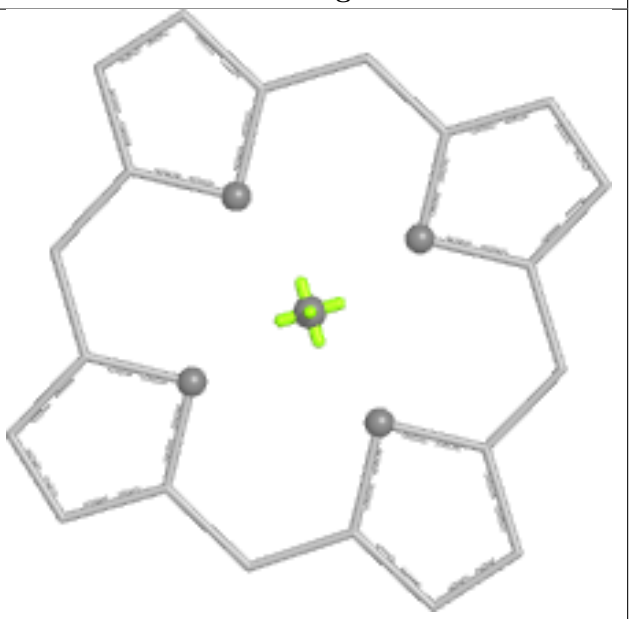
Bond lengths



Bond angles

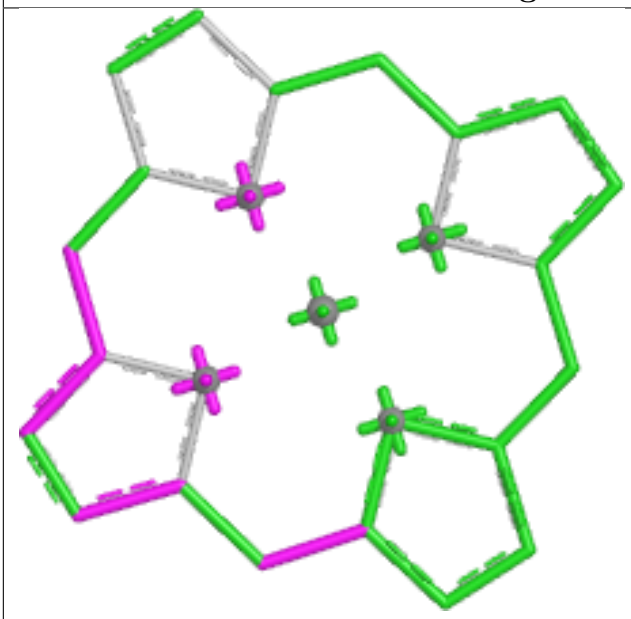


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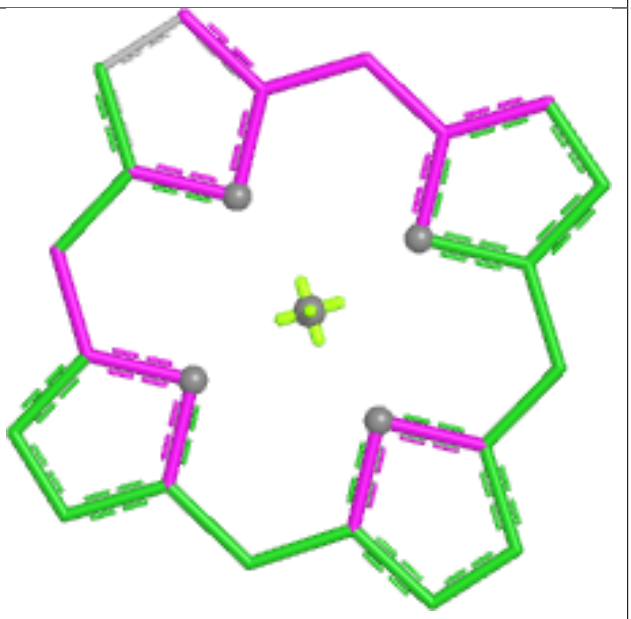


Rings

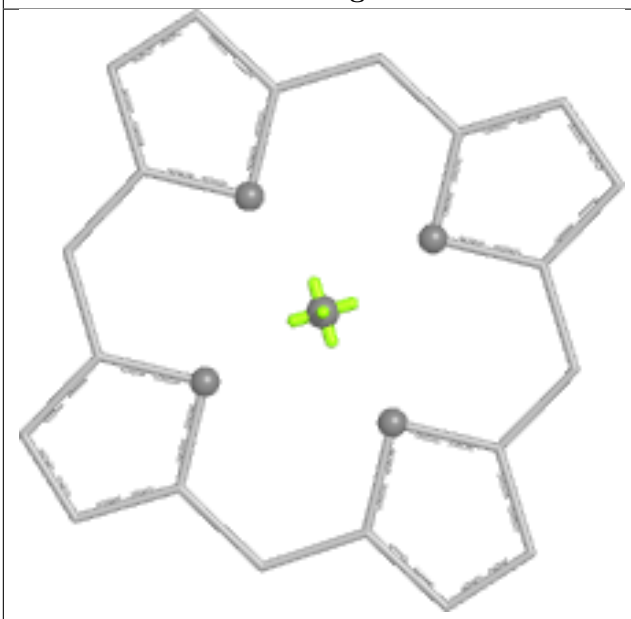
Ligand CLA 8 1013



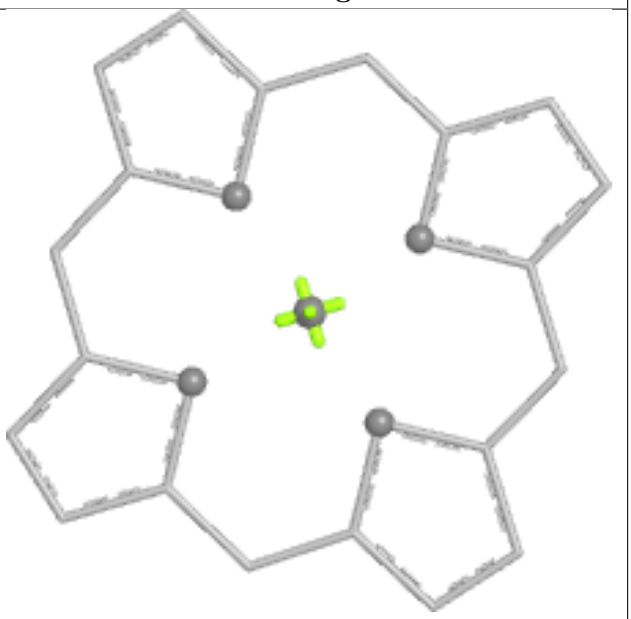
Bond lengths



Bond angles

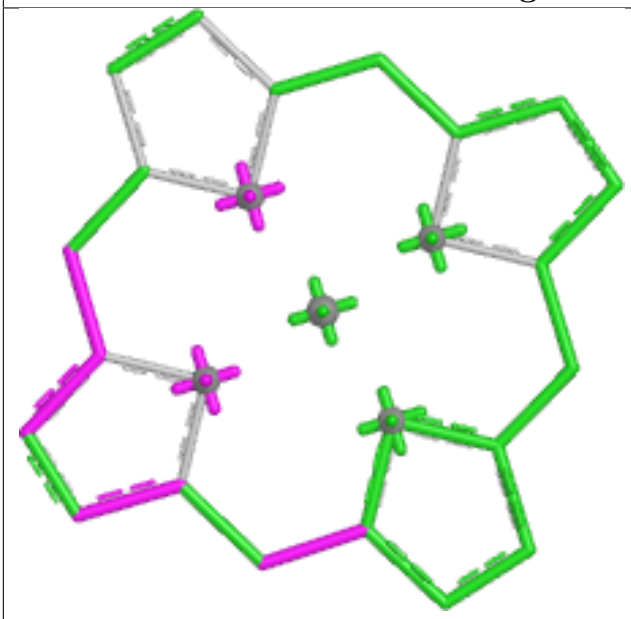


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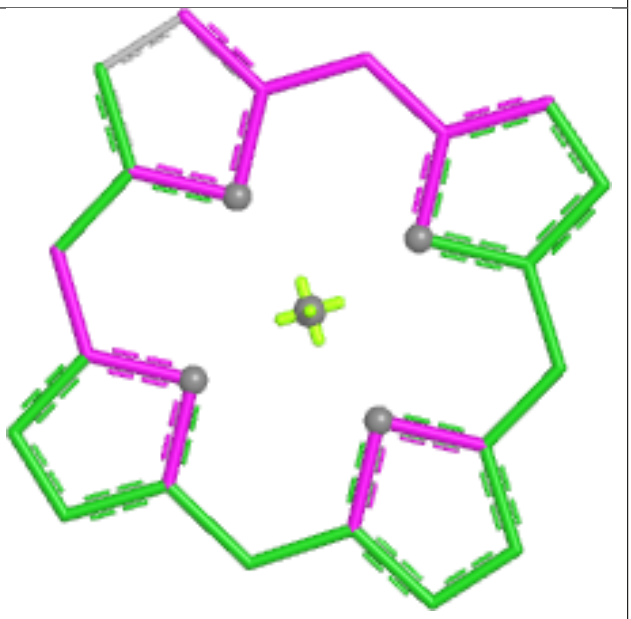


Rings

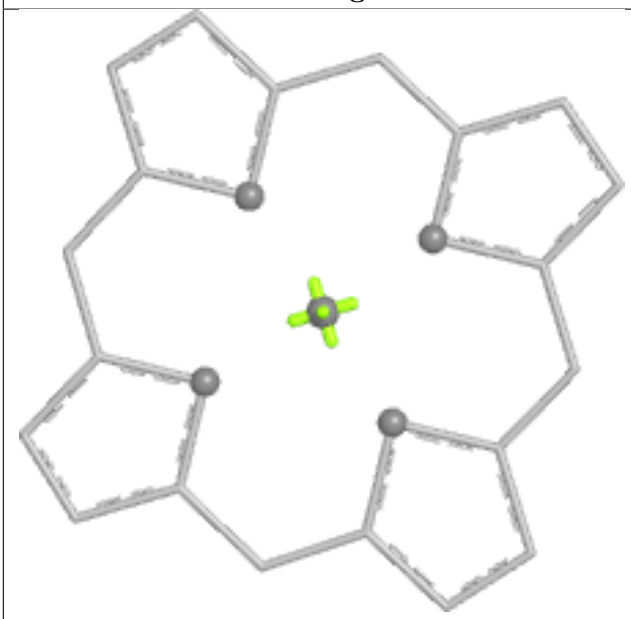
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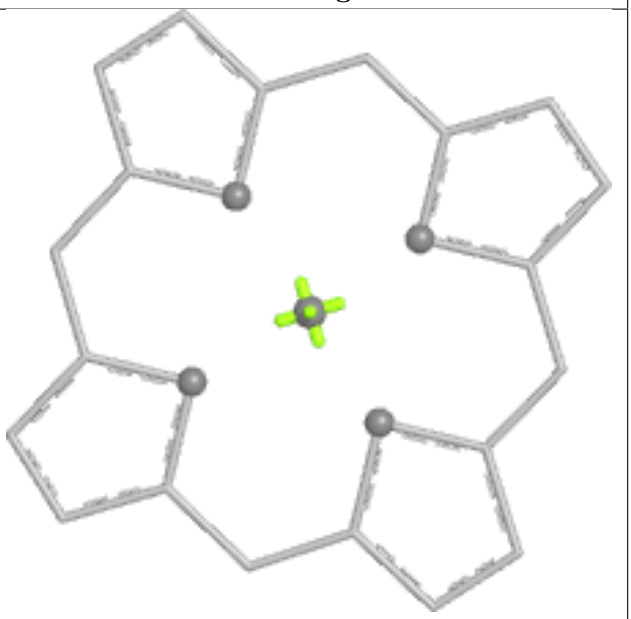
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Bond angles

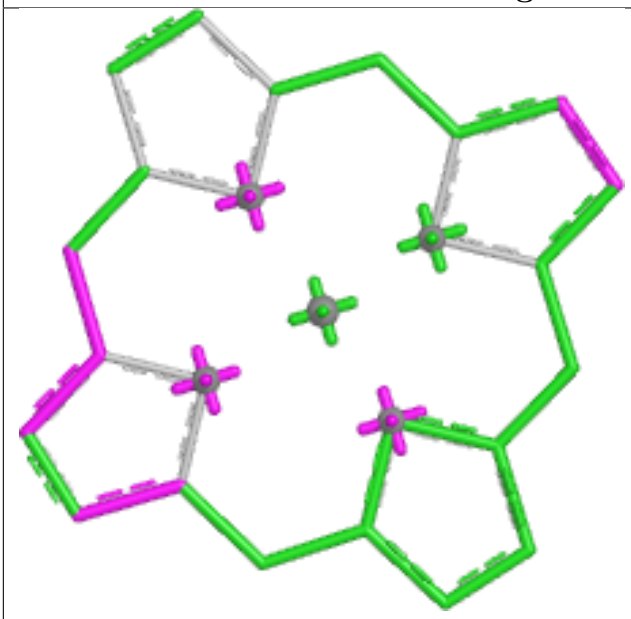


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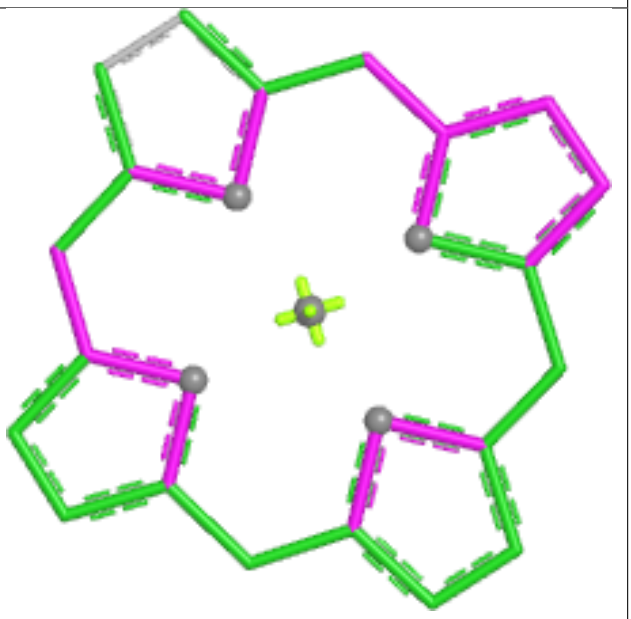


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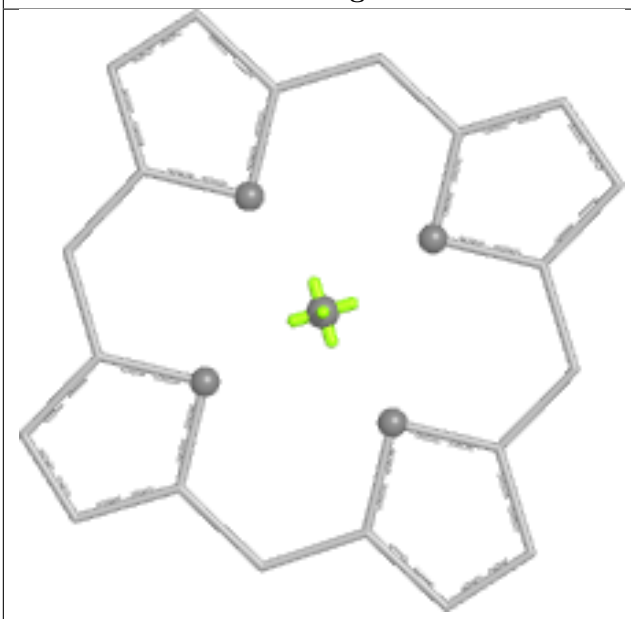
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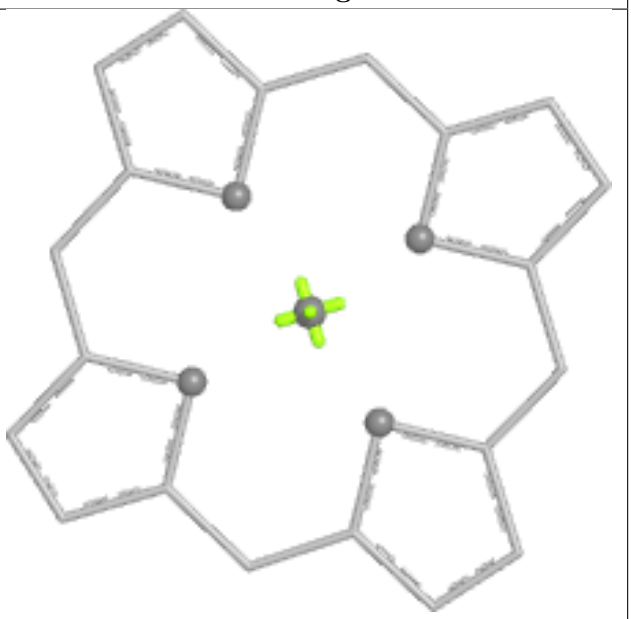
Bond lengths



Bond angles

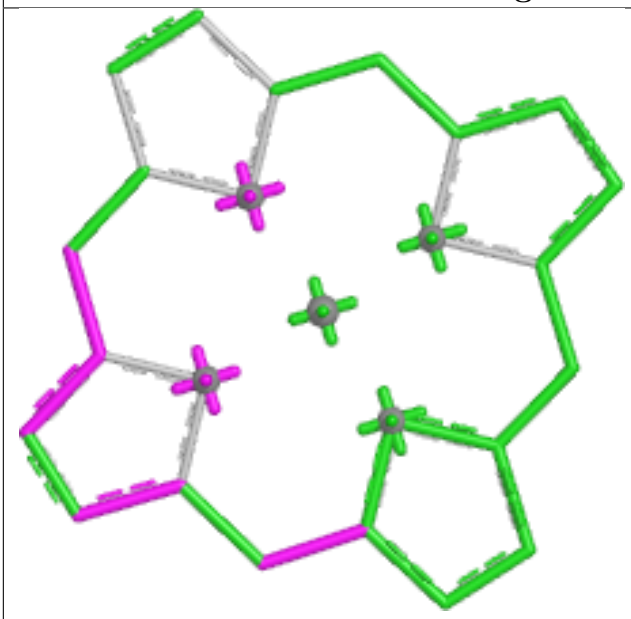


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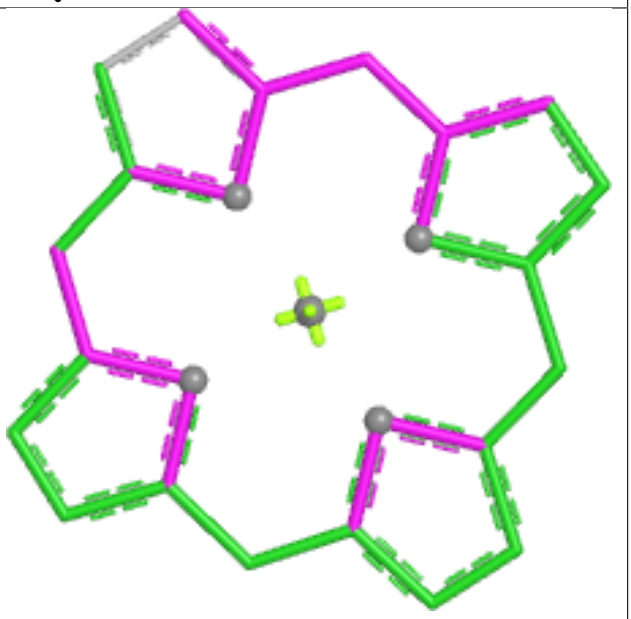


Rings

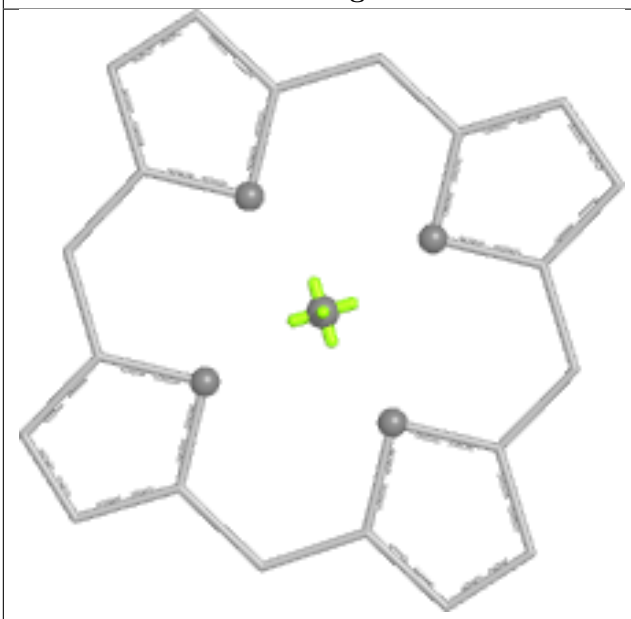
Ligand CLA Q 5240



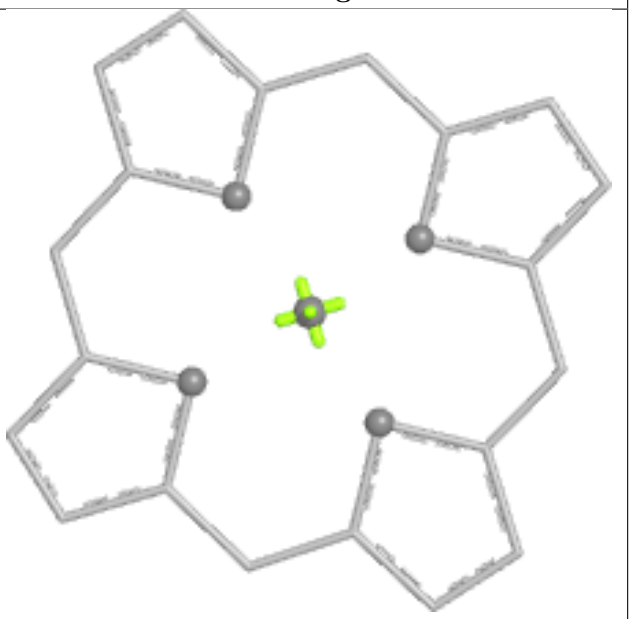
Bond lengths



Bond angles

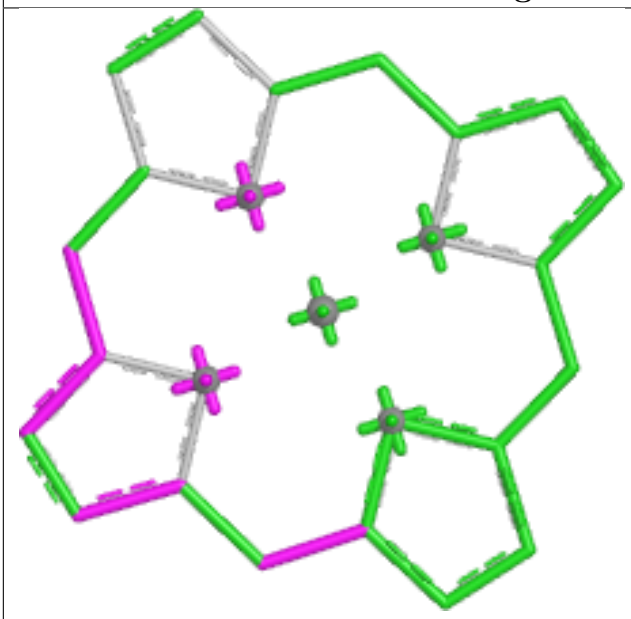


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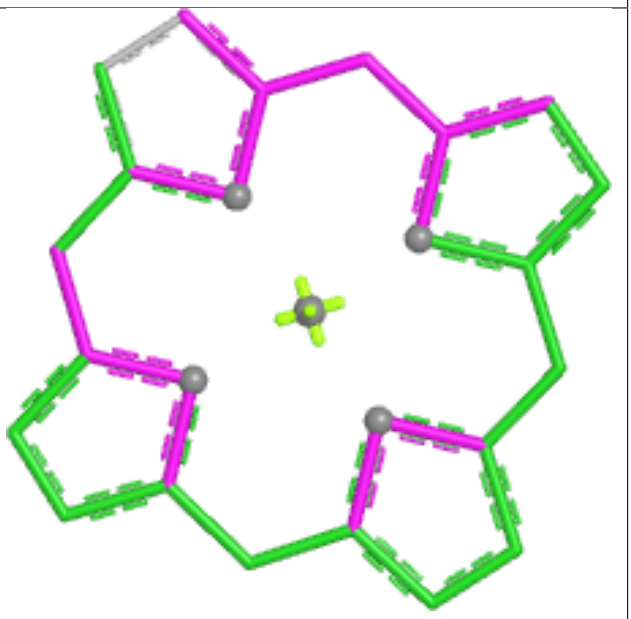


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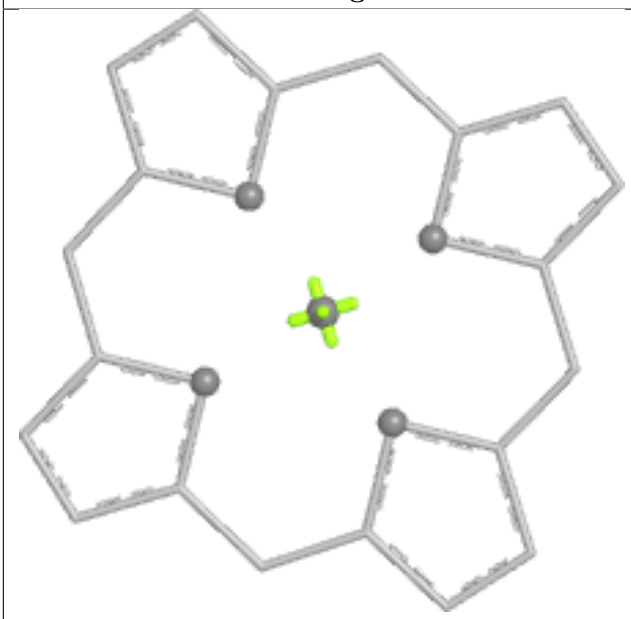
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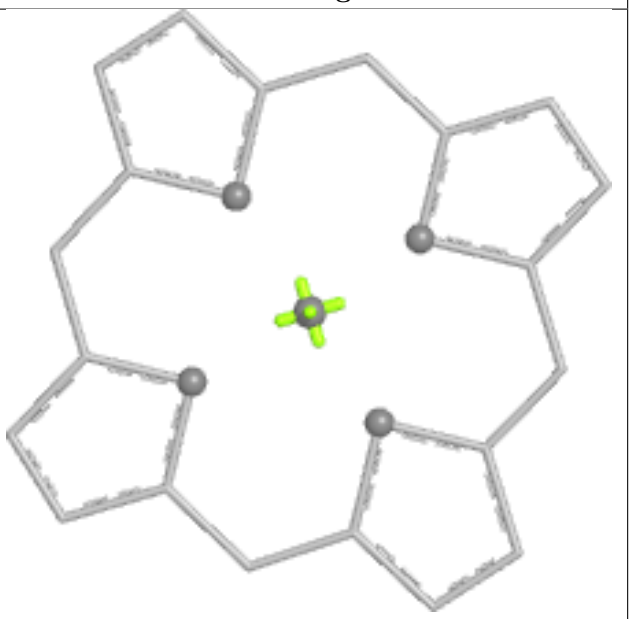
Bond lengths



Bond angles

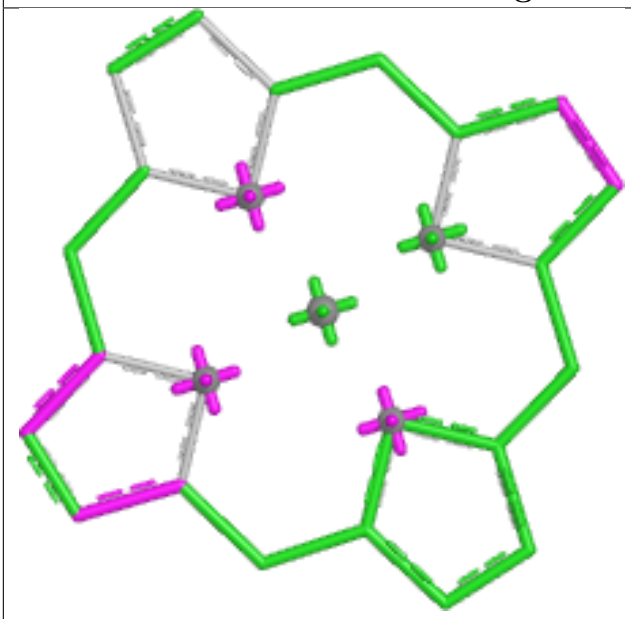


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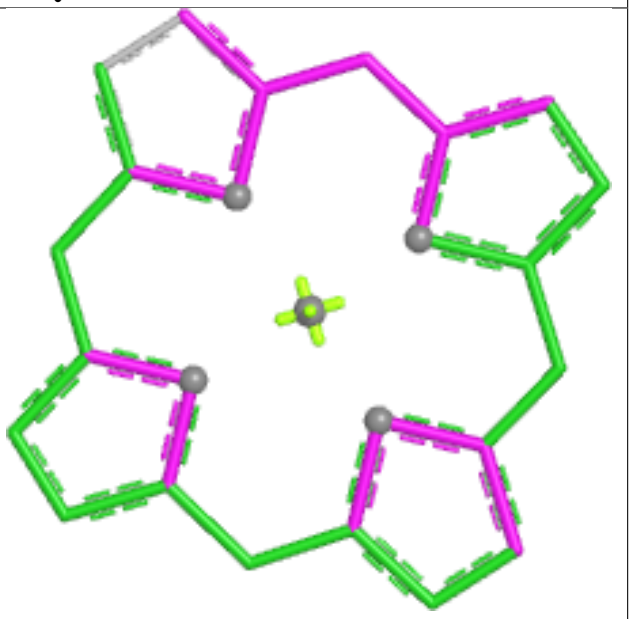


Rings

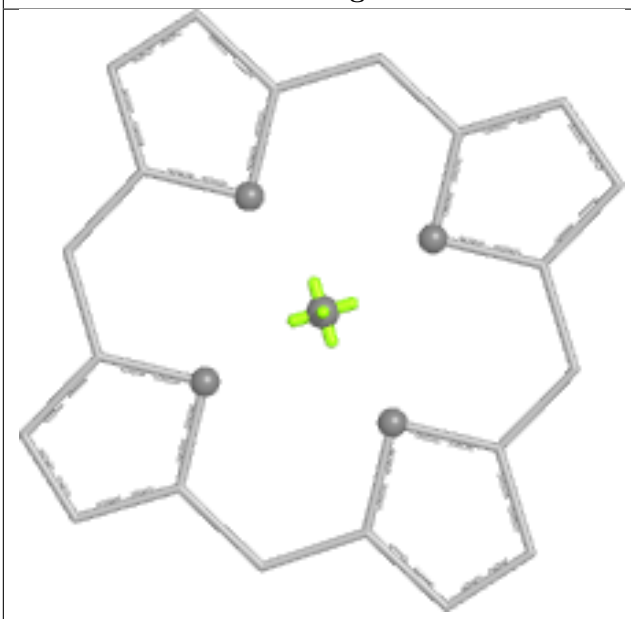
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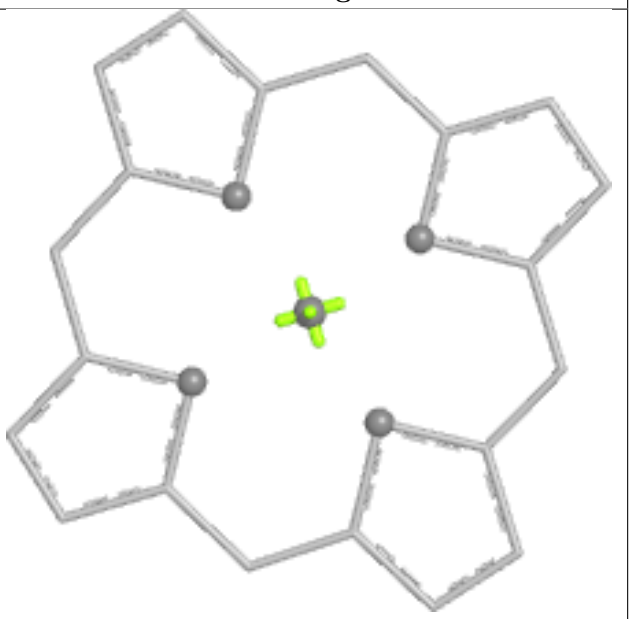
Bond lengths



Bond angles

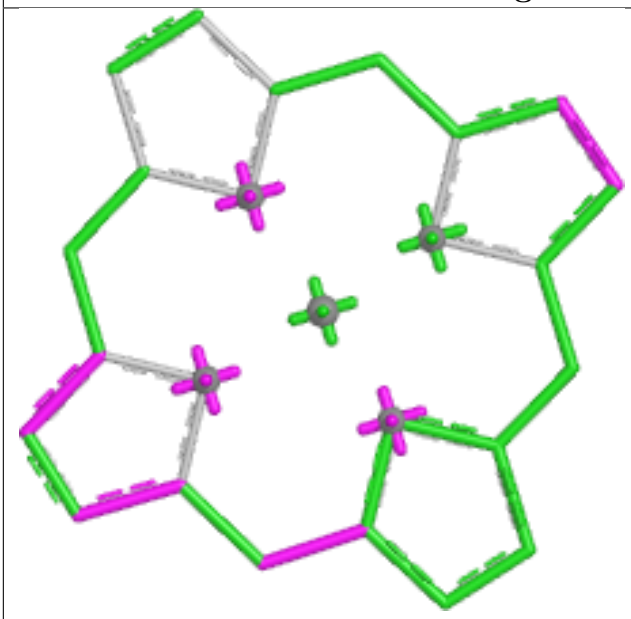


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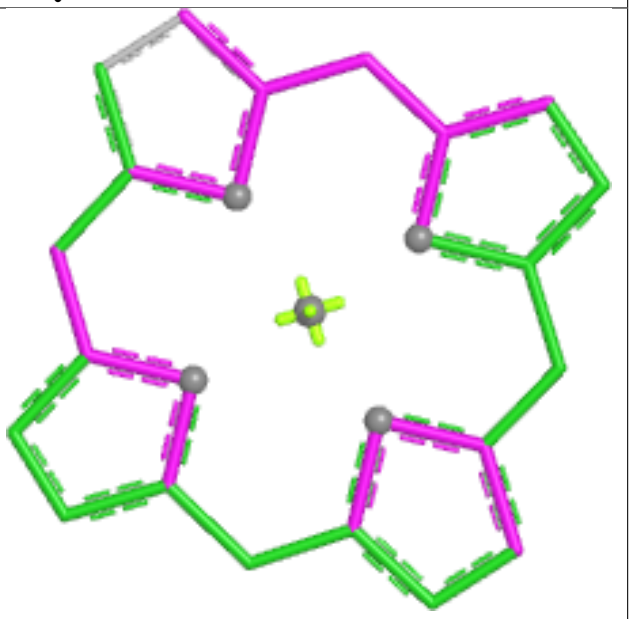


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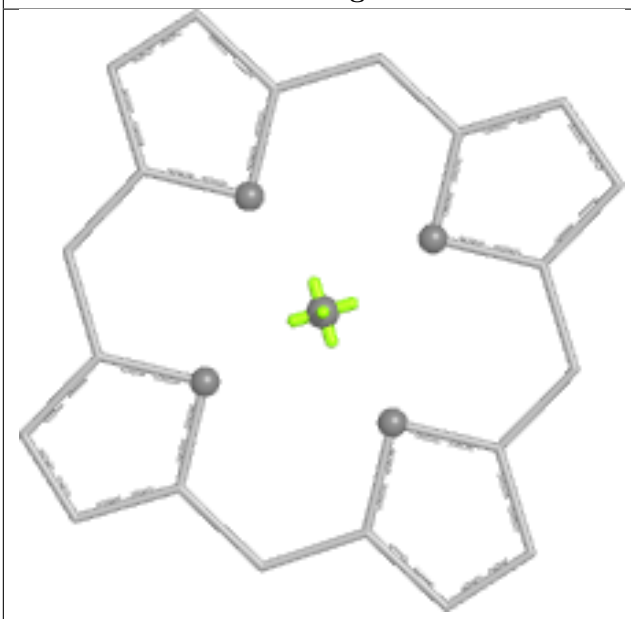
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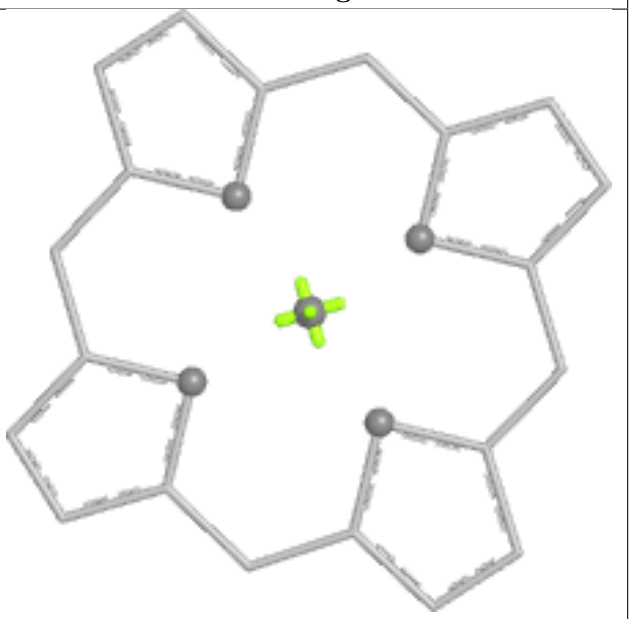
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Bond angles

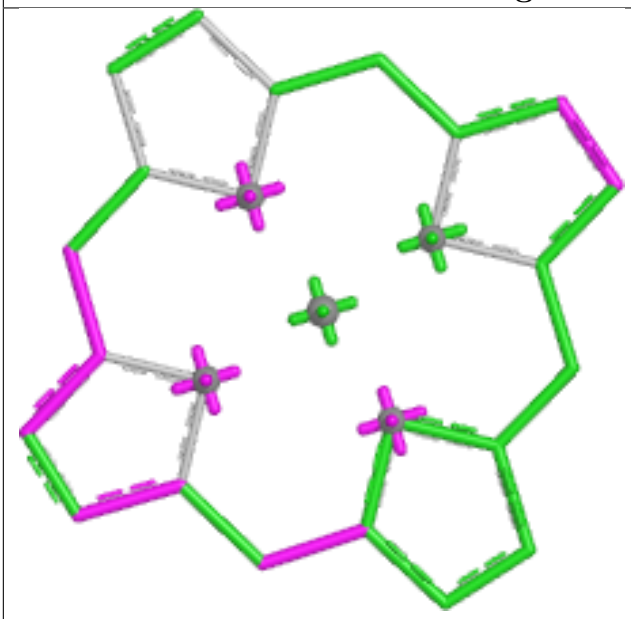


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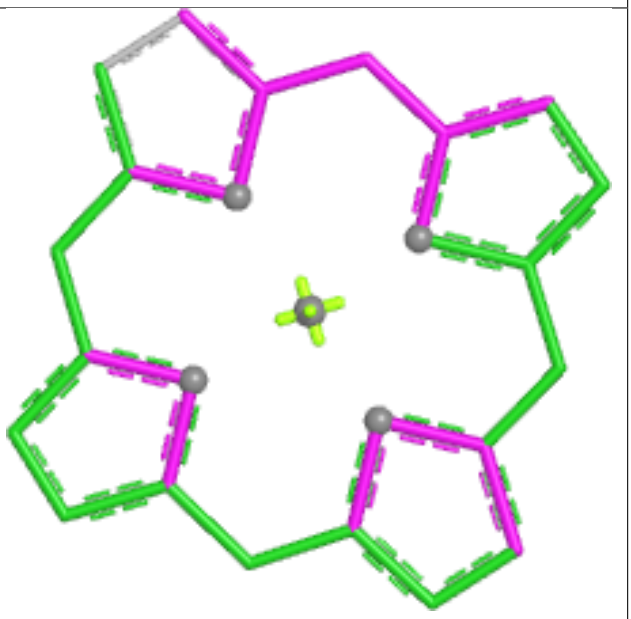


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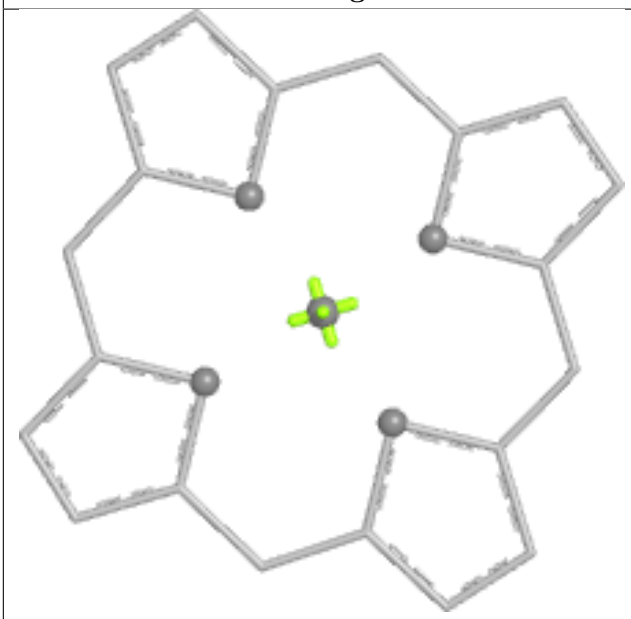
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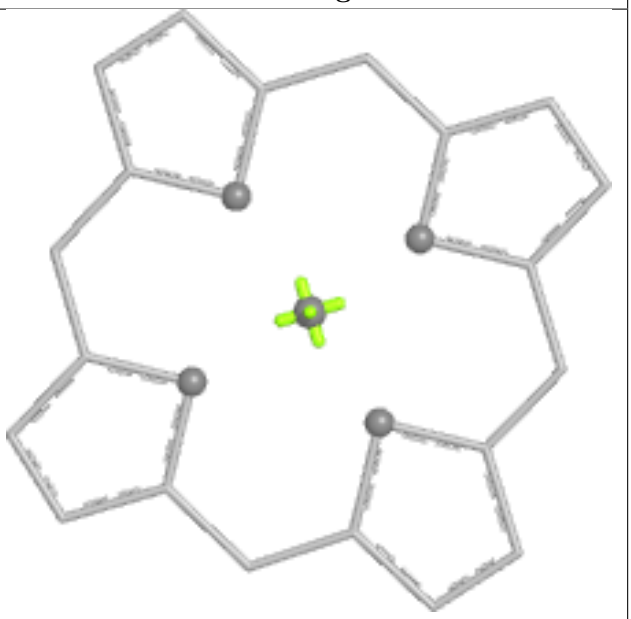
Bond lengths



Bond angles

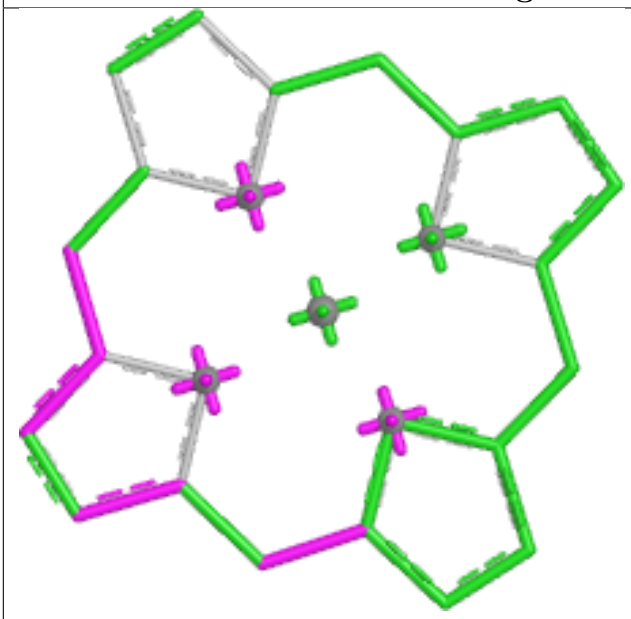


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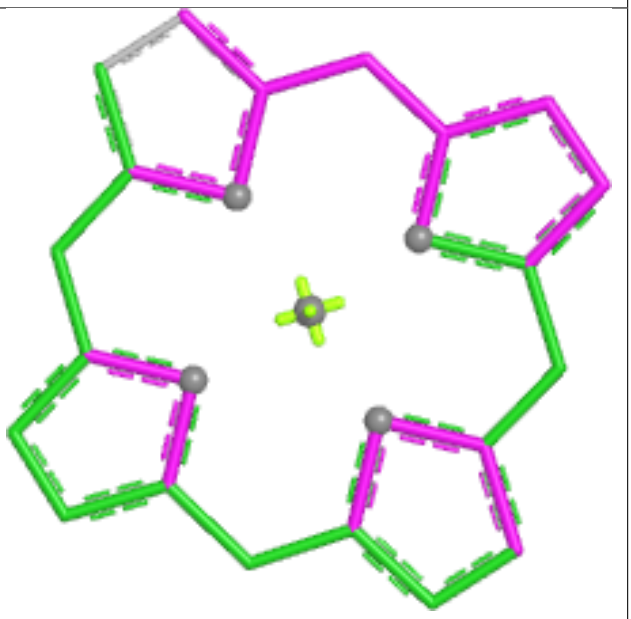


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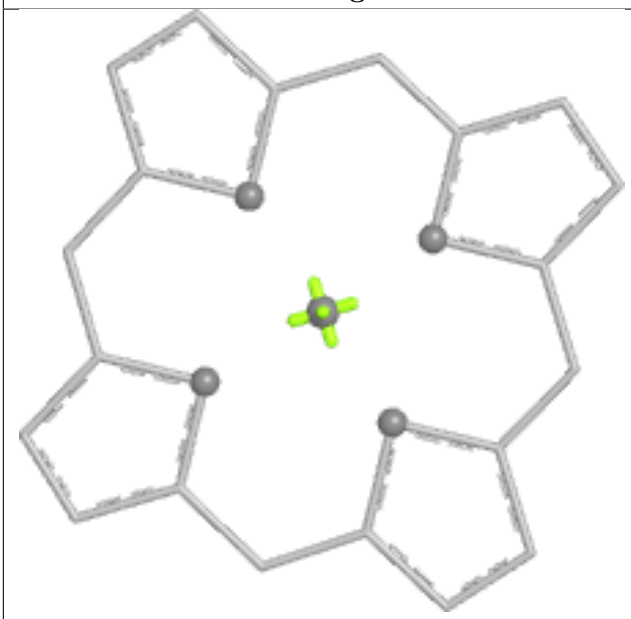
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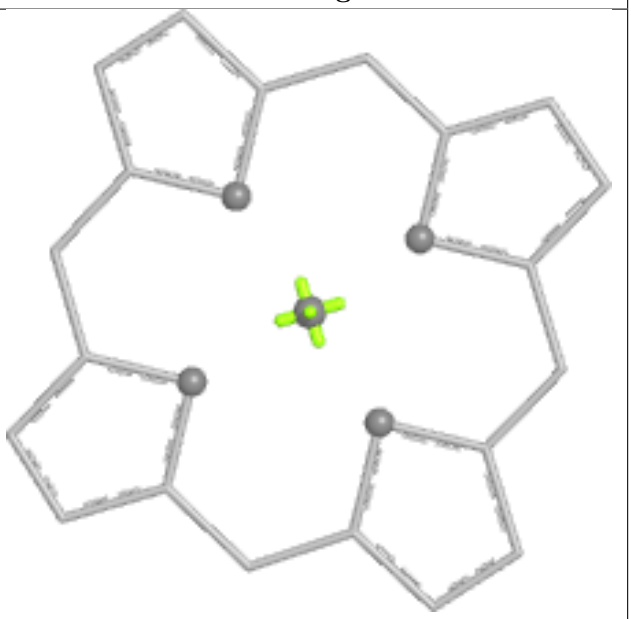
Bond lengths



Bond angles

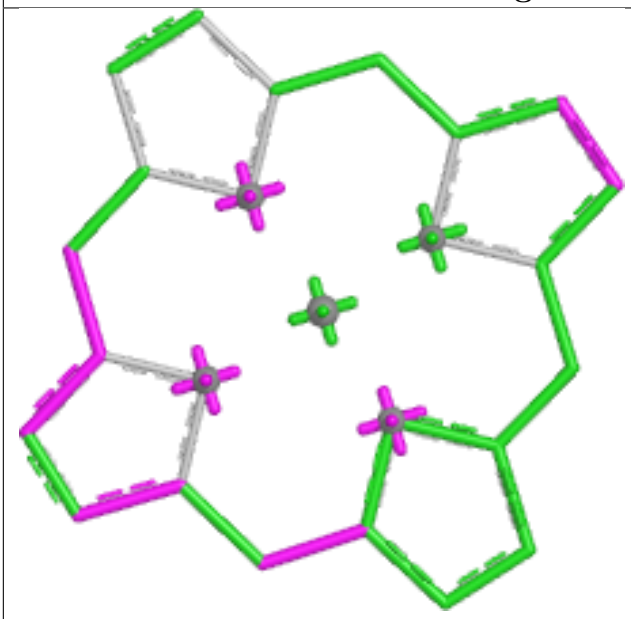


Torsions

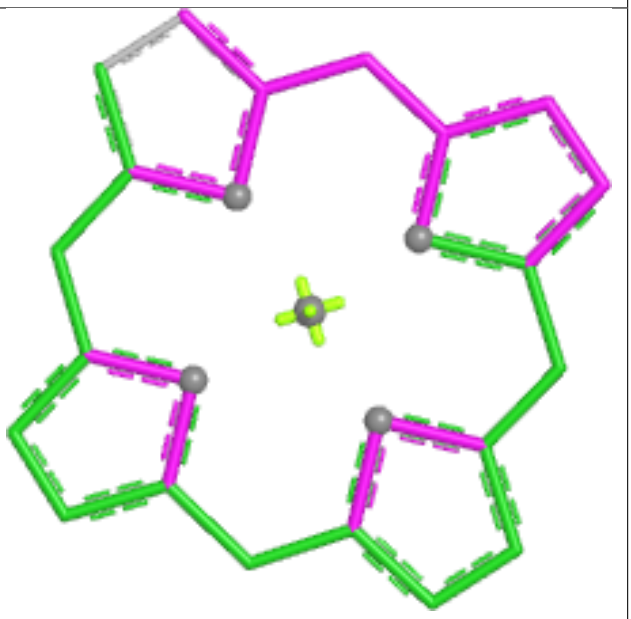


Rings

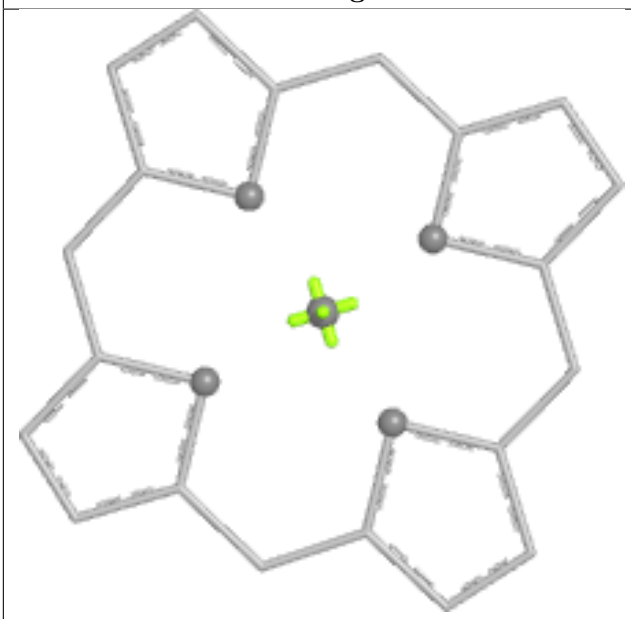
Ligand CLA A 1109



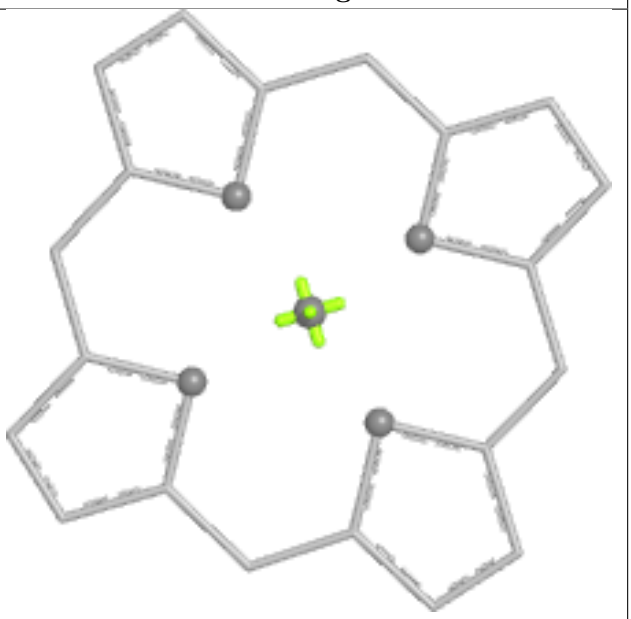
Bond lengths



Bond angles

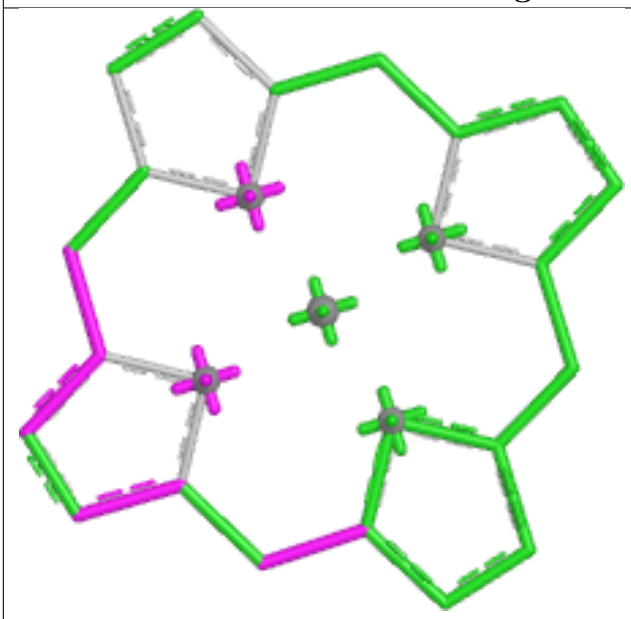


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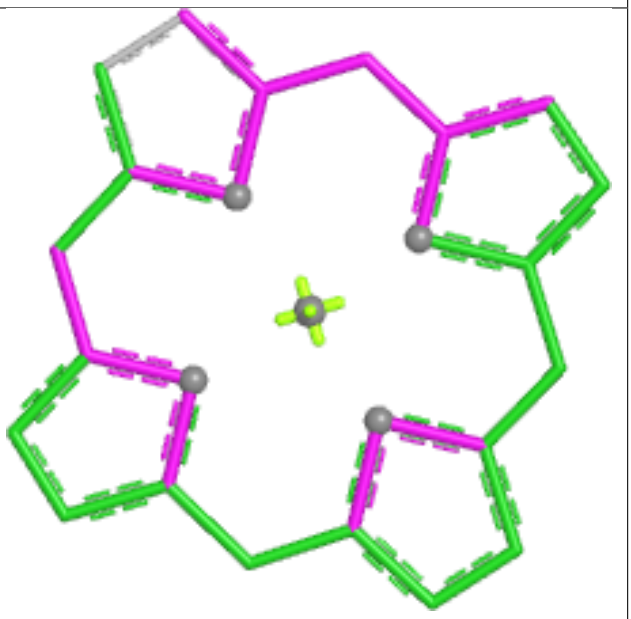


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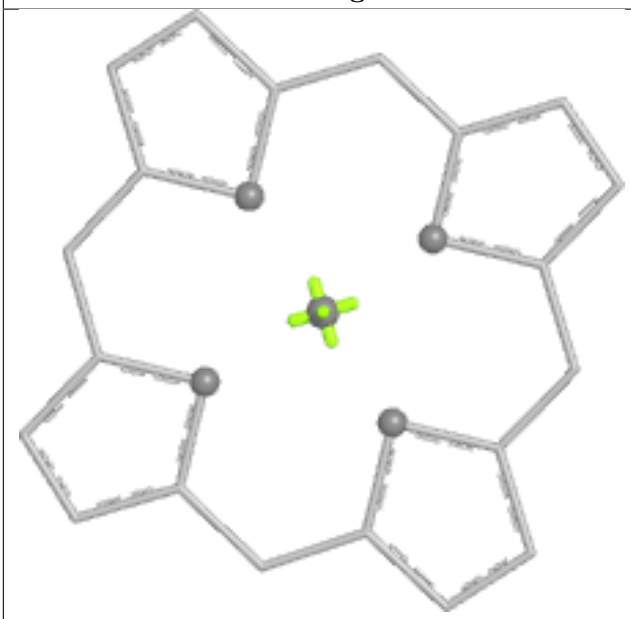
Ligand CLA G 1701



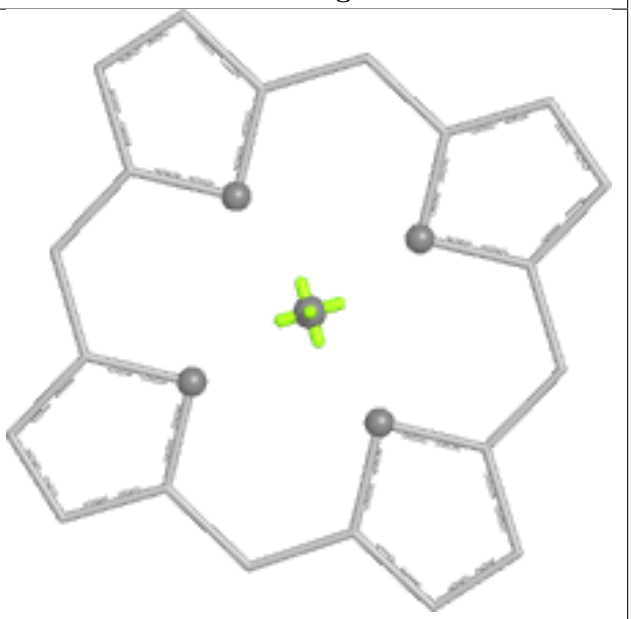
Bond lengths



Bond angles

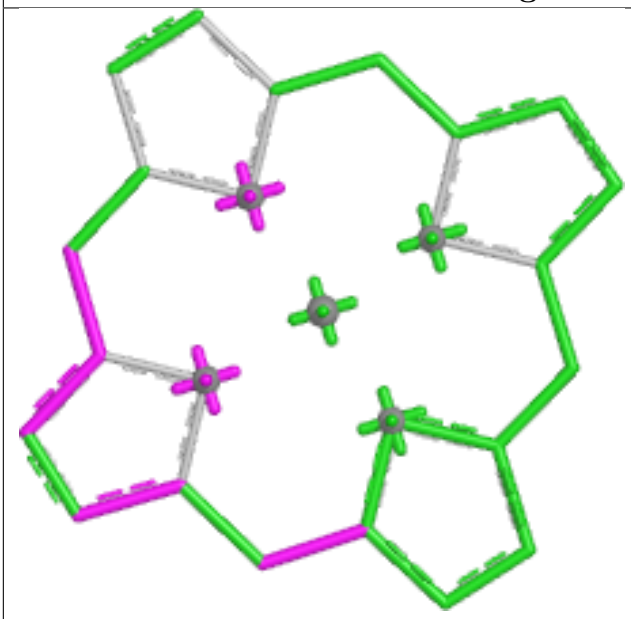


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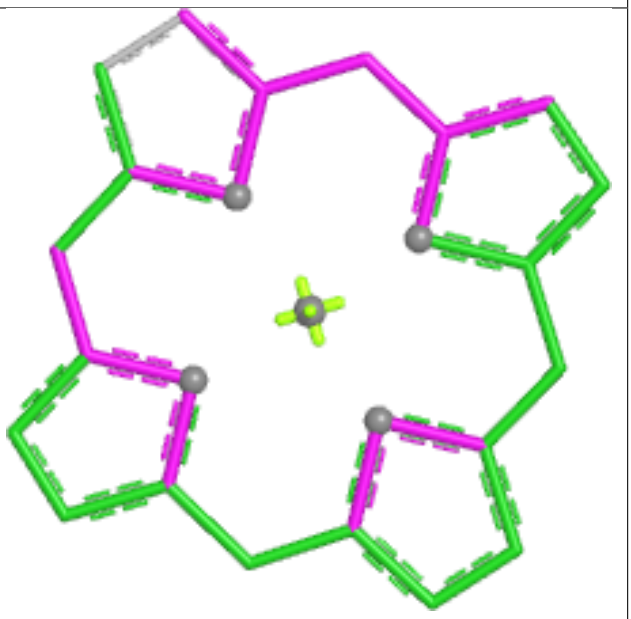


Rings

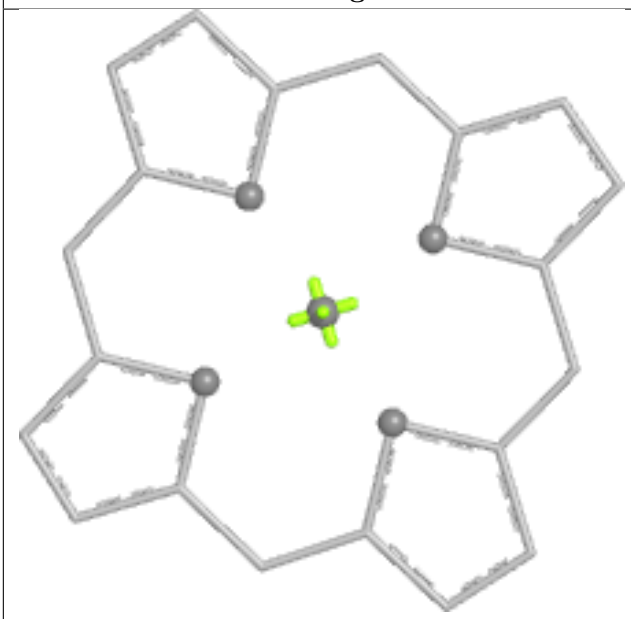
Ligand CLA 3 1031



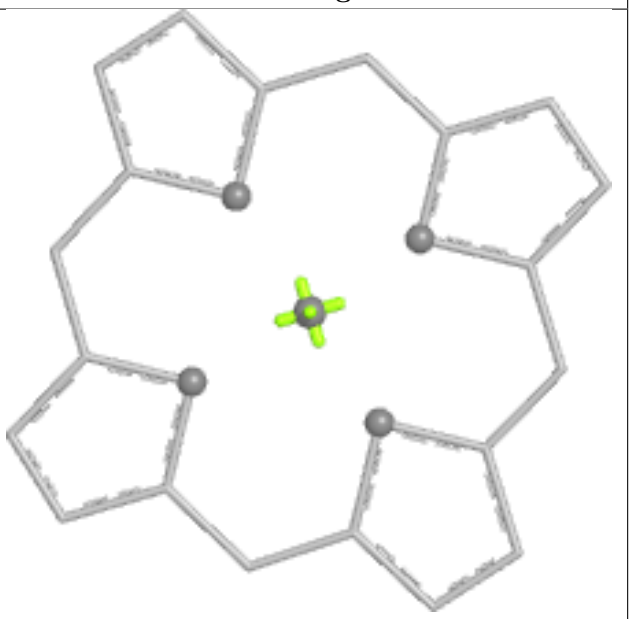
Bond lengths



Bond angles

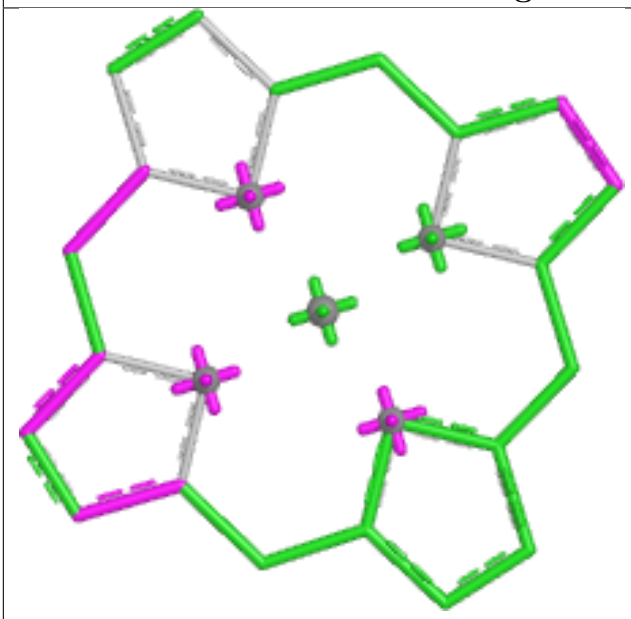


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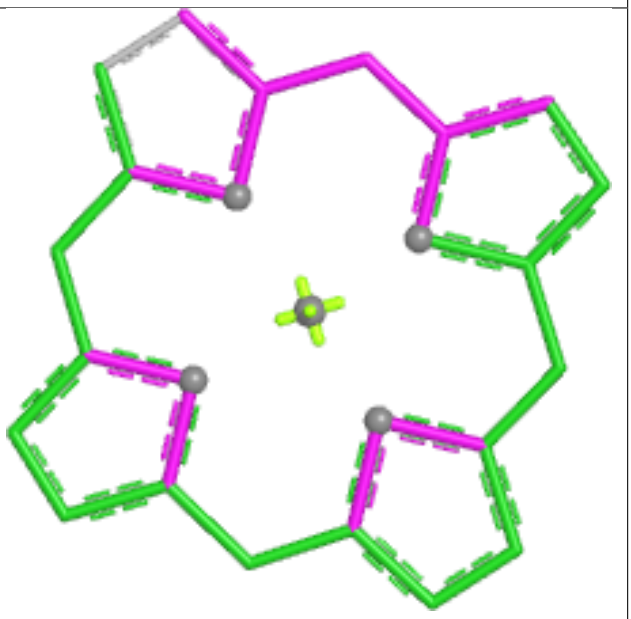


Rings

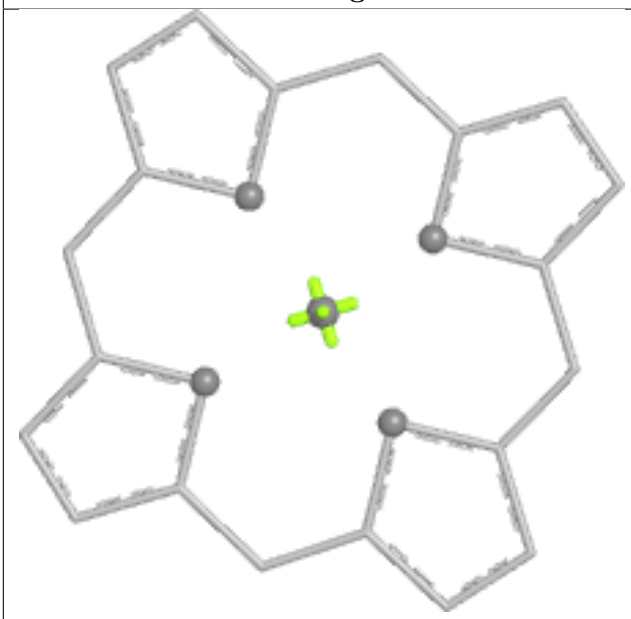
Ligand CLA A 1127



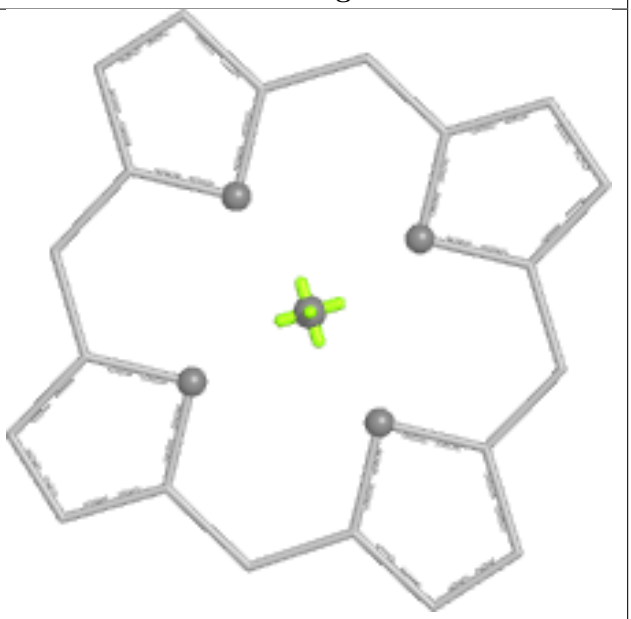
Bond lengths



Bond angles

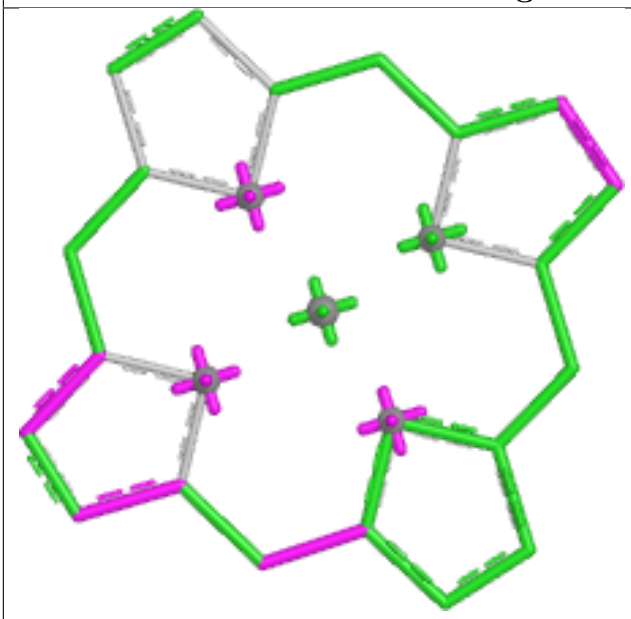


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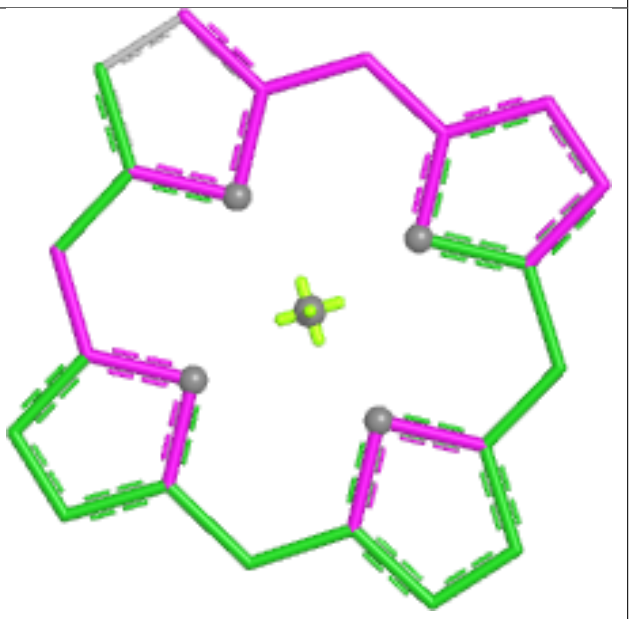


Rings

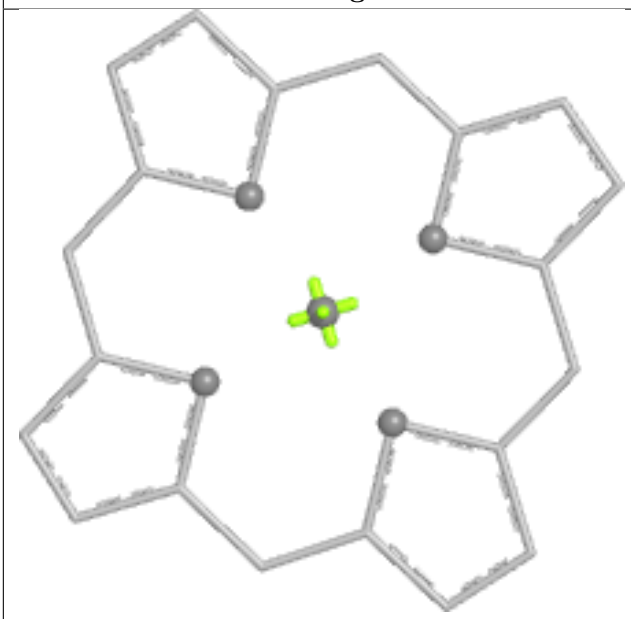
Ligand CLA P 5128



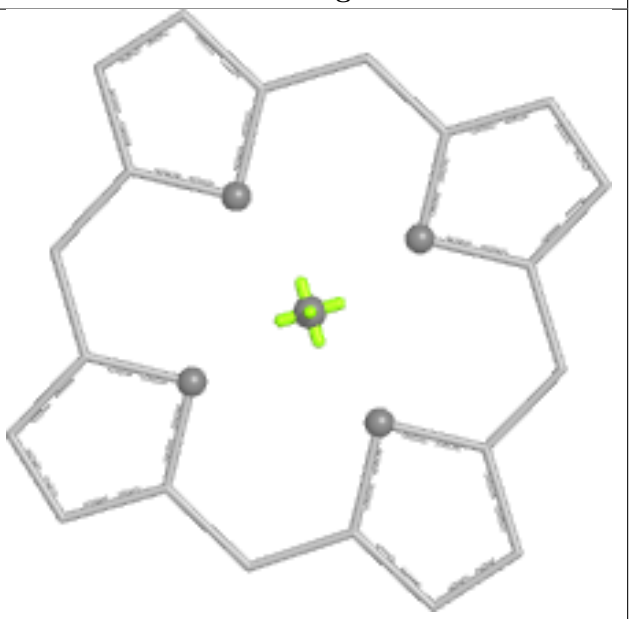
Bond lengths



Bond angles

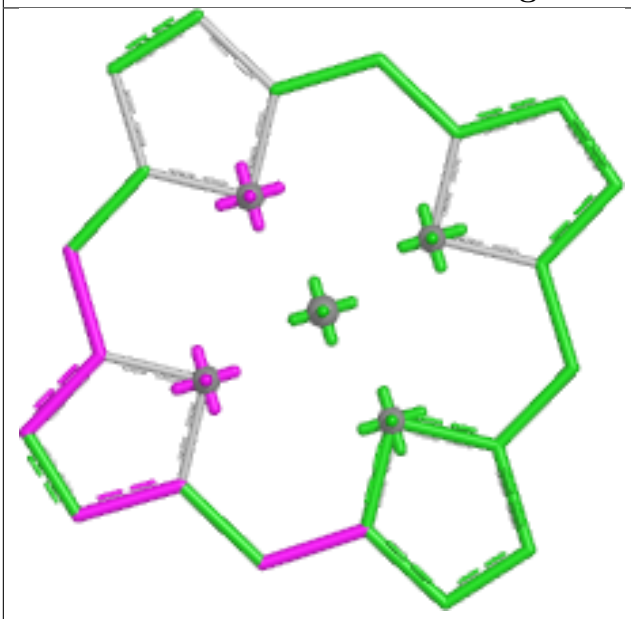


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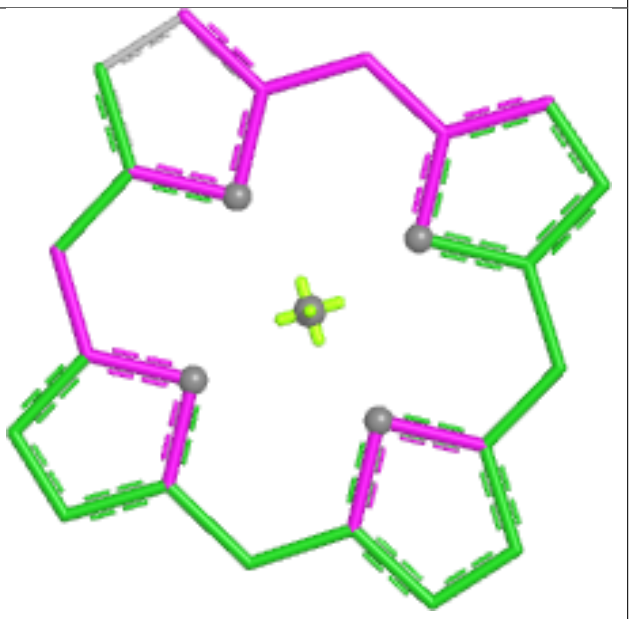


Rings

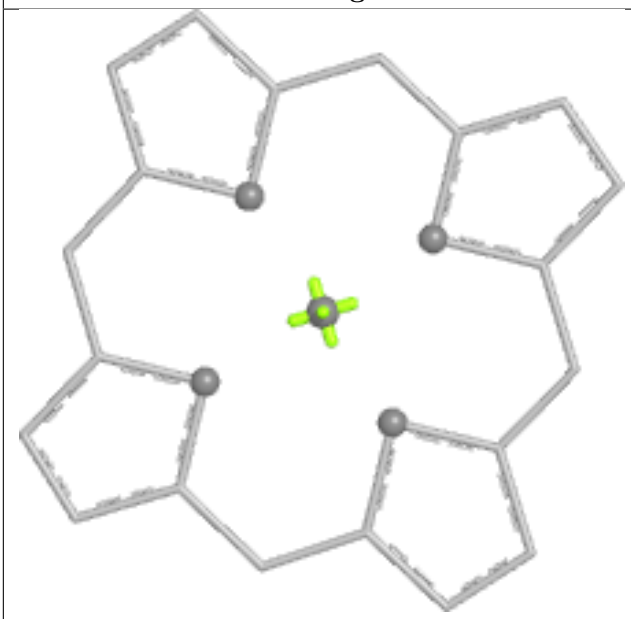
Ligand CLA 7 1016



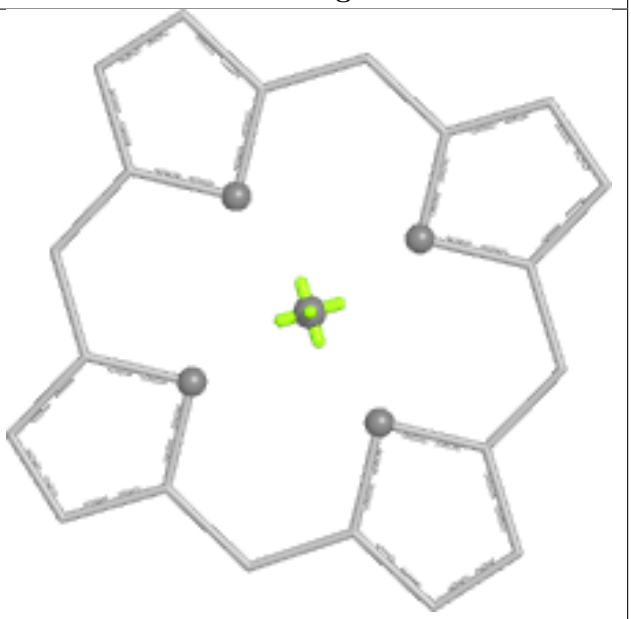
Bond lengths



Bond angles

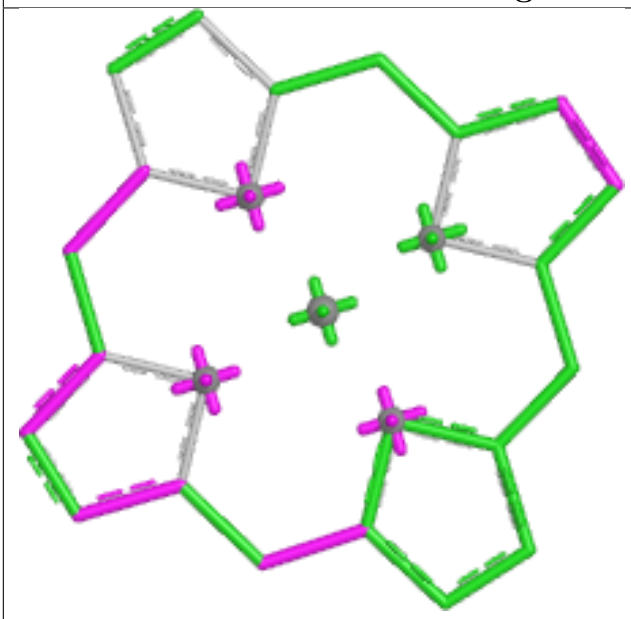


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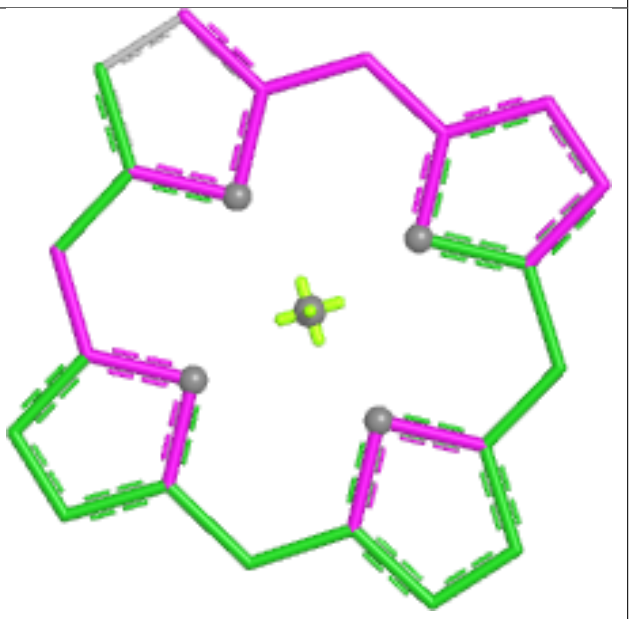


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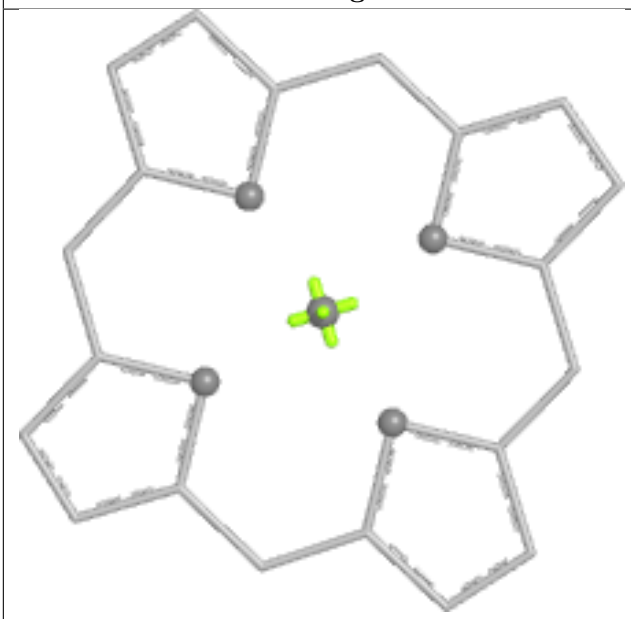
Ligand CLA B 1223



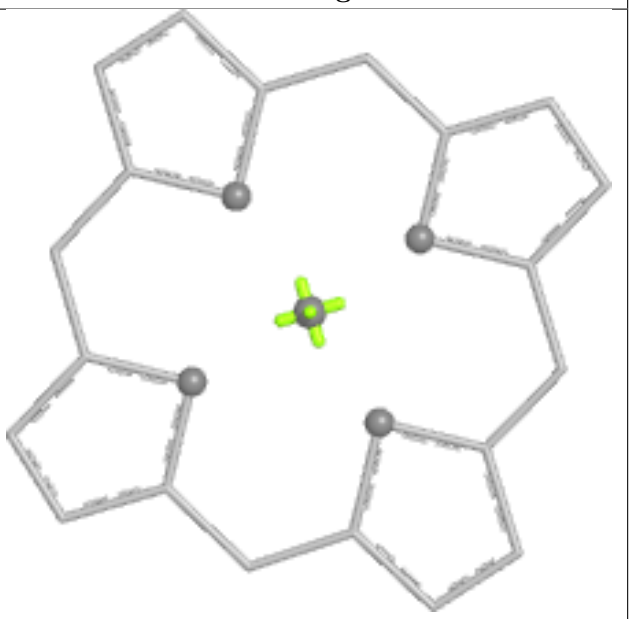
Bond lengths



Bond angles

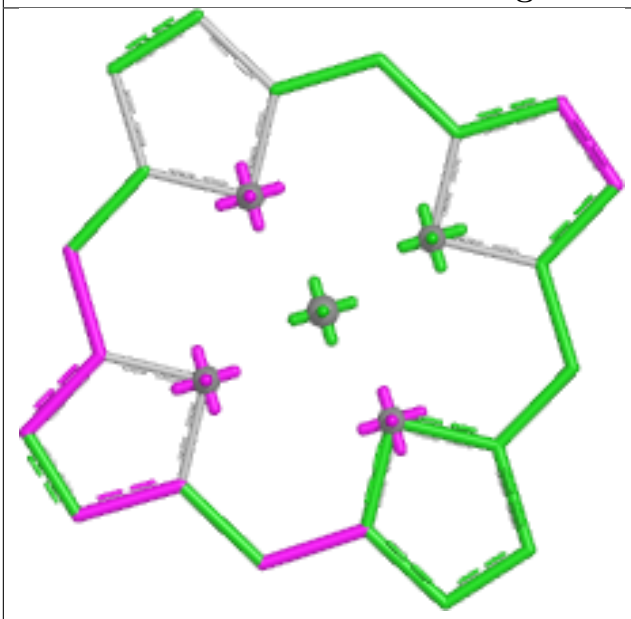


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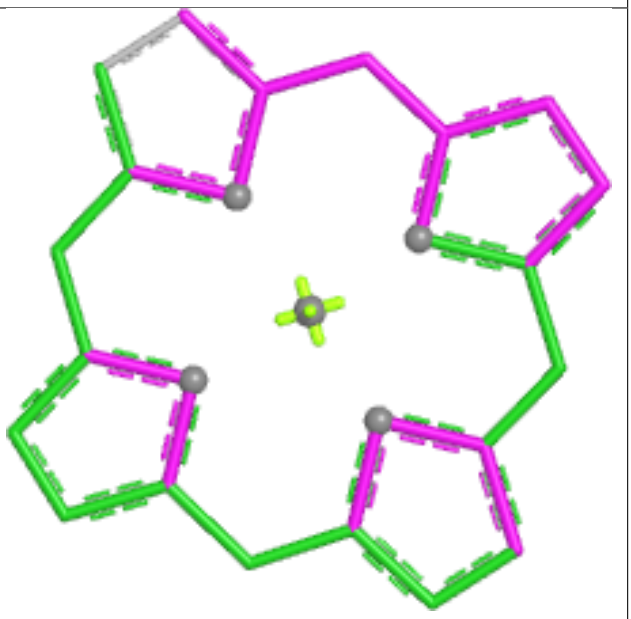


Rings

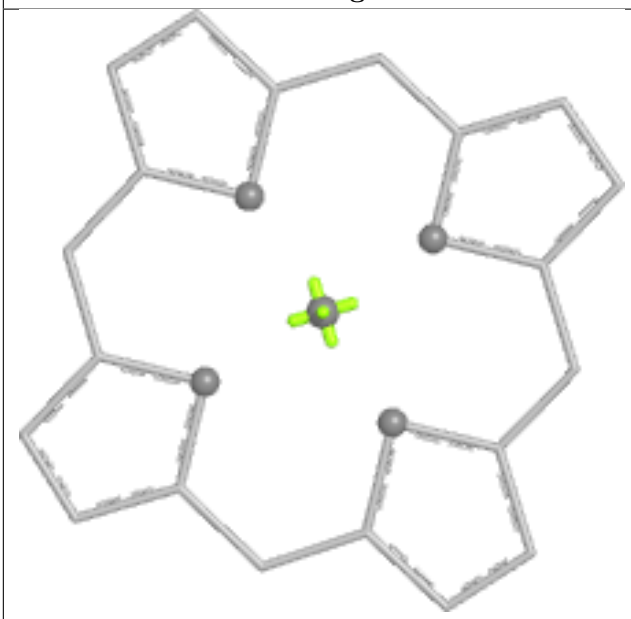
Ligand CLA P 5111



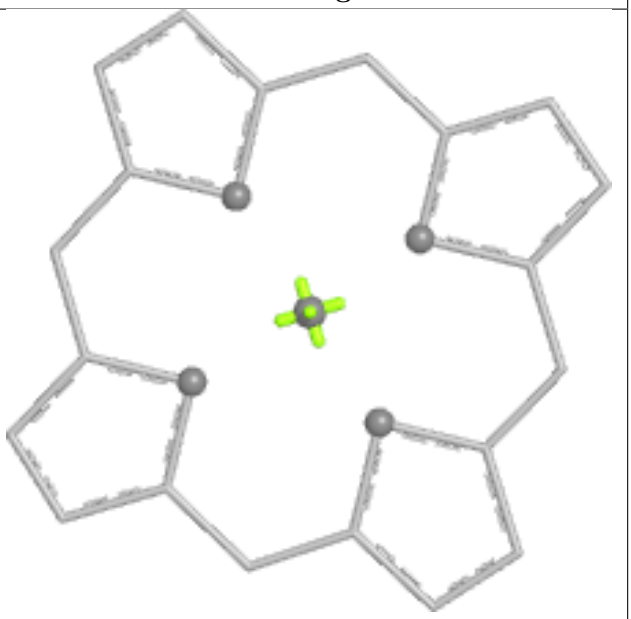
Bond lengths



Bond angles

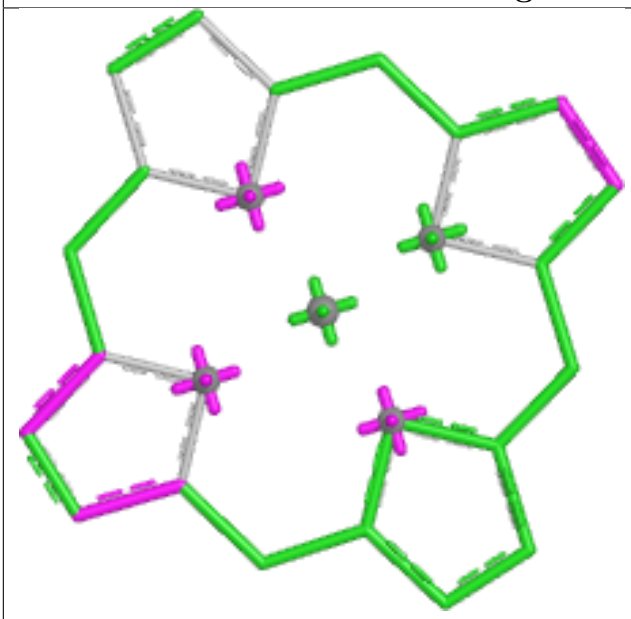


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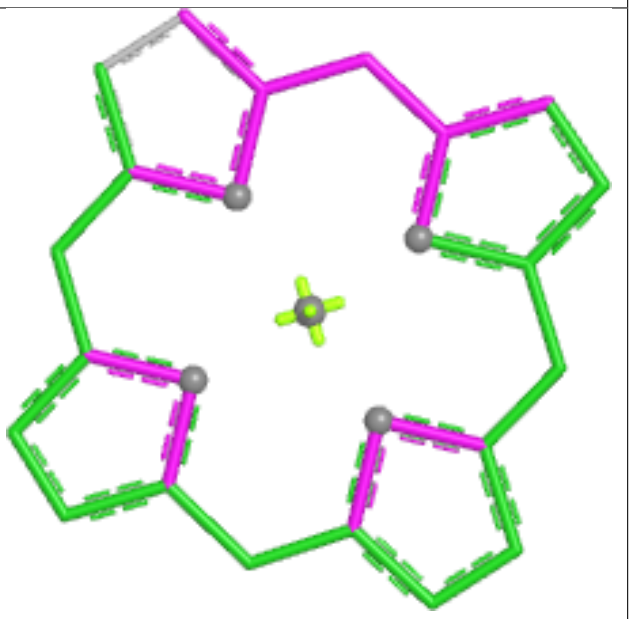


Rings

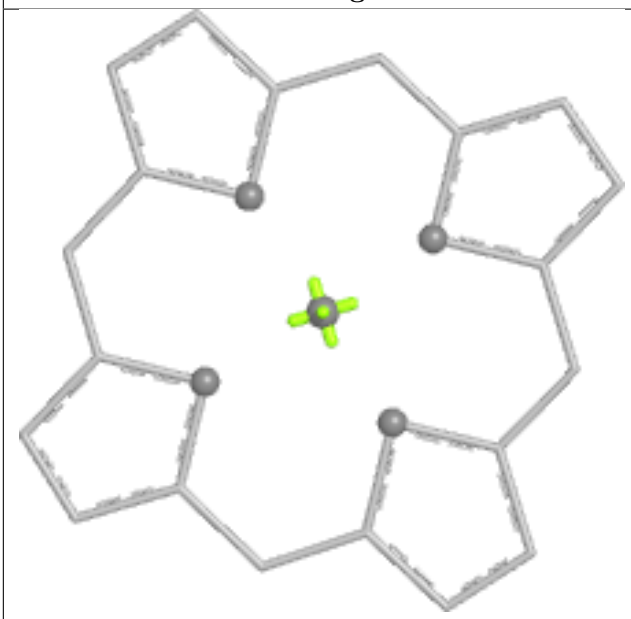
Ligand CLA B 1222



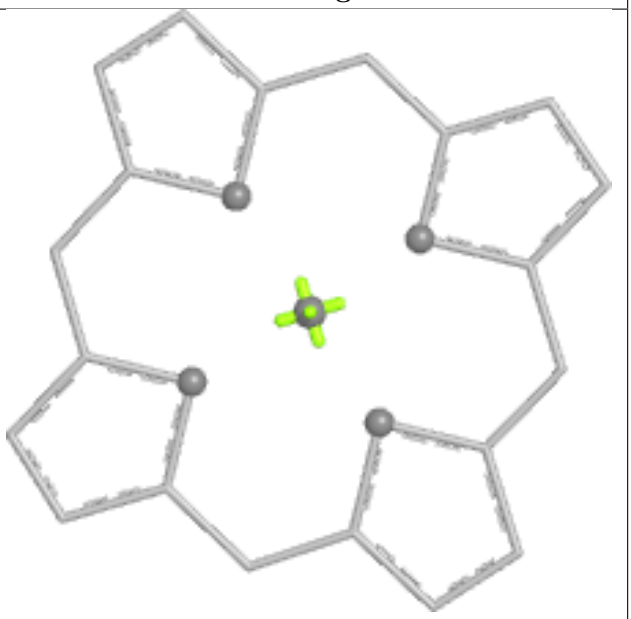
Bond lengths



Bond angles

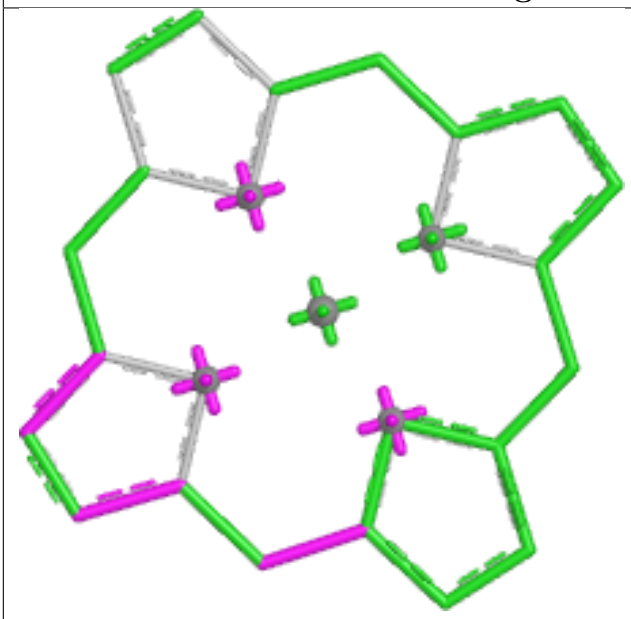


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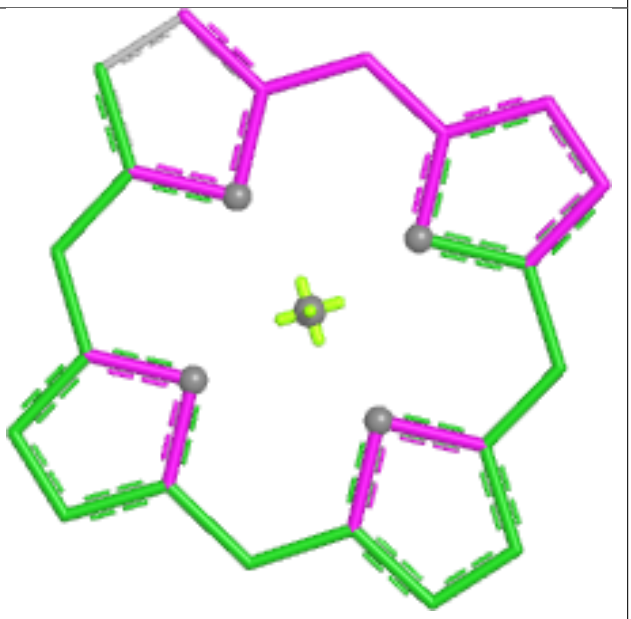


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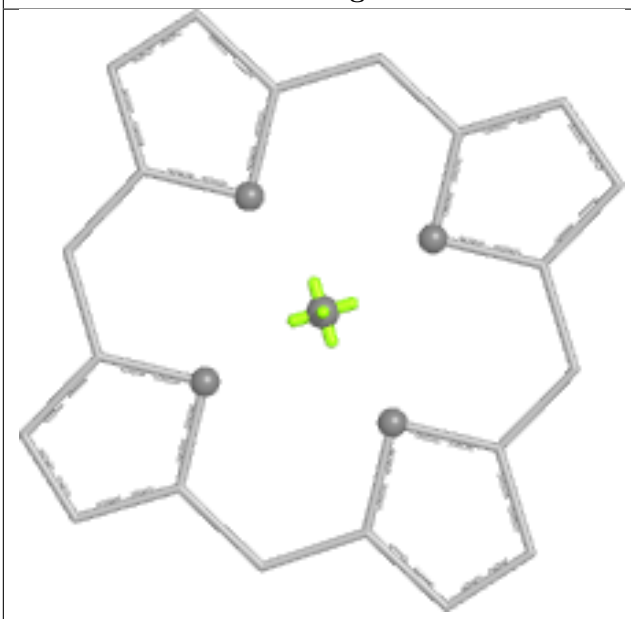
Ligand CLA A 1140



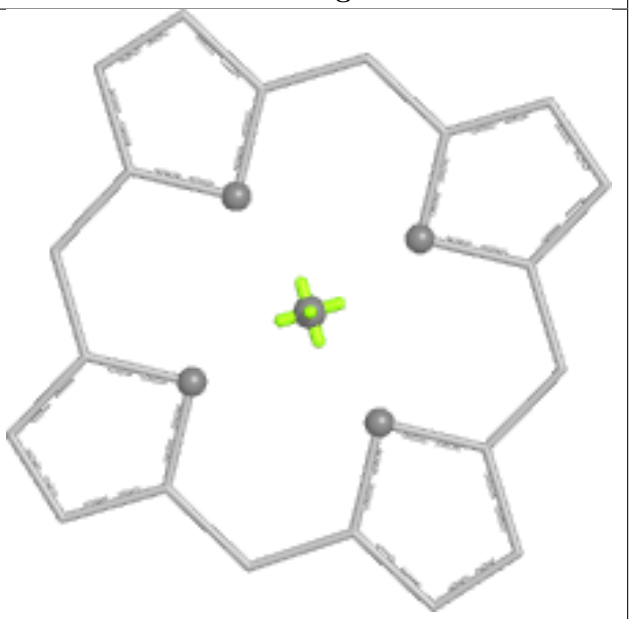
Bond lengths



Bond angles

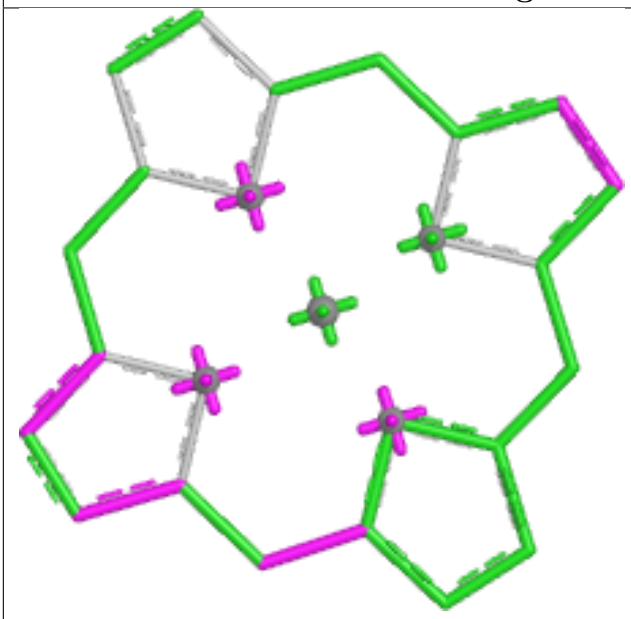


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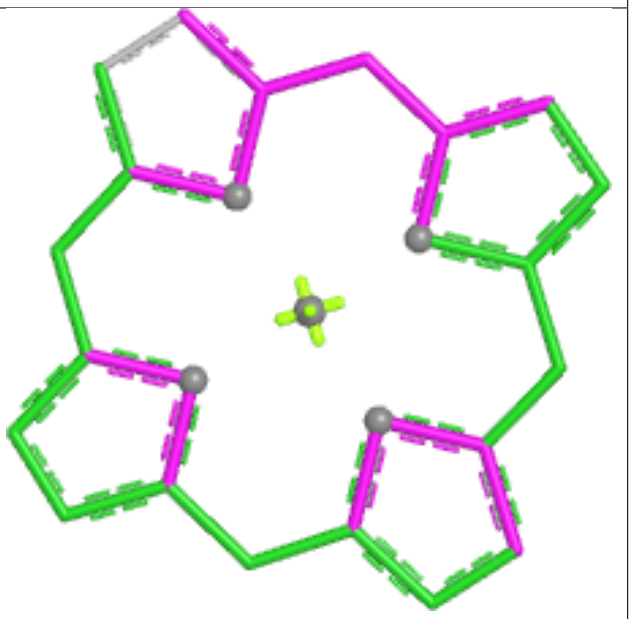


Rings

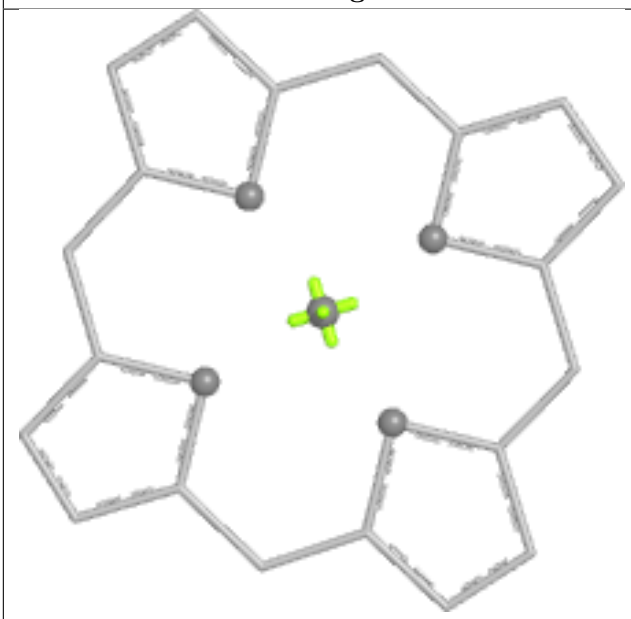
Ligand CLA P 5116



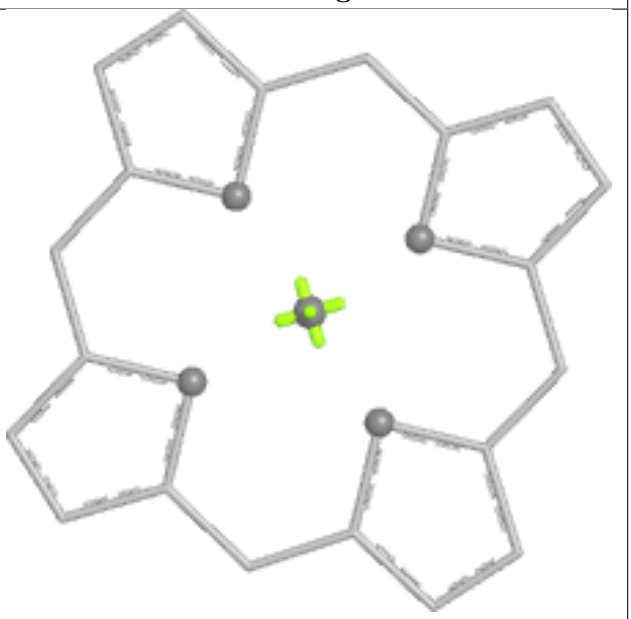
Bond lengths



Bond angles

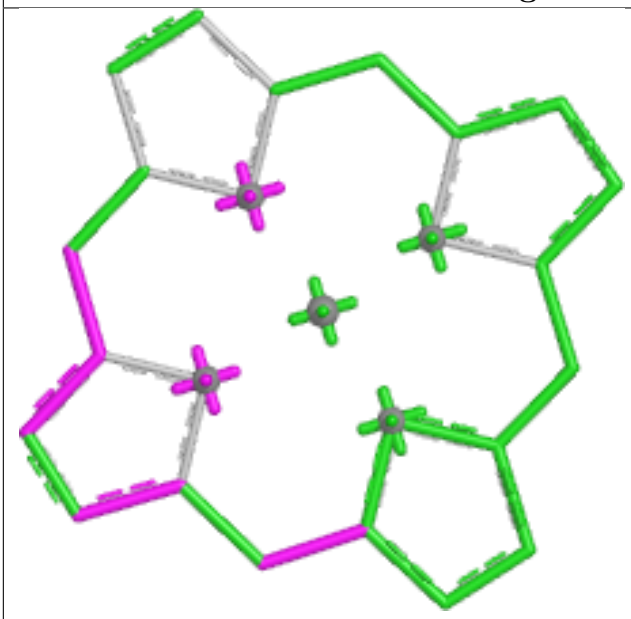


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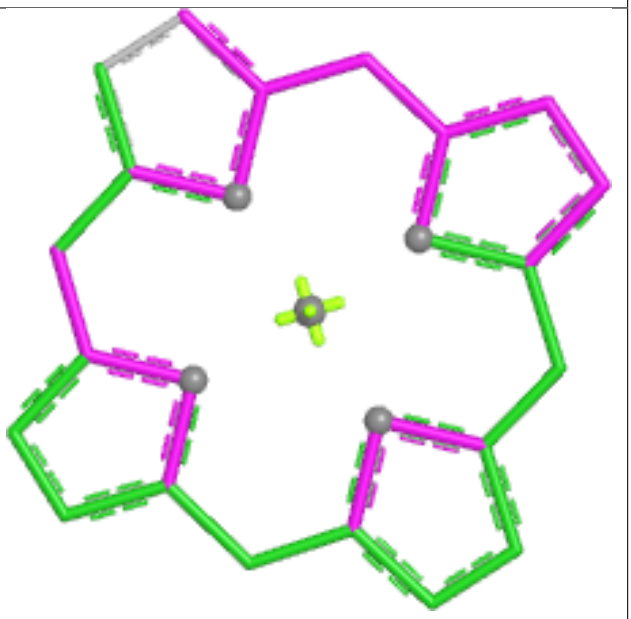


Rings

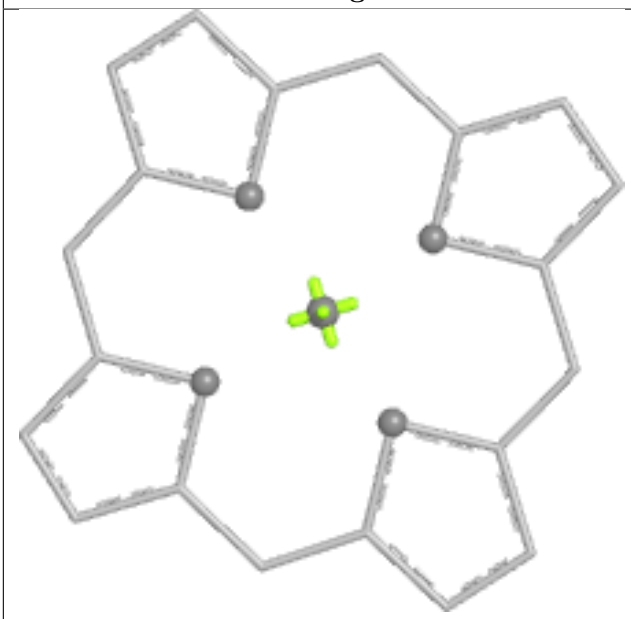
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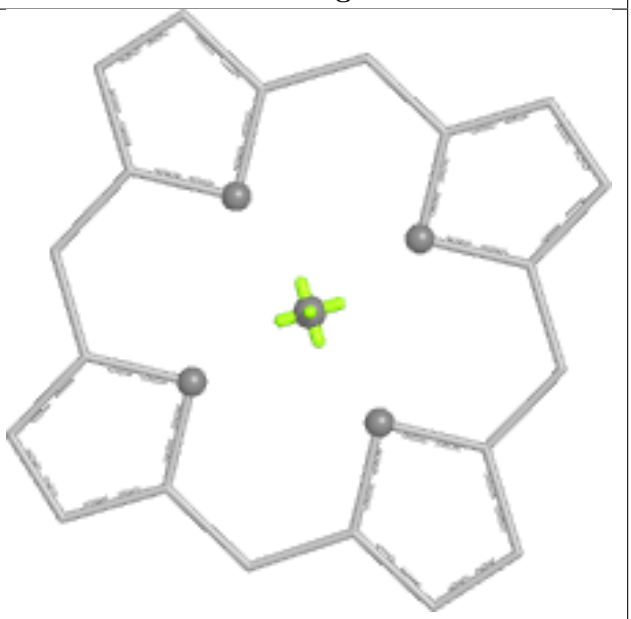
Bond lengths



Bond angles

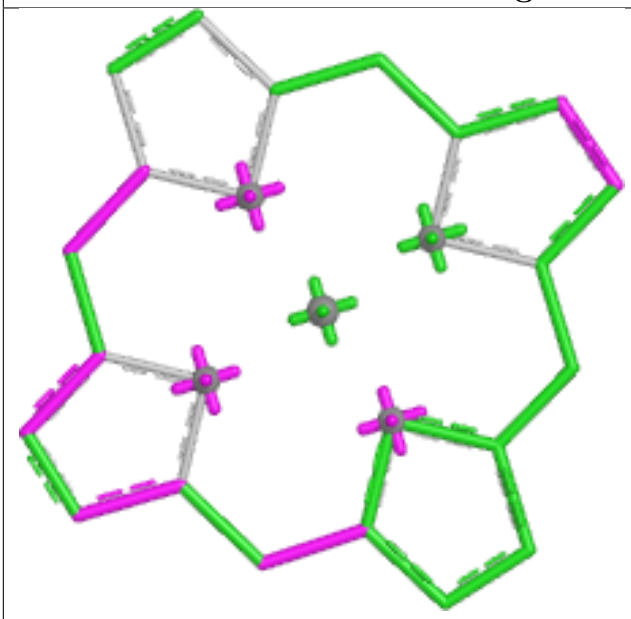


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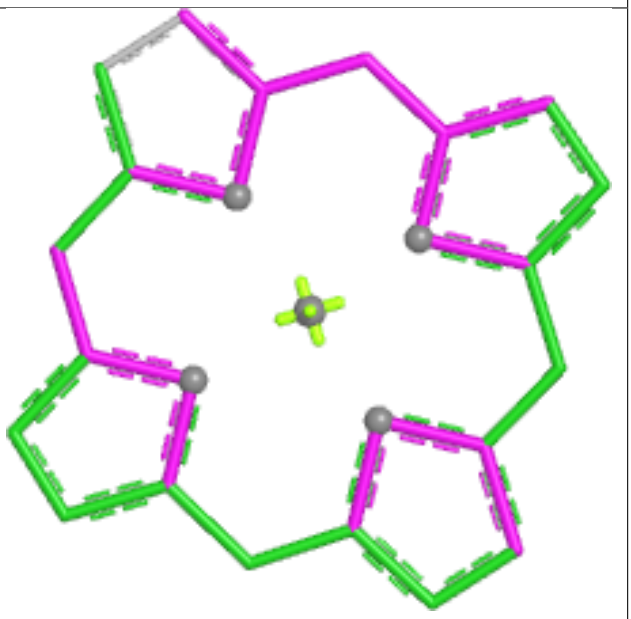


Rings

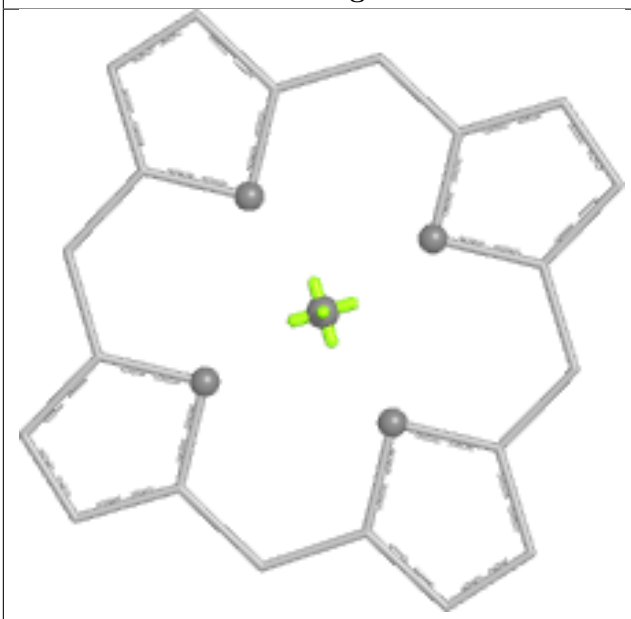
Ligand CLA B 1219



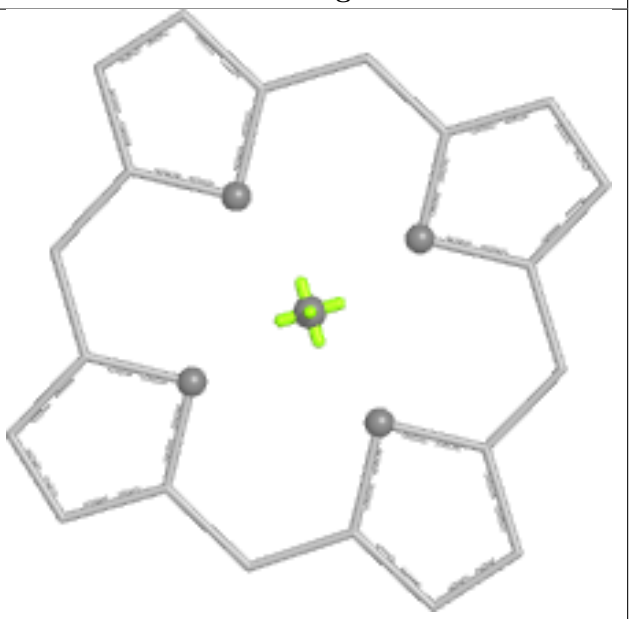
Bond lengths



Bond angles

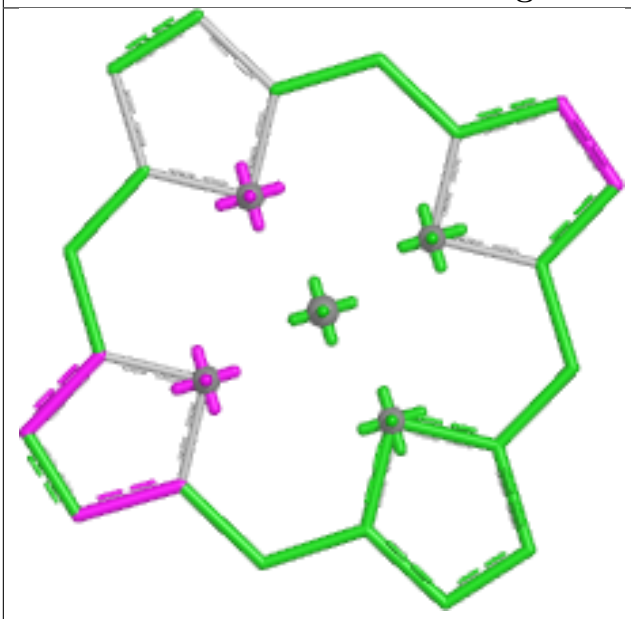


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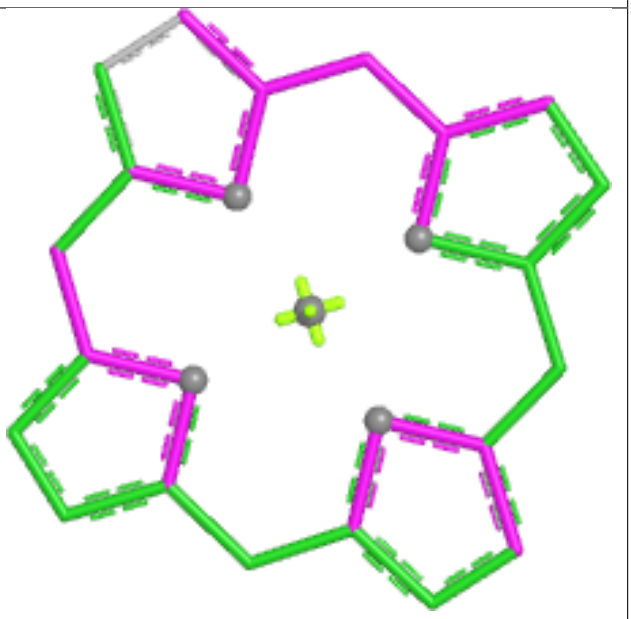


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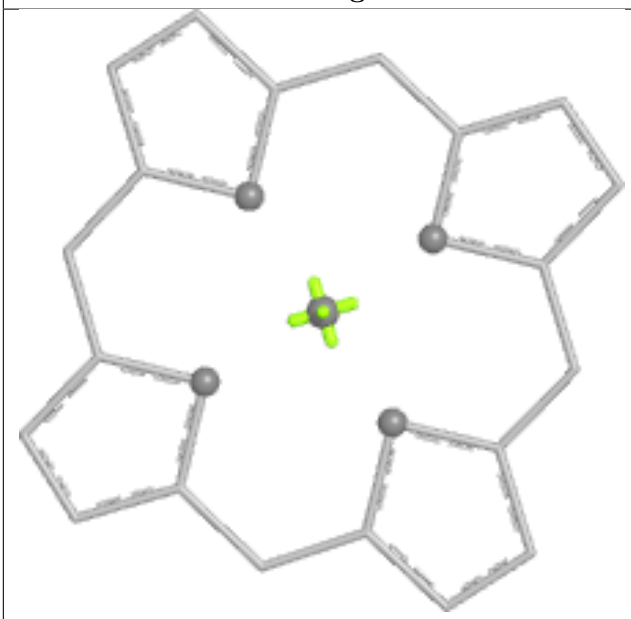
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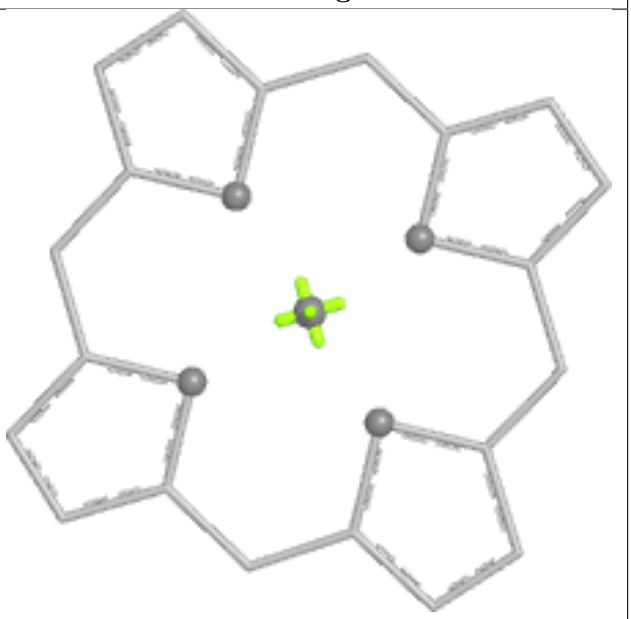
Bond lengths



Bond angles

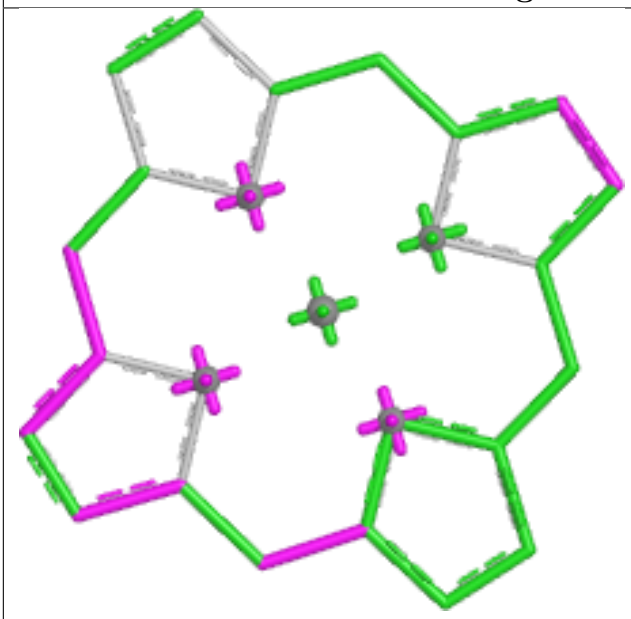


Torsions

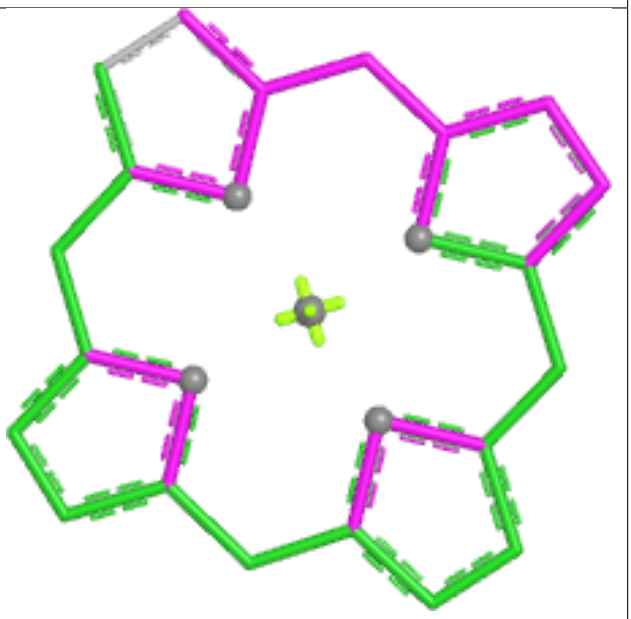


Rings

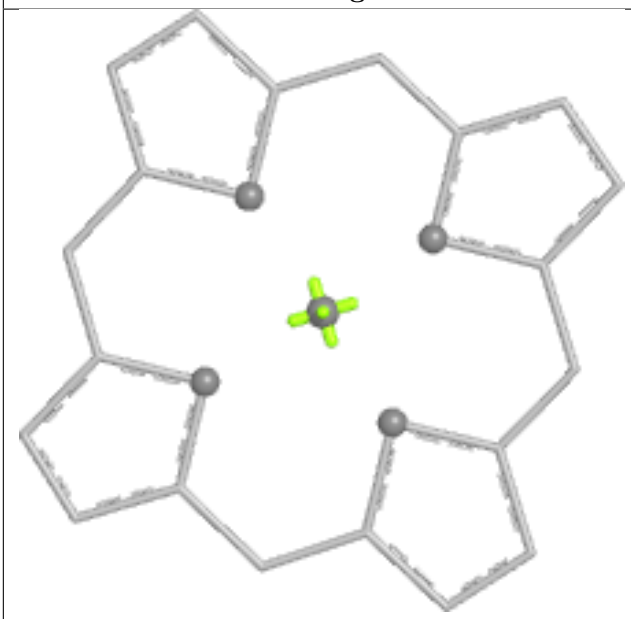
Ligand CLA P 5120



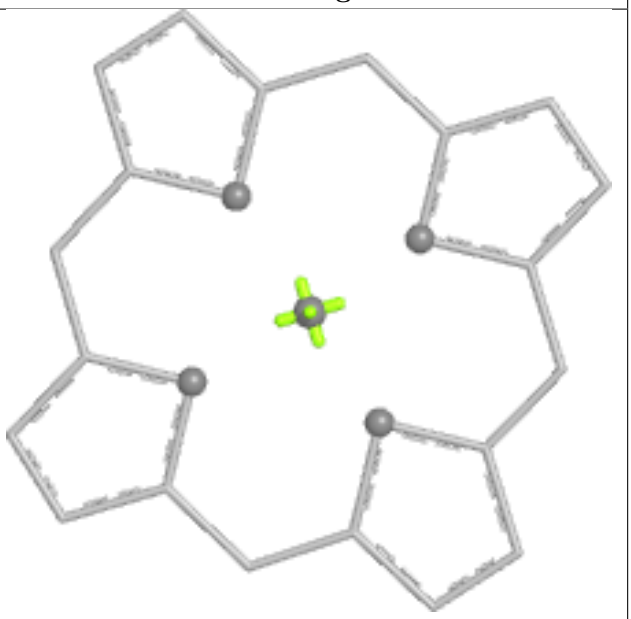
Bond lengths



Bond angles

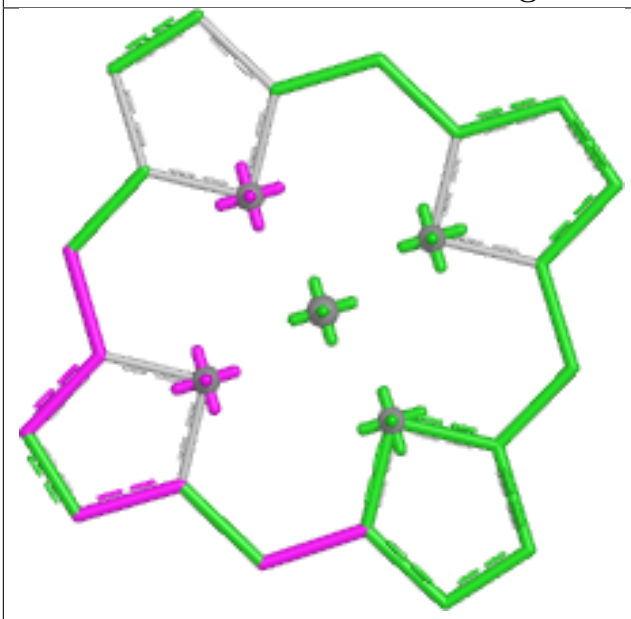


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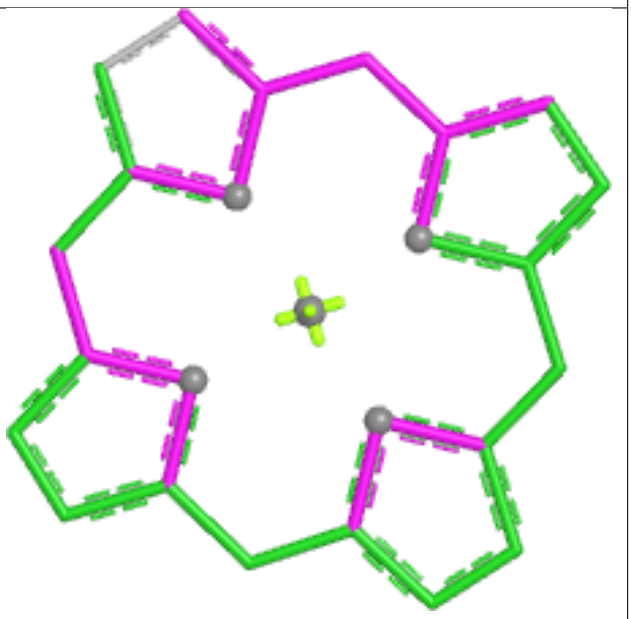


Rings

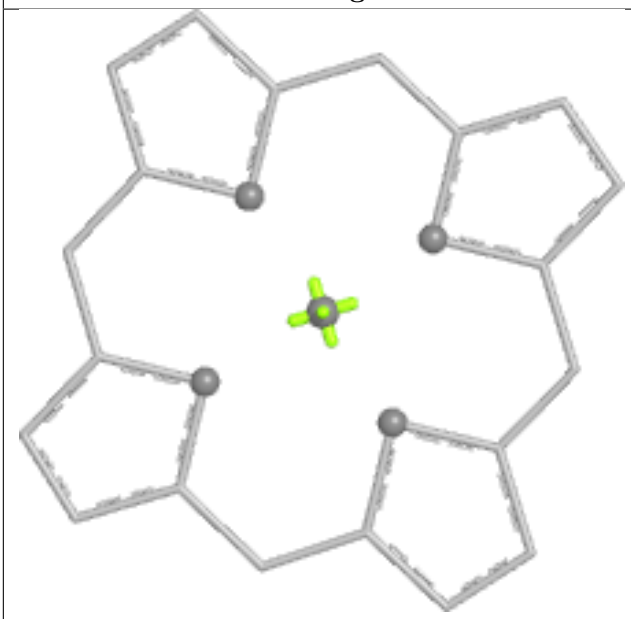
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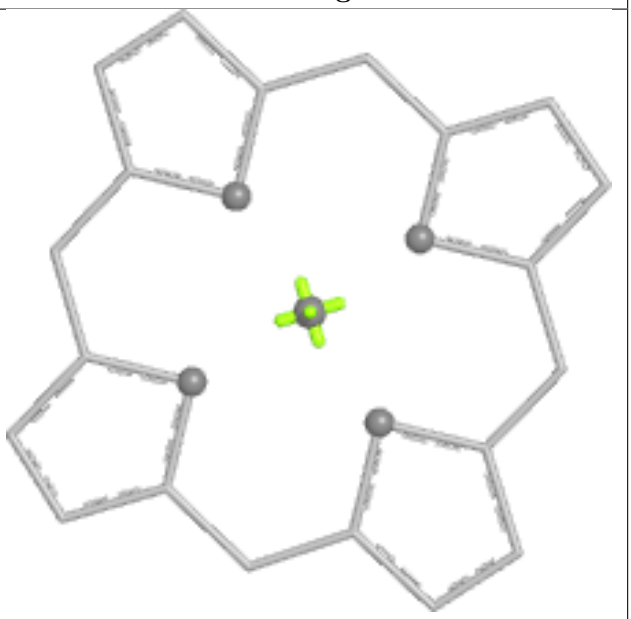
Bond lengths



Bond angles

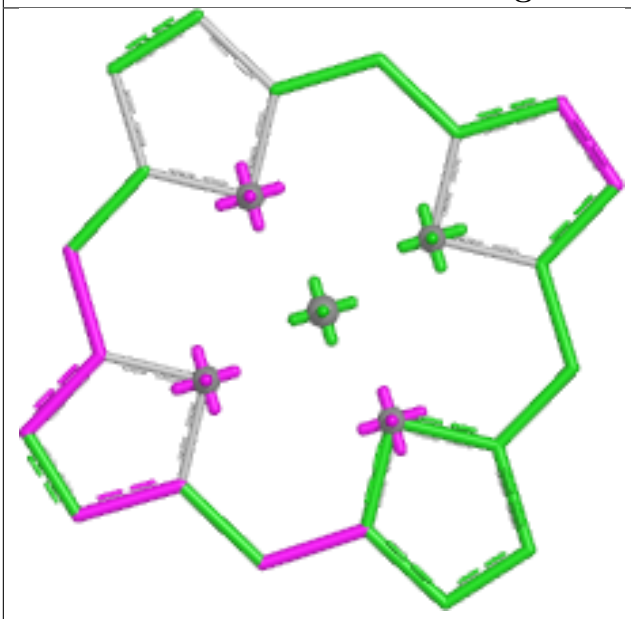


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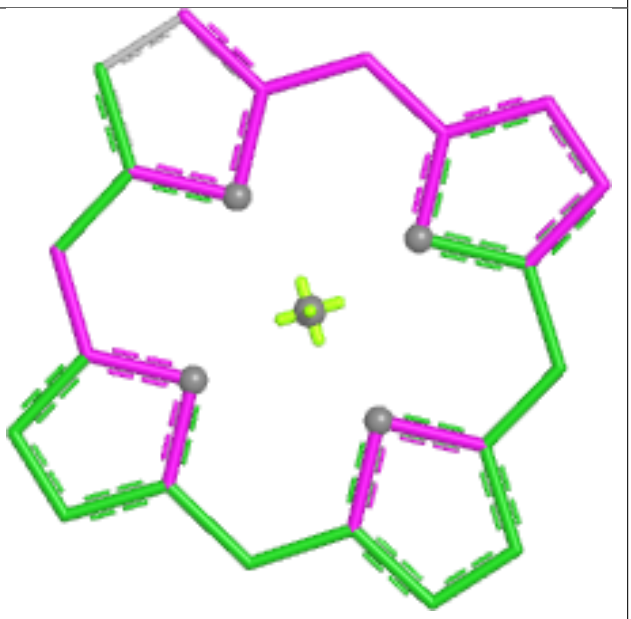


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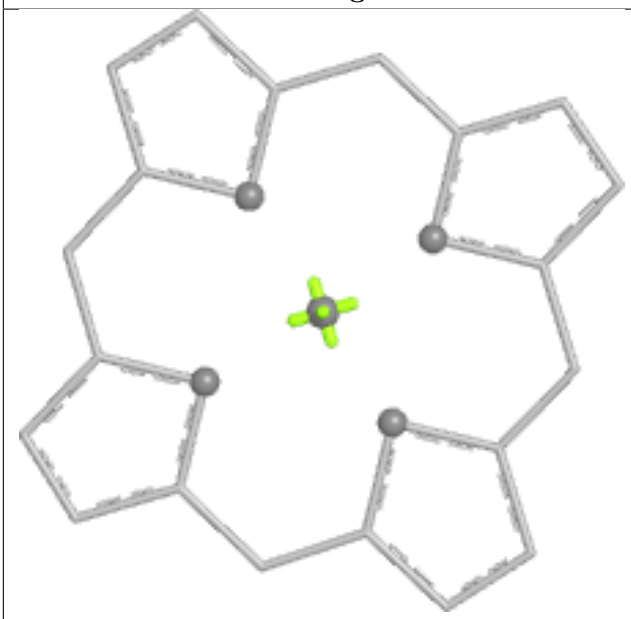
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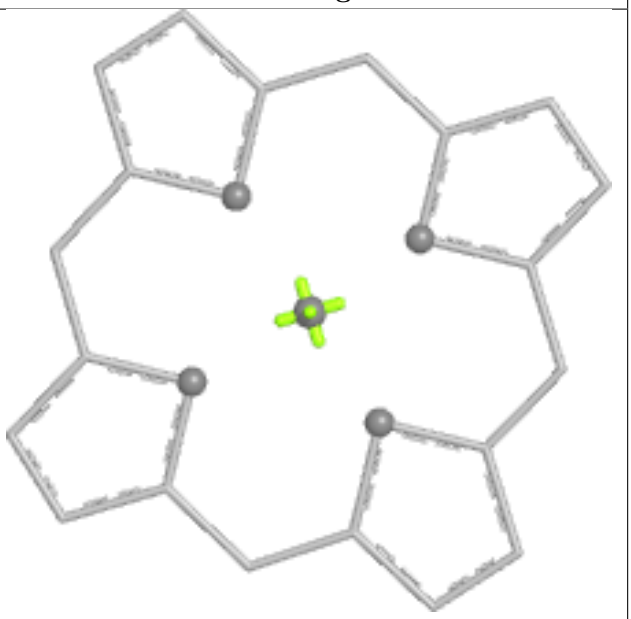
Bond lengths



Bond angles

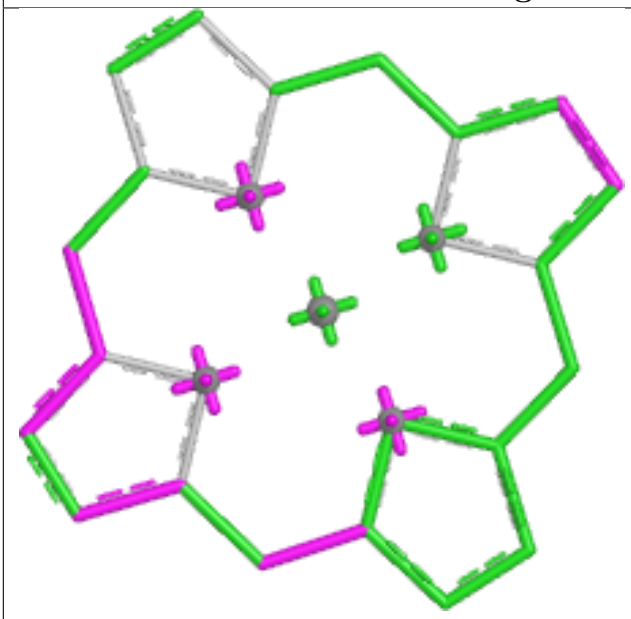


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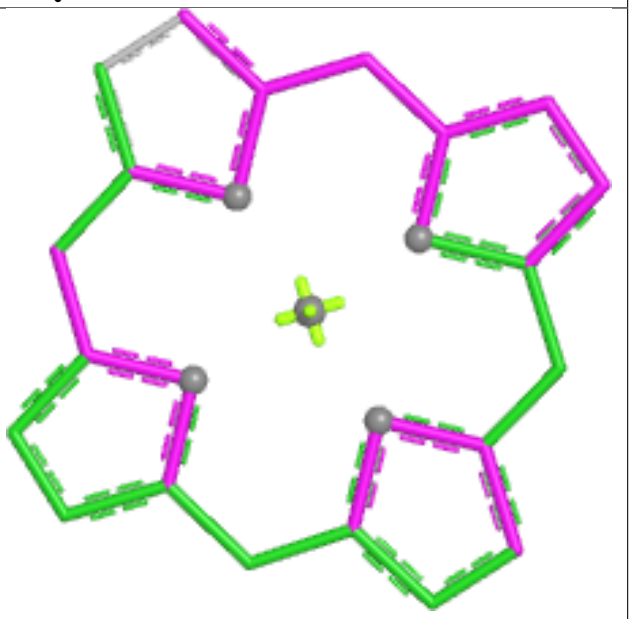


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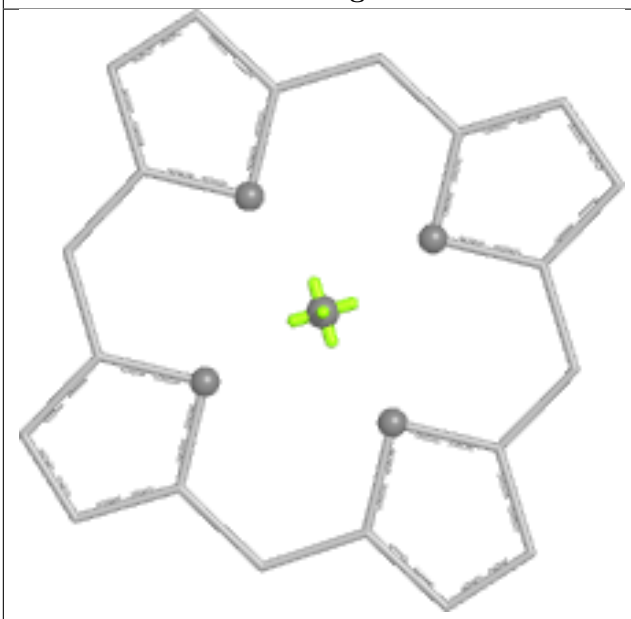
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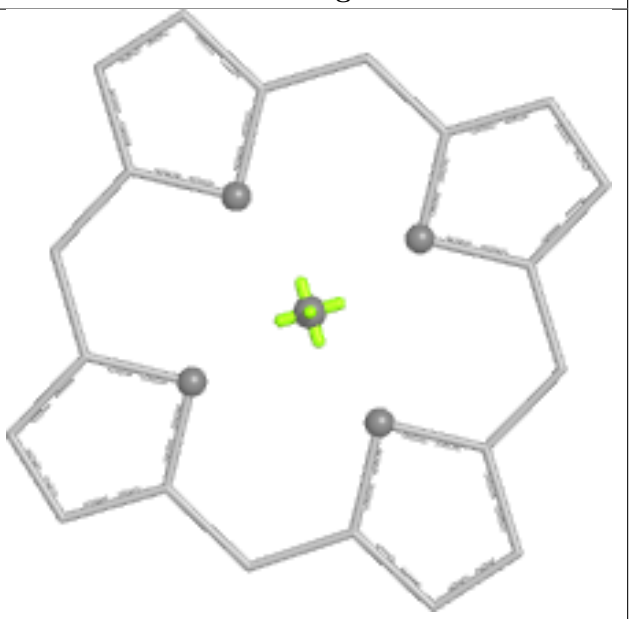
Bond lengths



Bond angles

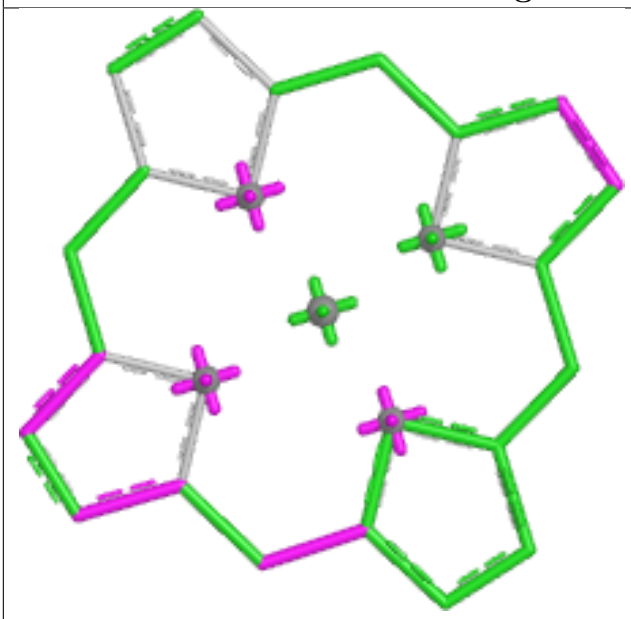


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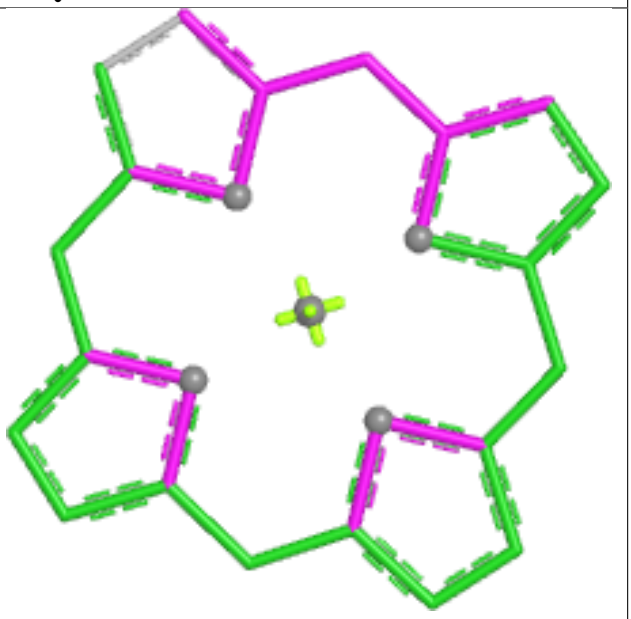


Rings

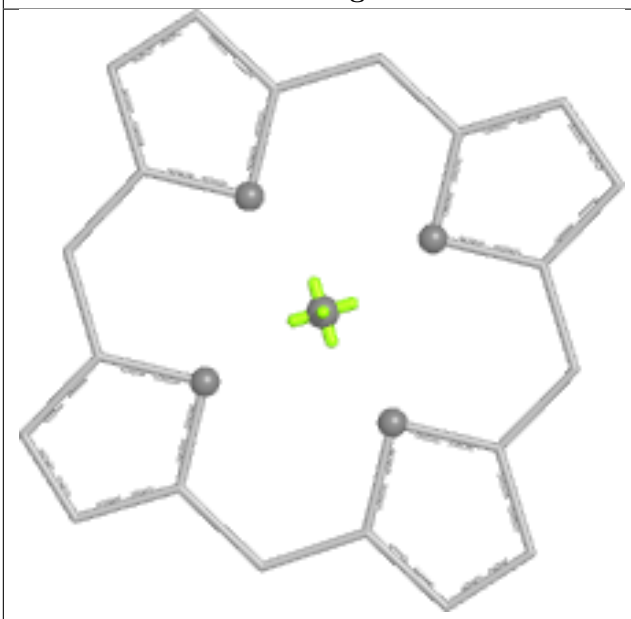
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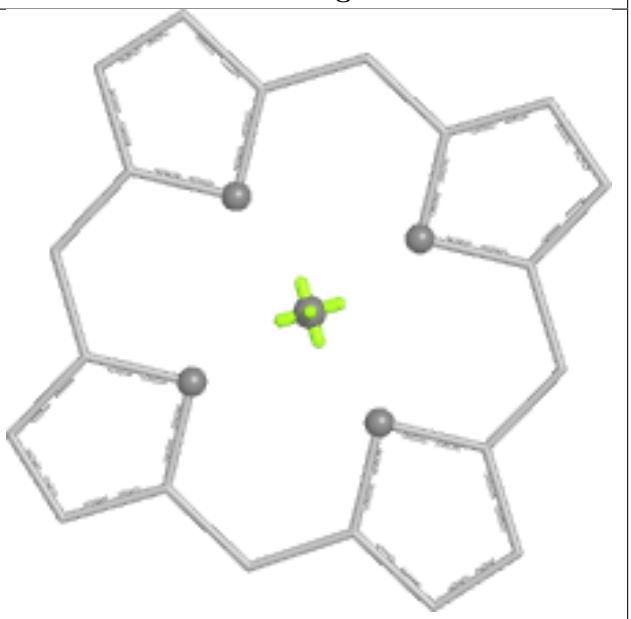
Bond lengths



Bond angles

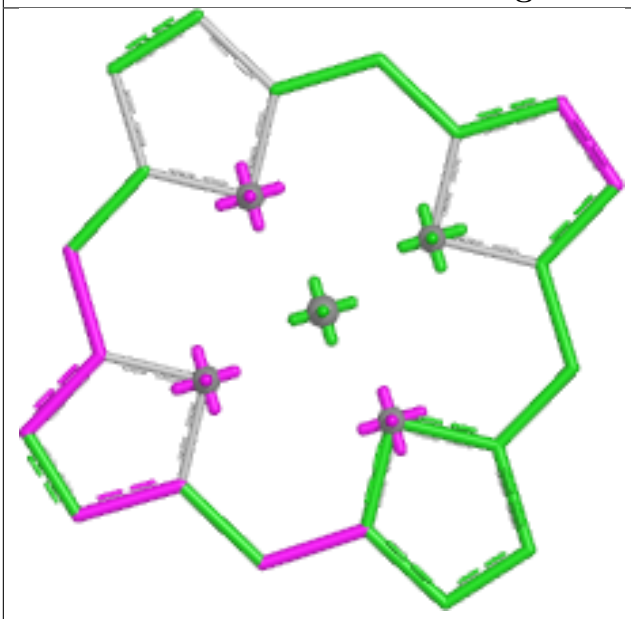


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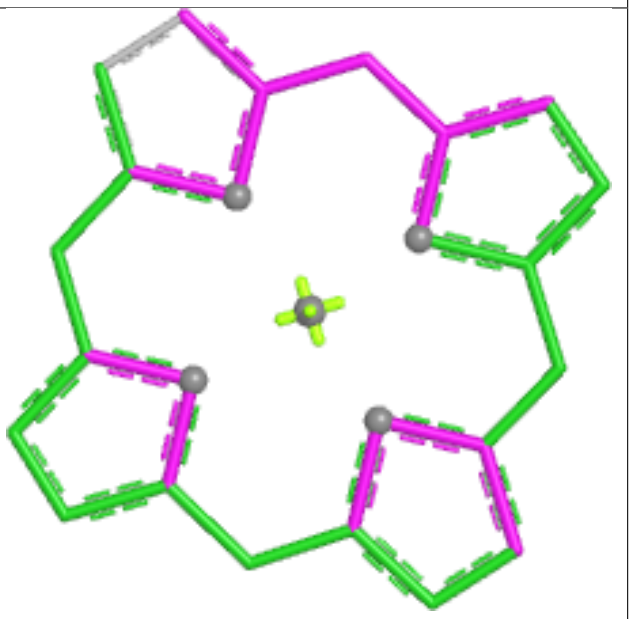


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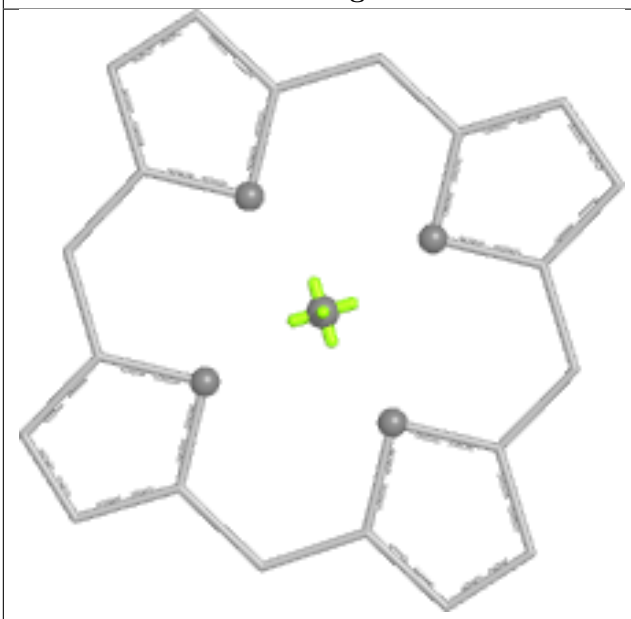
Ligand CLA B 1214



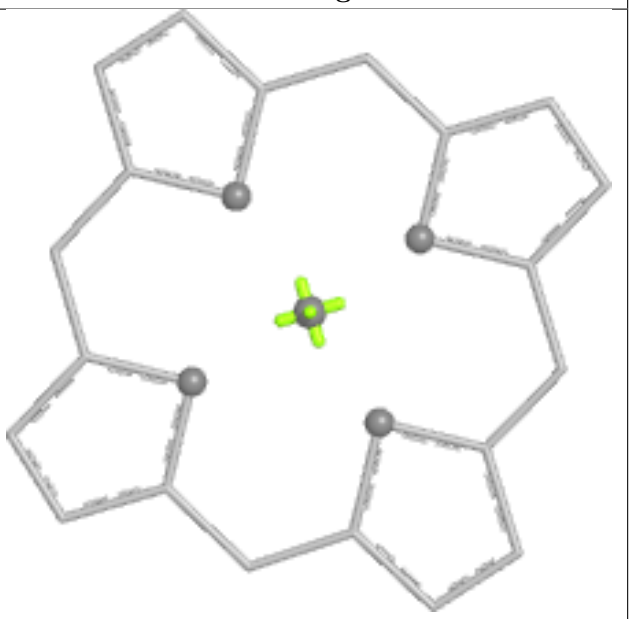
Bond lengths



Bond angles

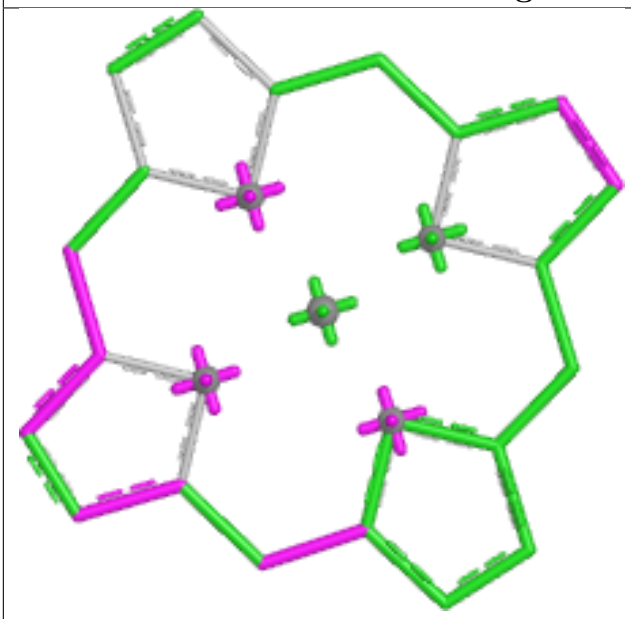


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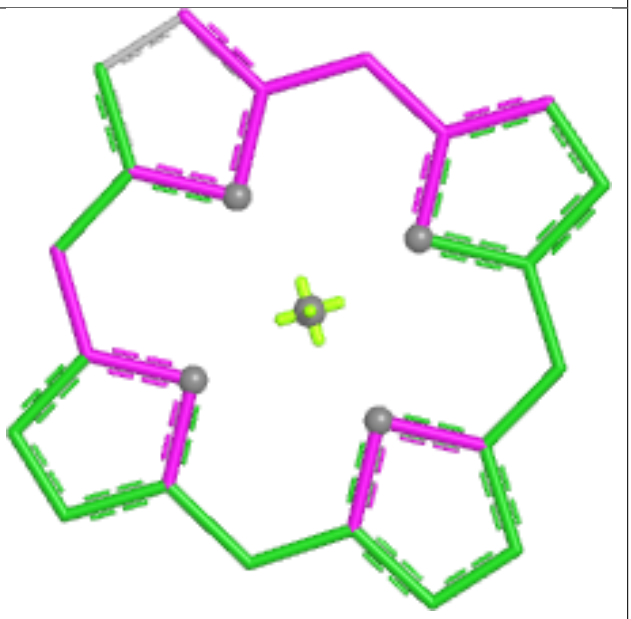


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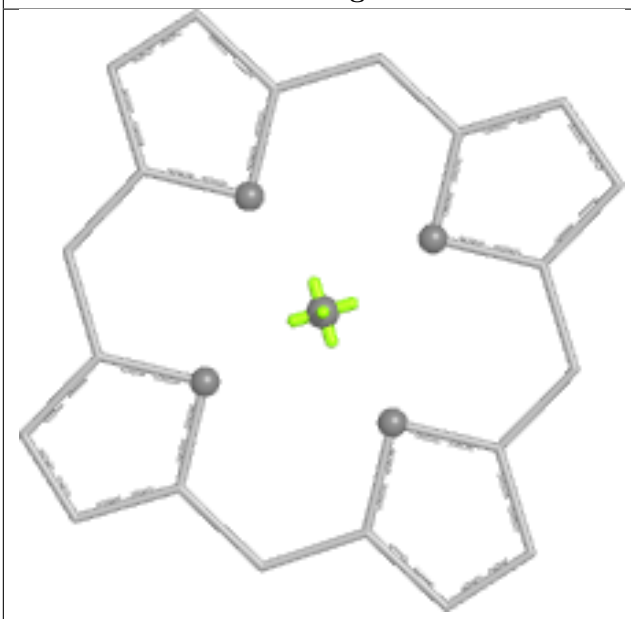
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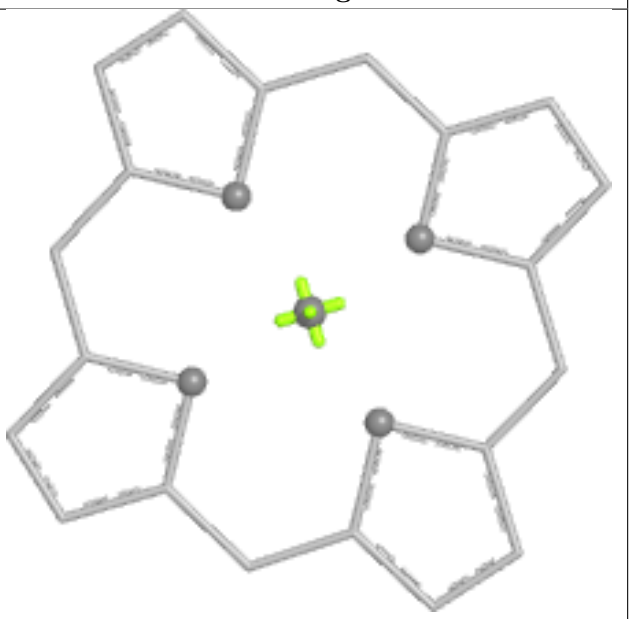
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Bond angles

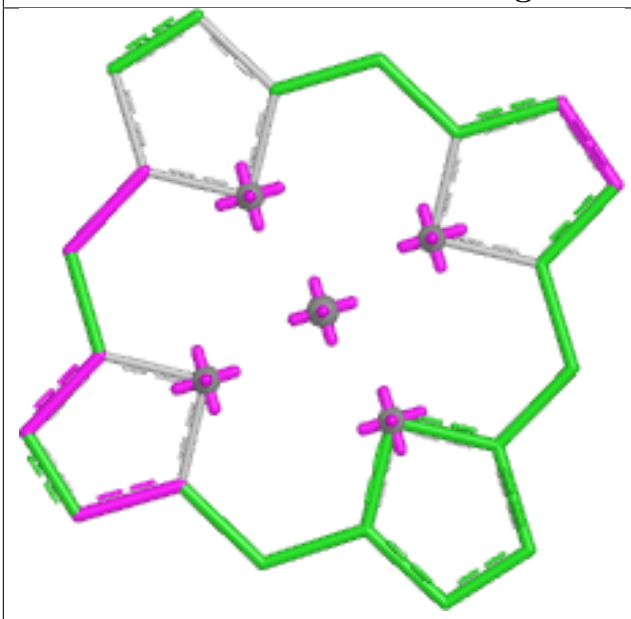


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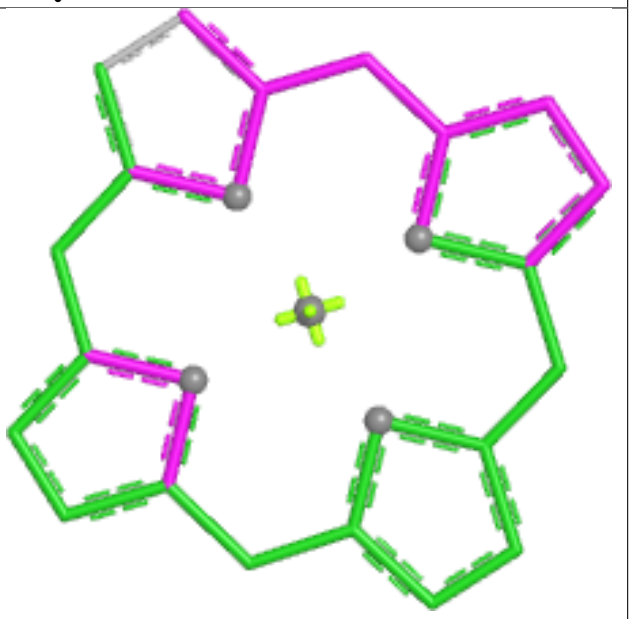


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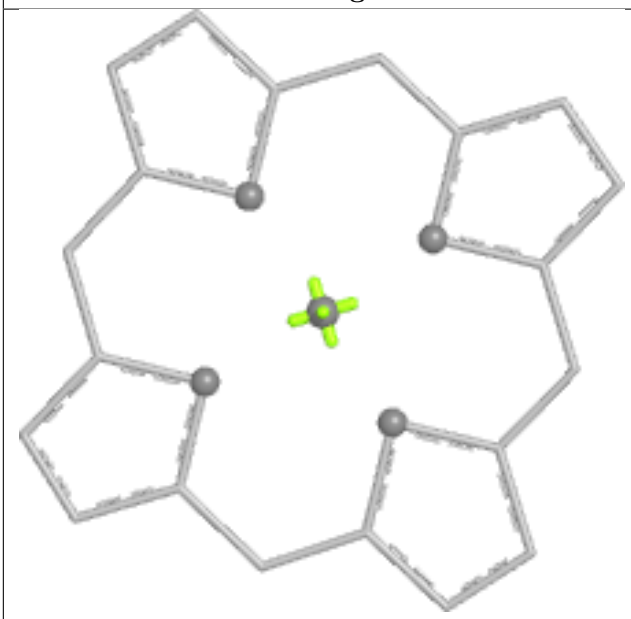
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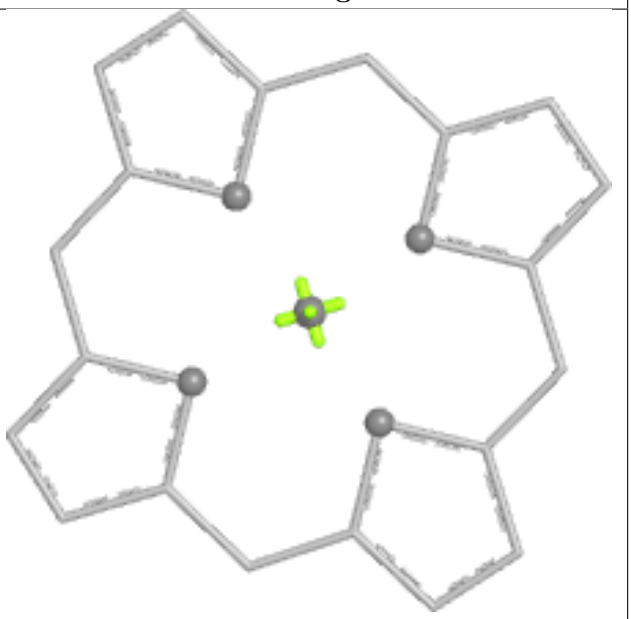
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Bond angles

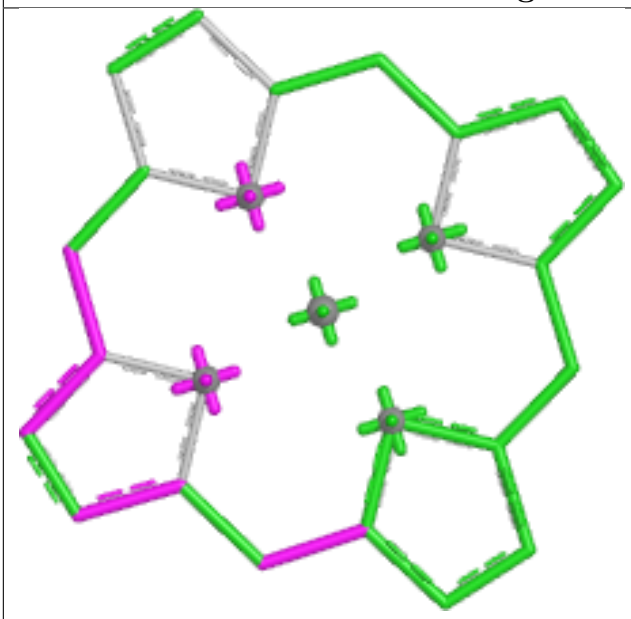


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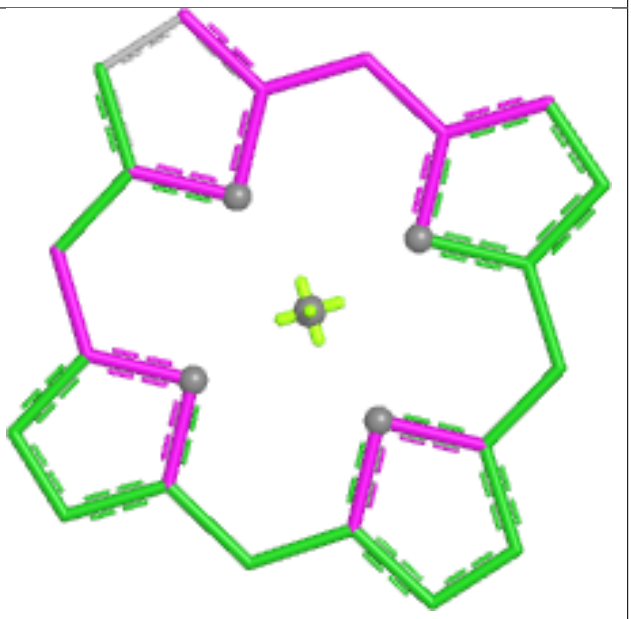


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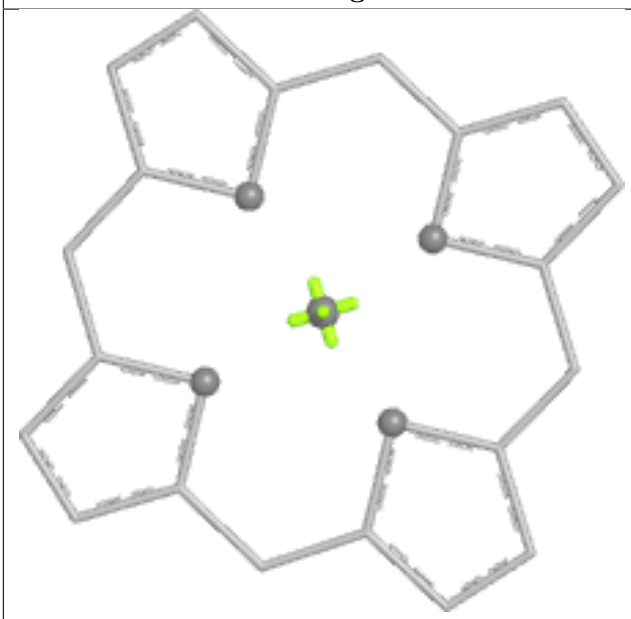
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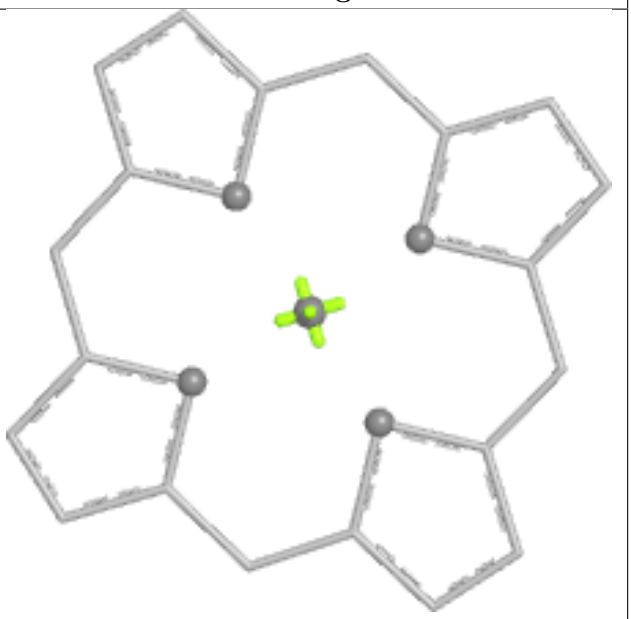
Bond lengths



Bond angles

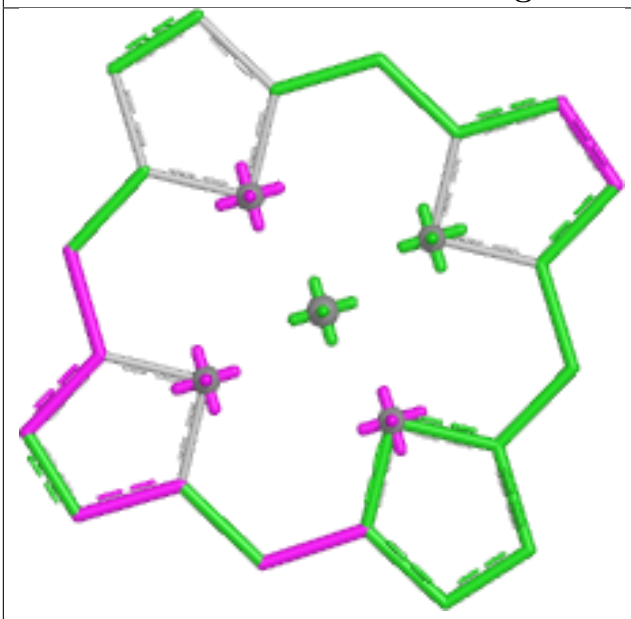


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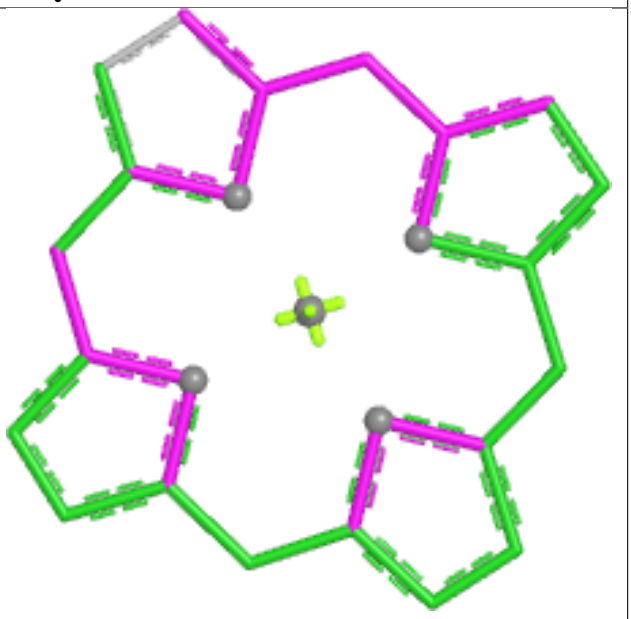


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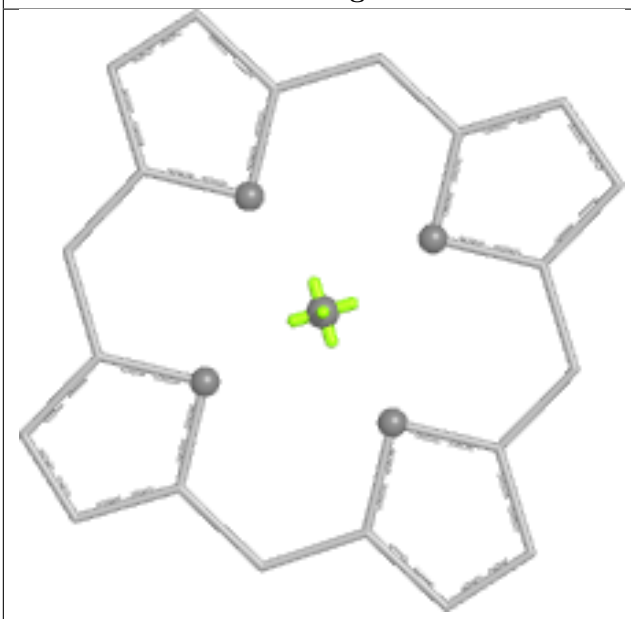
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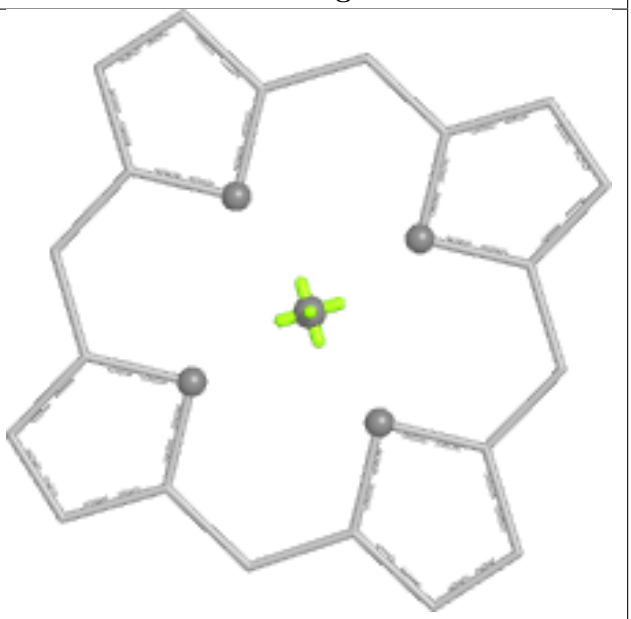
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Bond angles

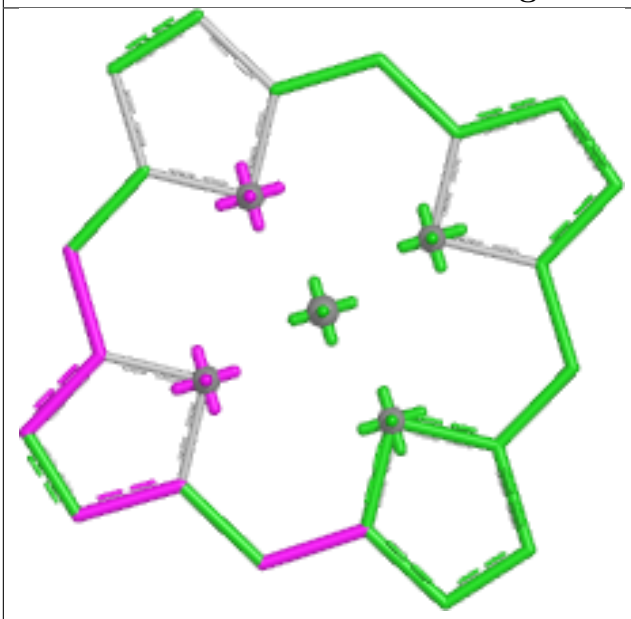


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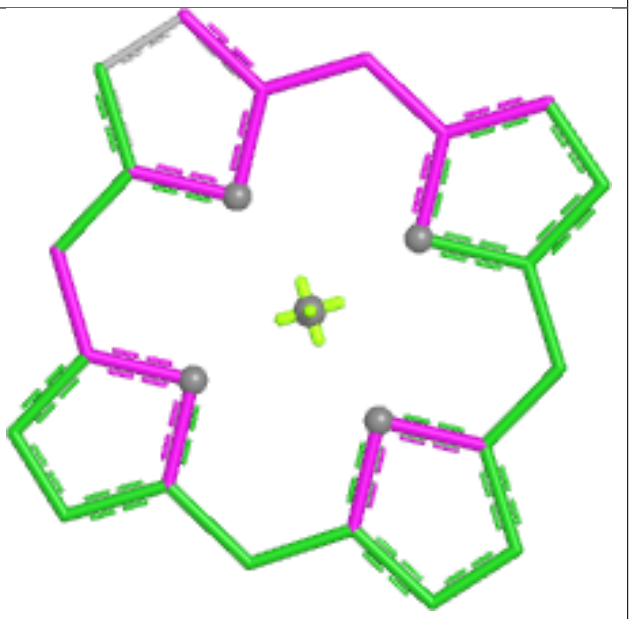


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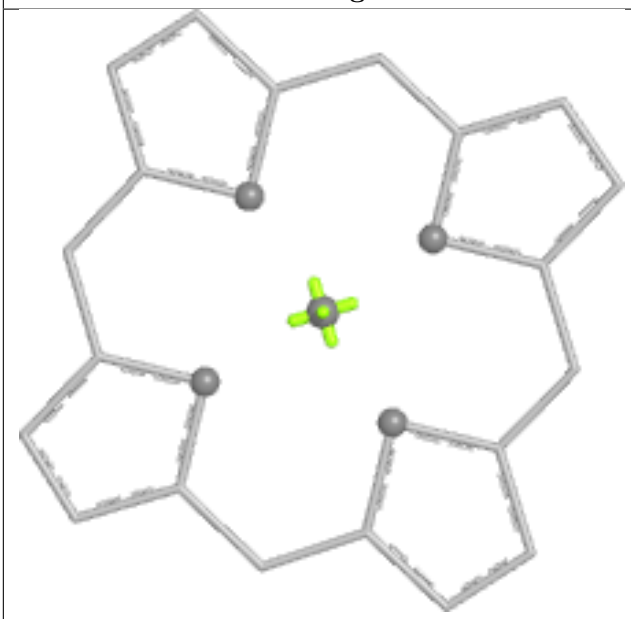
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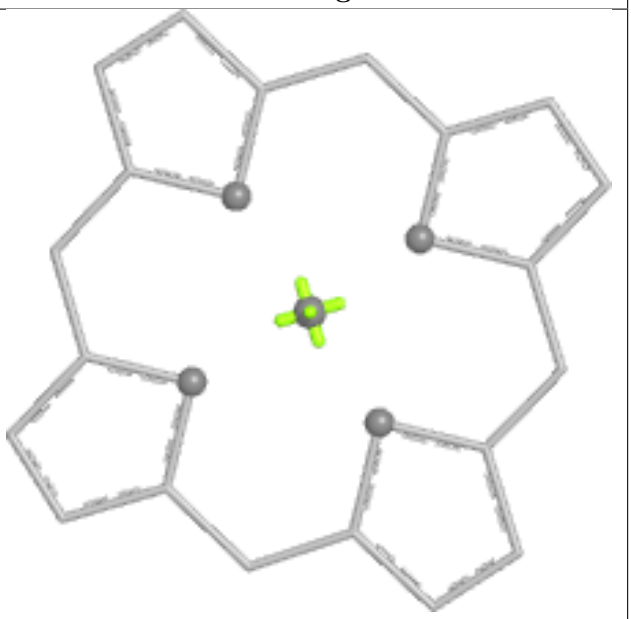
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Bond angles

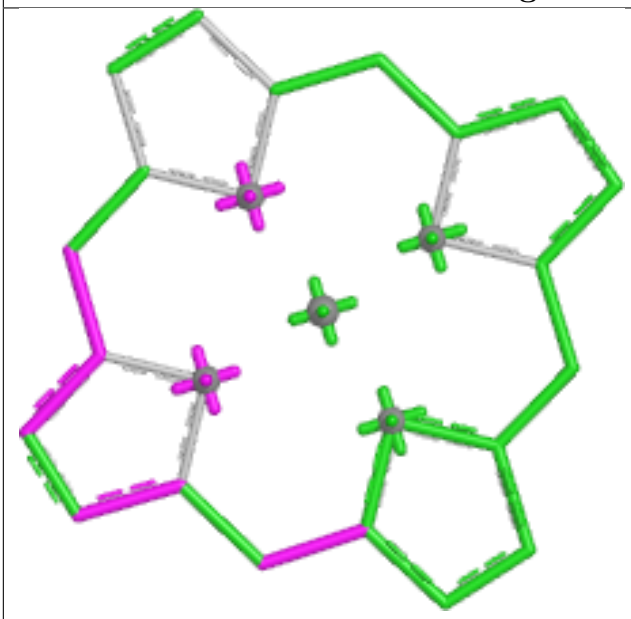


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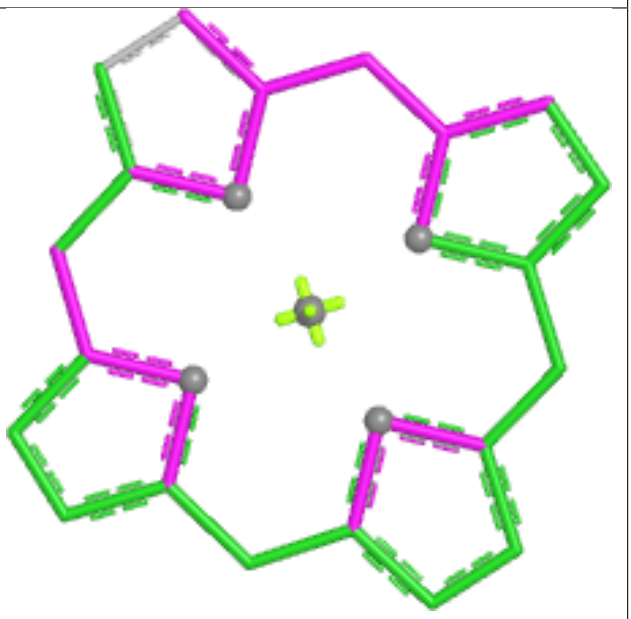


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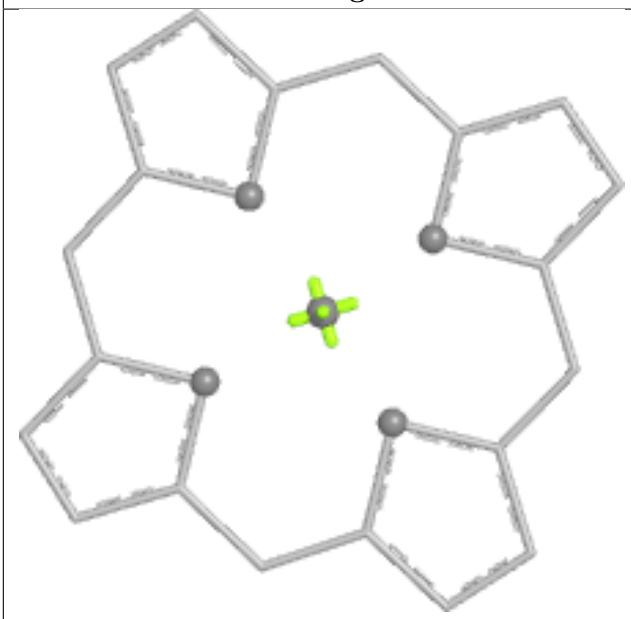
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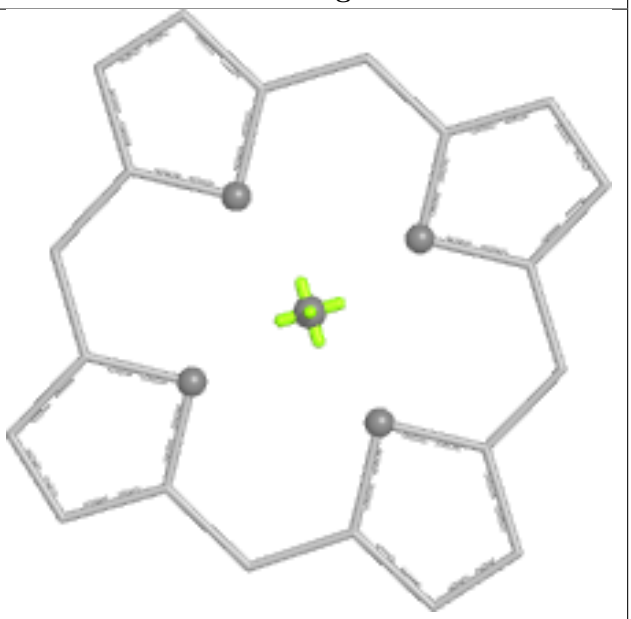
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Bond angles

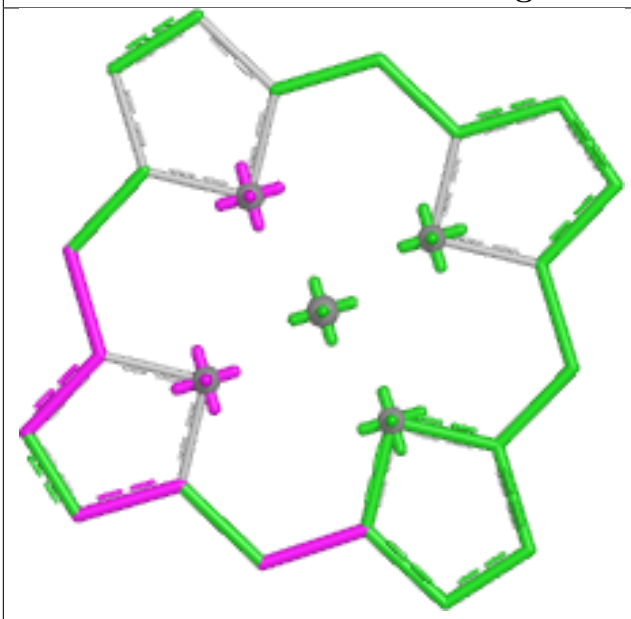


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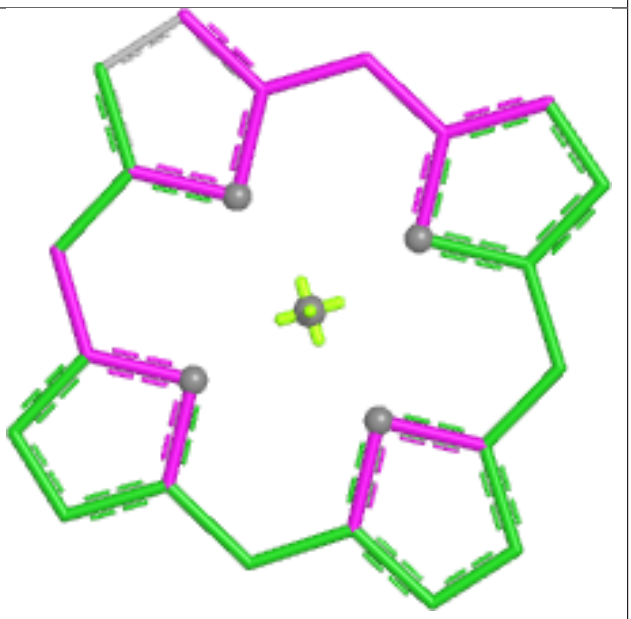


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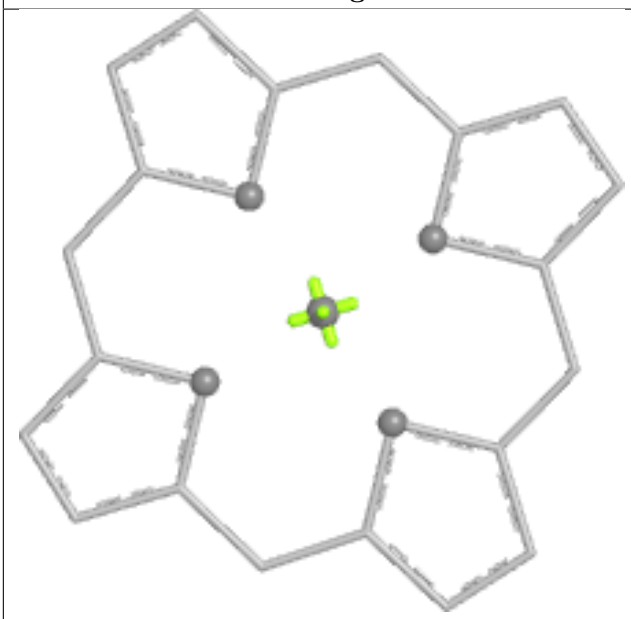
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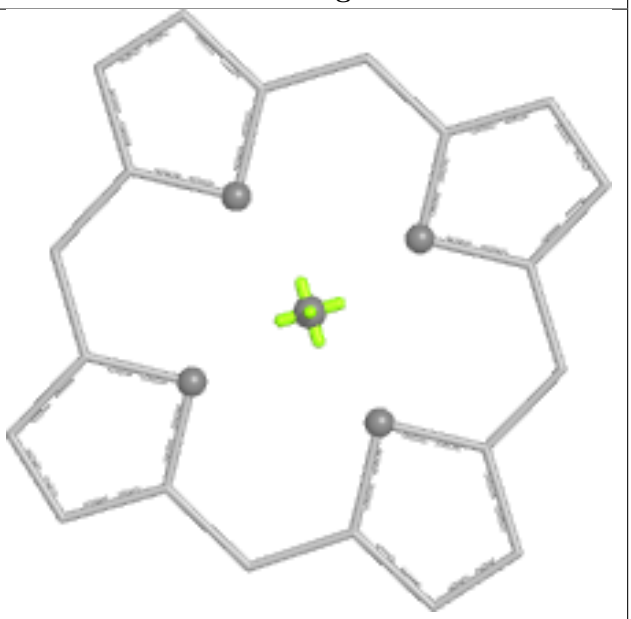
Bond lengths



Bond angles

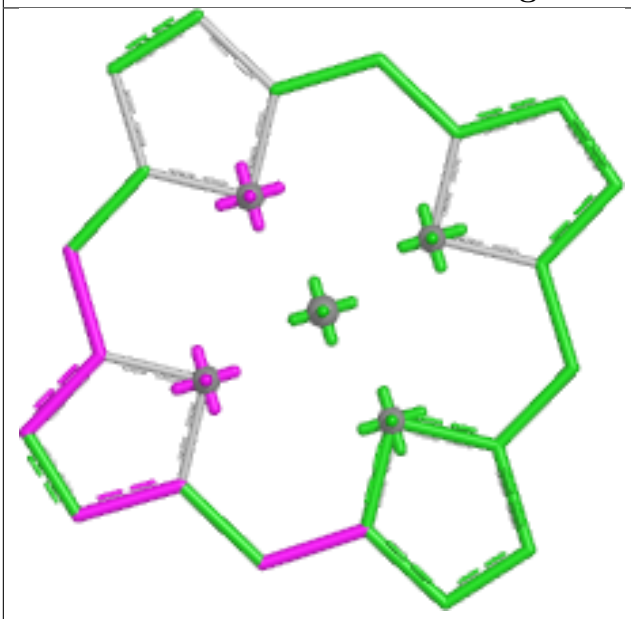


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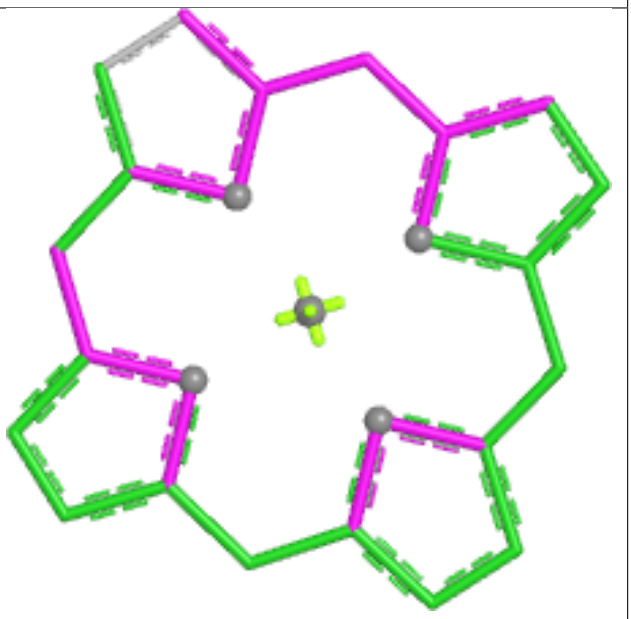


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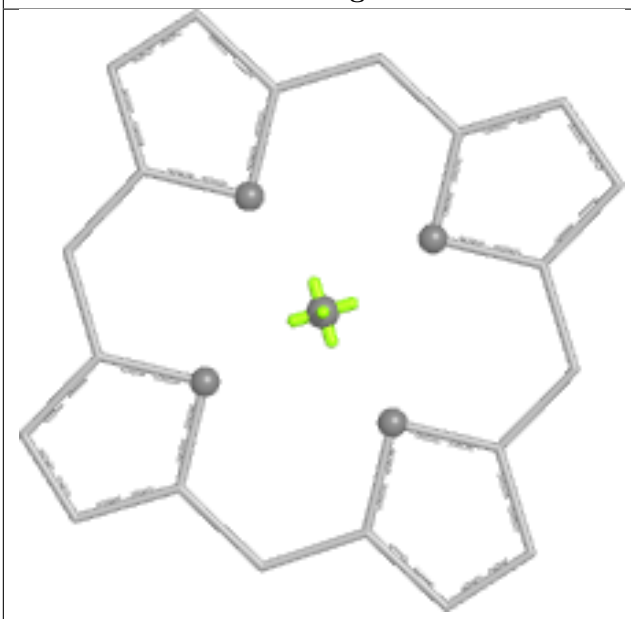
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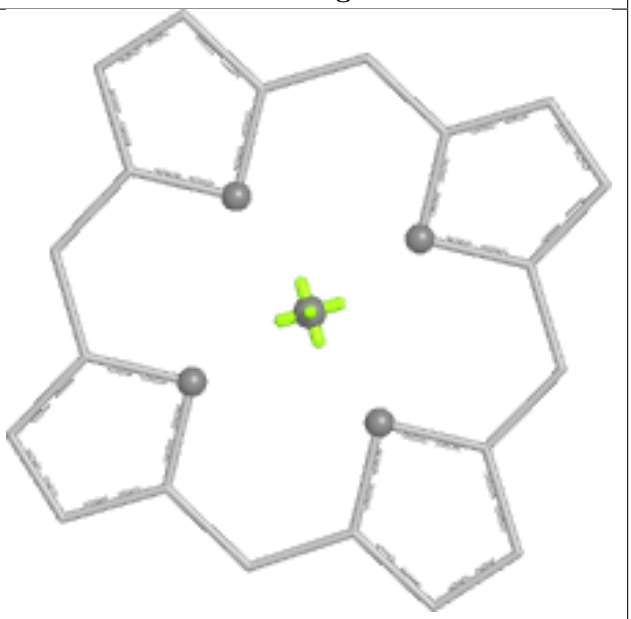
Bond lengths



Bond angles

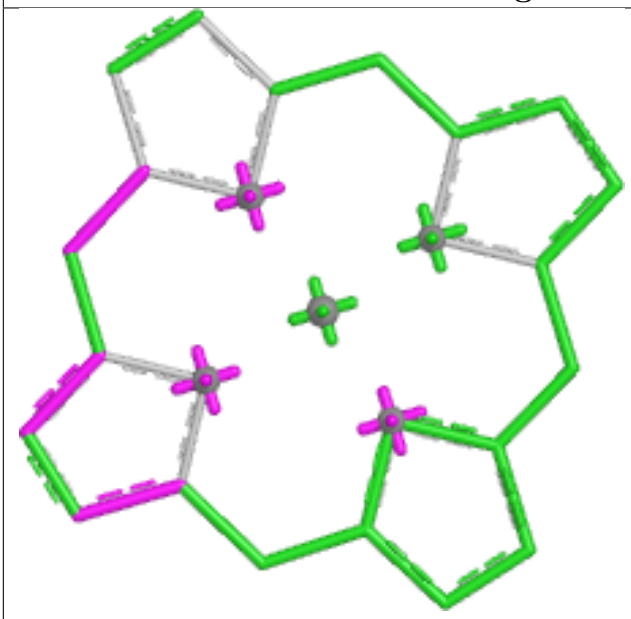


Torsions

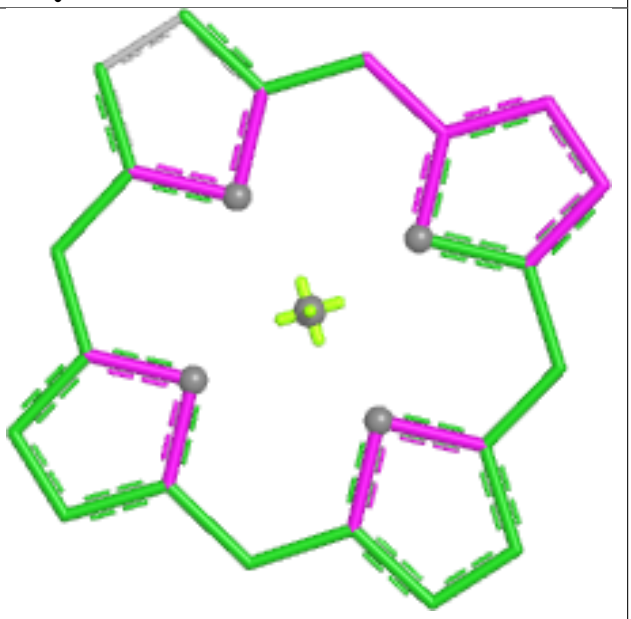


Rings

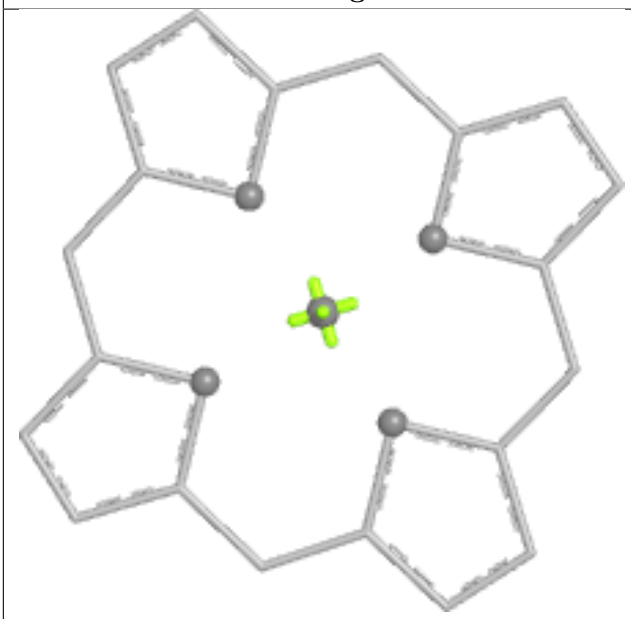
Ligand CLA Q 5239



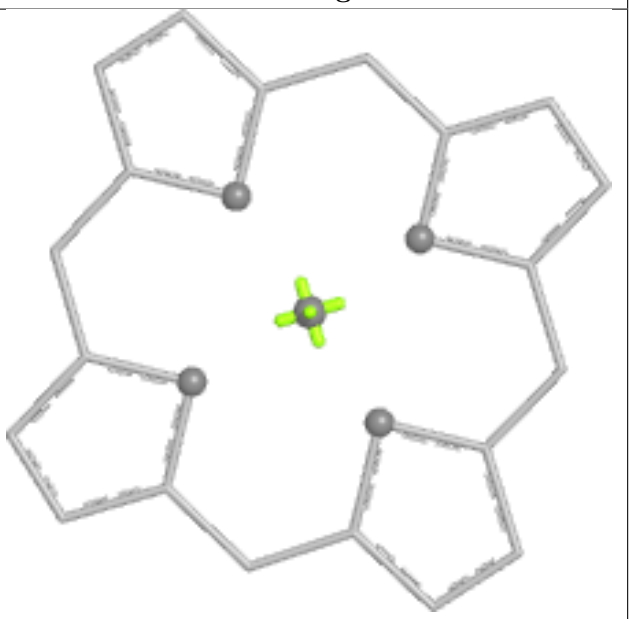
Bond lengths



Bond angles

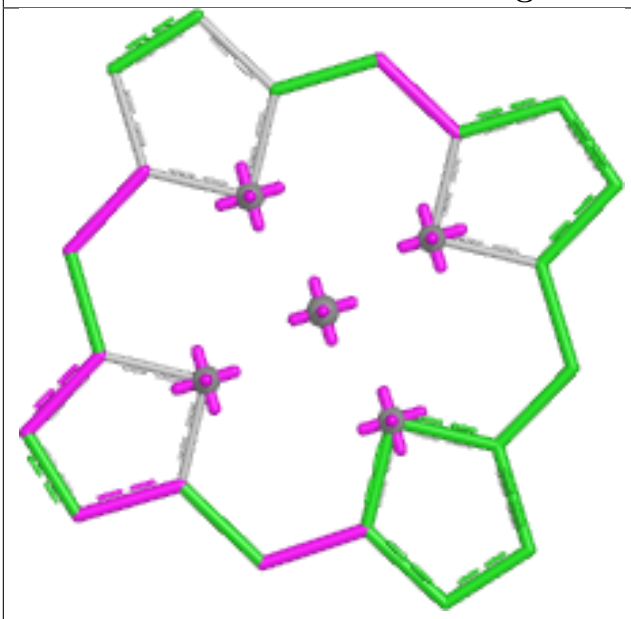


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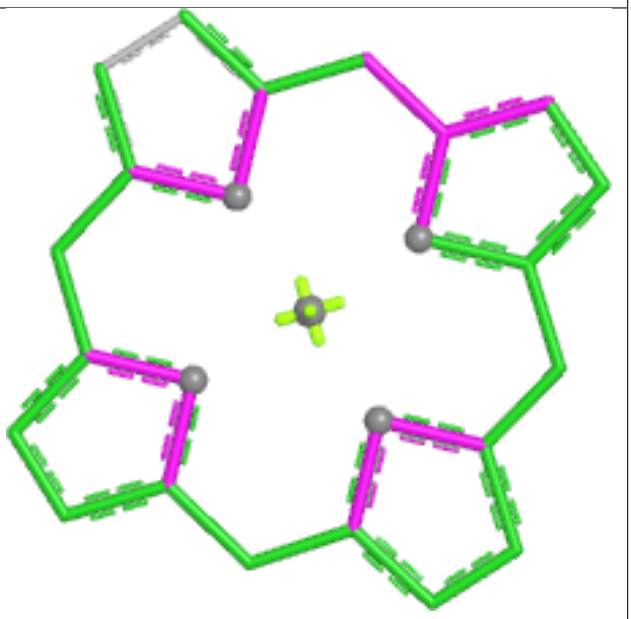


Rings

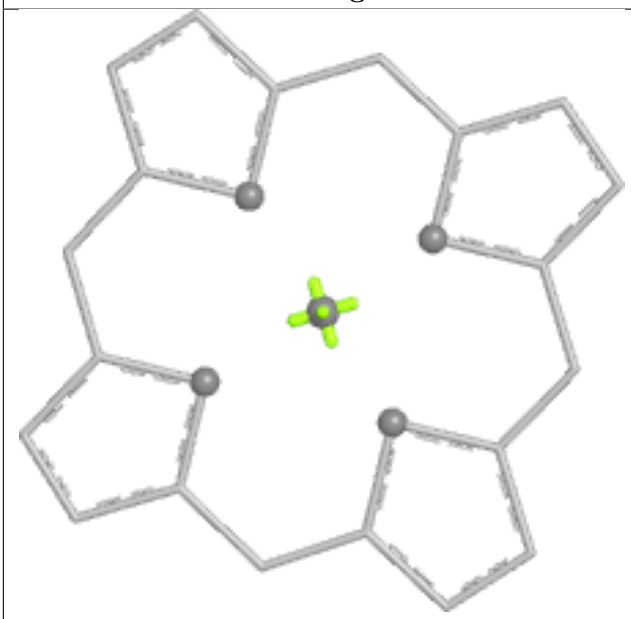
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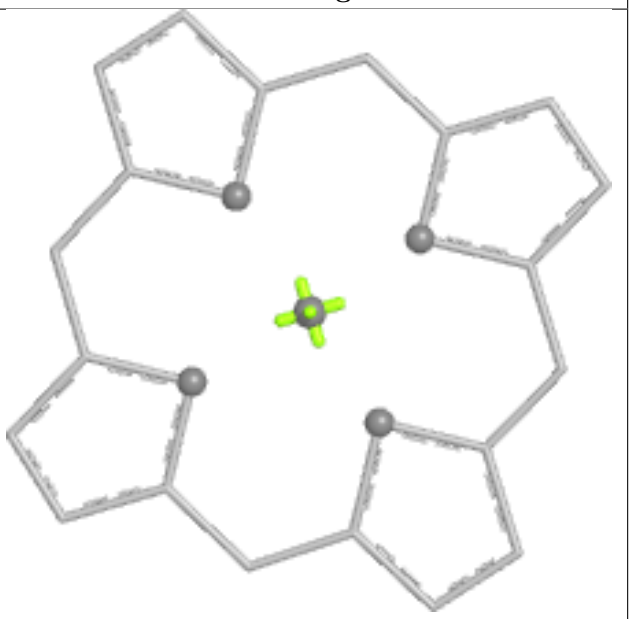
Bond lengths



Bond angles

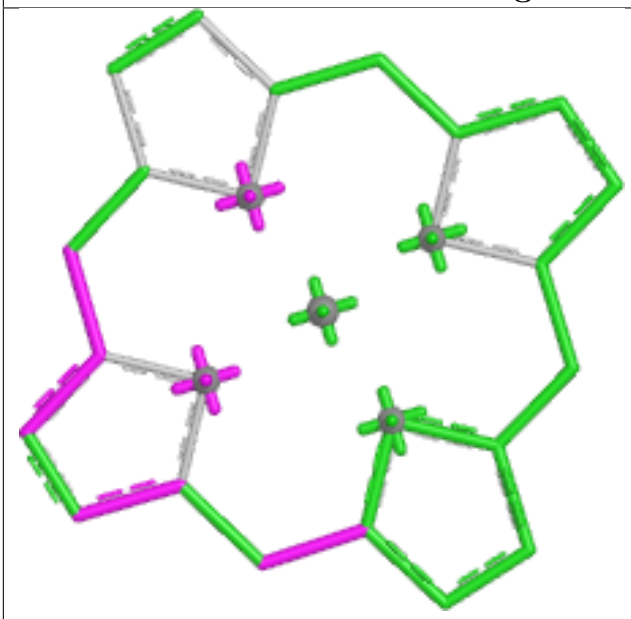


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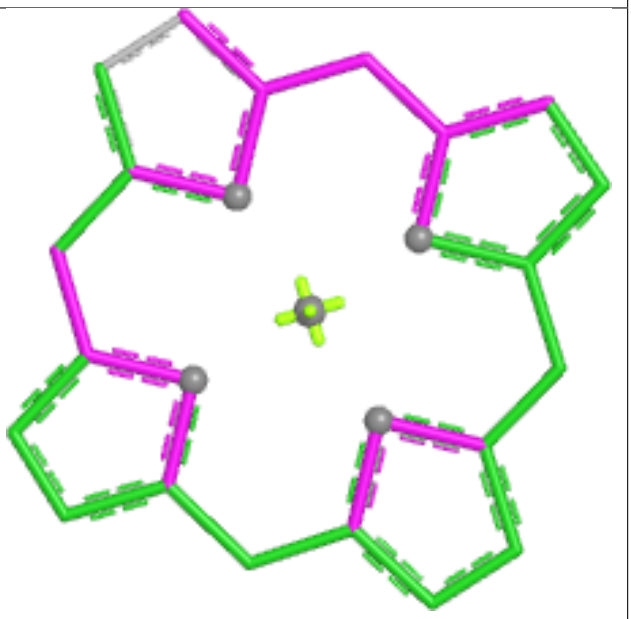


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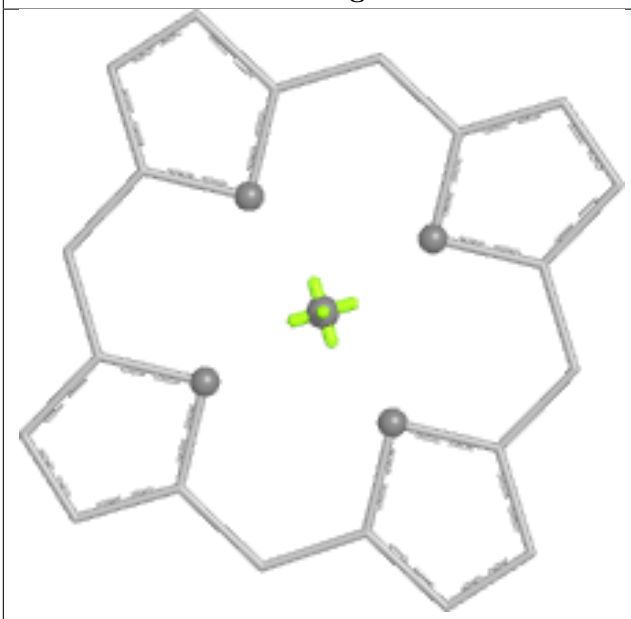
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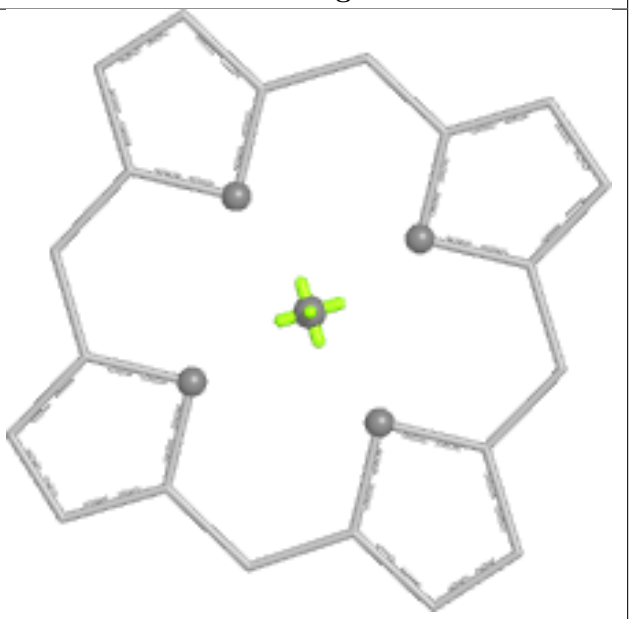
Bond lengths



Bond angles

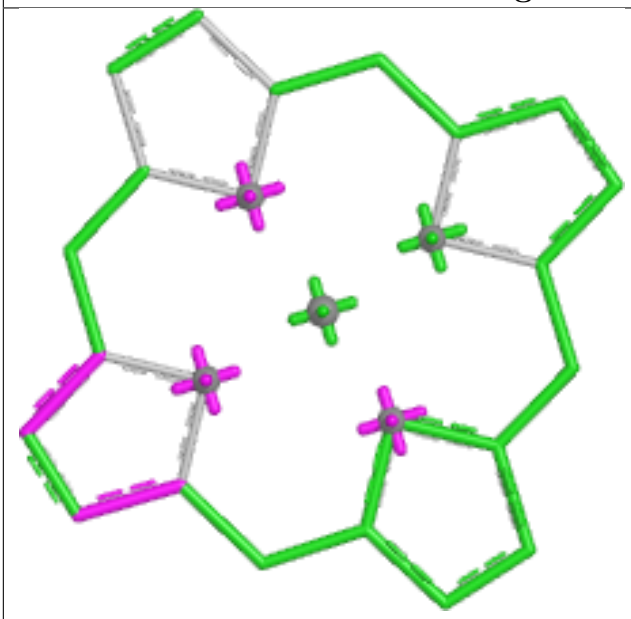


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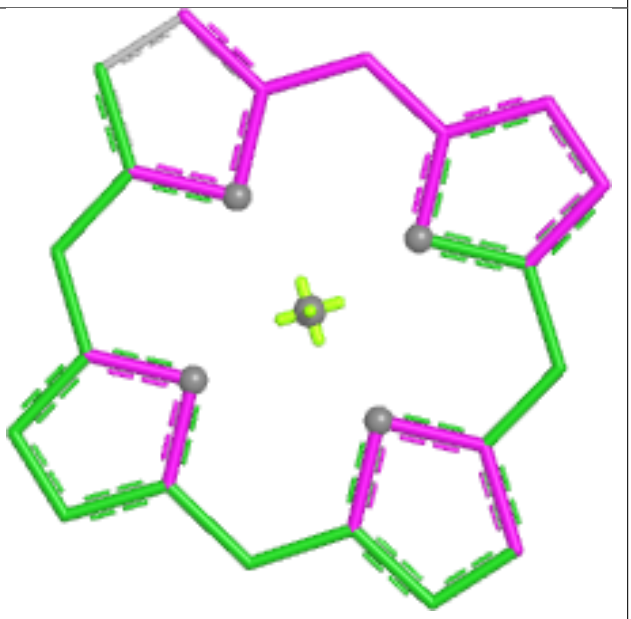


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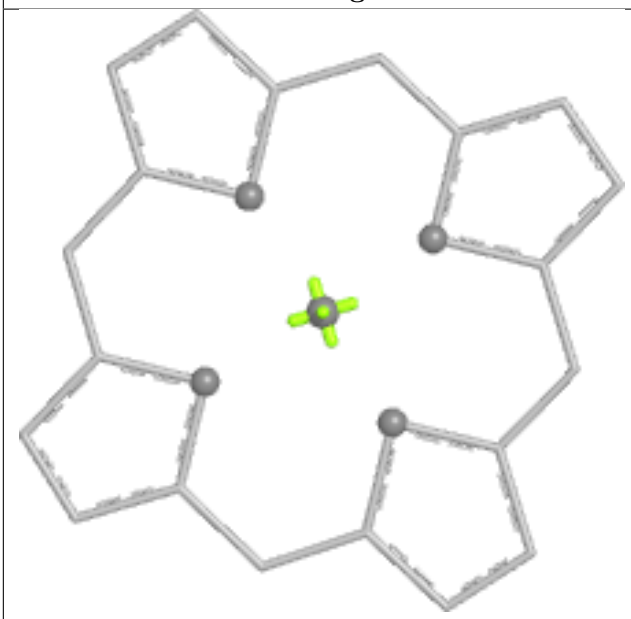
Ligand CLA A 1131



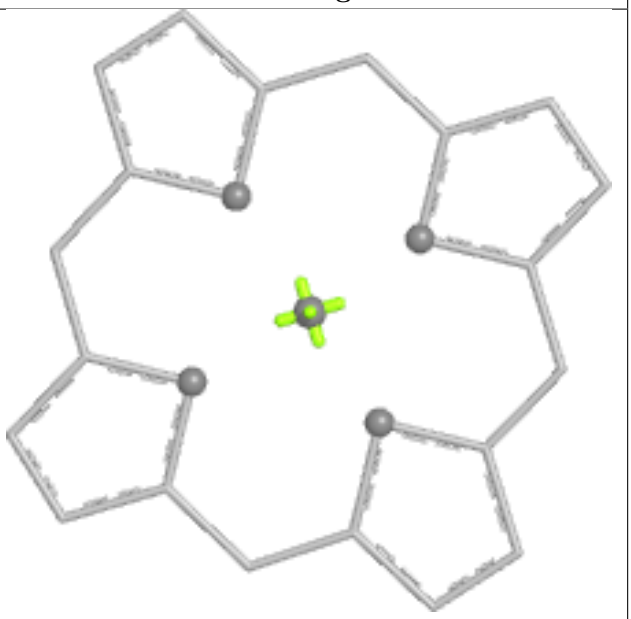
Bond lengths



Bond angles

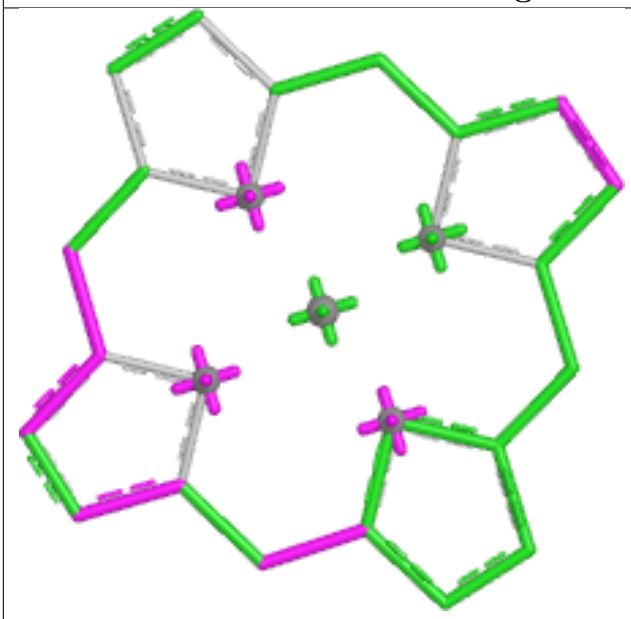


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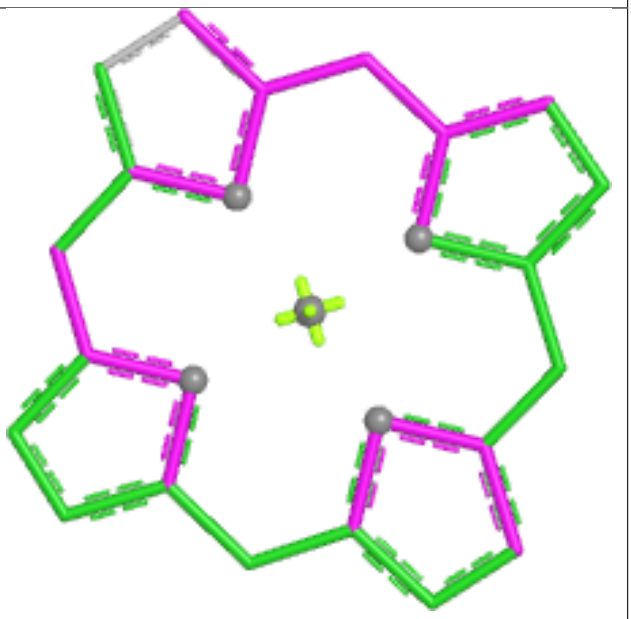


Rings

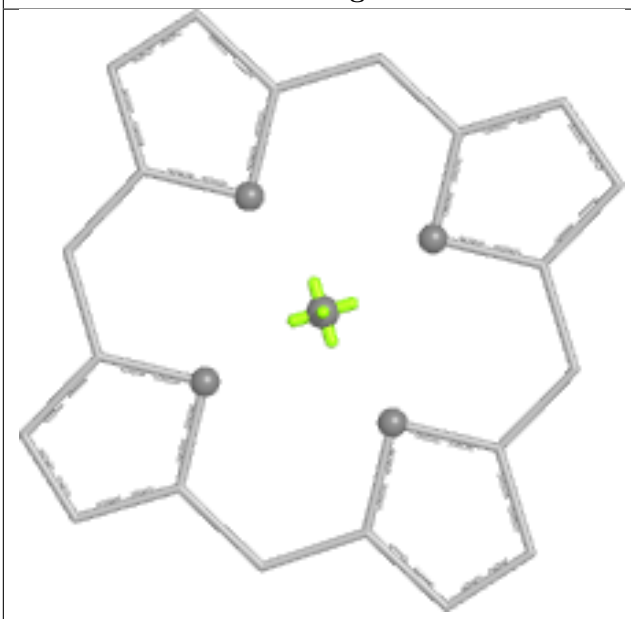
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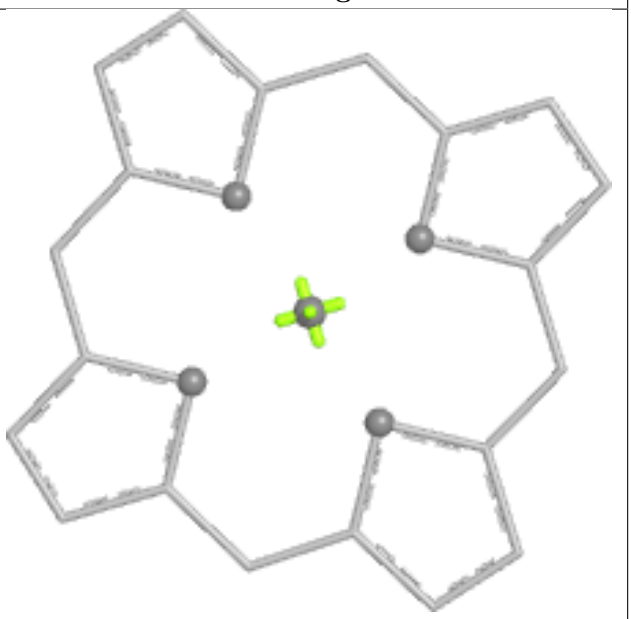
Bond lengths



Bond angles

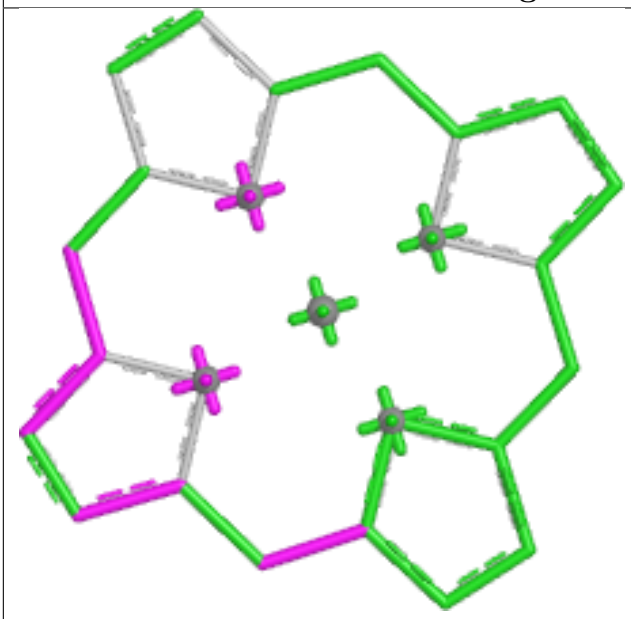


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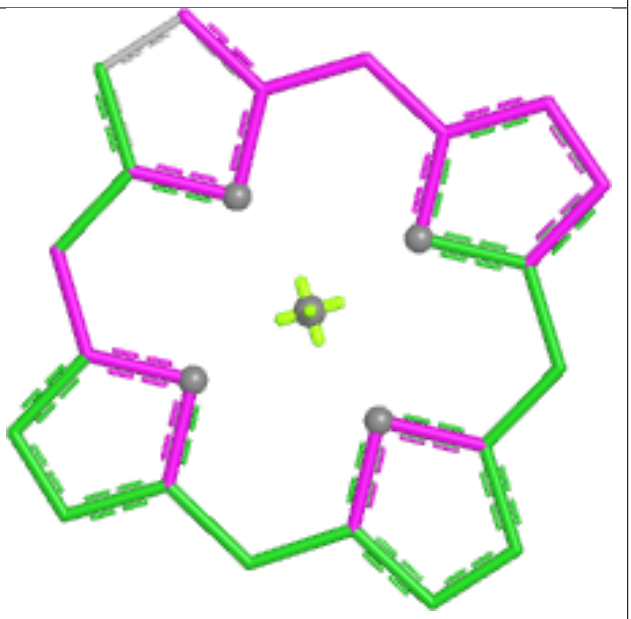


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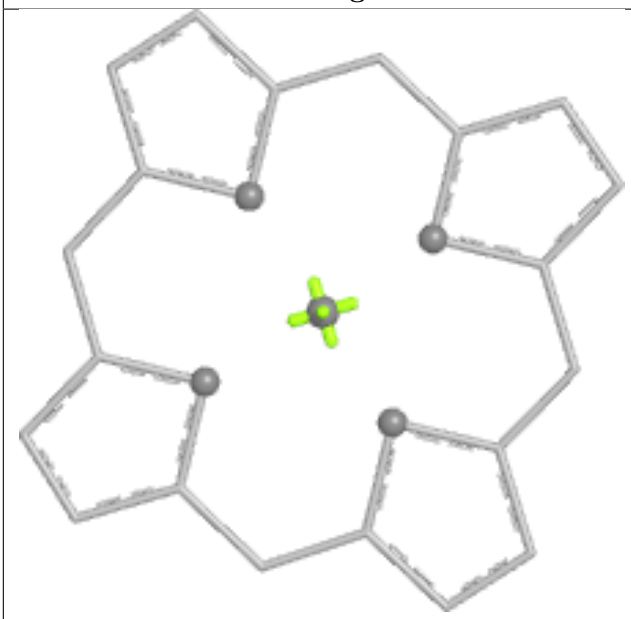
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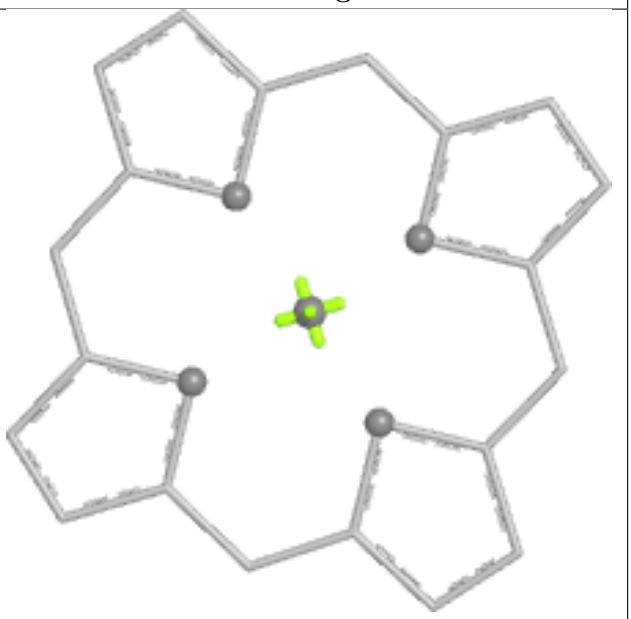
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Bond angles

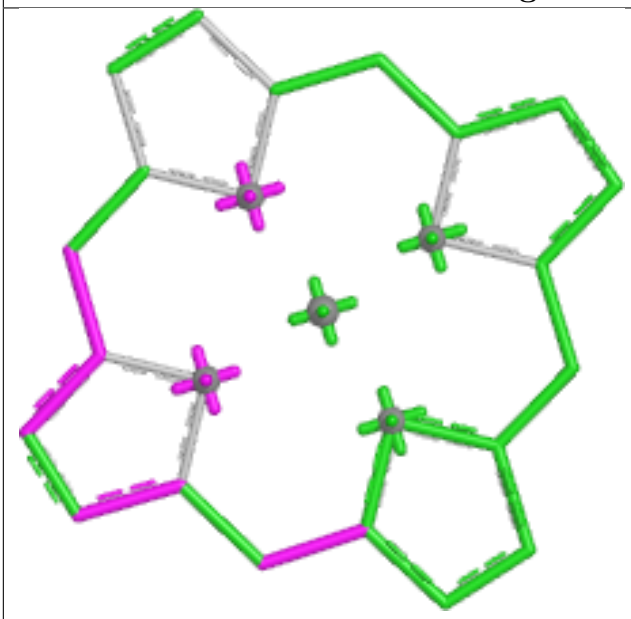


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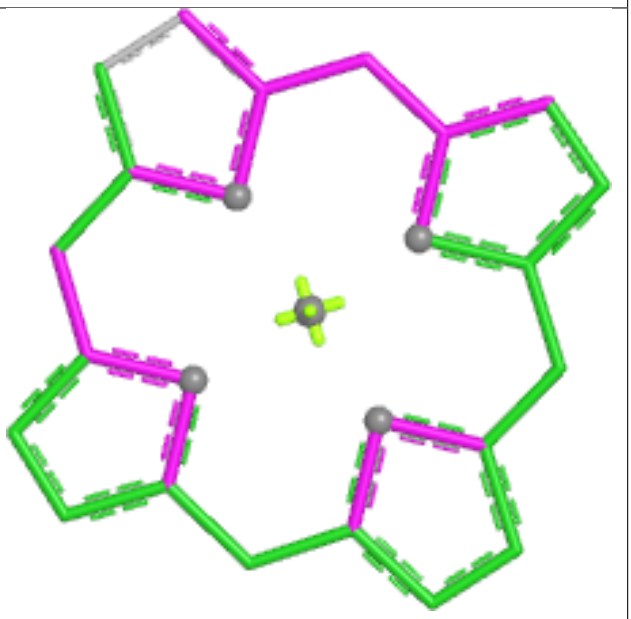


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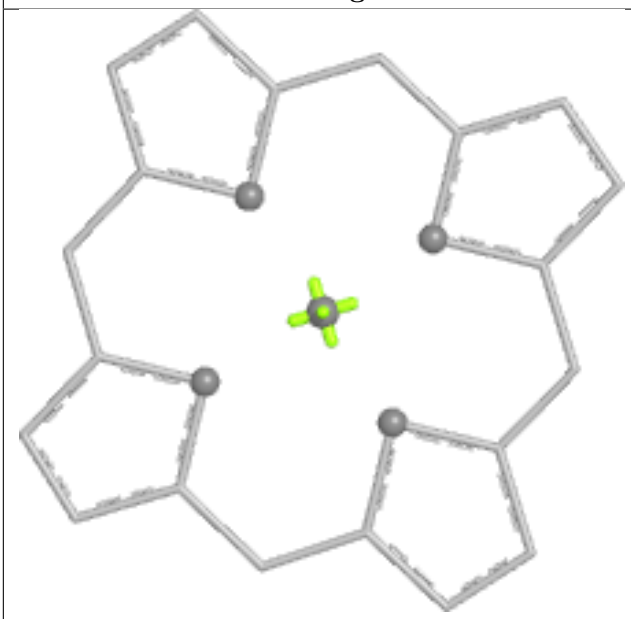
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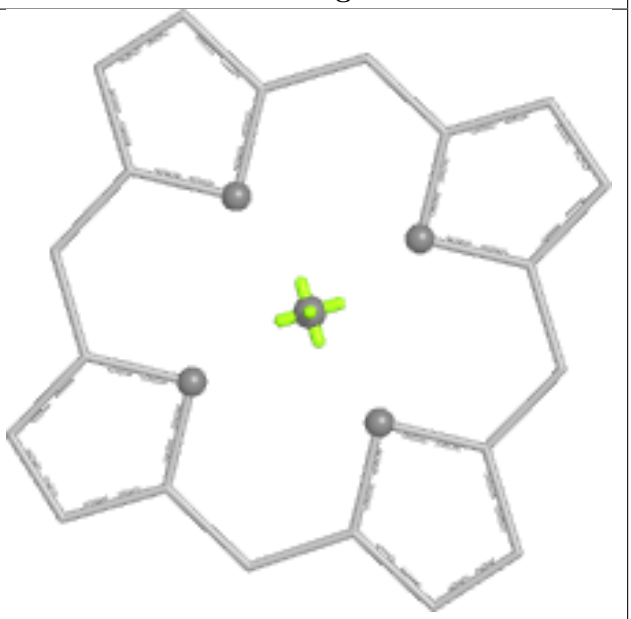
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Bond angles

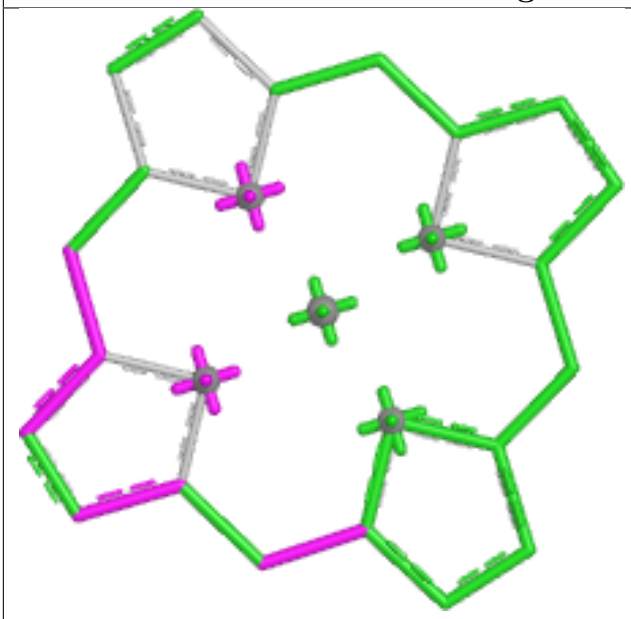


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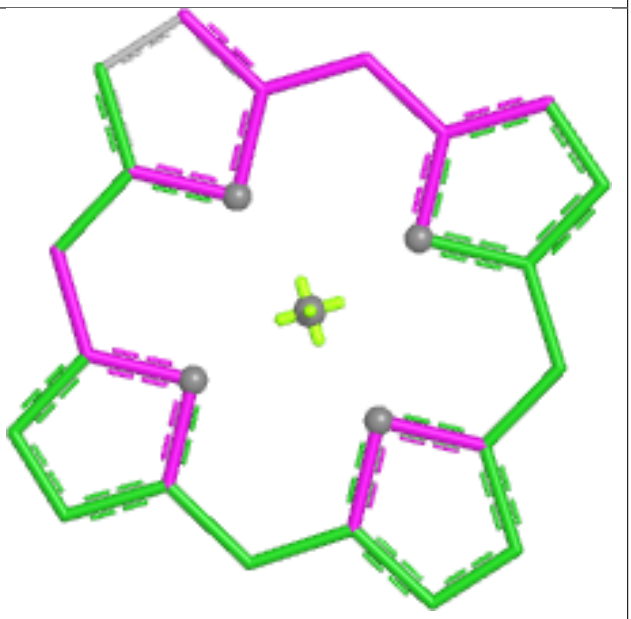


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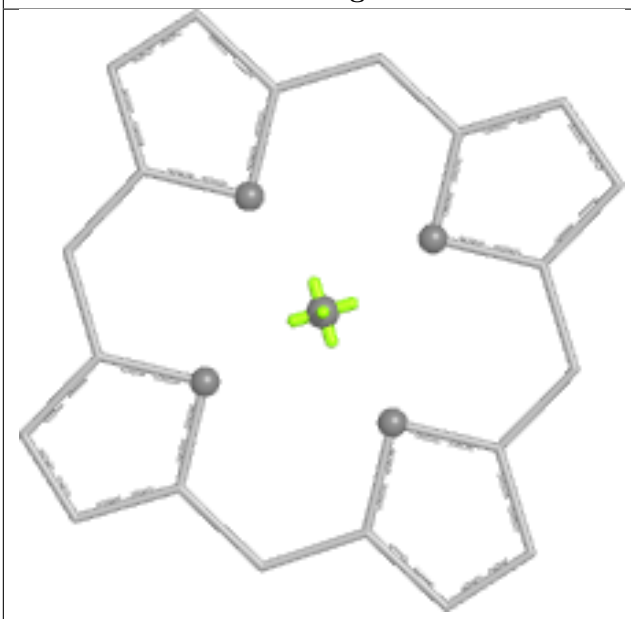
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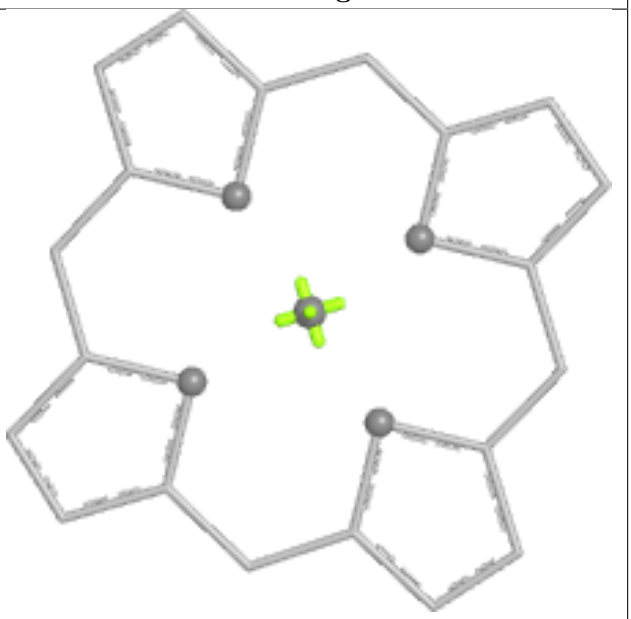
Bond lengths



Bond angles

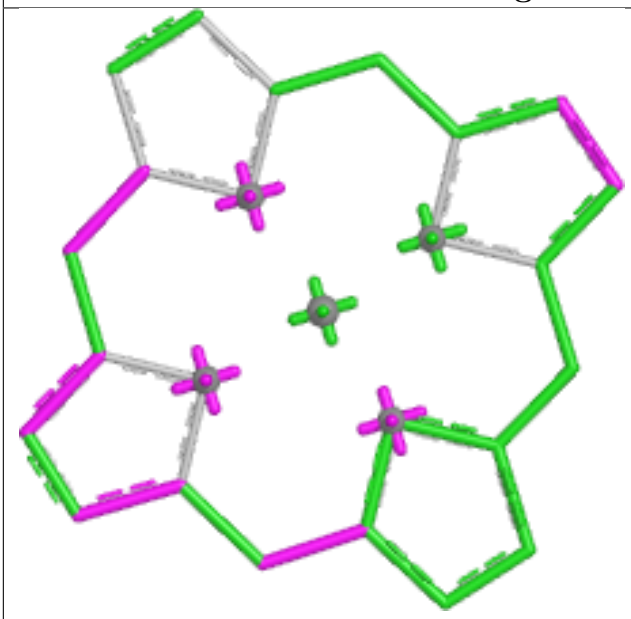


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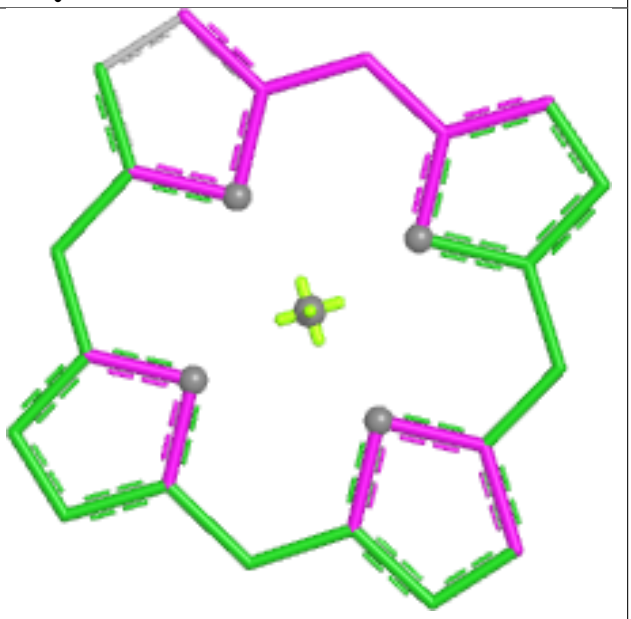


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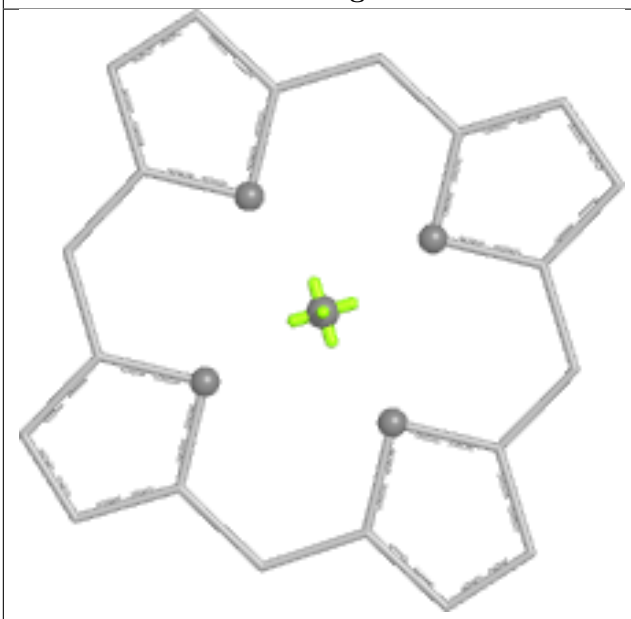
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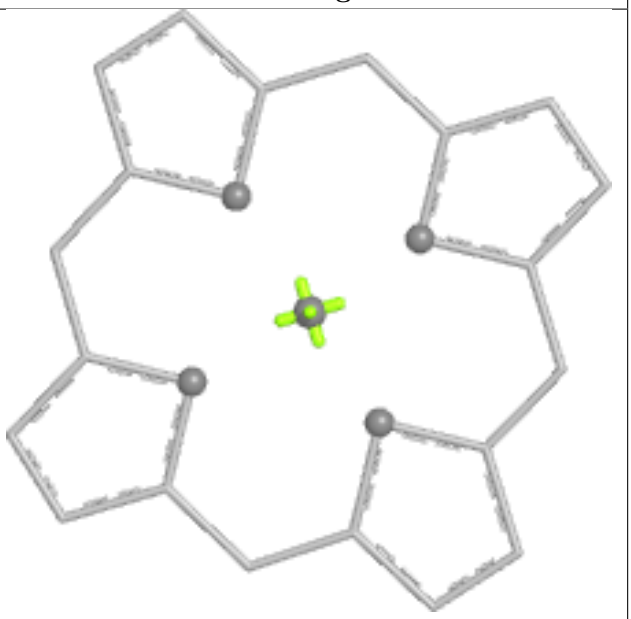
Bond lengths



Bond angles

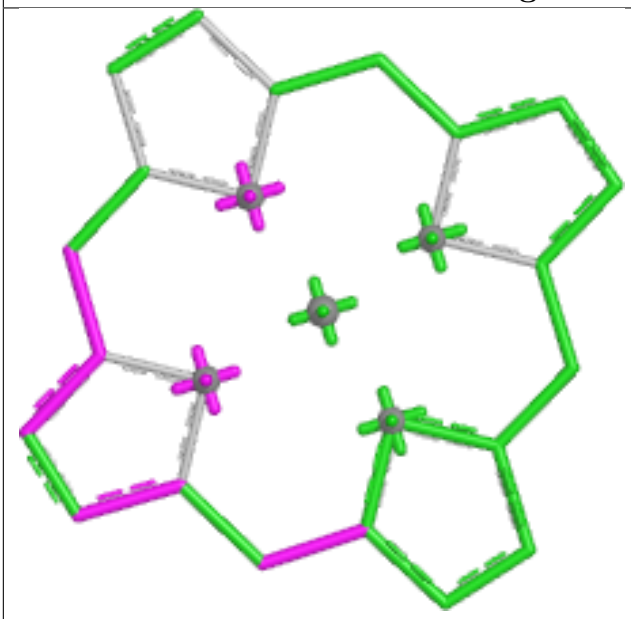


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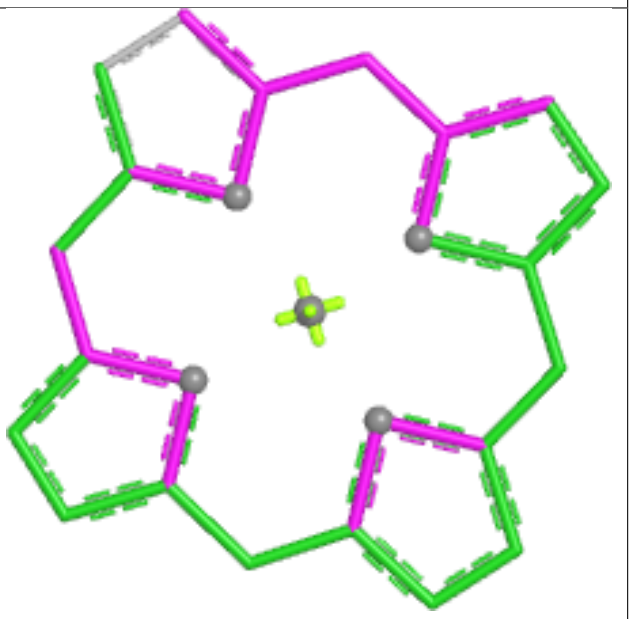


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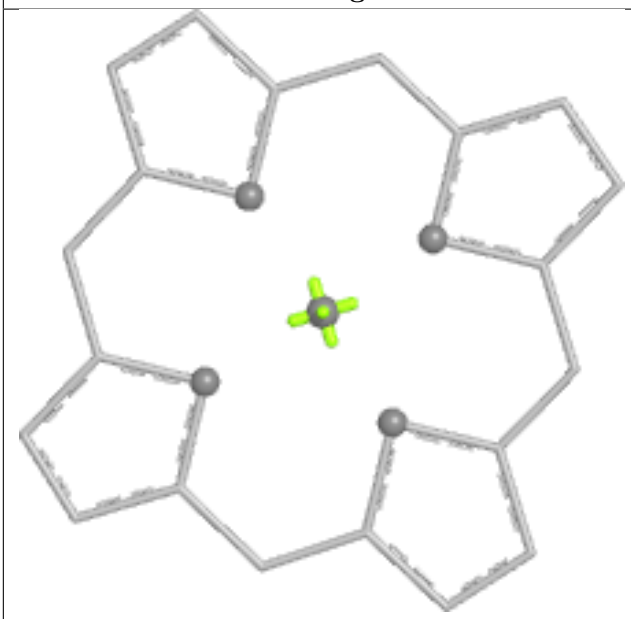
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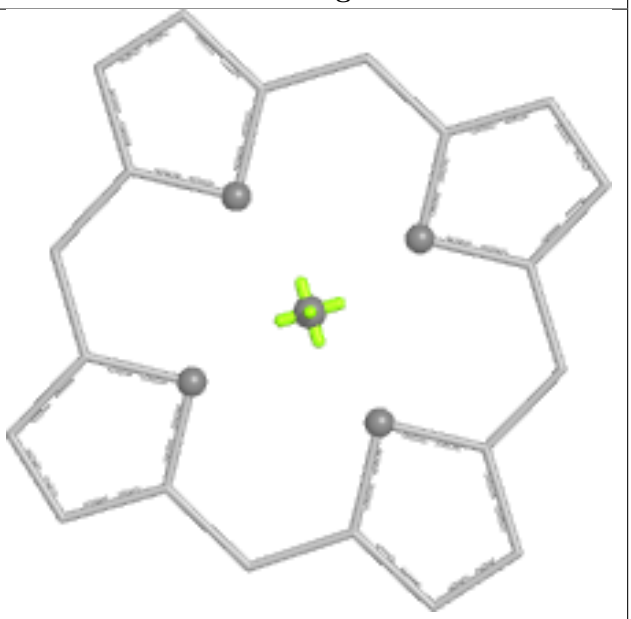
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Bond angles

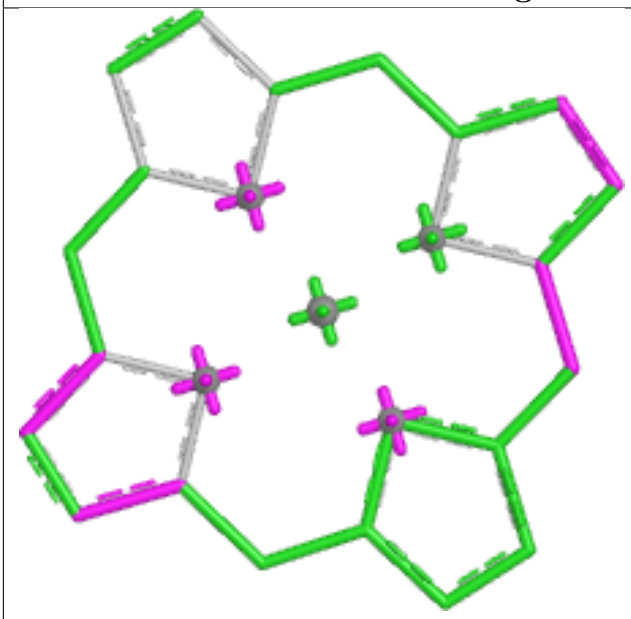


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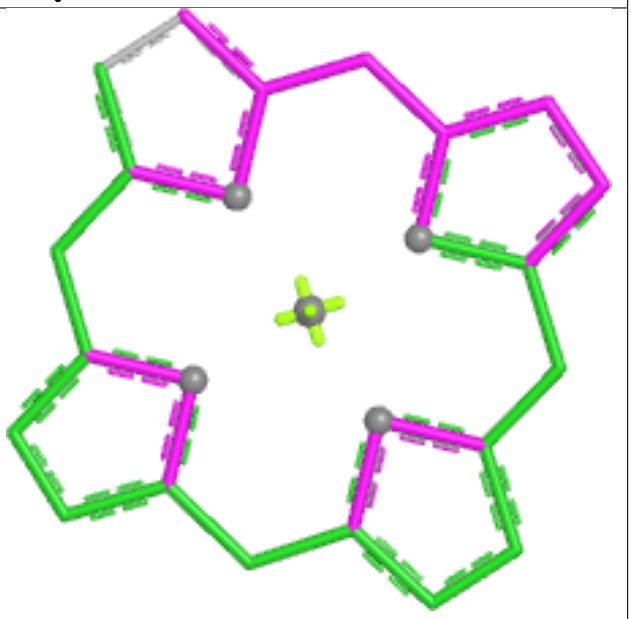


Rings

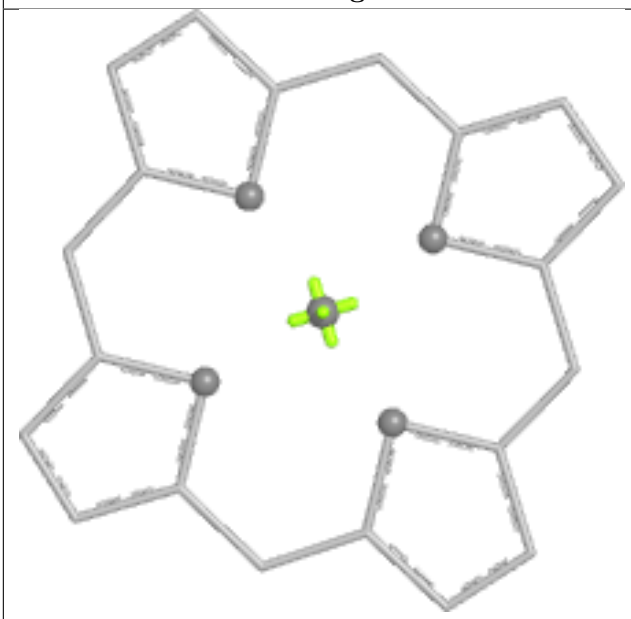
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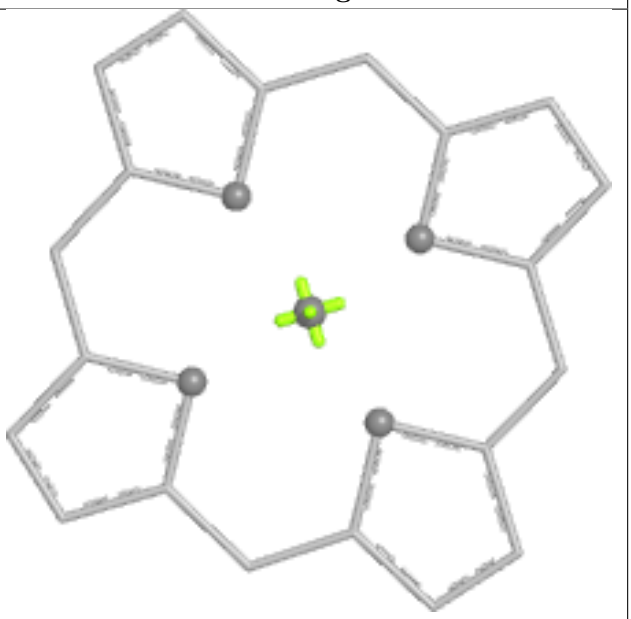
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Bond angles

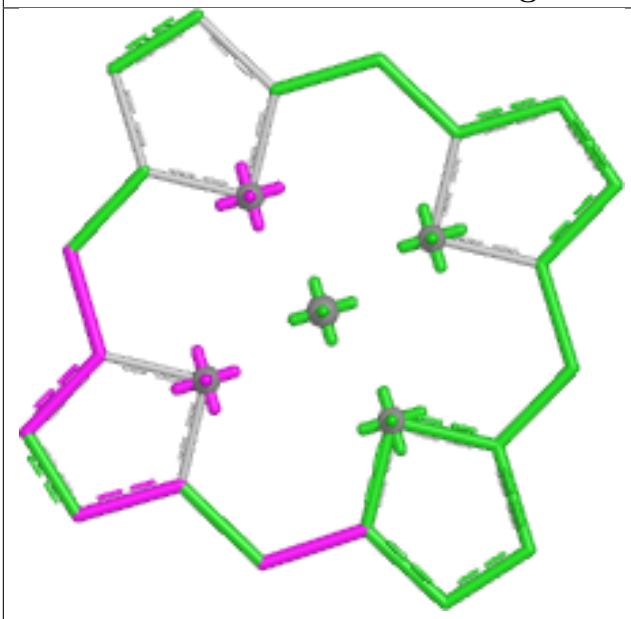


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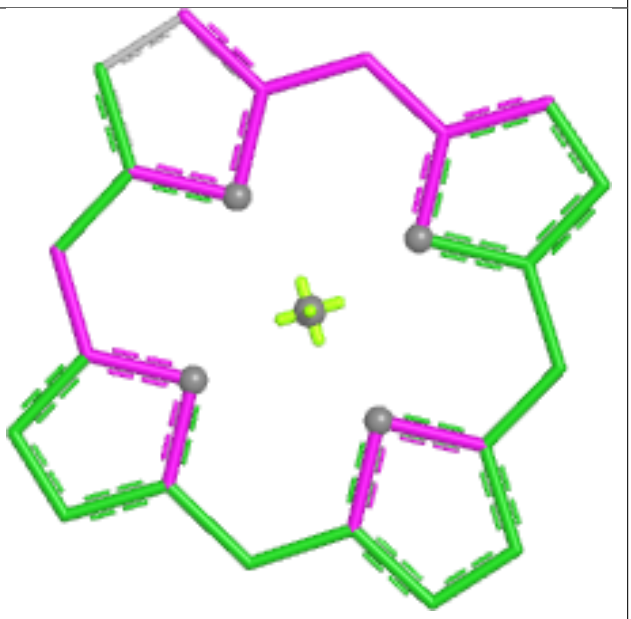


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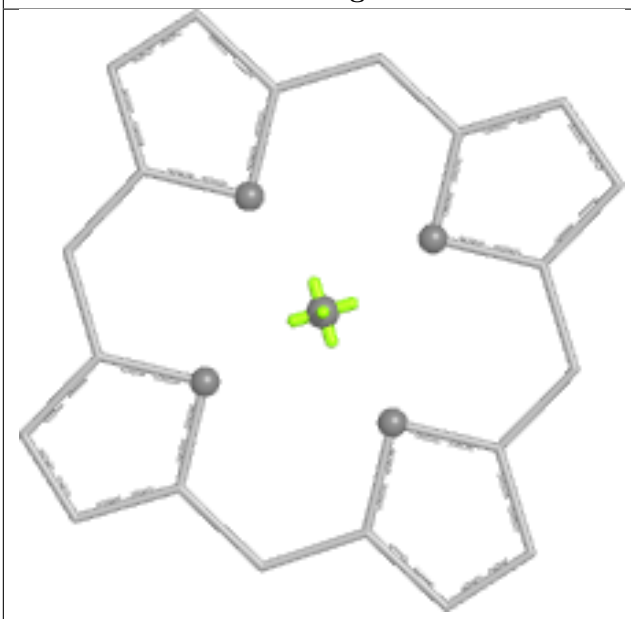
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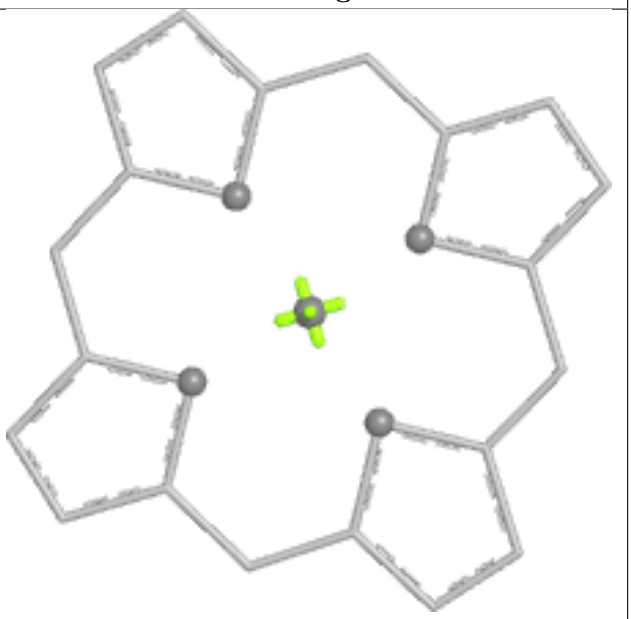
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Bond angles

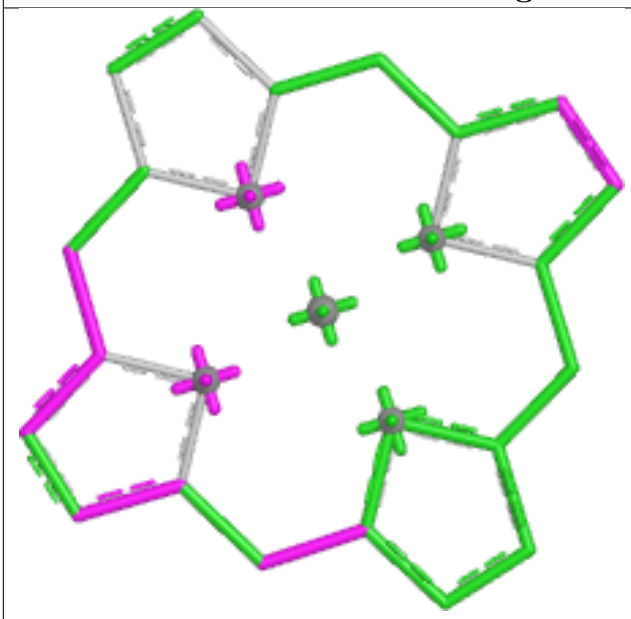


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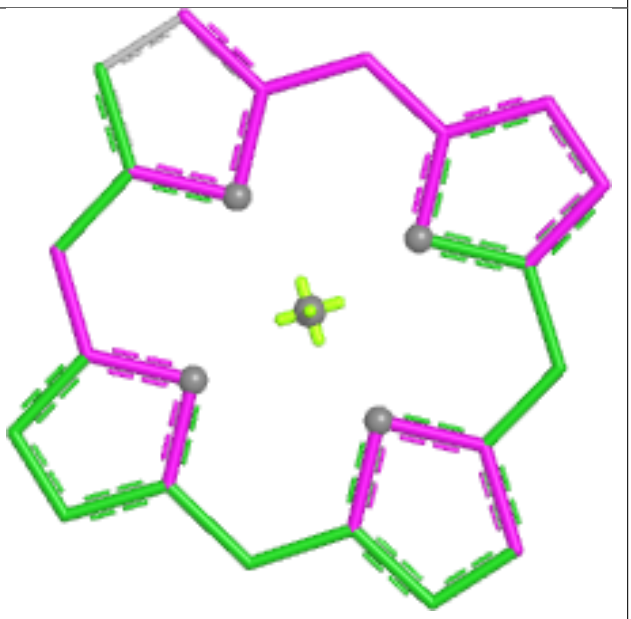


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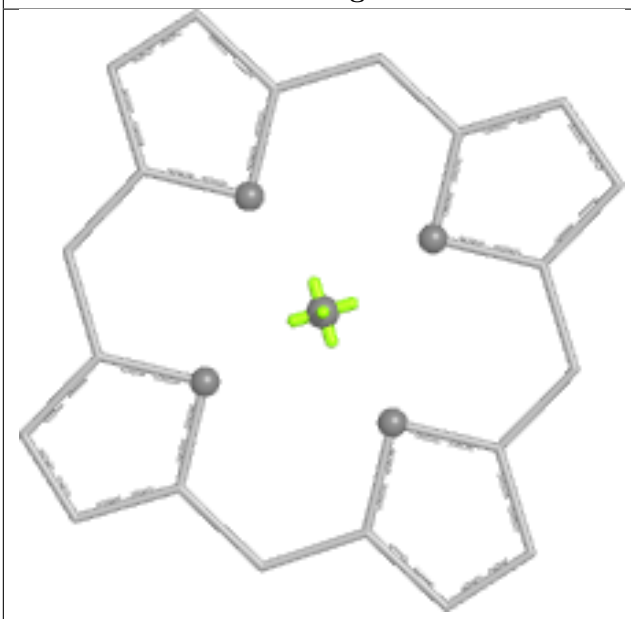
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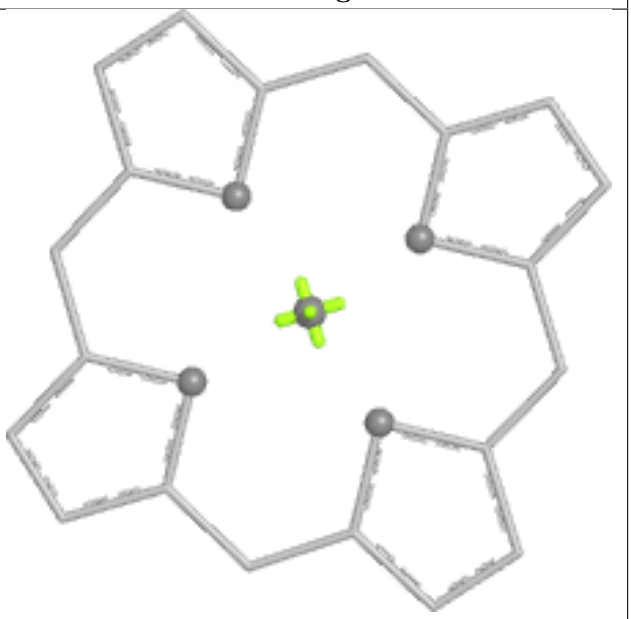
Bond lengths



Bond angles

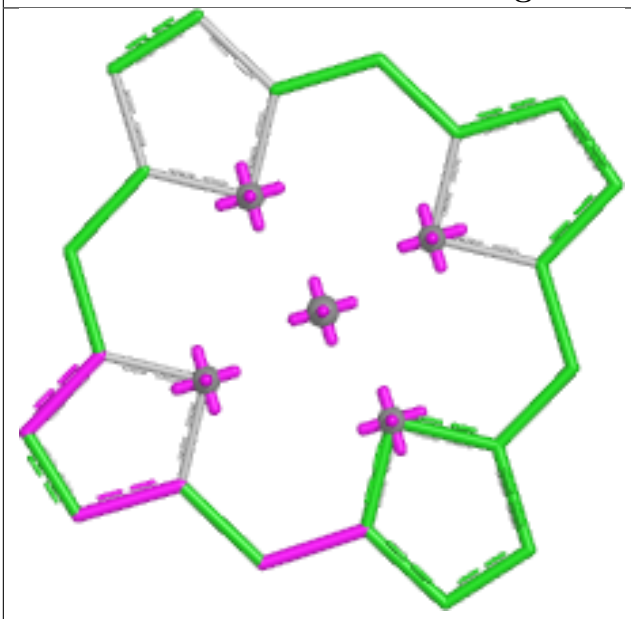


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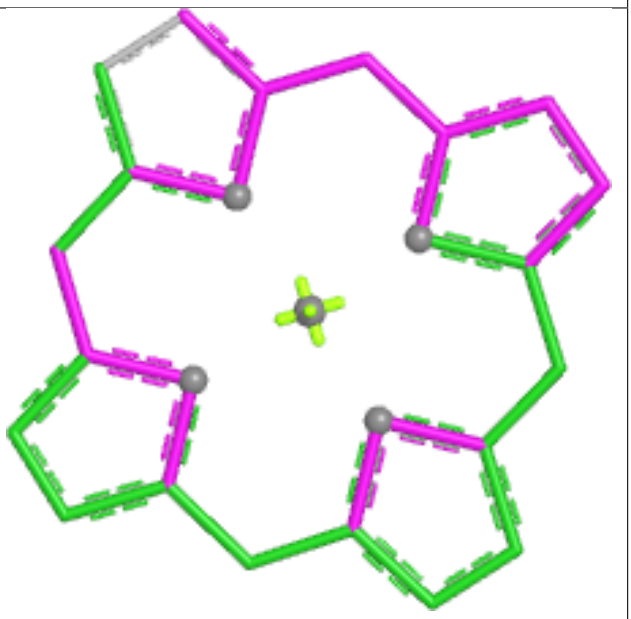


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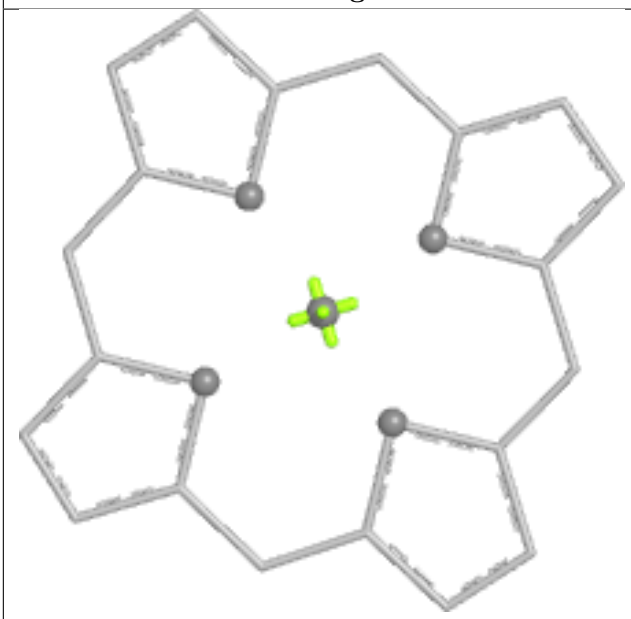
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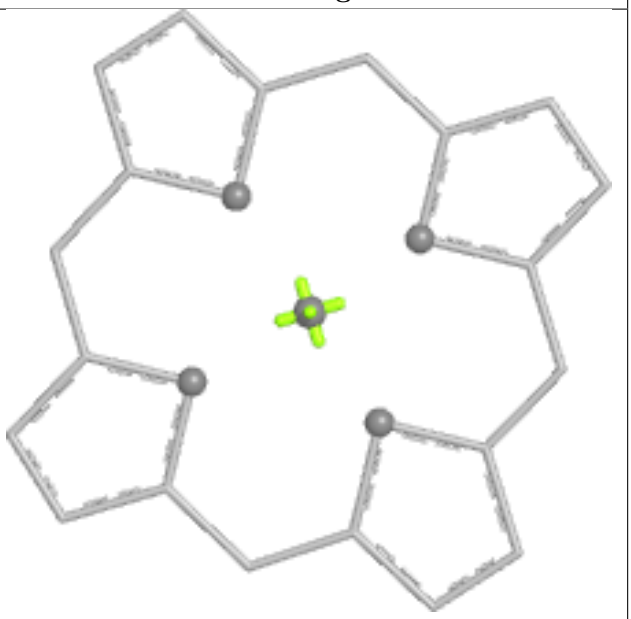
Bond lengths



Bond angles

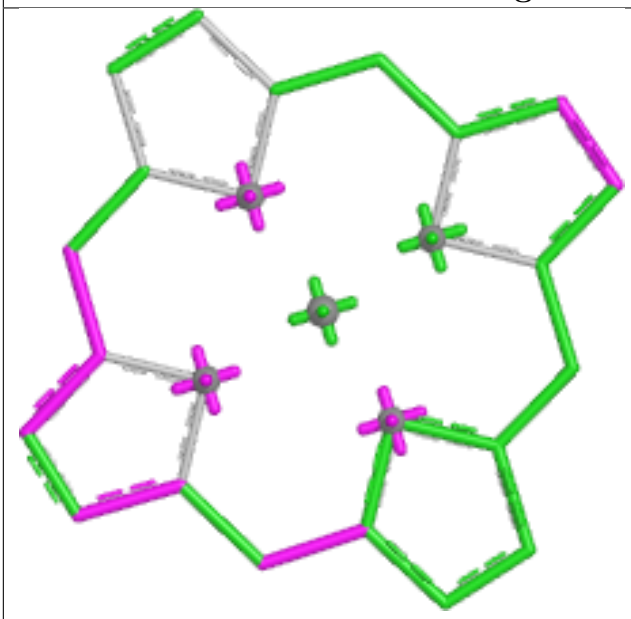


Torsions

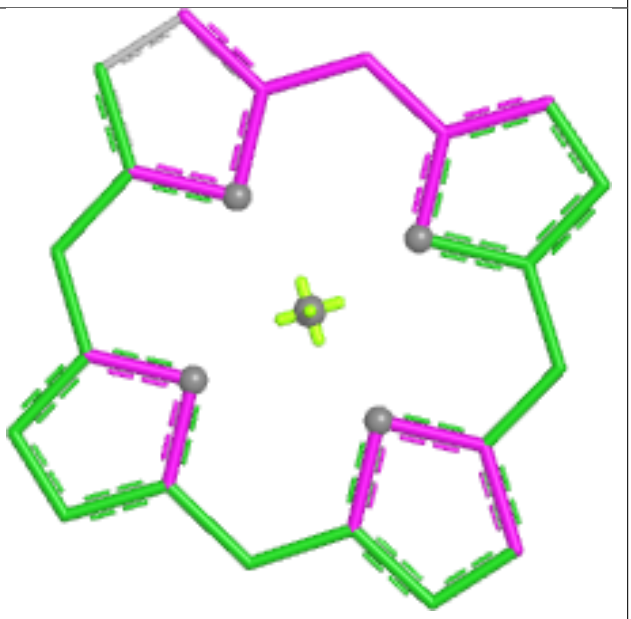


Rings

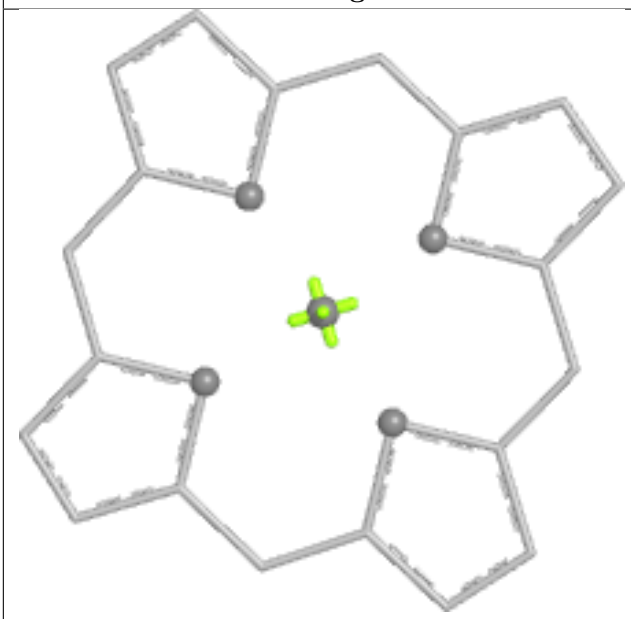
Ligand CLA A 1122



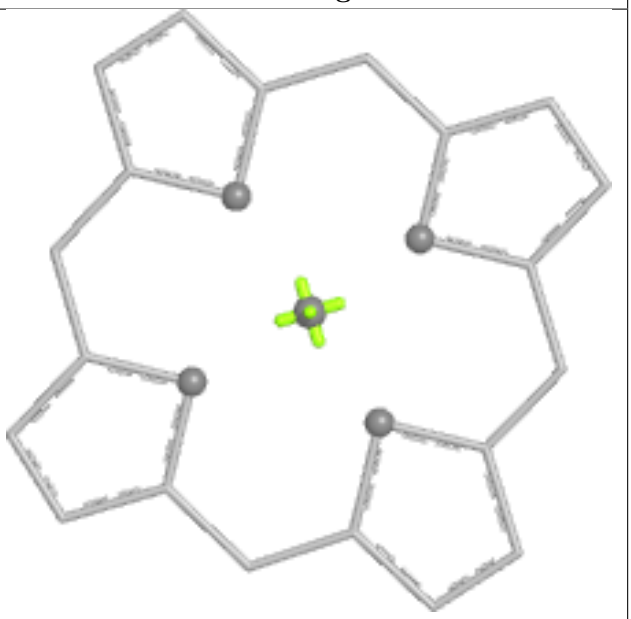
Bond lengths



Bond angles

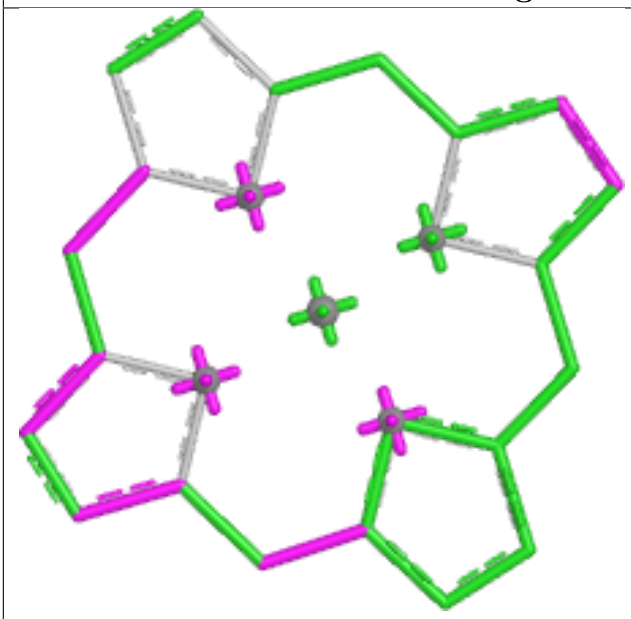


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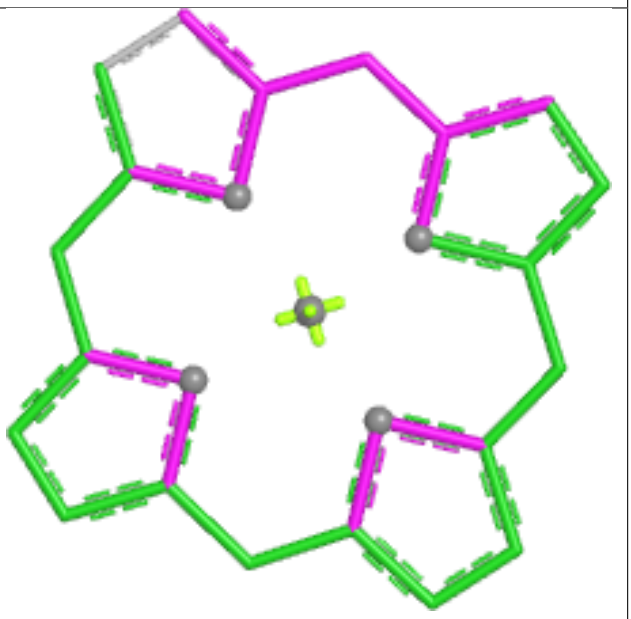


Rings

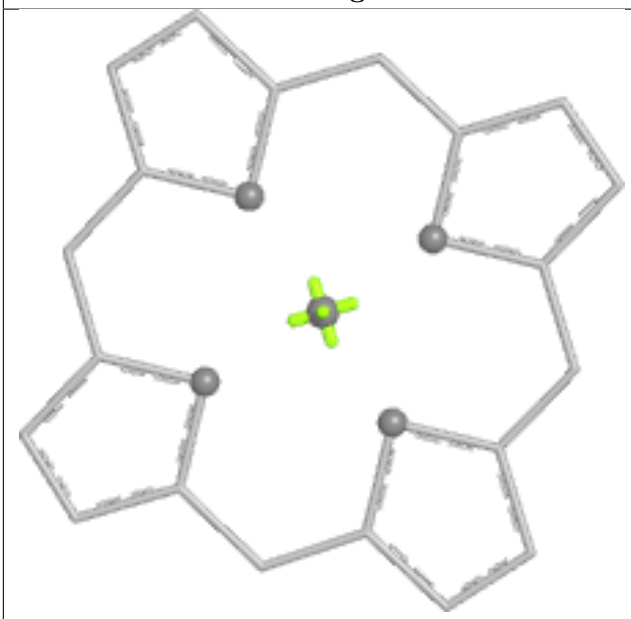
Ligand CLA B 1234



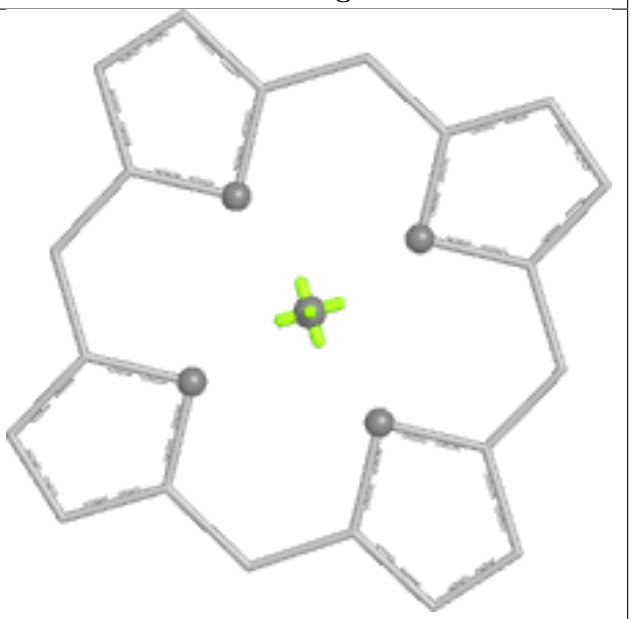
Bond lengths



Bond angles

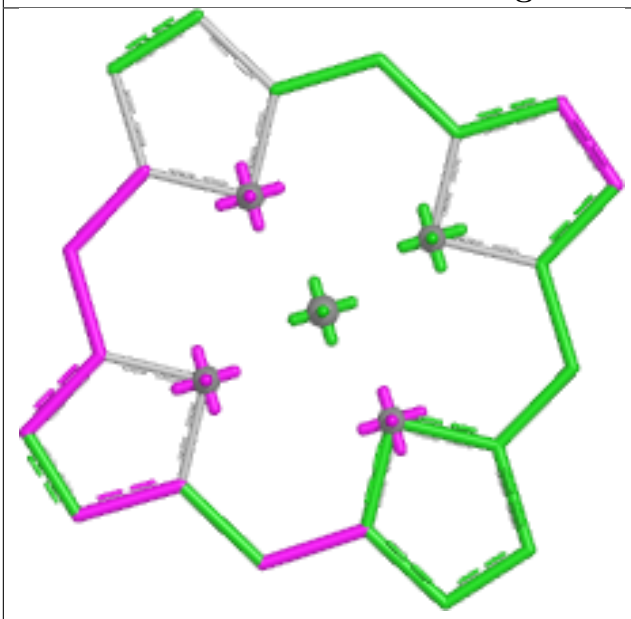


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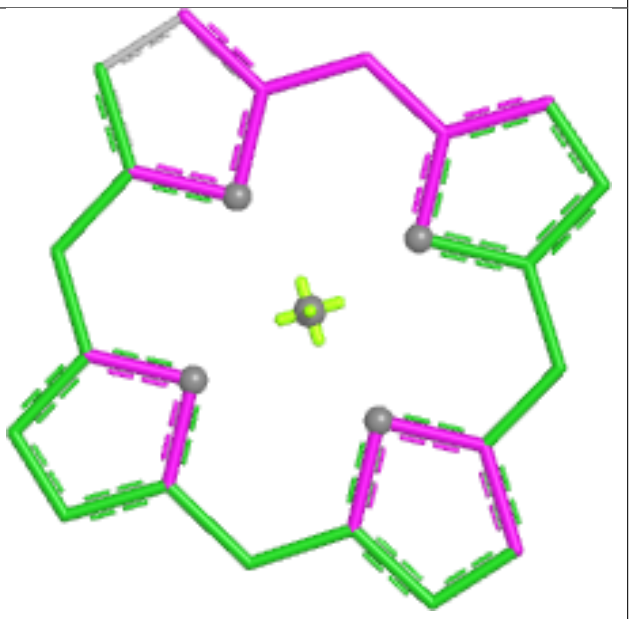


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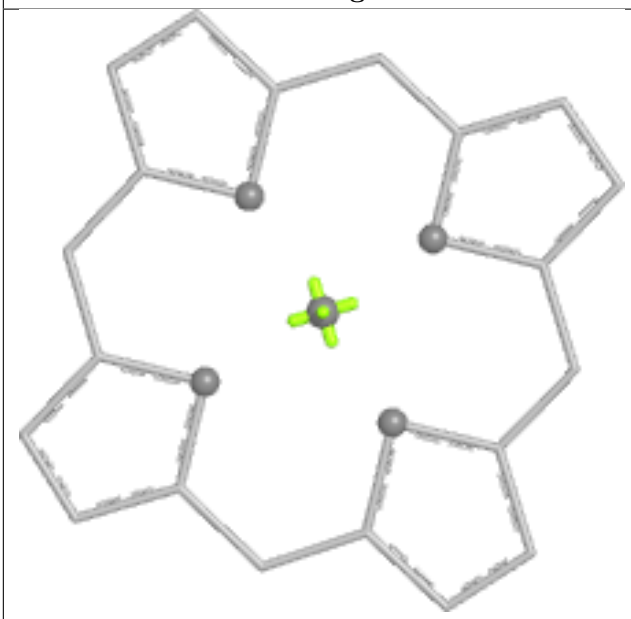
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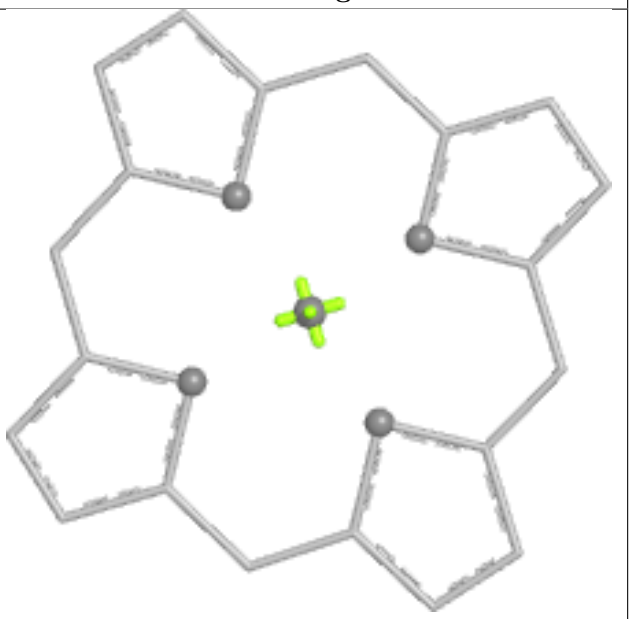
Bond lengths



Bond angles

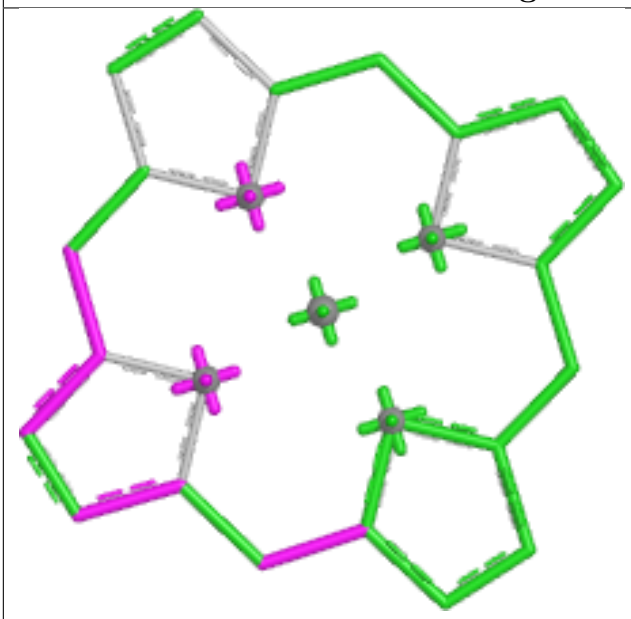


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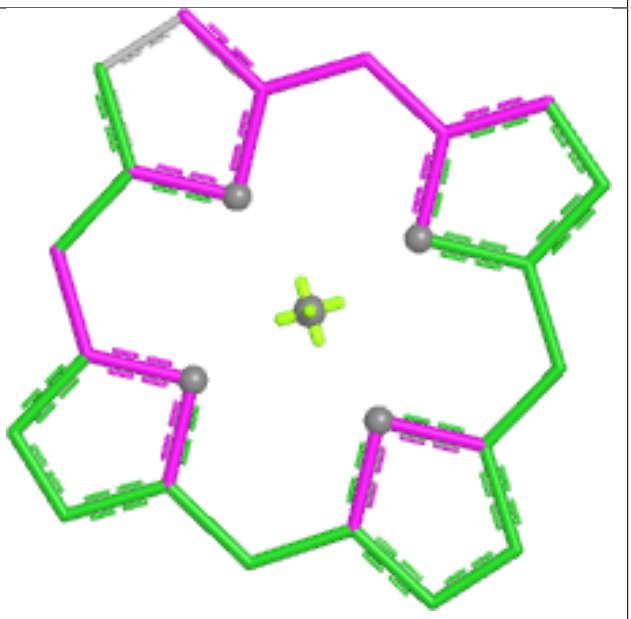


Rings

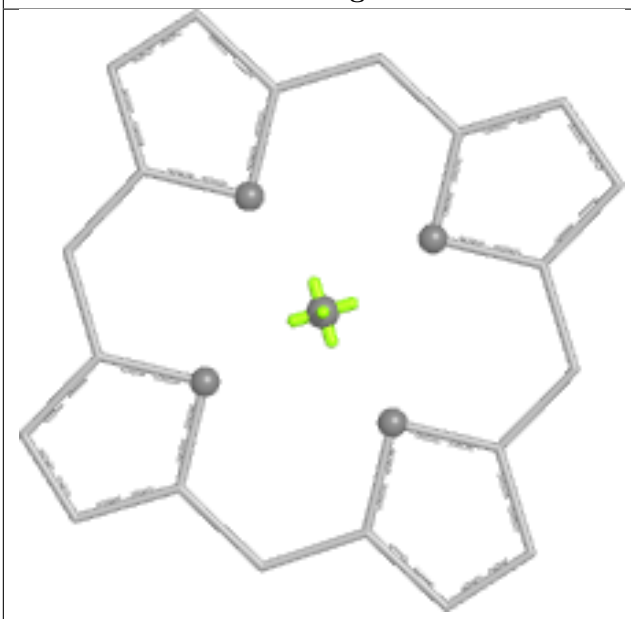
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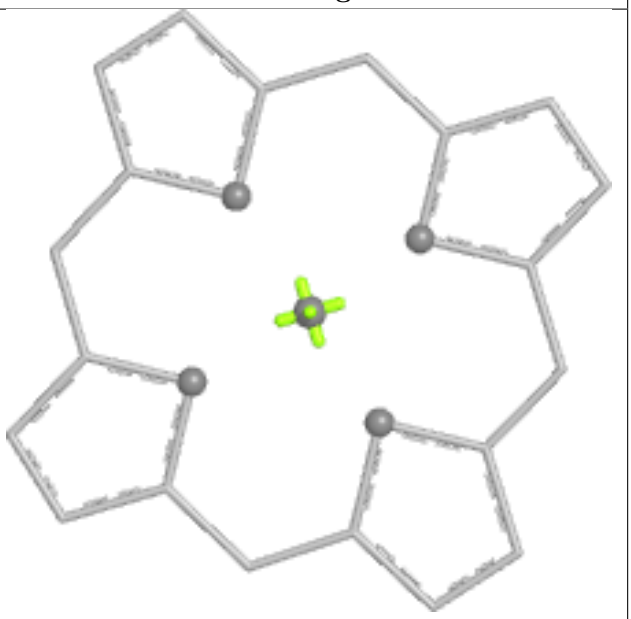
Bond lengths



Bond angles

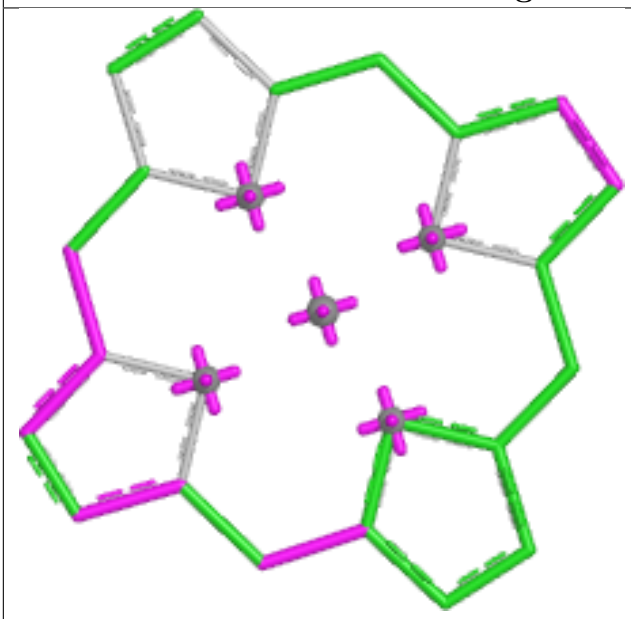


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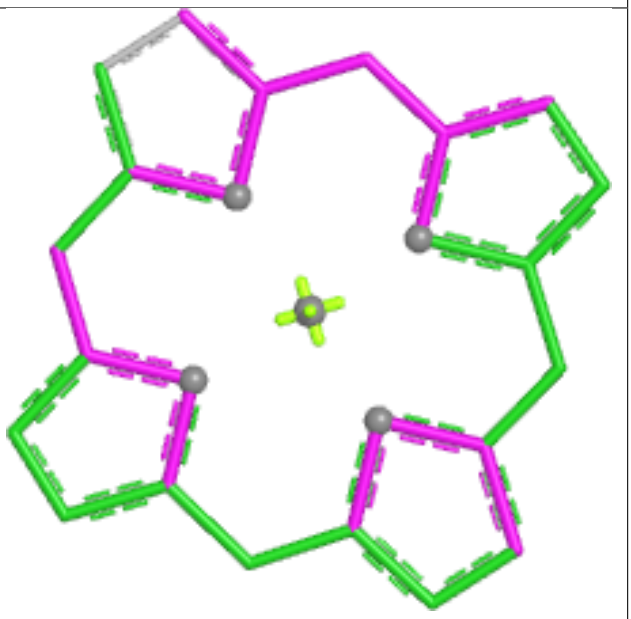


Rings

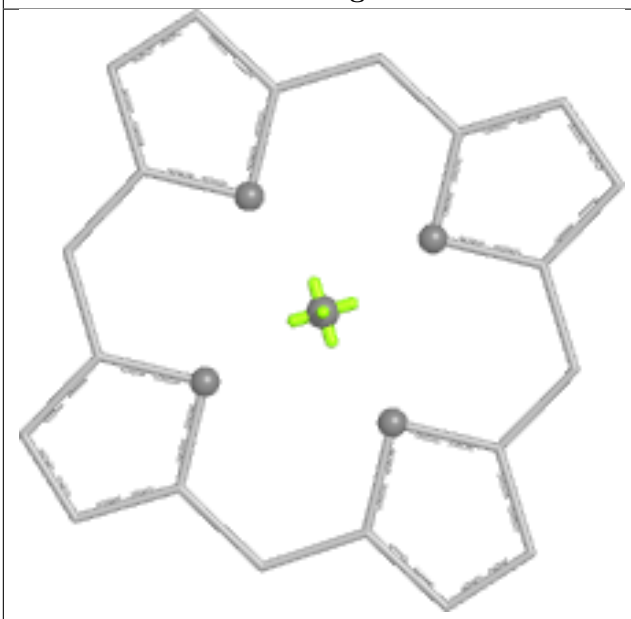
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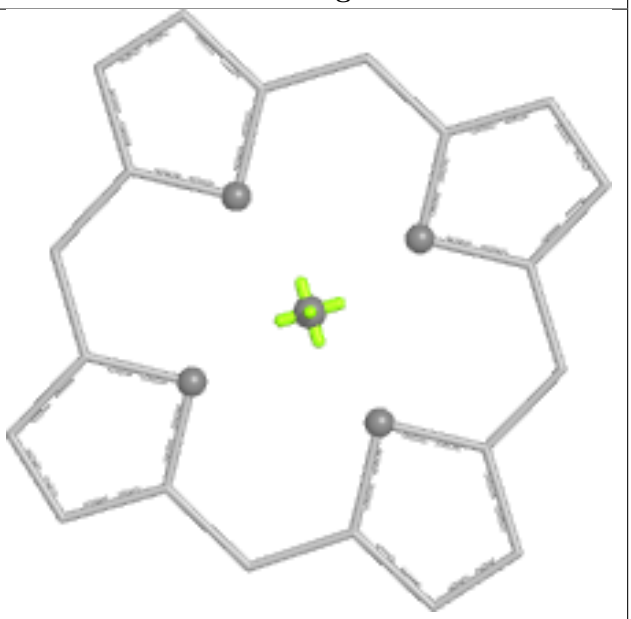
Bond lengths



Bond angles

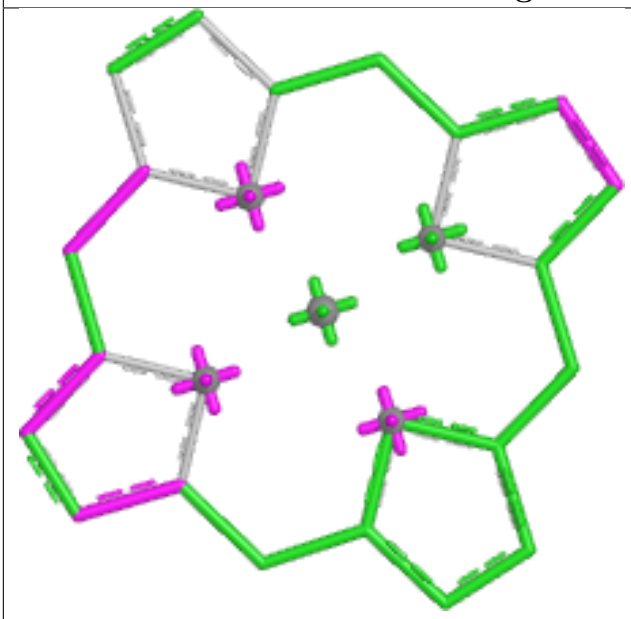


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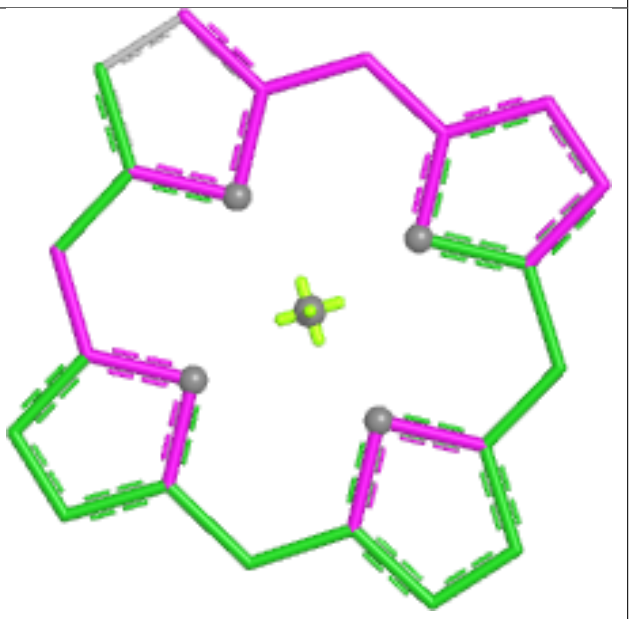


Rings

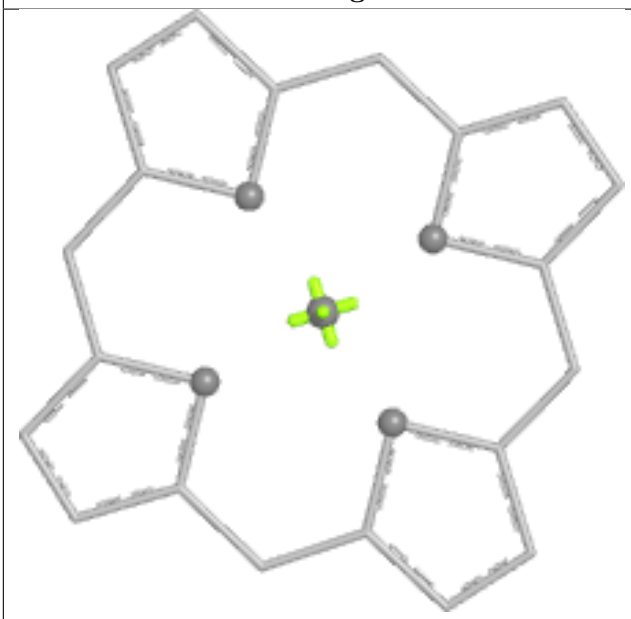
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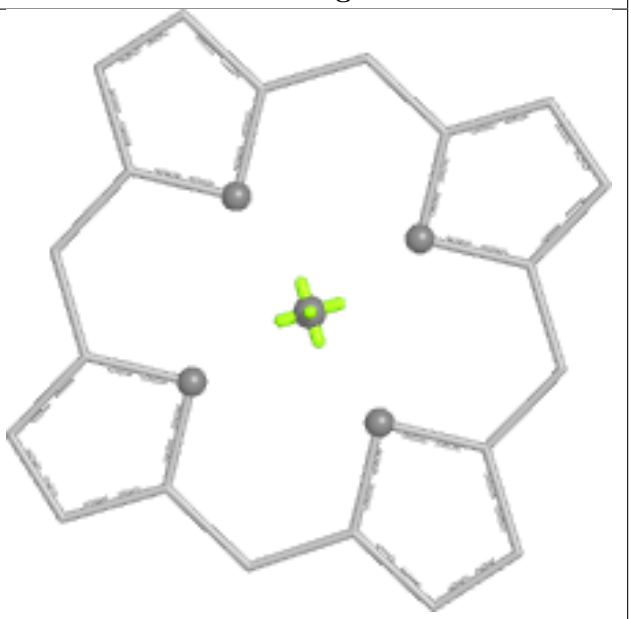
Bond lengths



Bond angles

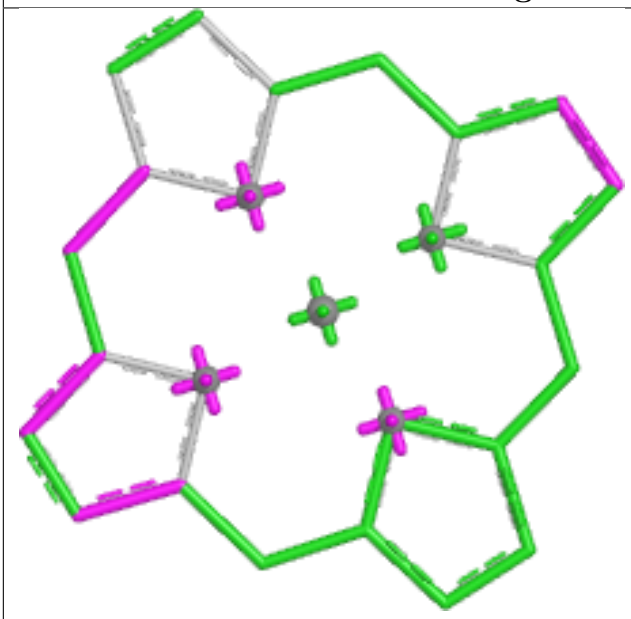


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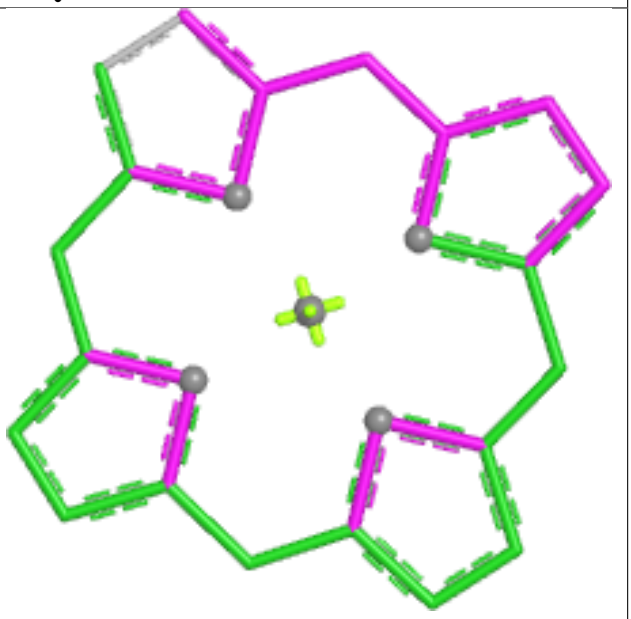


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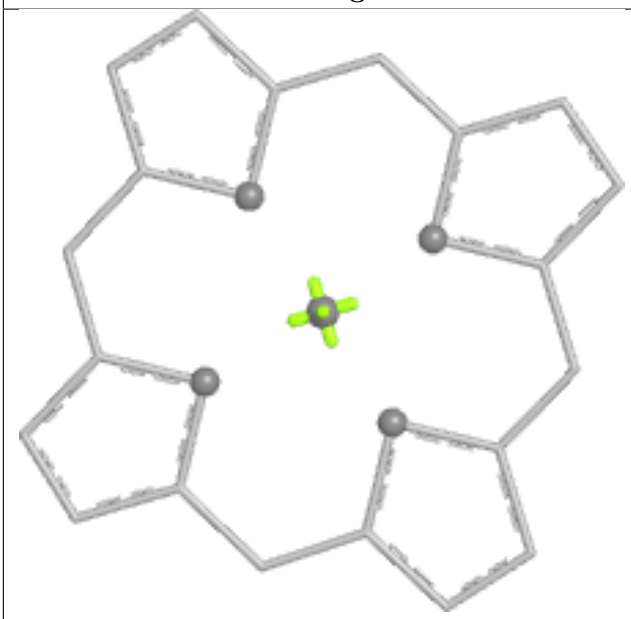
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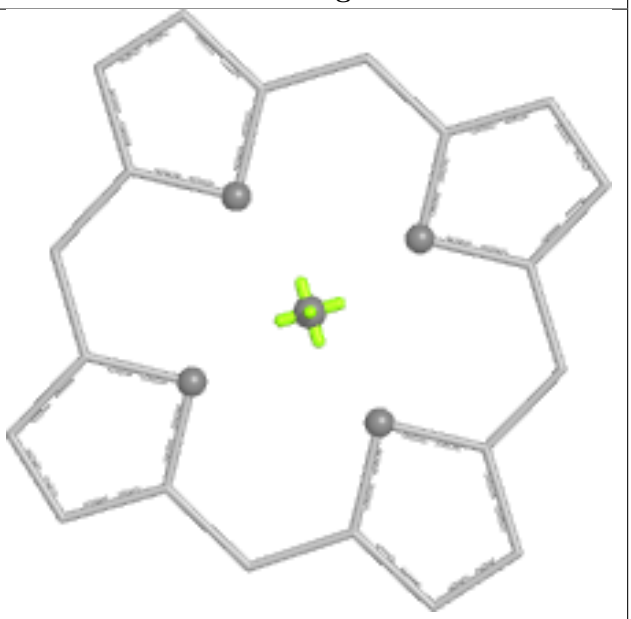
Bond lengths



Bond angles

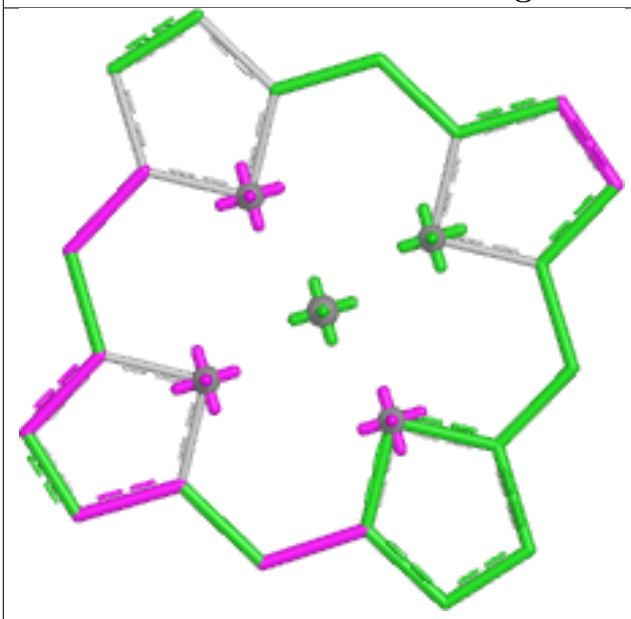


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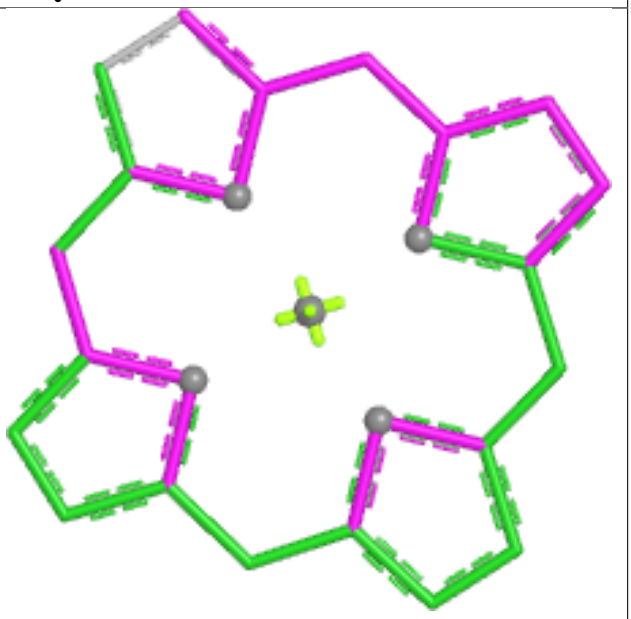


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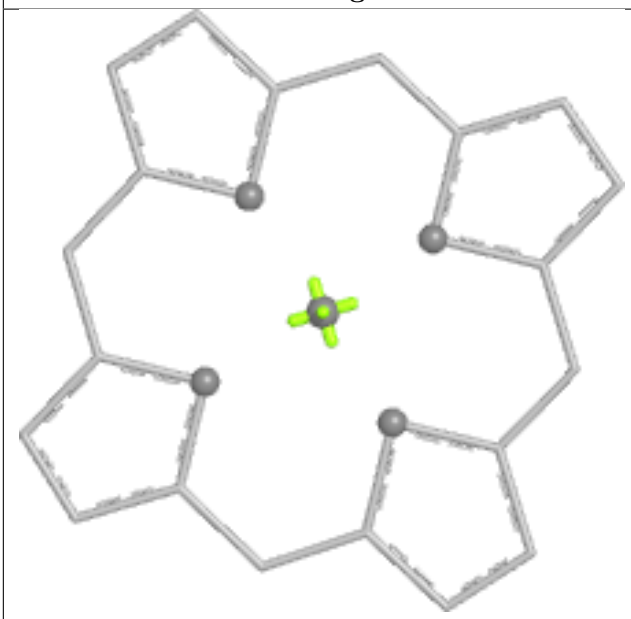
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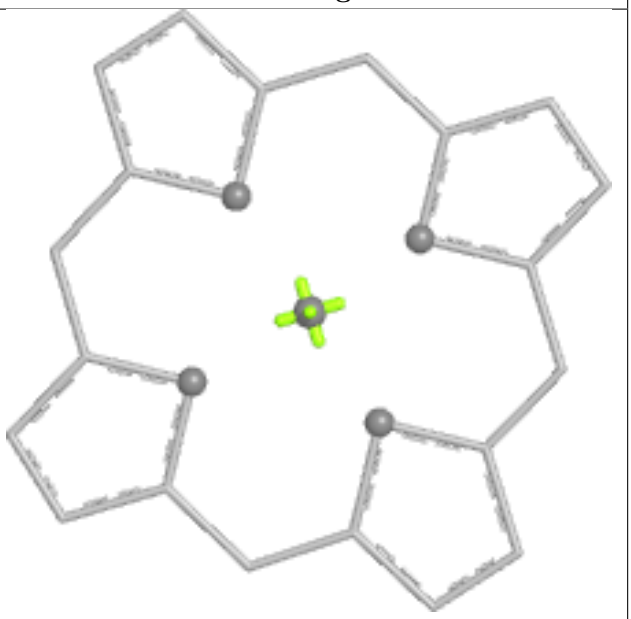
Bond lengths



Bond angles

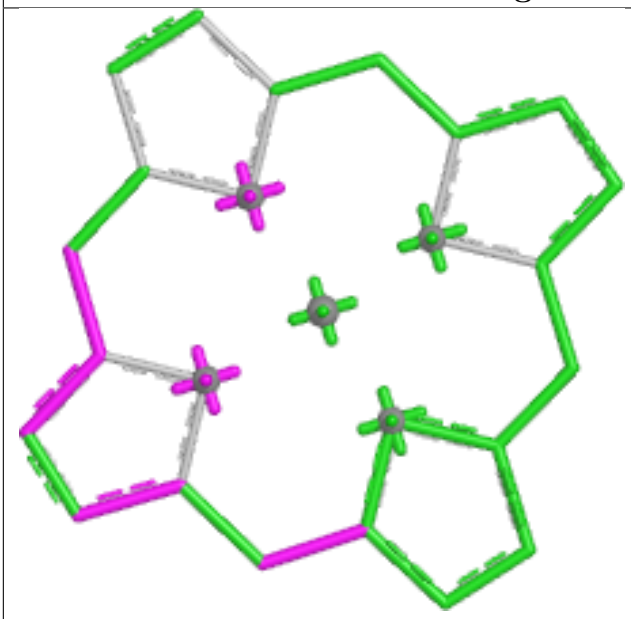


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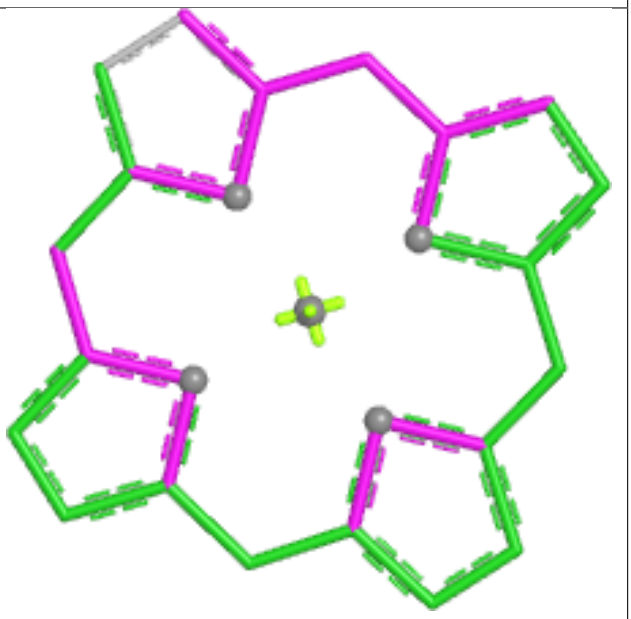


Rings

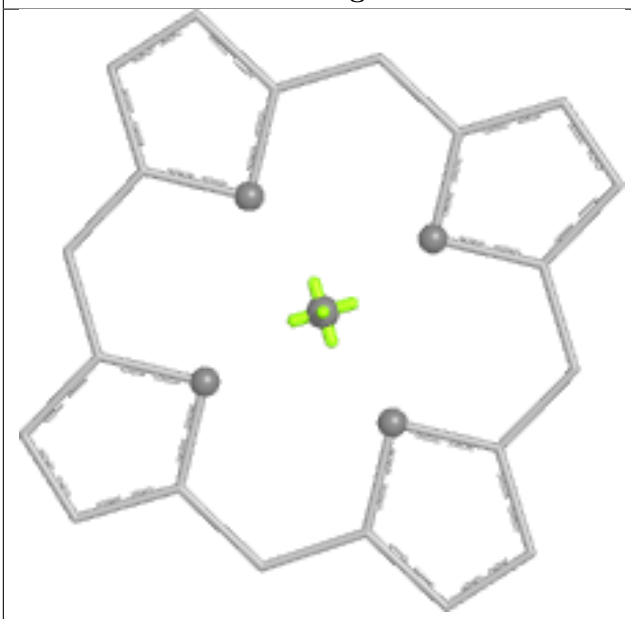
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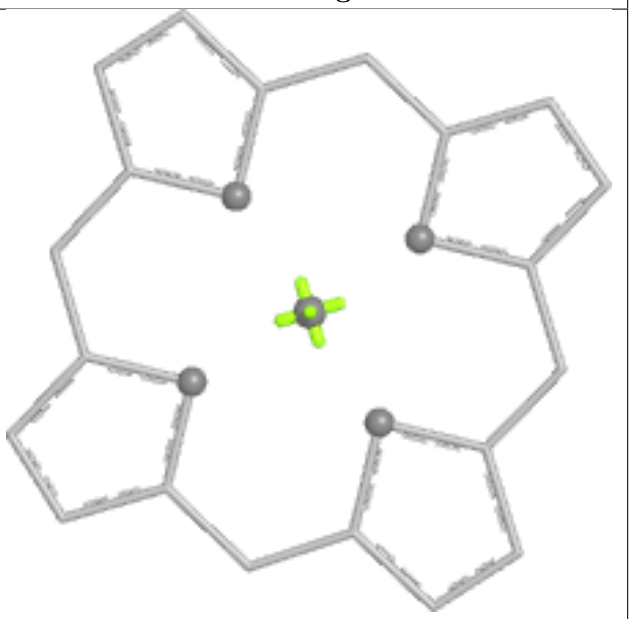
Bond lengths



Bond angles

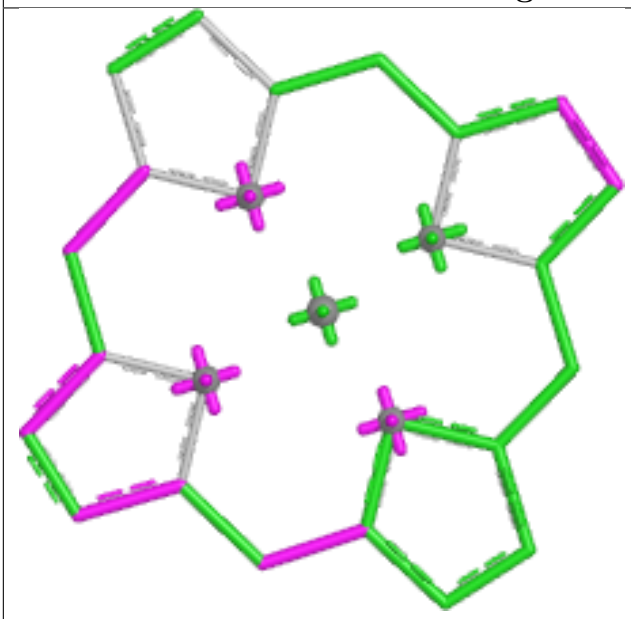


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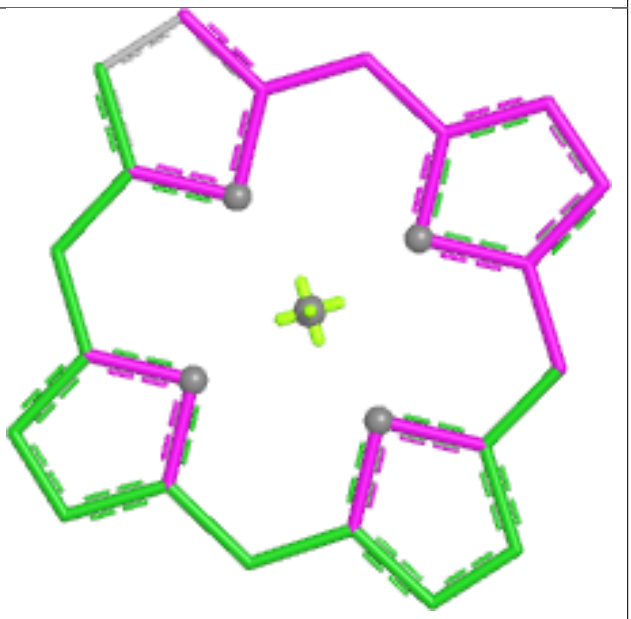


Rings

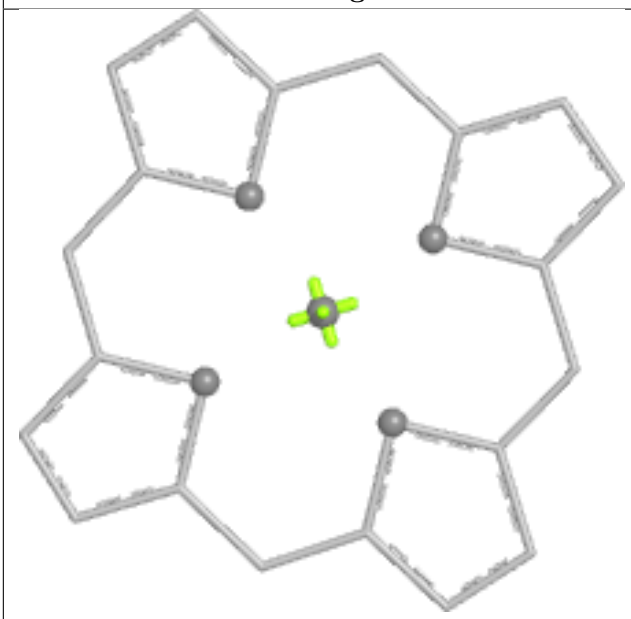
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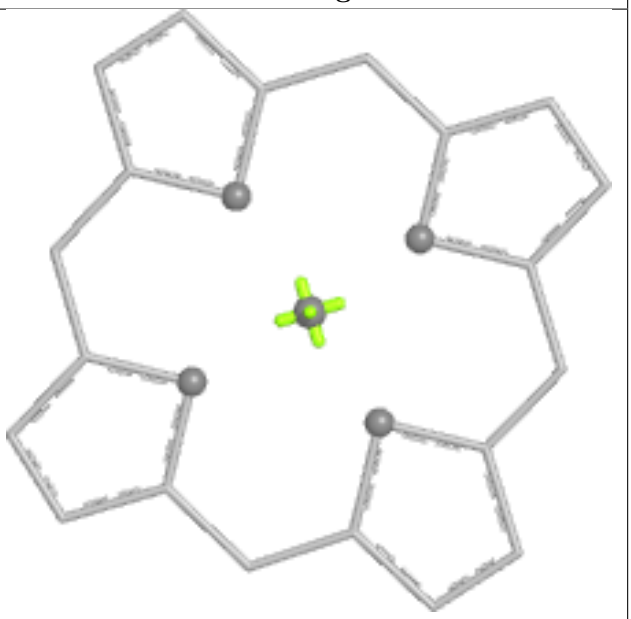
Bond lengths



Bond angles

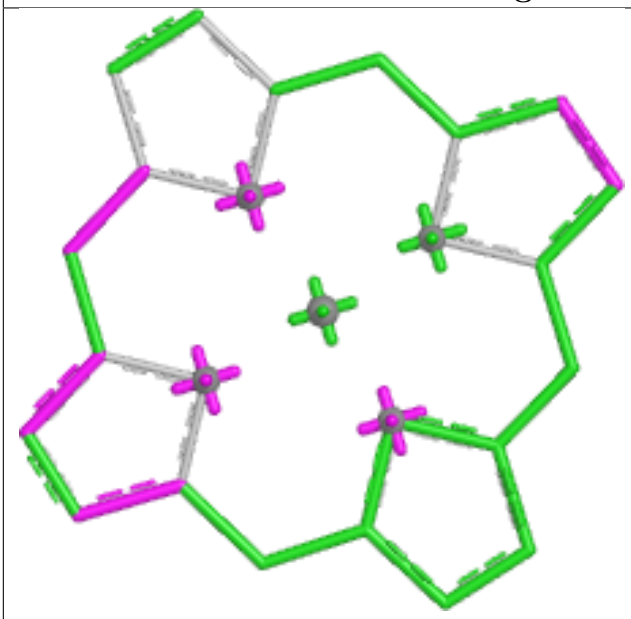


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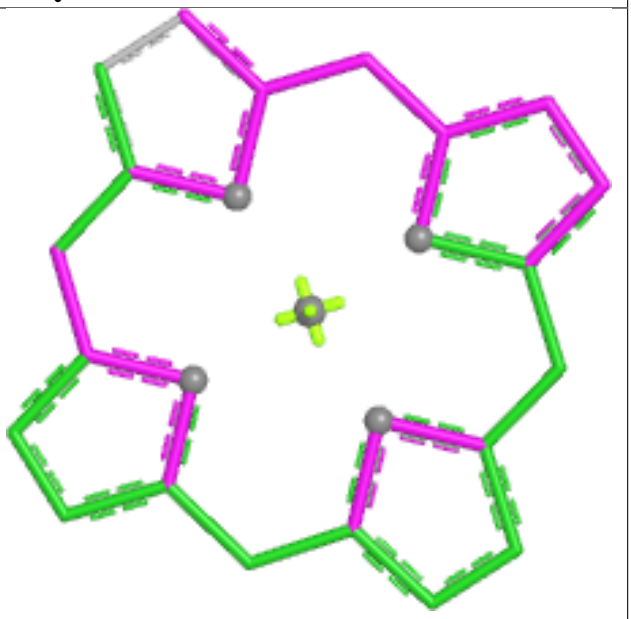


Rings

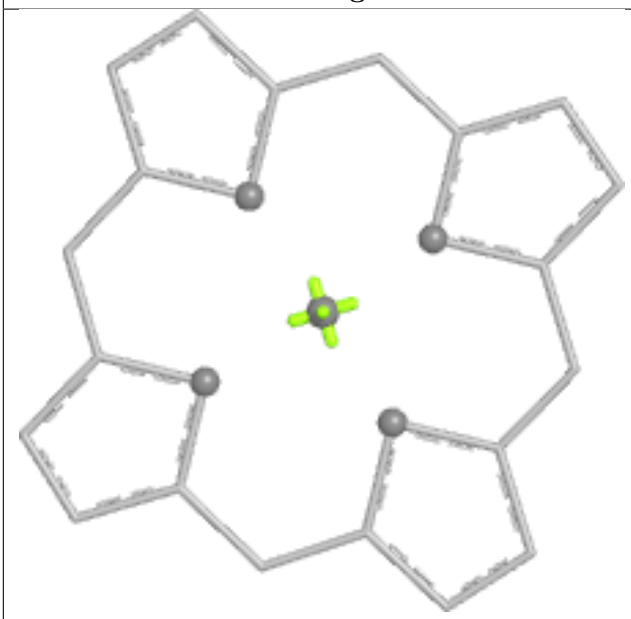
Ligand CLA Q 5226



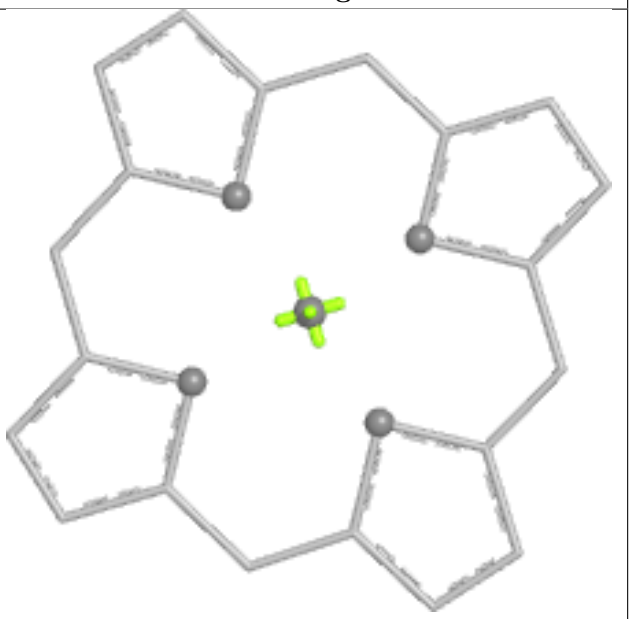
Bond lengths



Bond angles

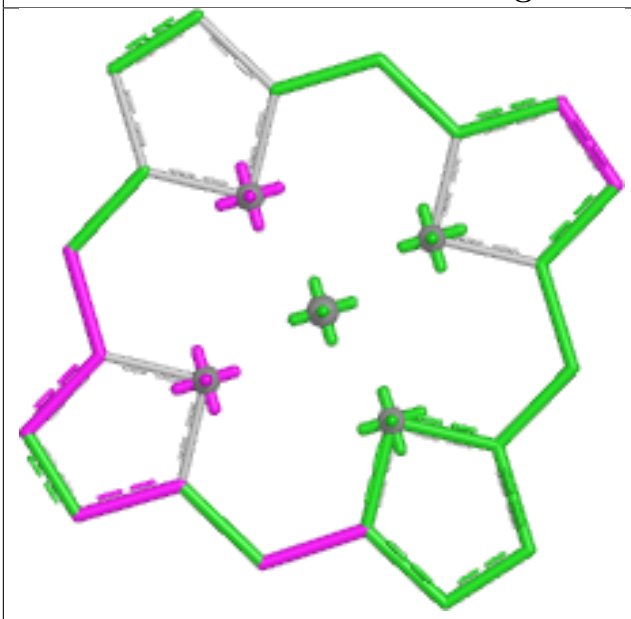


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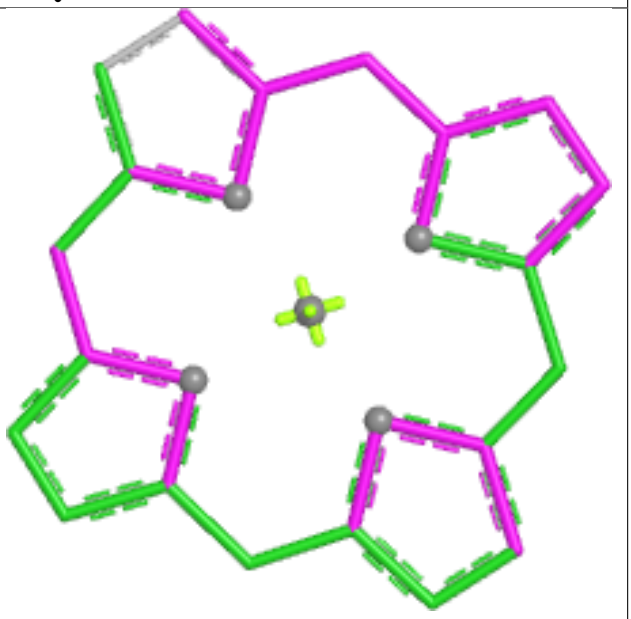


Rings

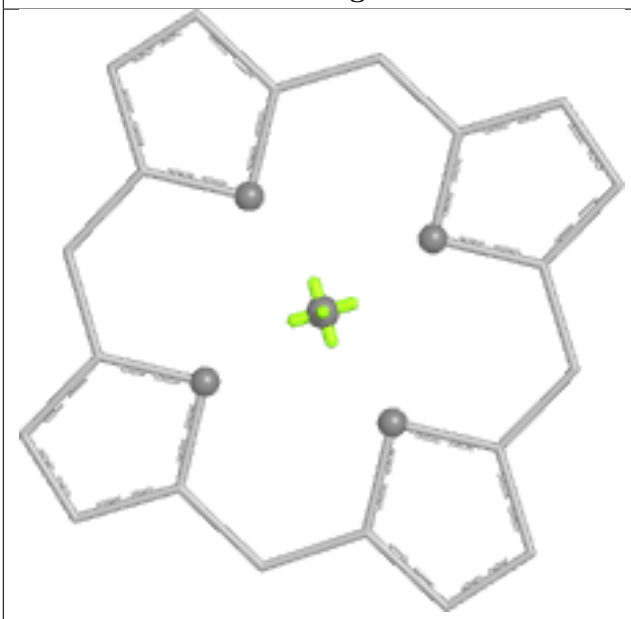
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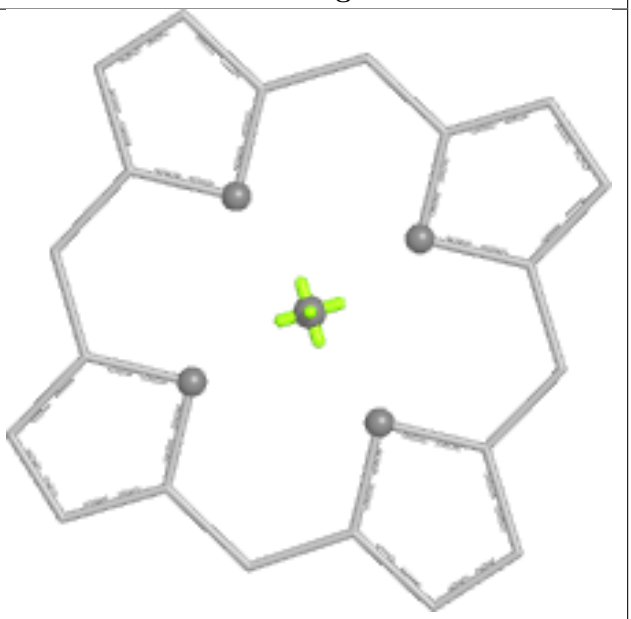
Bond lengths



Bond angles

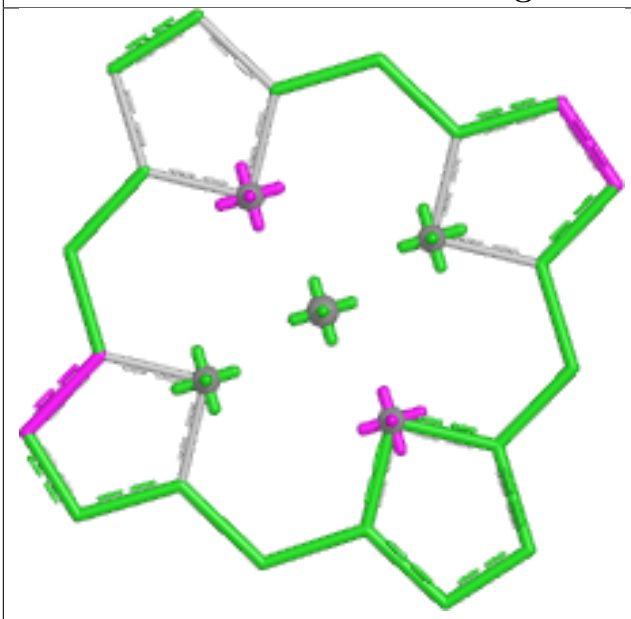


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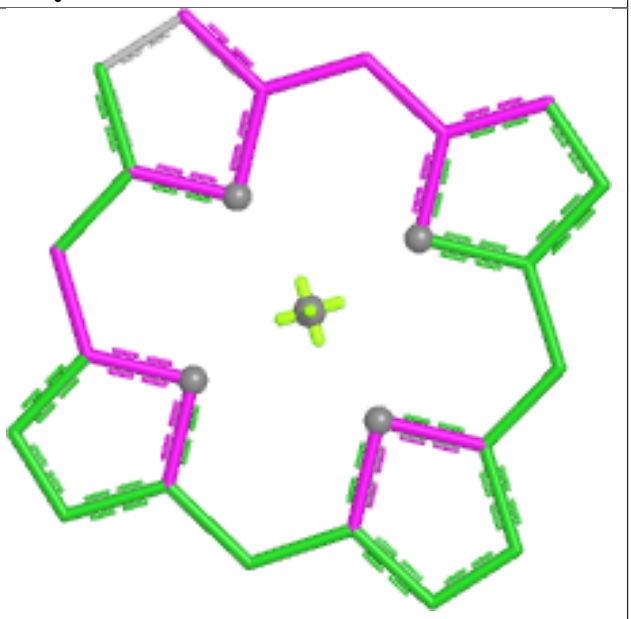


Rings

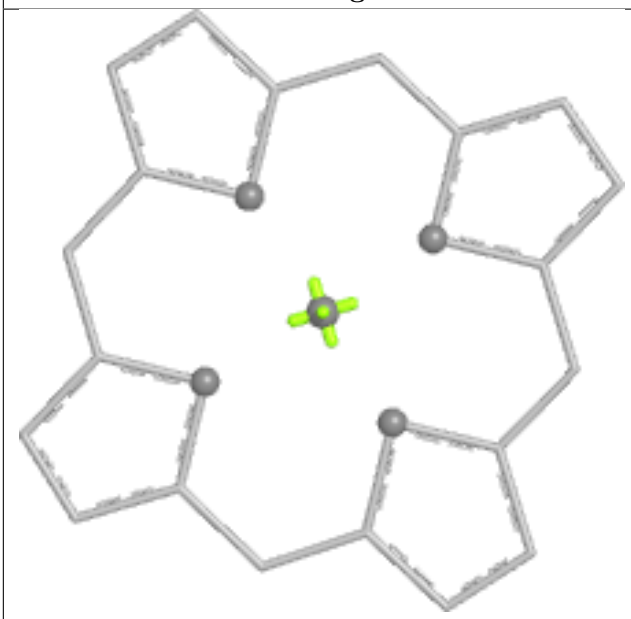
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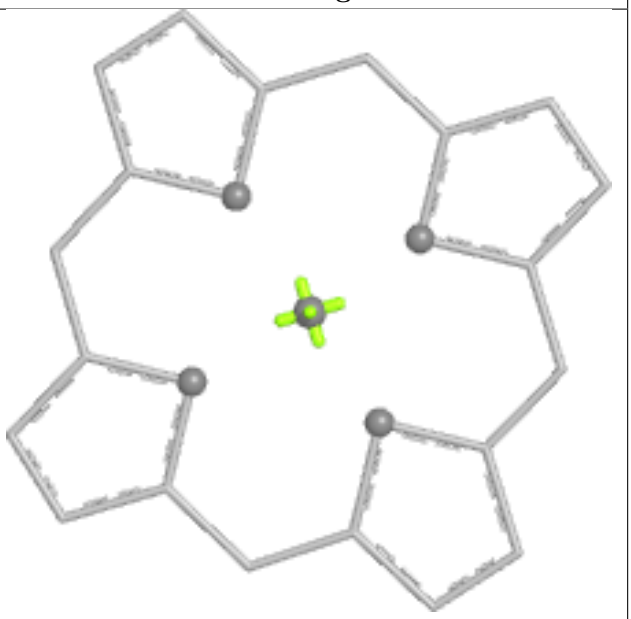
Bond lengths



Bond angles

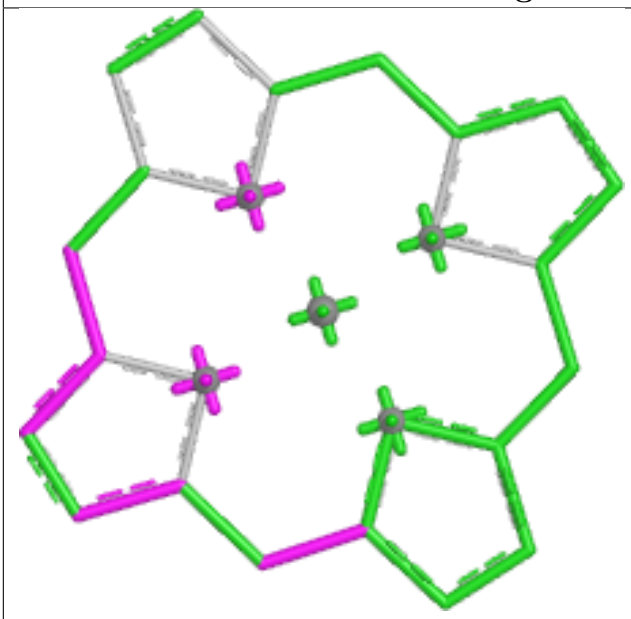


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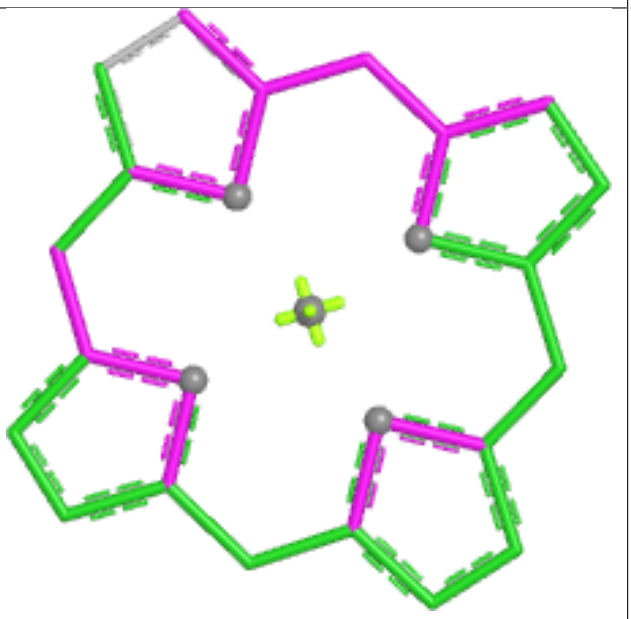


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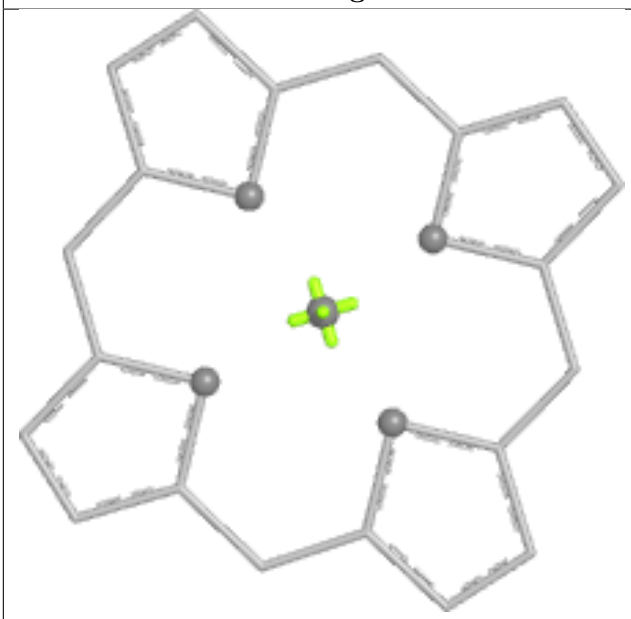
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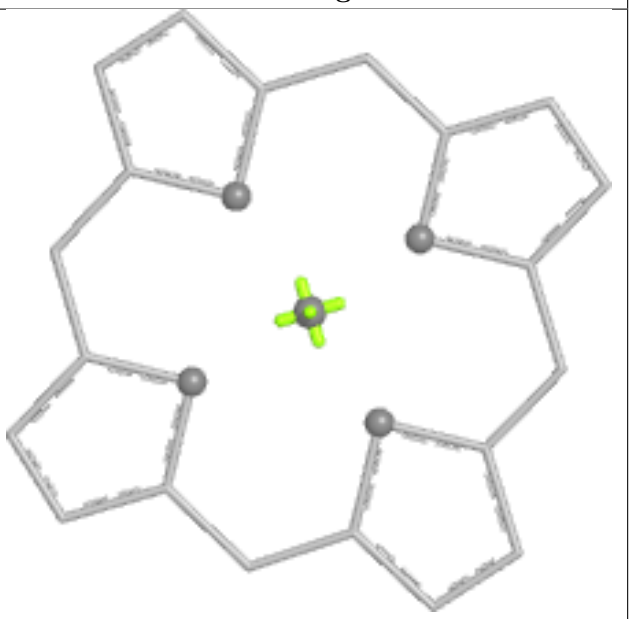
Bond lengths



Bond angles

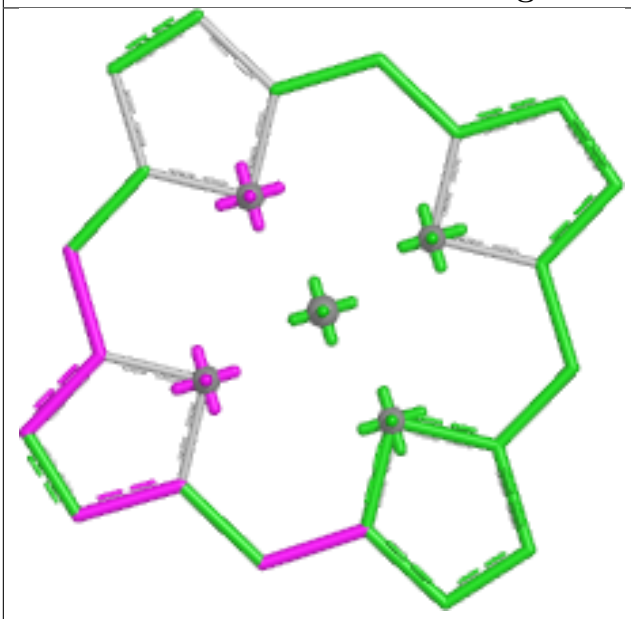


Torsions

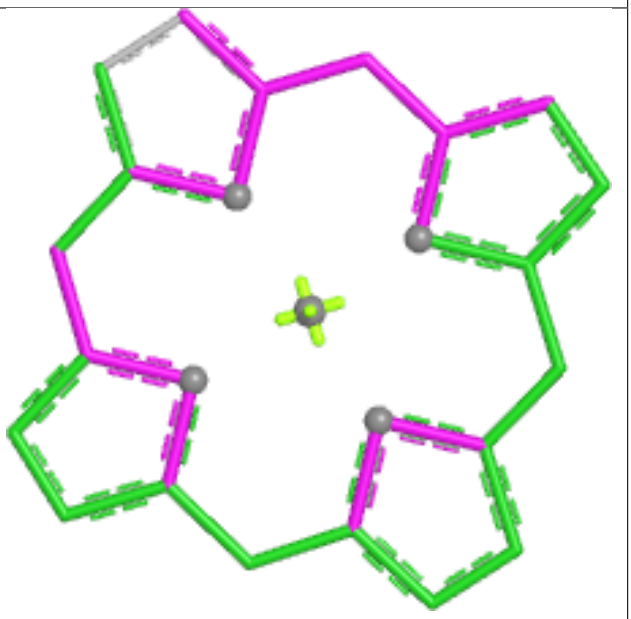


Rings

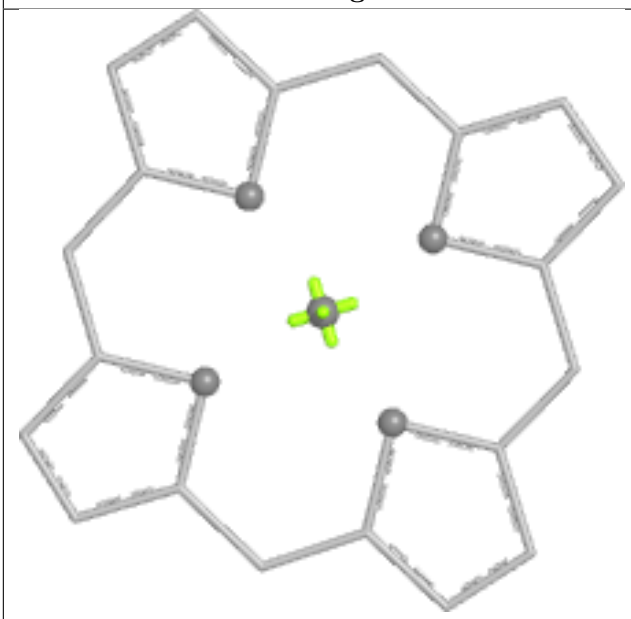
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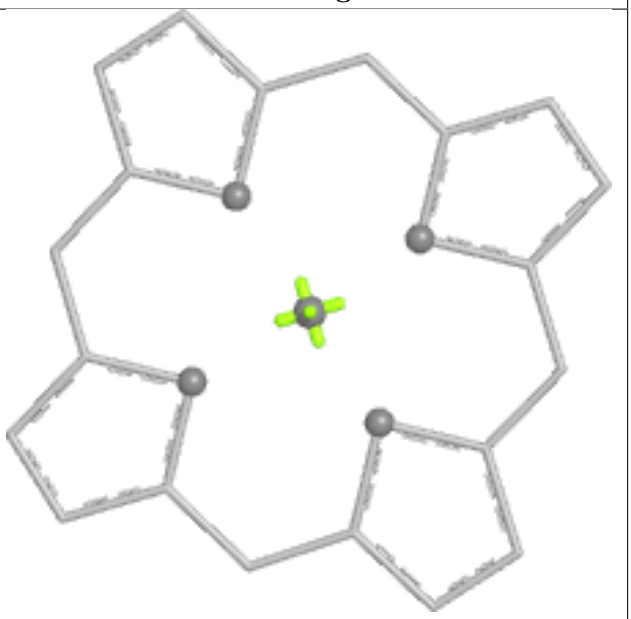
Bond lengths



Bond angles

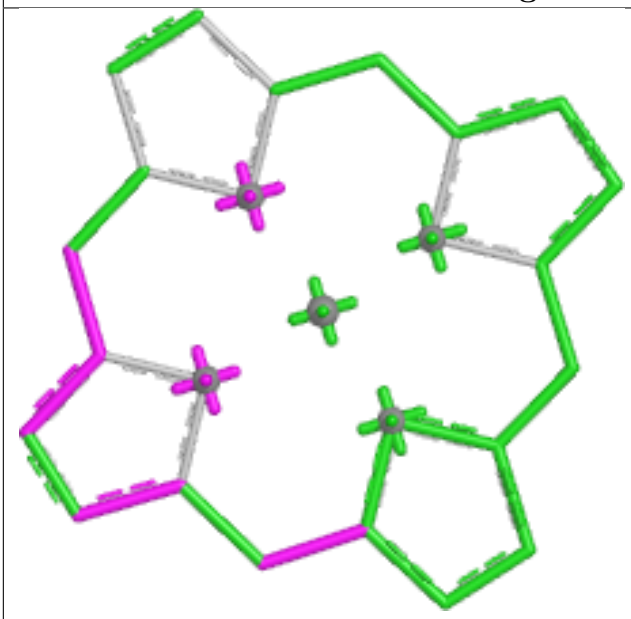


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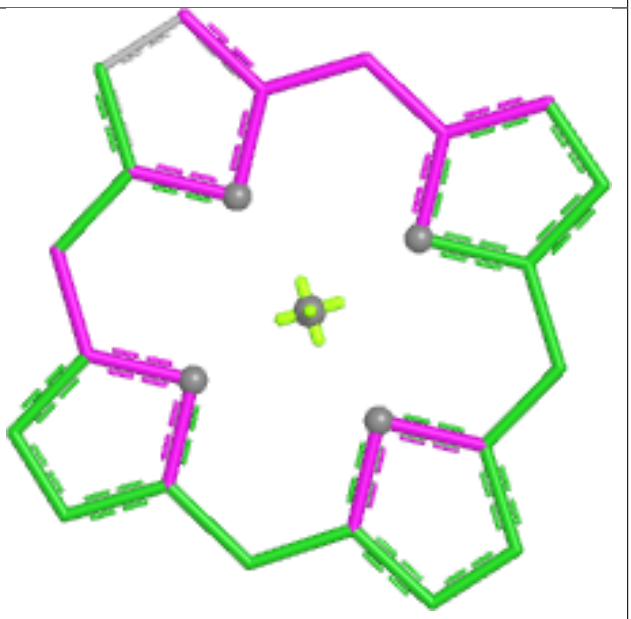


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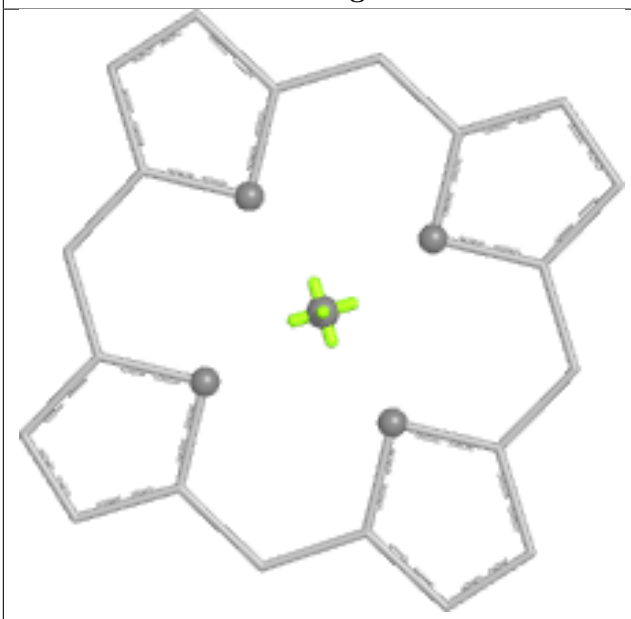
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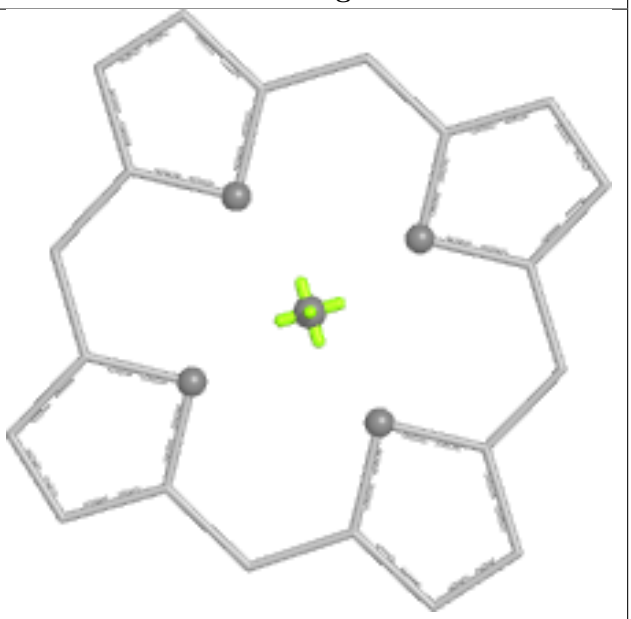
Bond lengths



Bond angles

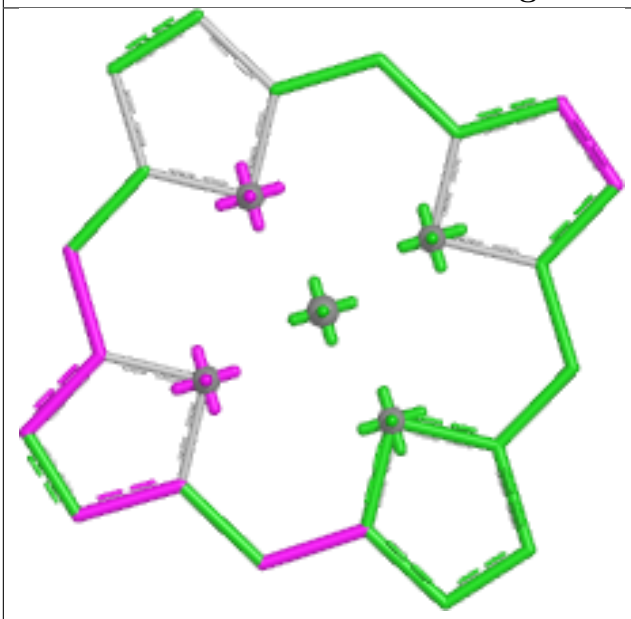


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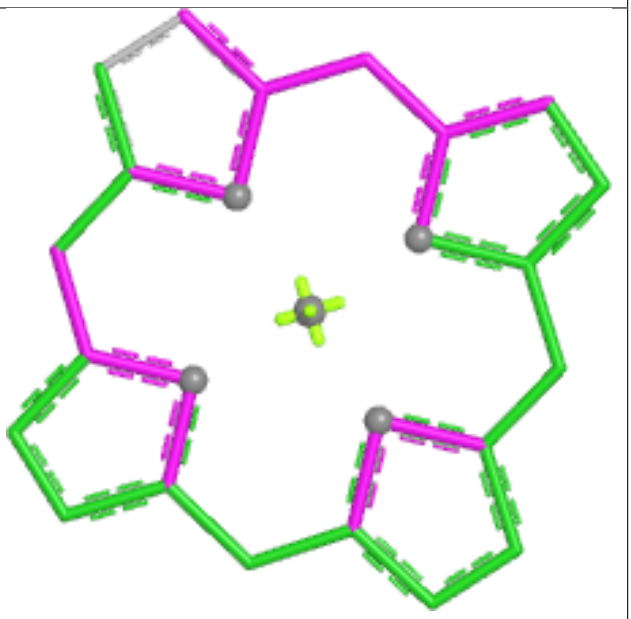


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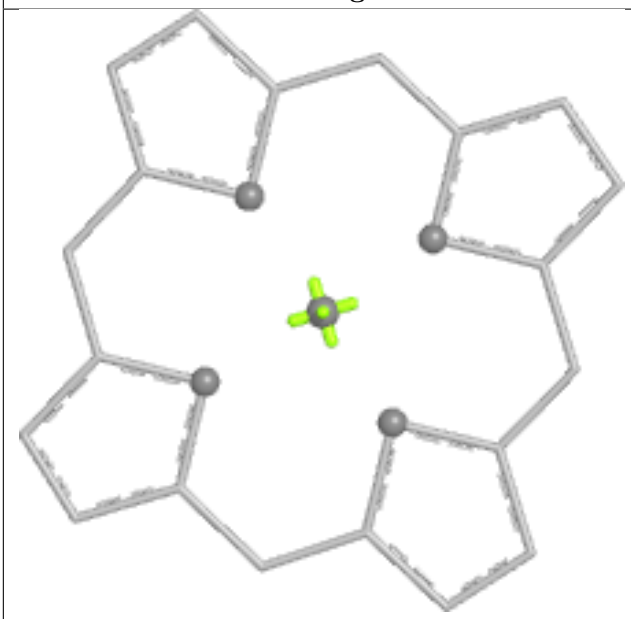
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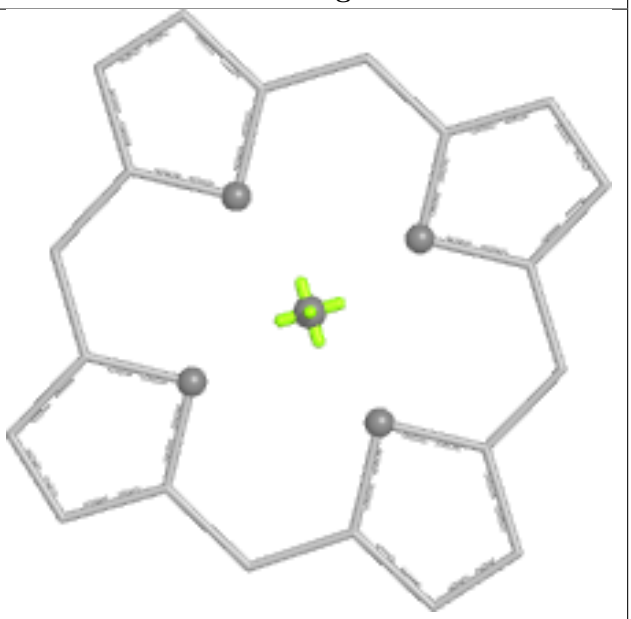
Bond lengths



Bond angles

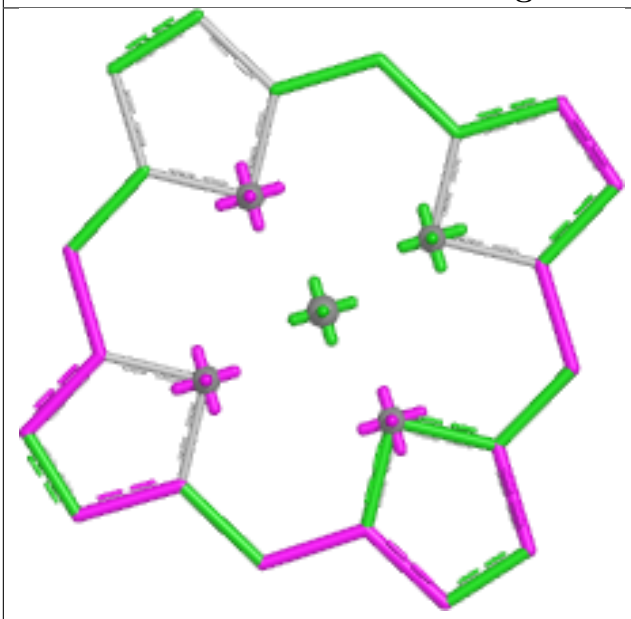


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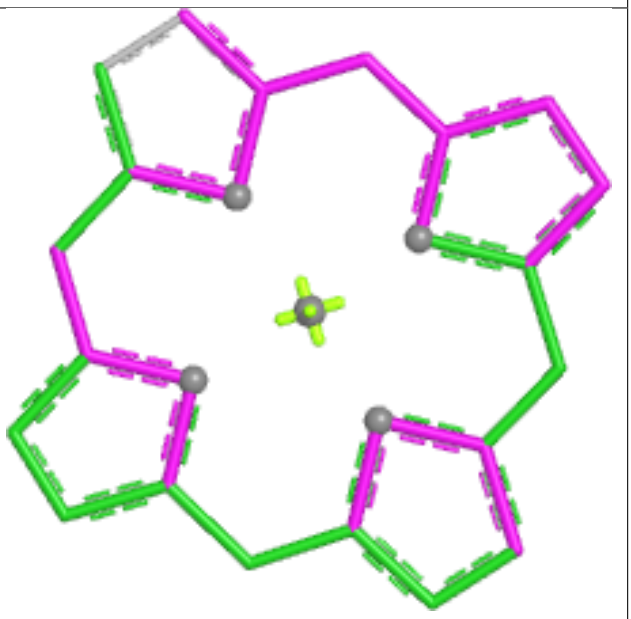


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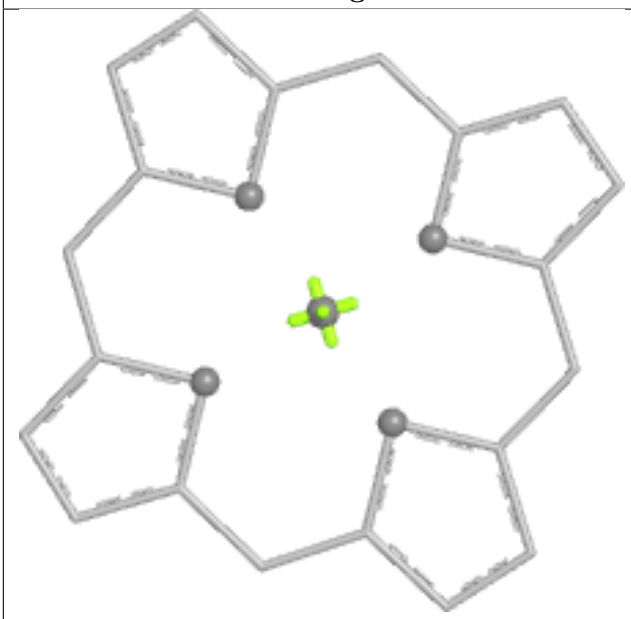
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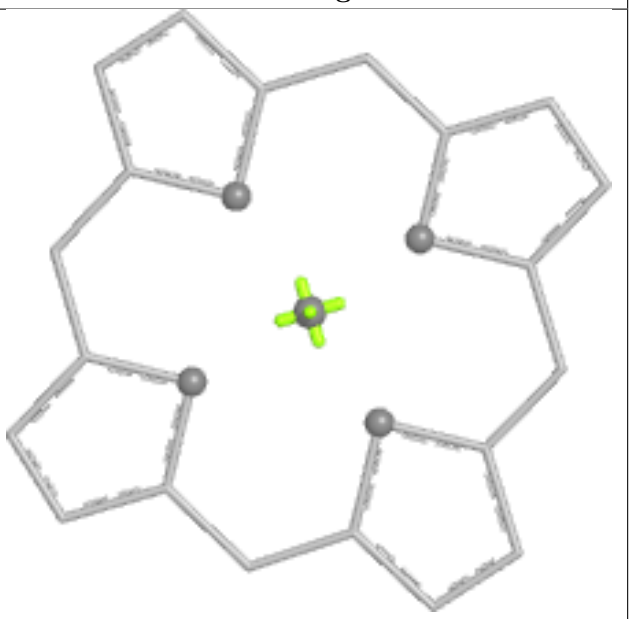
Bond lengths



Bond angles

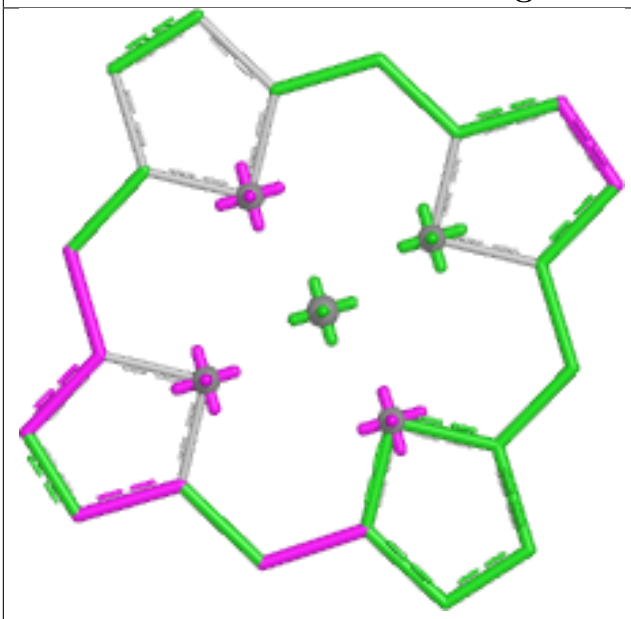


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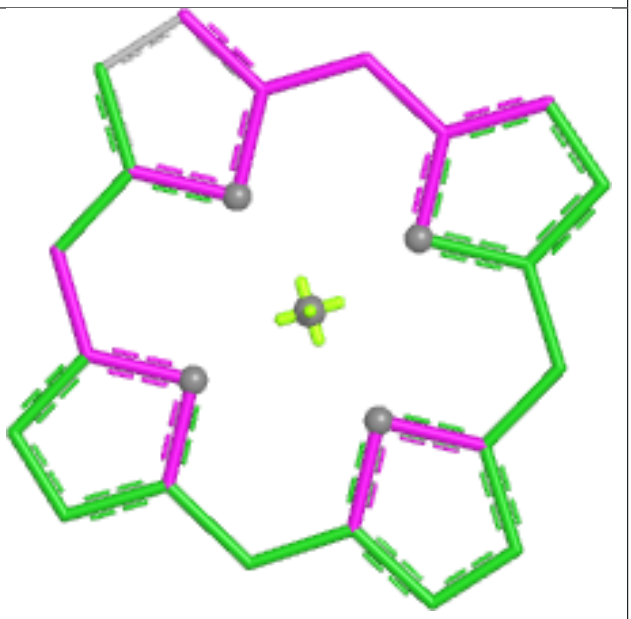


Rings

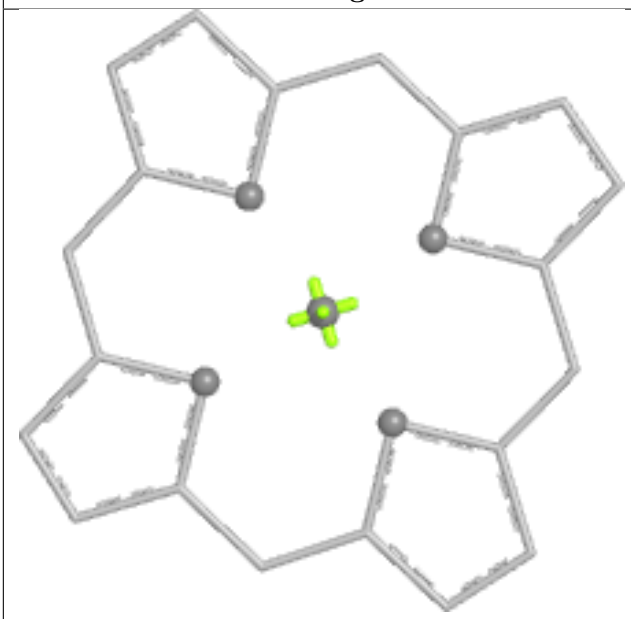
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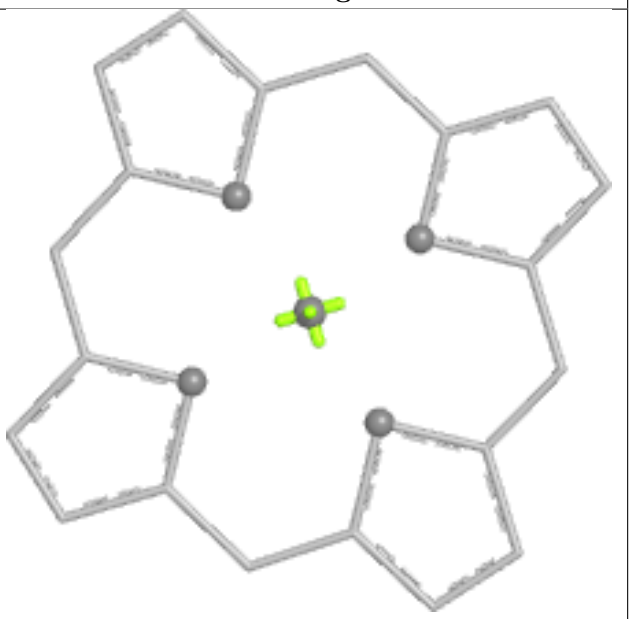
Bond lengths



Bond angles

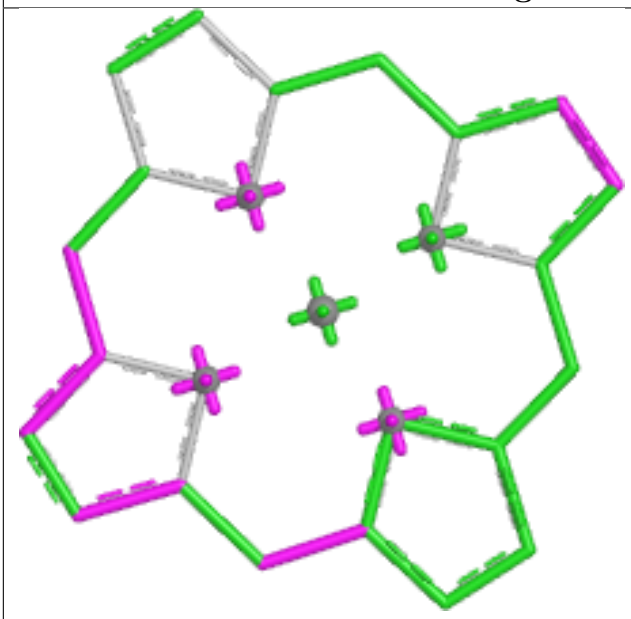


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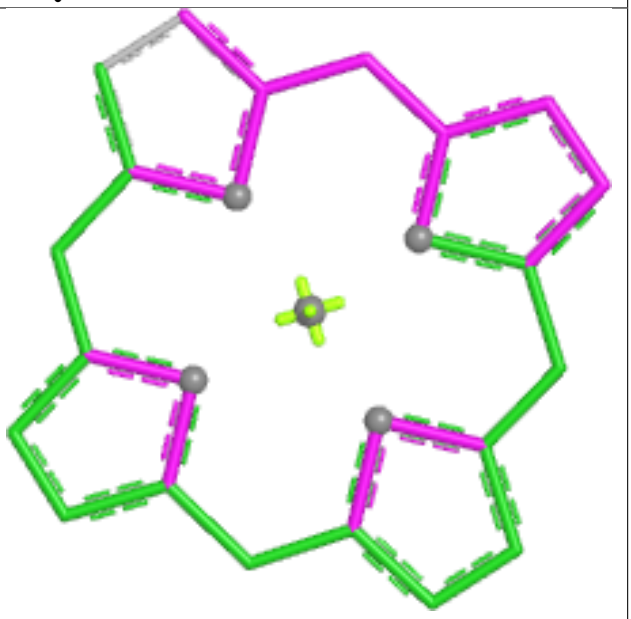


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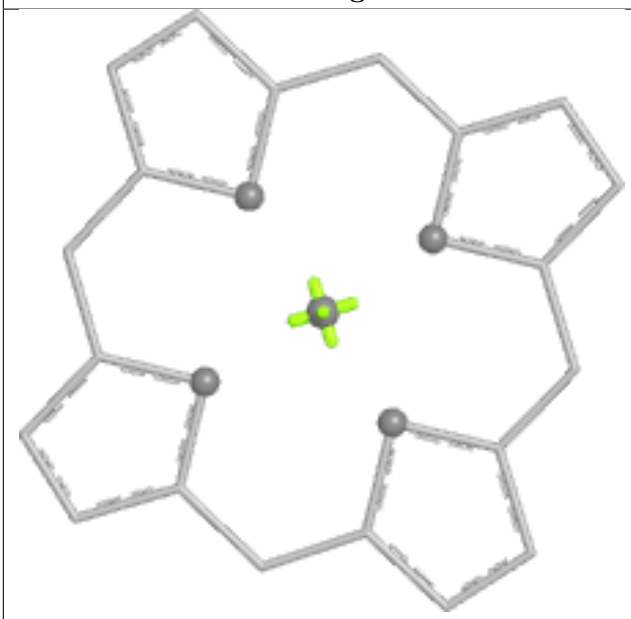
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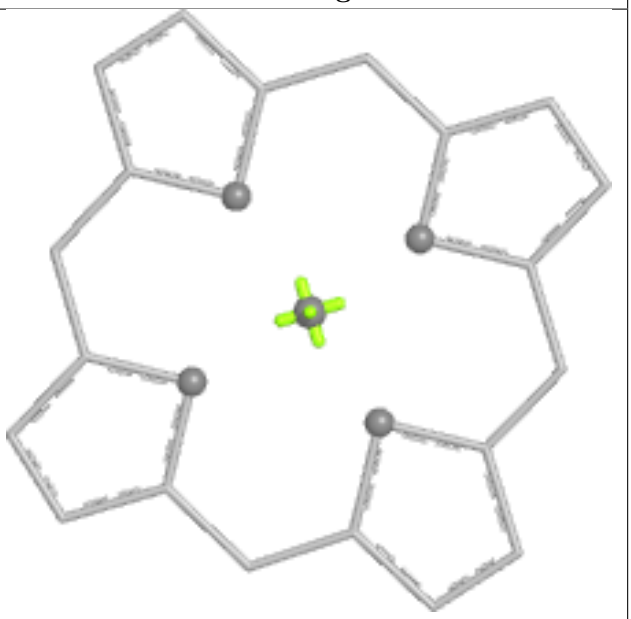
Bond lengths



Bond angles

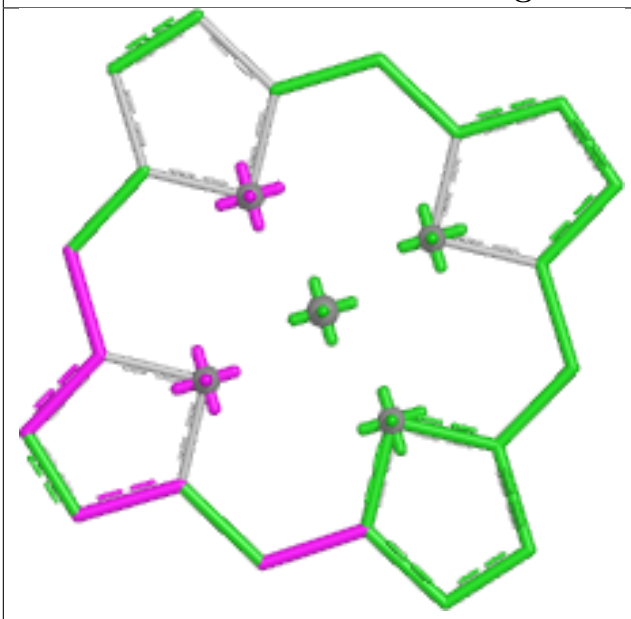


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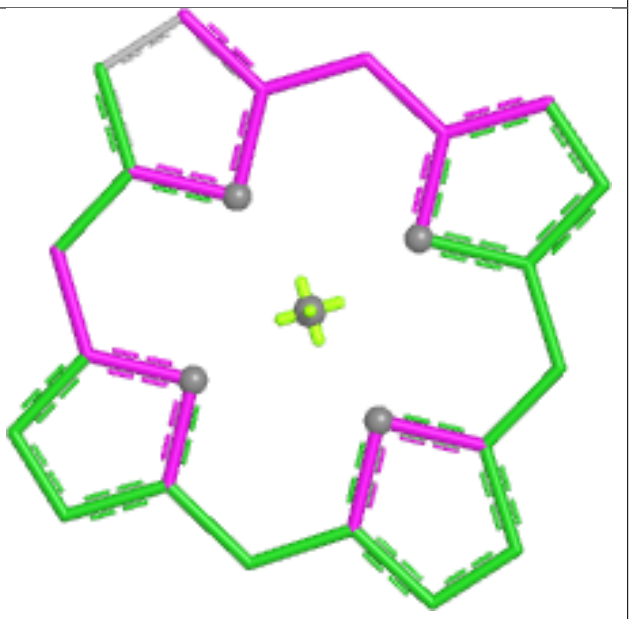


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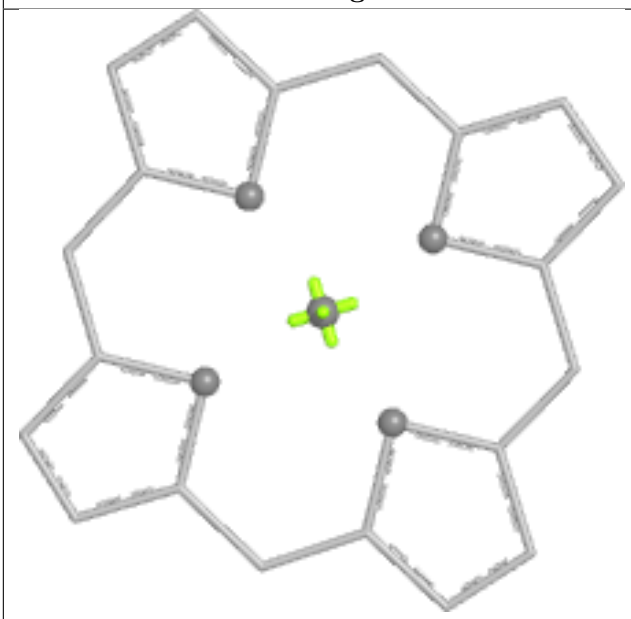
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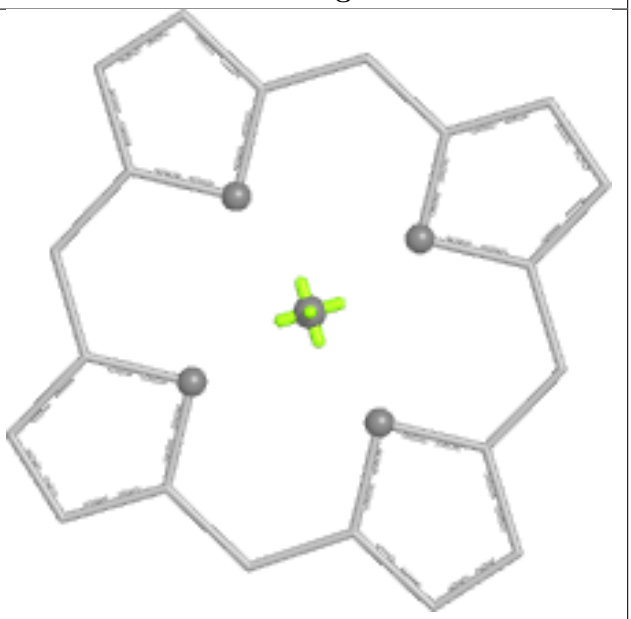
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Bond angles

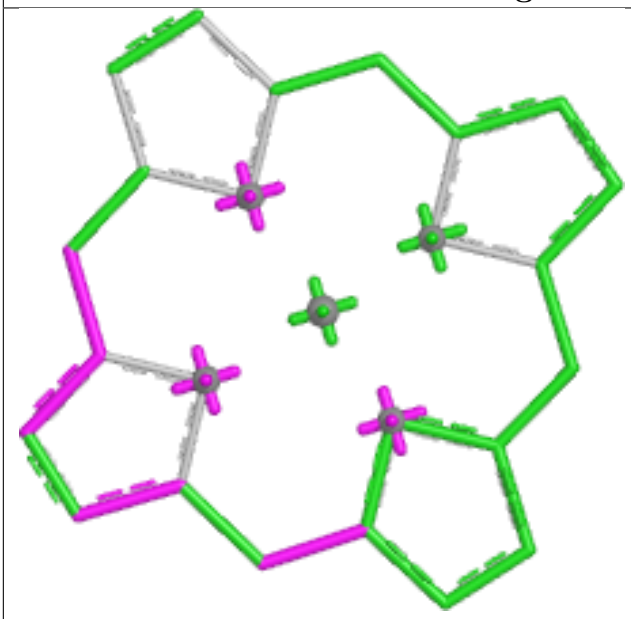


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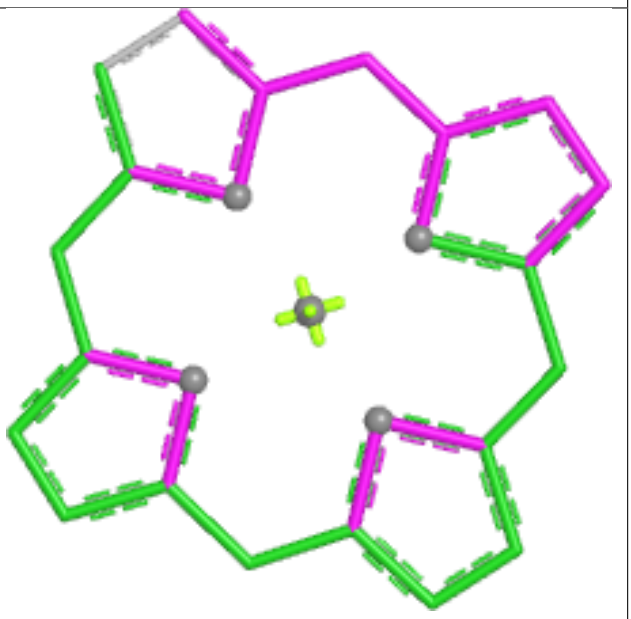


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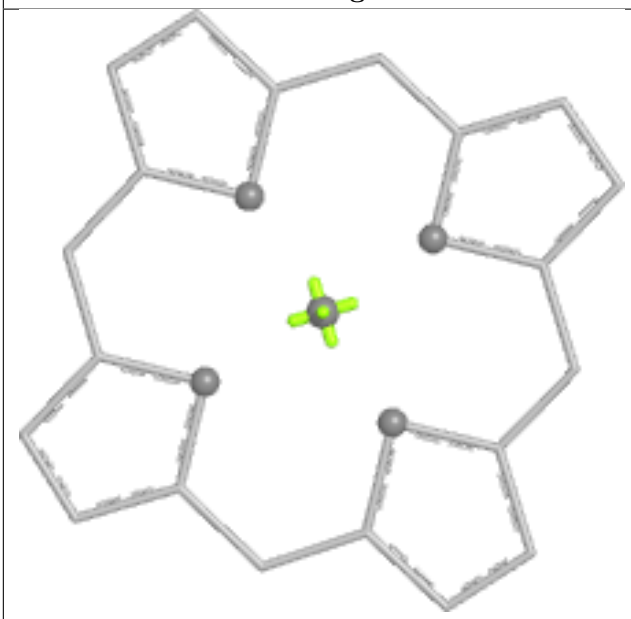
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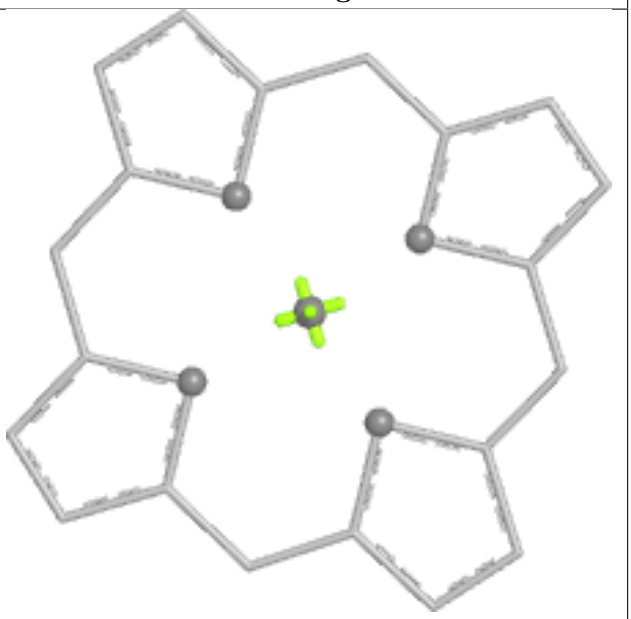
Bond lengths



Bond angles

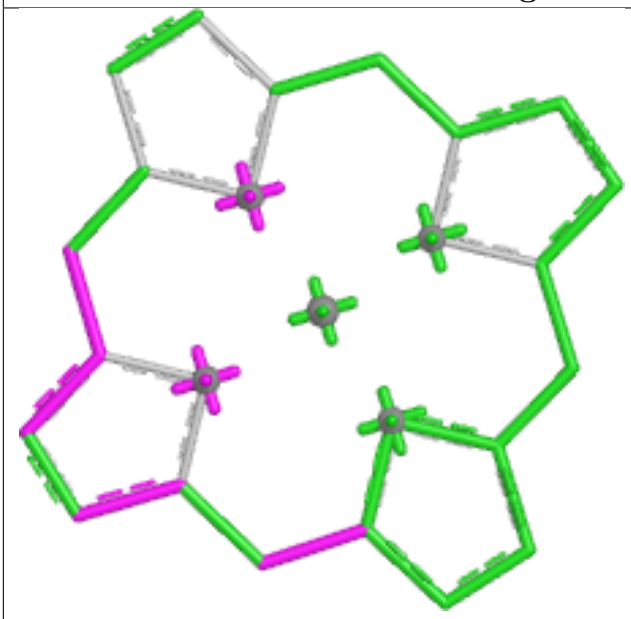


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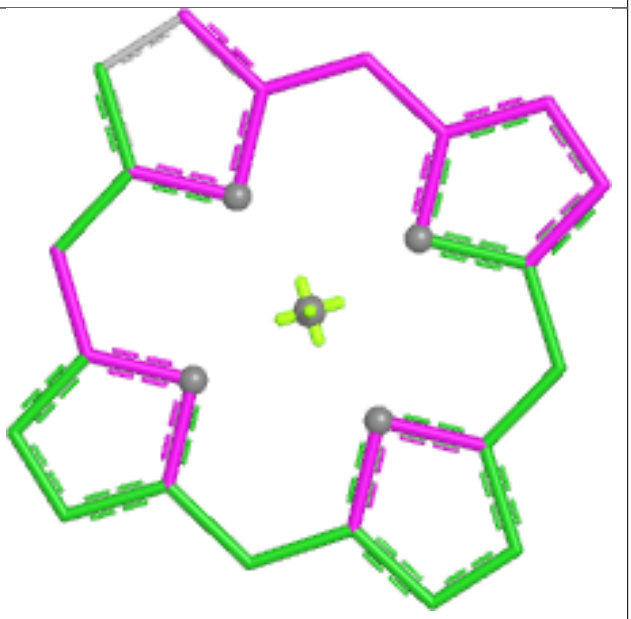


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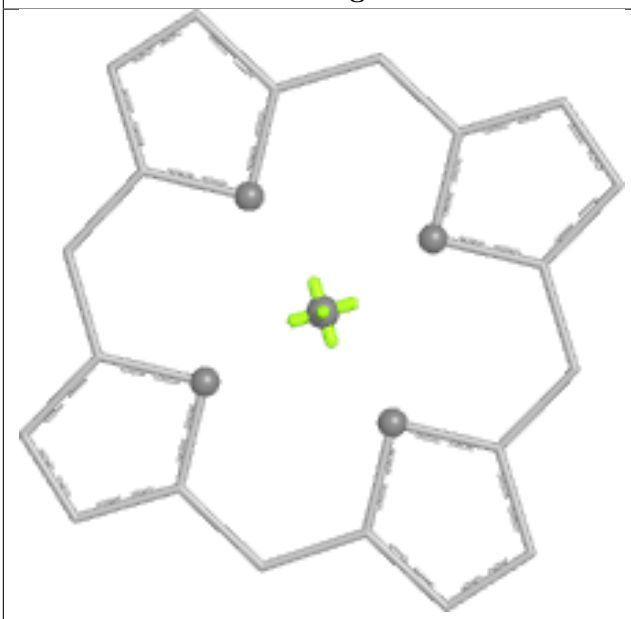
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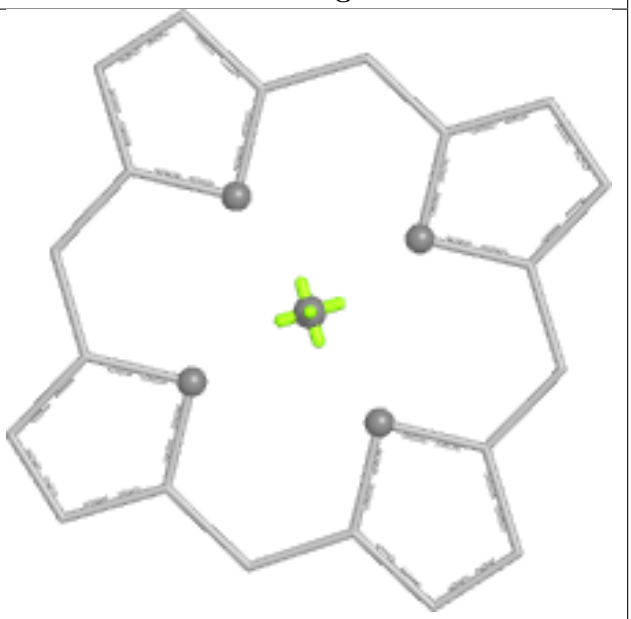
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Bond angles

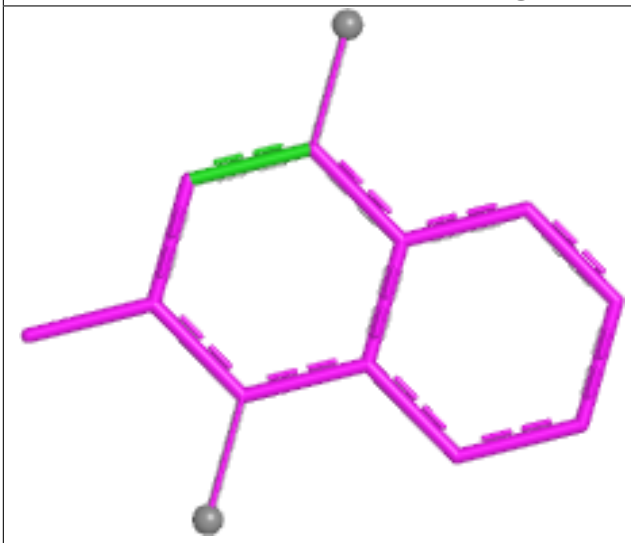


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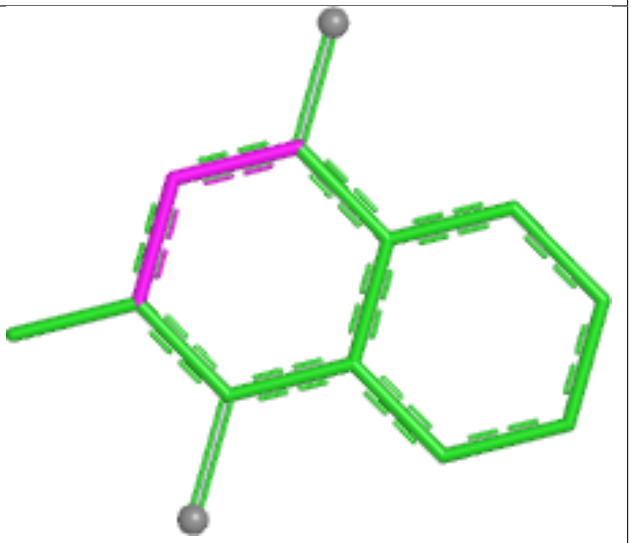


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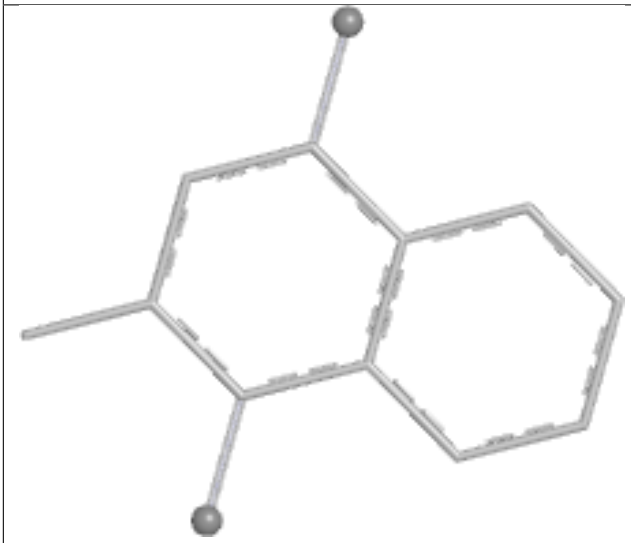
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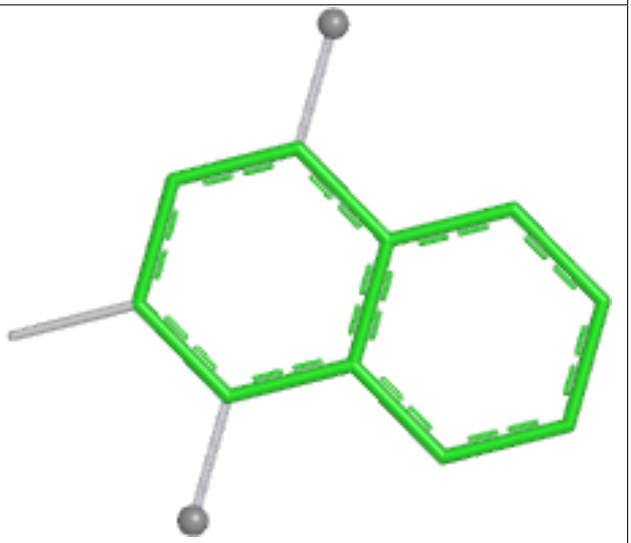
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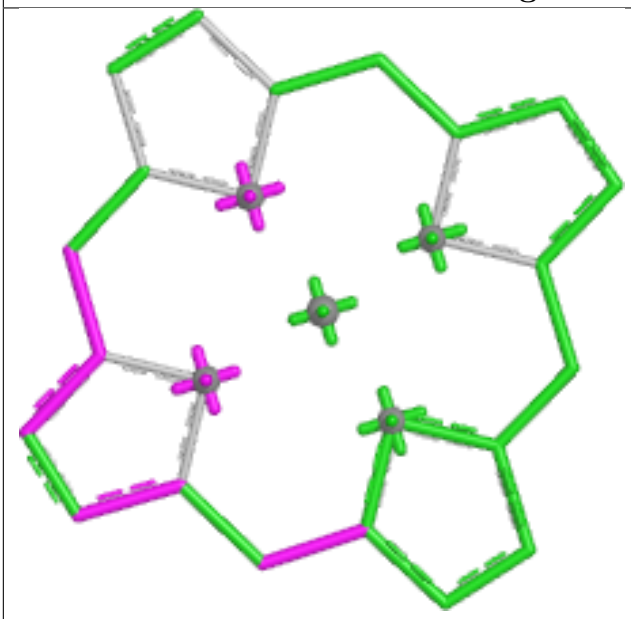


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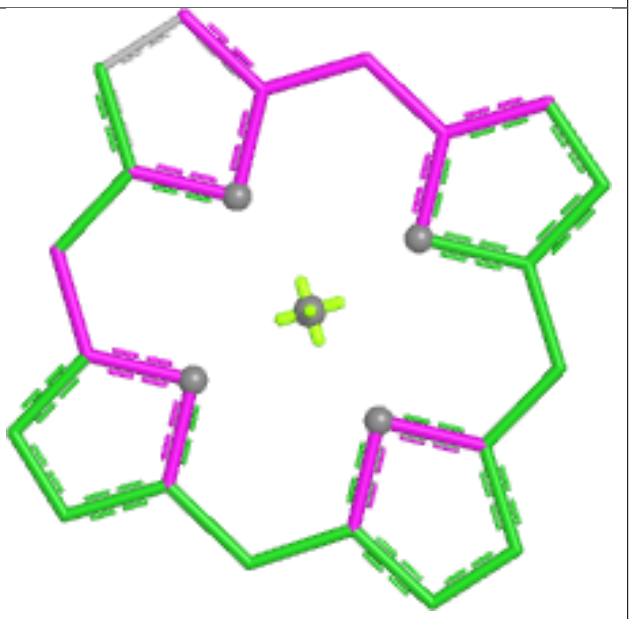


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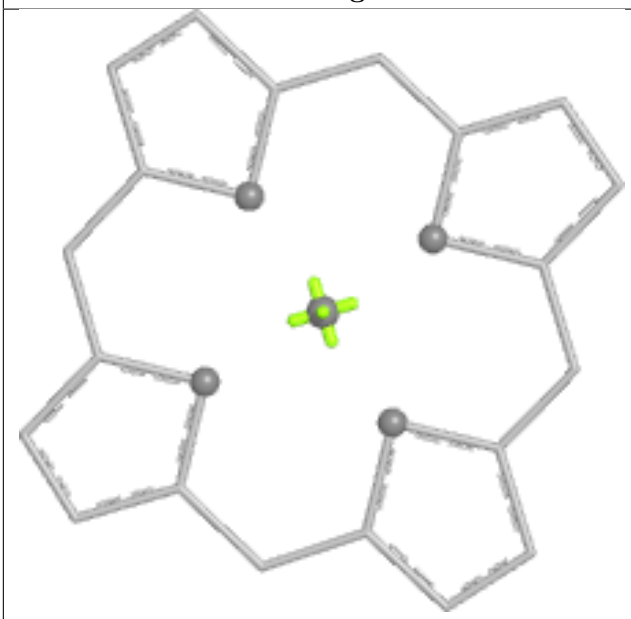
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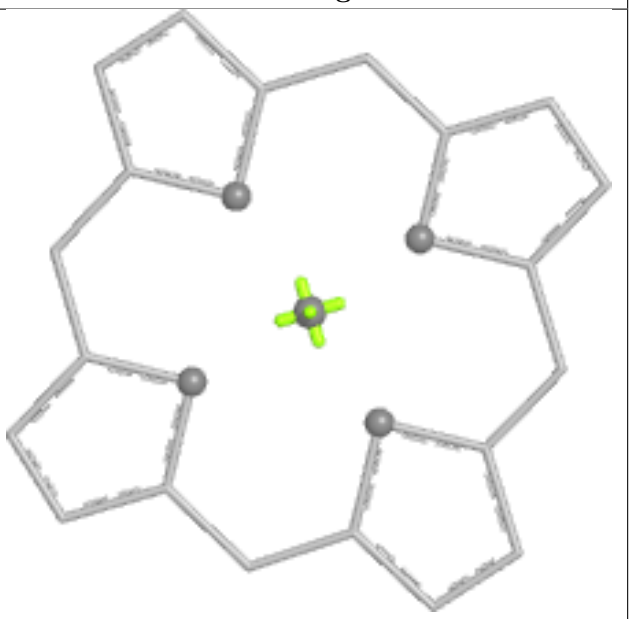
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Bond angles

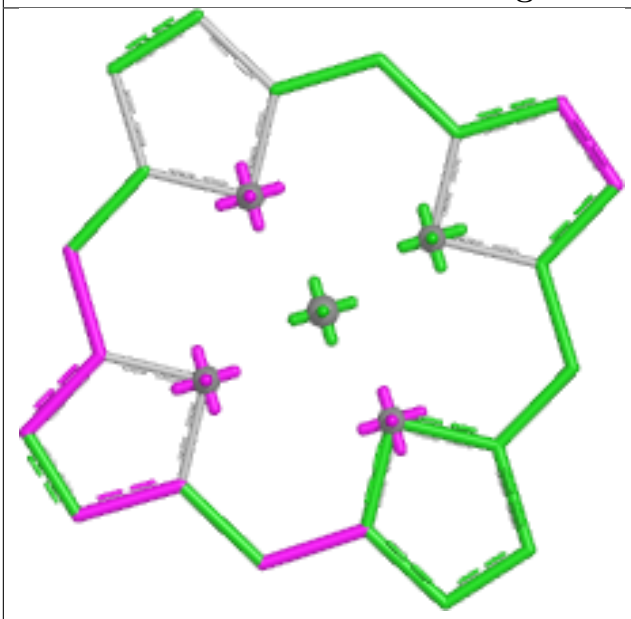


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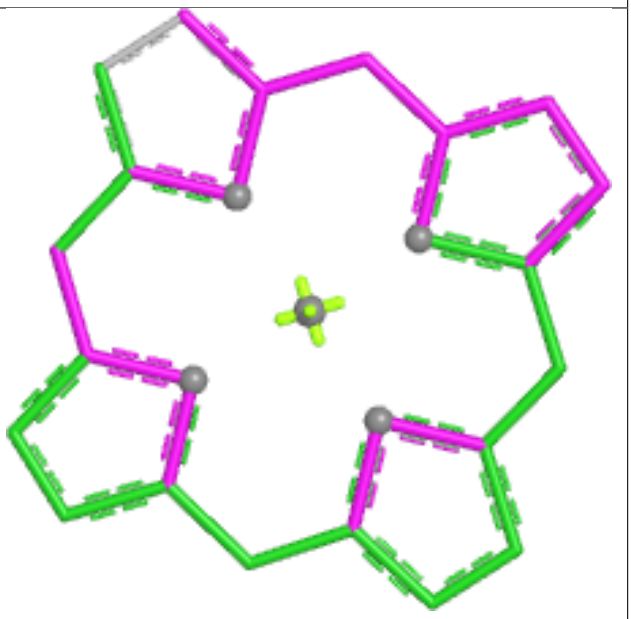


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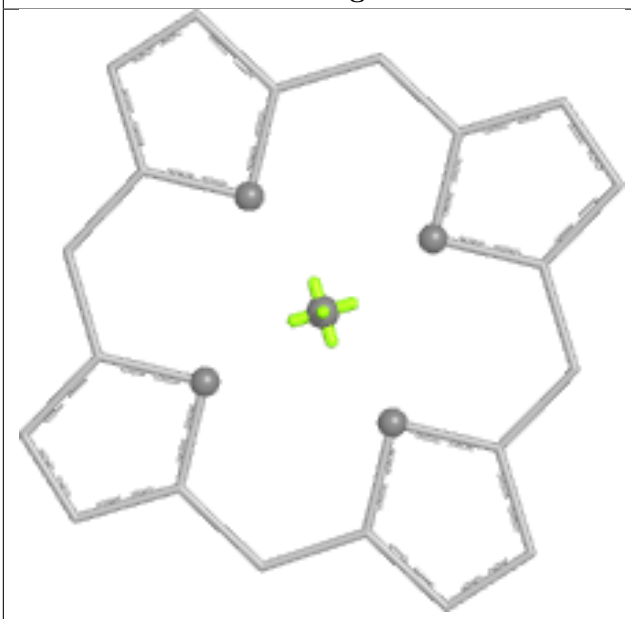
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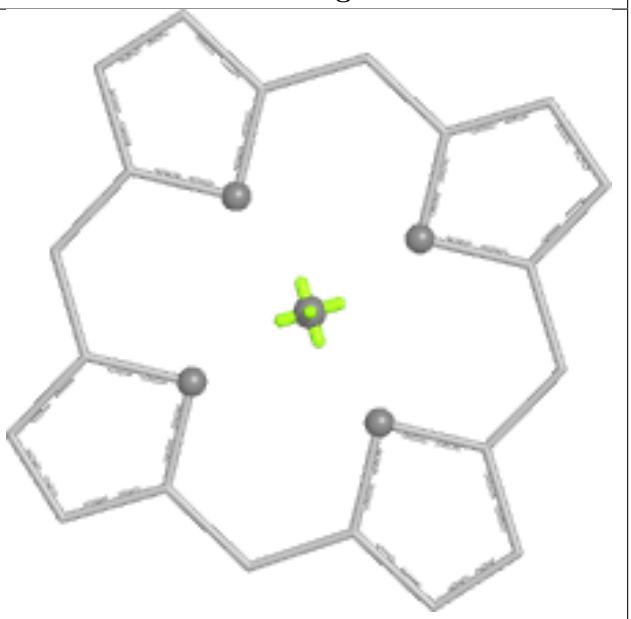
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Bond angles

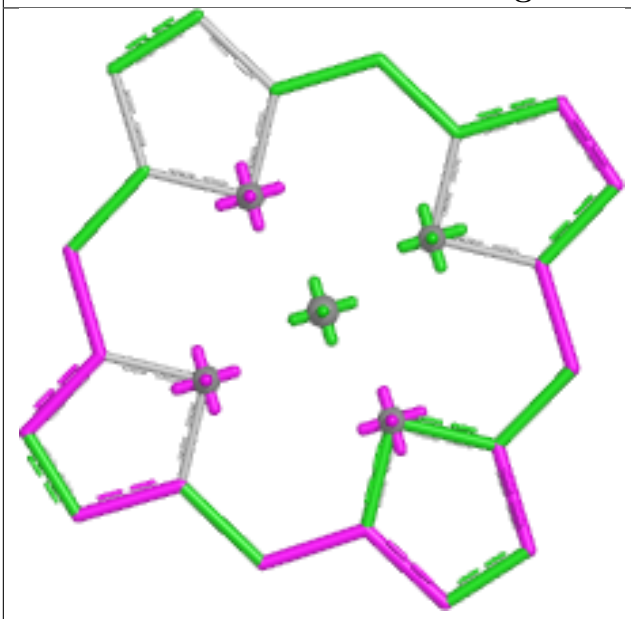


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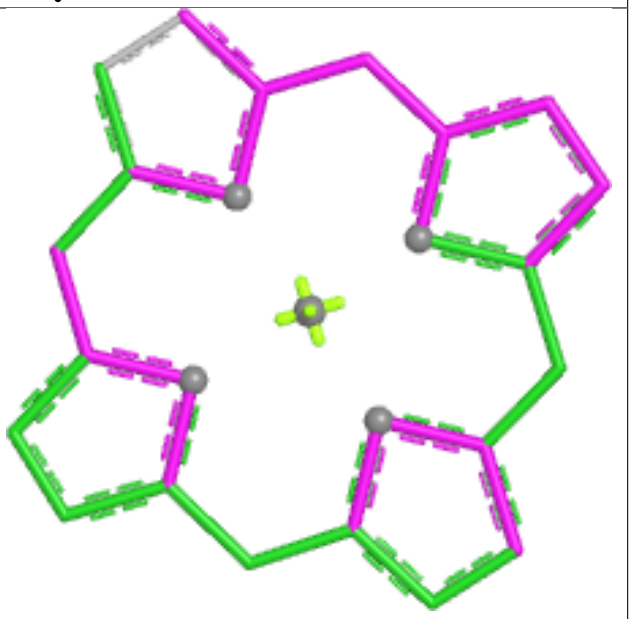


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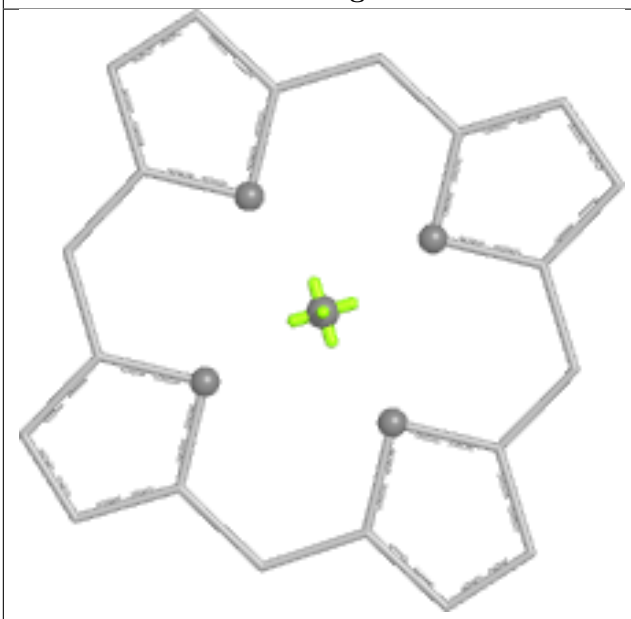
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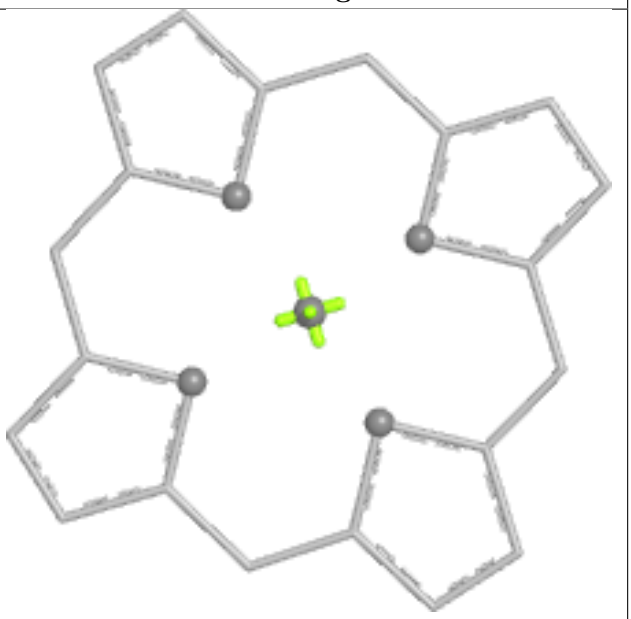
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Bond angles

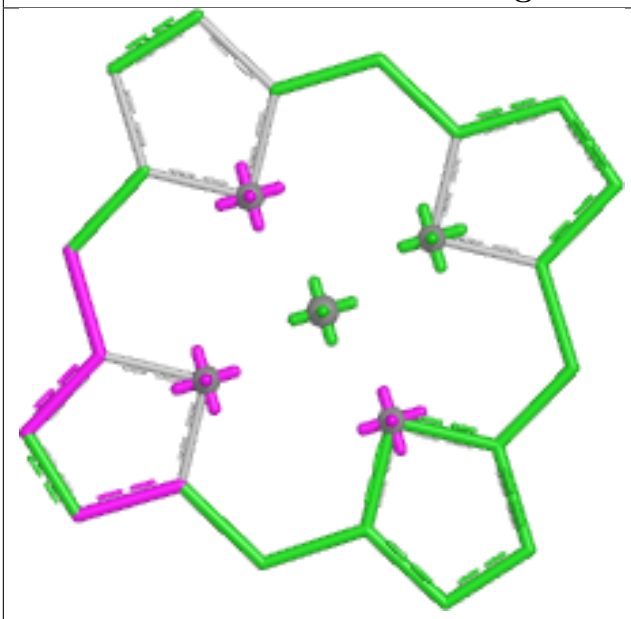


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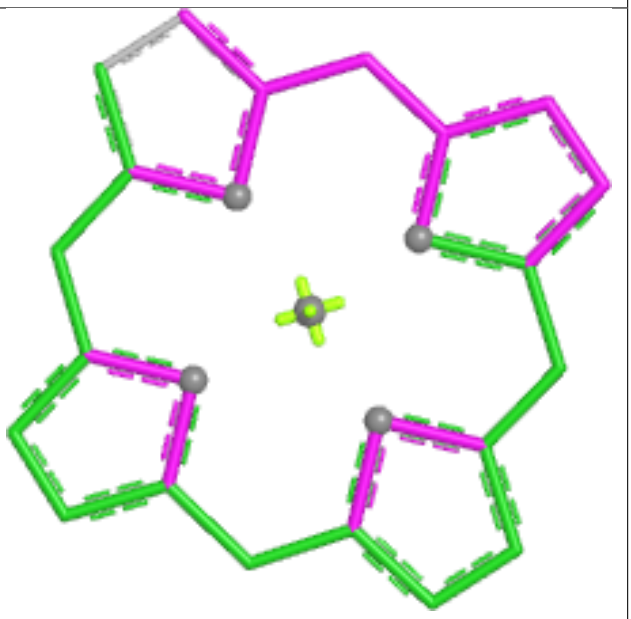


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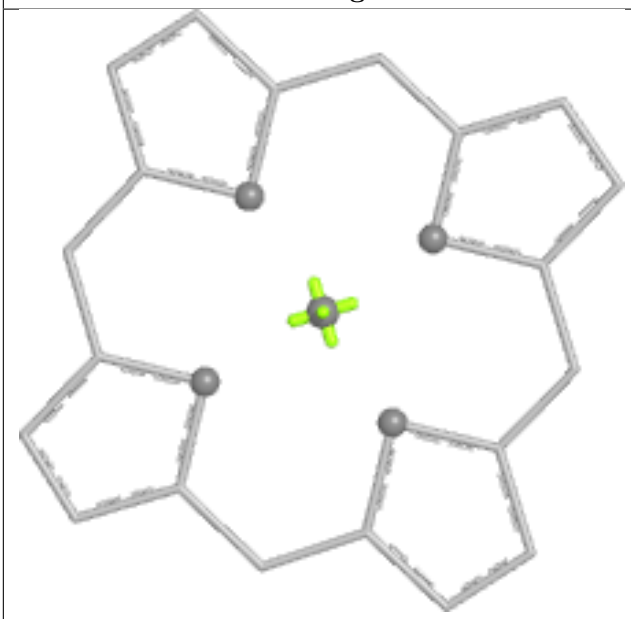
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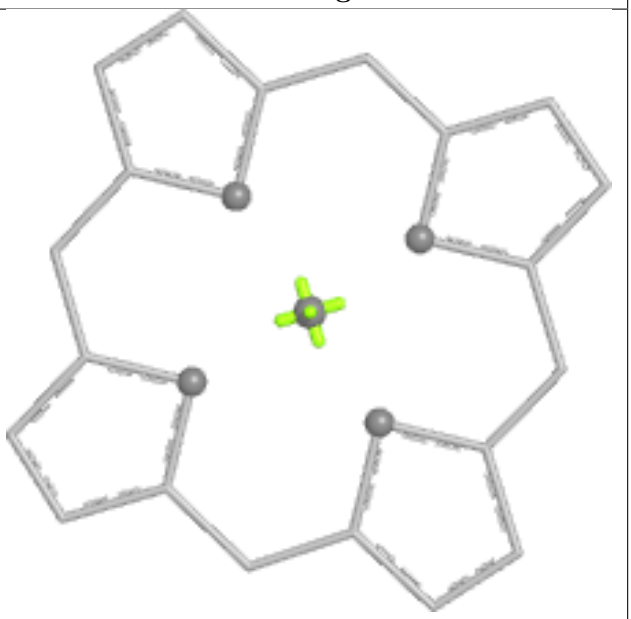
Bond lengths



Bond angles

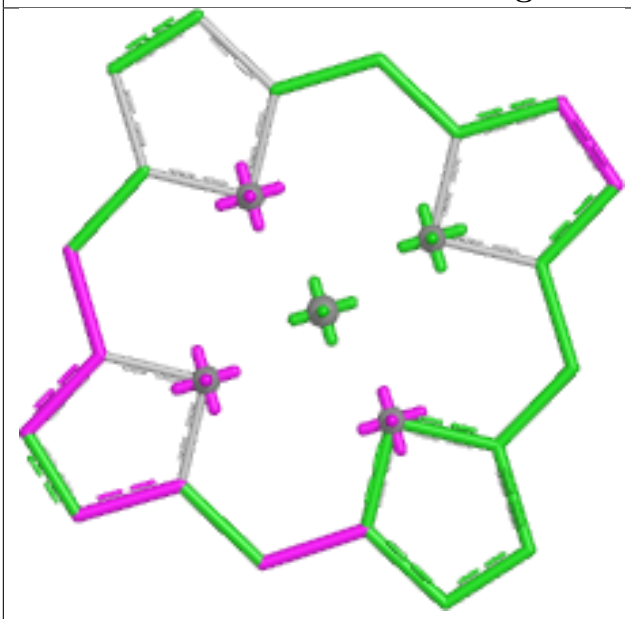


Torsions

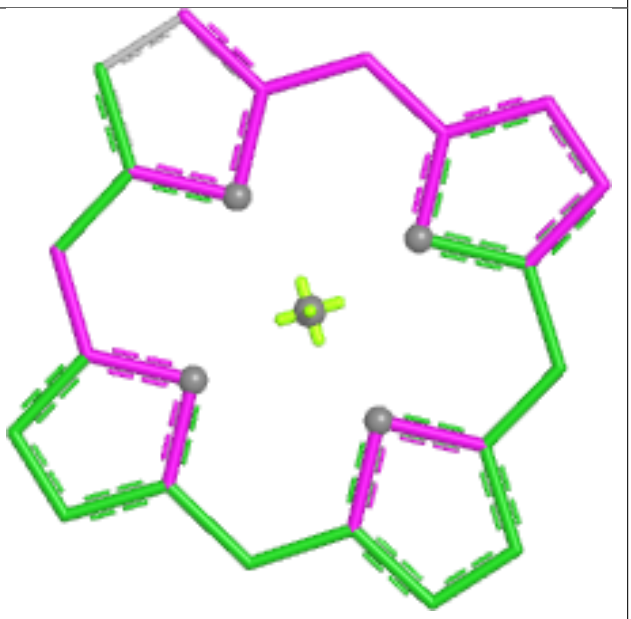


Rings

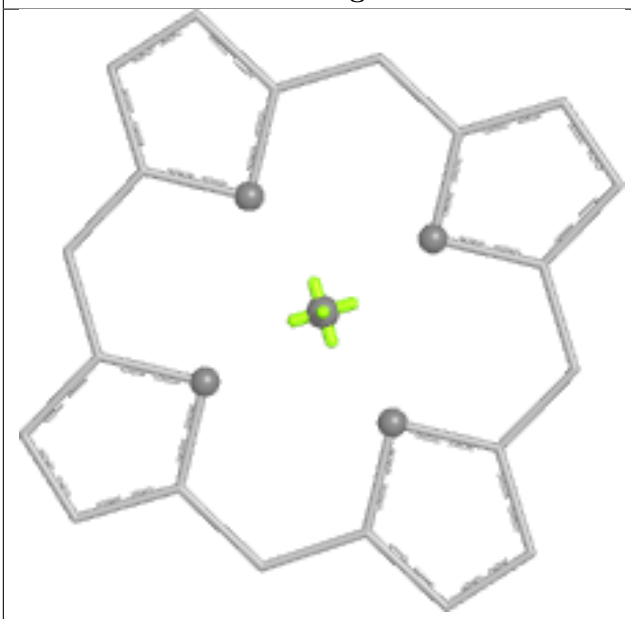
Ligand CLA B 1210



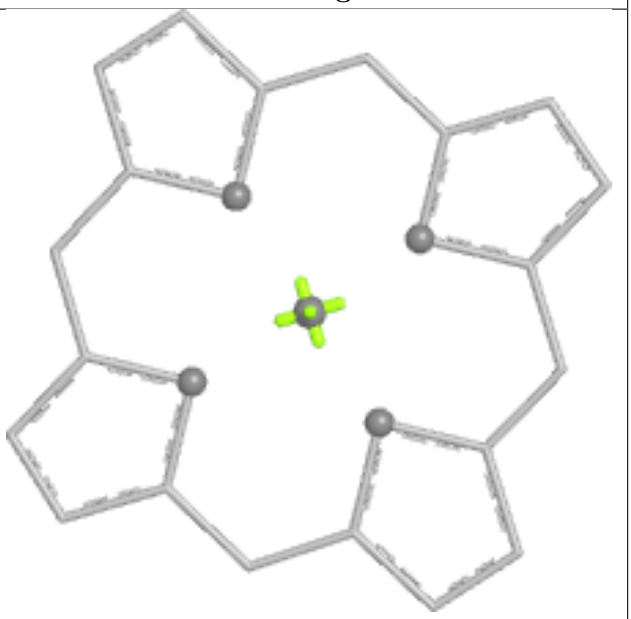
Bond lengths



Bond angles

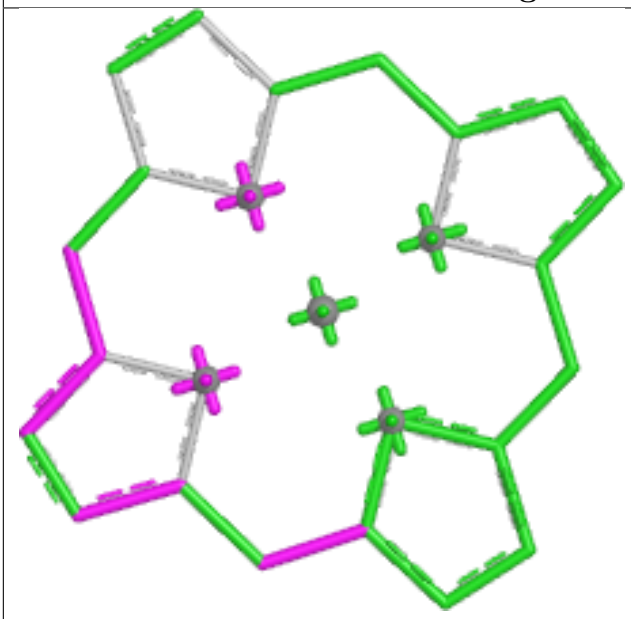


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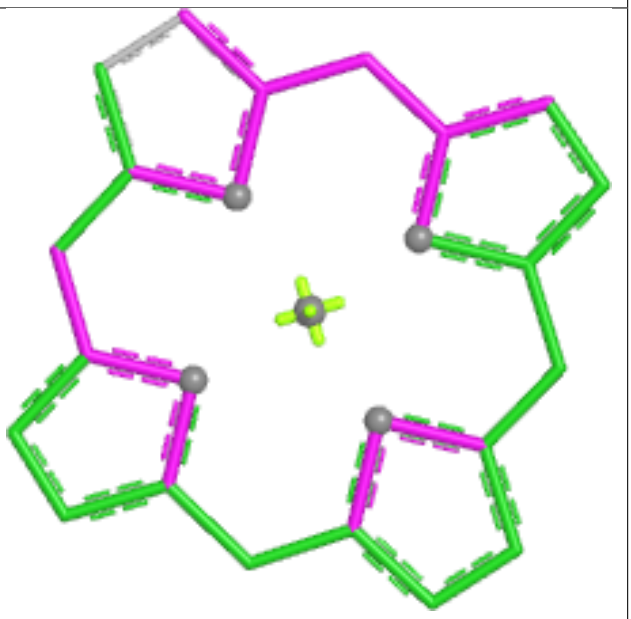


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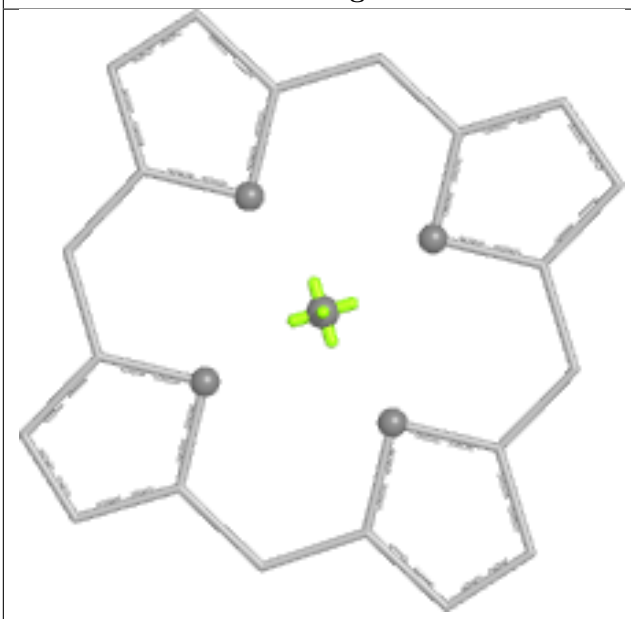
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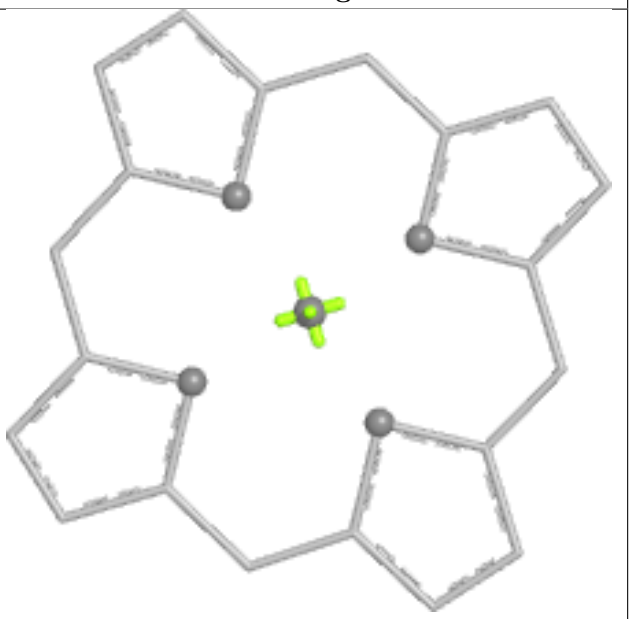
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Bond angles

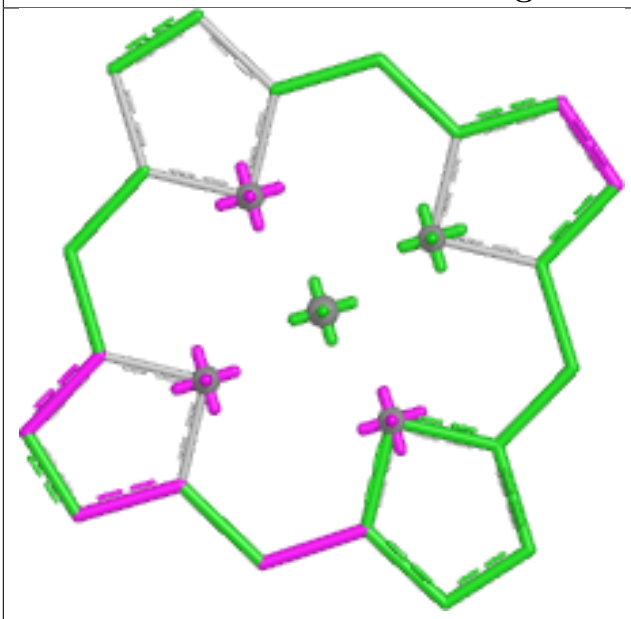


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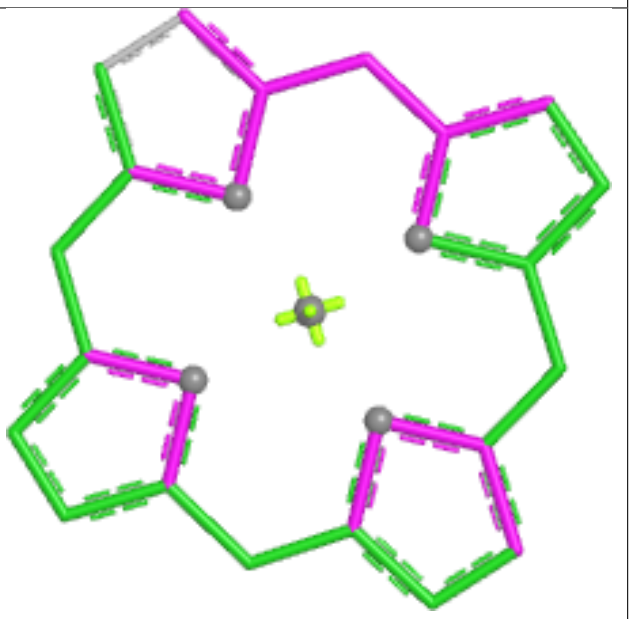


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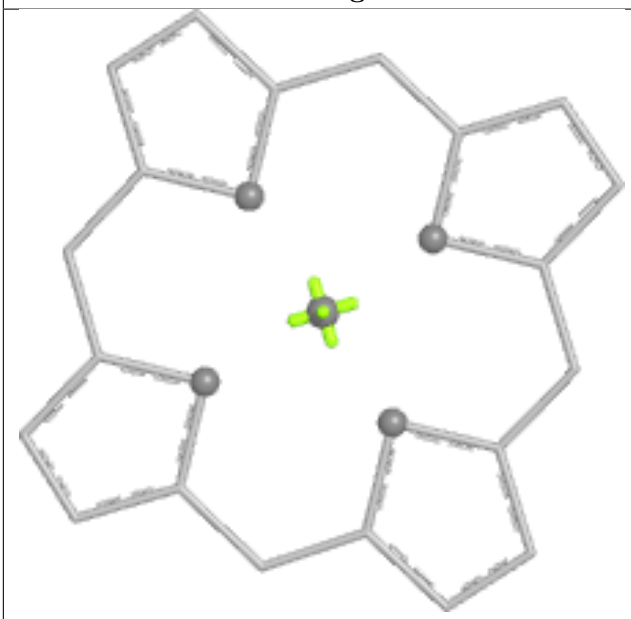
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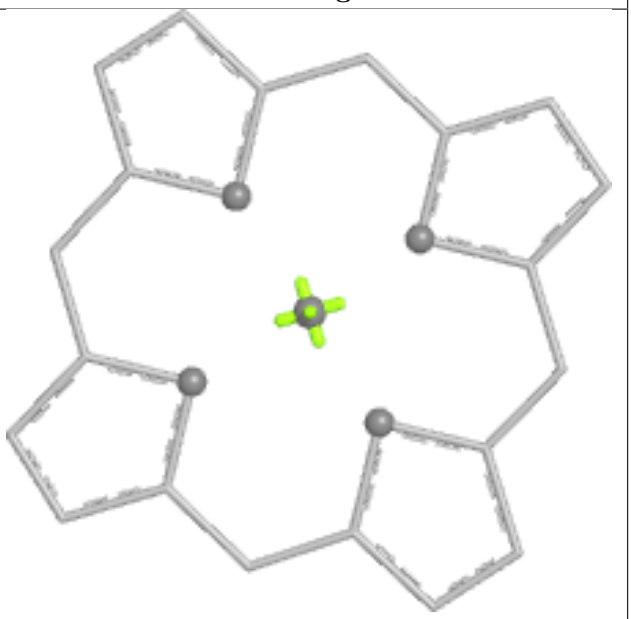
Bond lengths



Bond angles

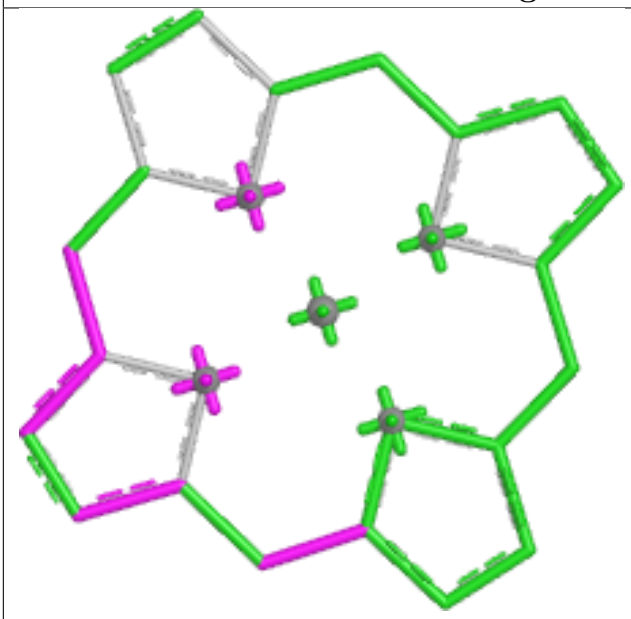


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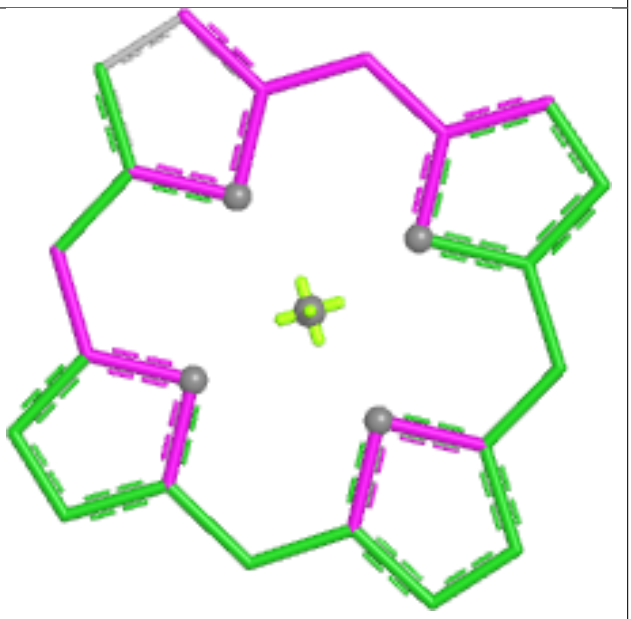


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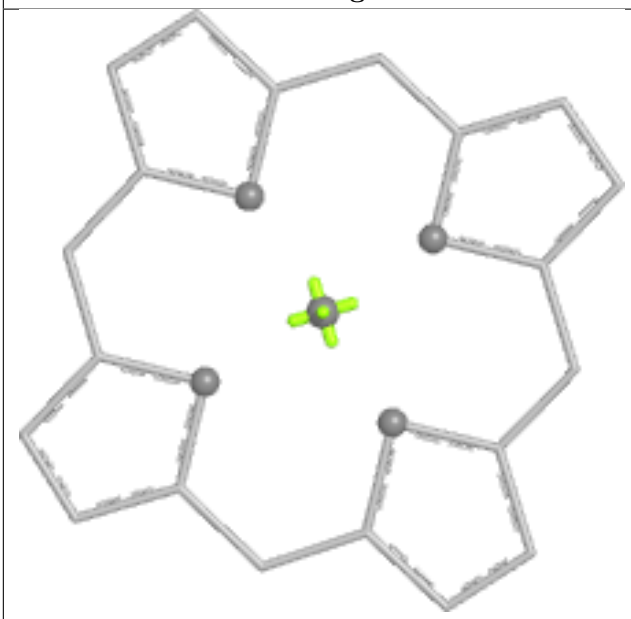
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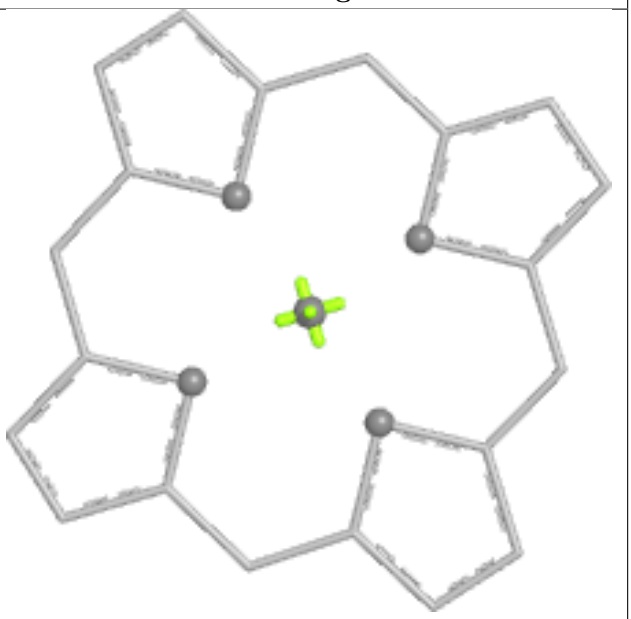
Bond lengths



Bond angles

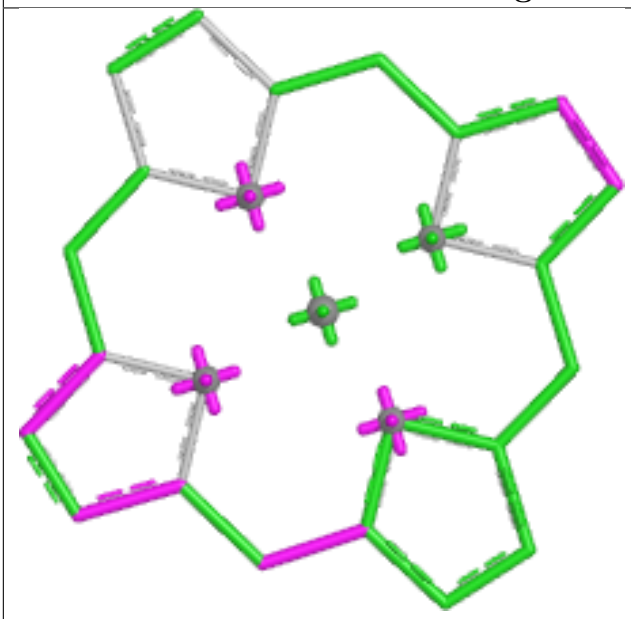


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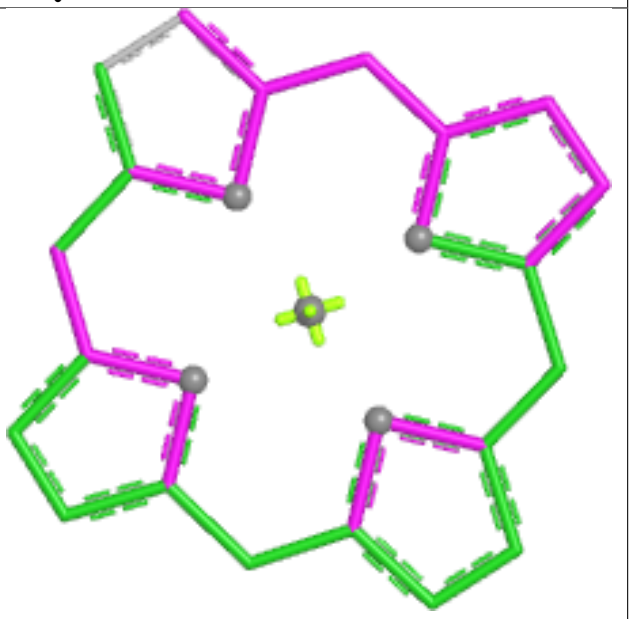


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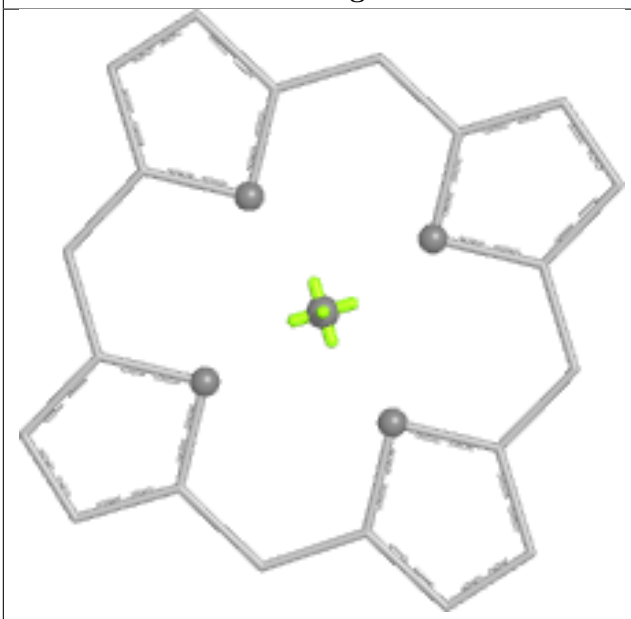
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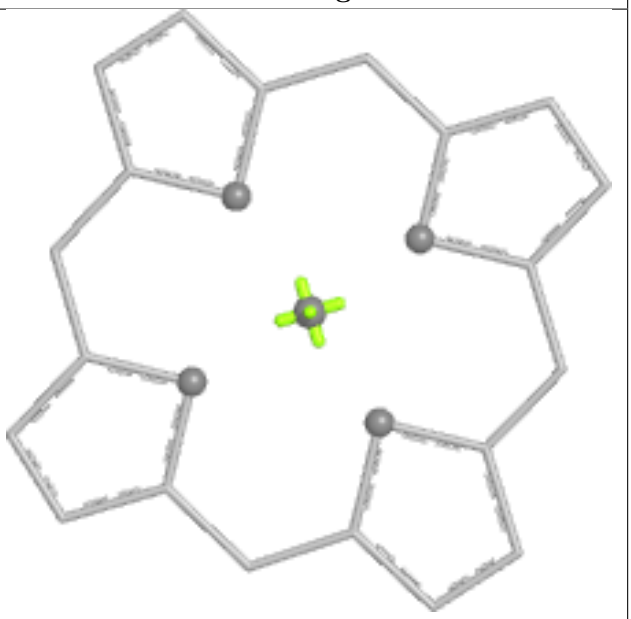
Bond lengths



Bond angles

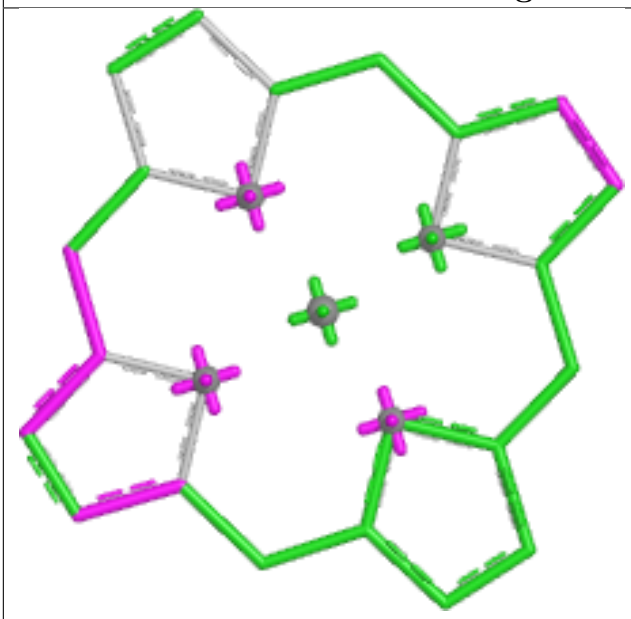


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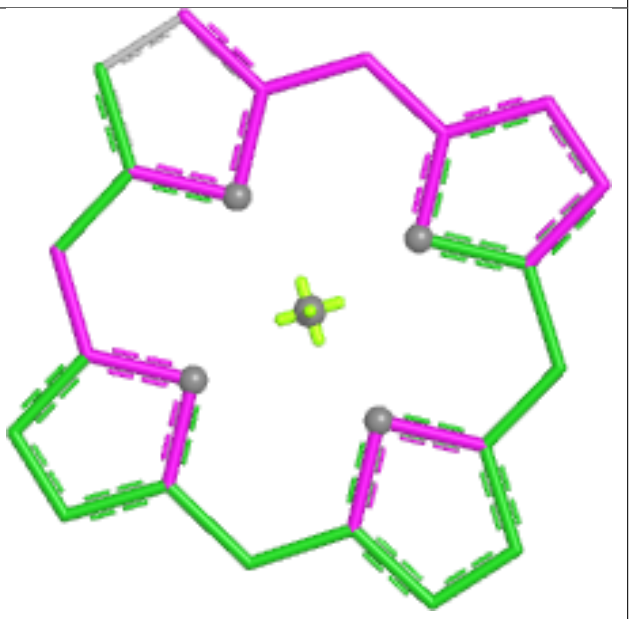


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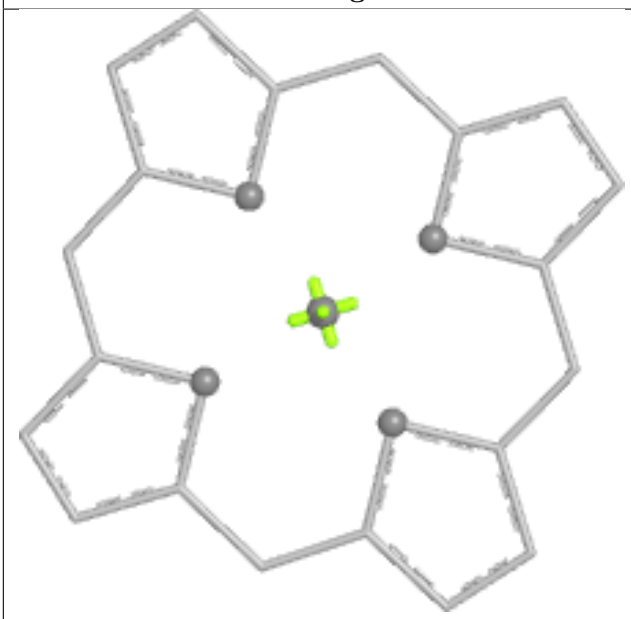
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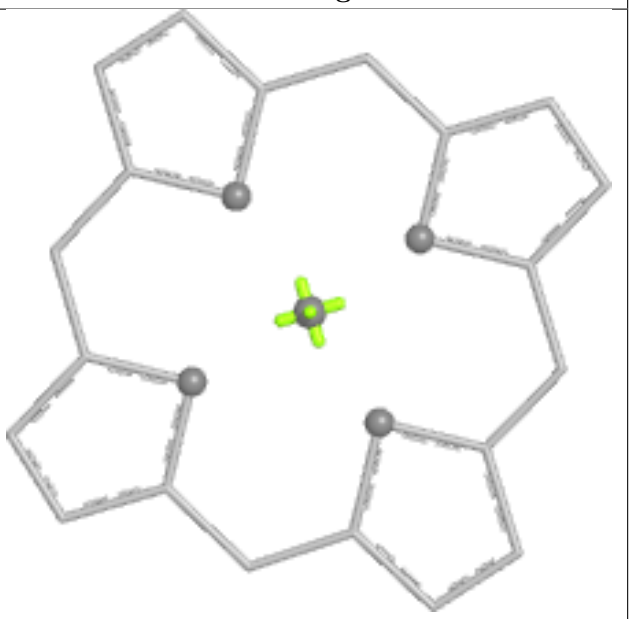
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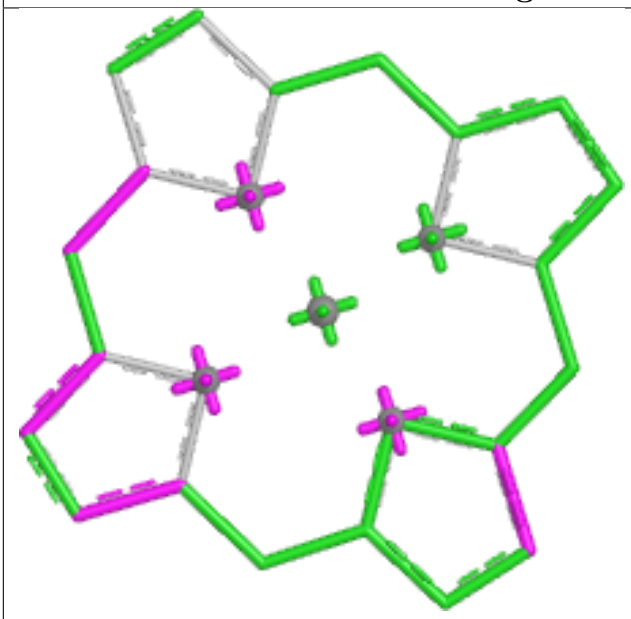


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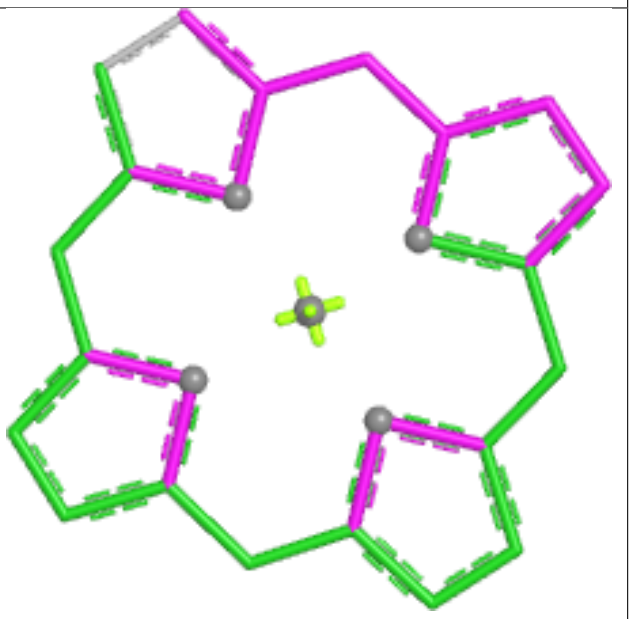


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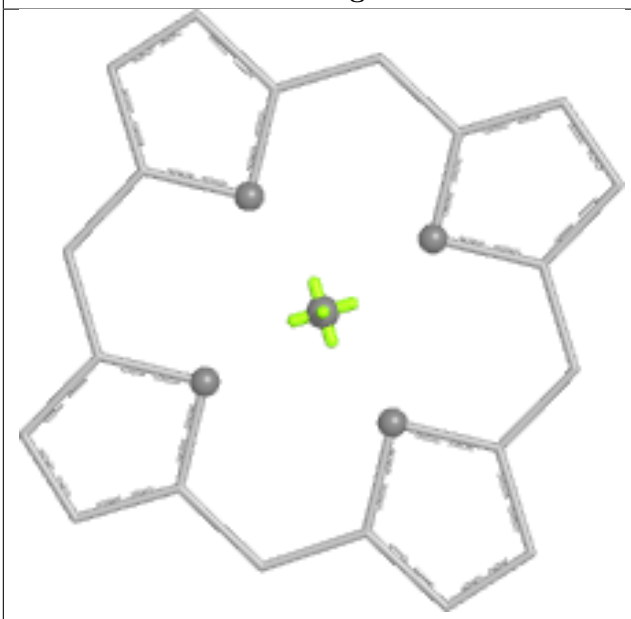
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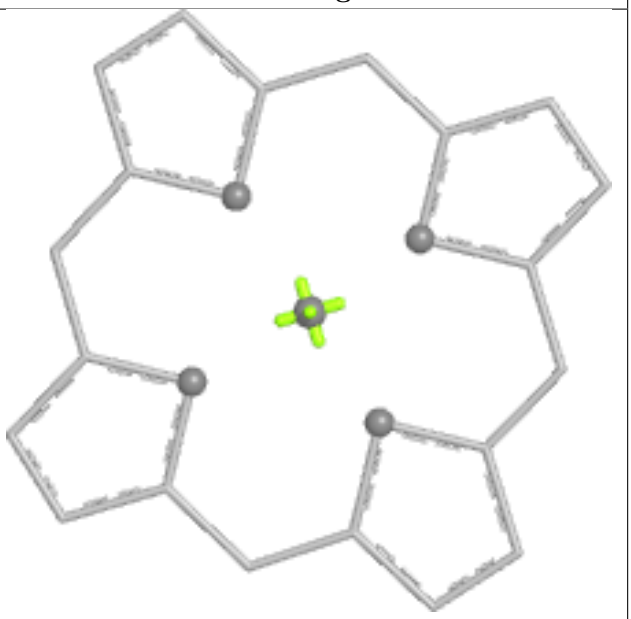
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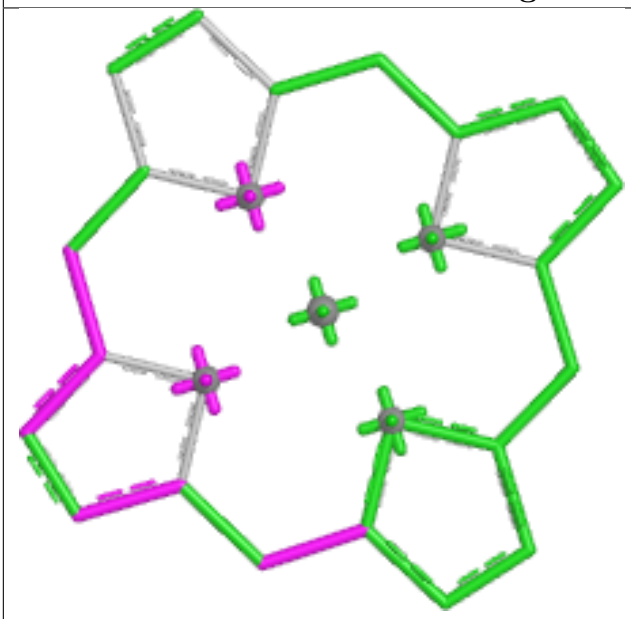


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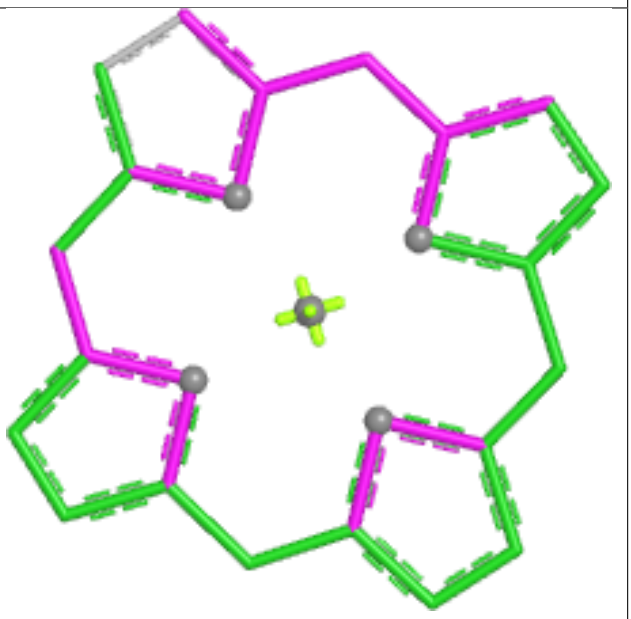


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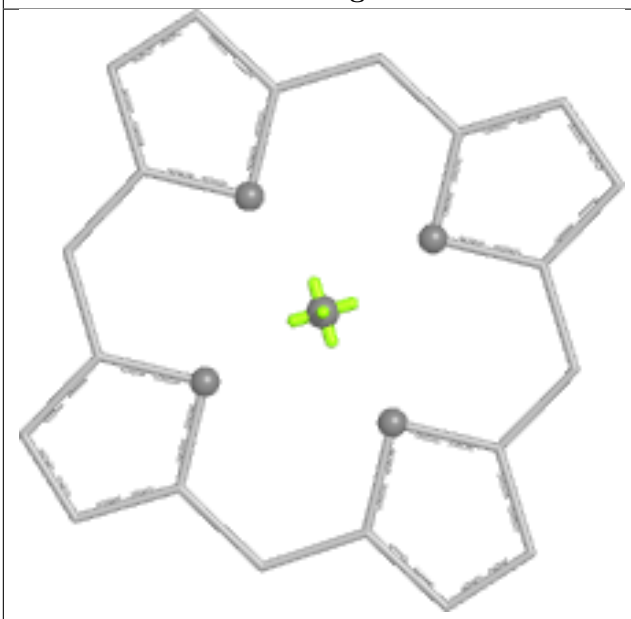
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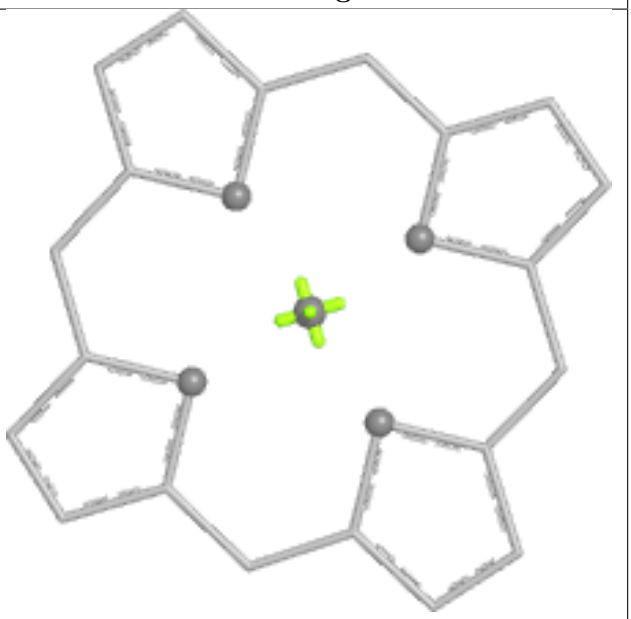
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Bond angles

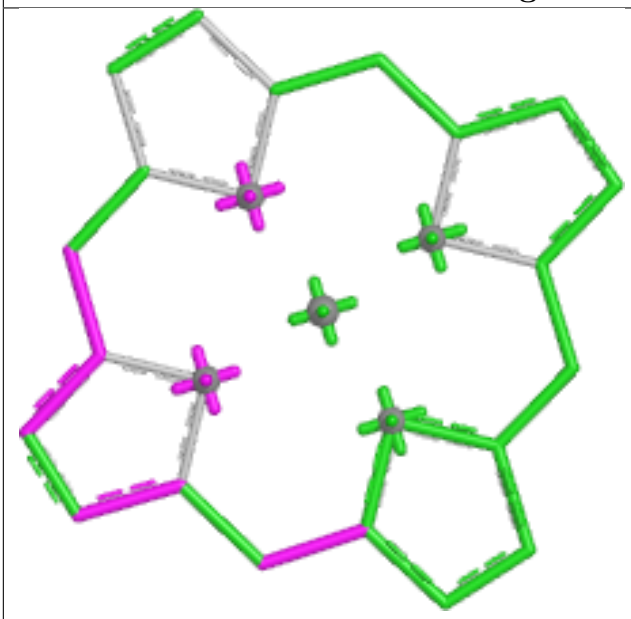


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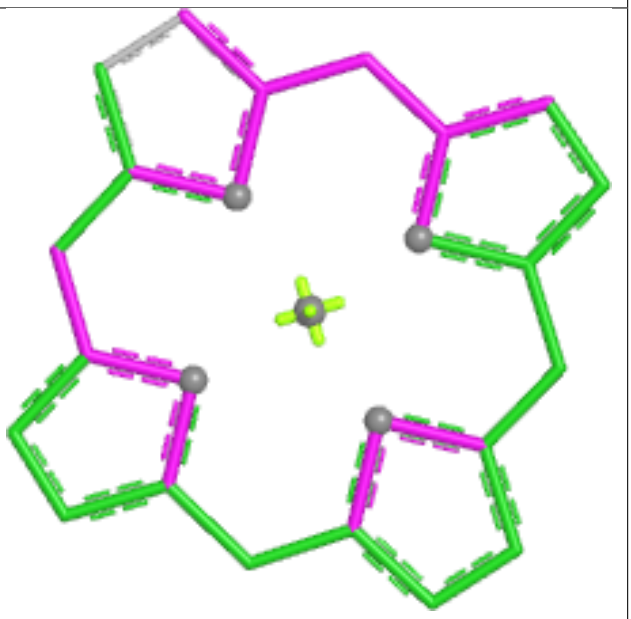


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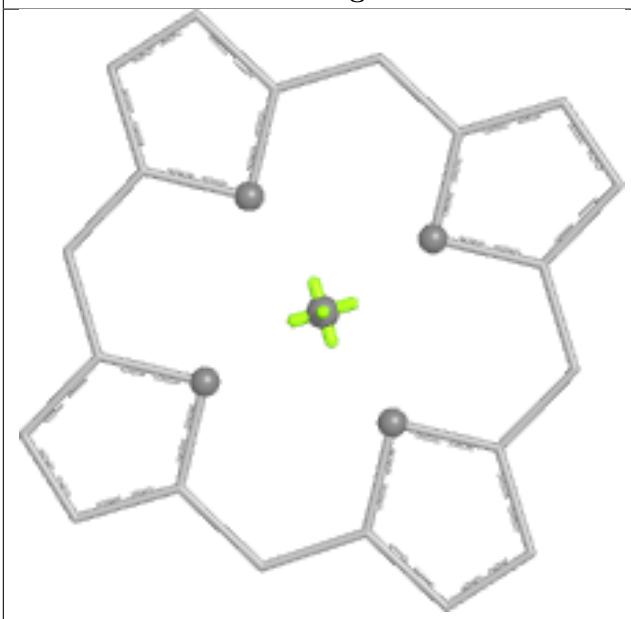
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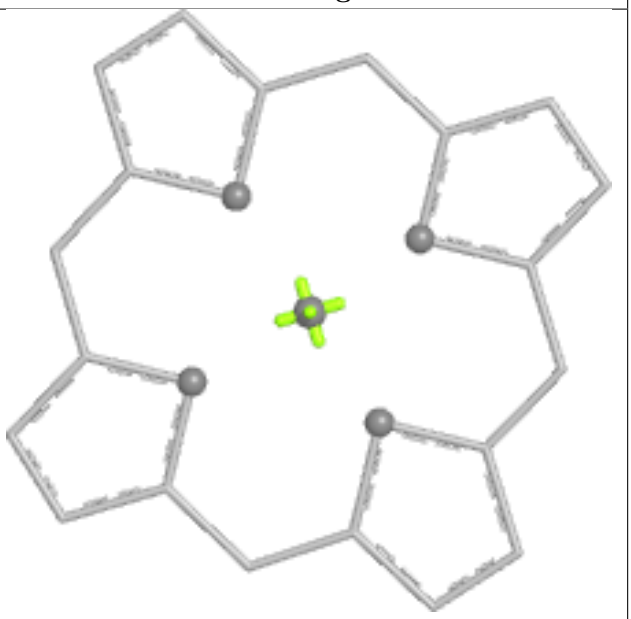
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Bond angles

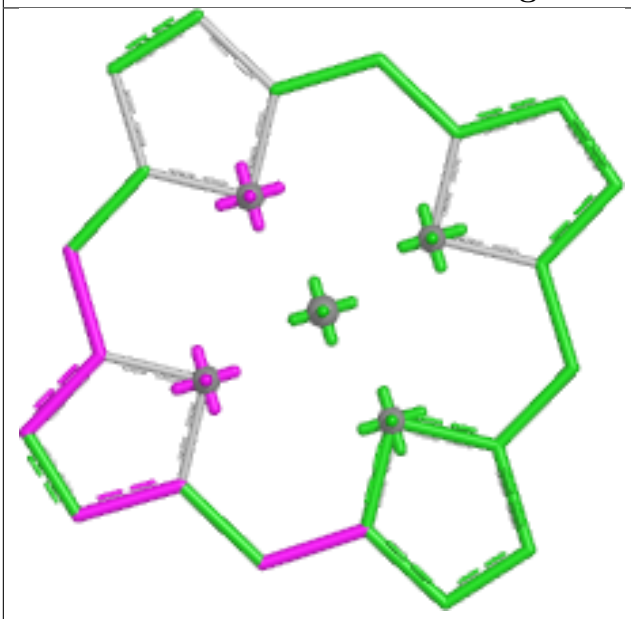


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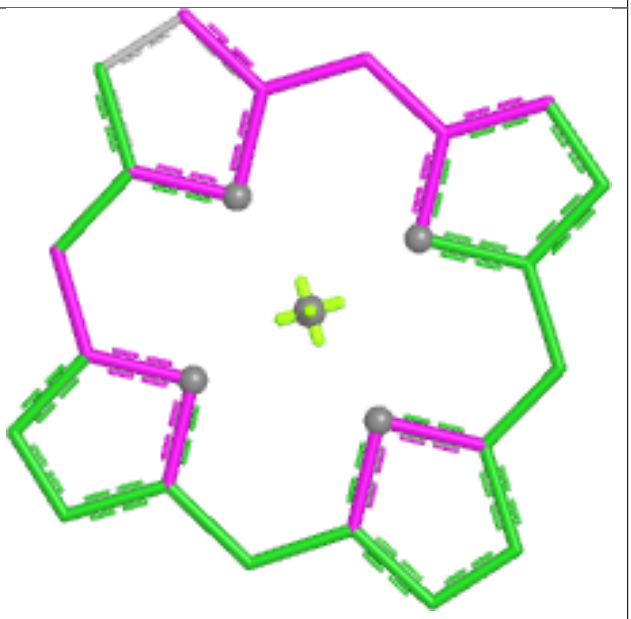


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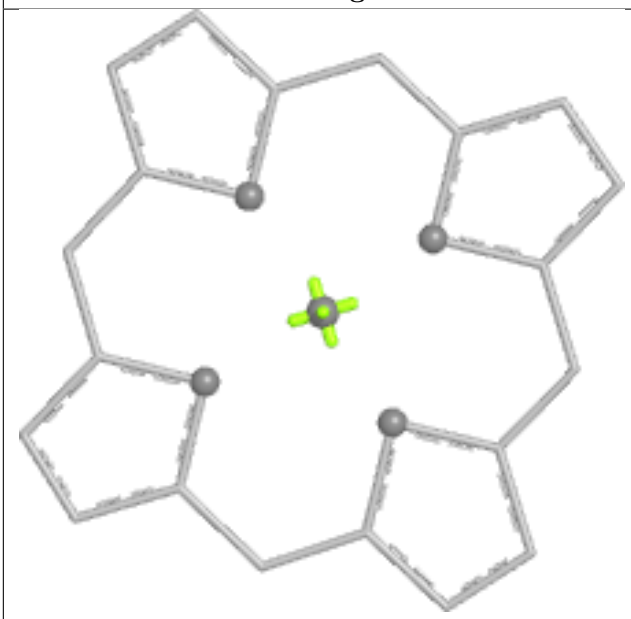
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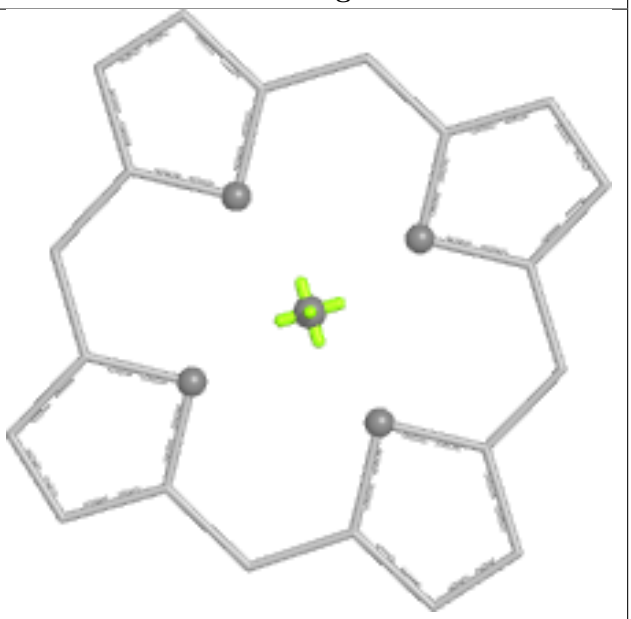
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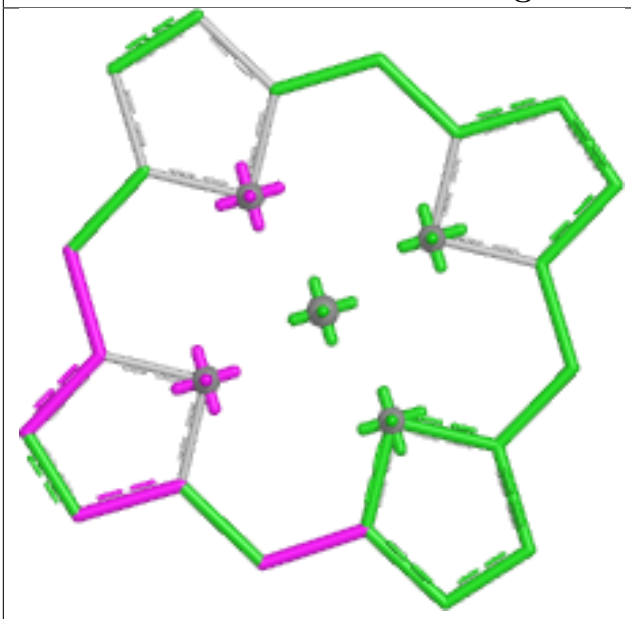


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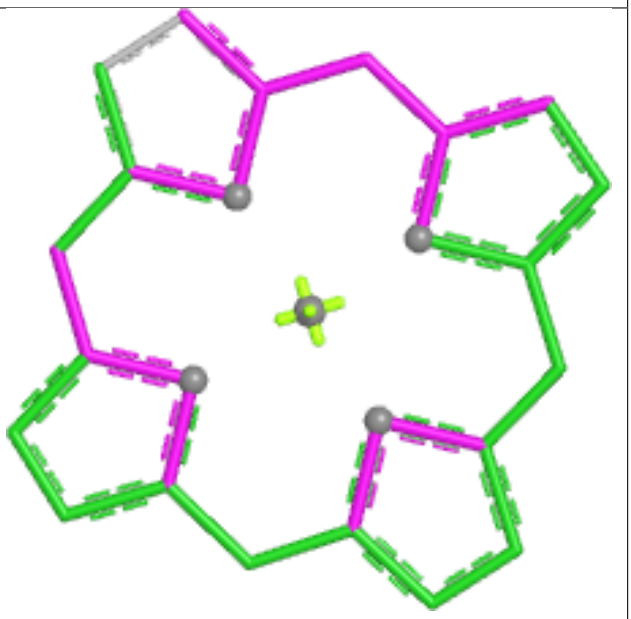


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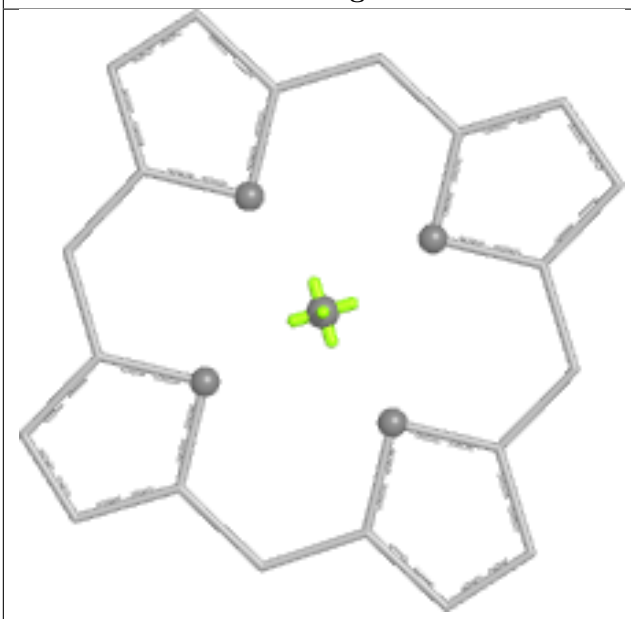
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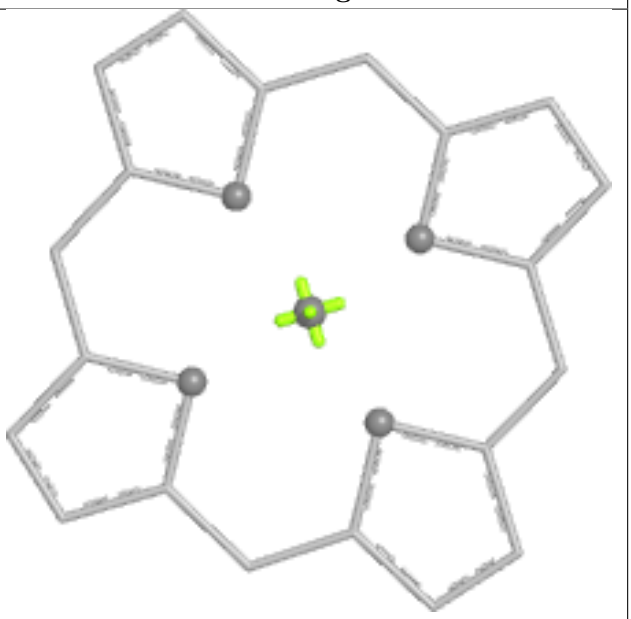
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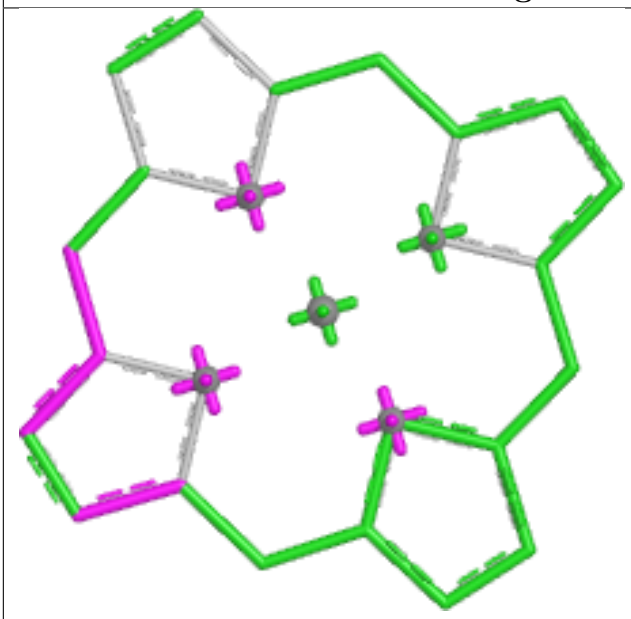


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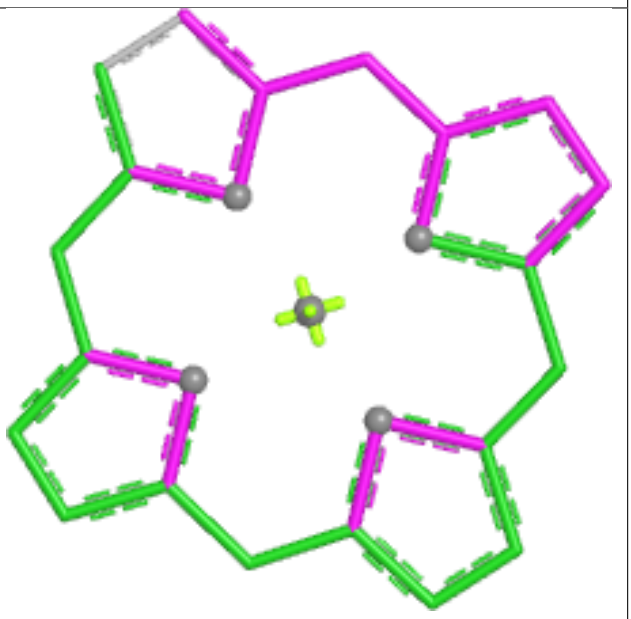


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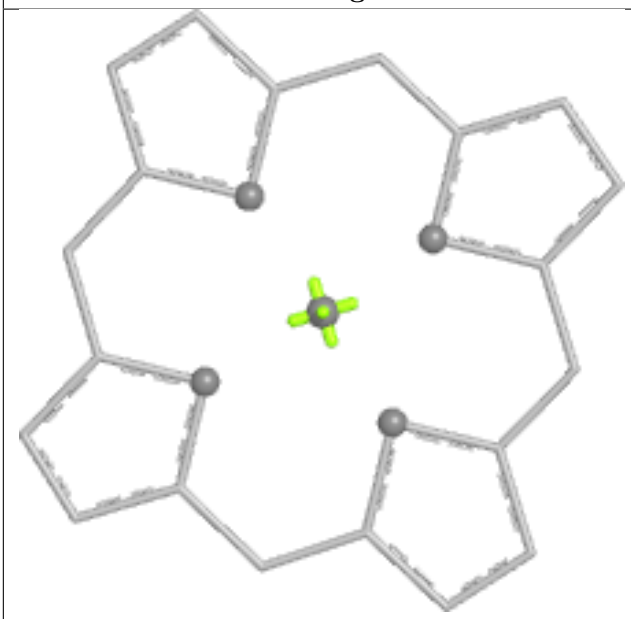
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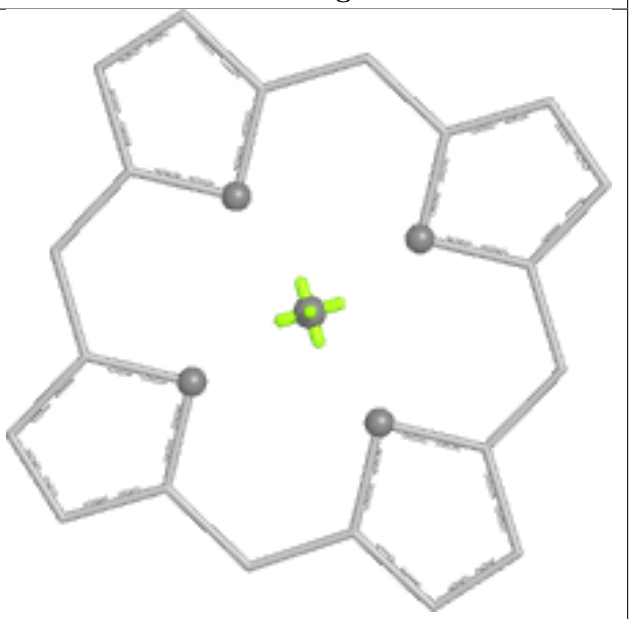
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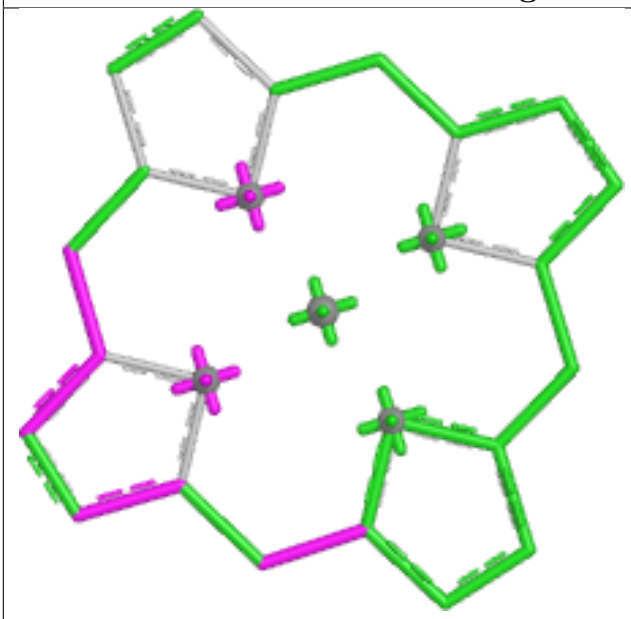


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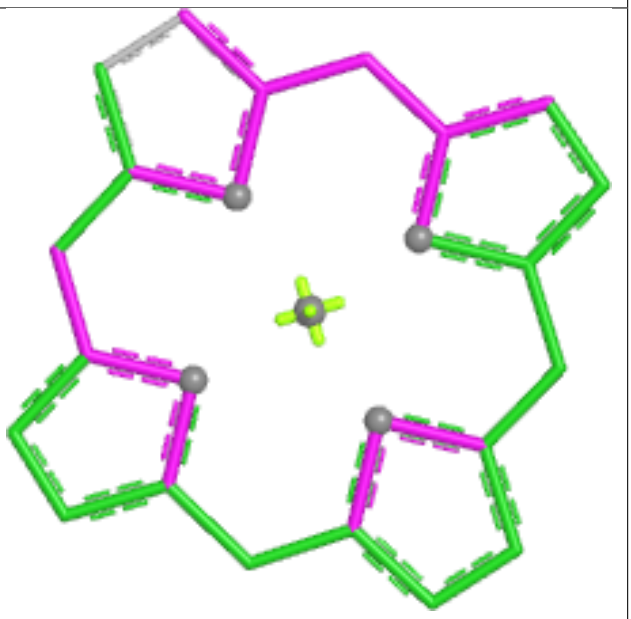


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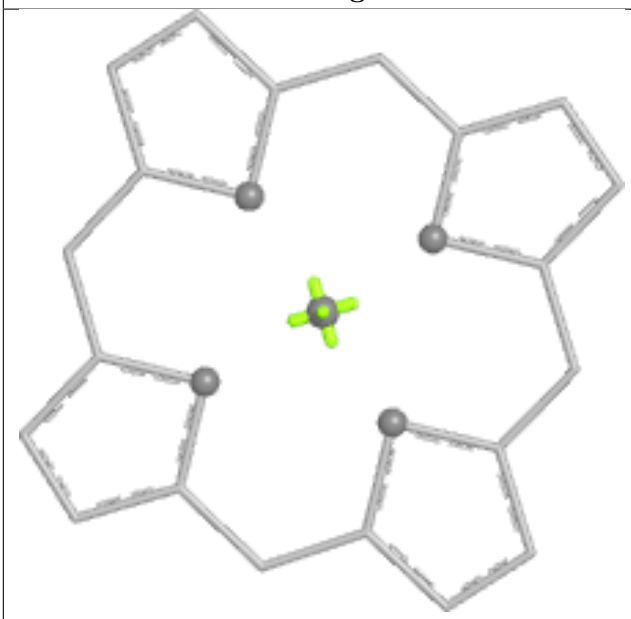
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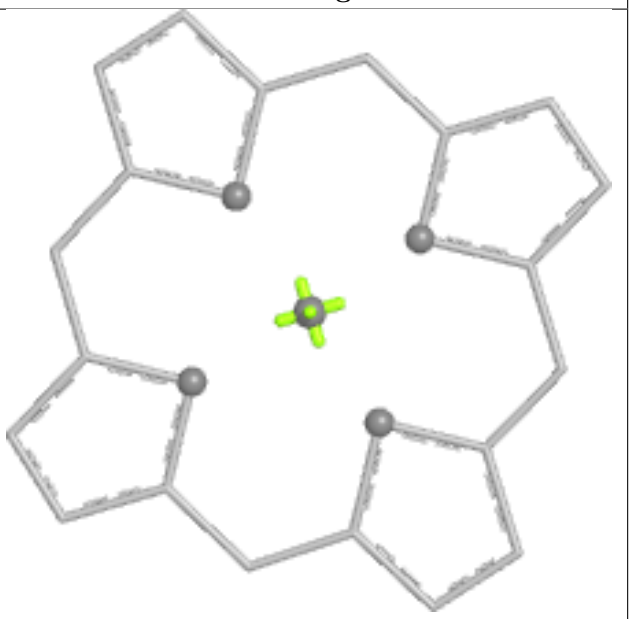
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Bond angles

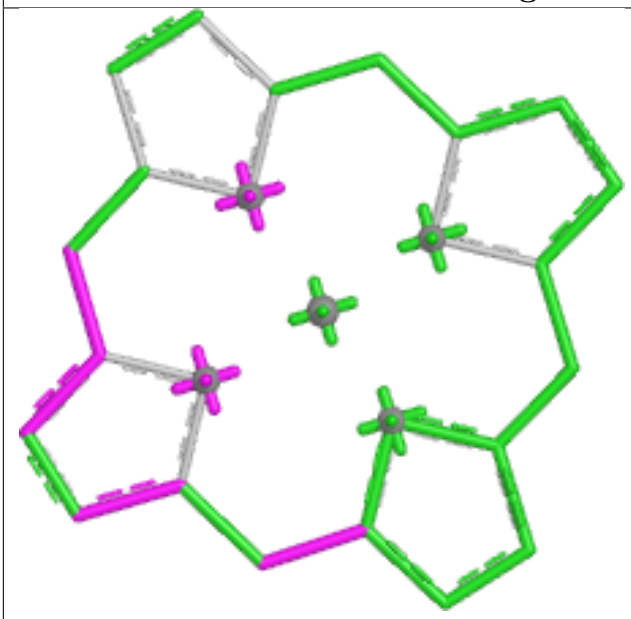


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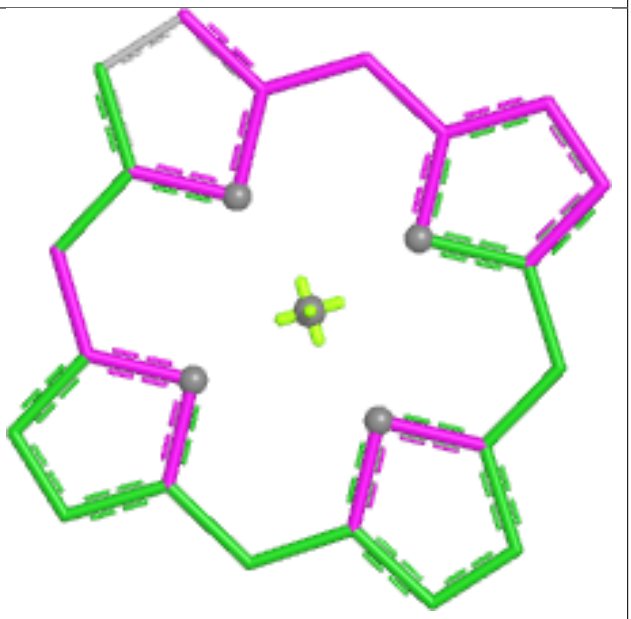


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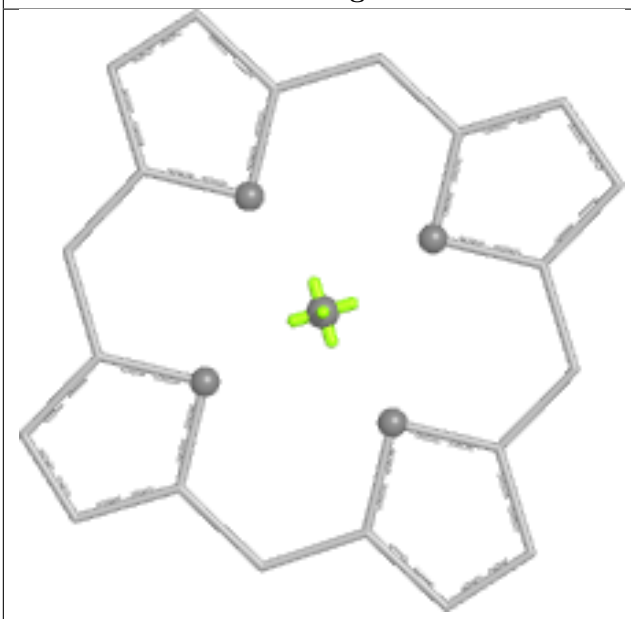
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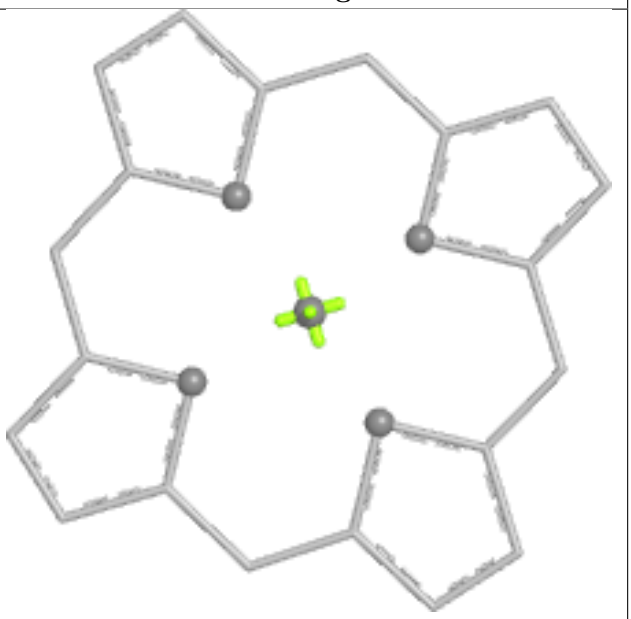
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Bond angles

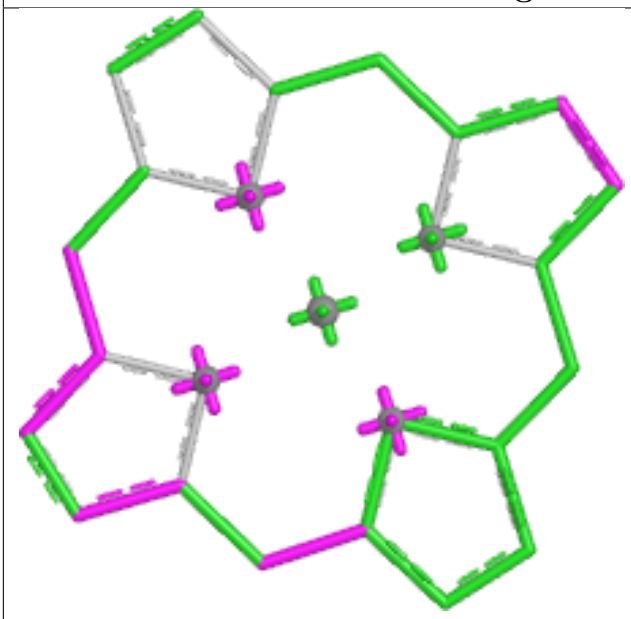


Torsions

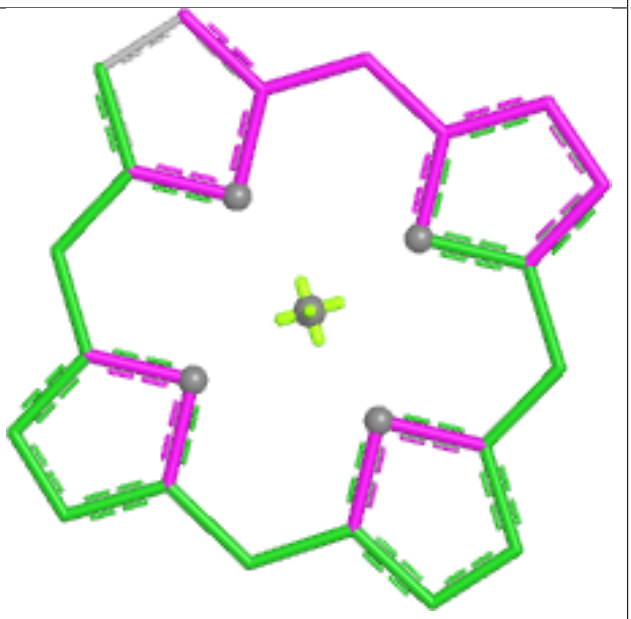


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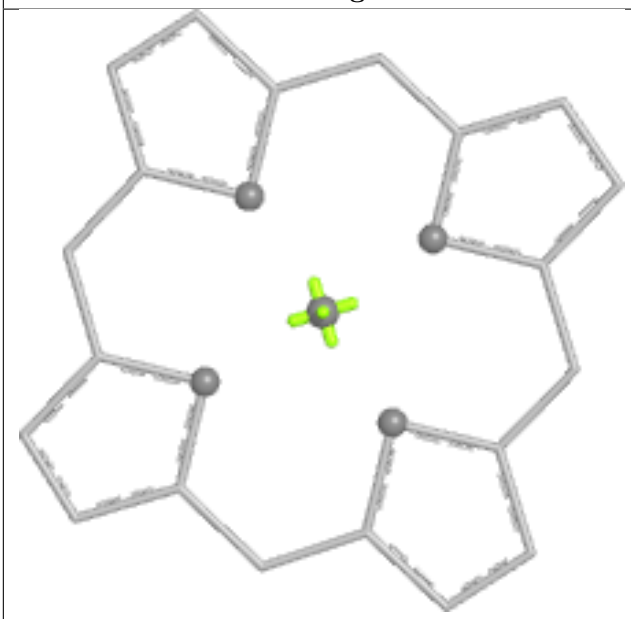
Ligand CLA B 1208



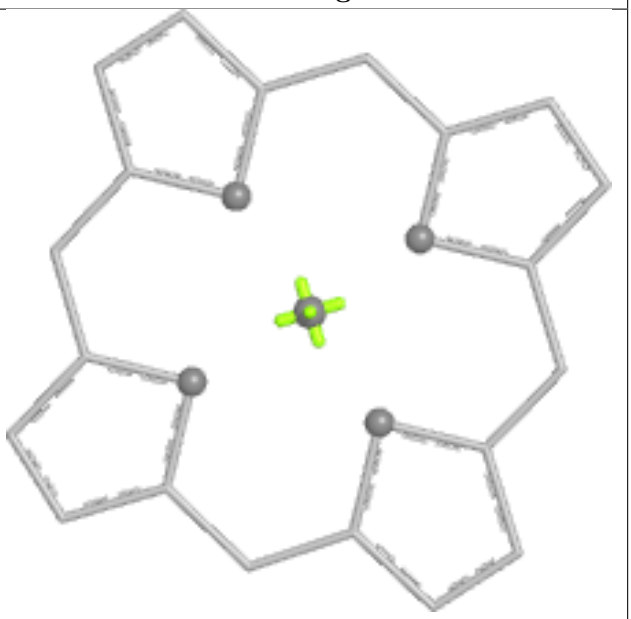
Bond lengths



Bond angles

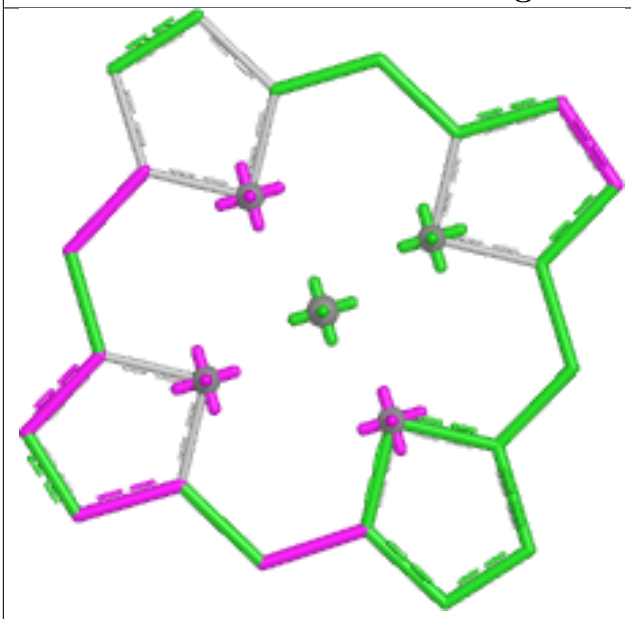


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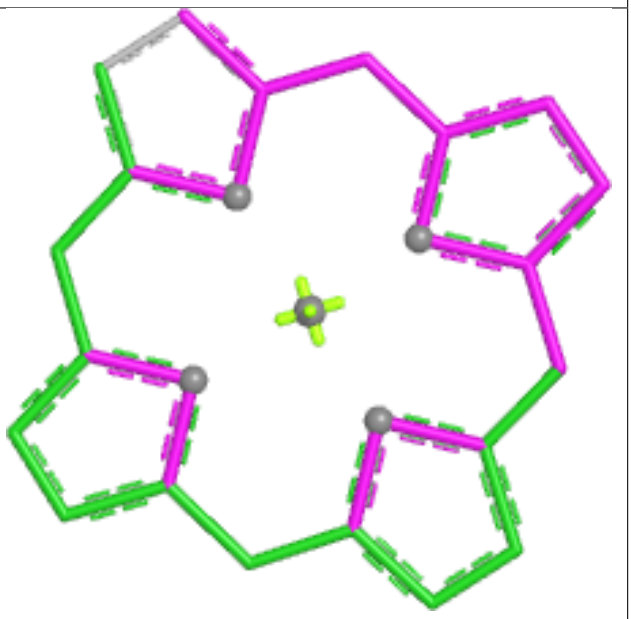


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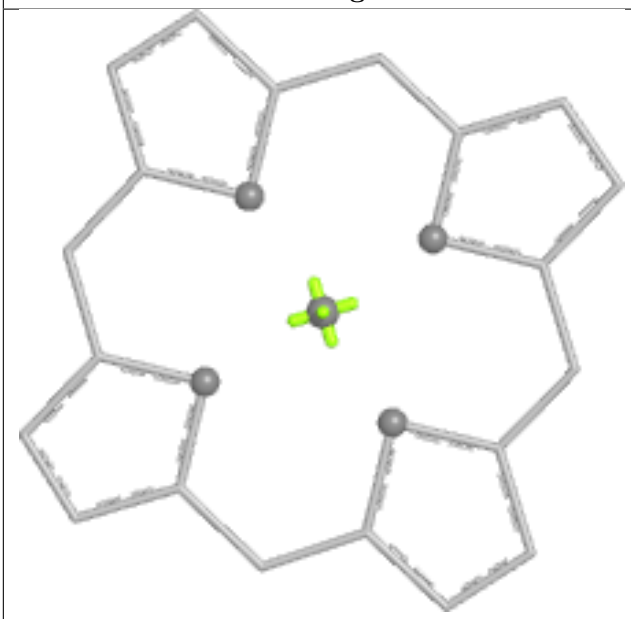
Ligand CLA A 1134



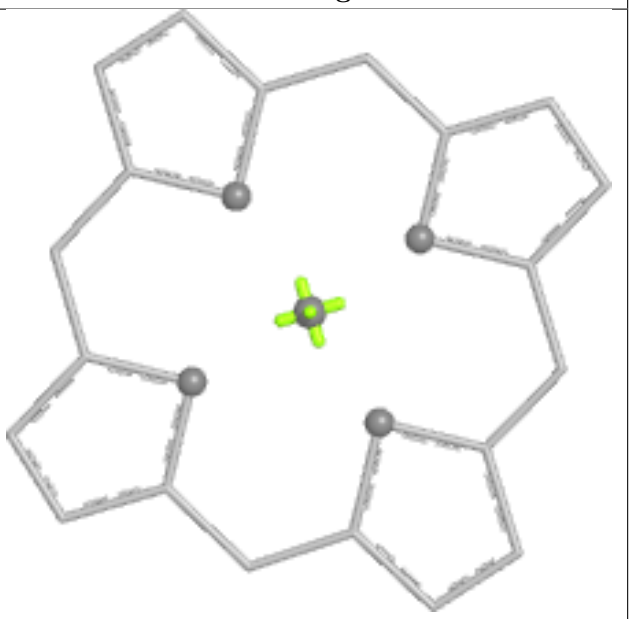
Bond lengths



Bond angles

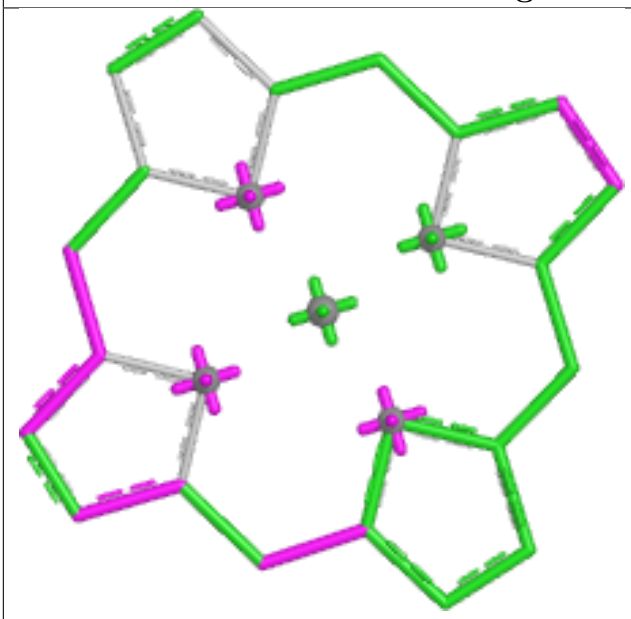


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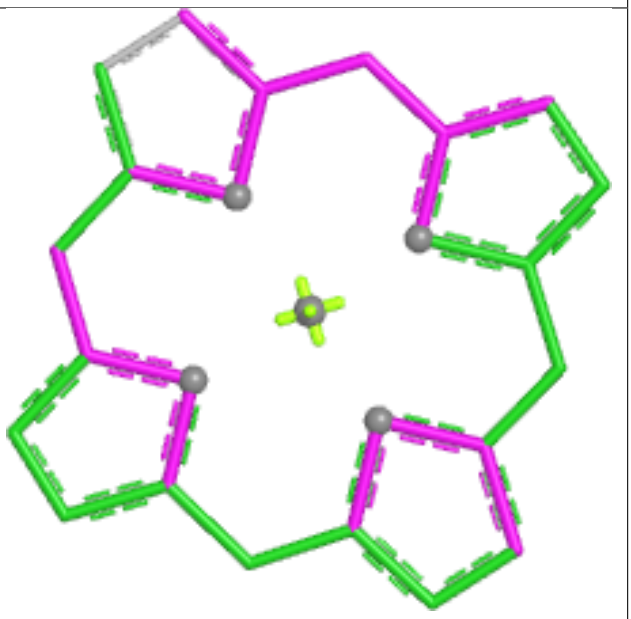


Rings

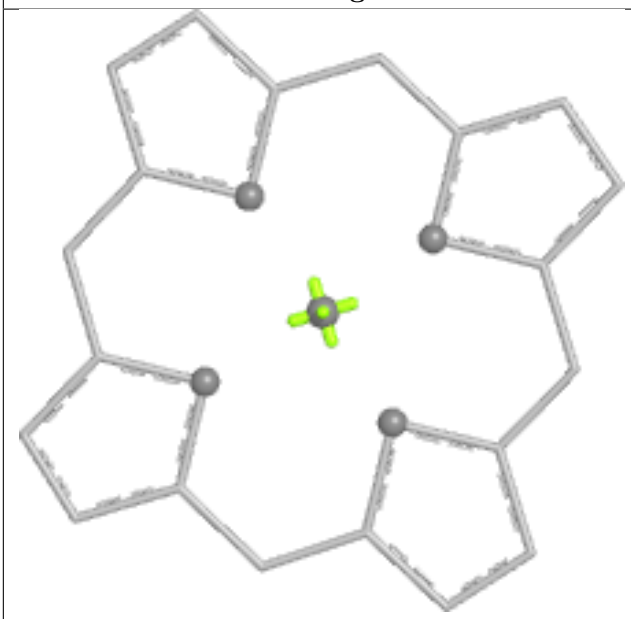
Ligand CLA P 5112



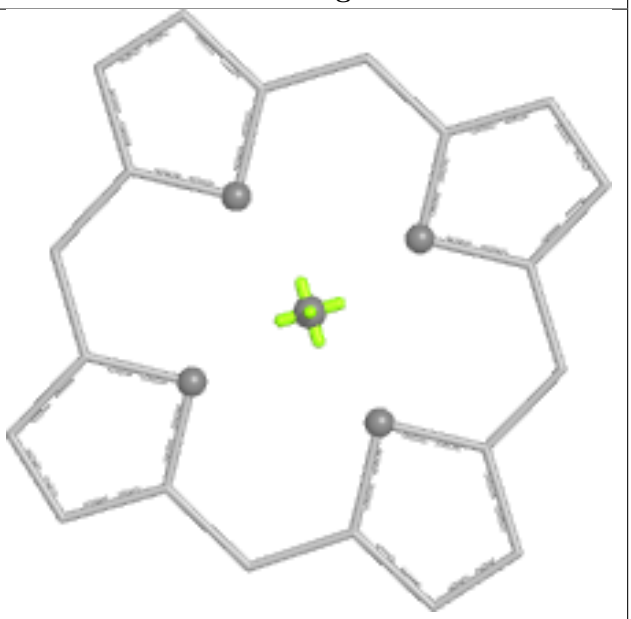
Bond lengths



Bond angles

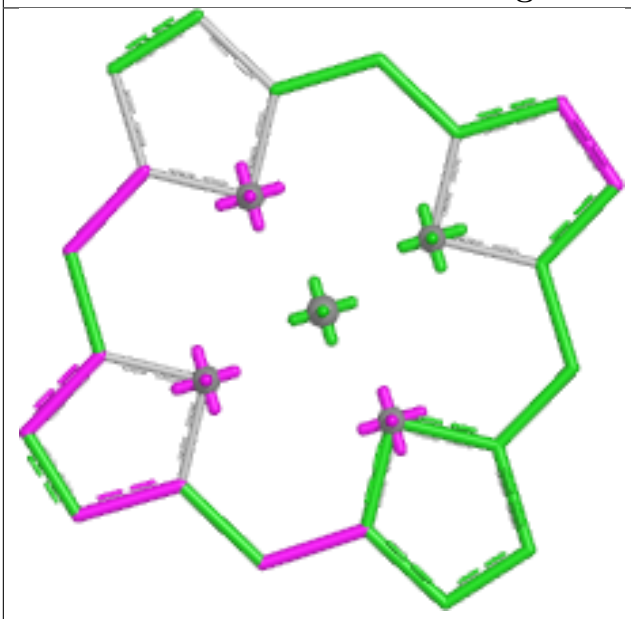


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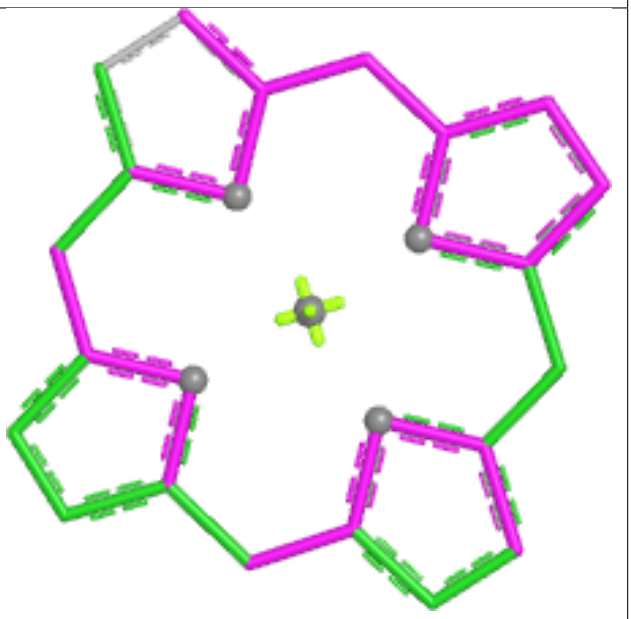


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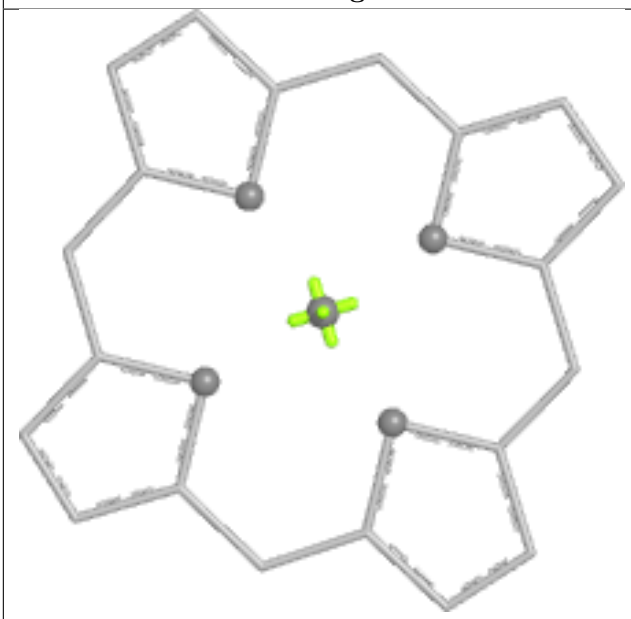
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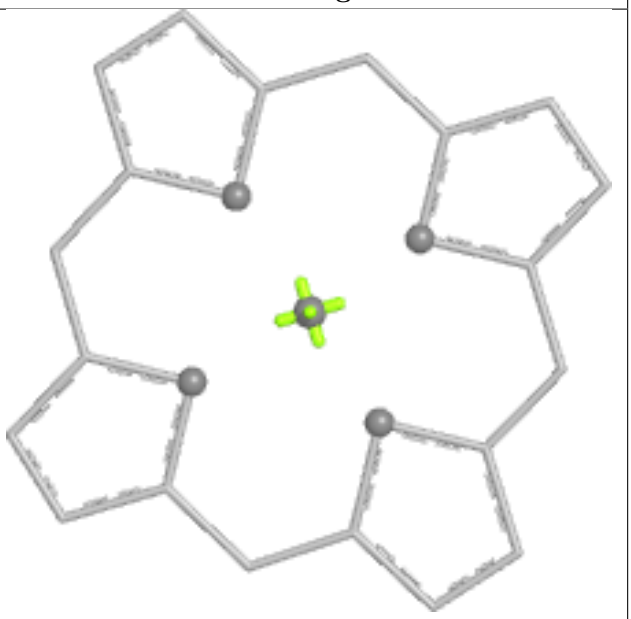
Bond lengths



Bond angles

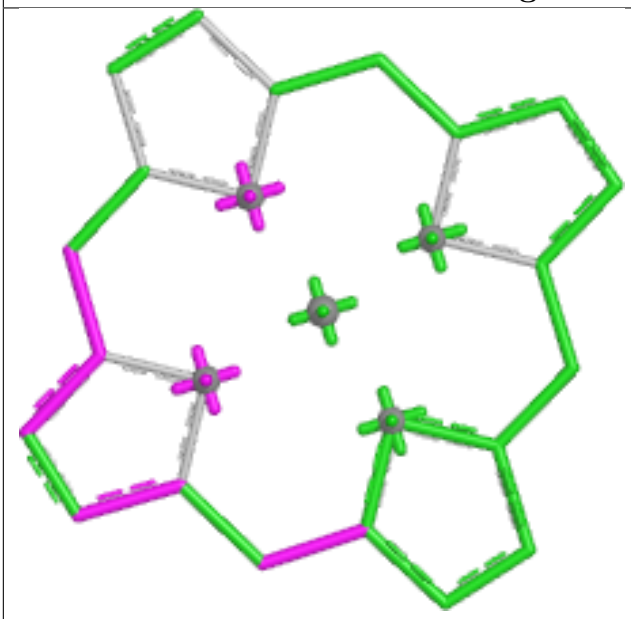


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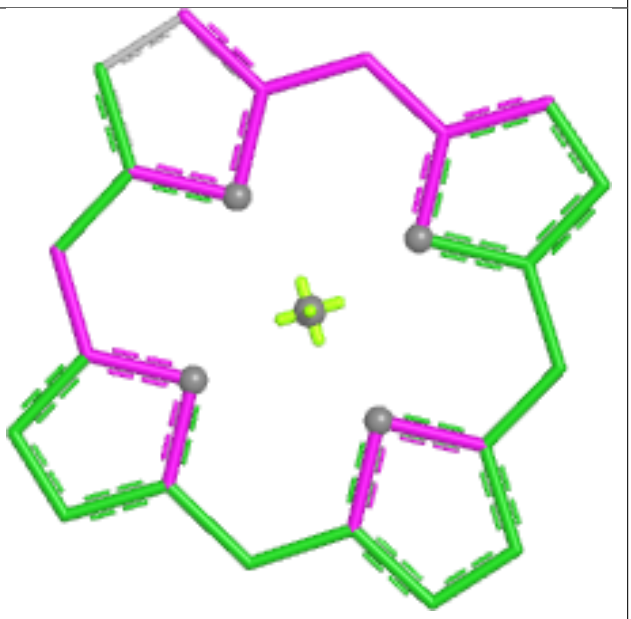


Rings

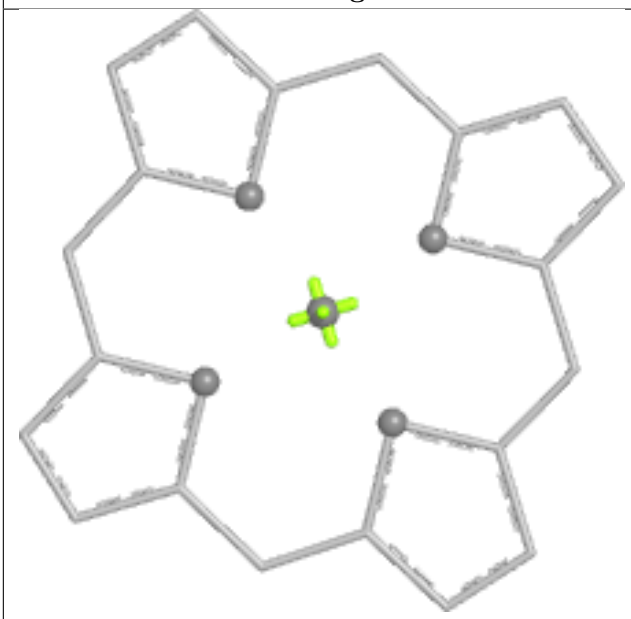
Ligand CLA 8 1011



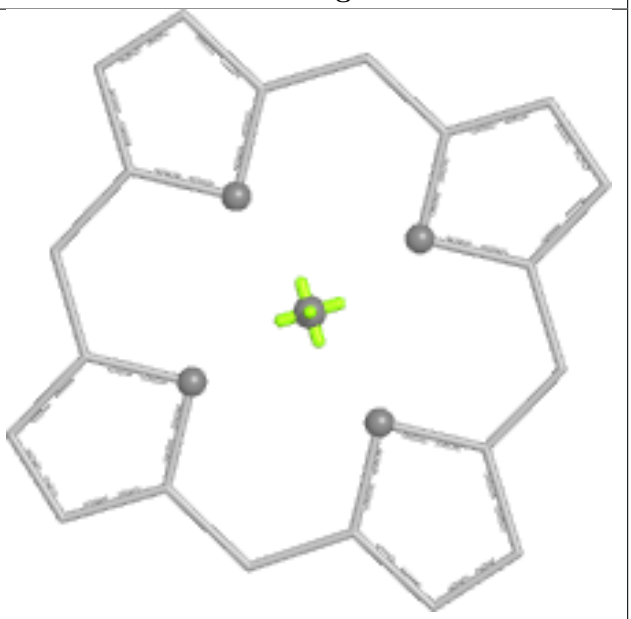
Bond lengths



Bond angles

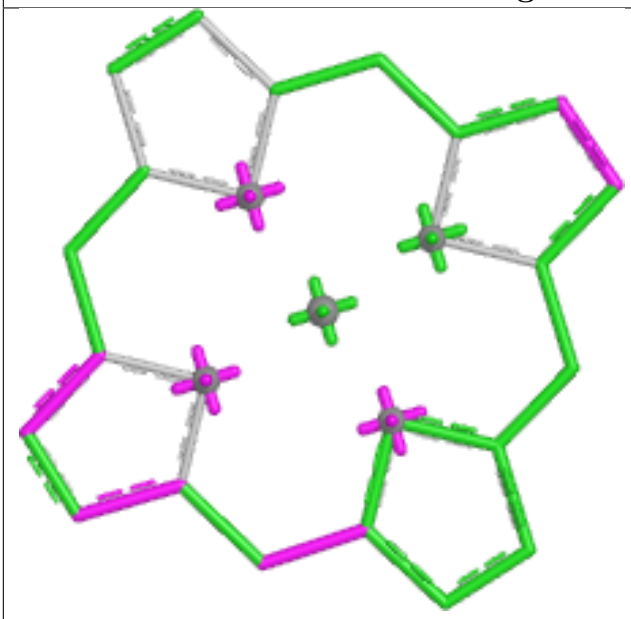


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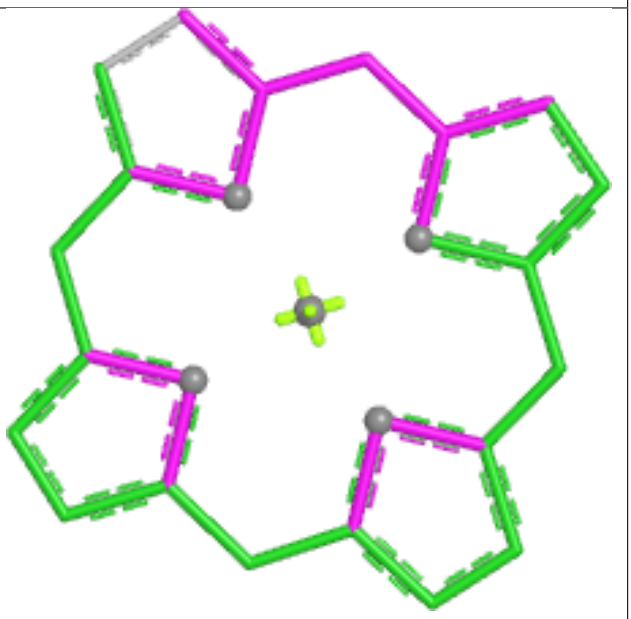


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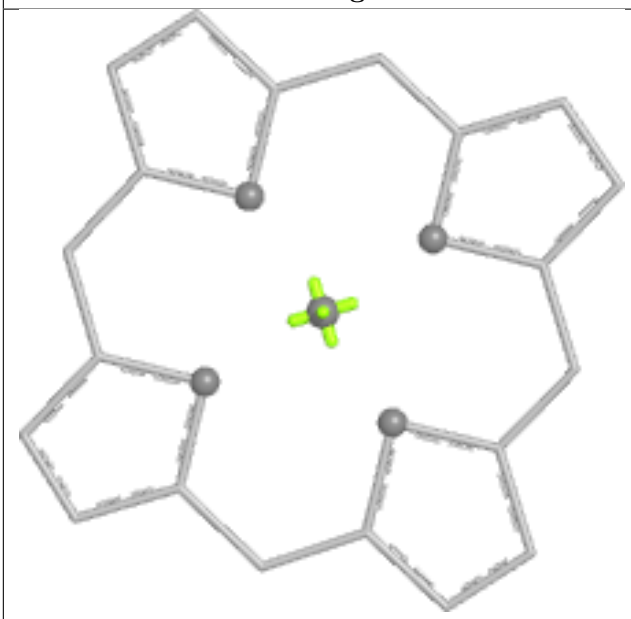
Ligand CLA F 1301



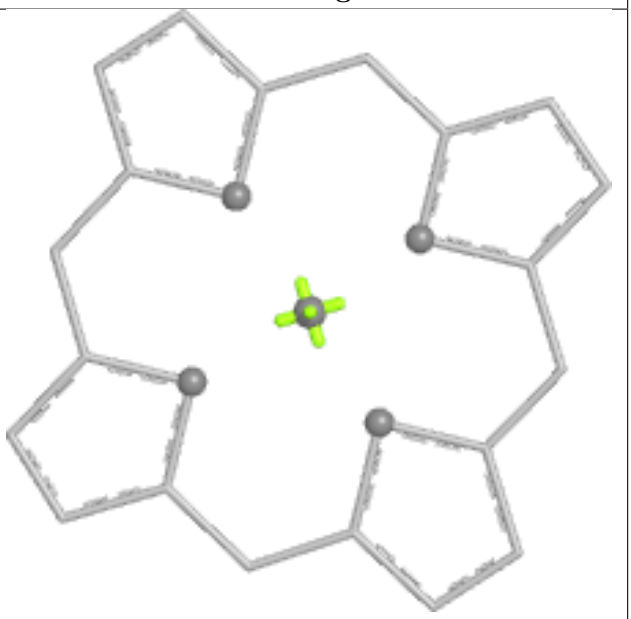
Bond lengths



Bond angles

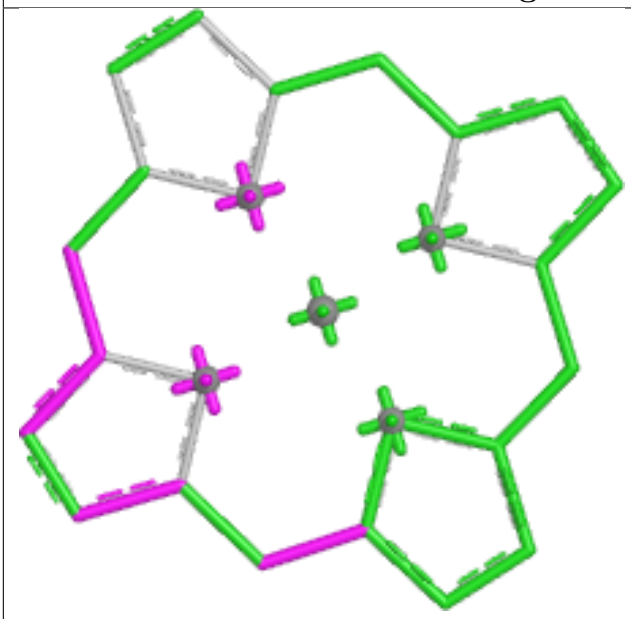


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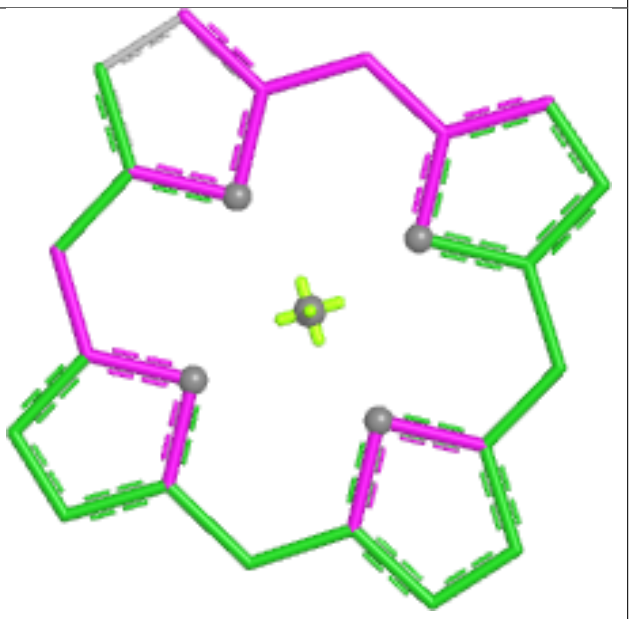


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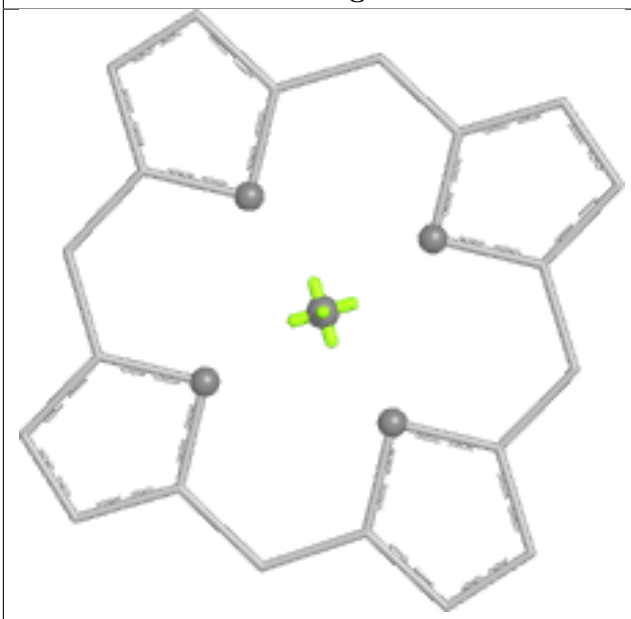
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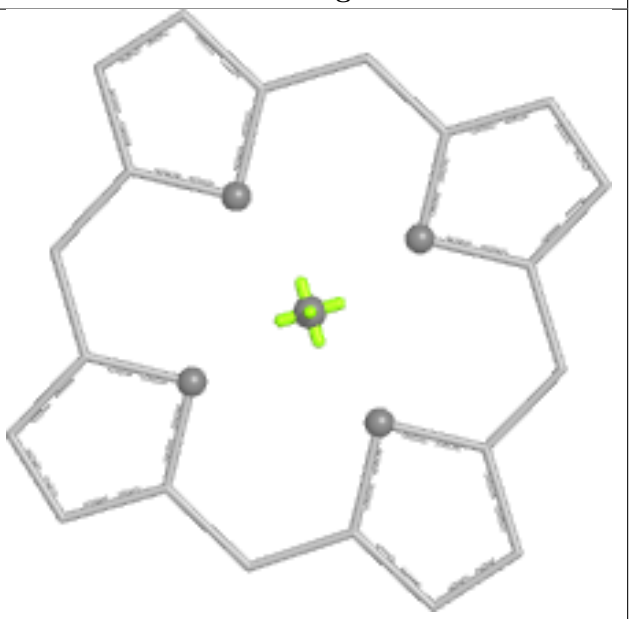
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Bond angles

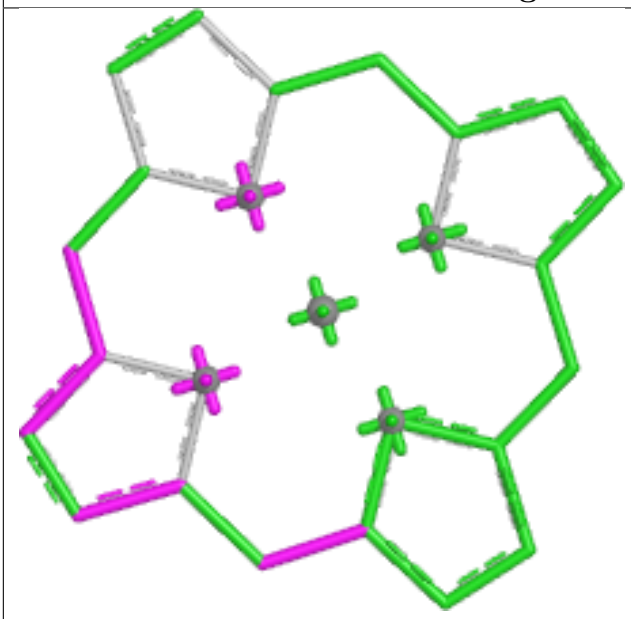


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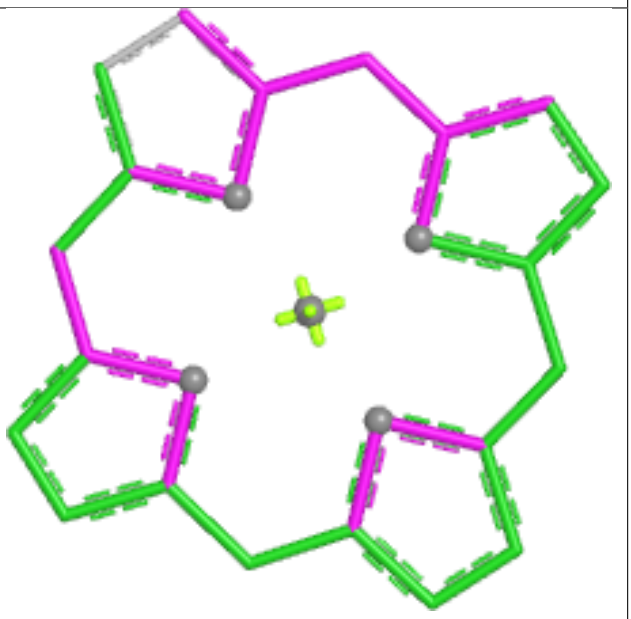


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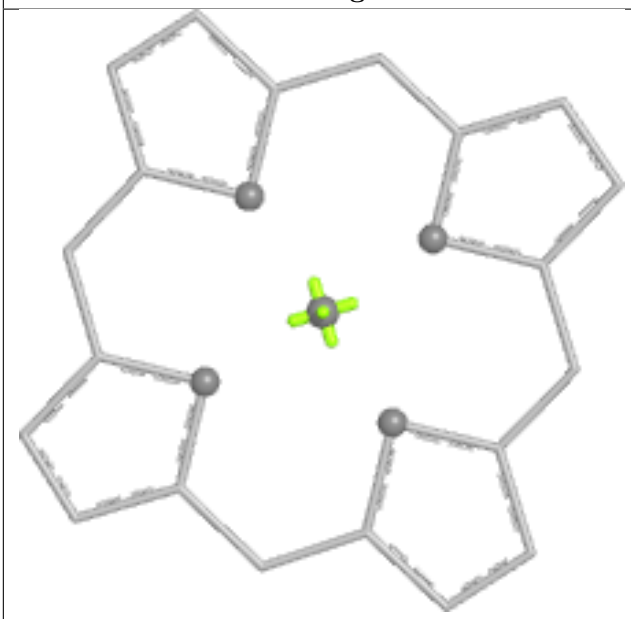
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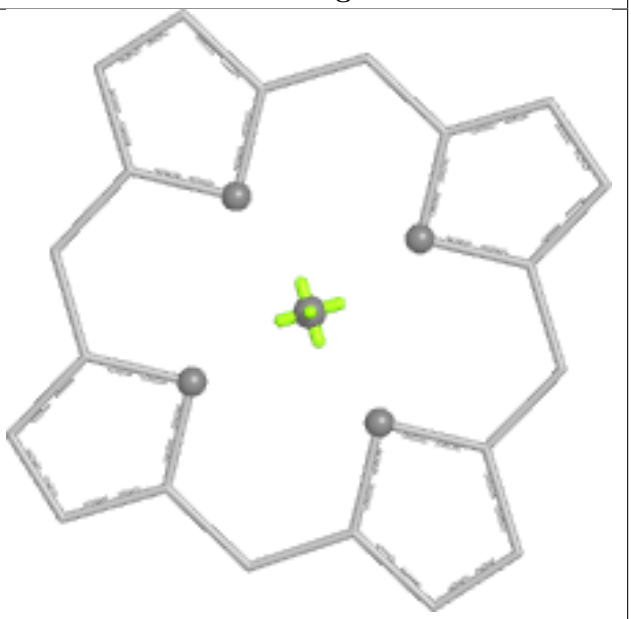
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Bond angles

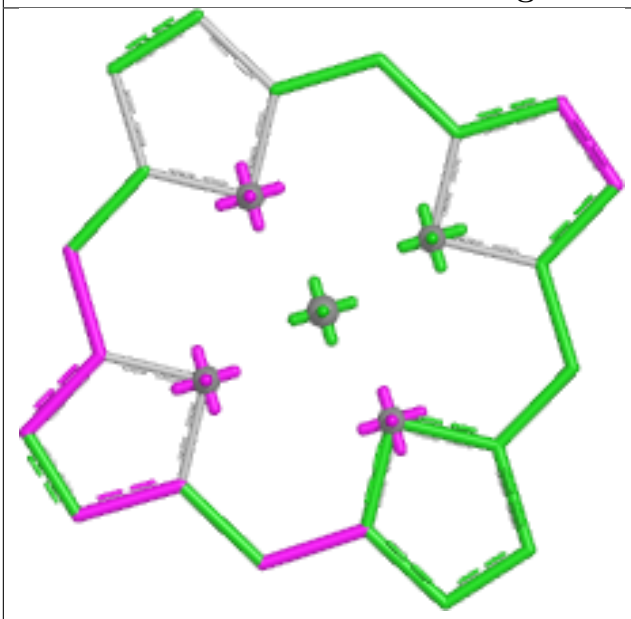


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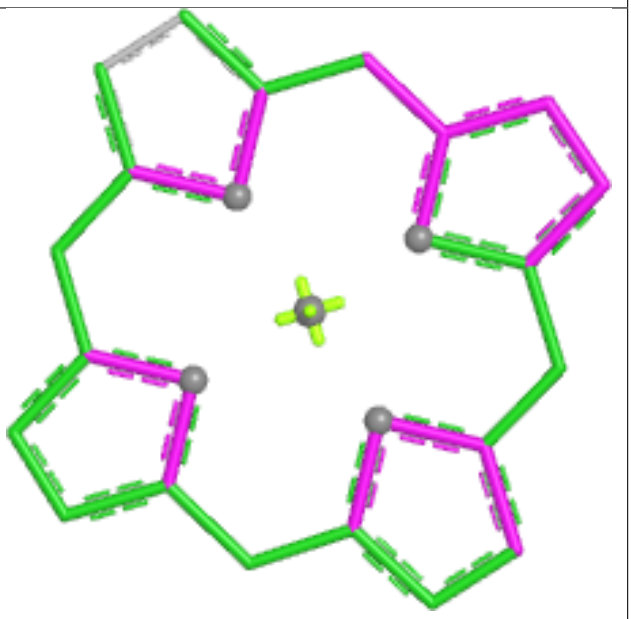


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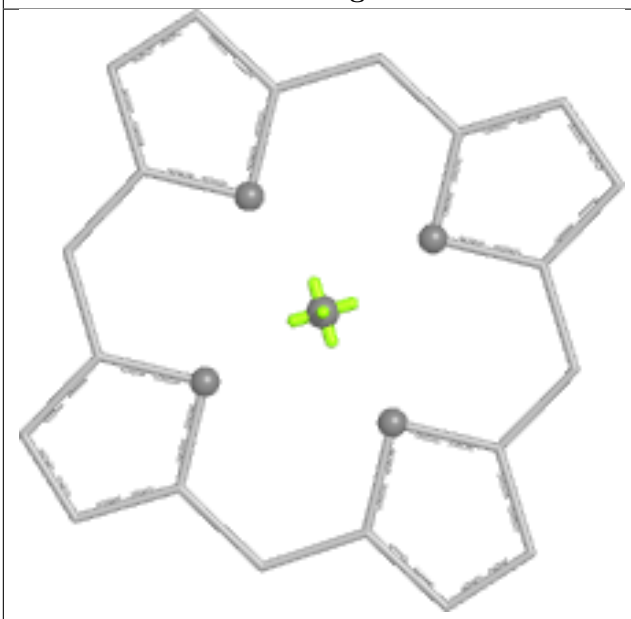
Ligand CLA F 1229



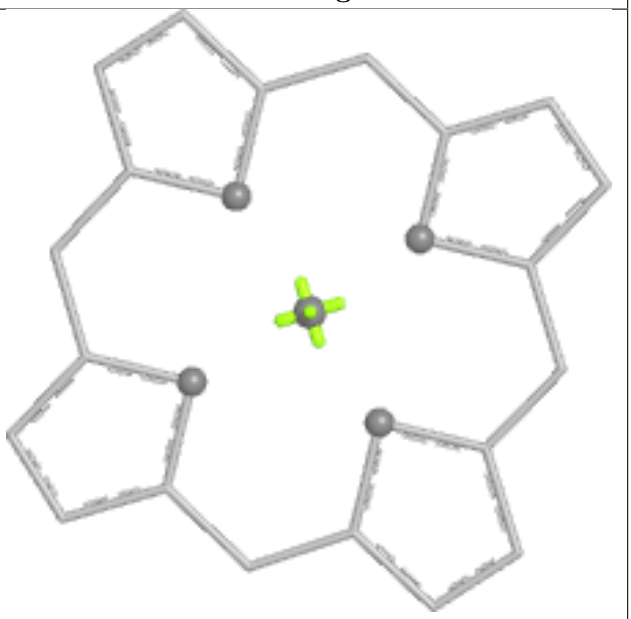
Bond lengths



Bond angles

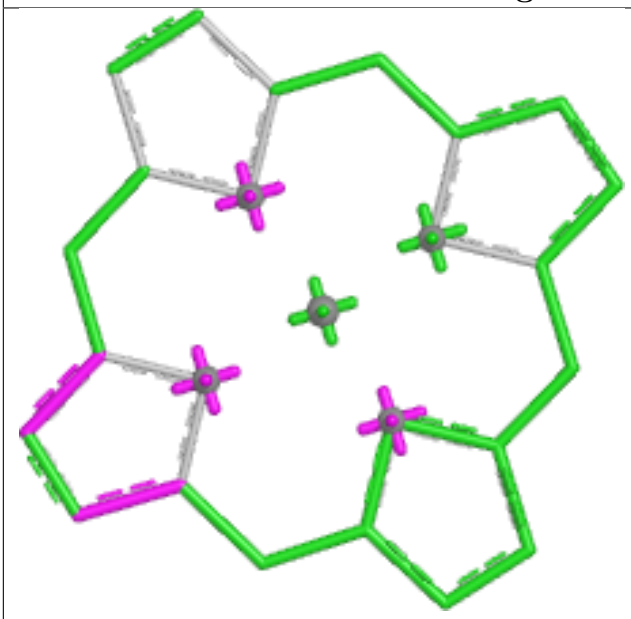


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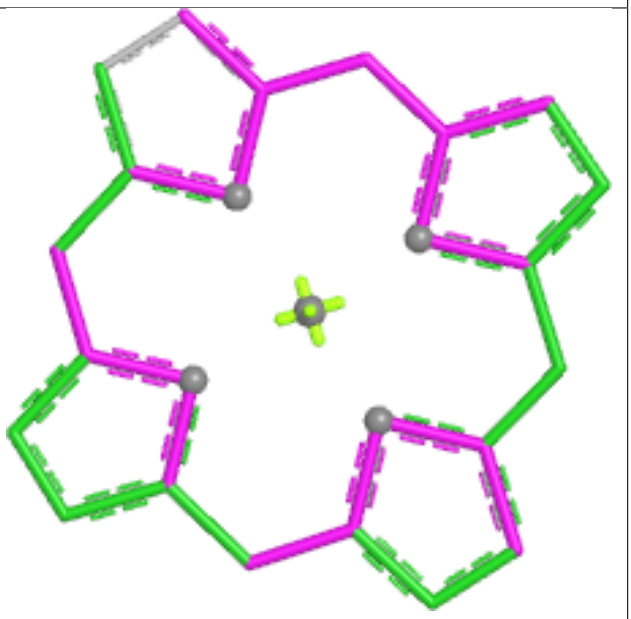


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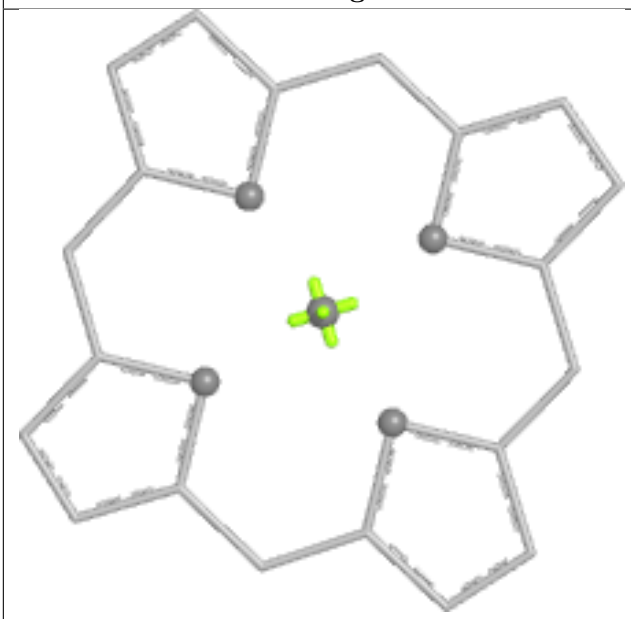
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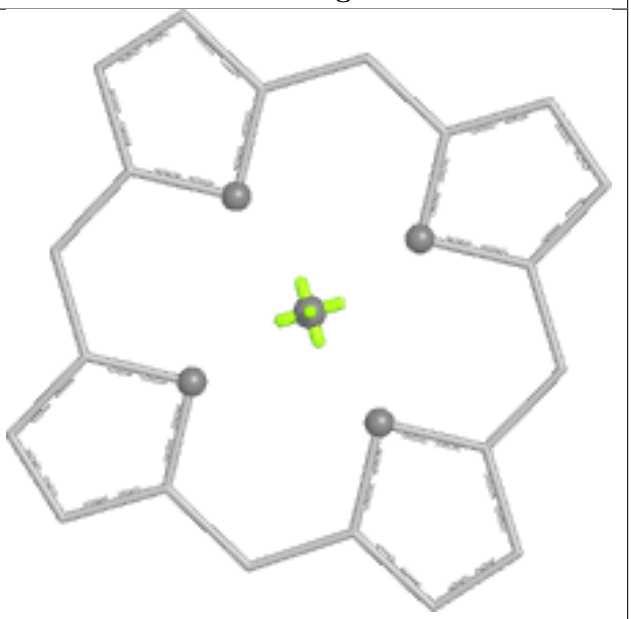
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Bond angles

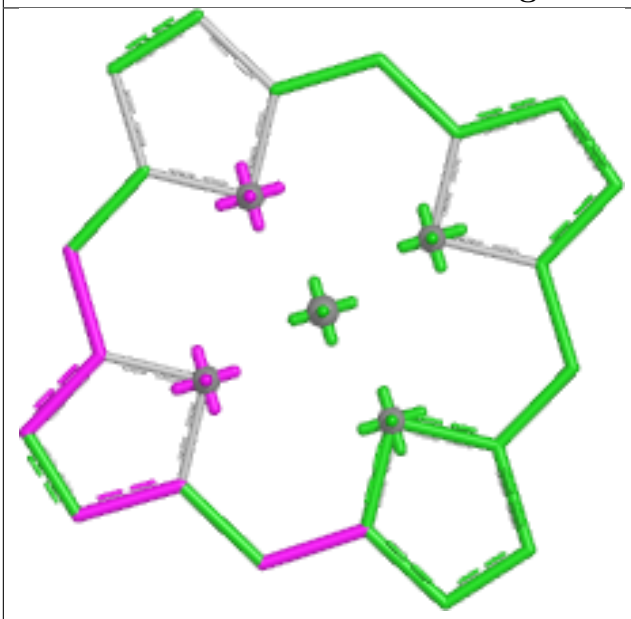


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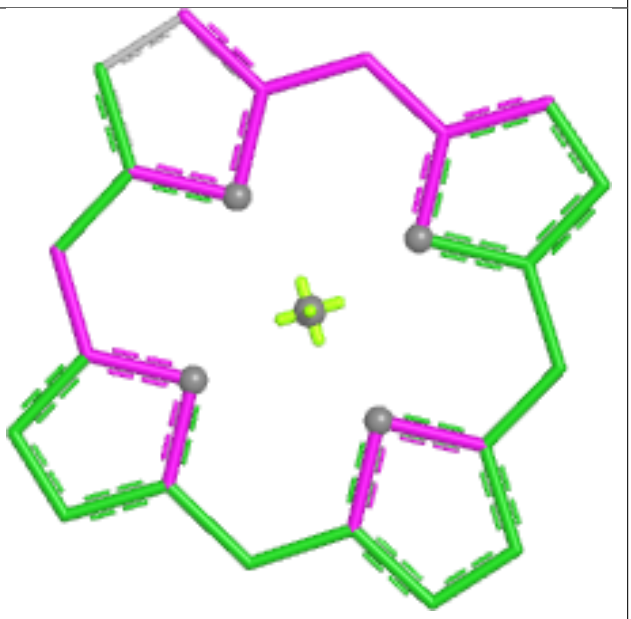


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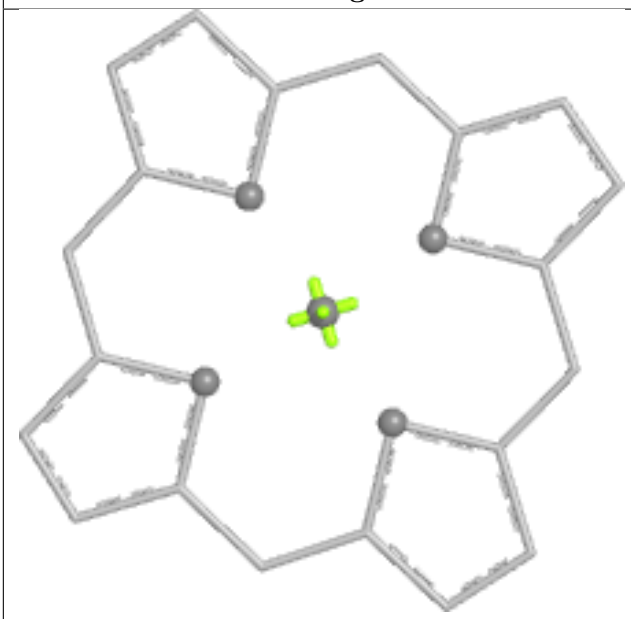
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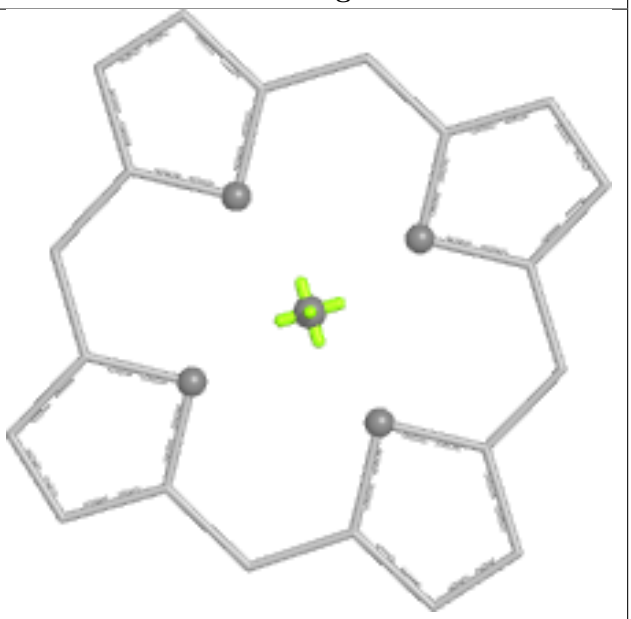
Bond lengths



Bond angles

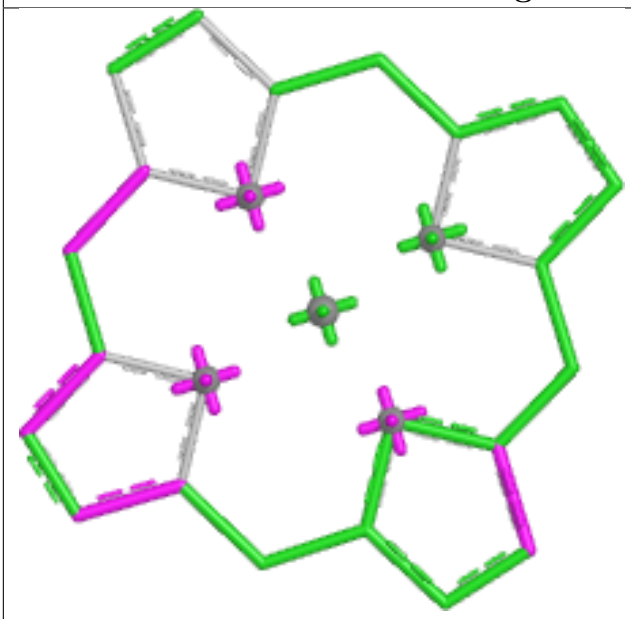


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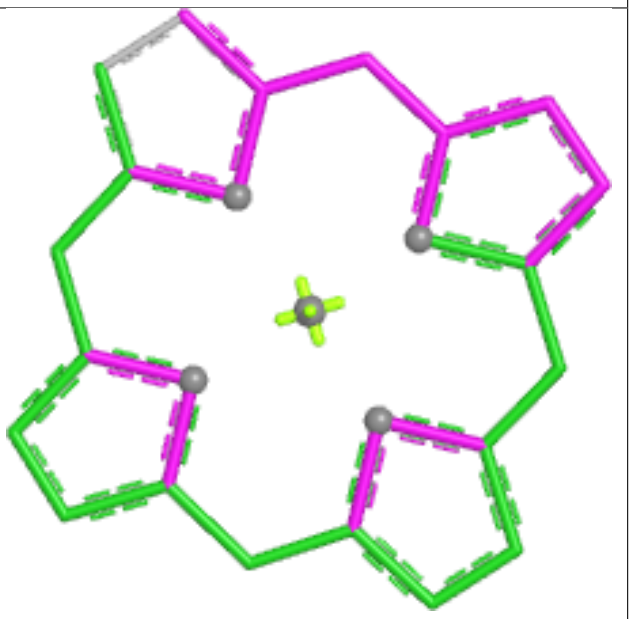


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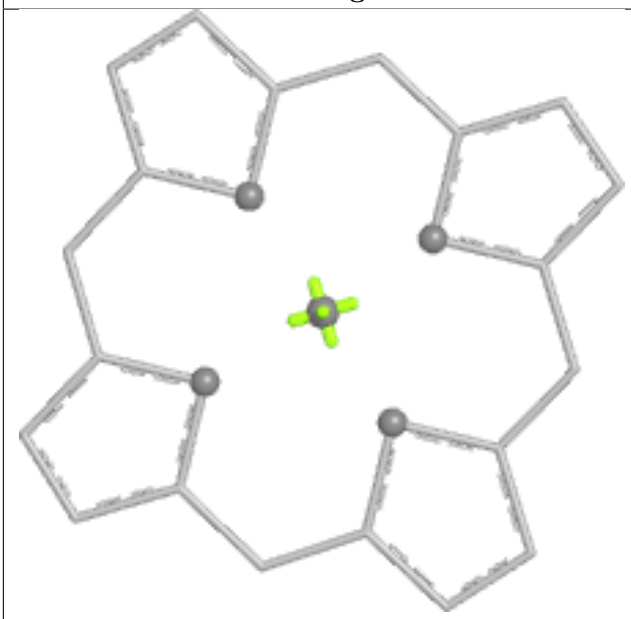
Ligand CLA A 1135



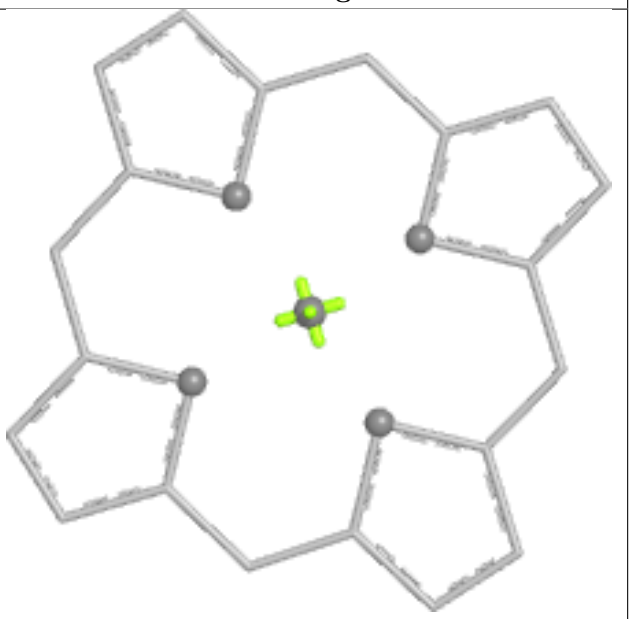
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Bond angles

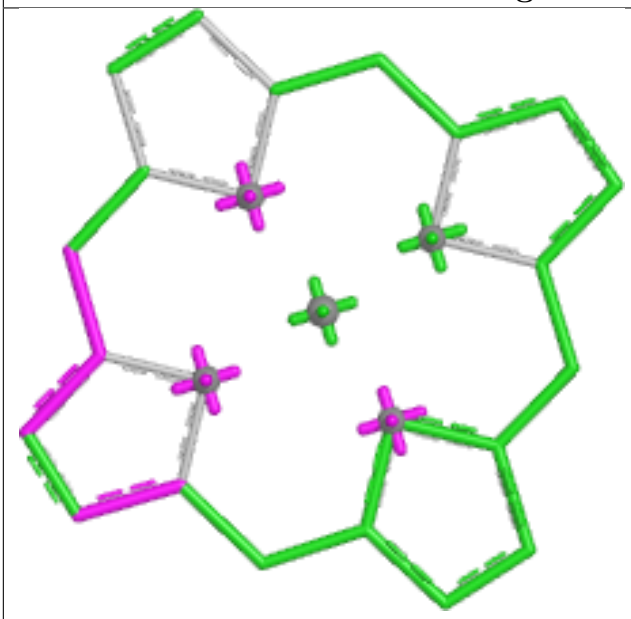


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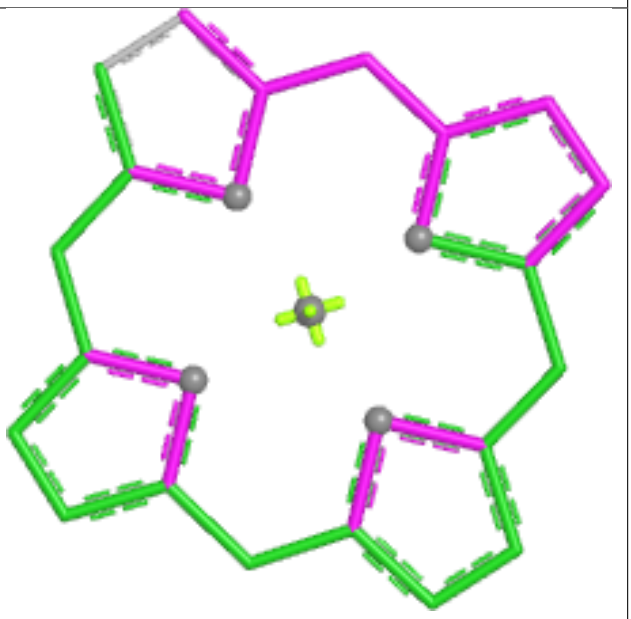


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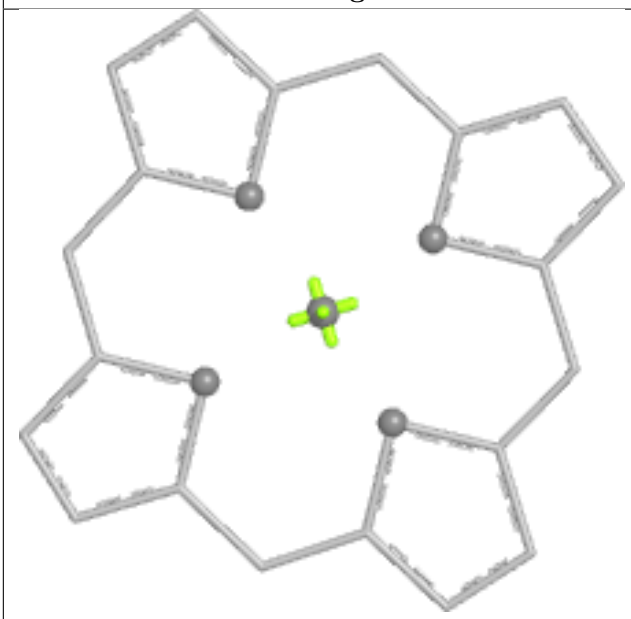
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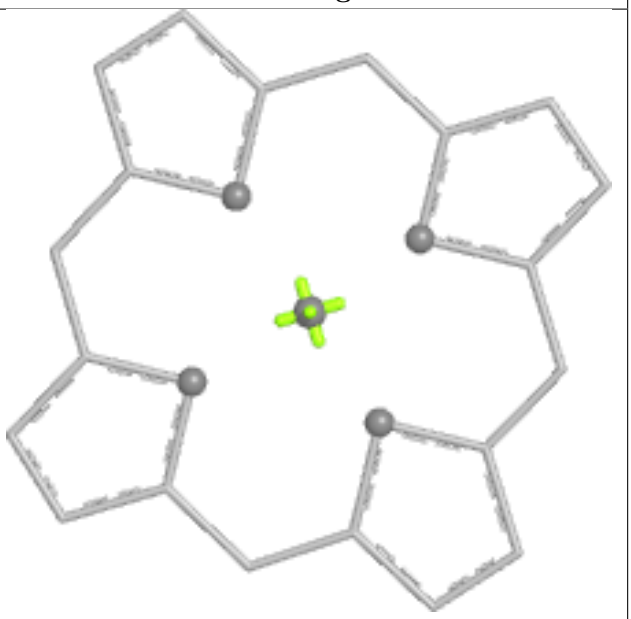
Bond lengths



Bond angles

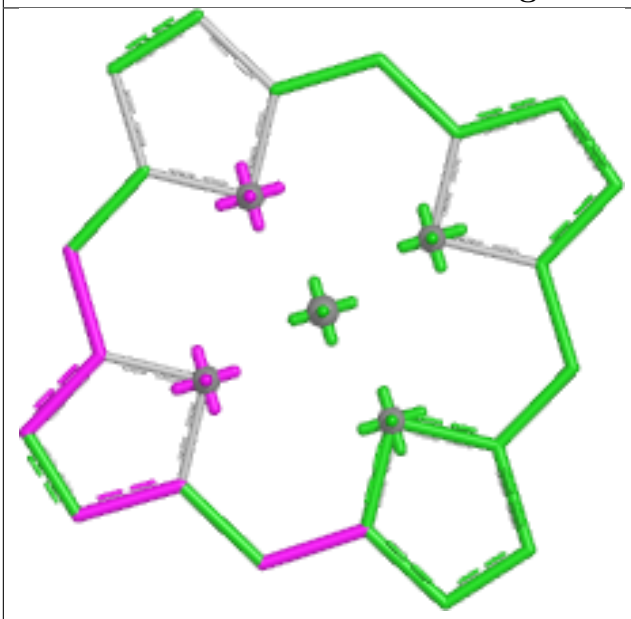


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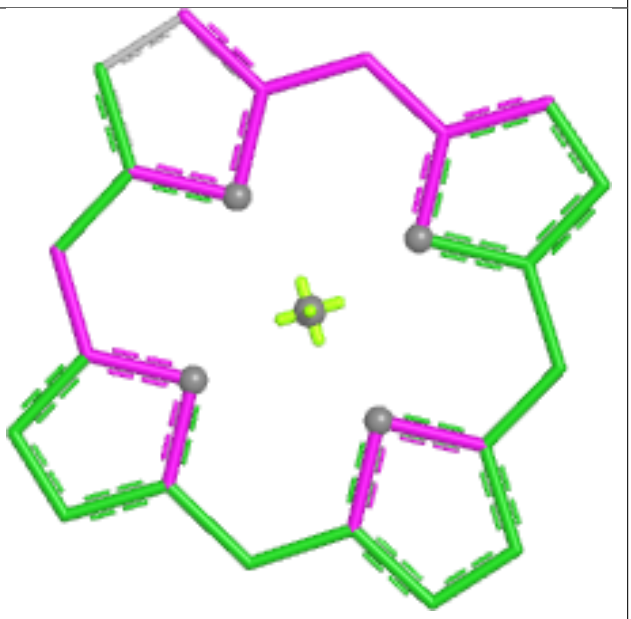


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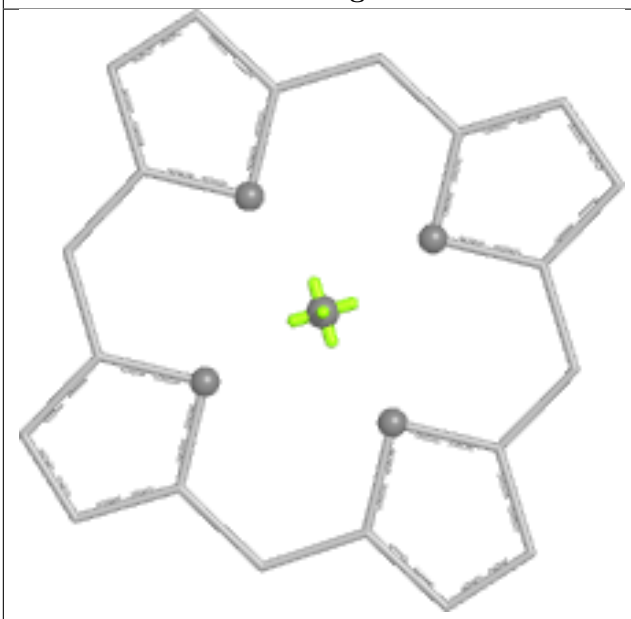
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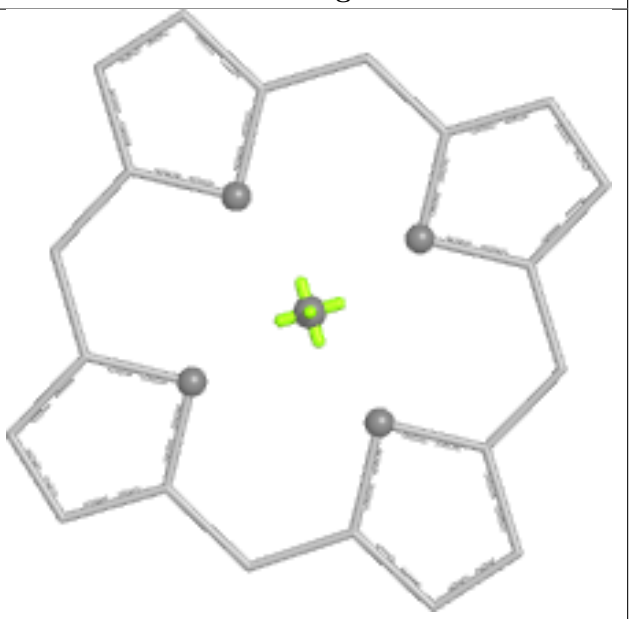
Bond lengths



Bond angles

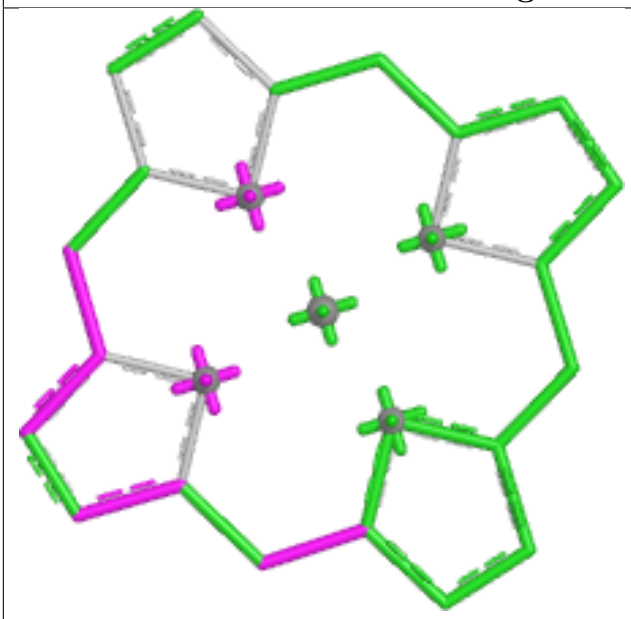


Torsions

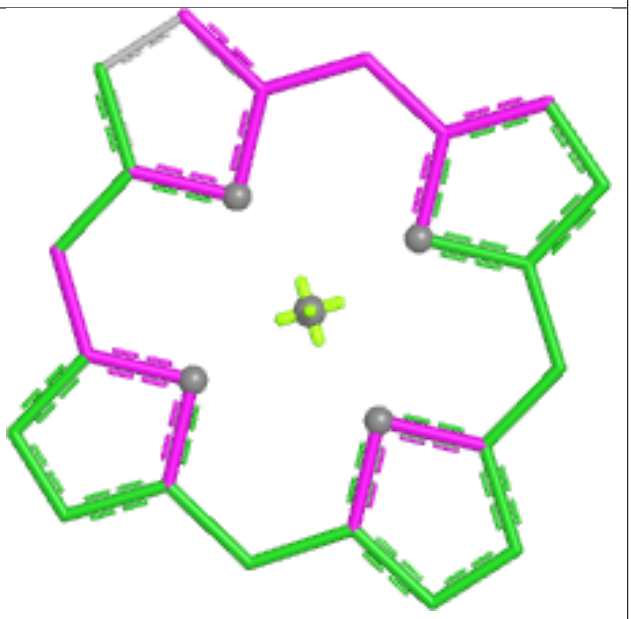


Rings

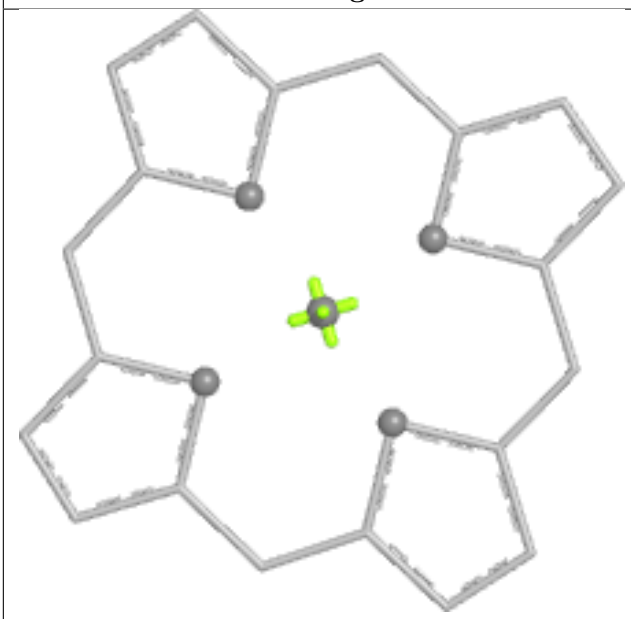
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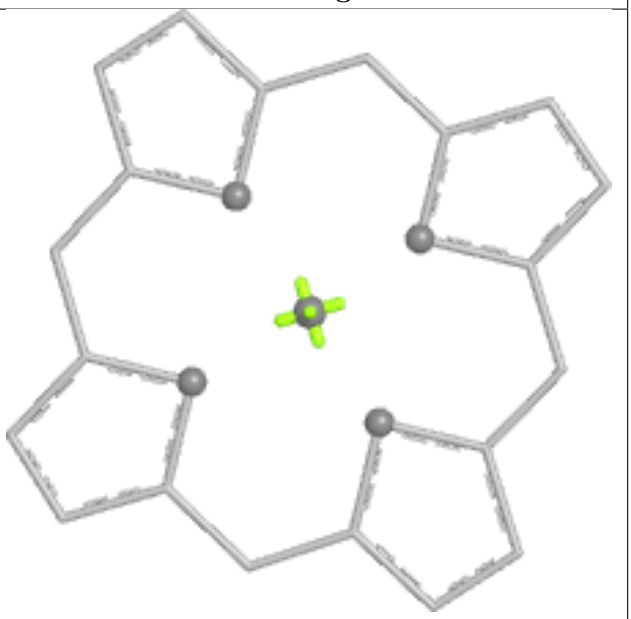
Bond lengths



Bond angles

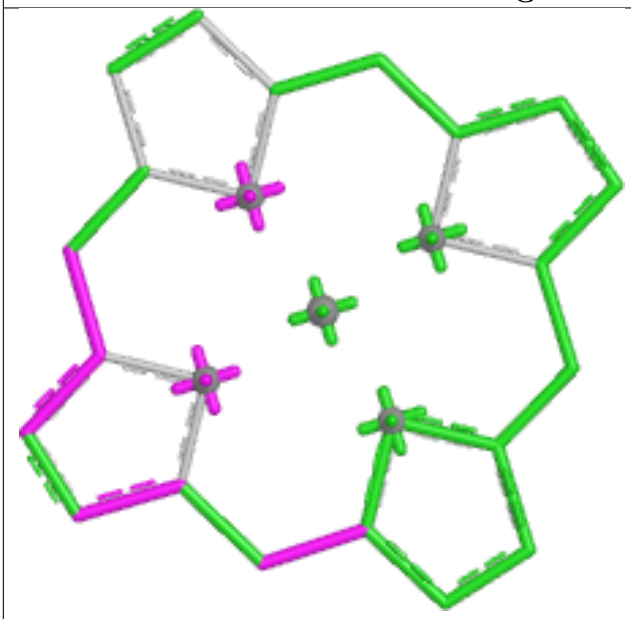


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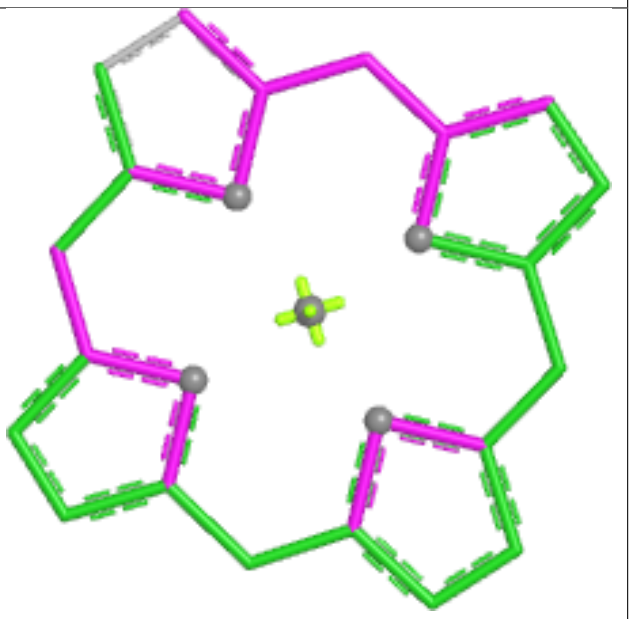


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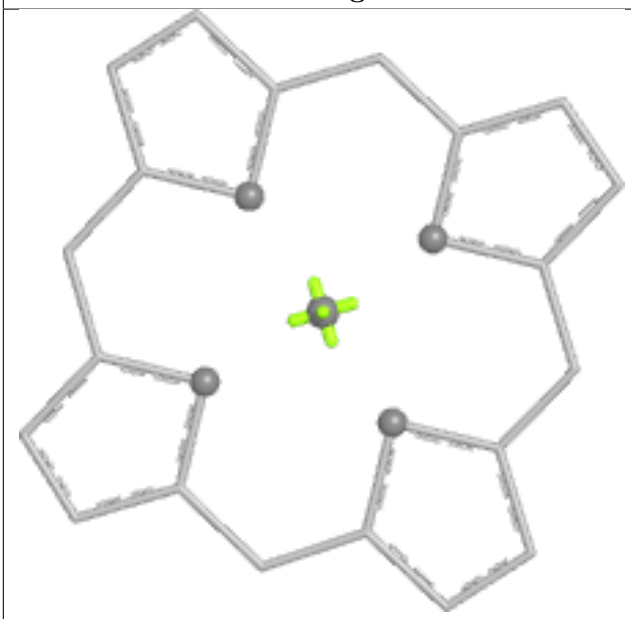
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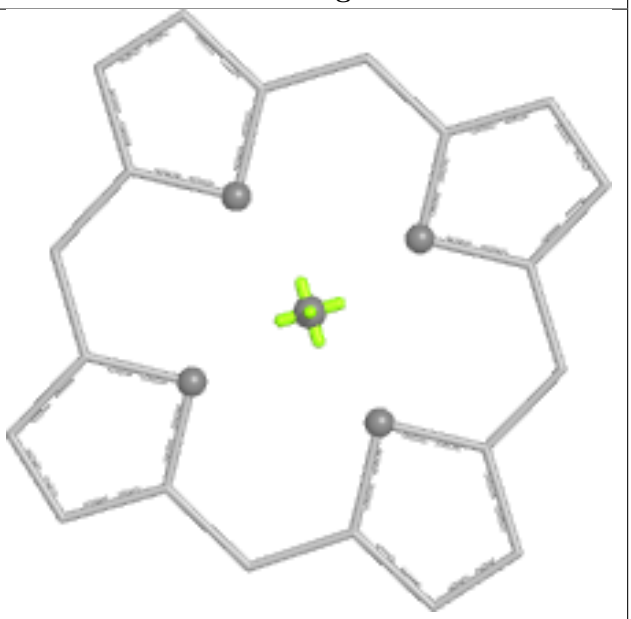
Bond lengths



Bond angles

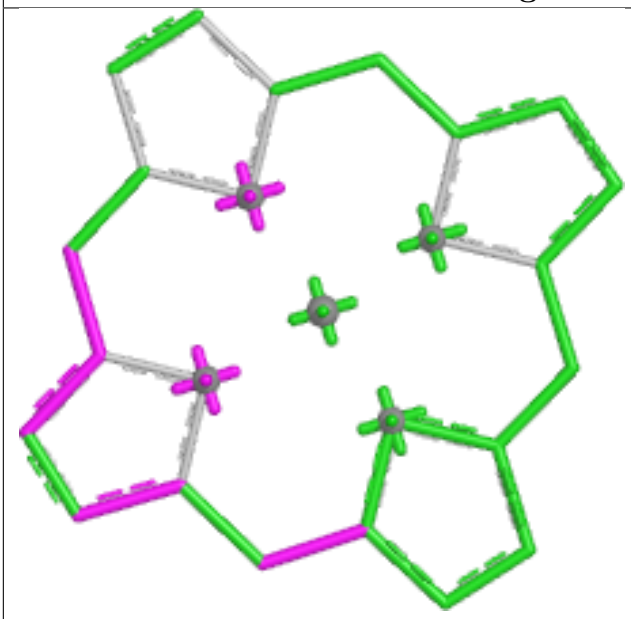


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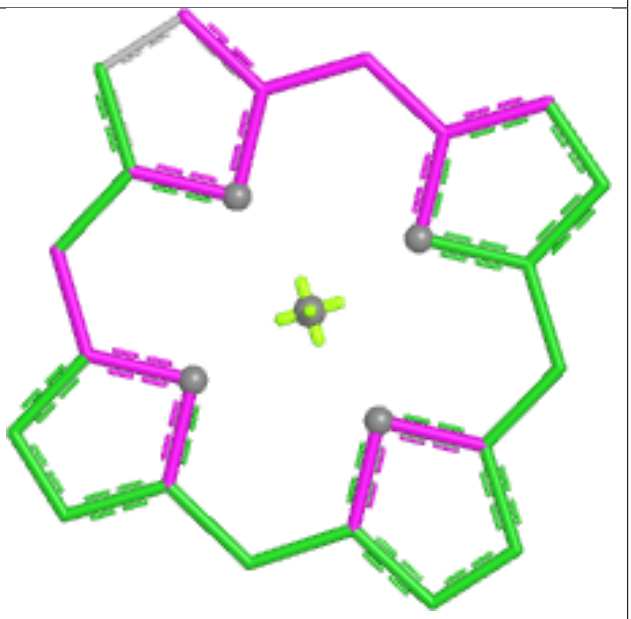


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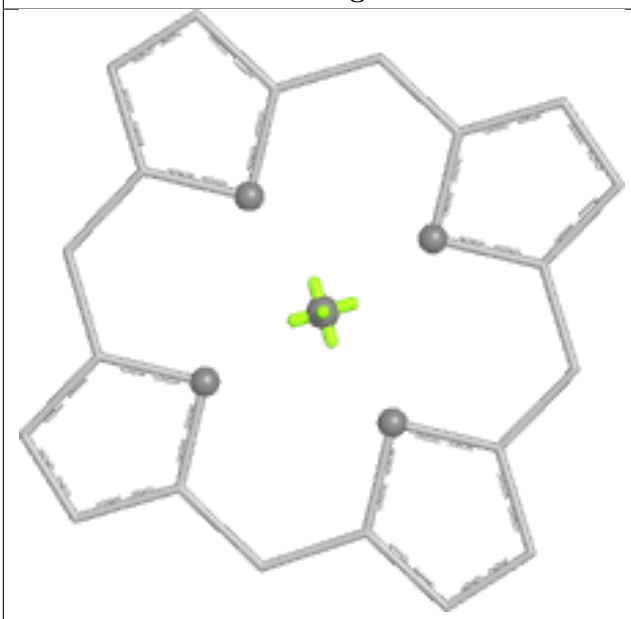
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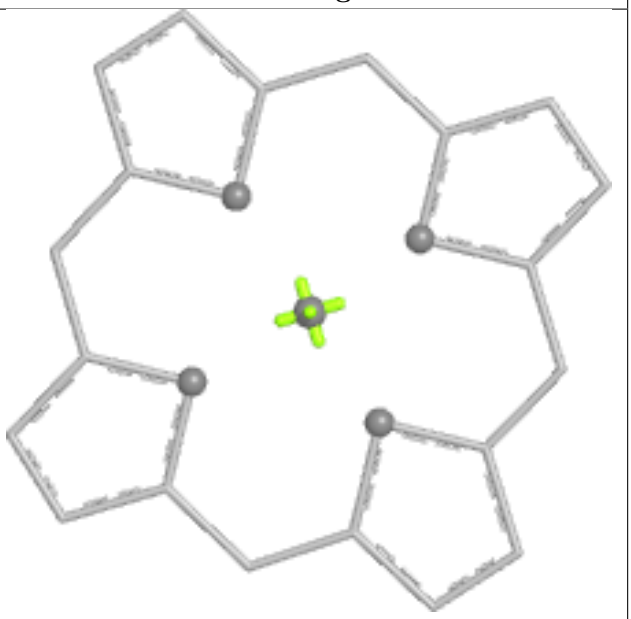
Bond lengths



Bond angles

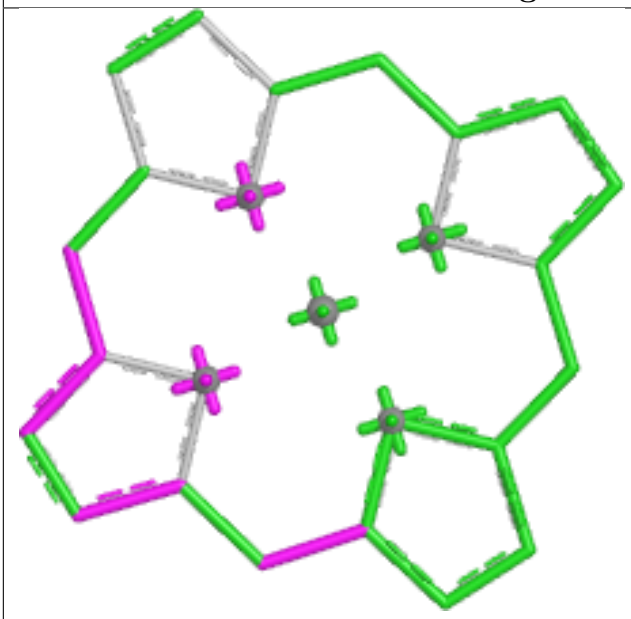


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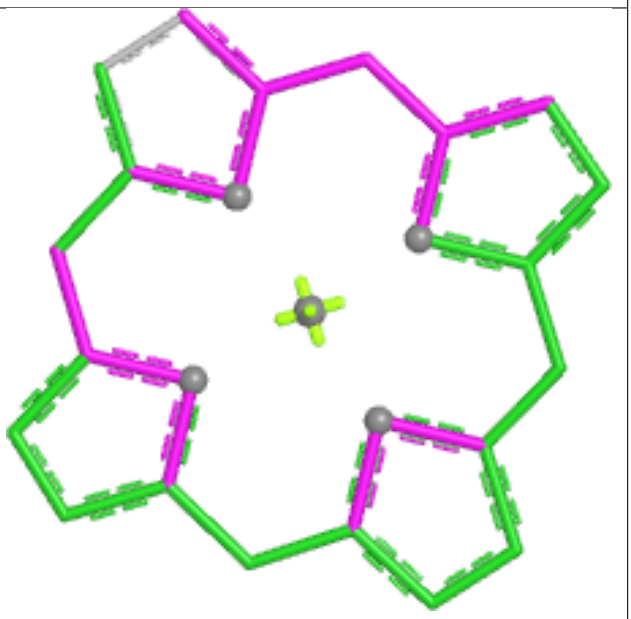


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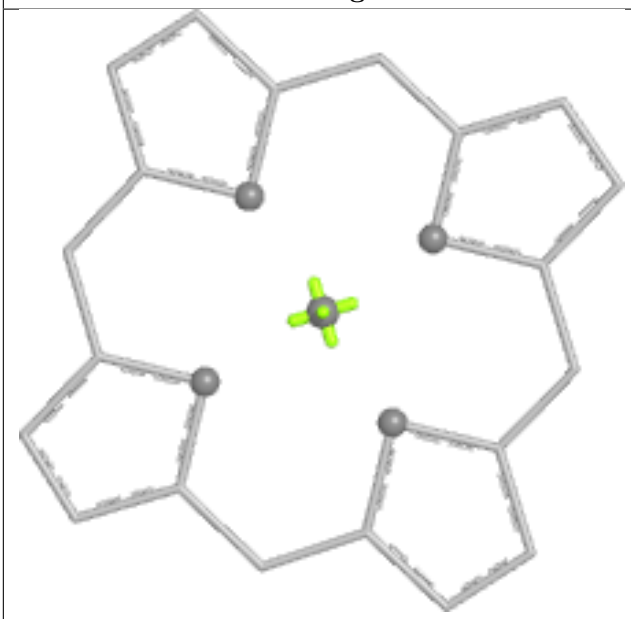
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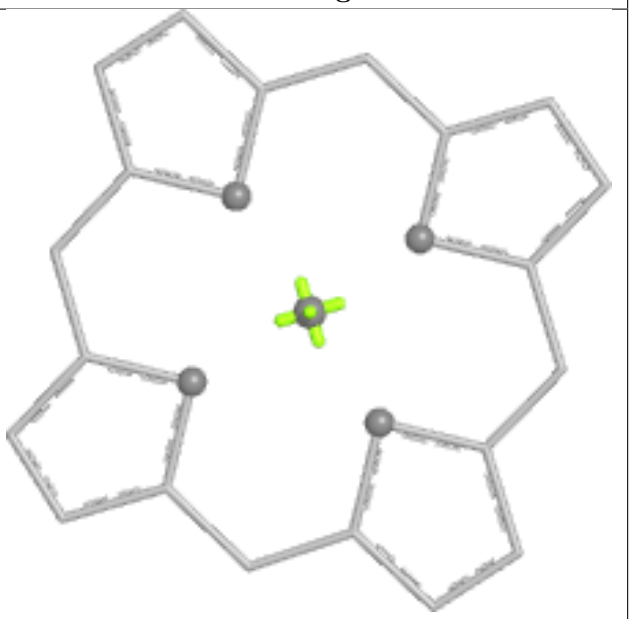
Bond lengths



Bond angles

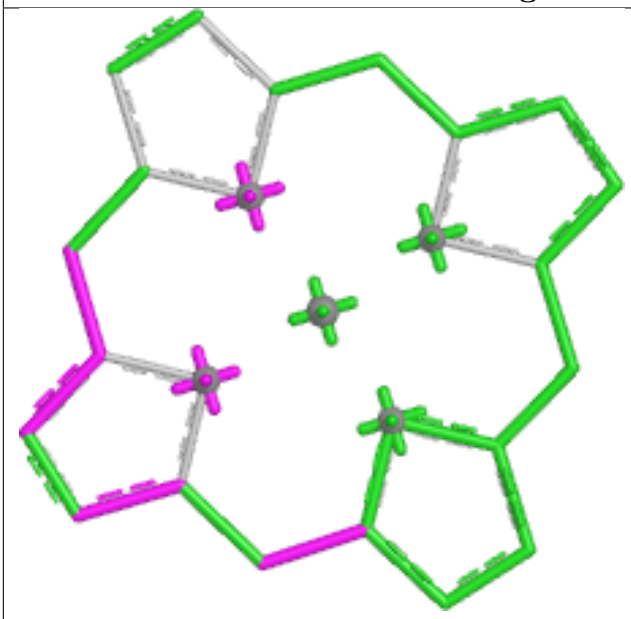


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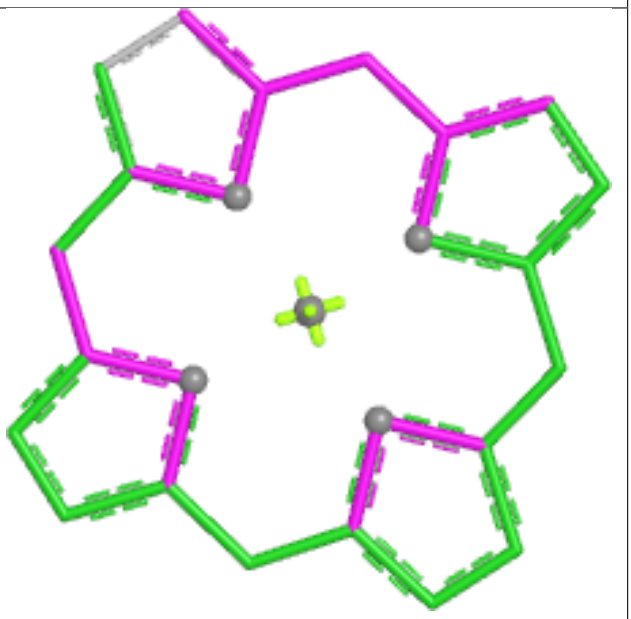


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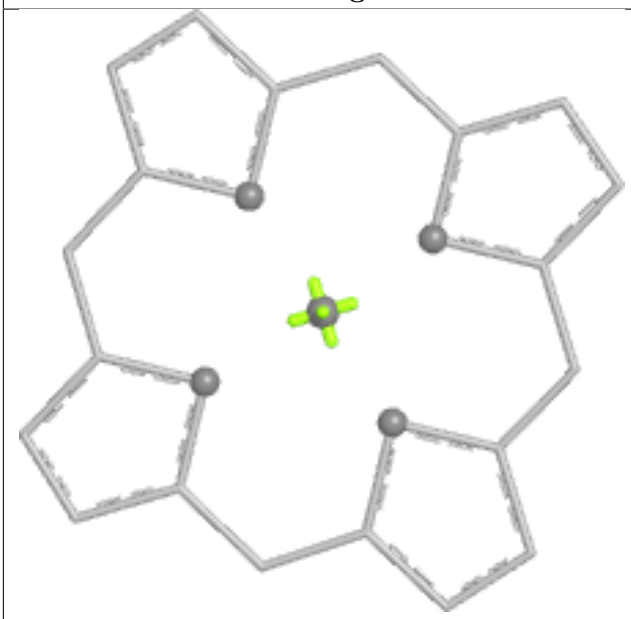
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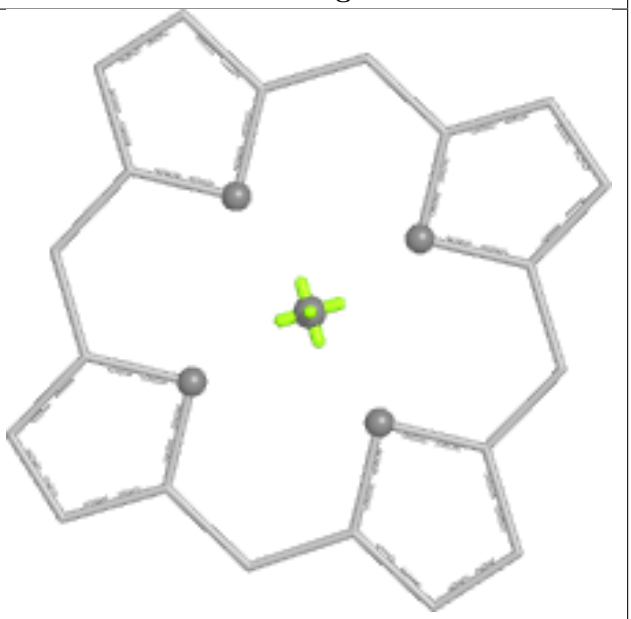
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Bond angles

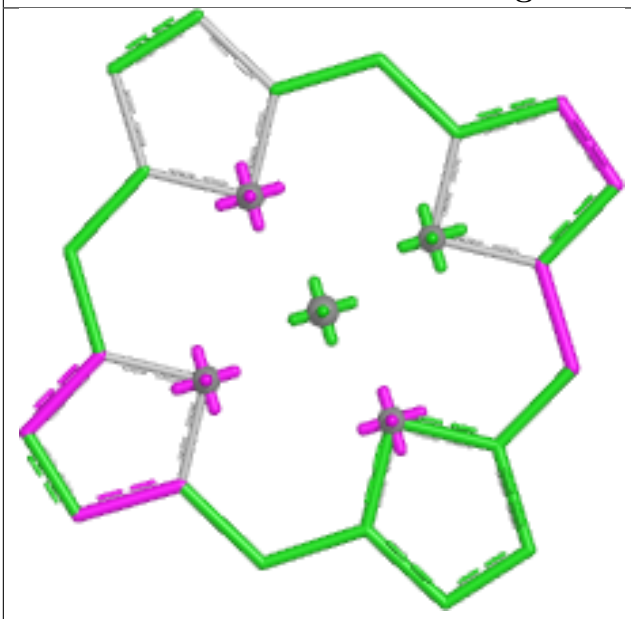


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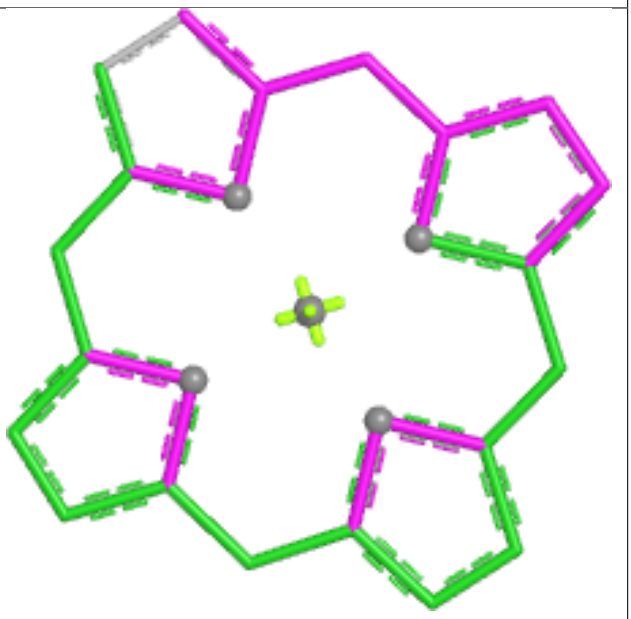


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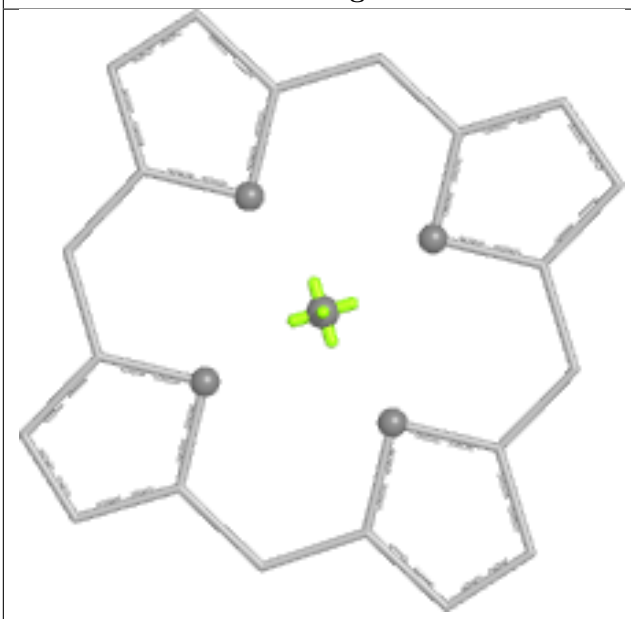
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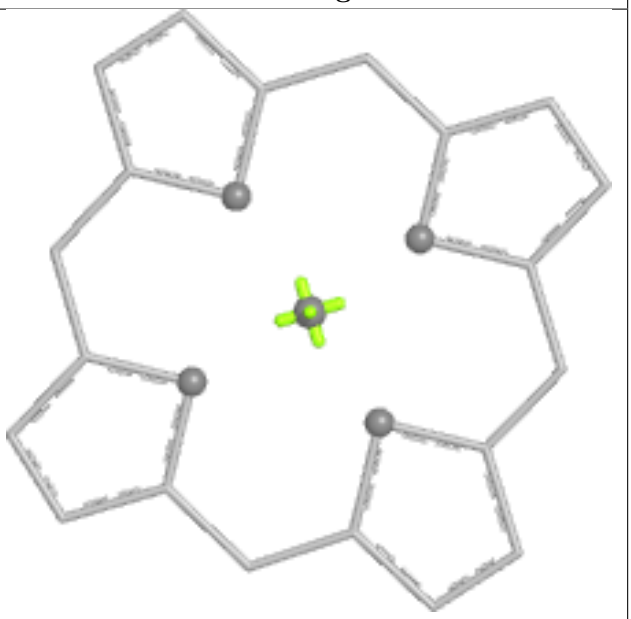
Bond lengths



Bond angles

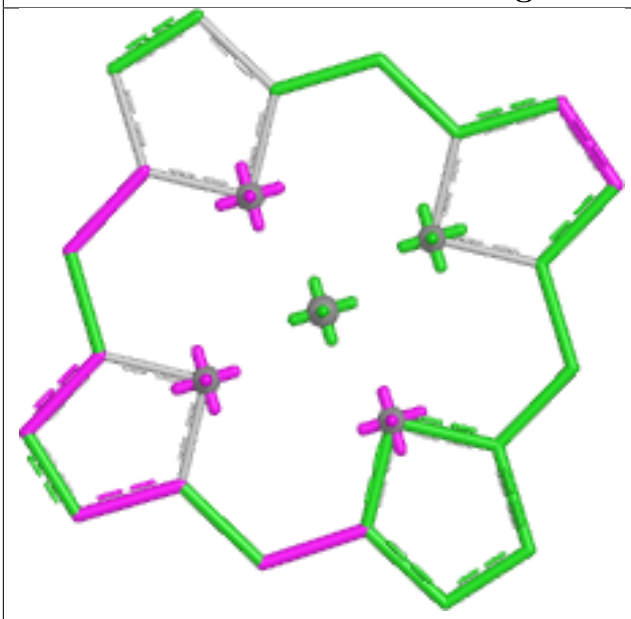


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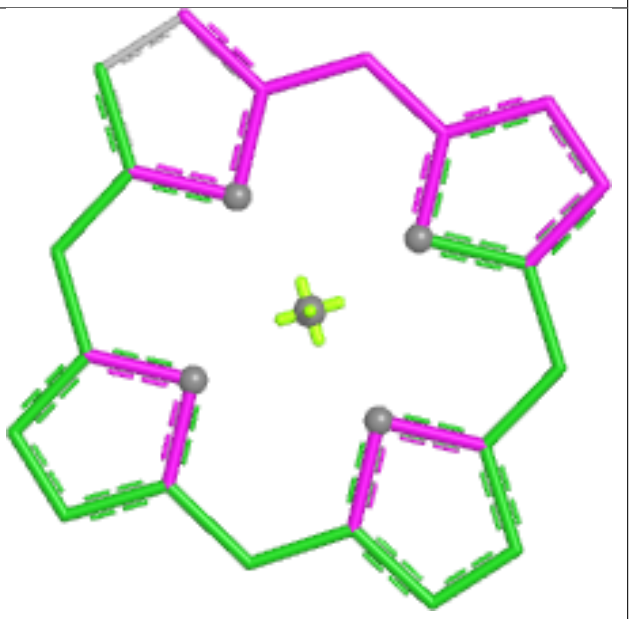


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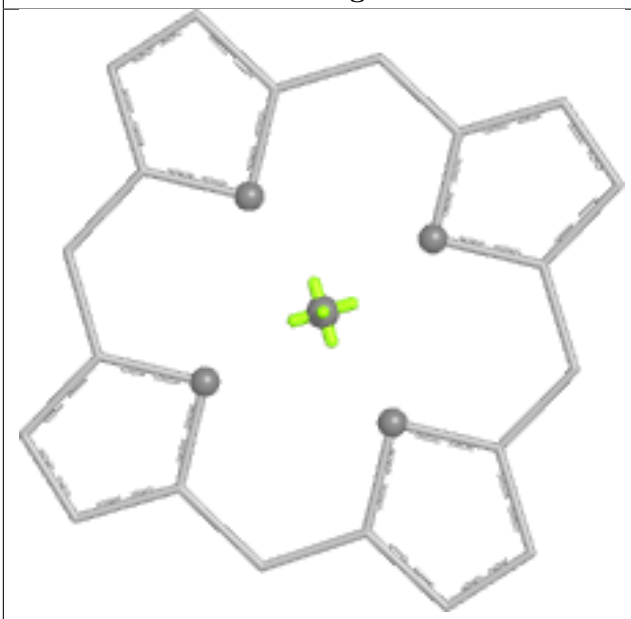
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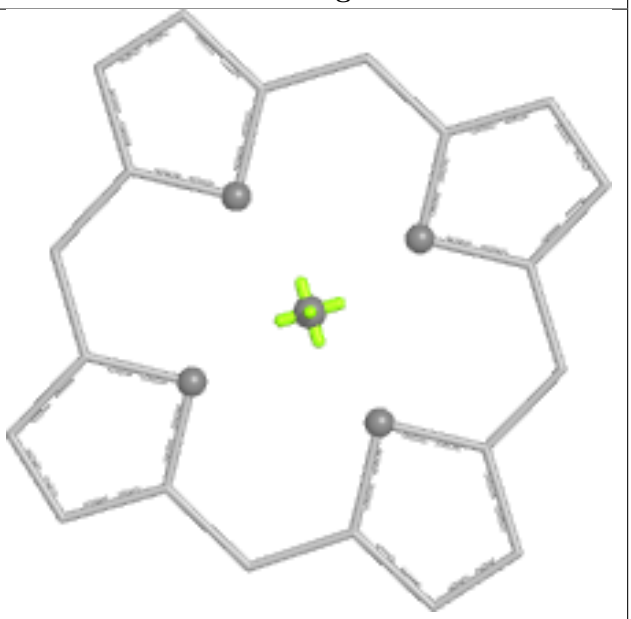
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Bond angles

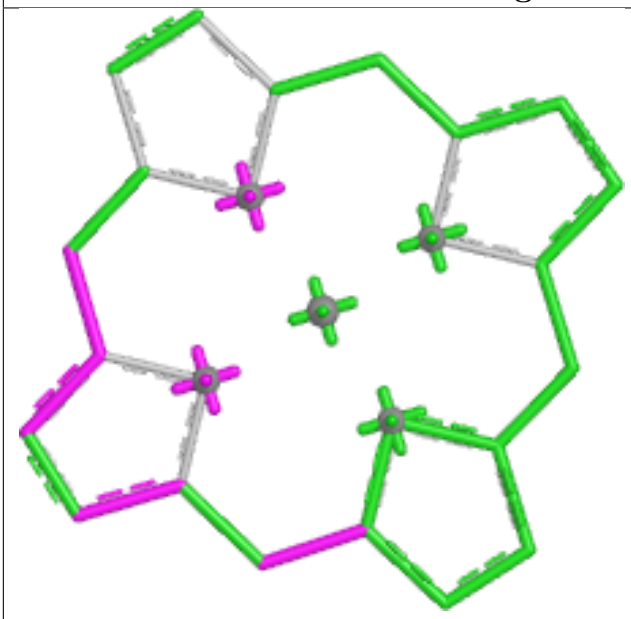


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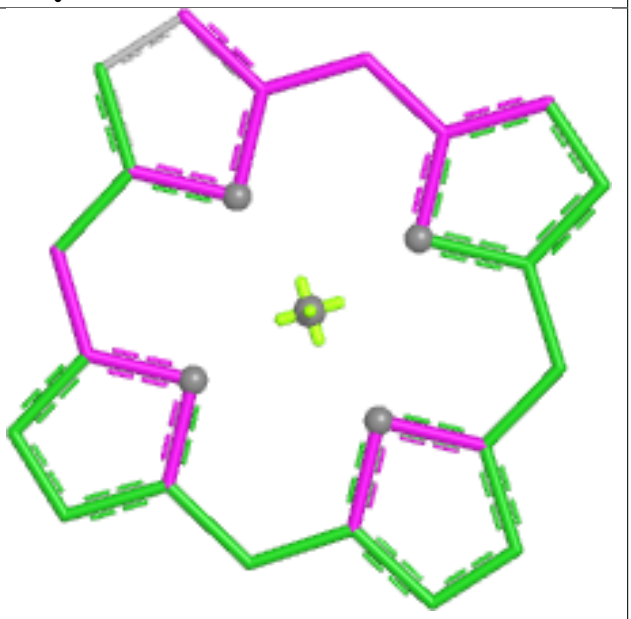


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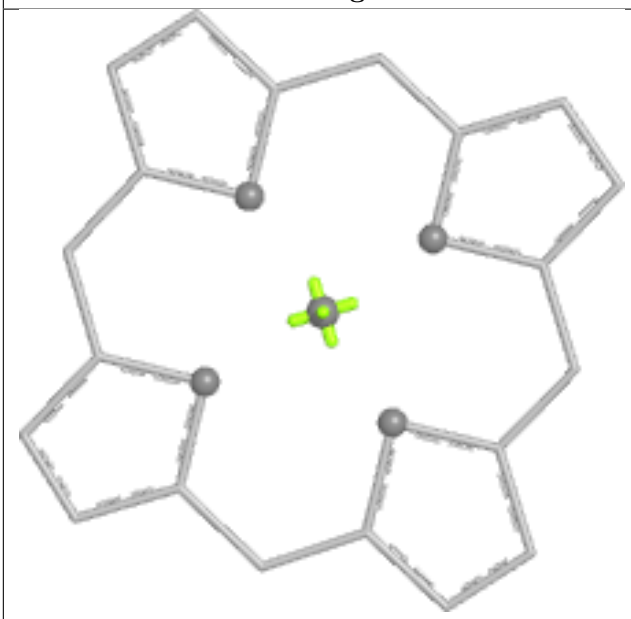
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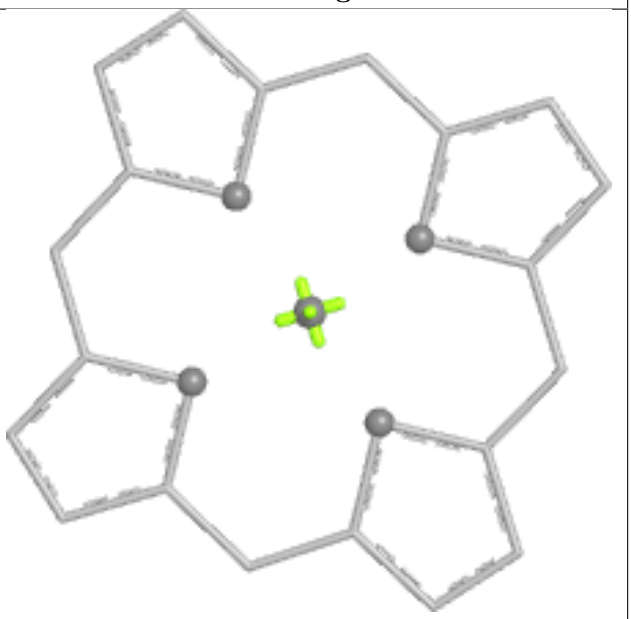
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Bond angles

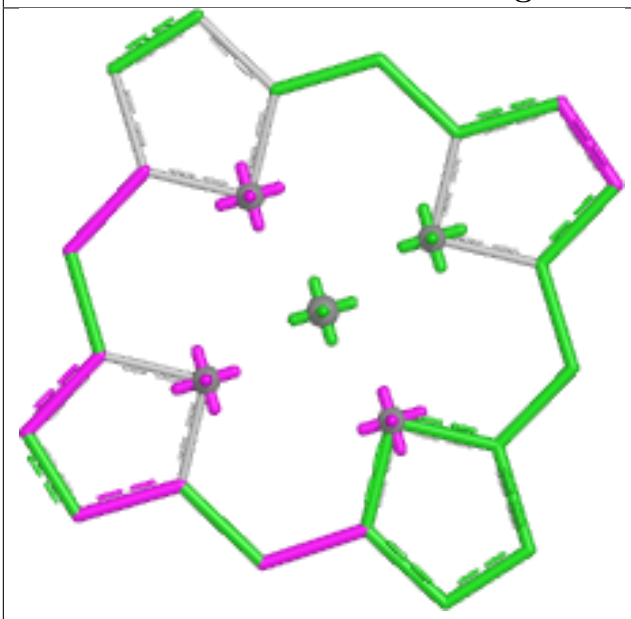


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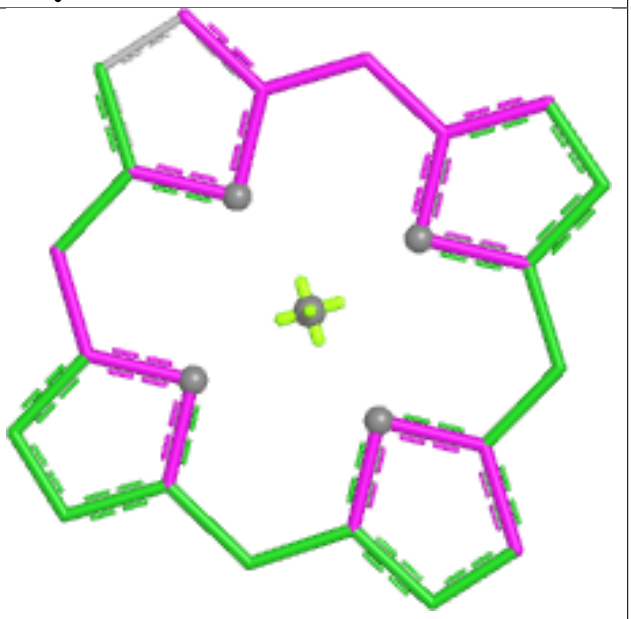


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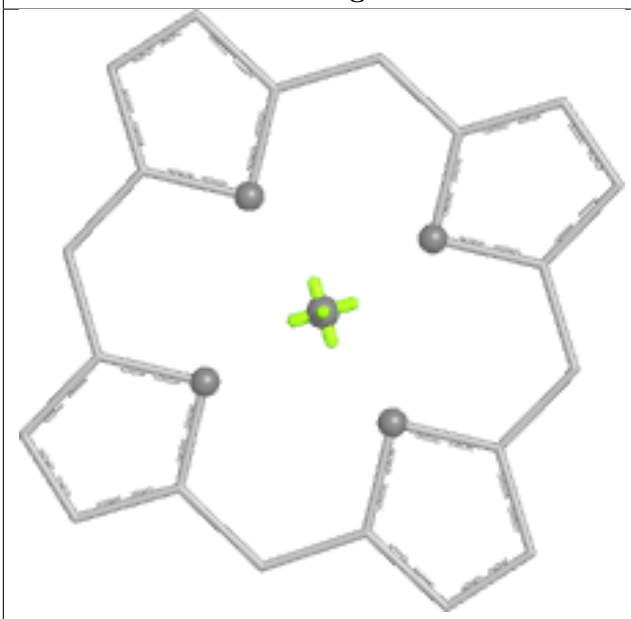
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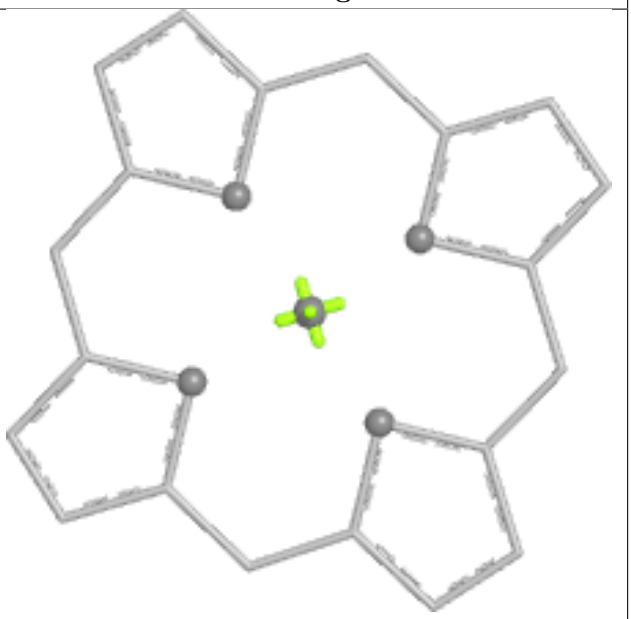
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Bond angles

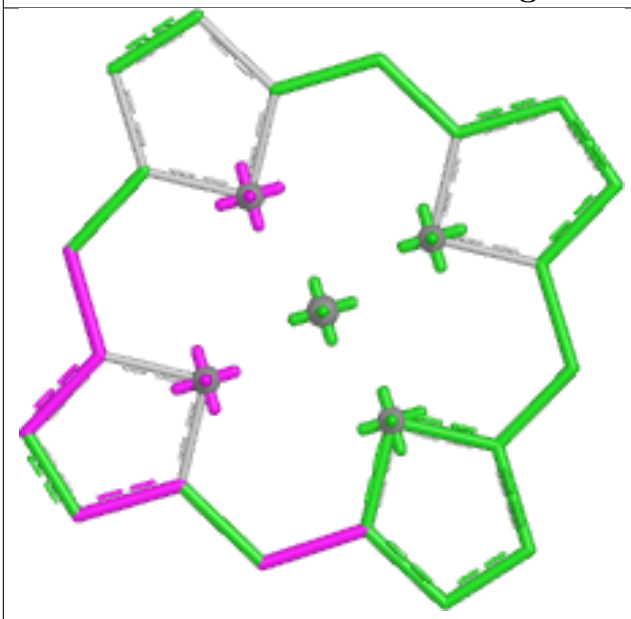


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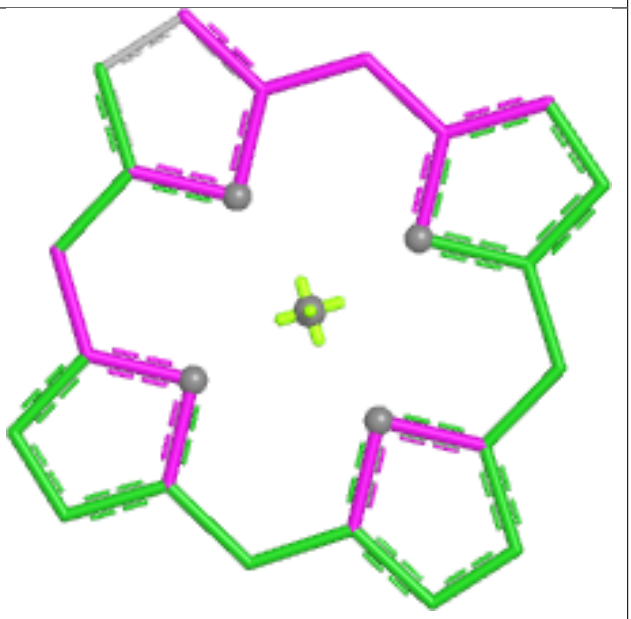


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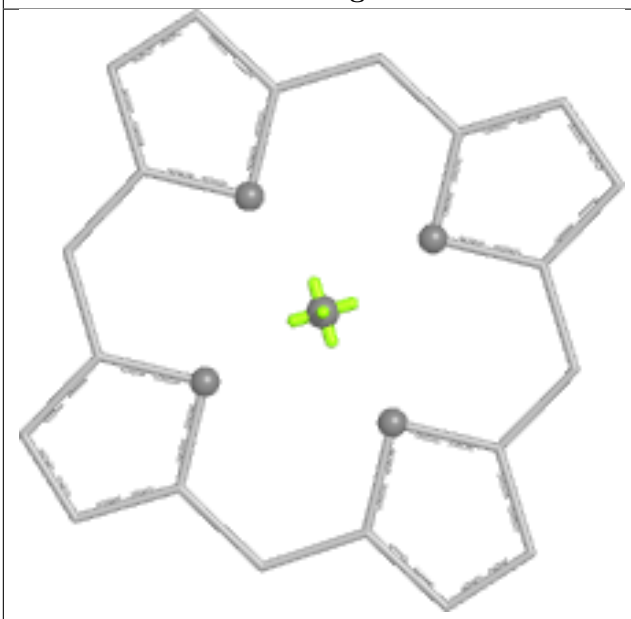
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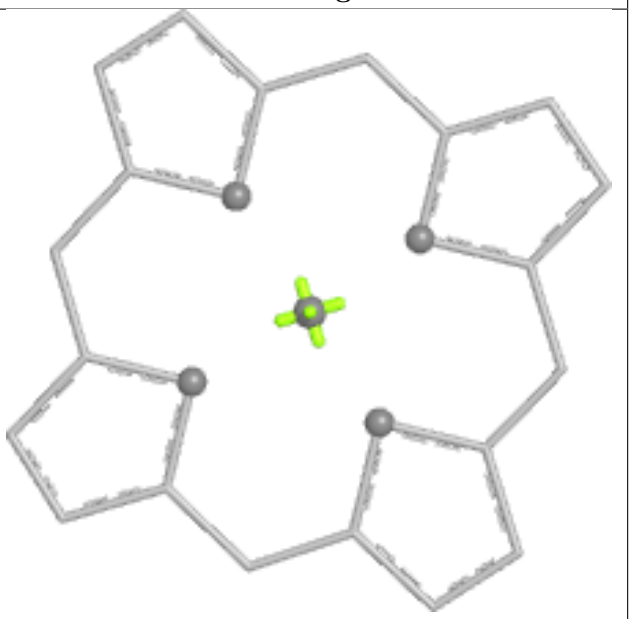
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Bond angles

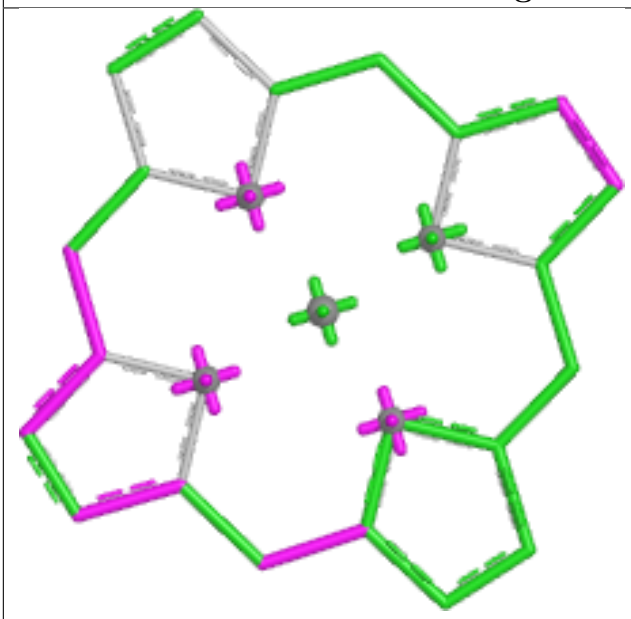


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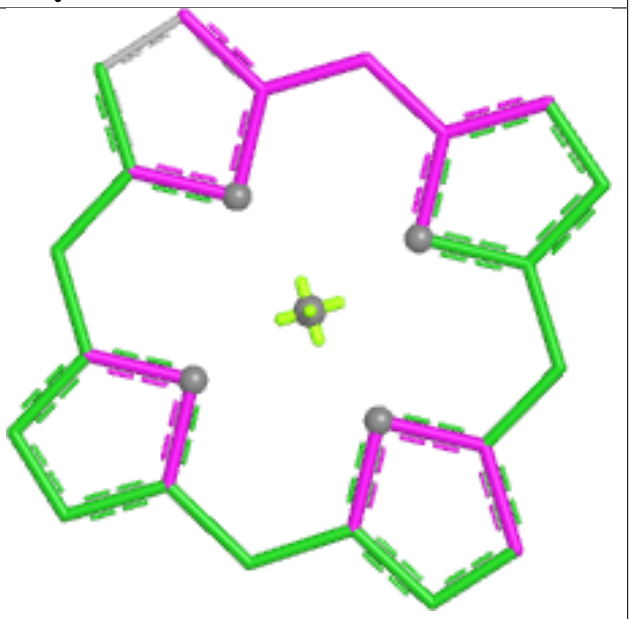


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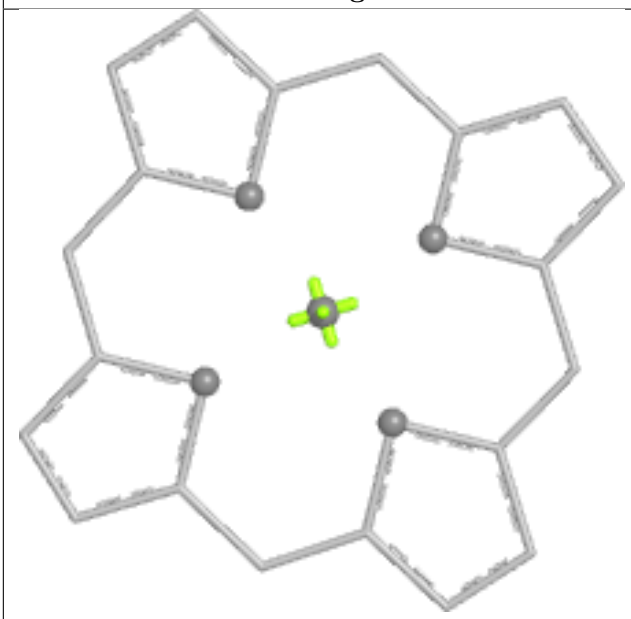
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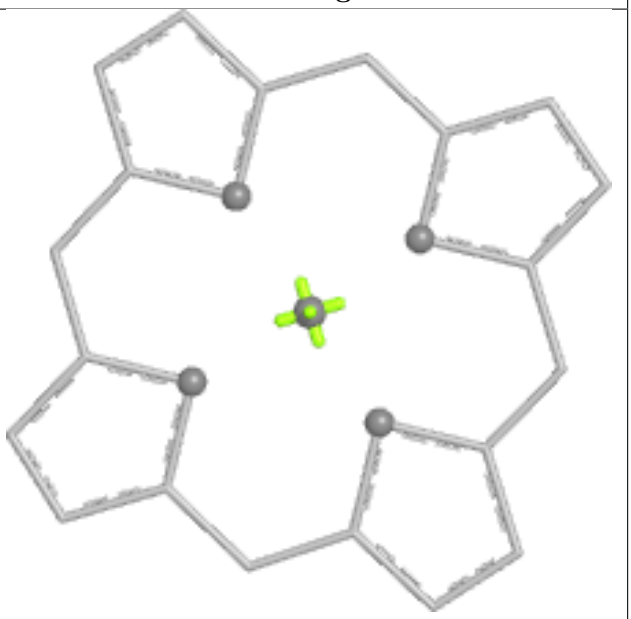
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Bond angles

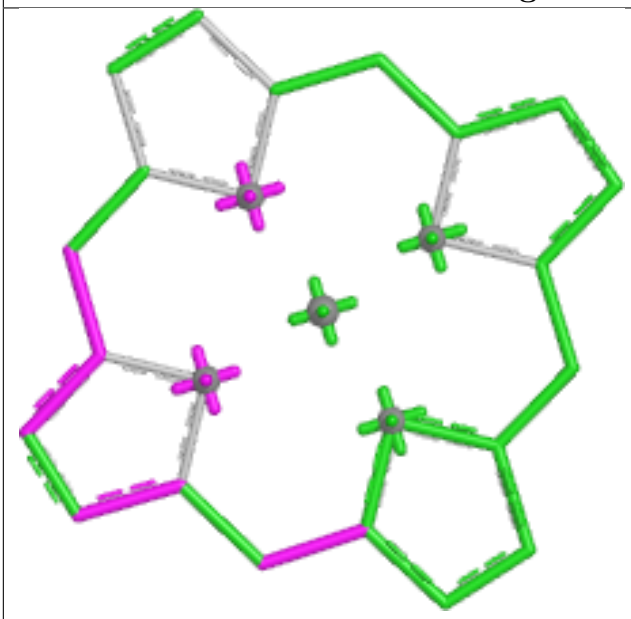


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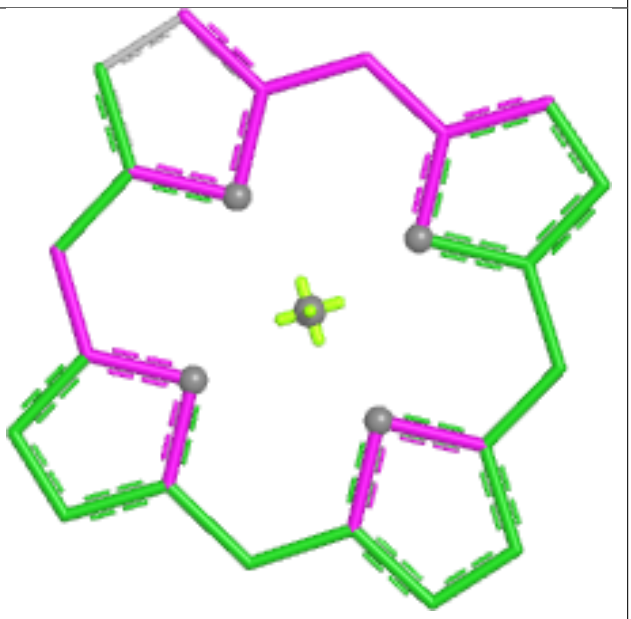


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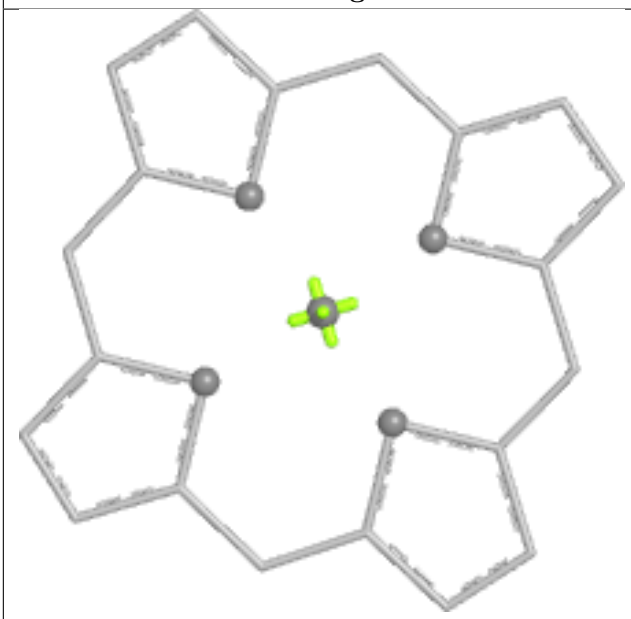
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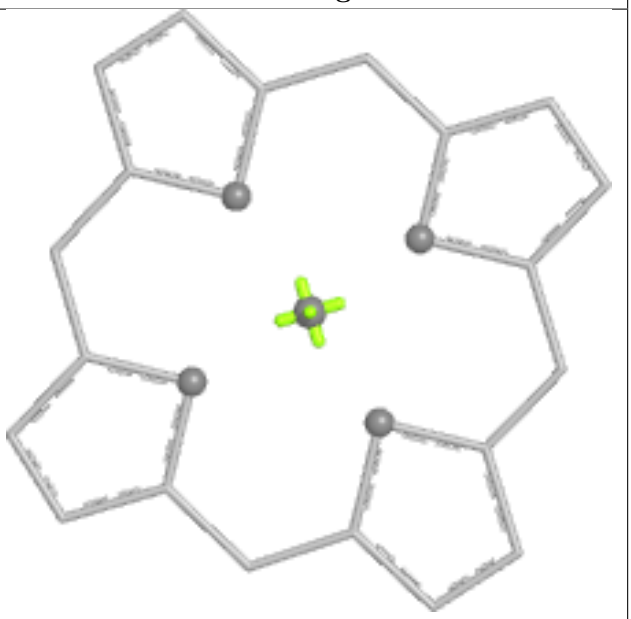
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Bond angles

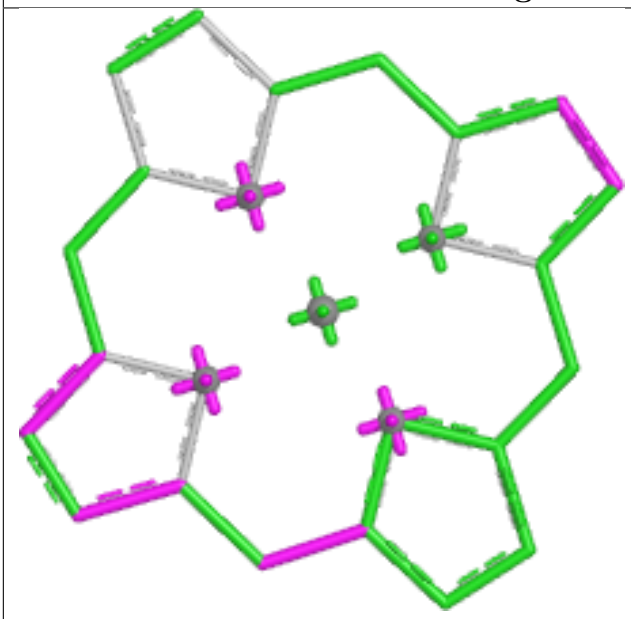


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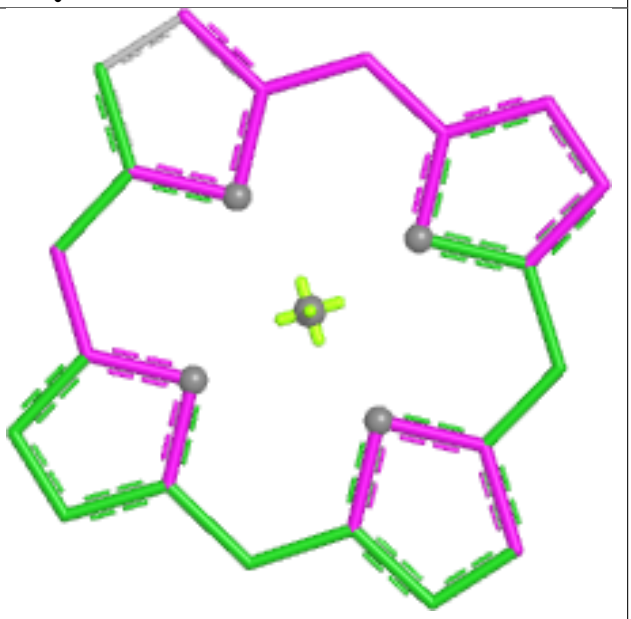


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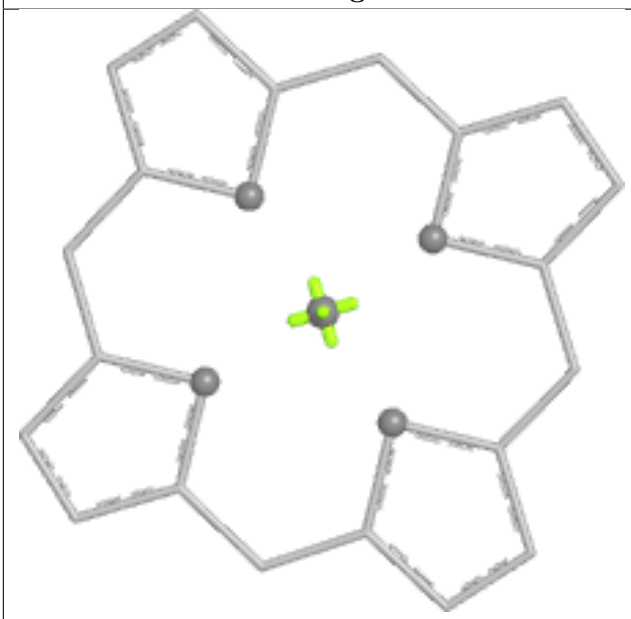
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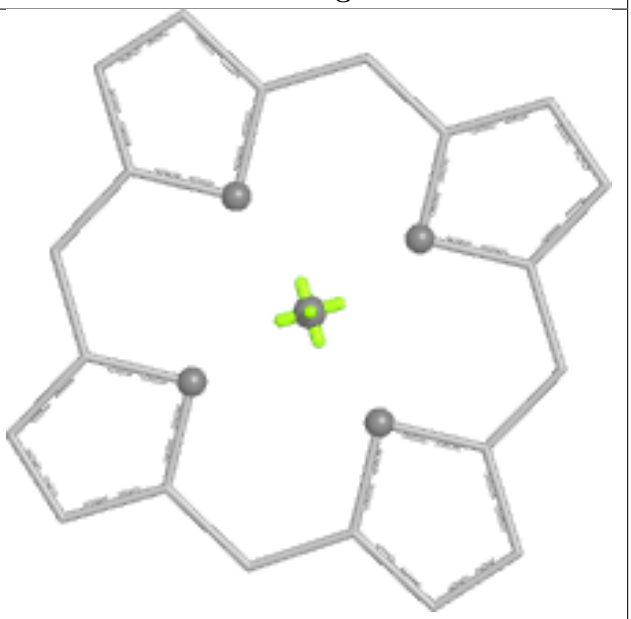
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Bond angles

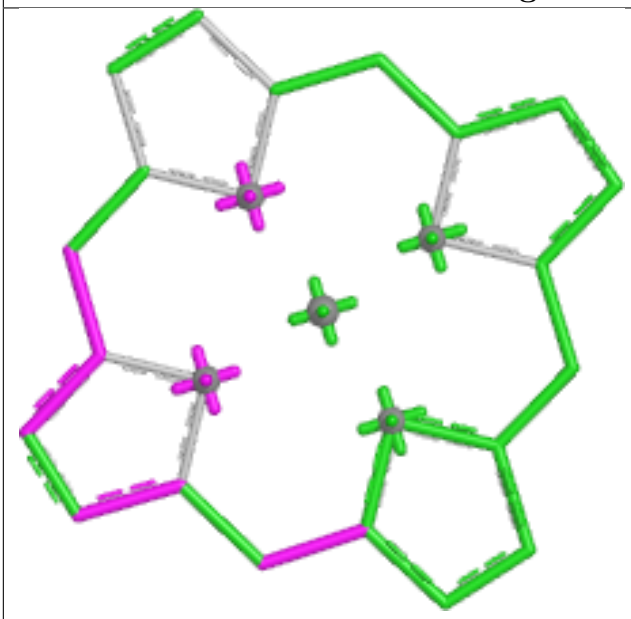


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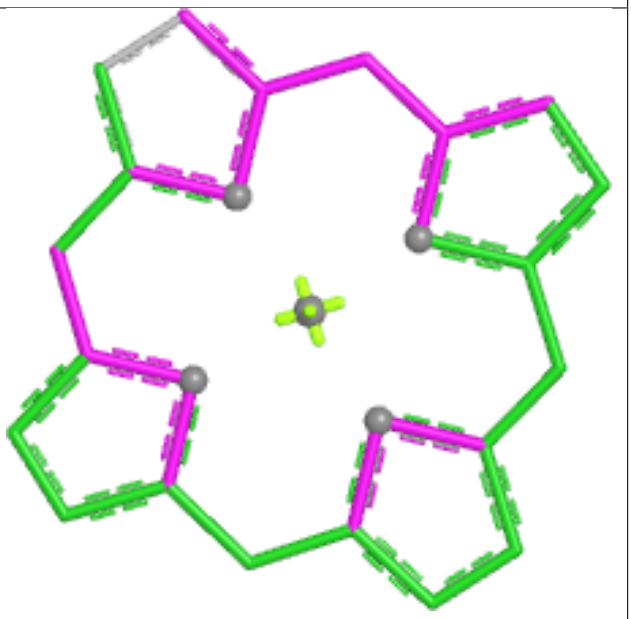


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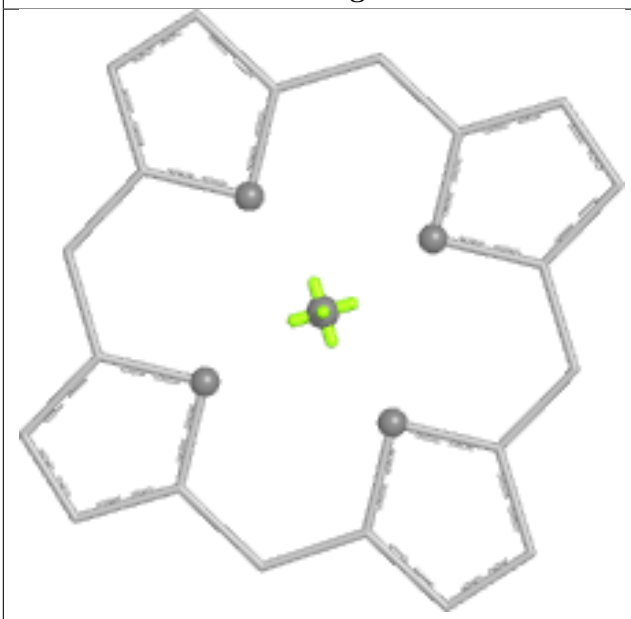
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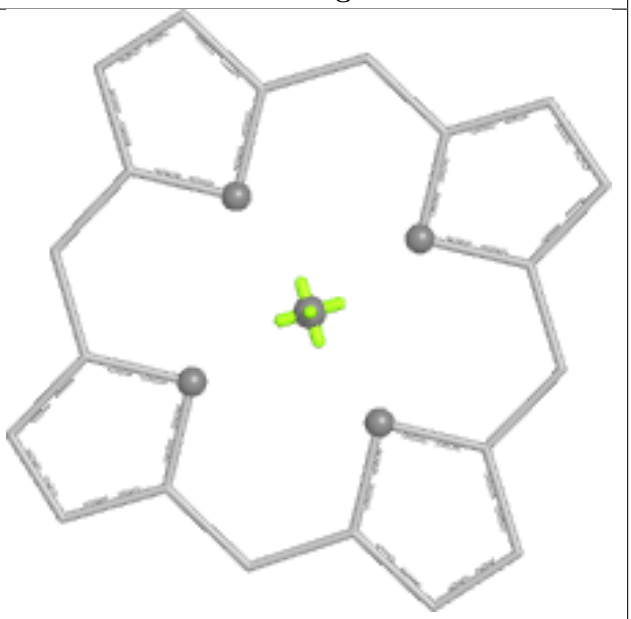
Bond lengths



Bond angles

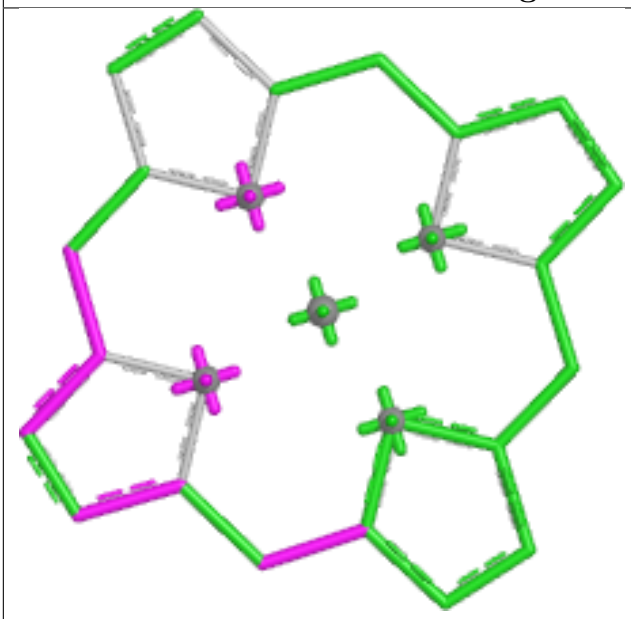


Torsions

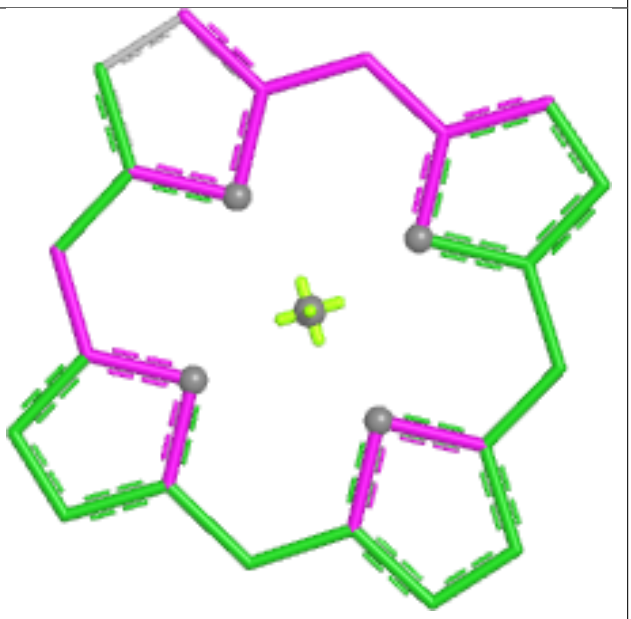


Rings

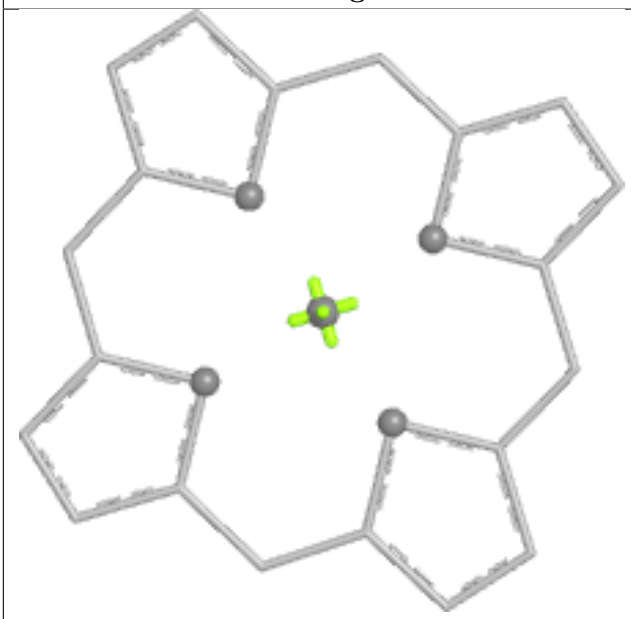
Ligand CLA 9 1015



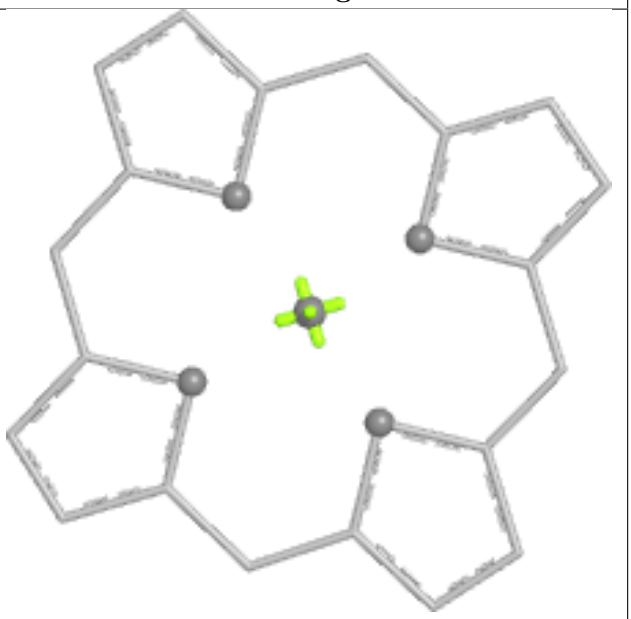
Bond lengths



Bond angles

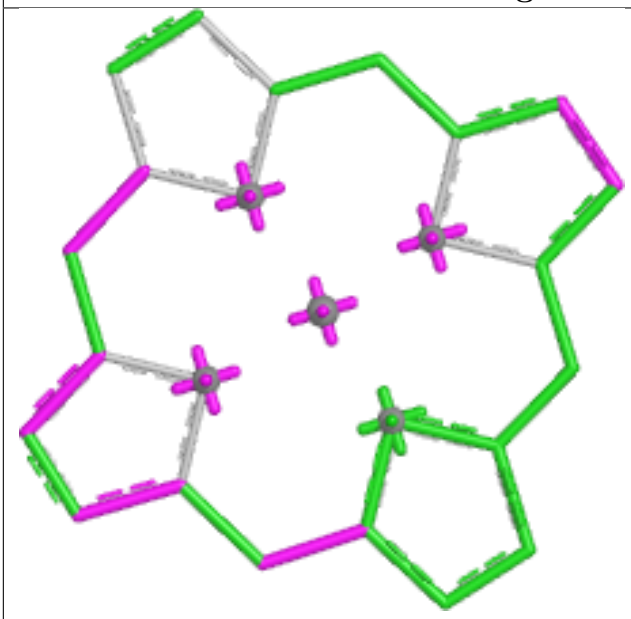


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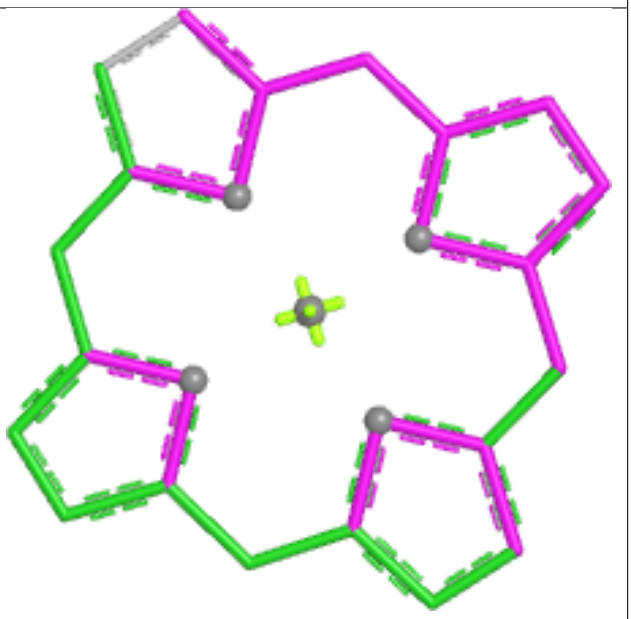


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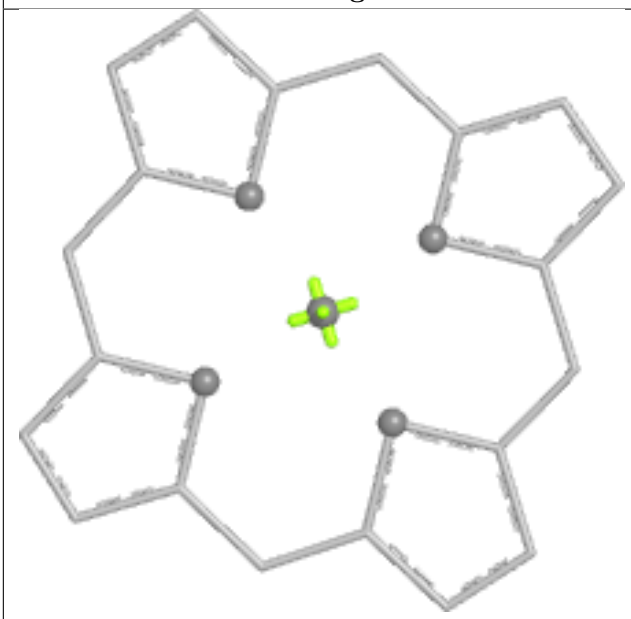
Ligand CLA P 5118



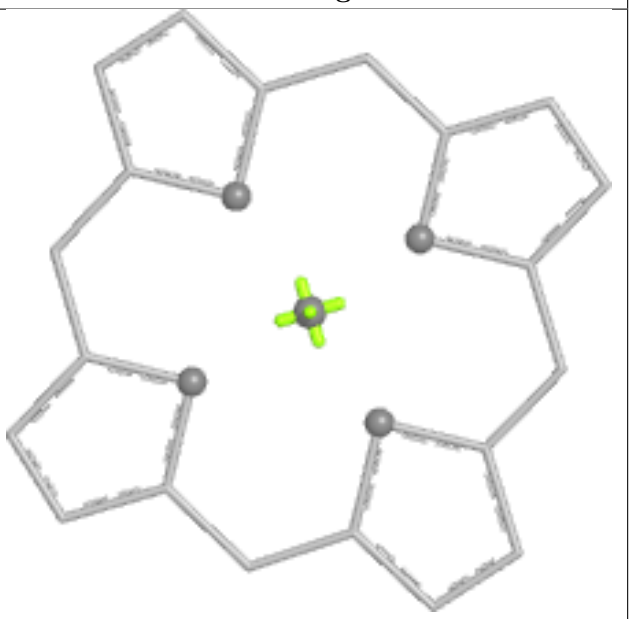
Bond lengths



Bond angles

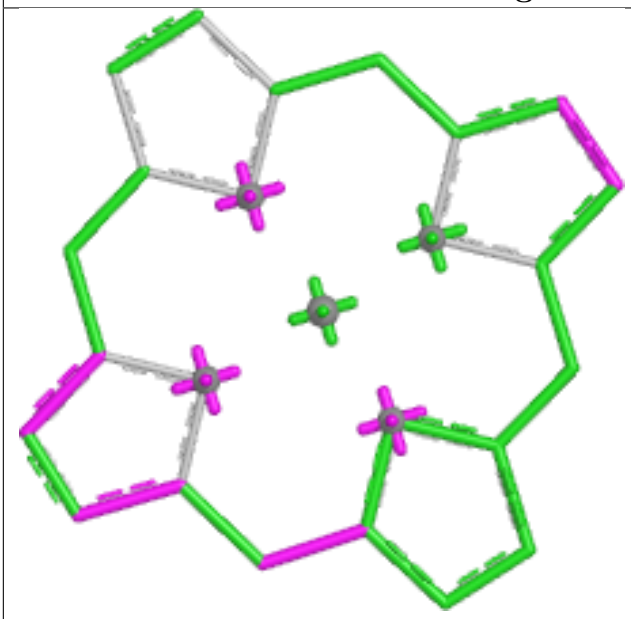


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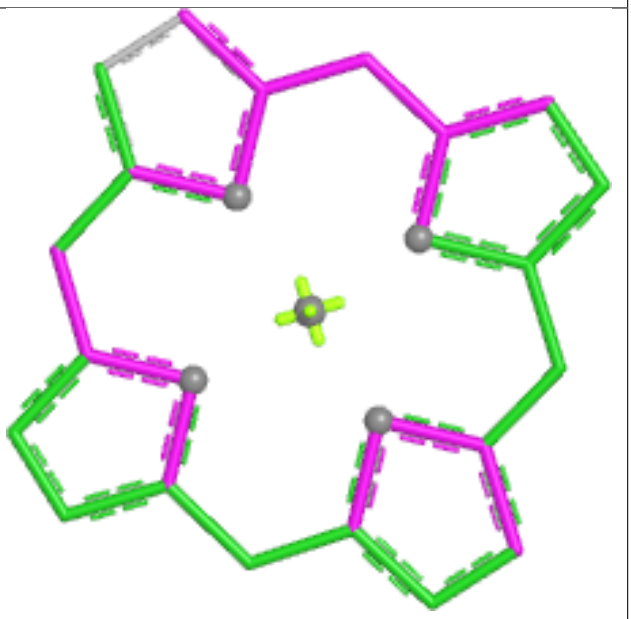


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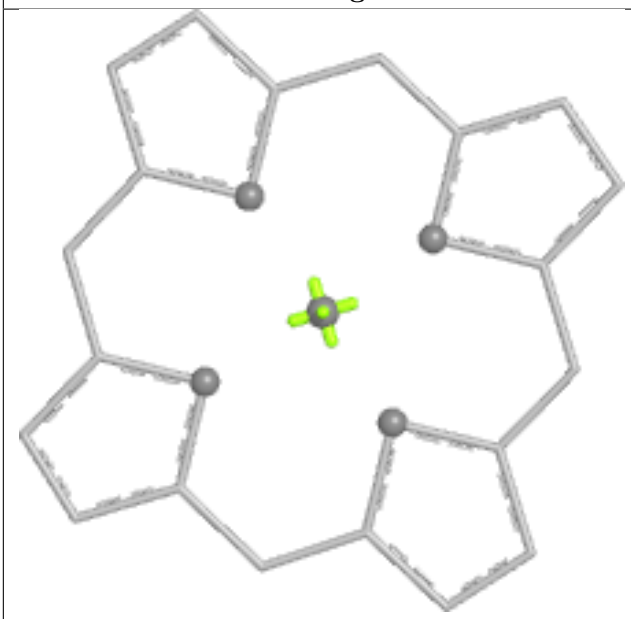
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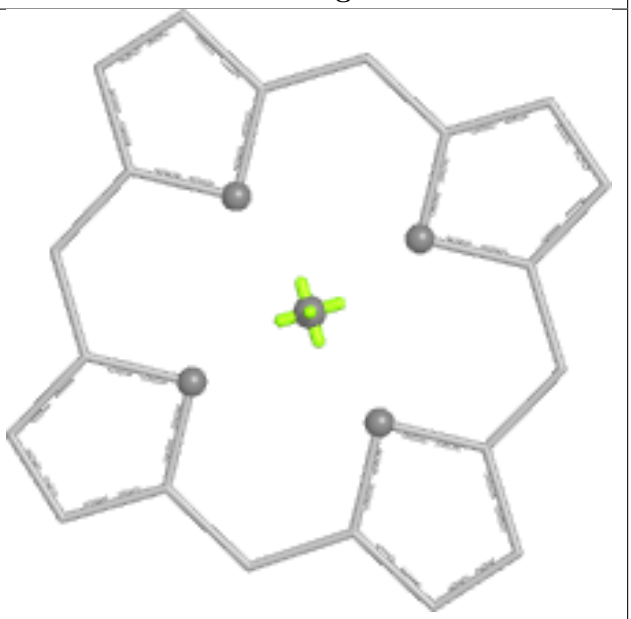
Bond lengths



Bond angles

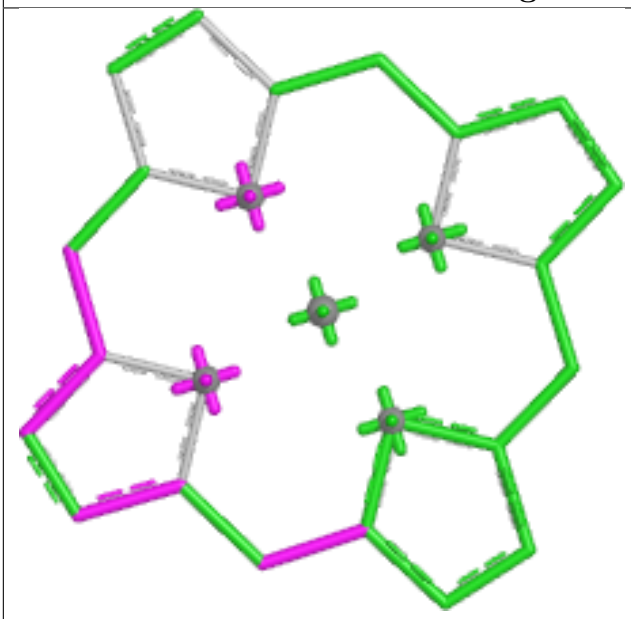


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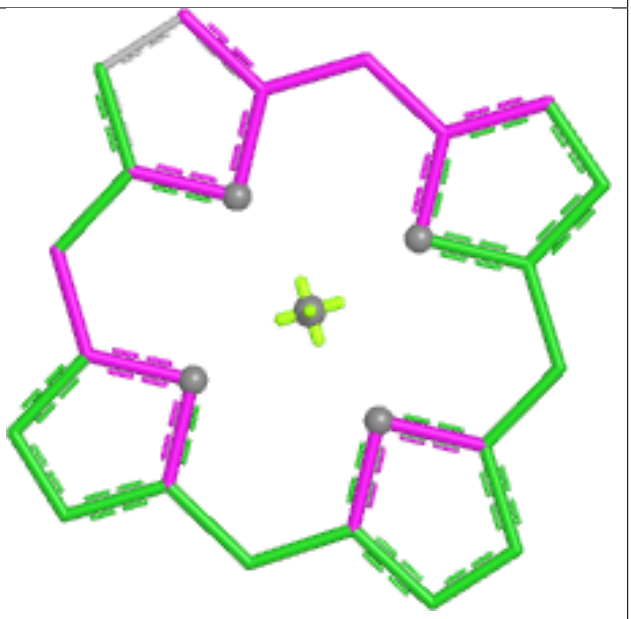


Rings

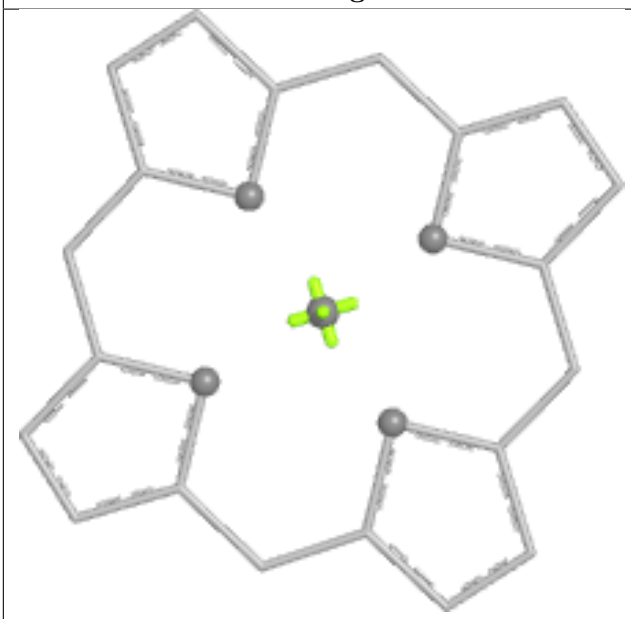
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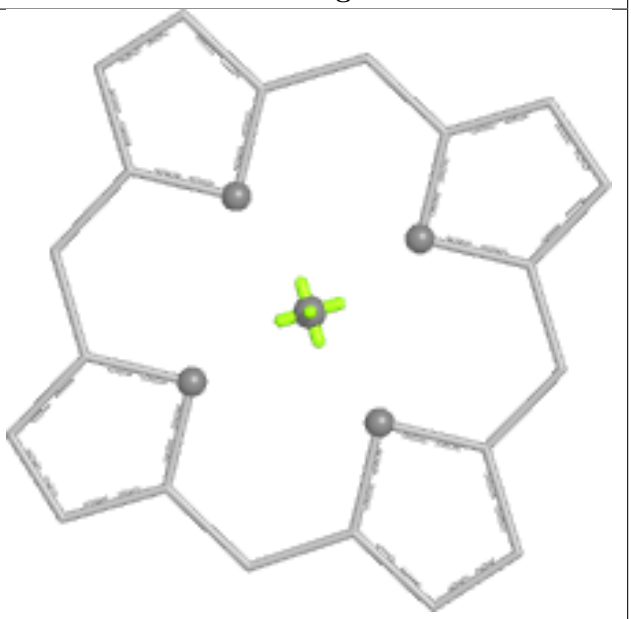
Bond lengths



Bond angles

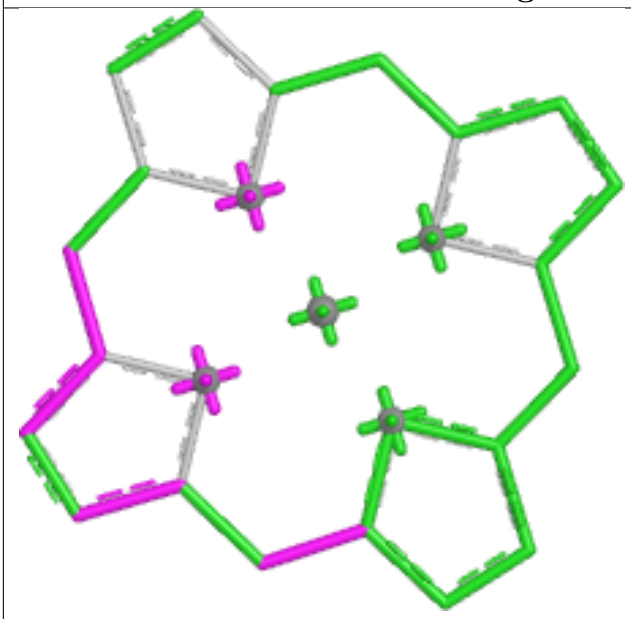


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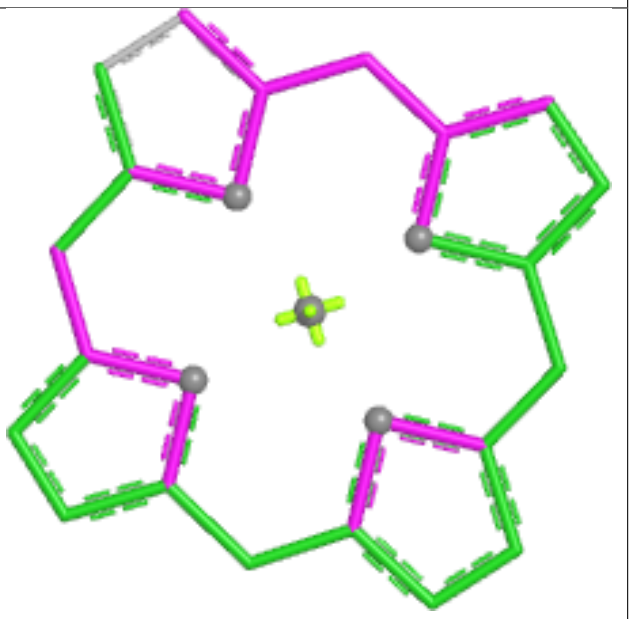


Rings

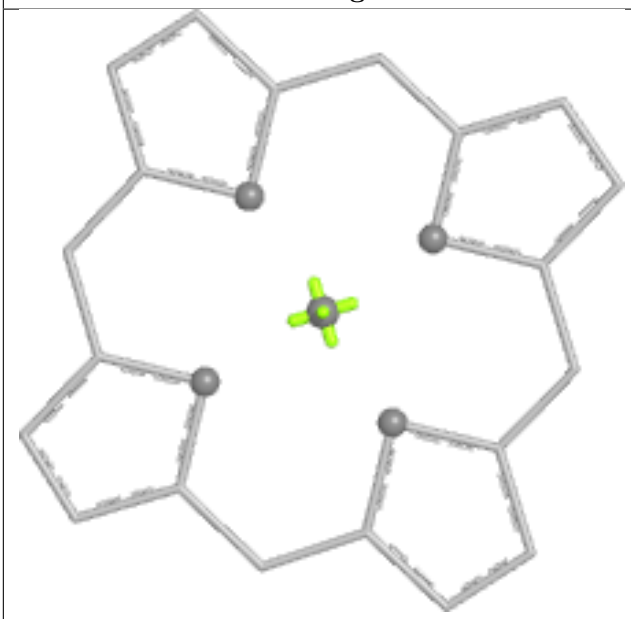
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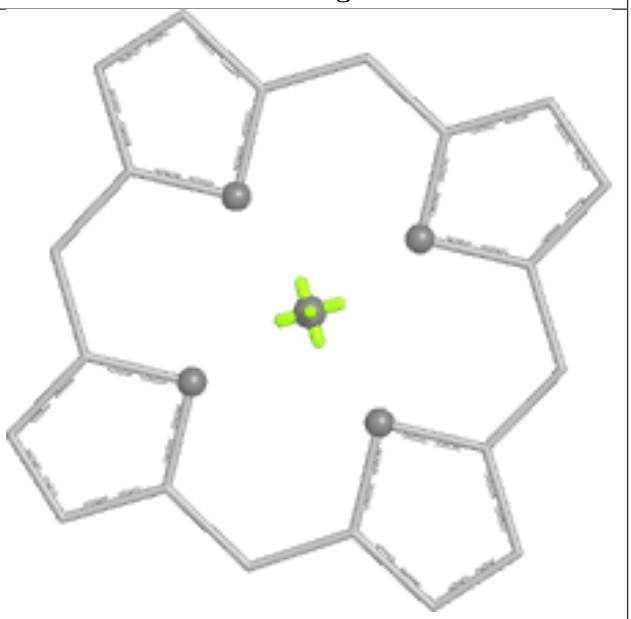
Bond lengths



Bond angles

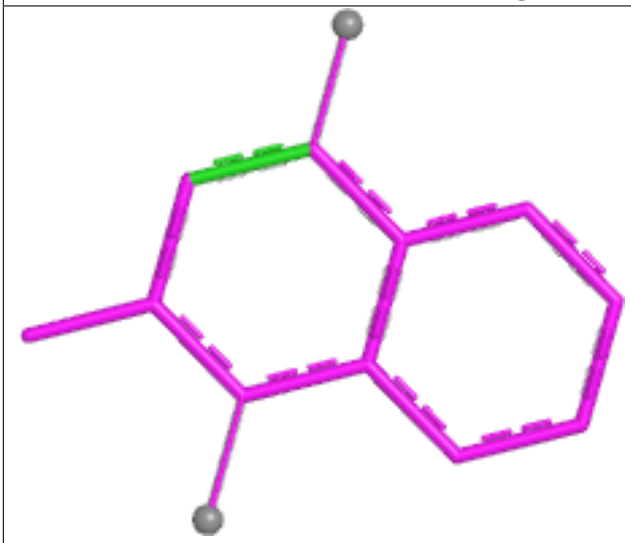


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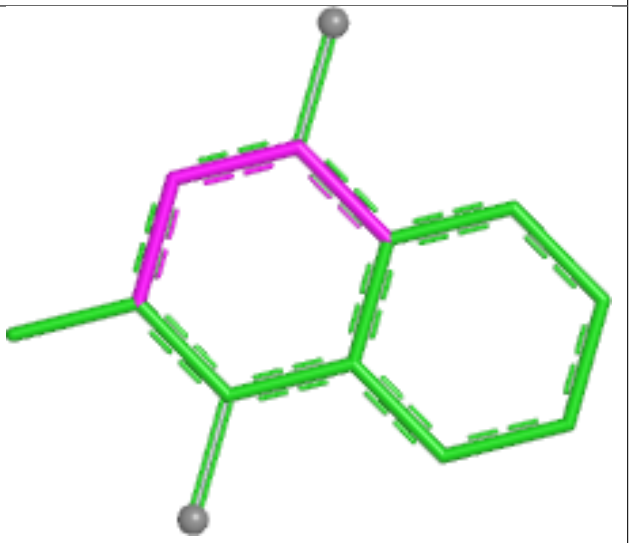


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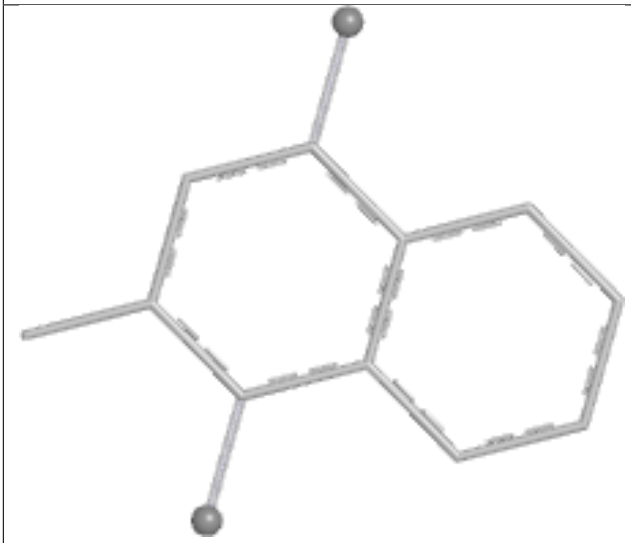
Ligand PQN B 2002



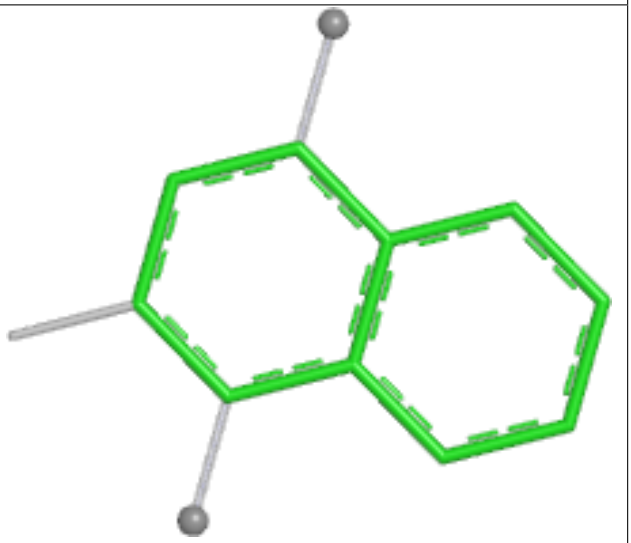
Bond lengths



Bond angles

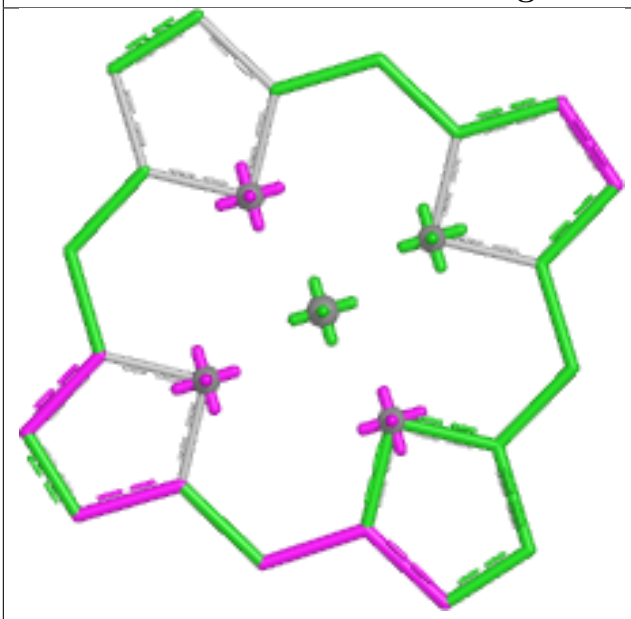


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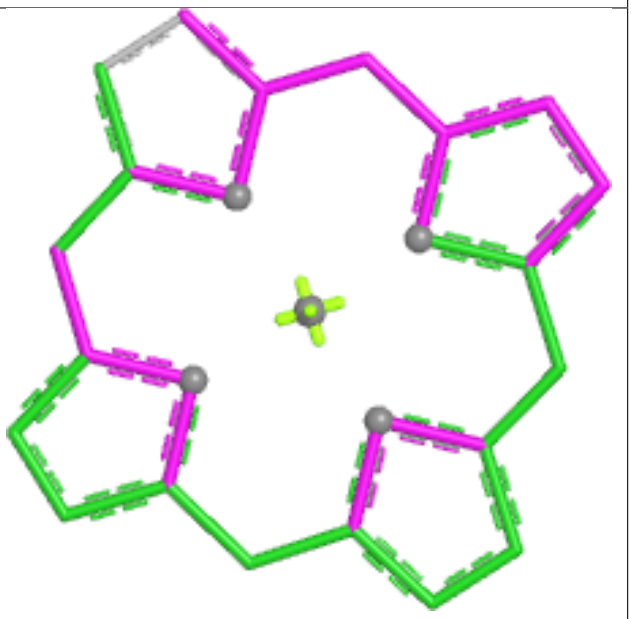


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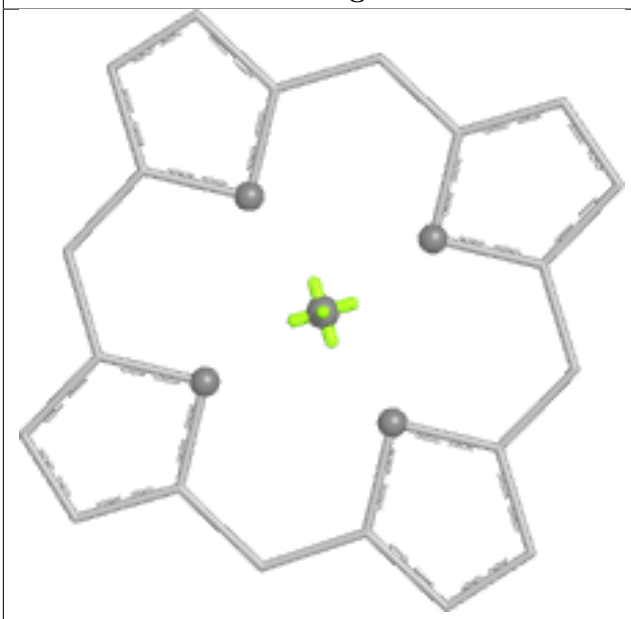
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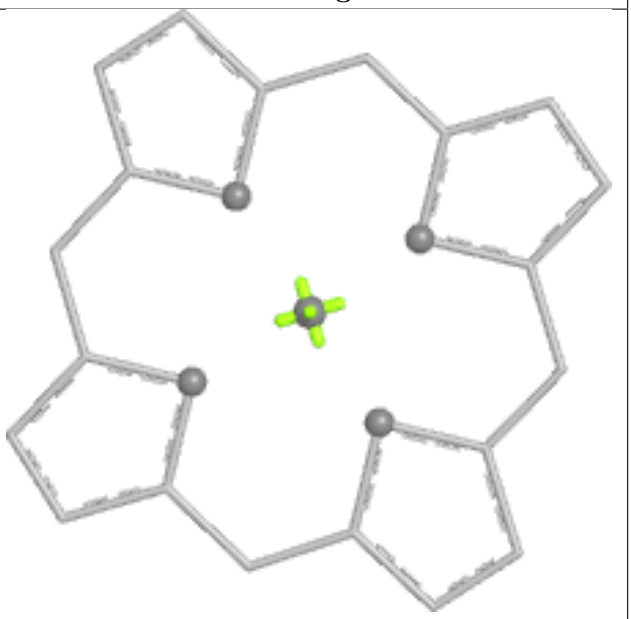
Bond lengths



Bond angles

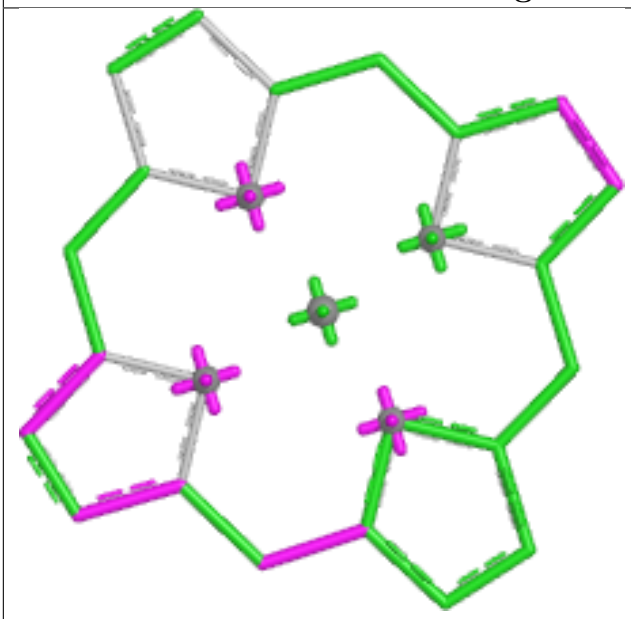


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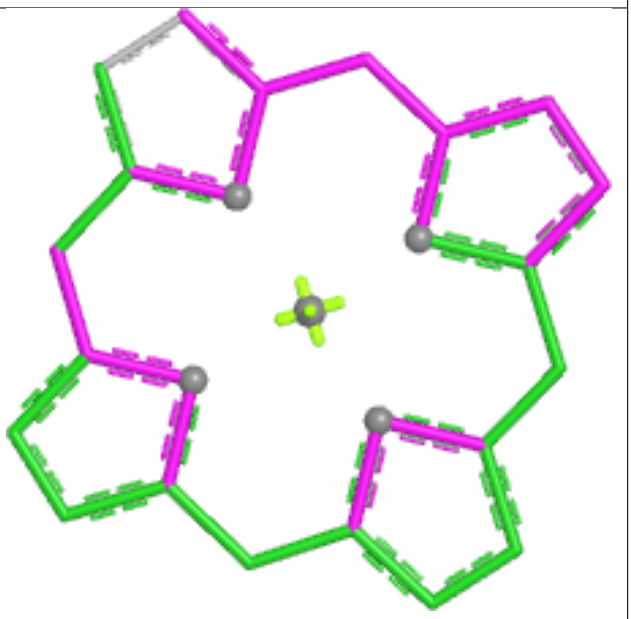


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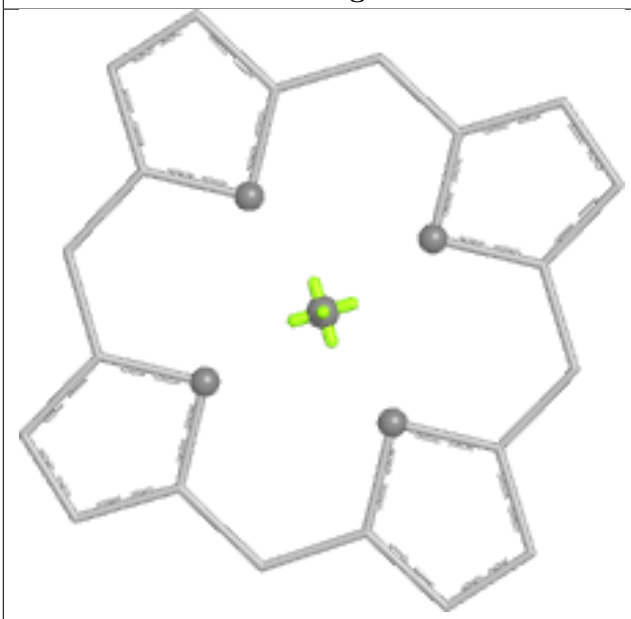
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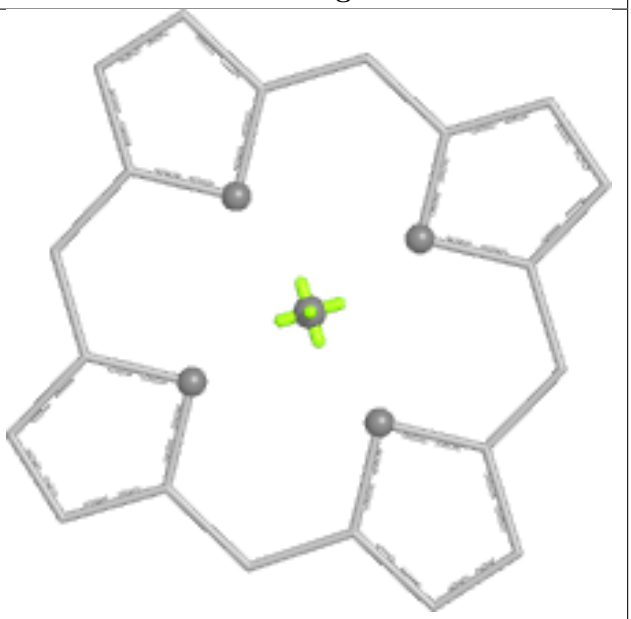
Bond lengths



Bond angles

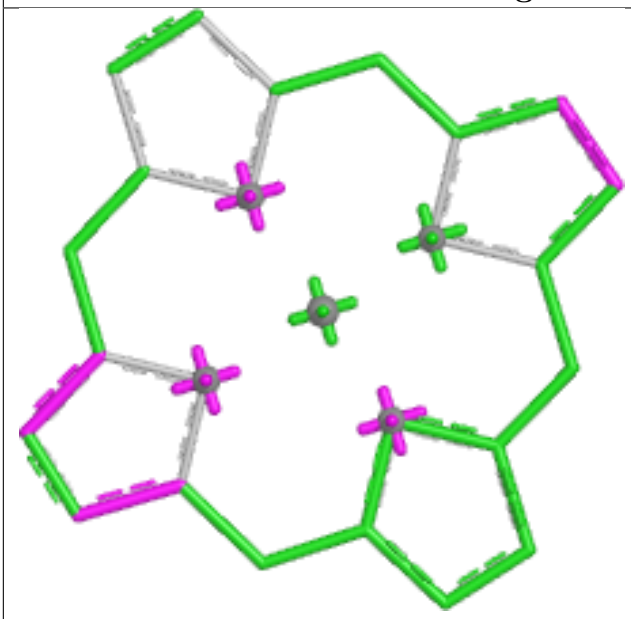


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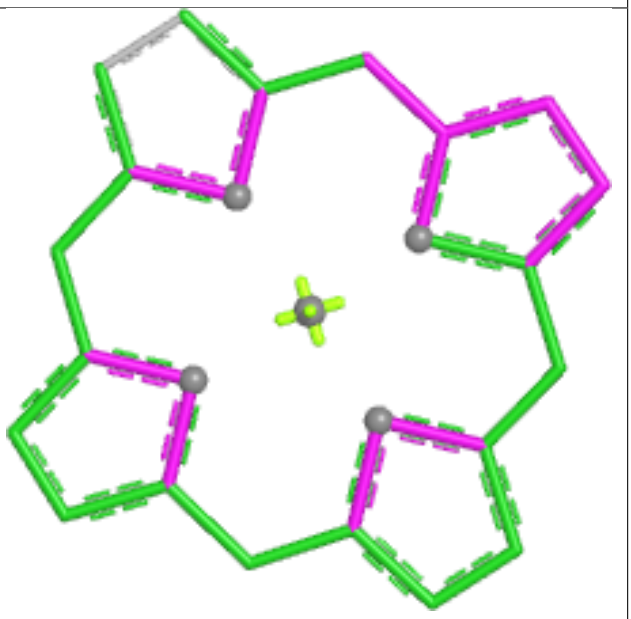


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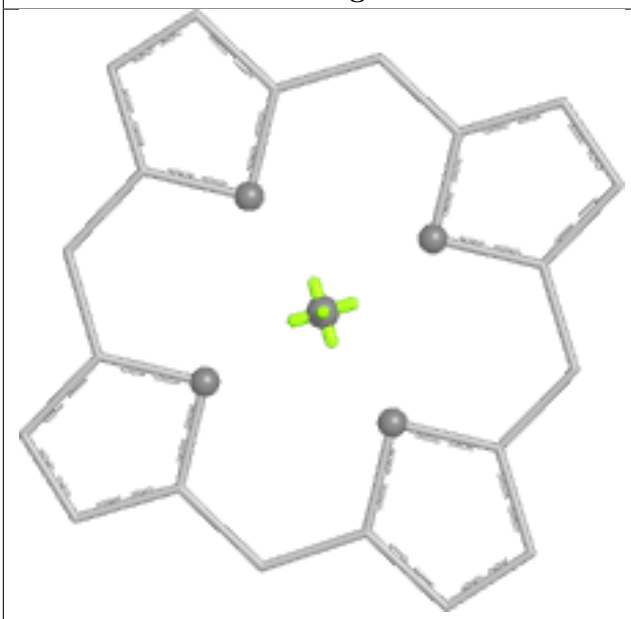
Ligand CLA B 1202



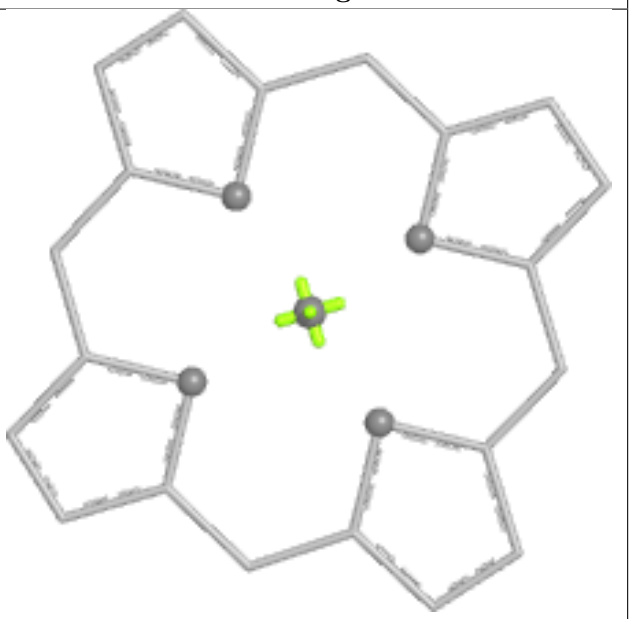
Bond lengths



Bond angles

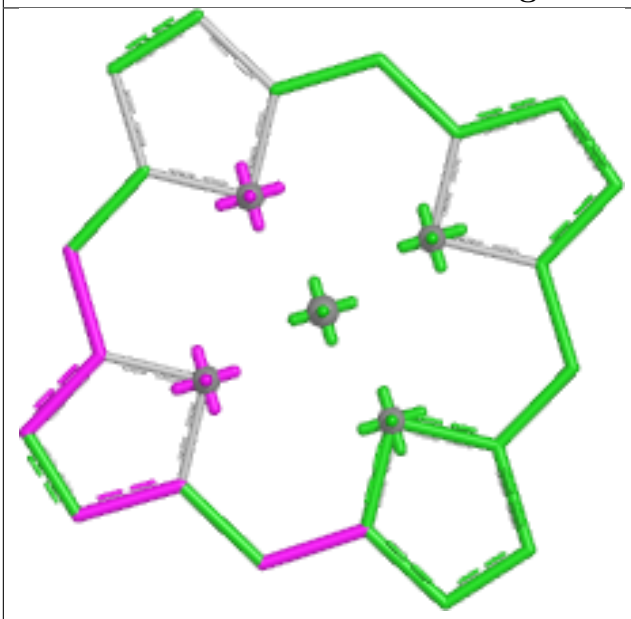


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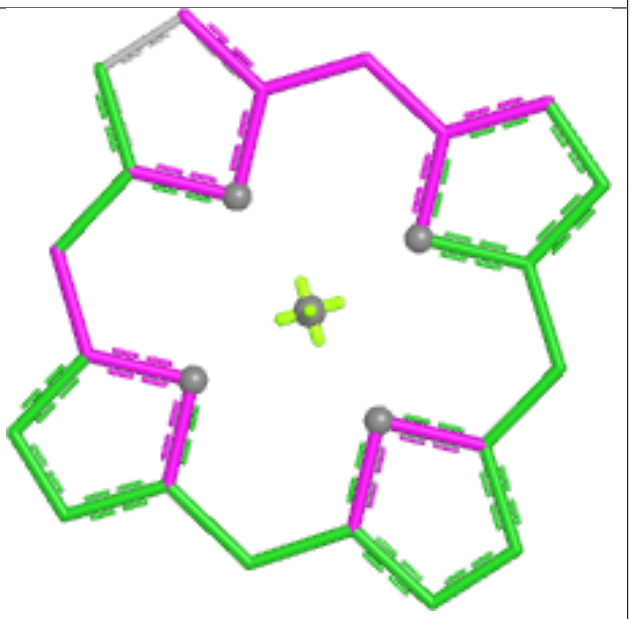


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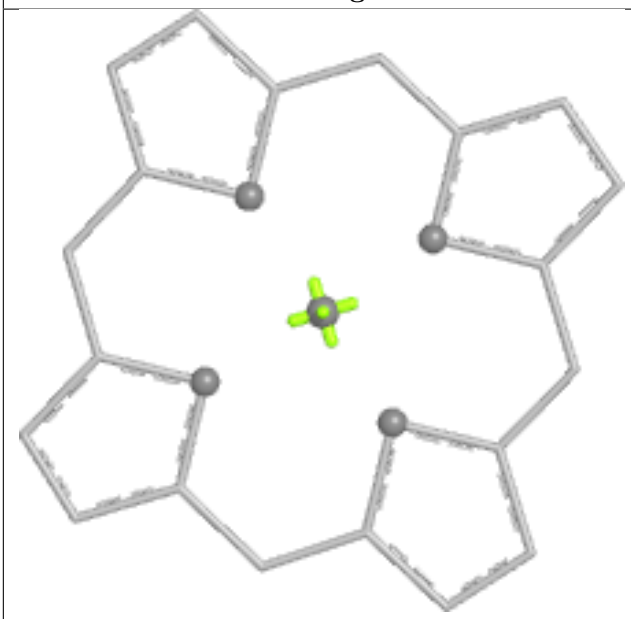
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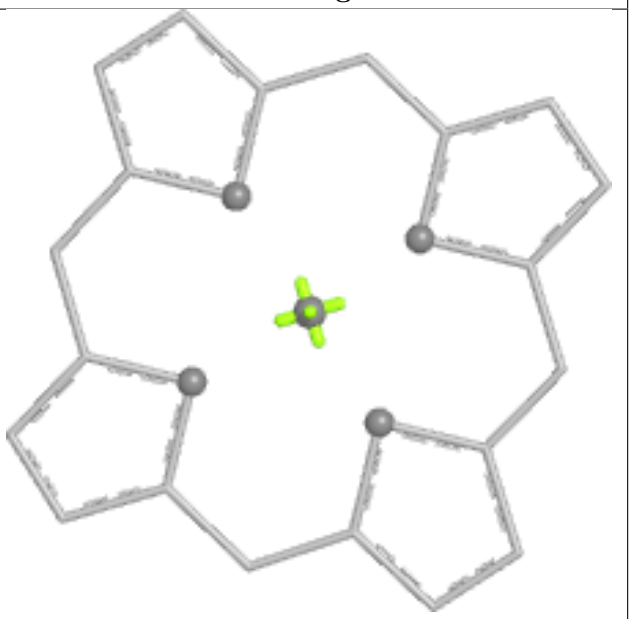
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Bond angles

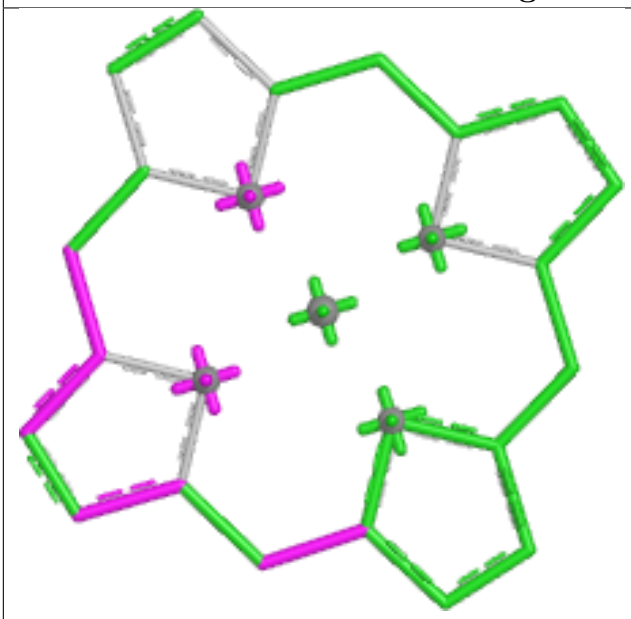


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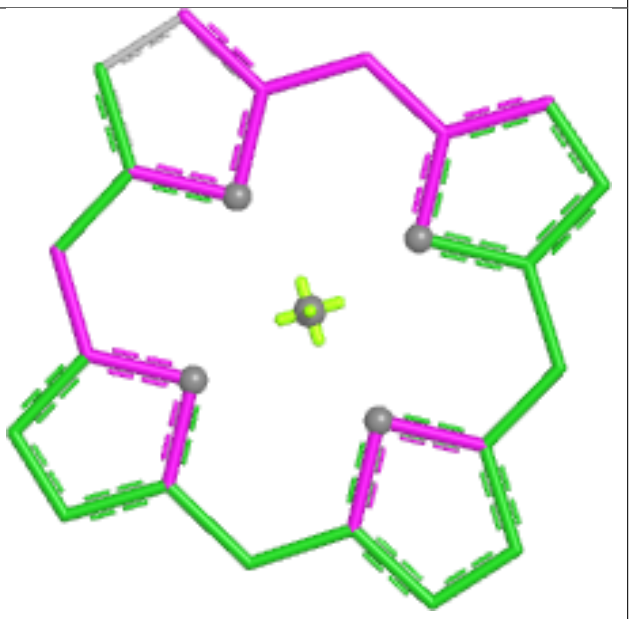


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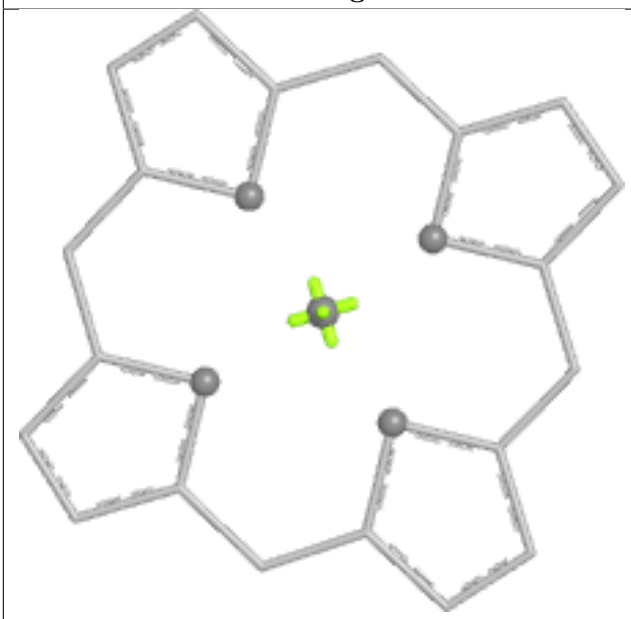
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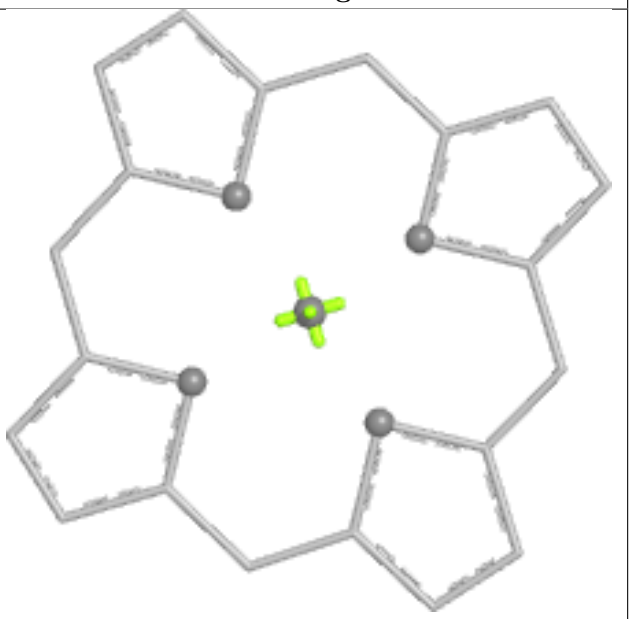
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Bond angles

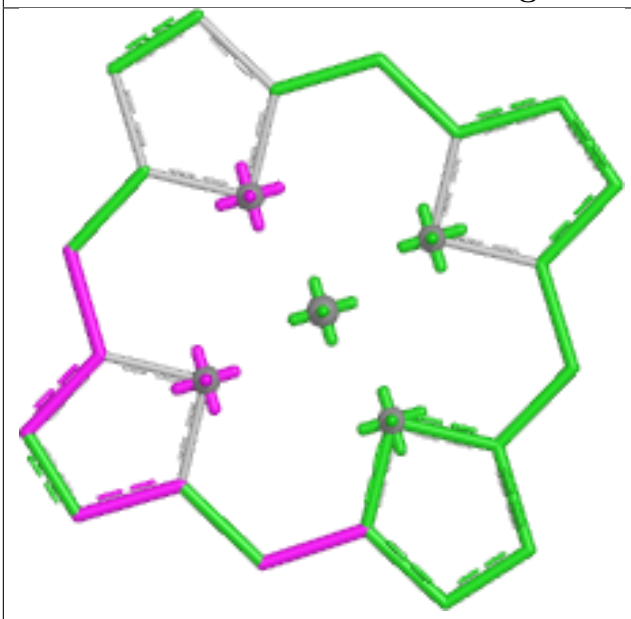


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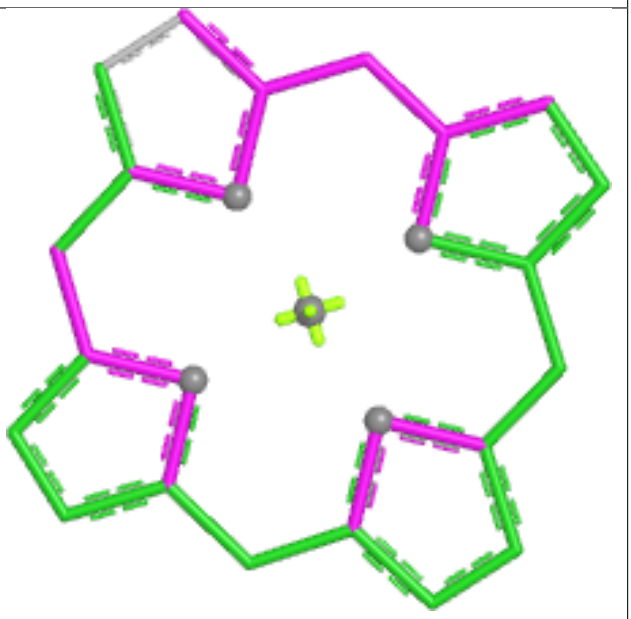


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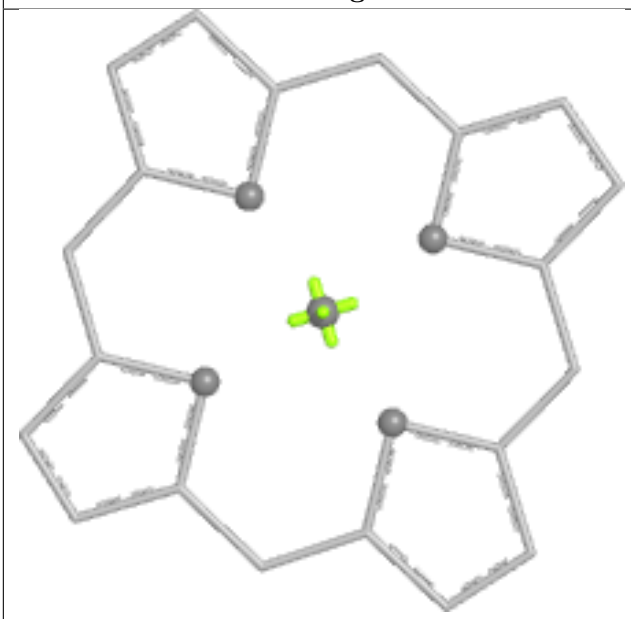
Ligand CLA 8 1017



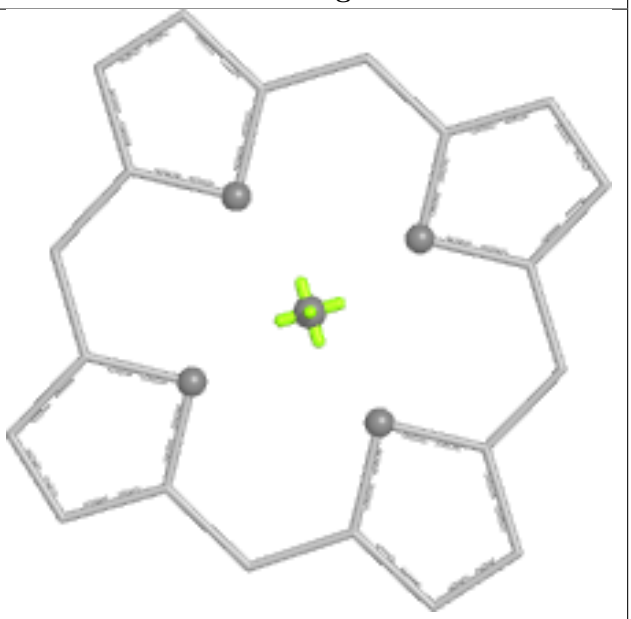
Bond lengths



Bond angles

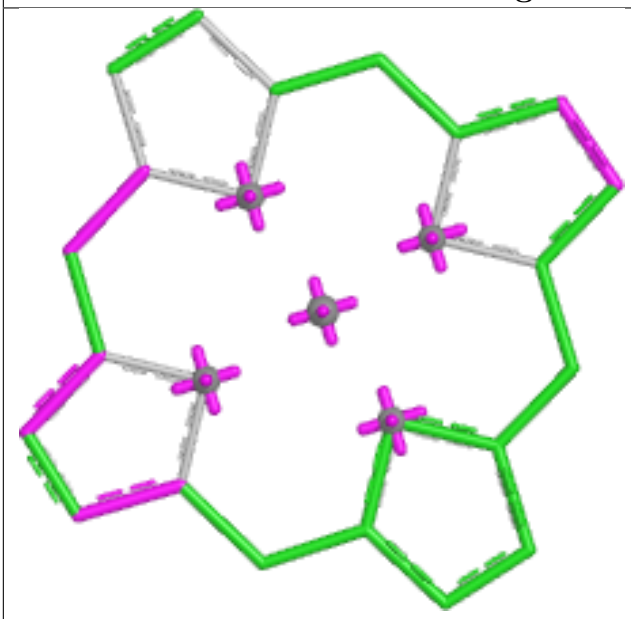


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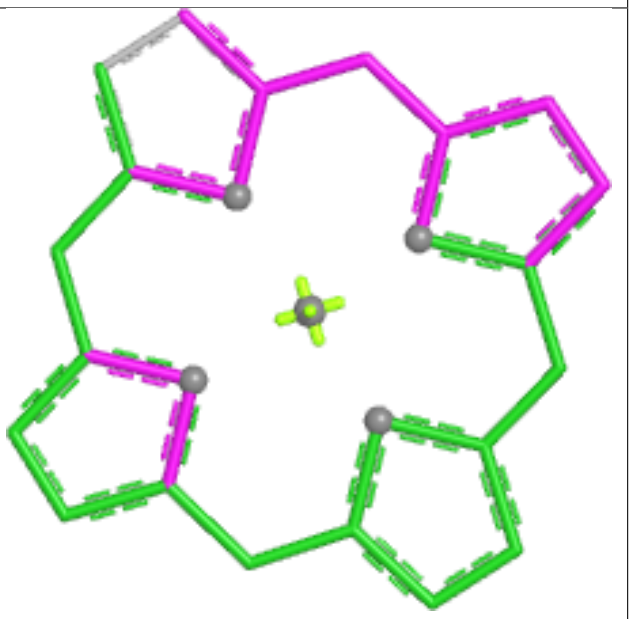


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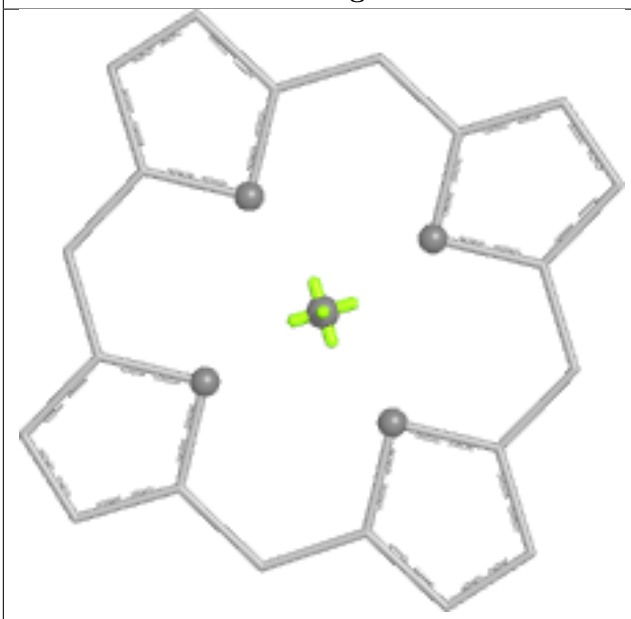
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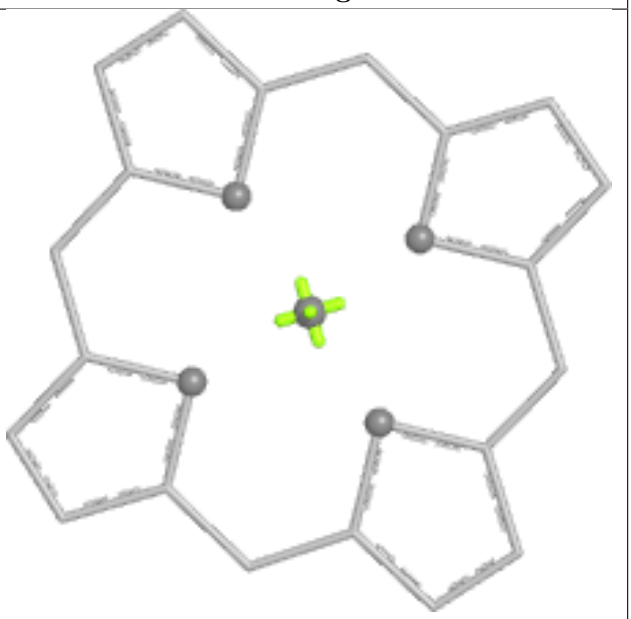
Bond lengths



Bond angles

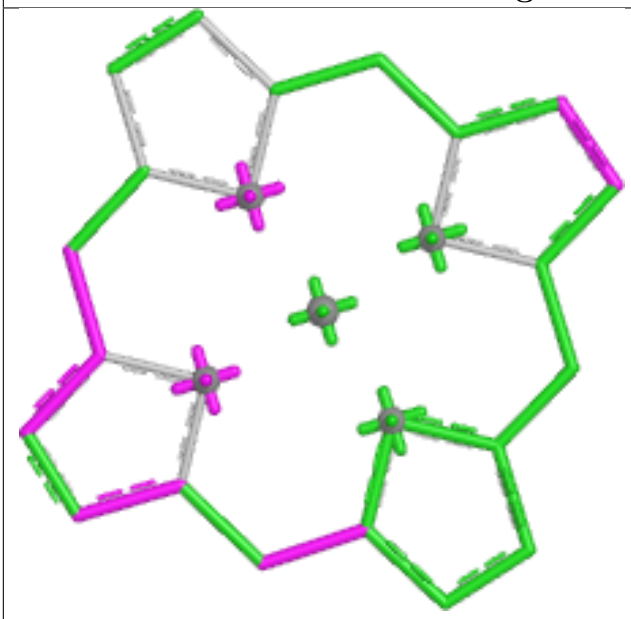


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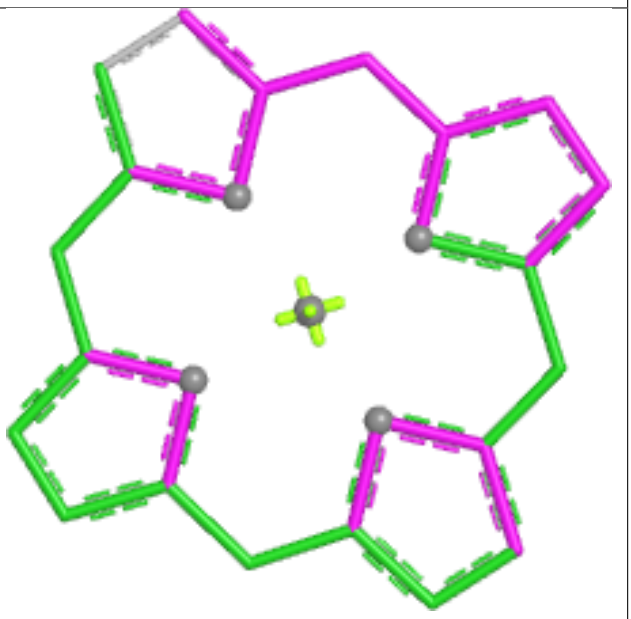


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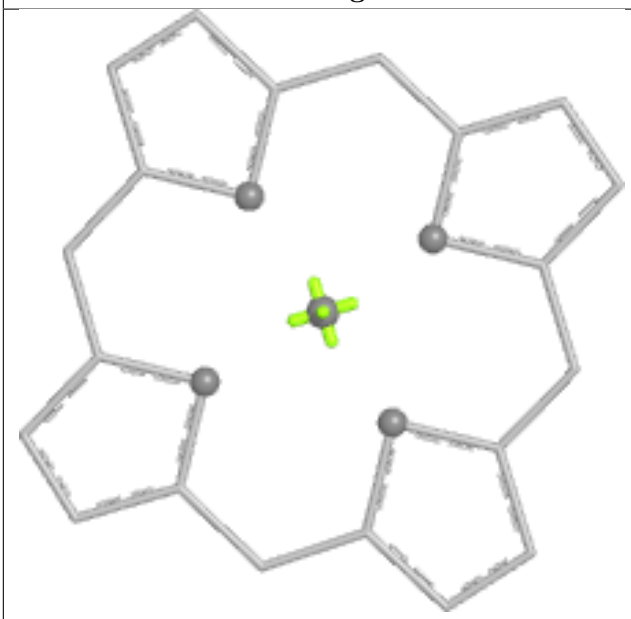
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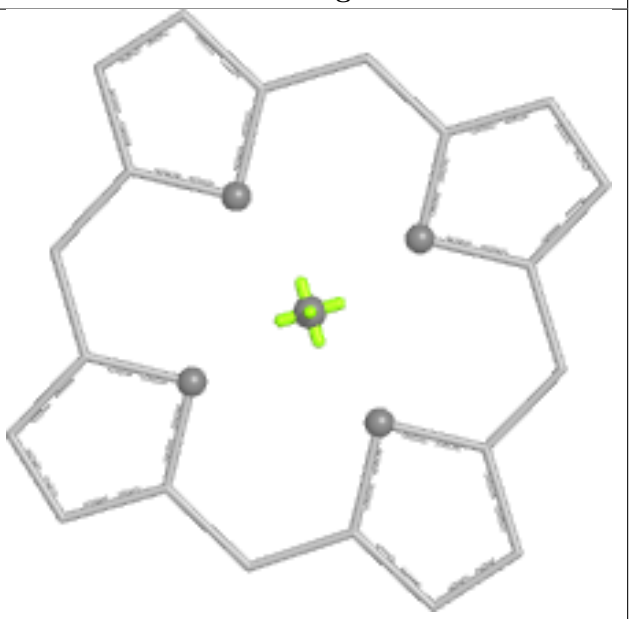
Bond lengths



Bond angles

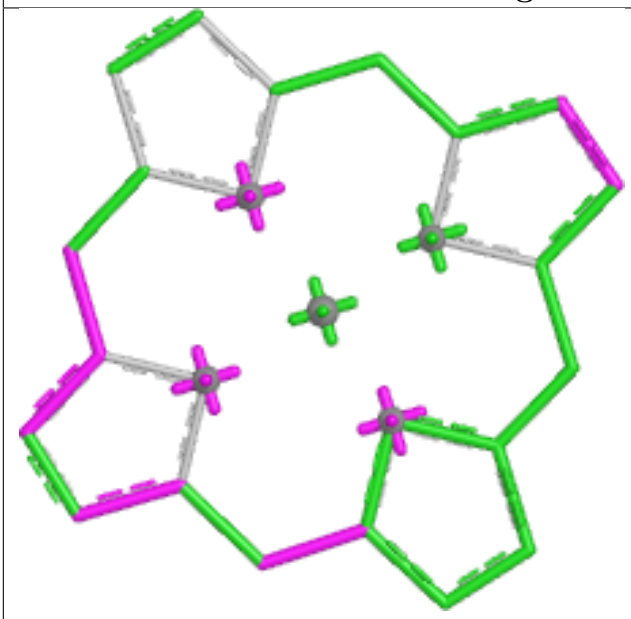


Torsions

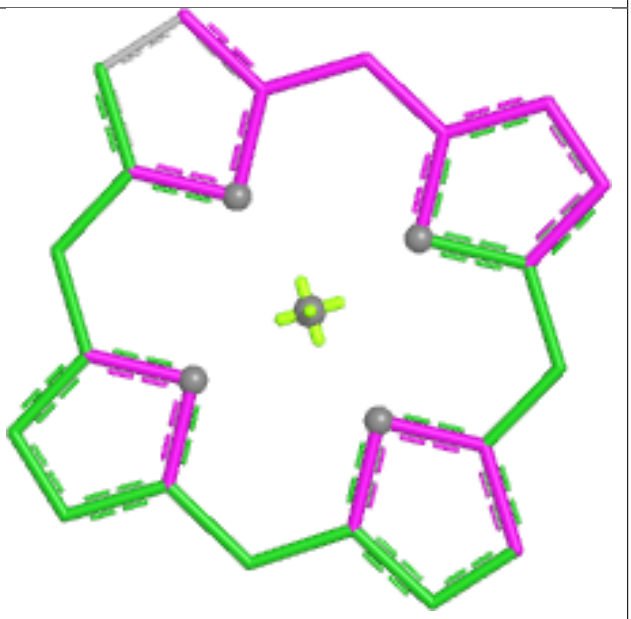


Rings

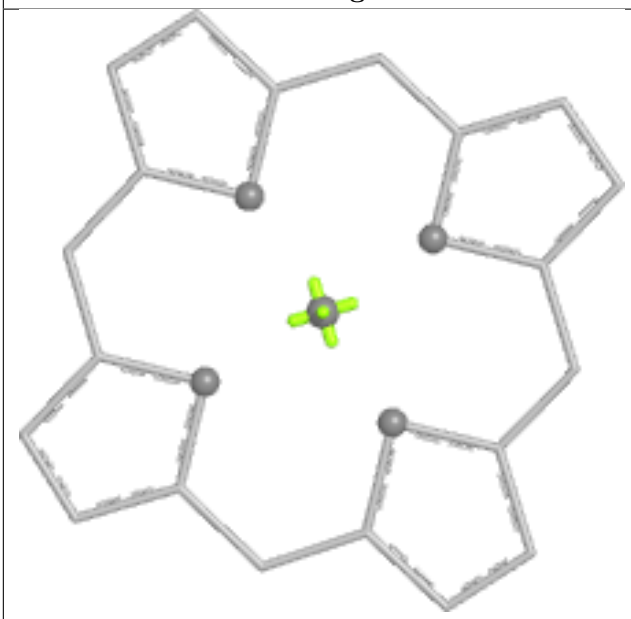
Ligand CLA P 5013



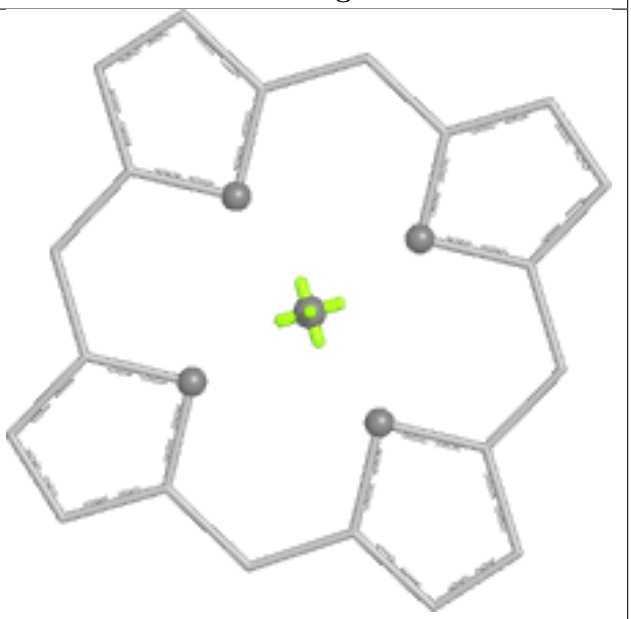
Bond lengths



Bond angles

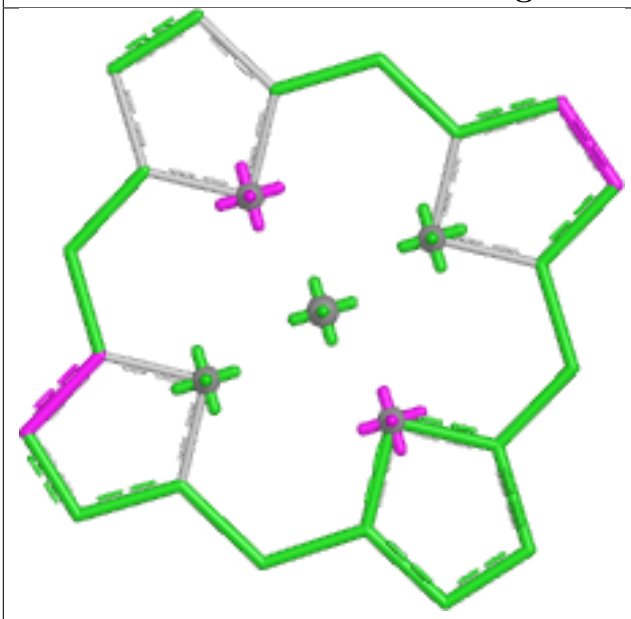


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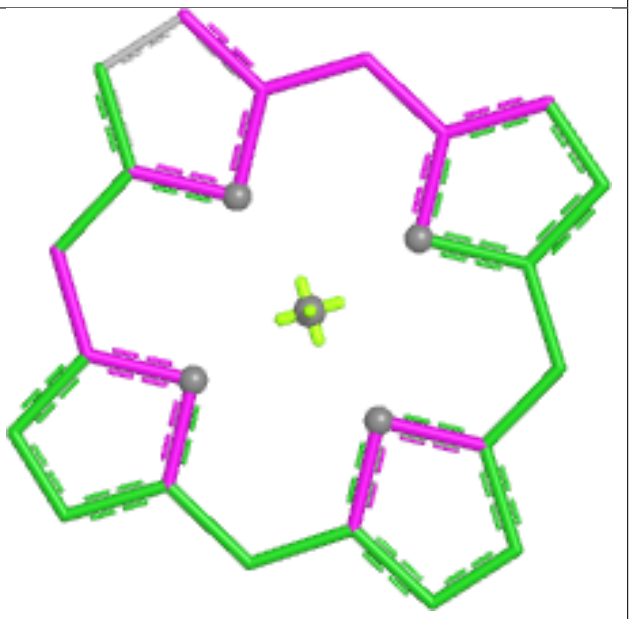


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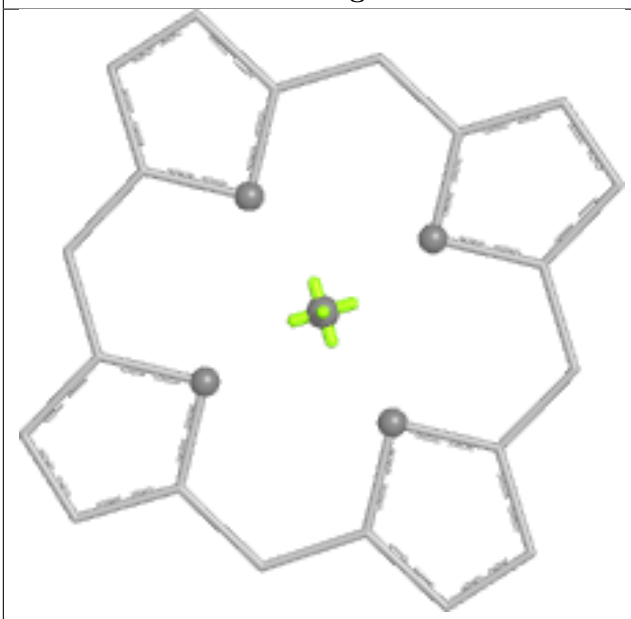
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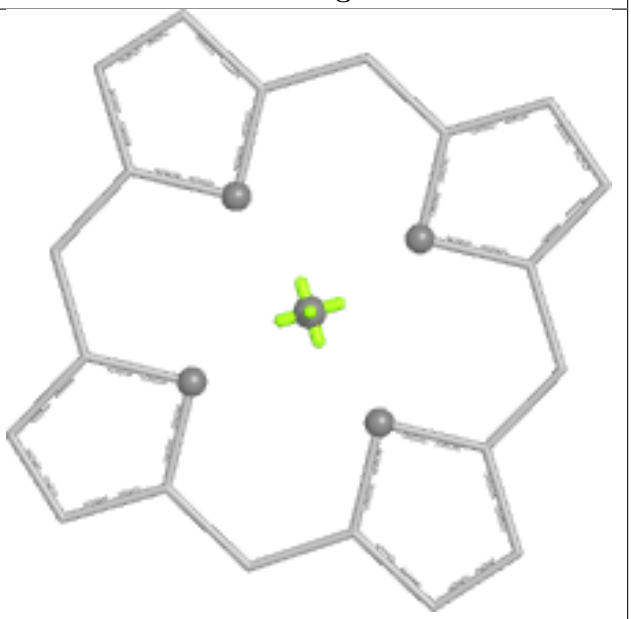
Bond lengths



Bond angles

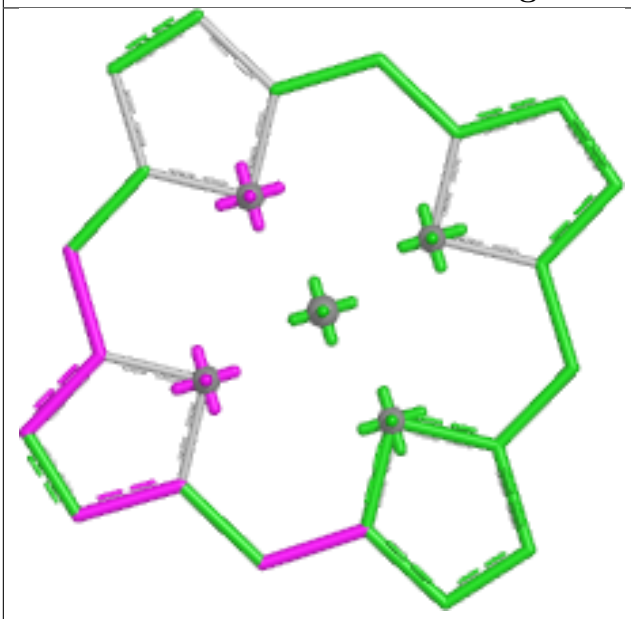


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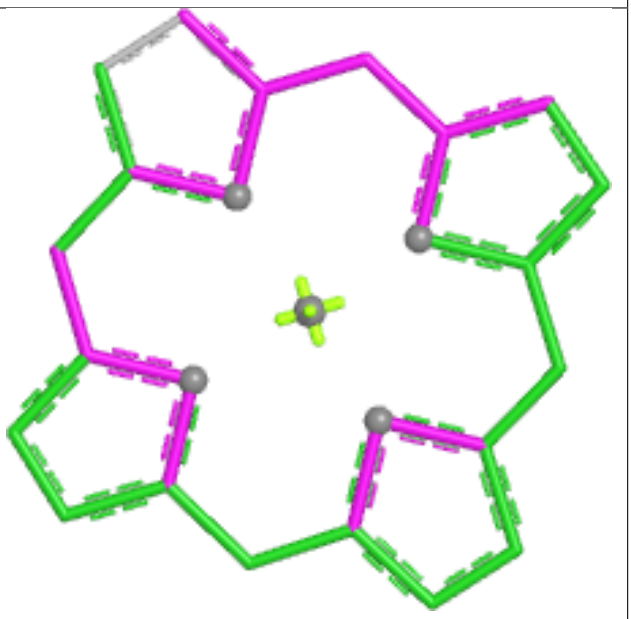


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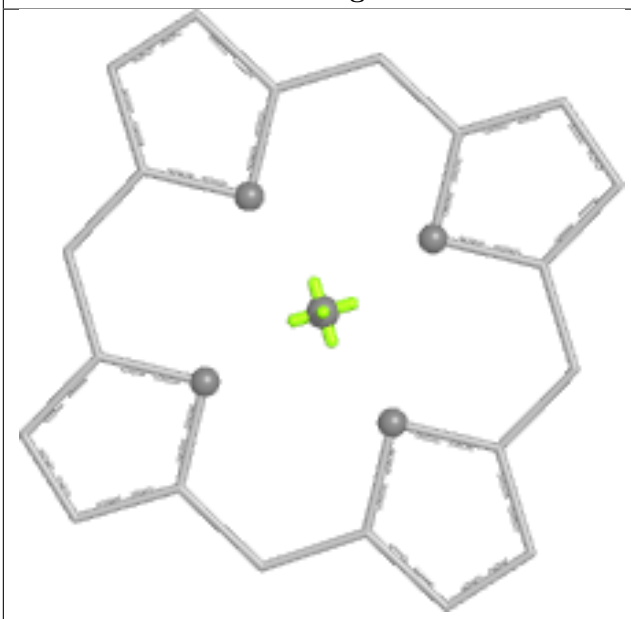
Ligand CLA 3 1011



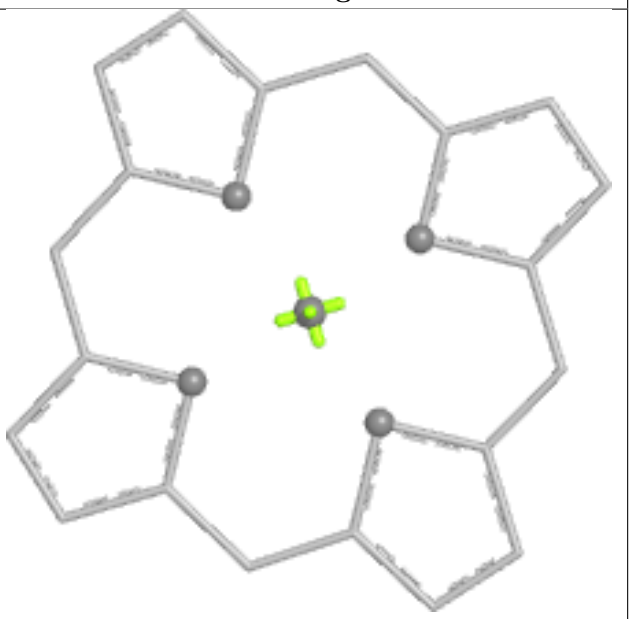
Bond lengths



Bond angles

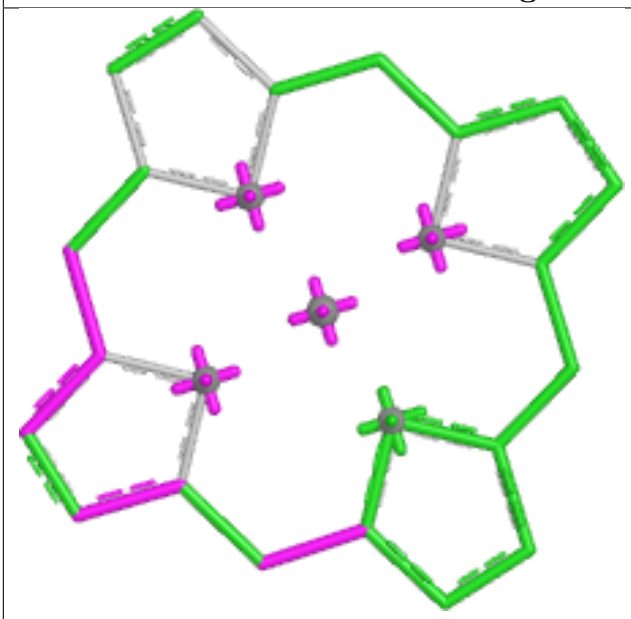


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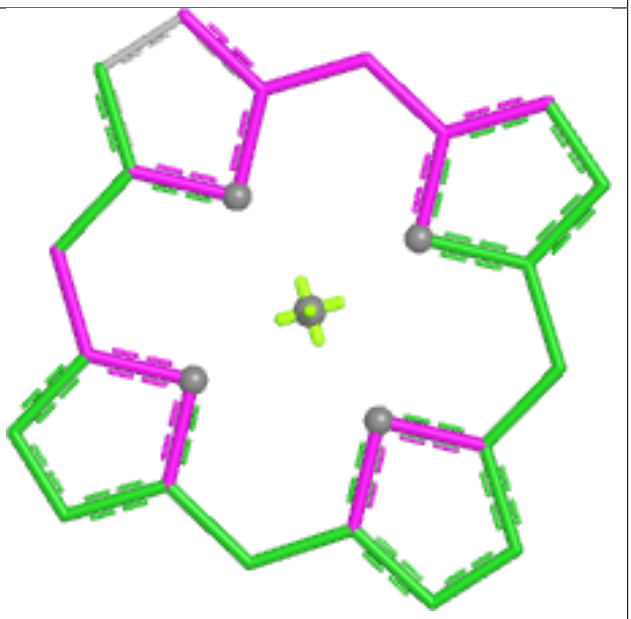


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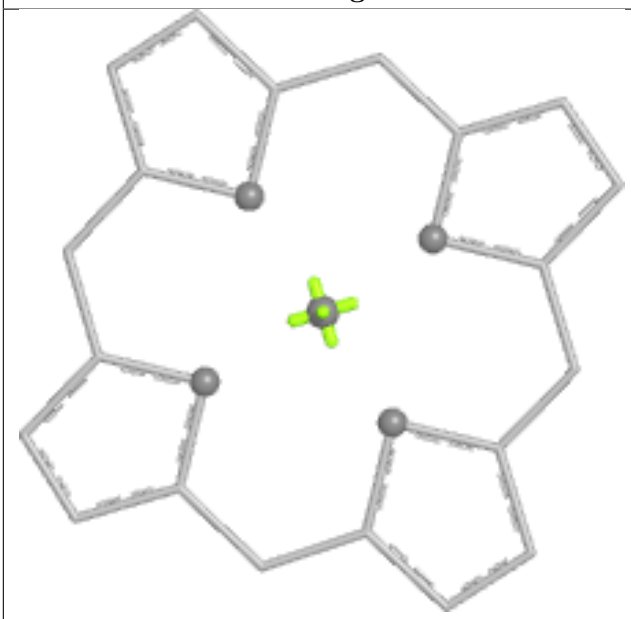
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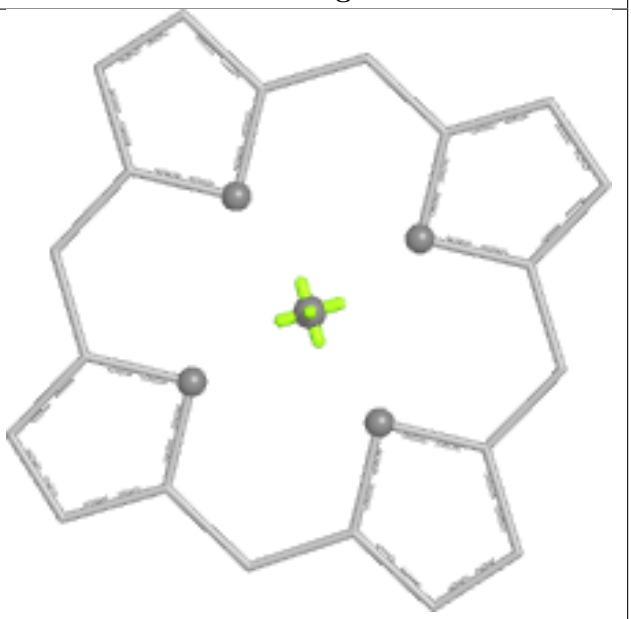
Bond lengths



Bond angles

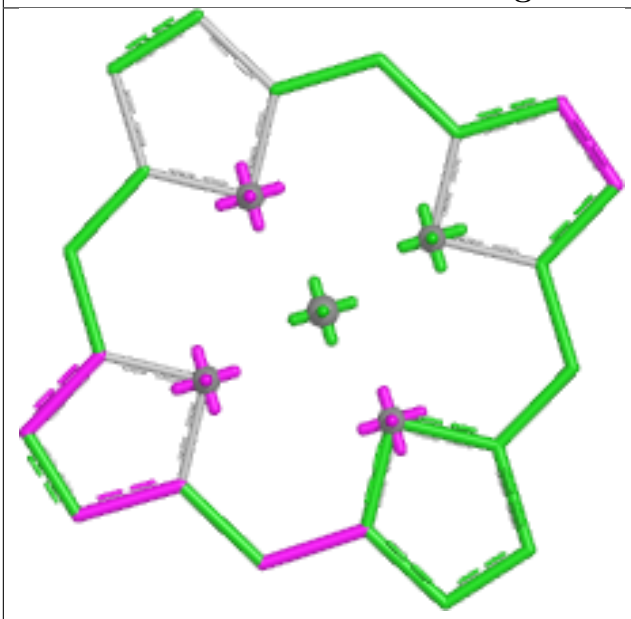


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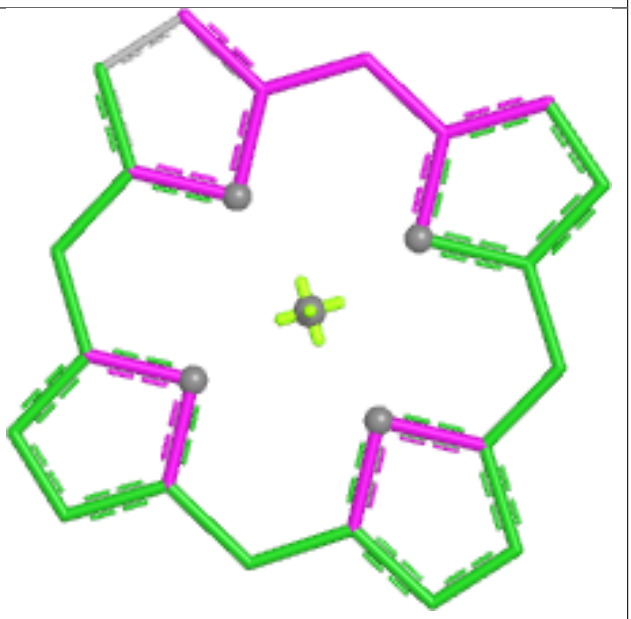


Rings

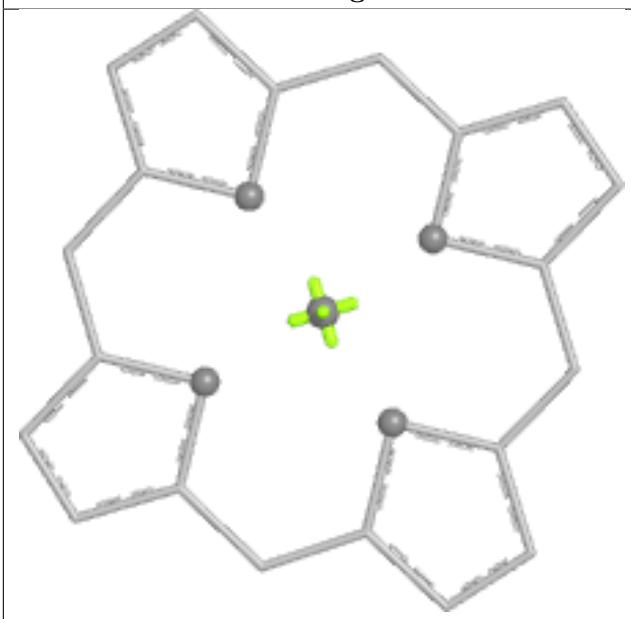
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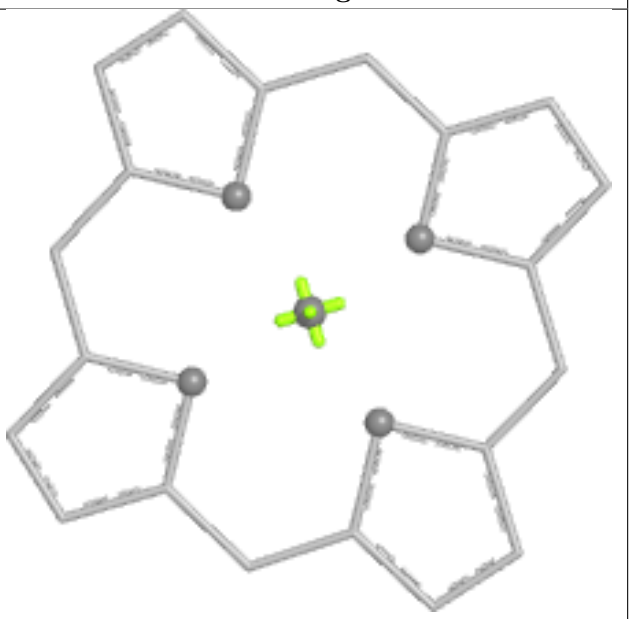
Bond lengths



Bond angles

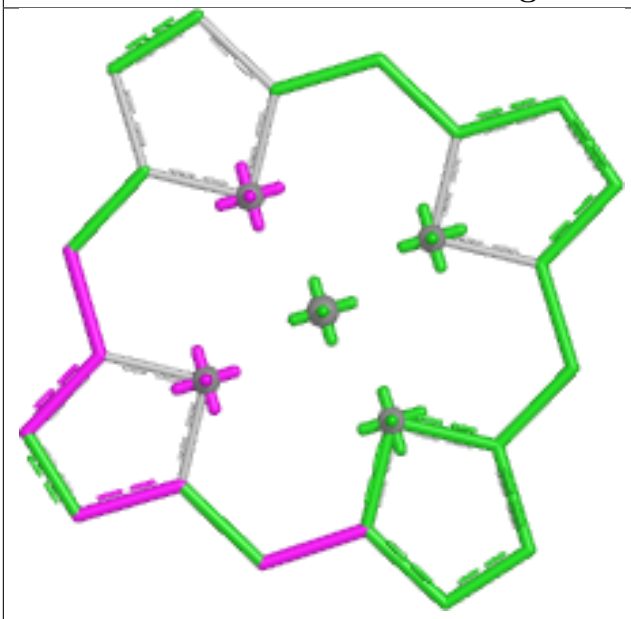


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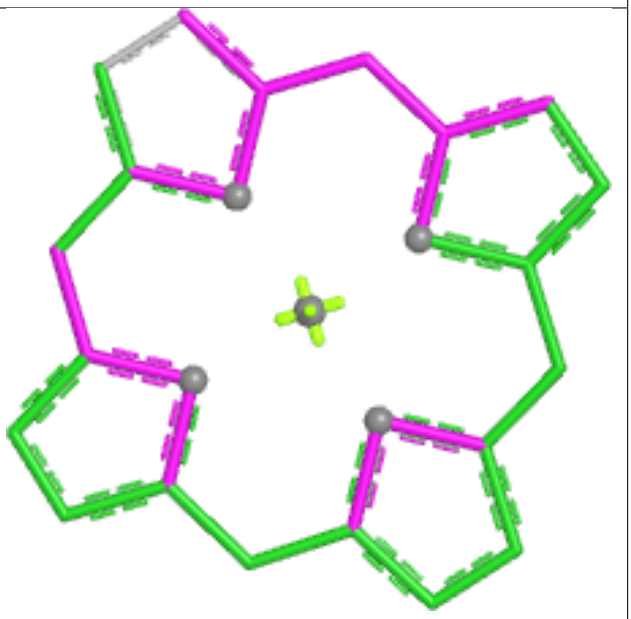


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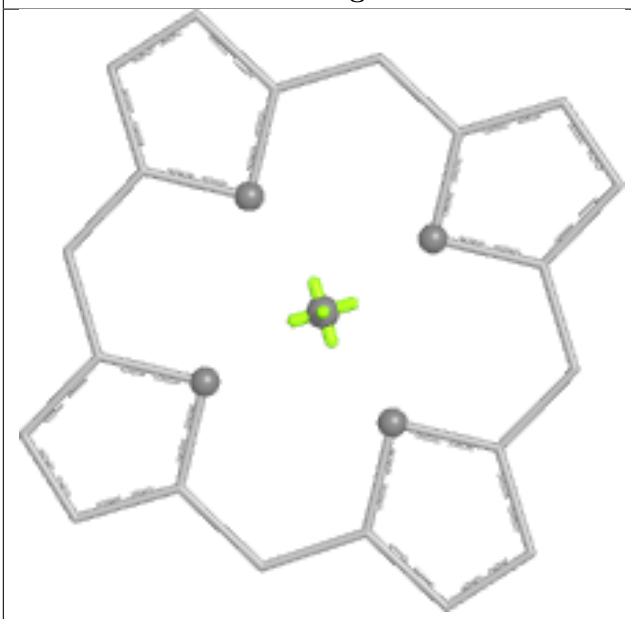
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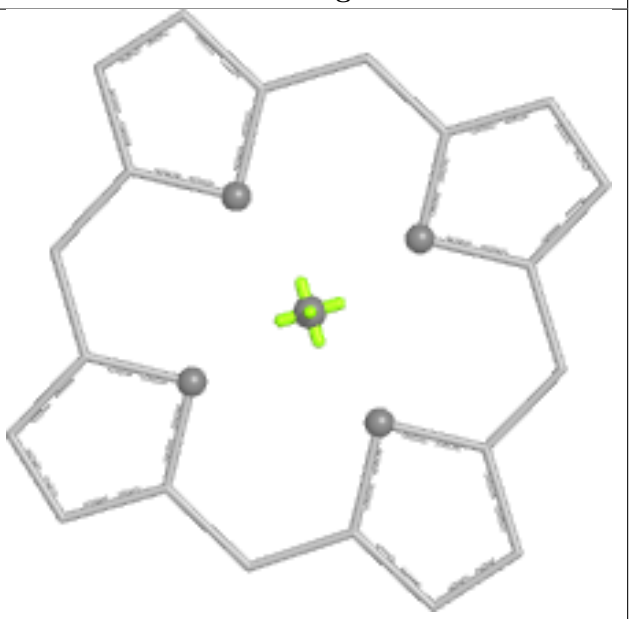
Bond lengths



Bond angles

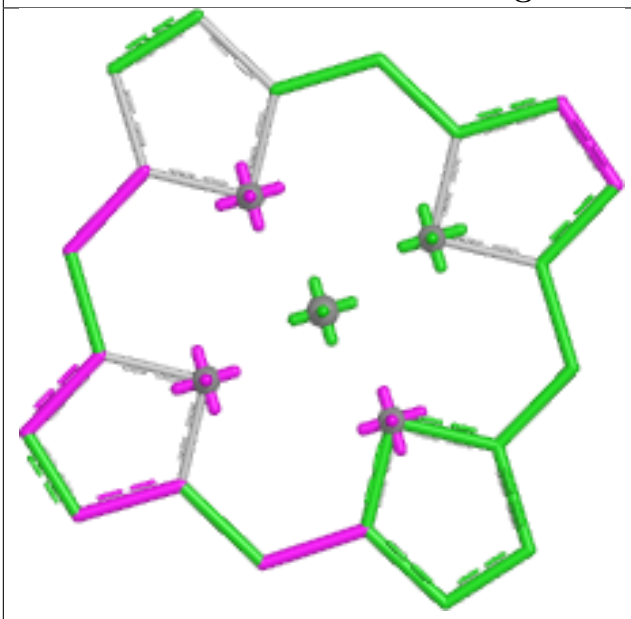


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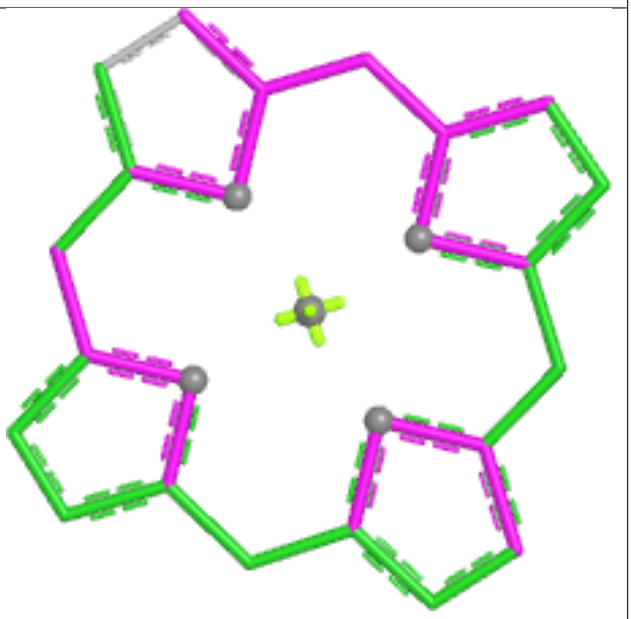


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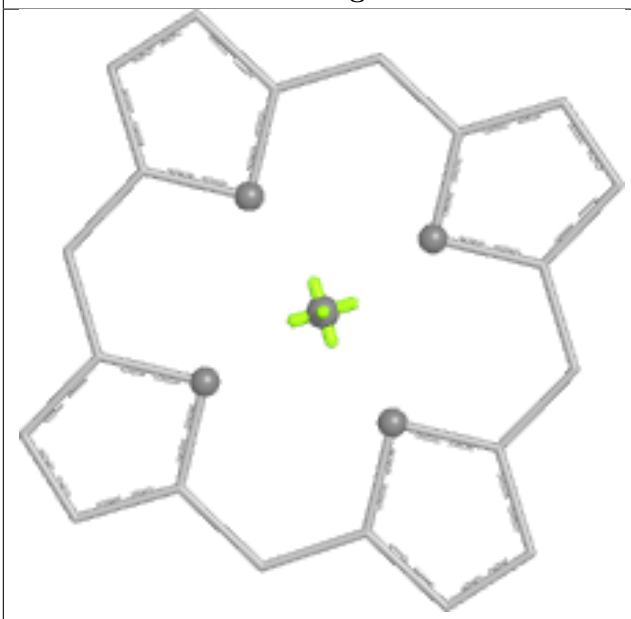
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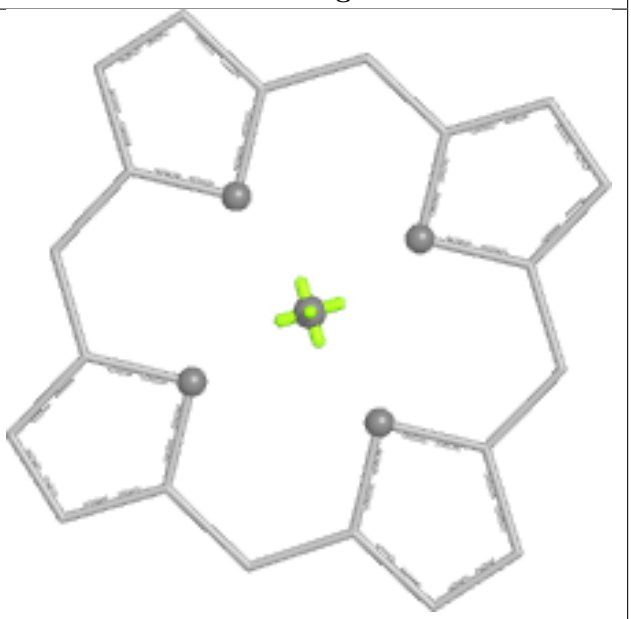
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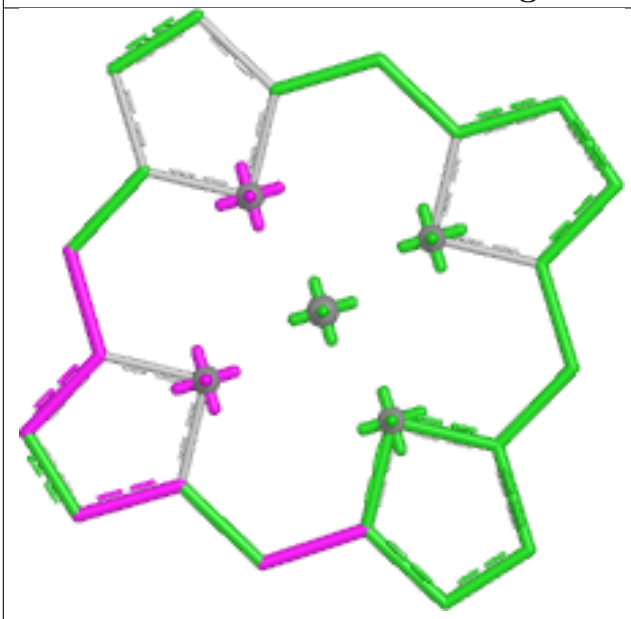


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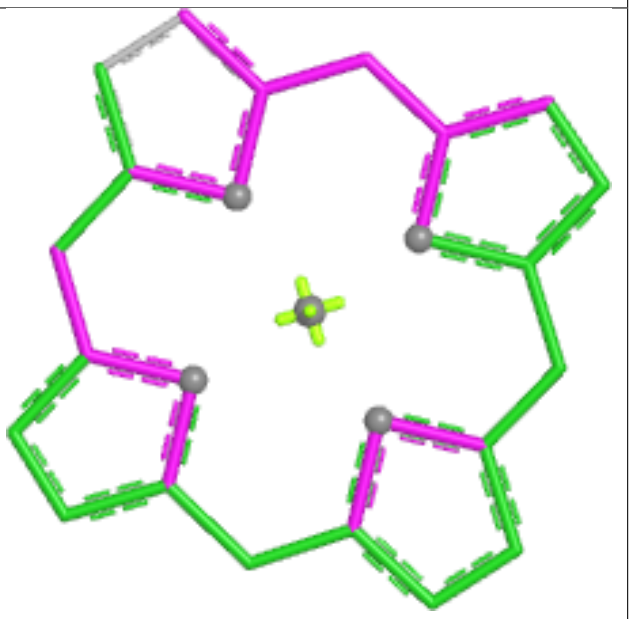


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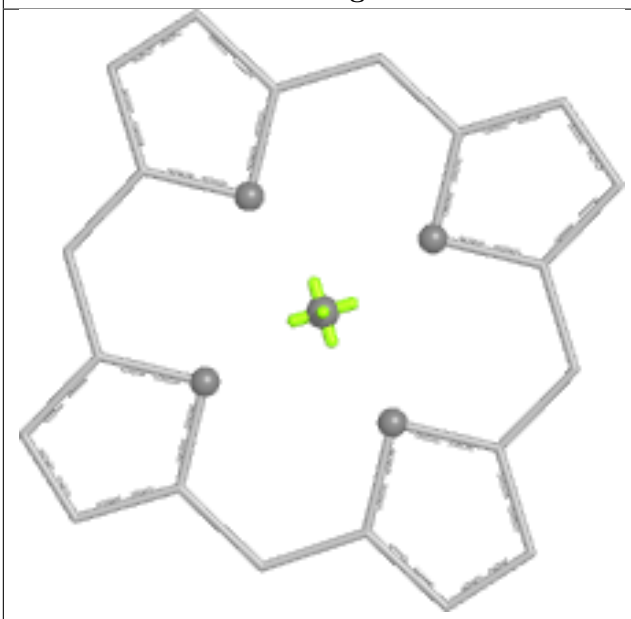
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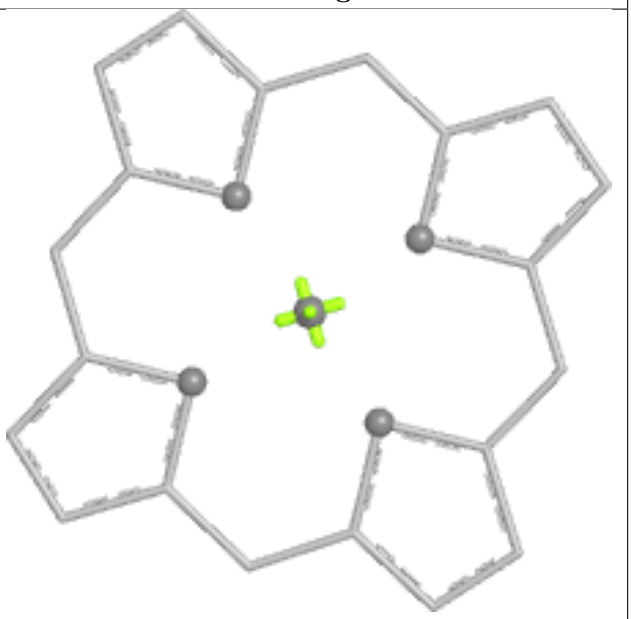
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Bond angles

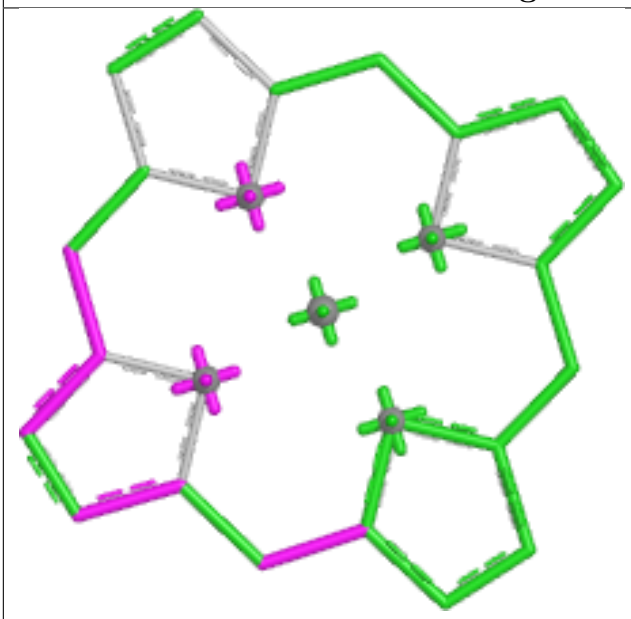


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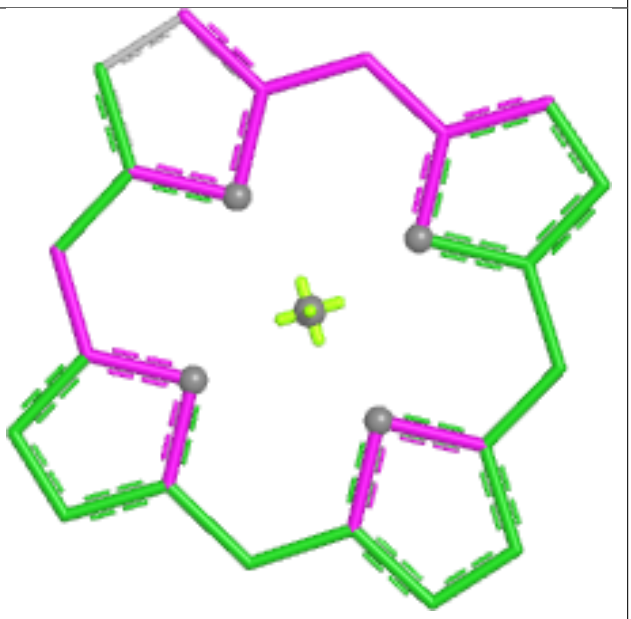


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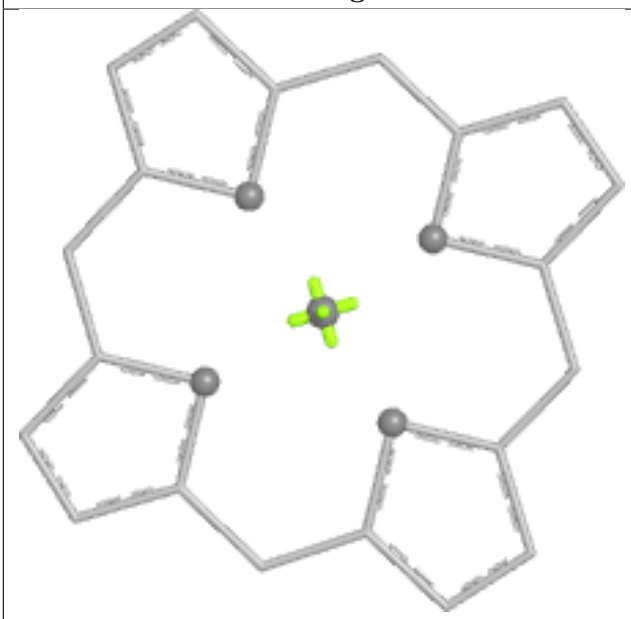
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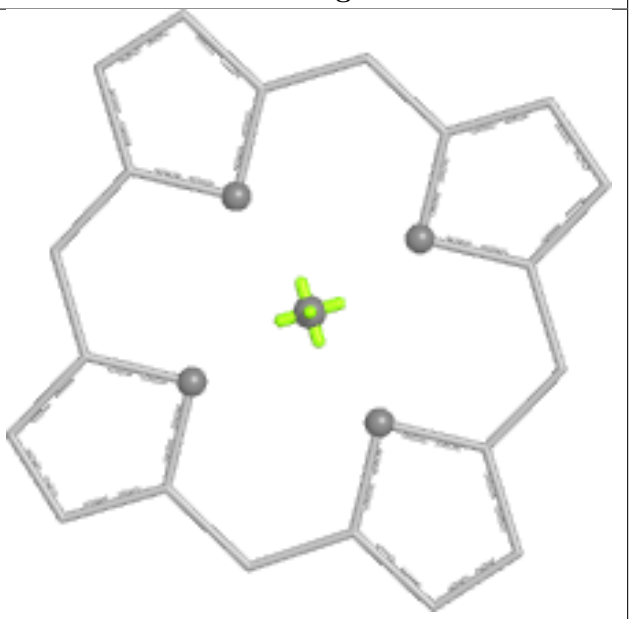
Bond lengths



Bond angles

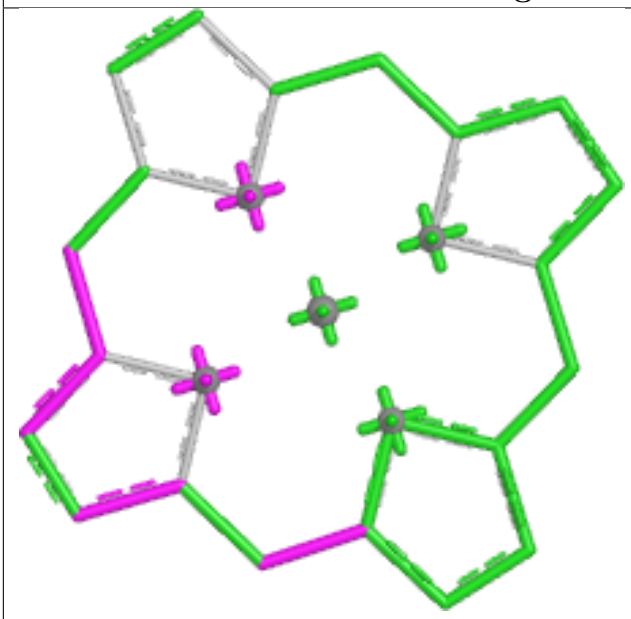


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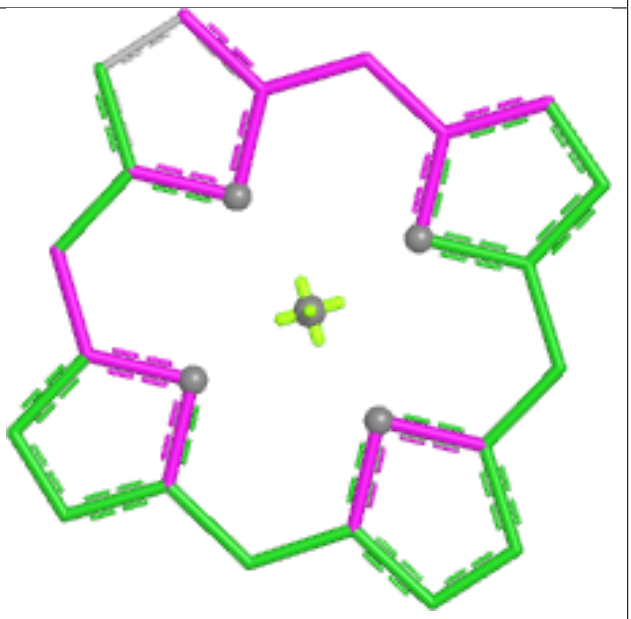


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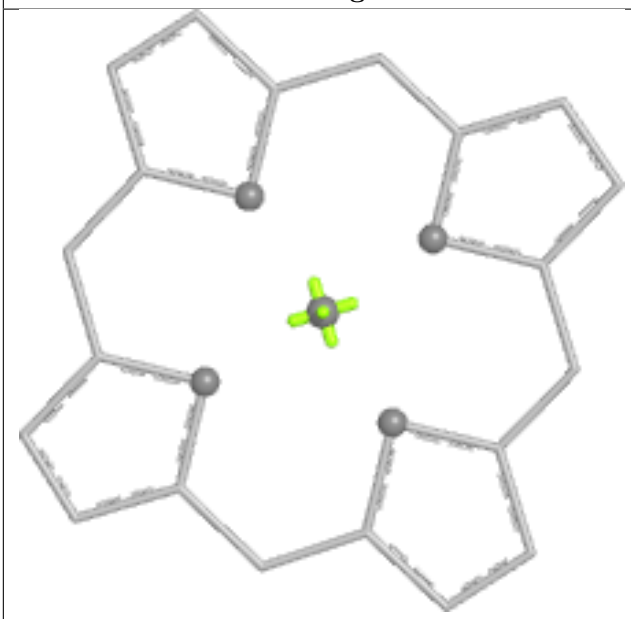
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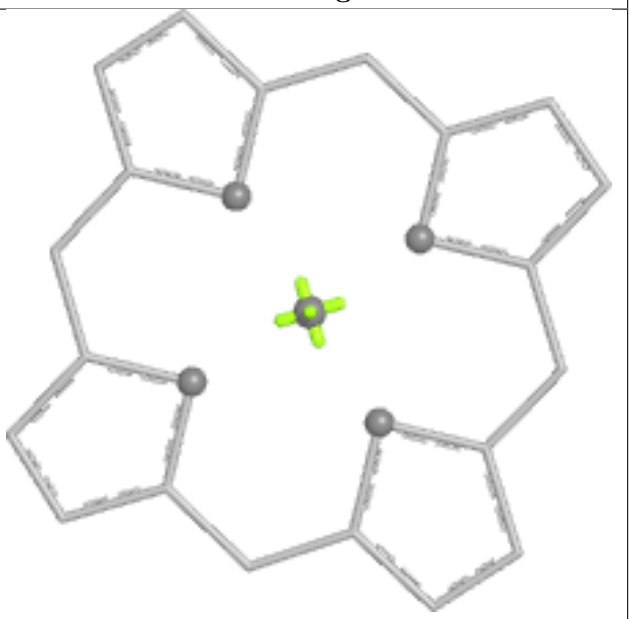
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Bond angles

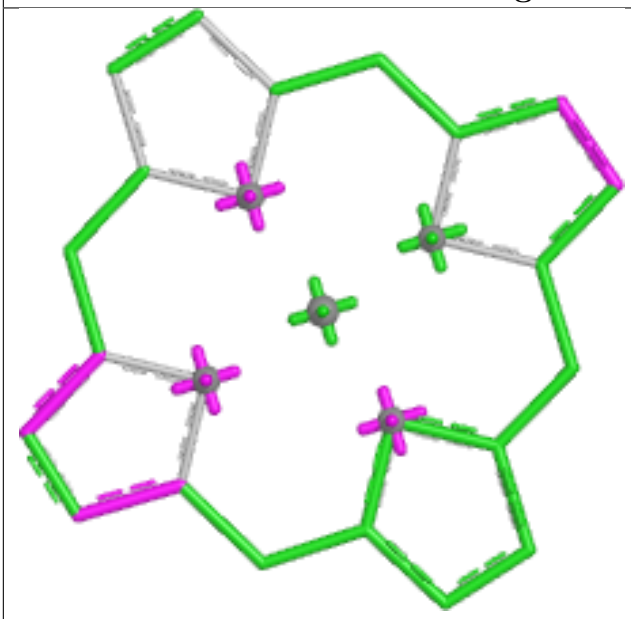


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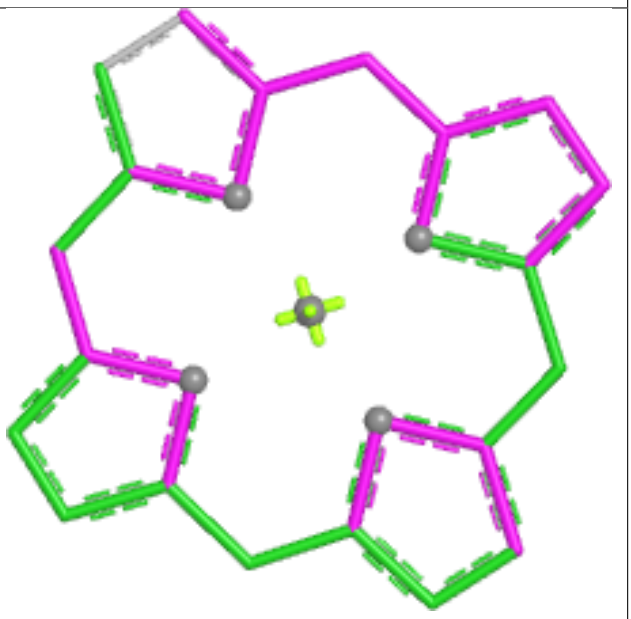


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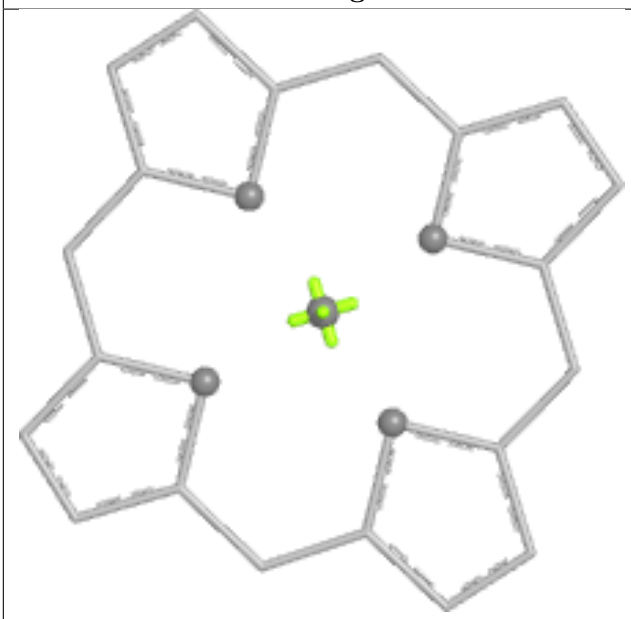
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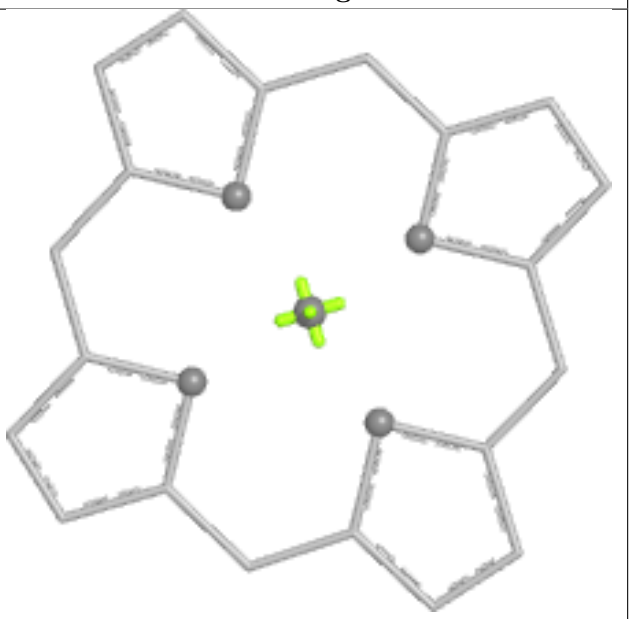
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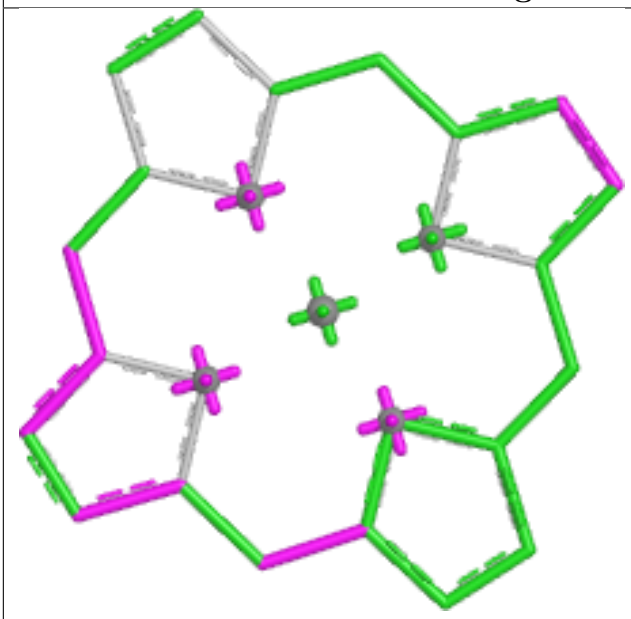


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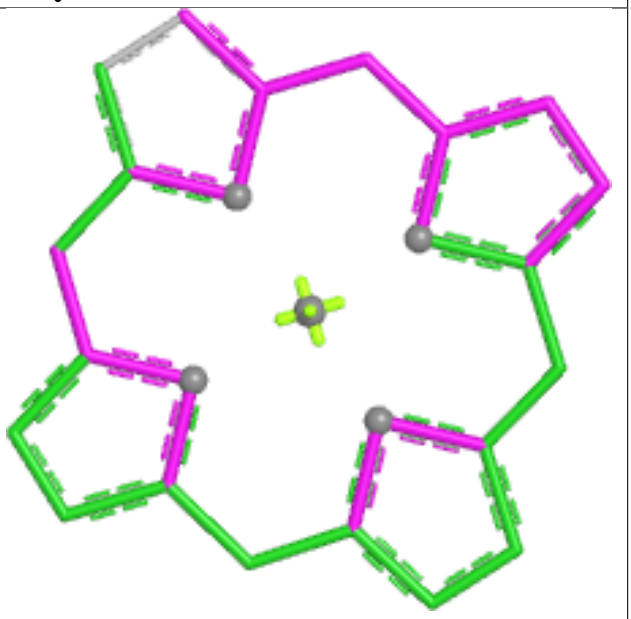


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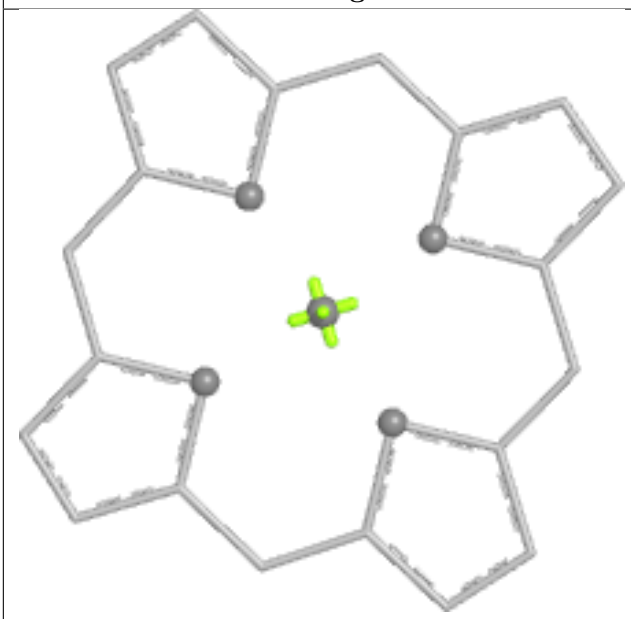
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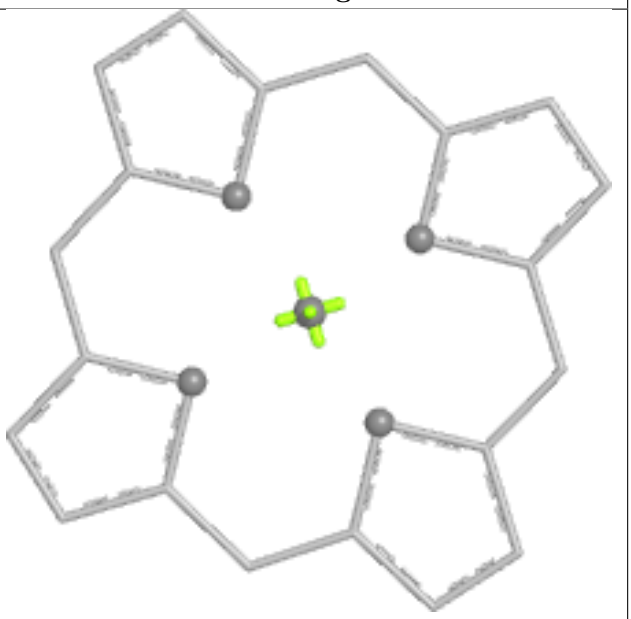
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Bond angles

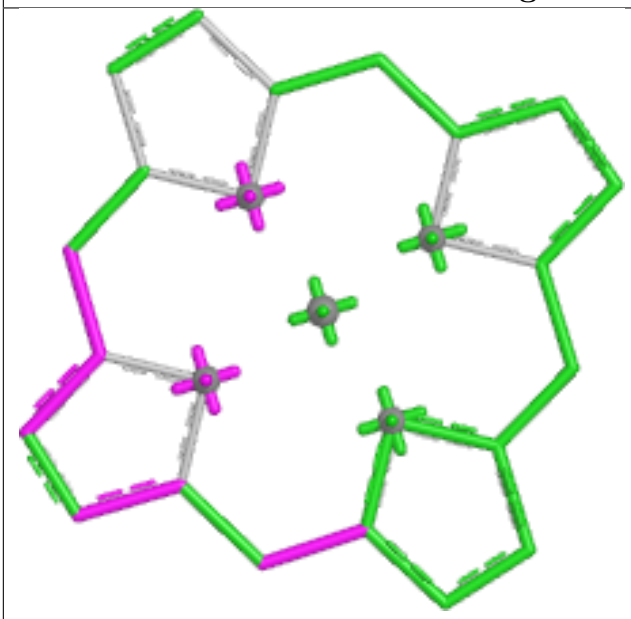


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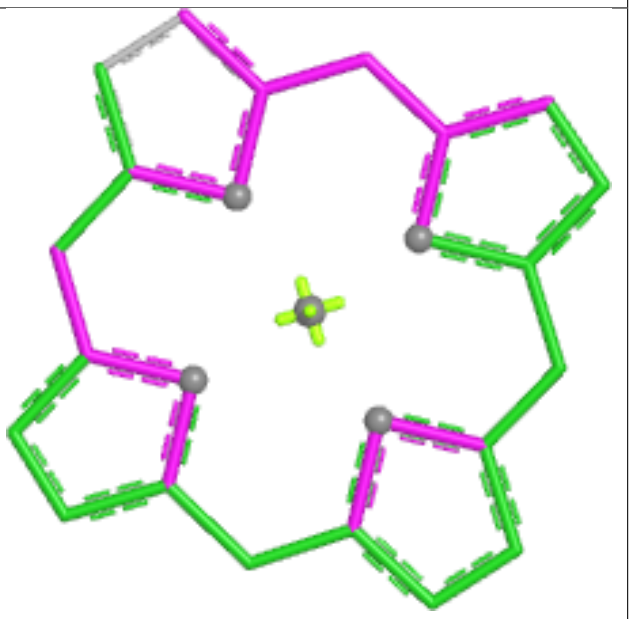


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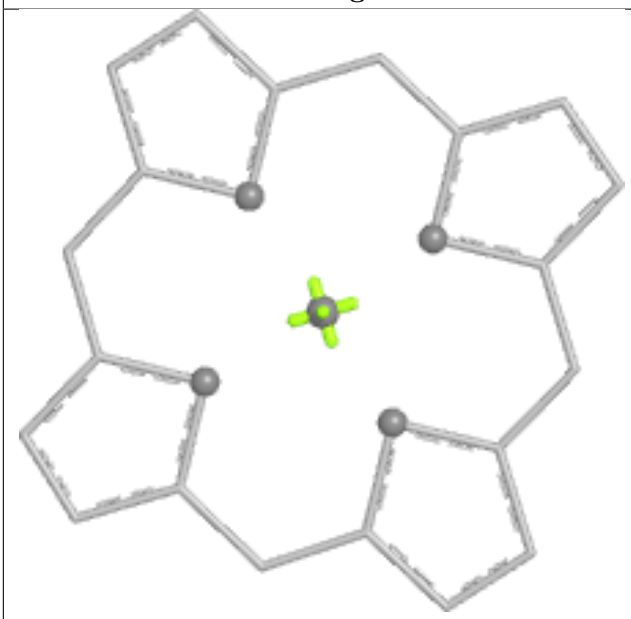
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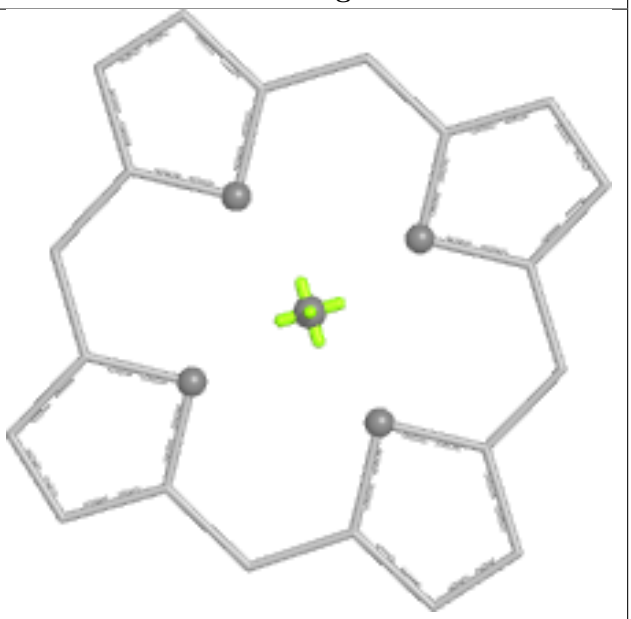
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Bond angles

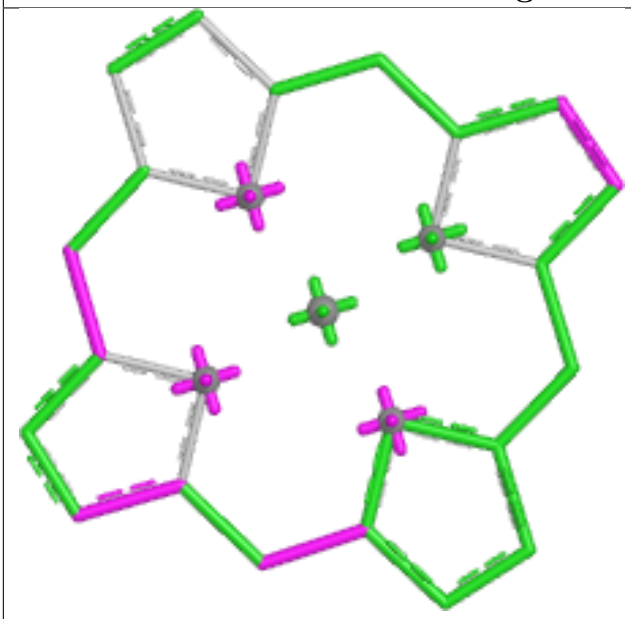


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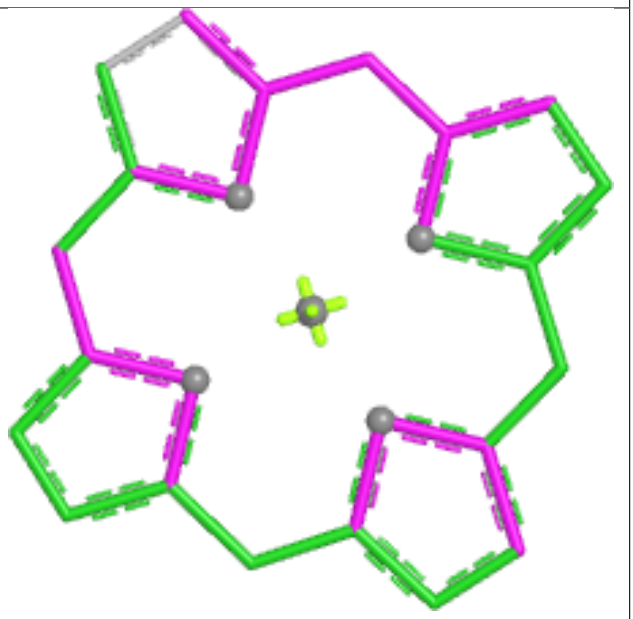


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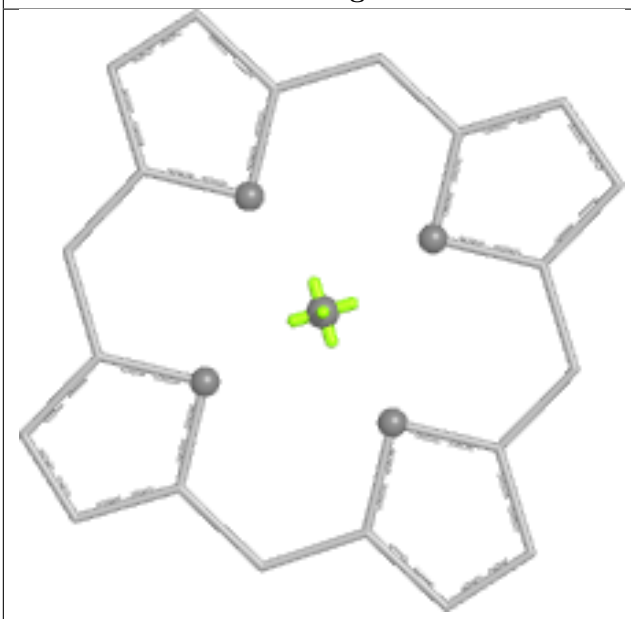
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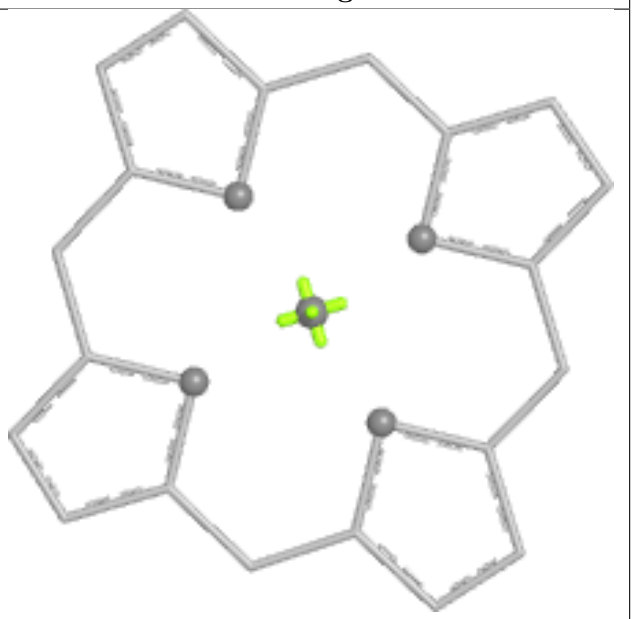
Bond lengths



Bond angles

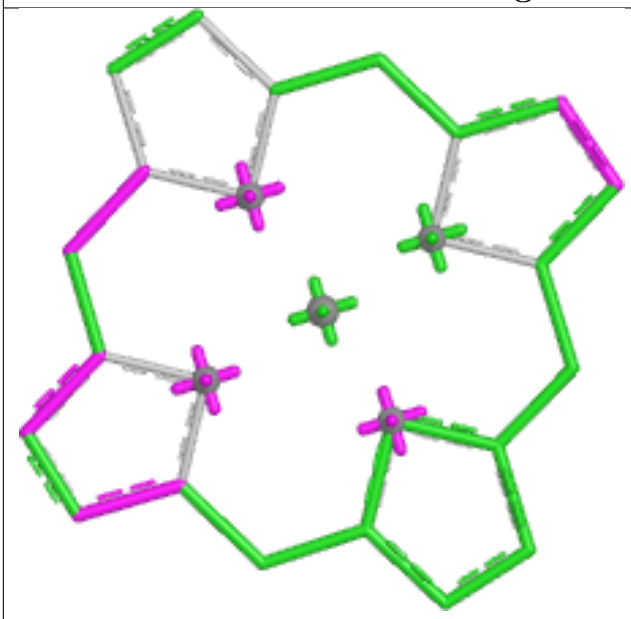


Torsions

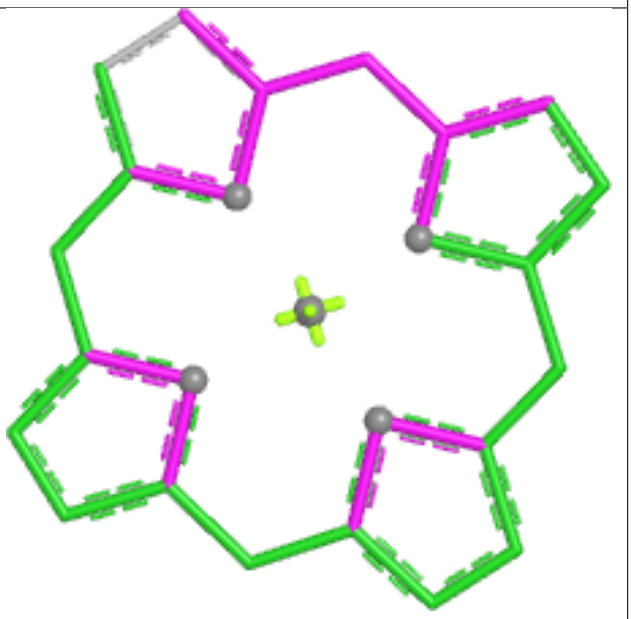


Rings

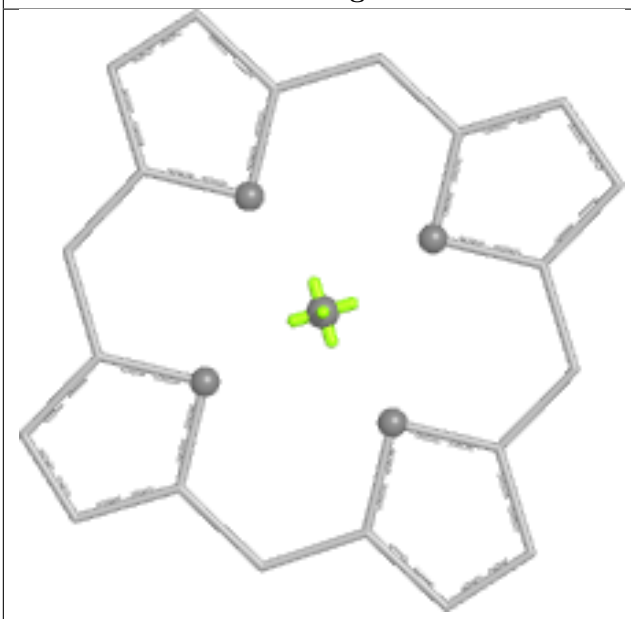
Ligand CLA A 1139



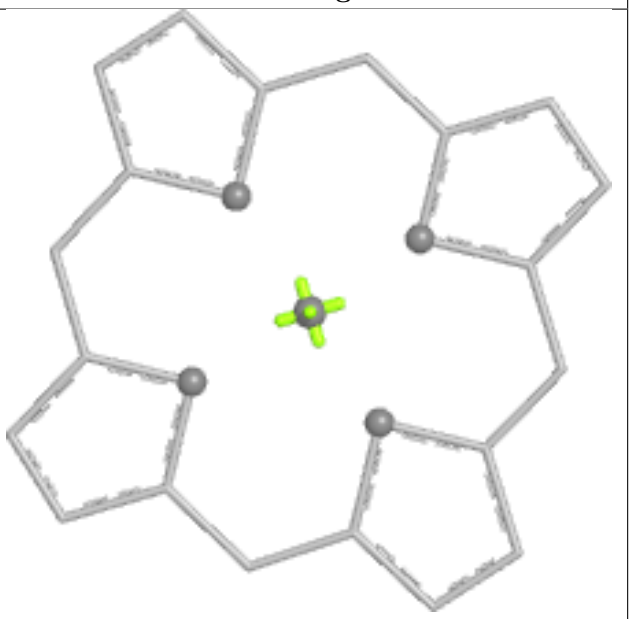
Bond lengths



Bond angles

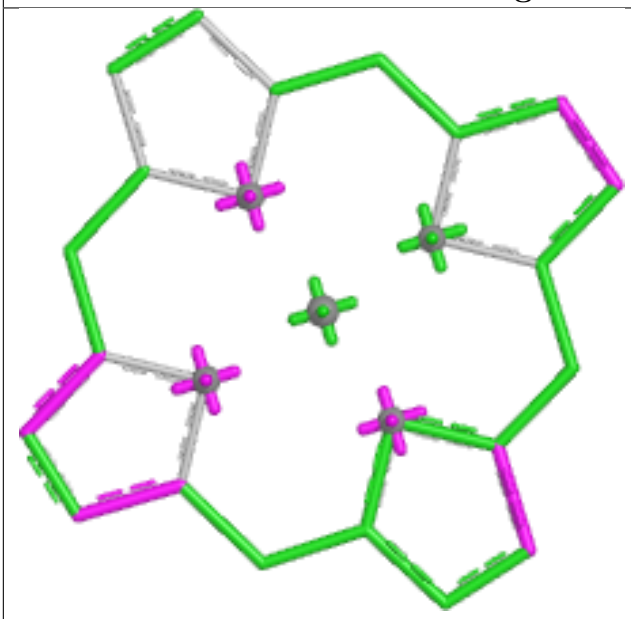


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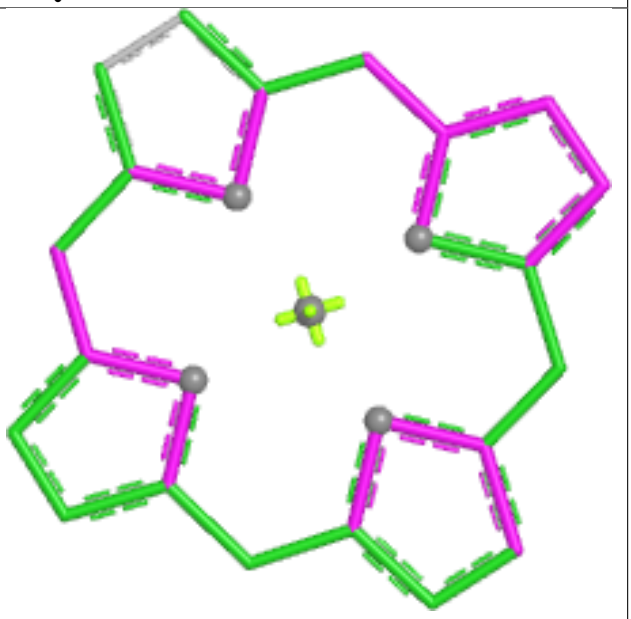


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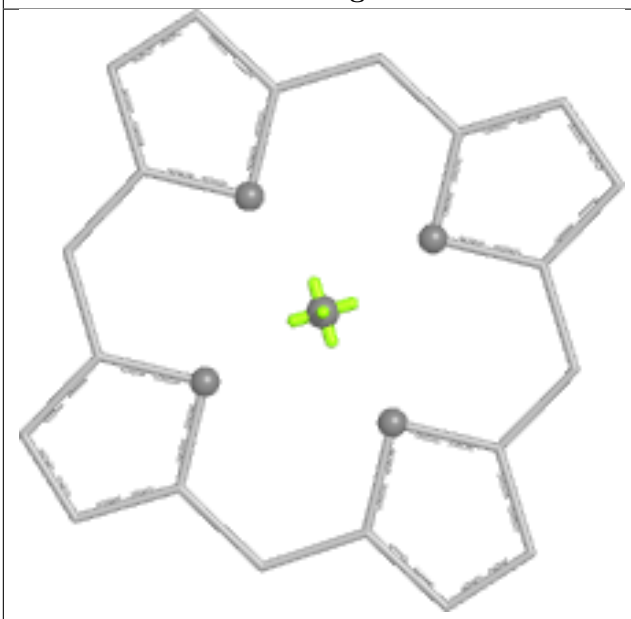
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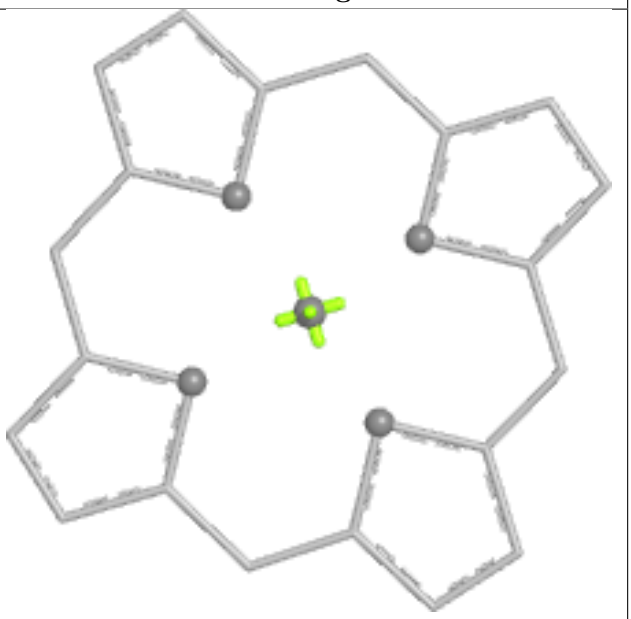
Bond lengths



Bond angles

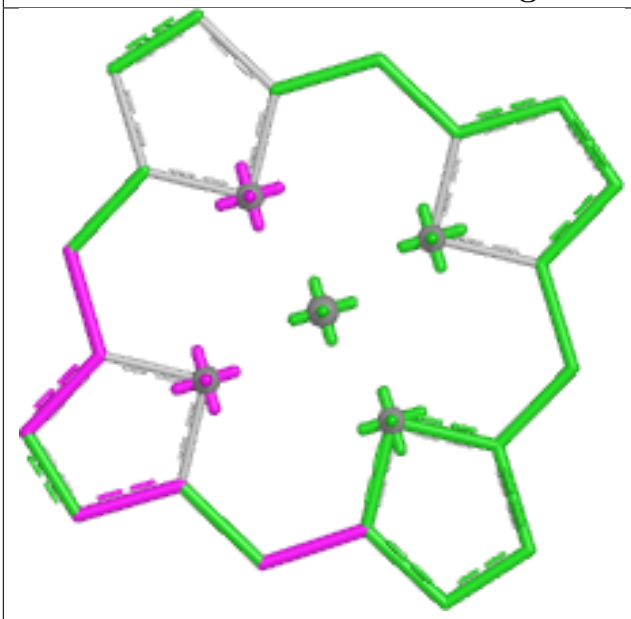


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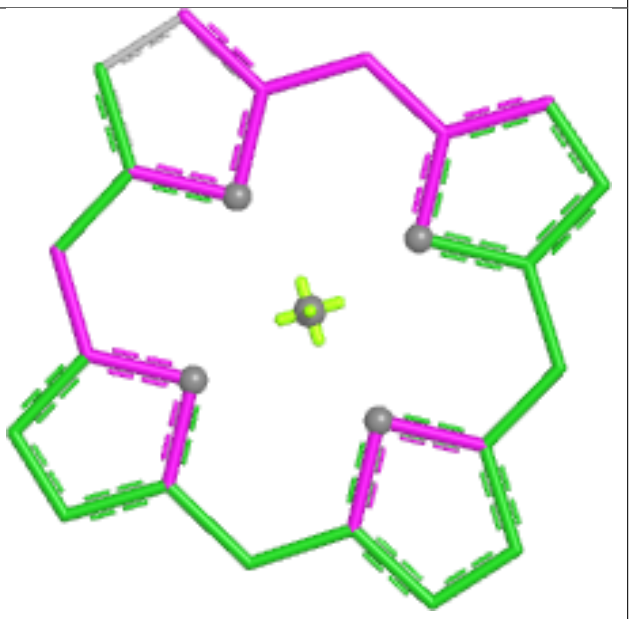


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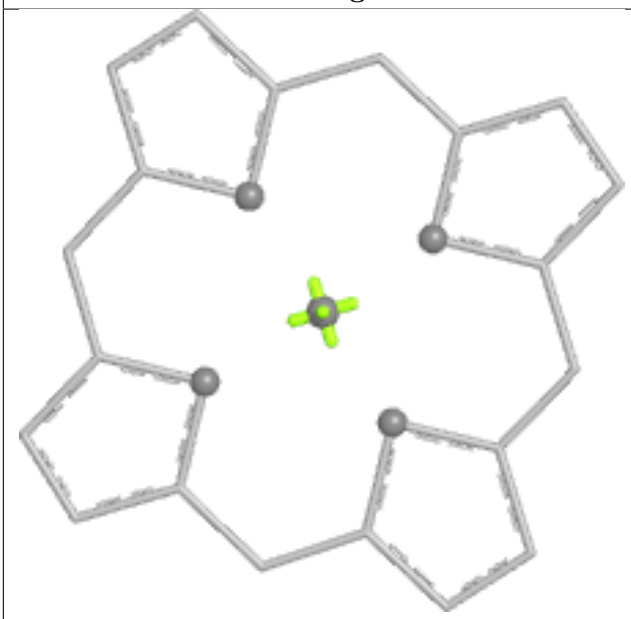
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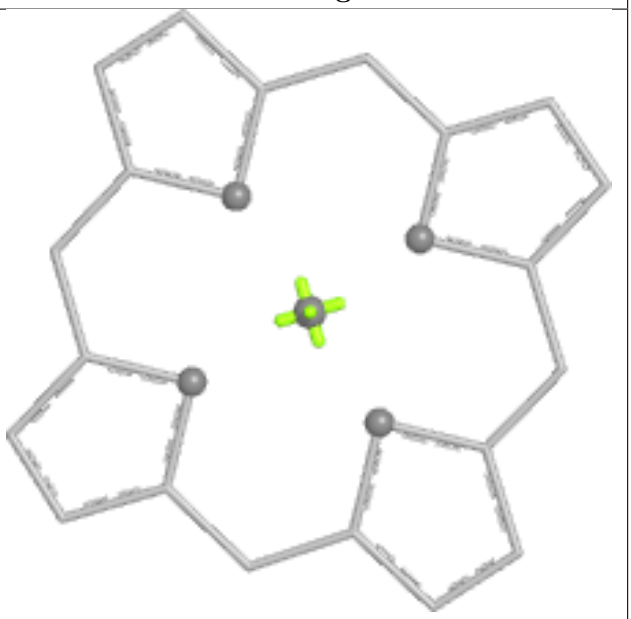
Bond lengths



Bond angles

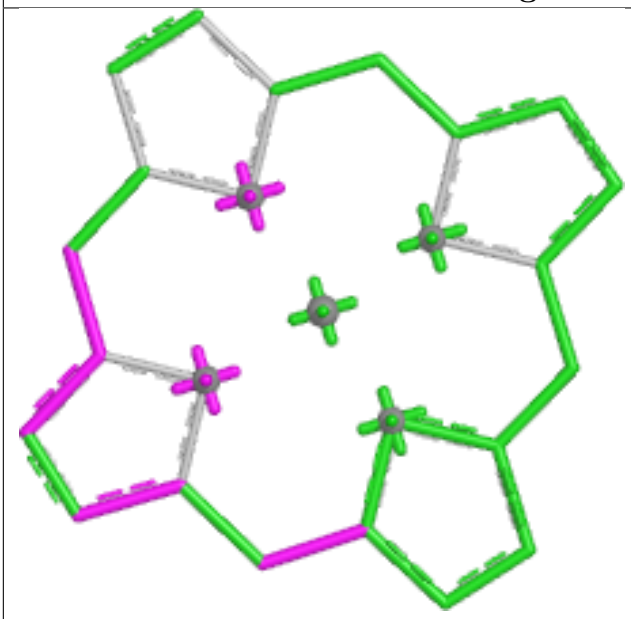


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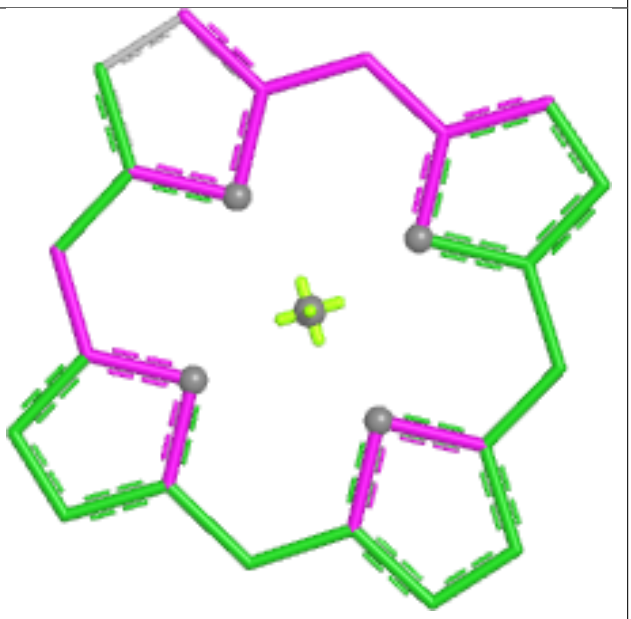


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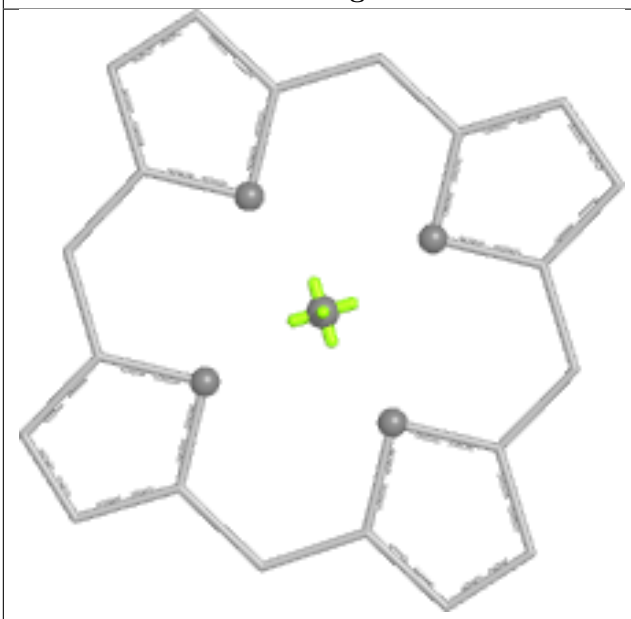
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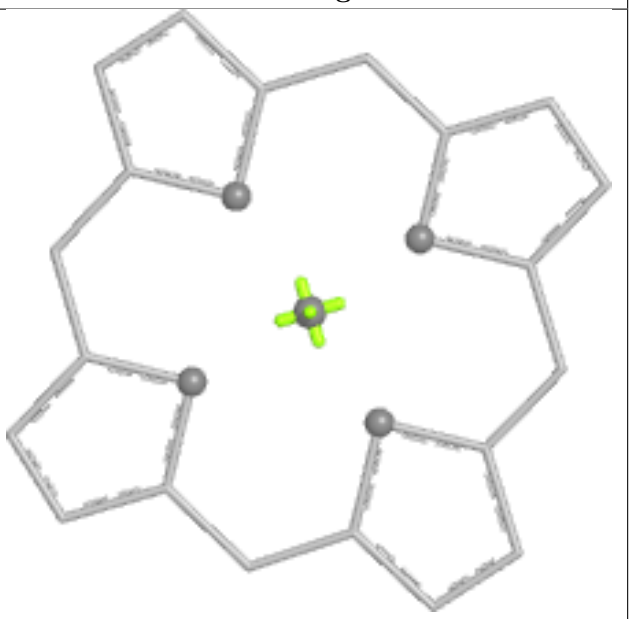
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Bond angles

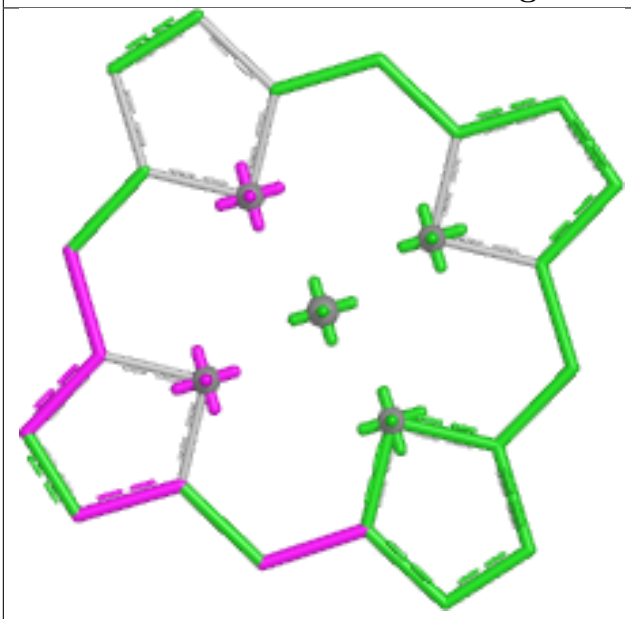


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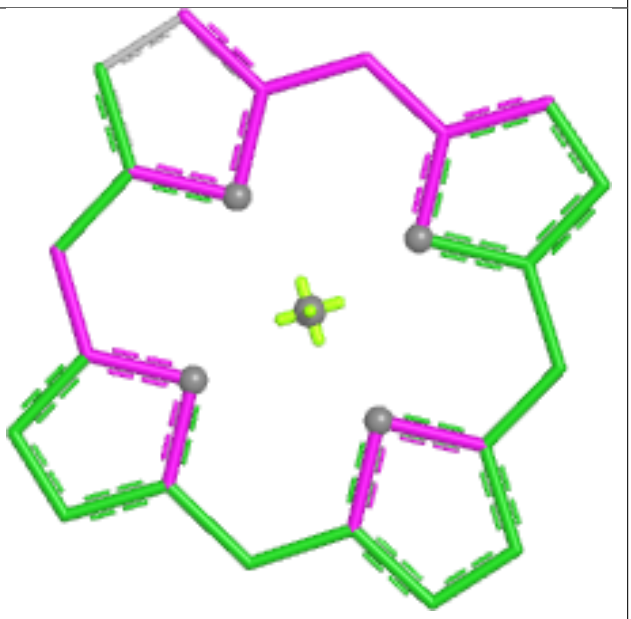


Rings

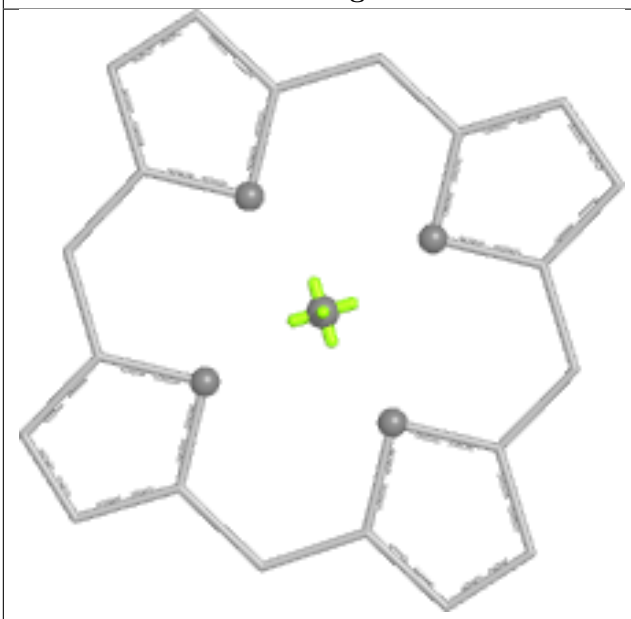
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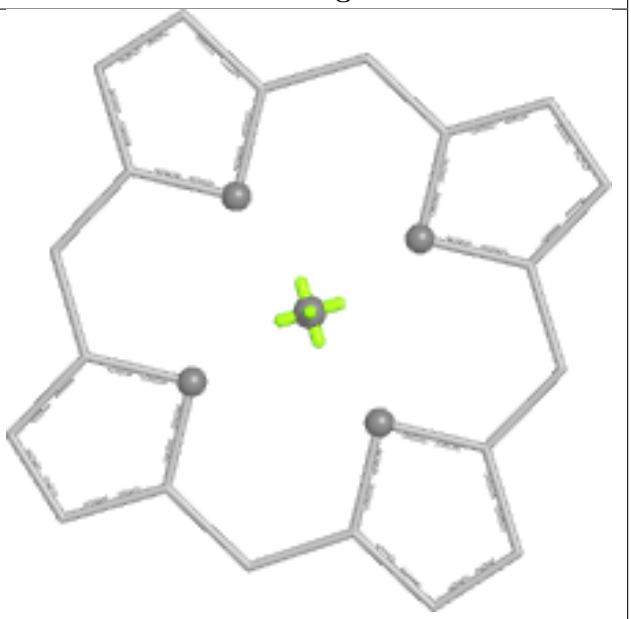
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Bond angles

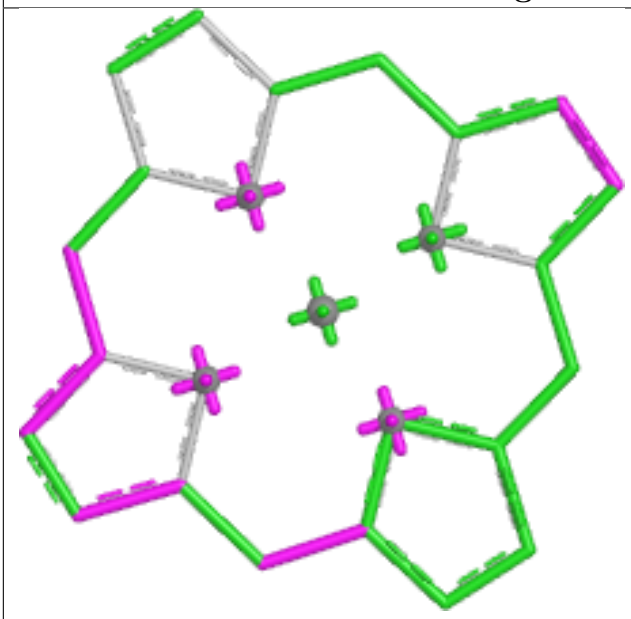


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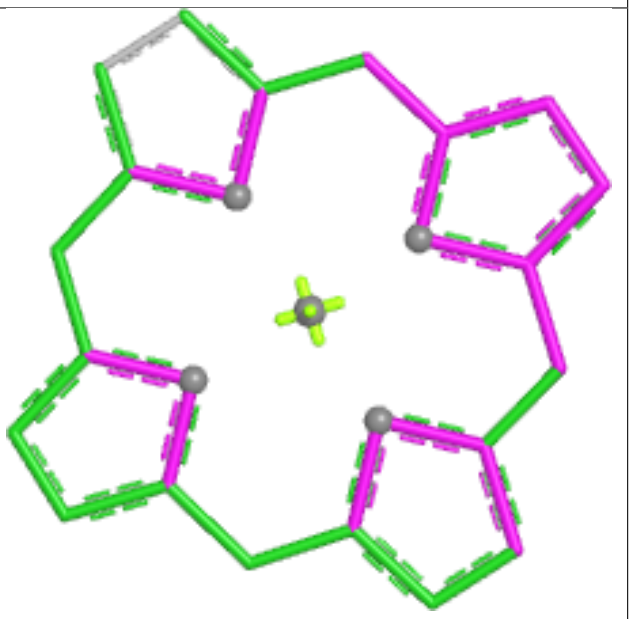


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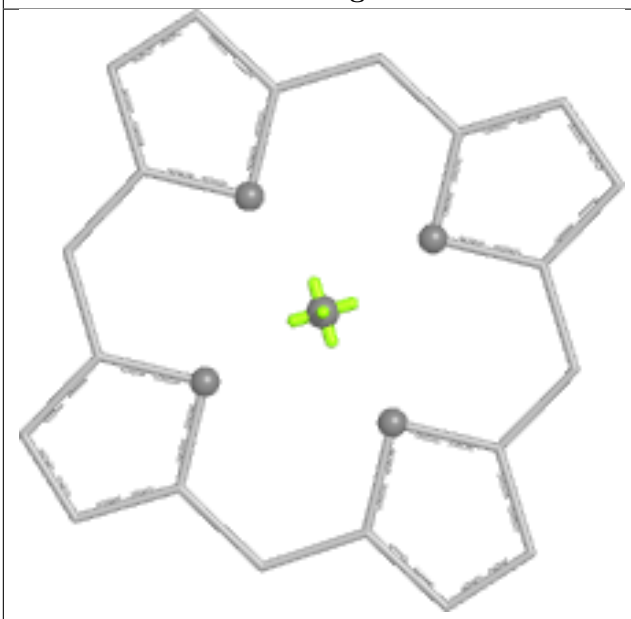
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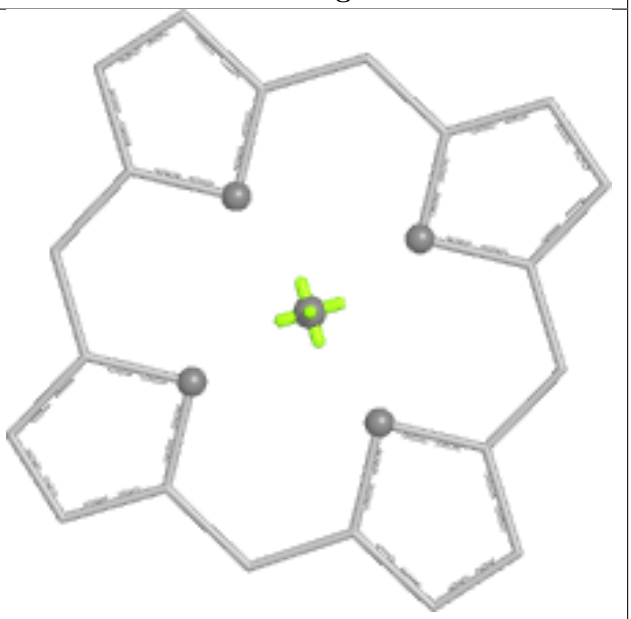
Bond lengths



Bond angles

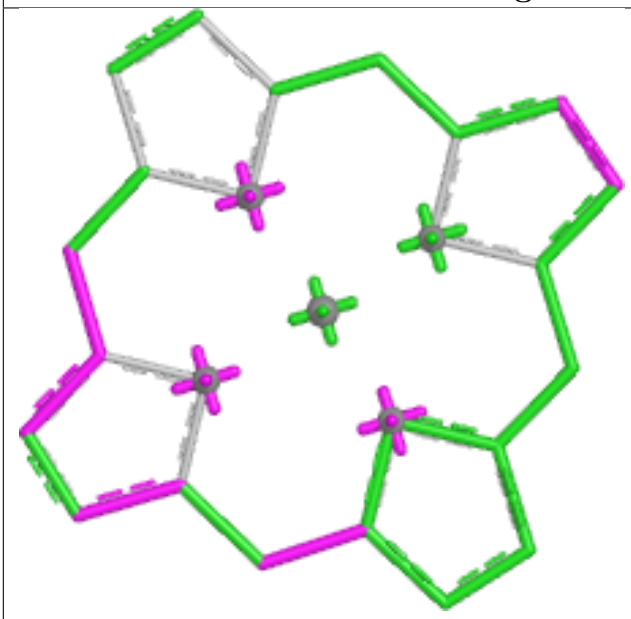


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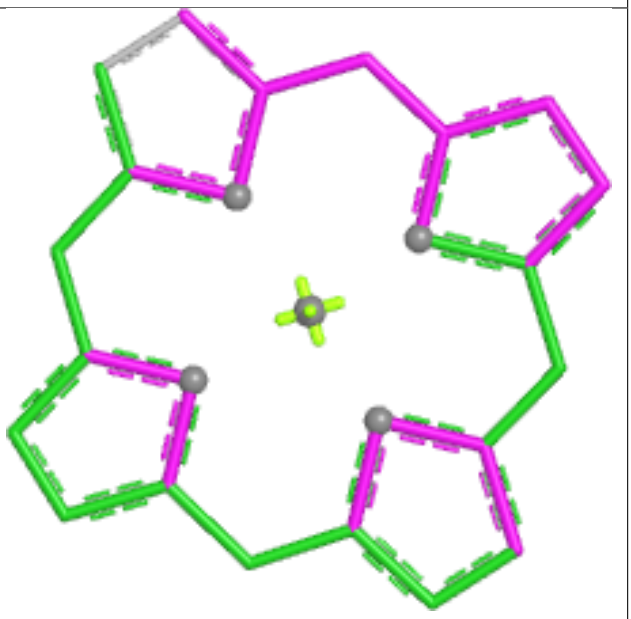


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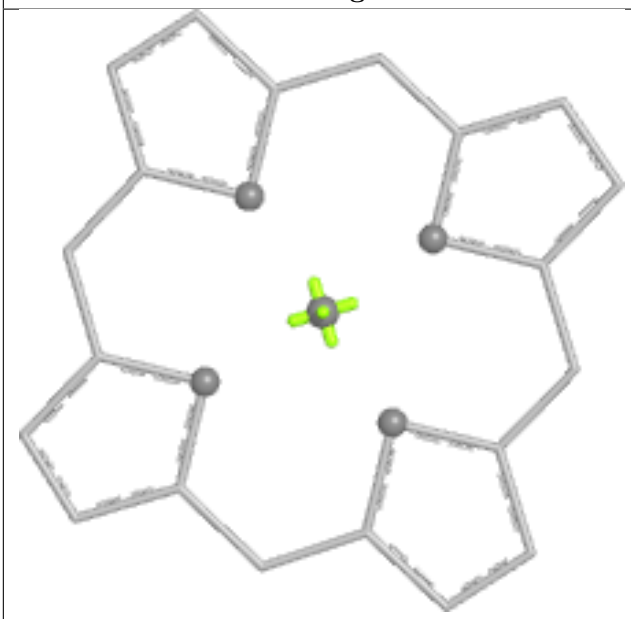
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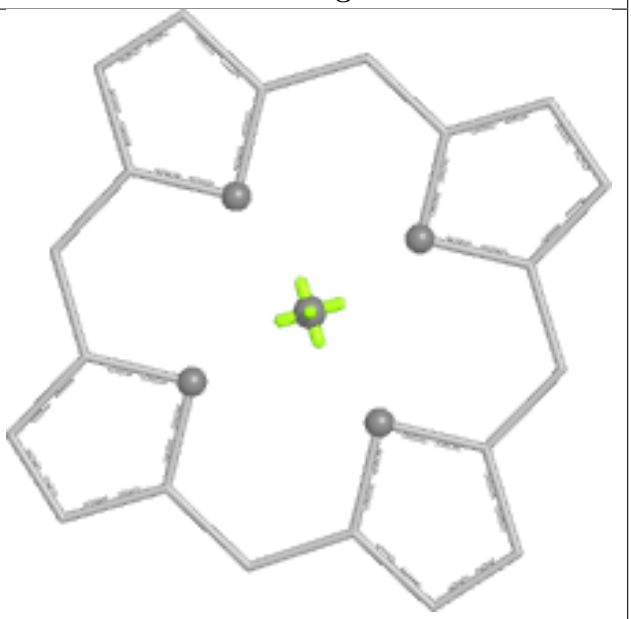
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Bond angles

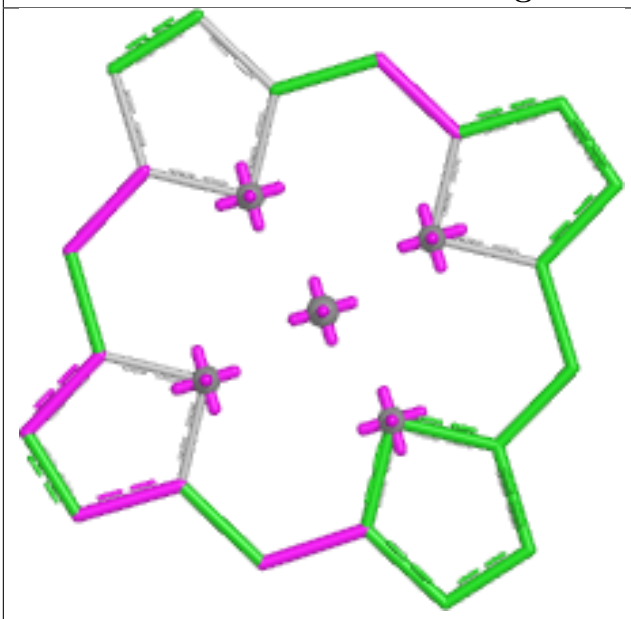


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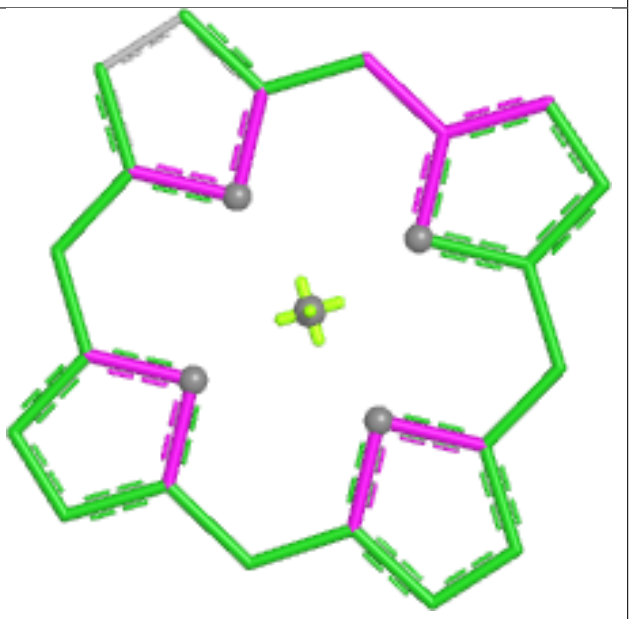


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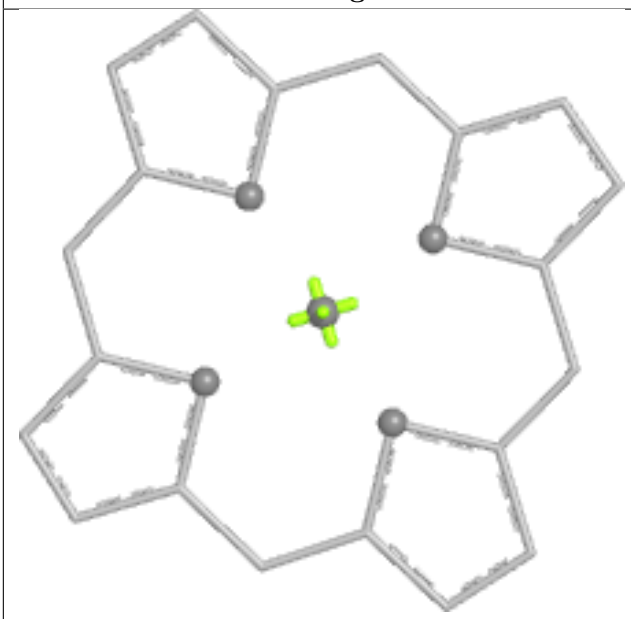
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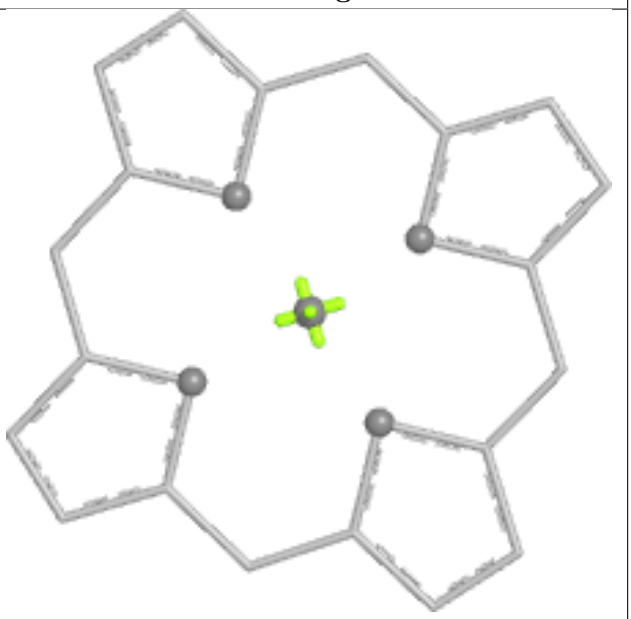
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Bond angles

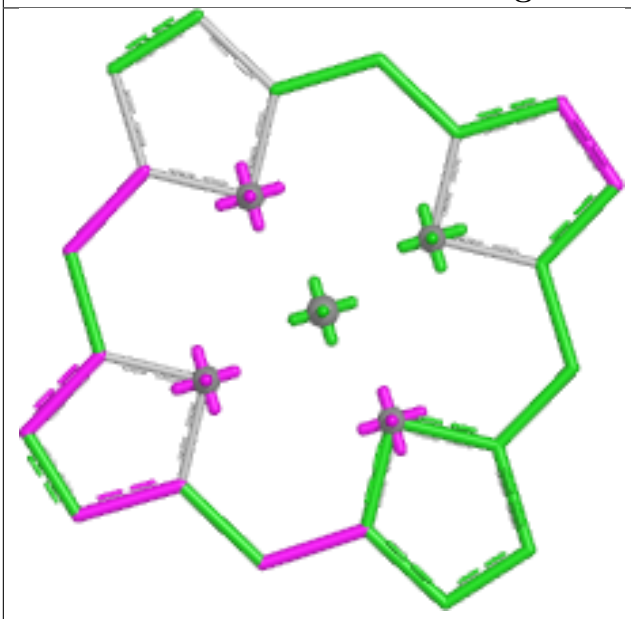


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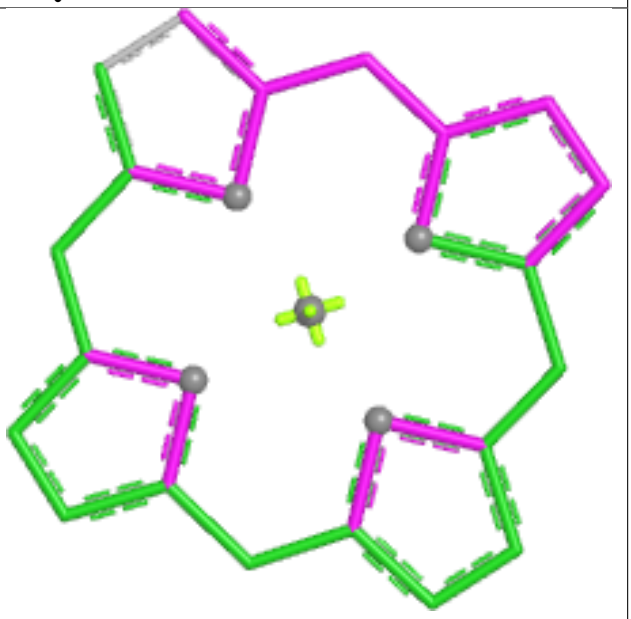


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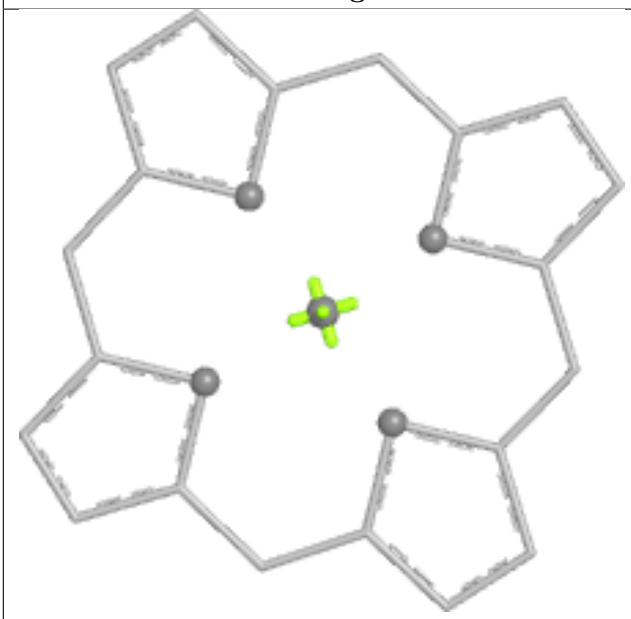
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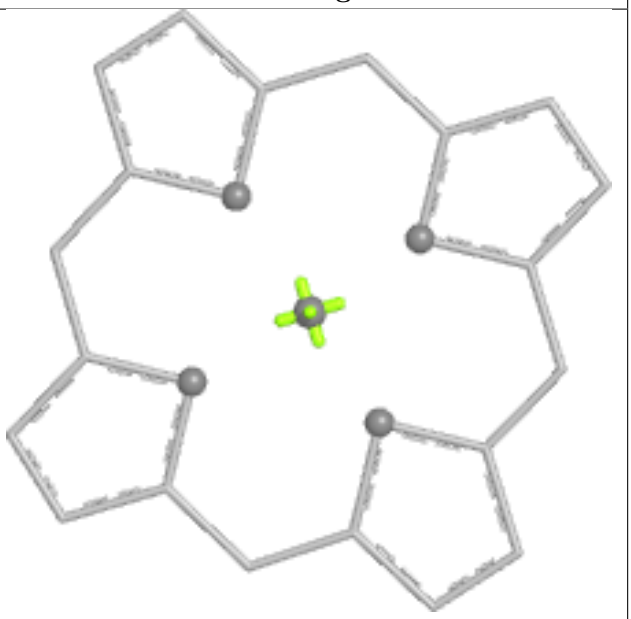
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Bond angles

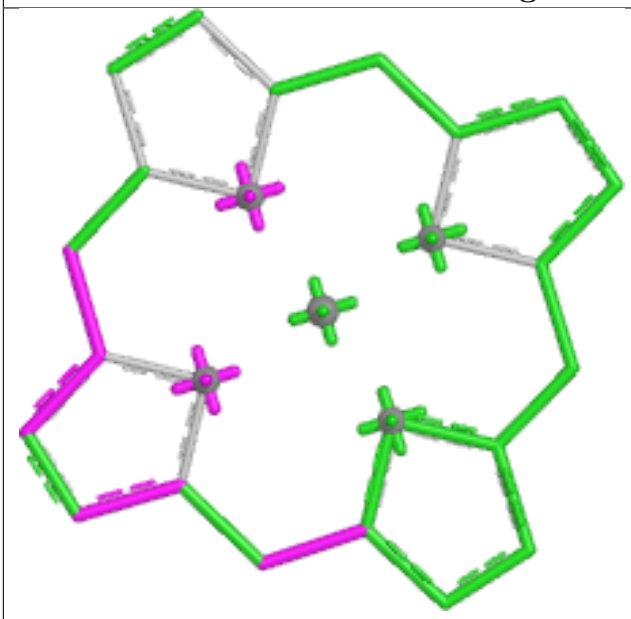


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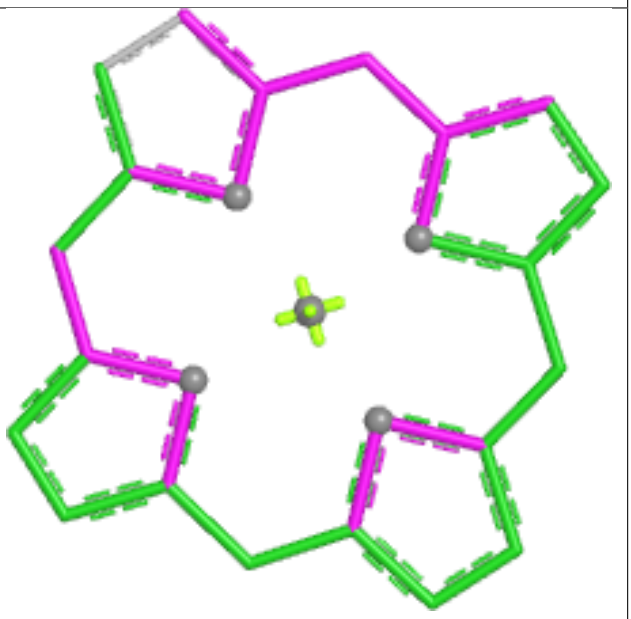


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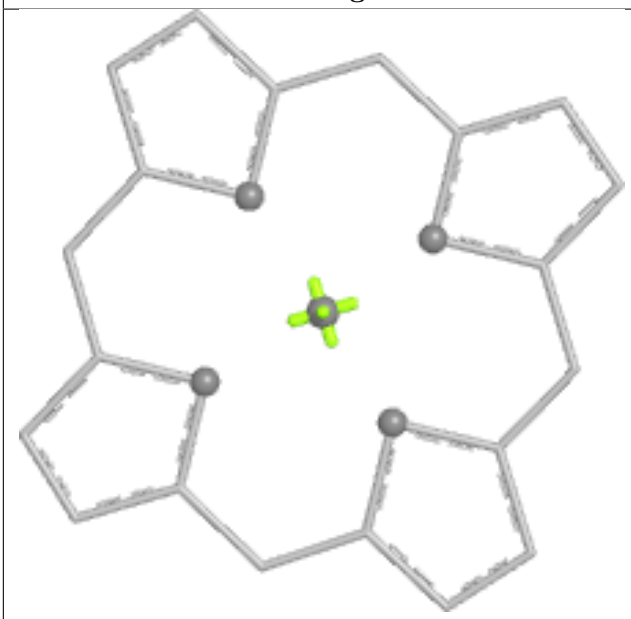
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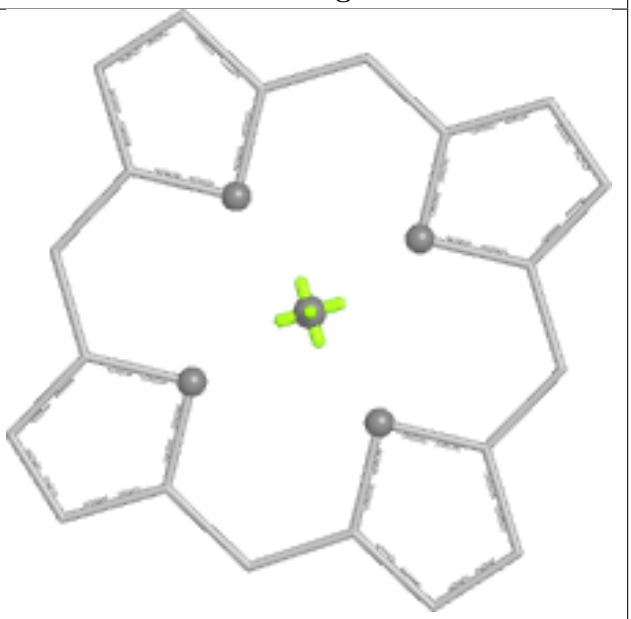
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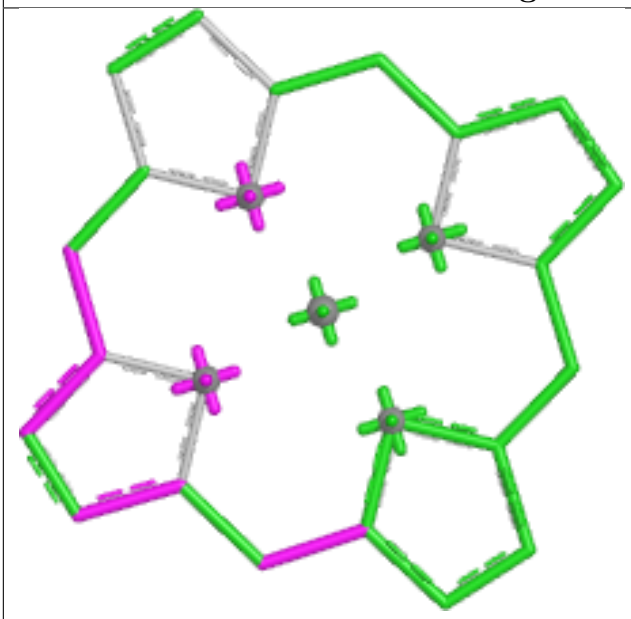


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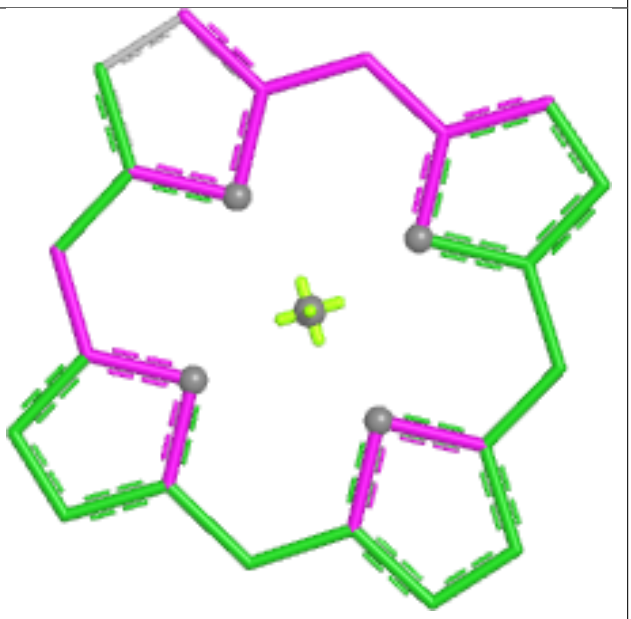


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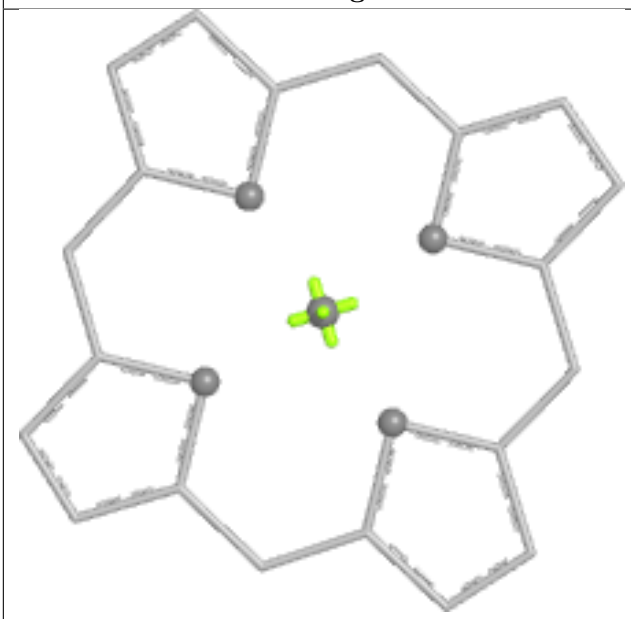
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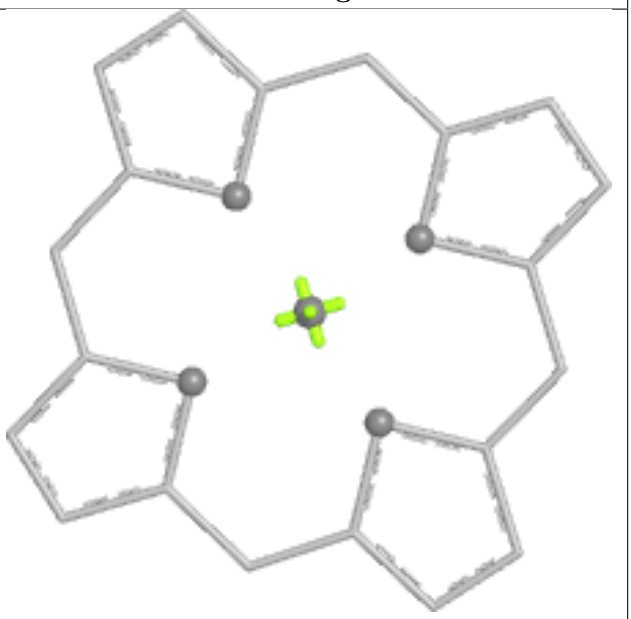
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Bond angles

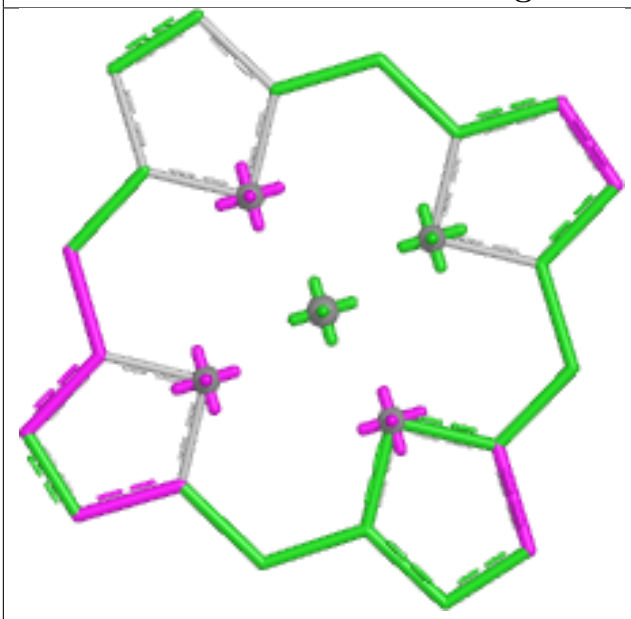


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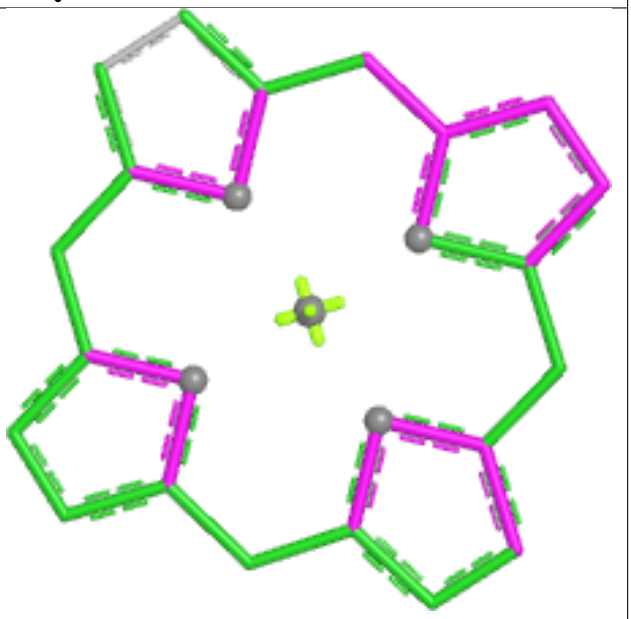


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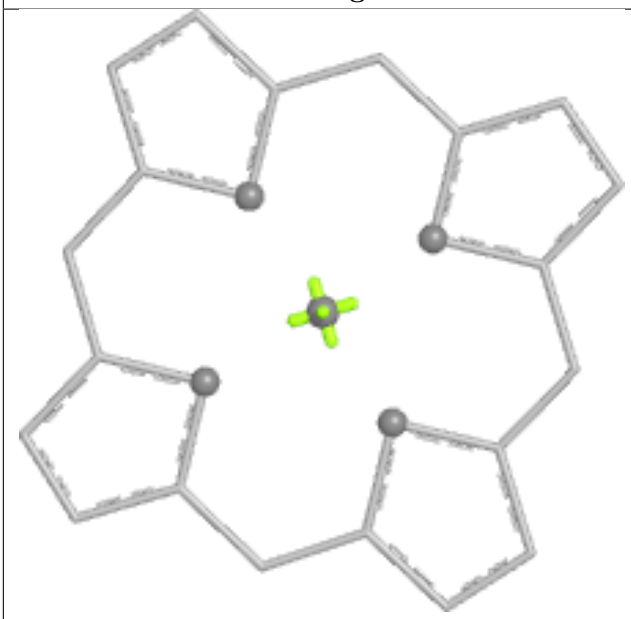
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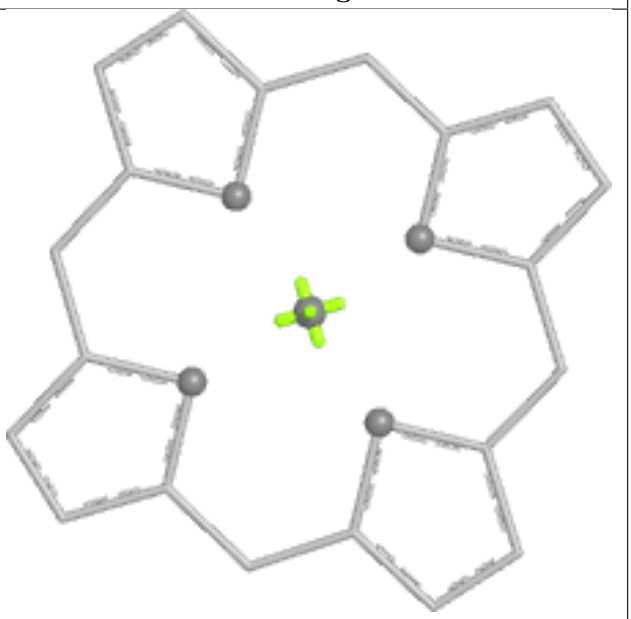
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Bond angles

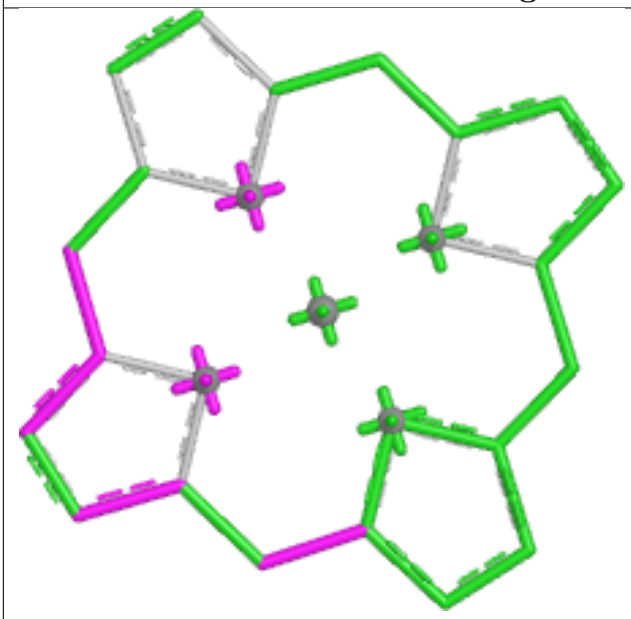


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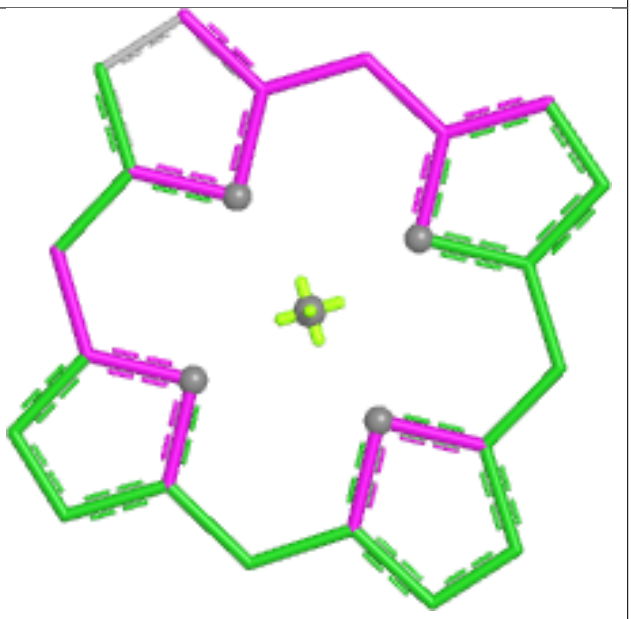


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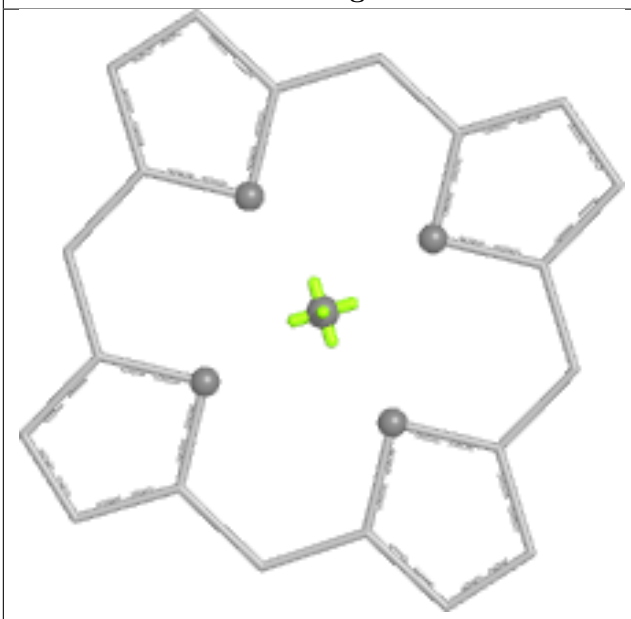
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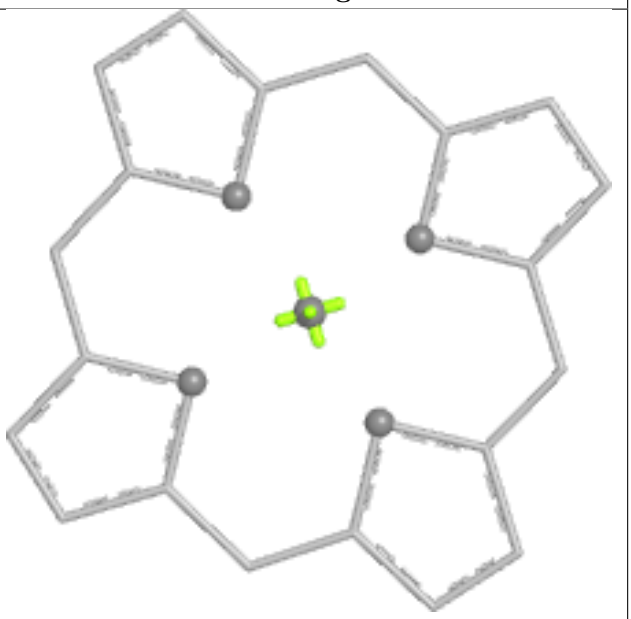
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Bond angles

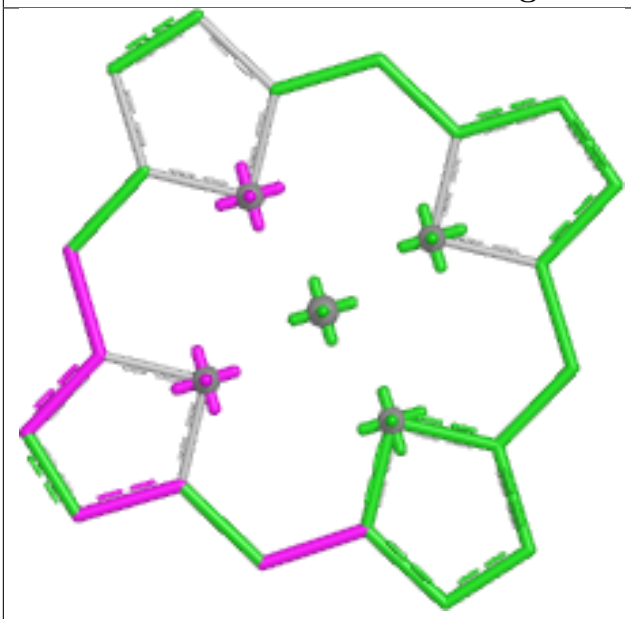


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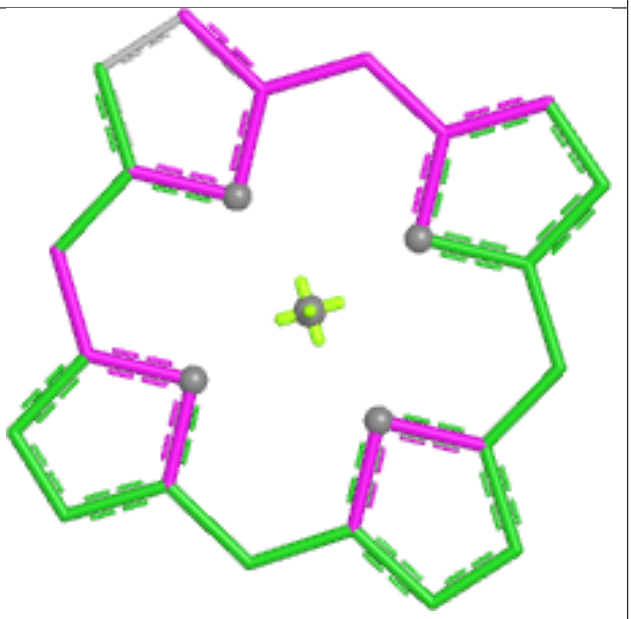


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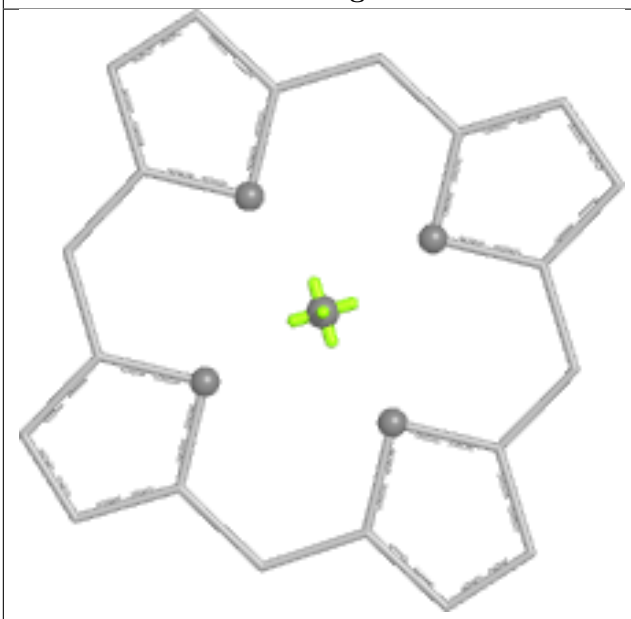
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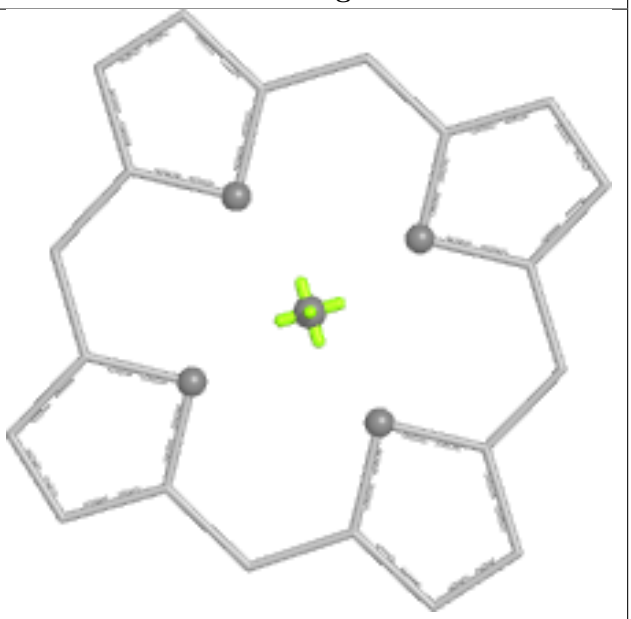
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Bond angles

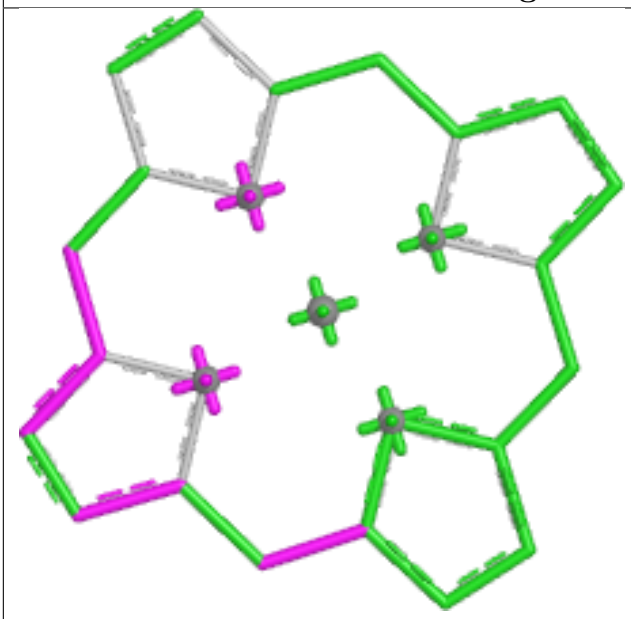


Torsions

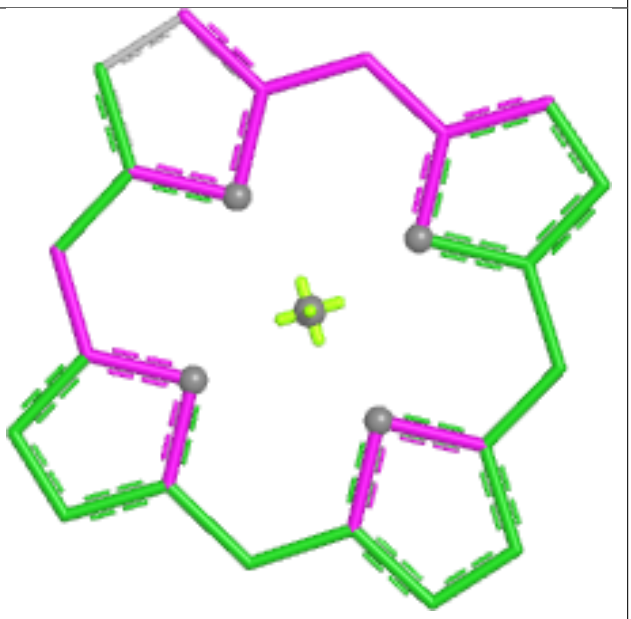


Rings

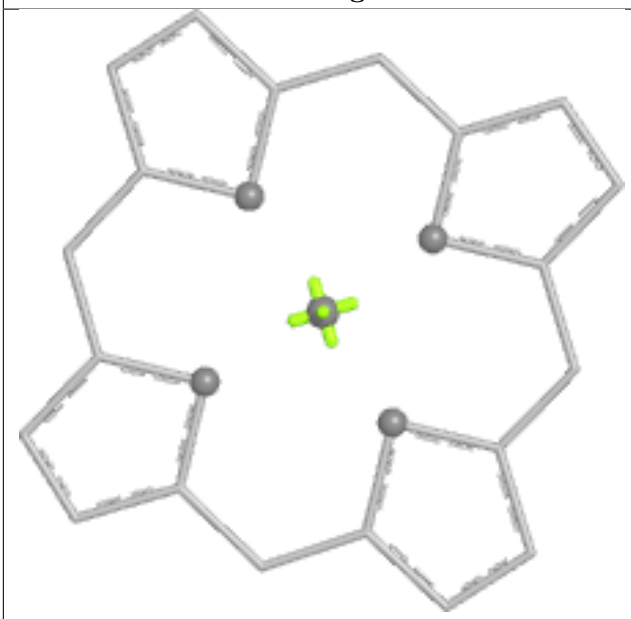
Ligand CLA 5 5404



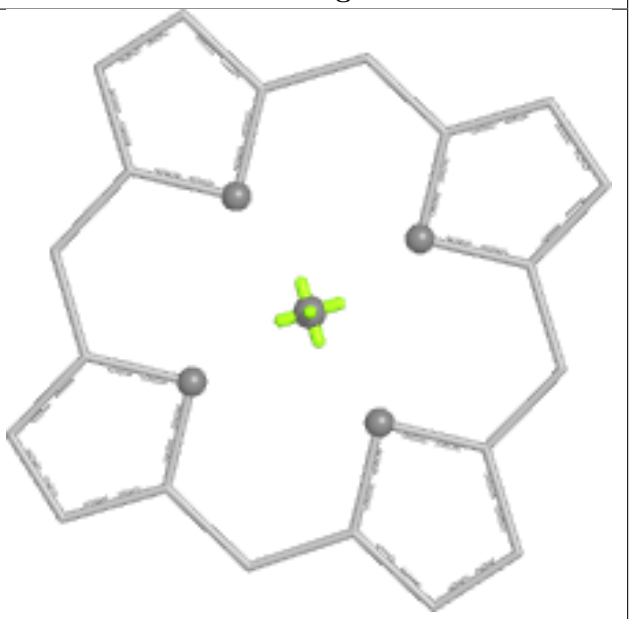
Bond lengths



Bond angles

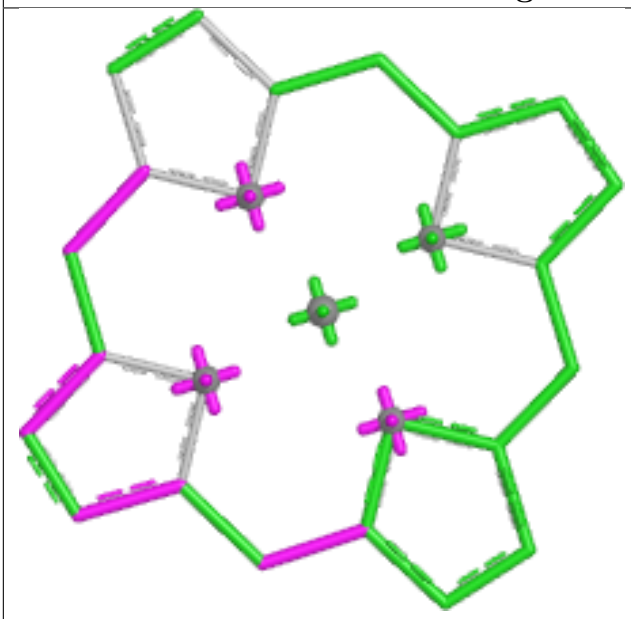


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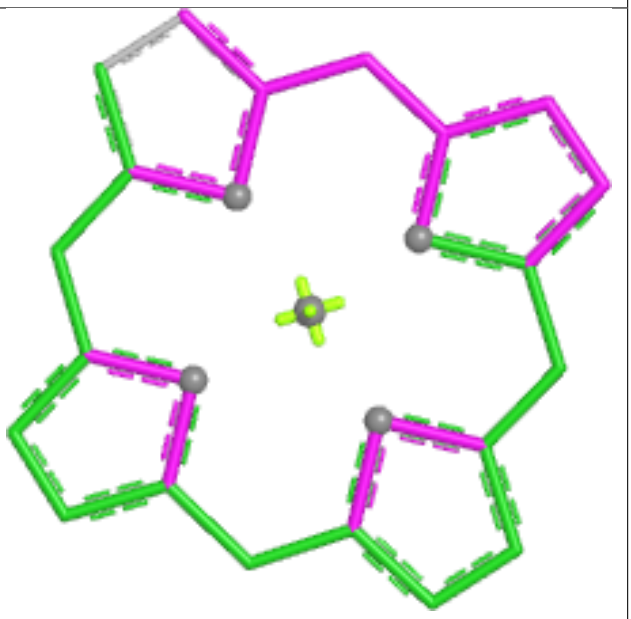


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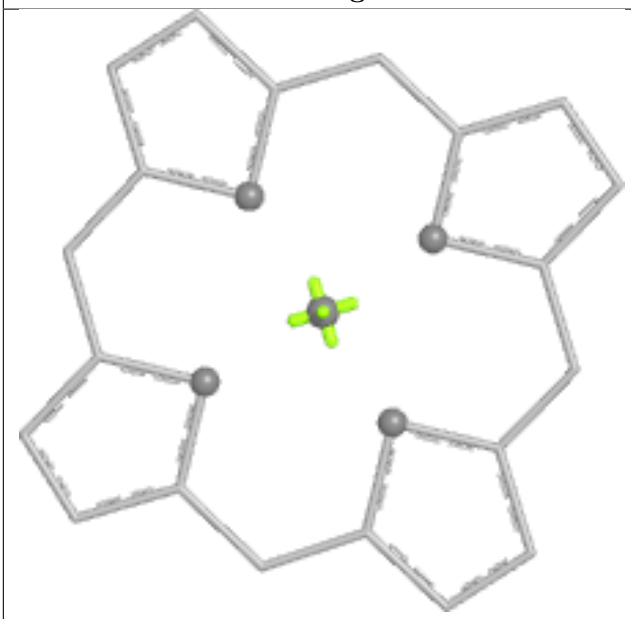
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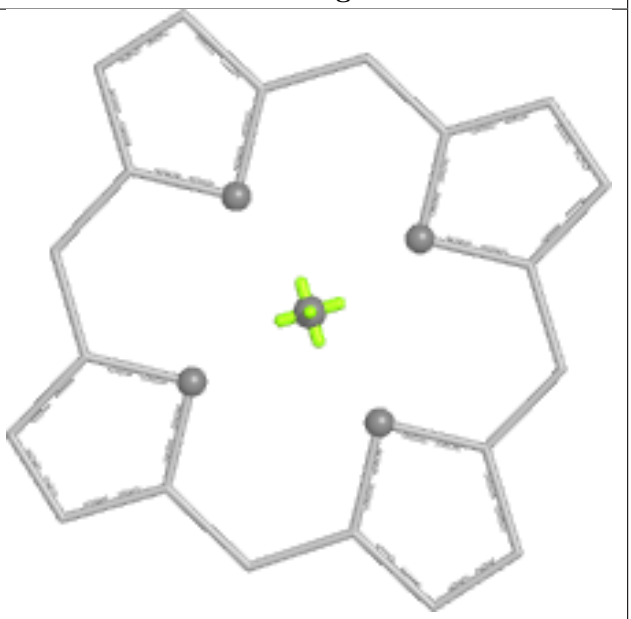
Bond lengths



Bond angles

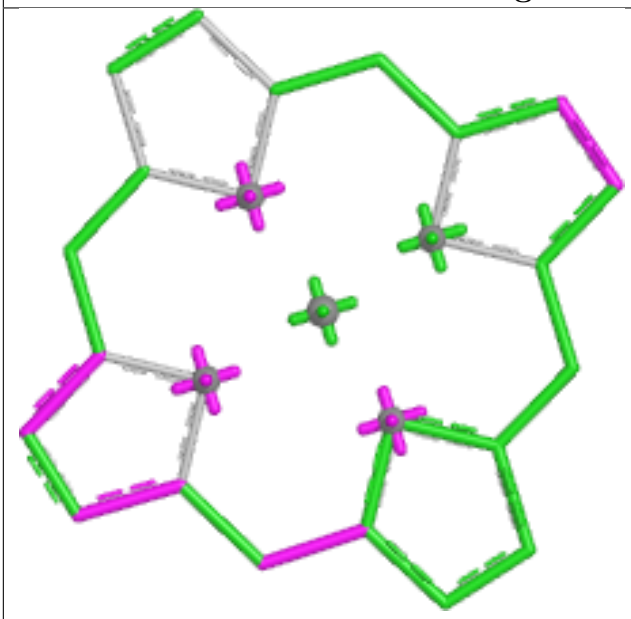


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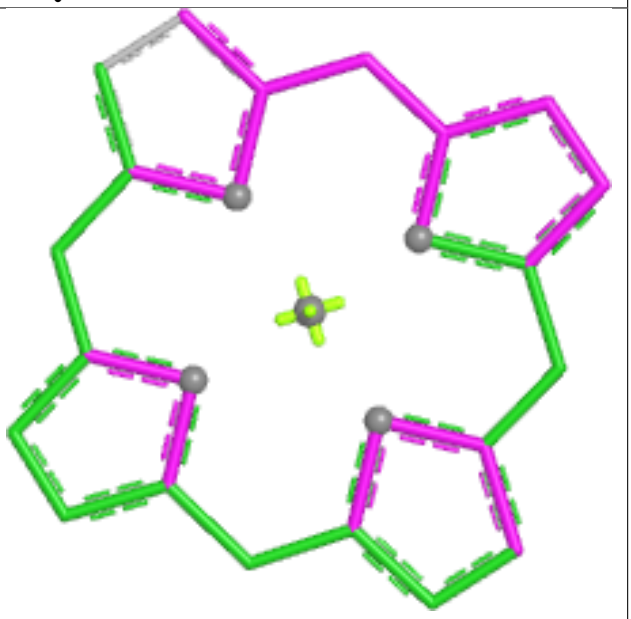


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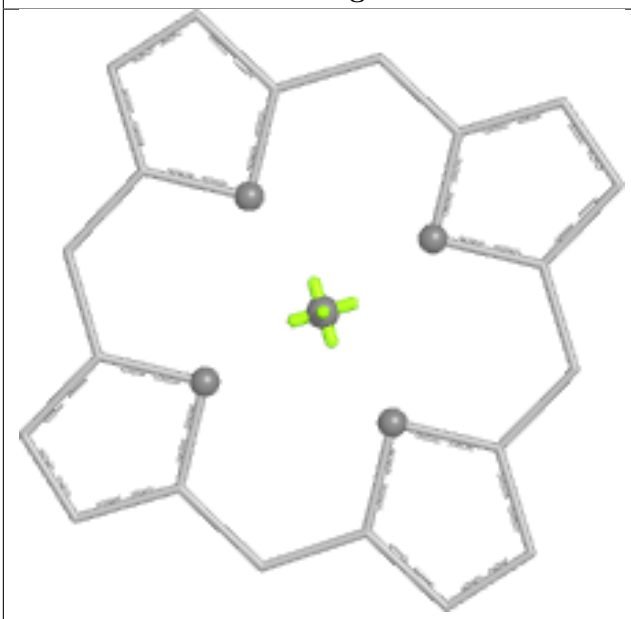
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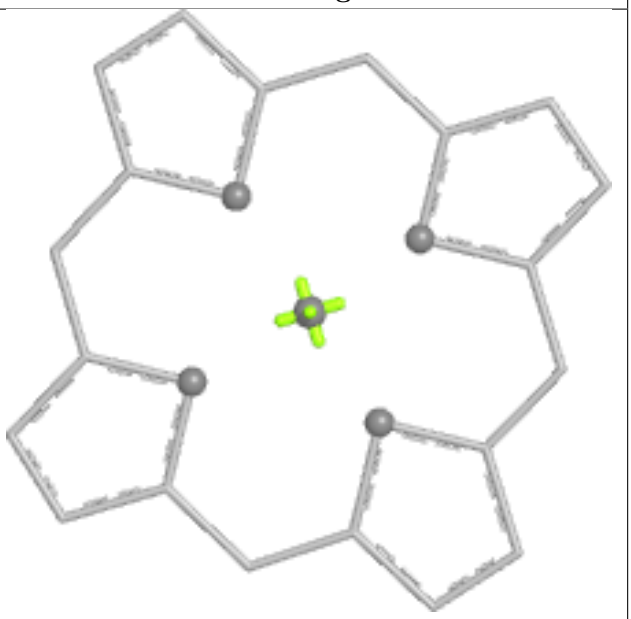
Bond lengths



Bond angles

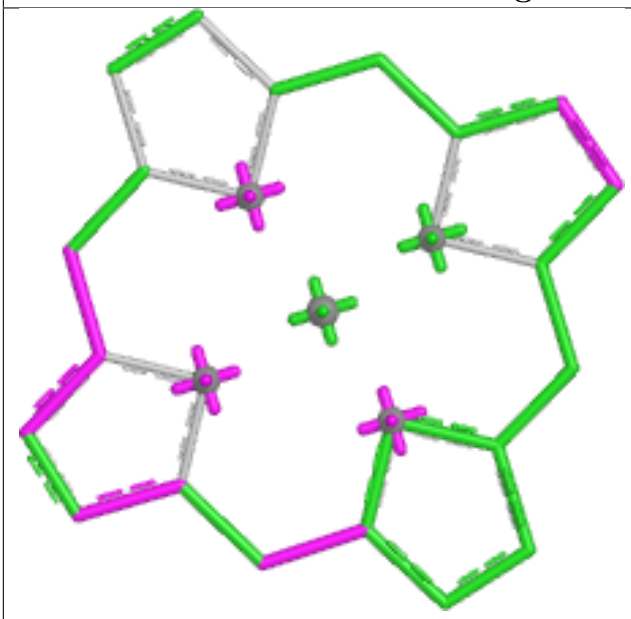


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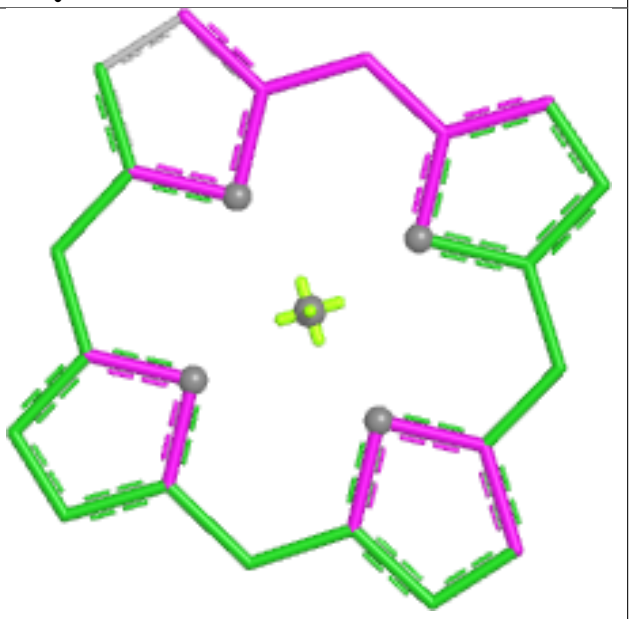


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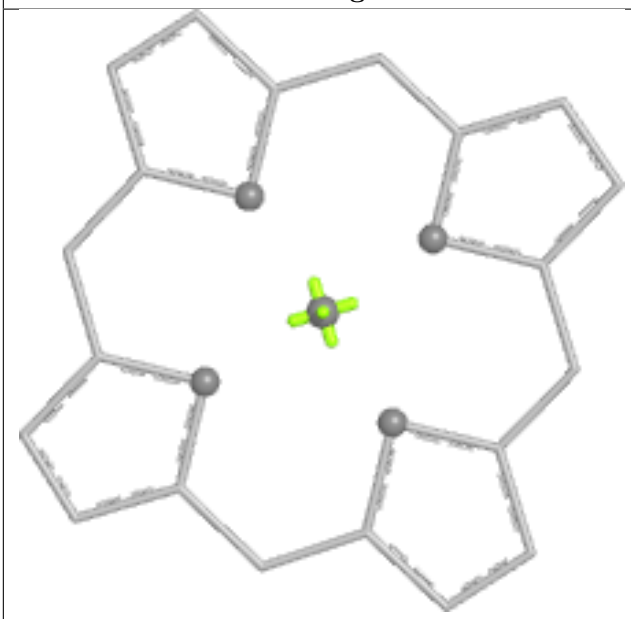
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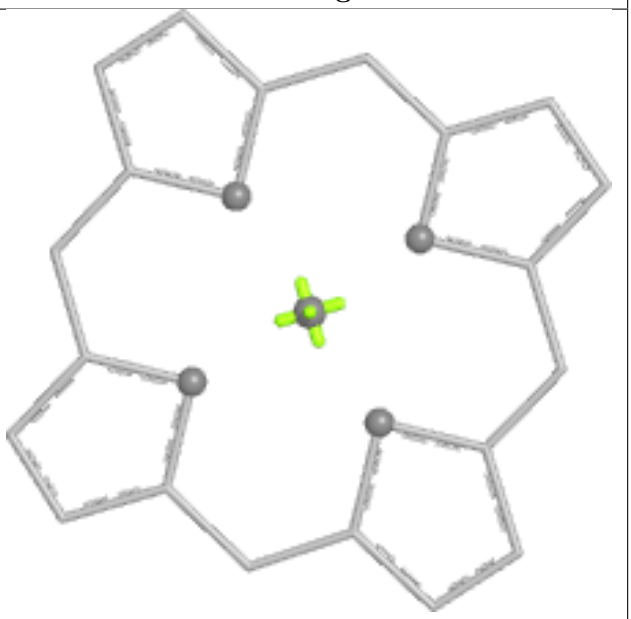
Bond lengths



Bond angles

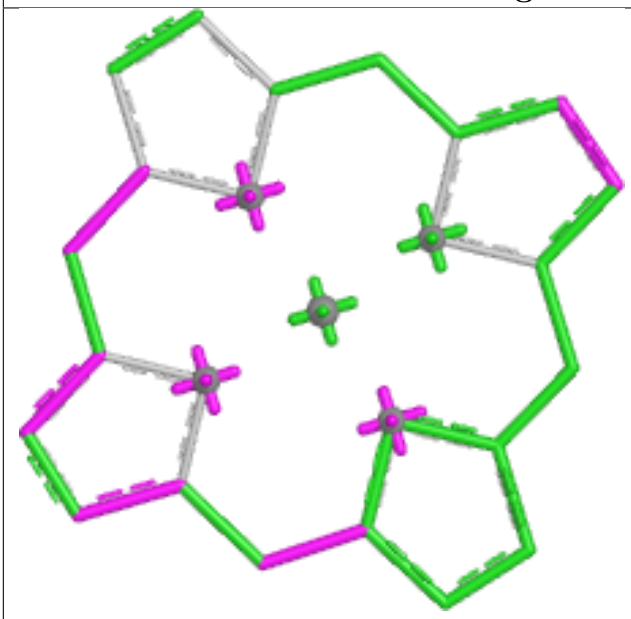


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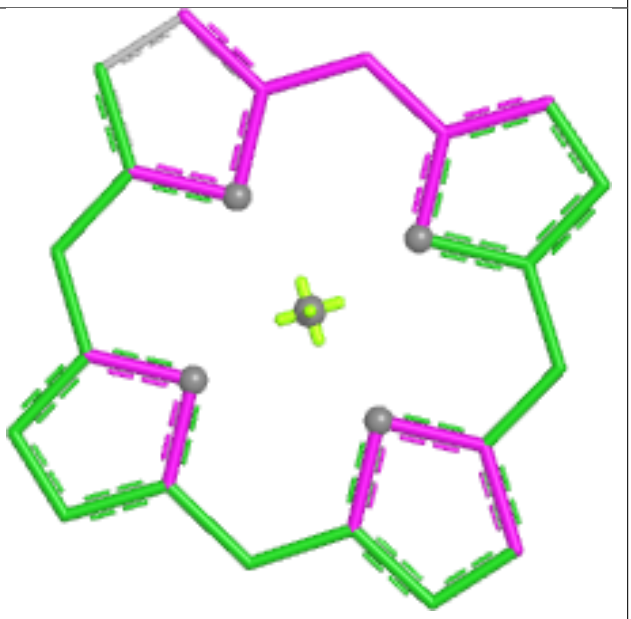


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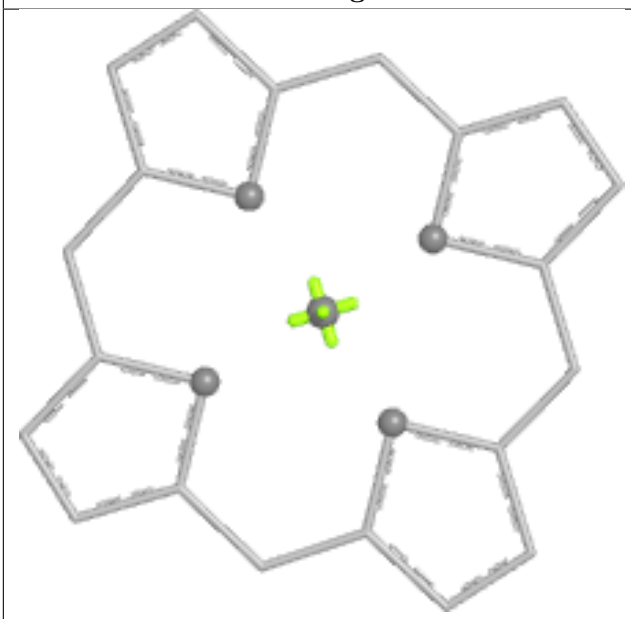
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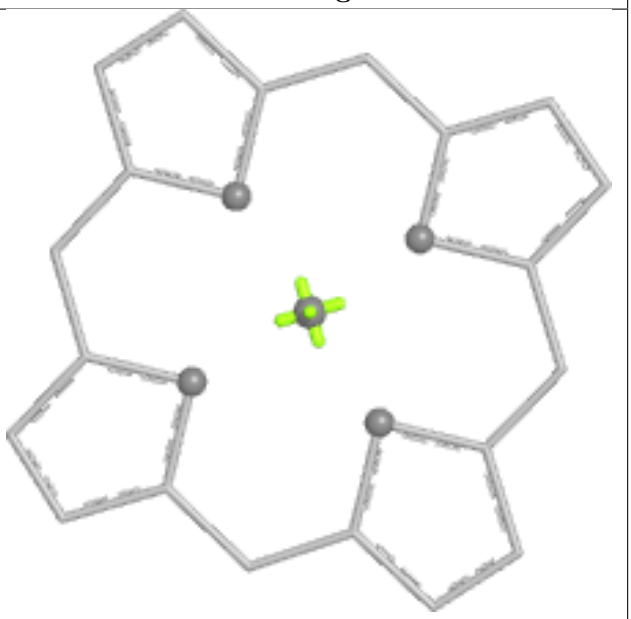
Bond lengths



Bond angles

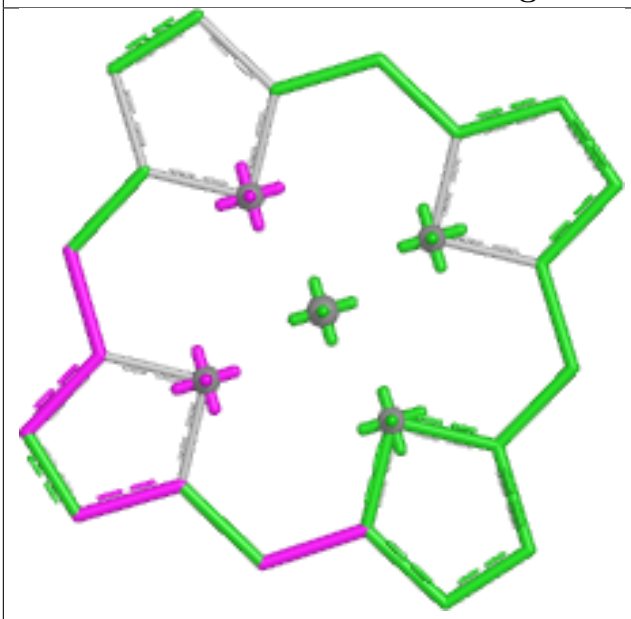


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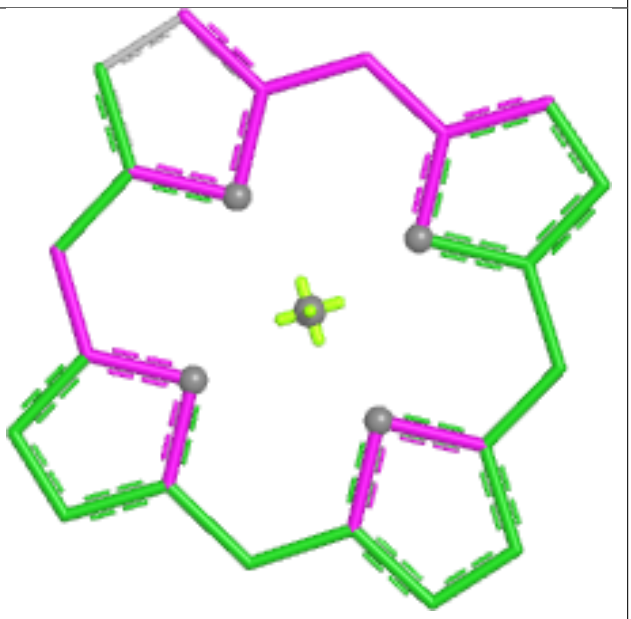


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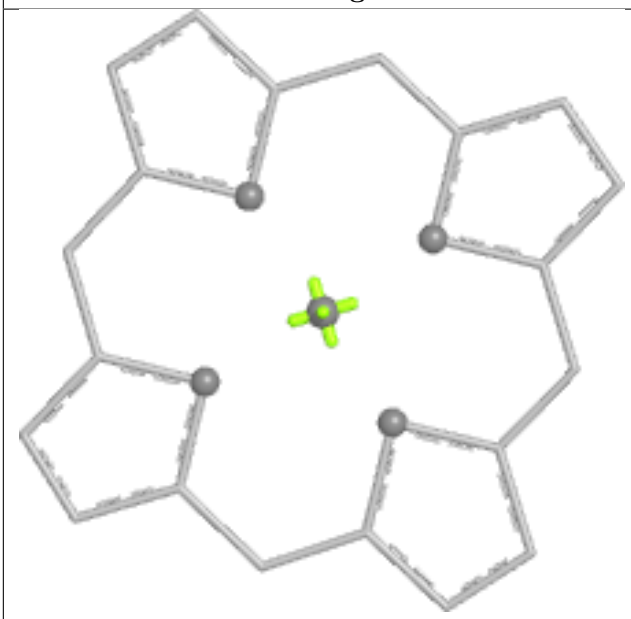
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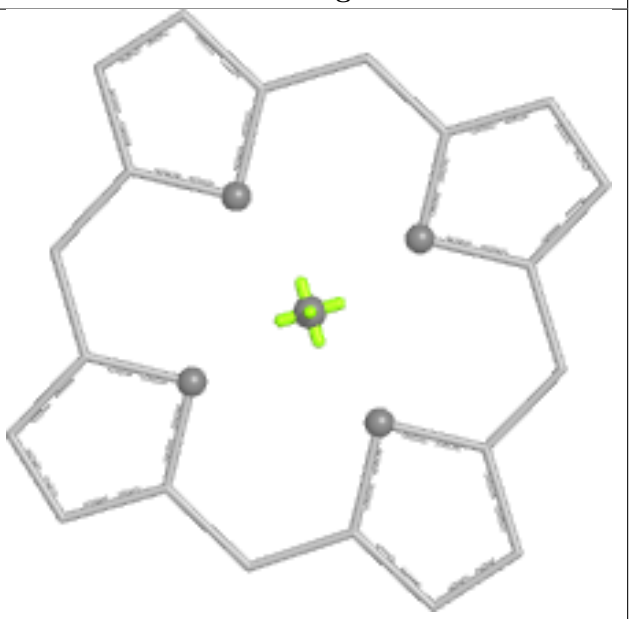
Bond lengths



Bond angles

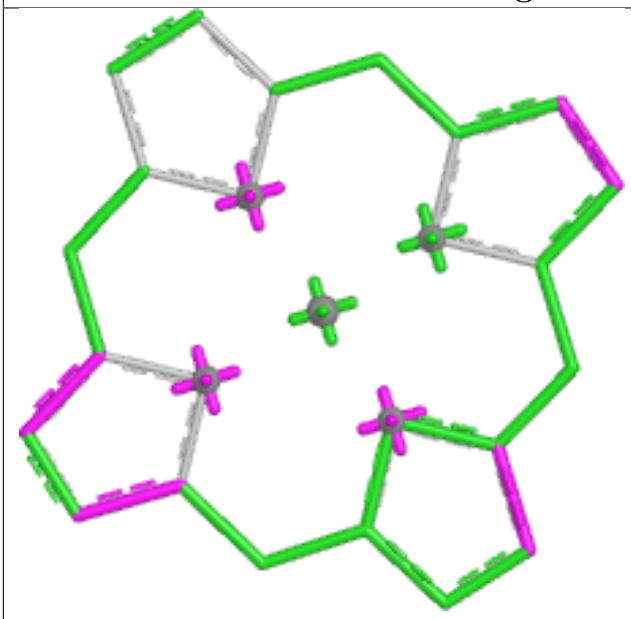


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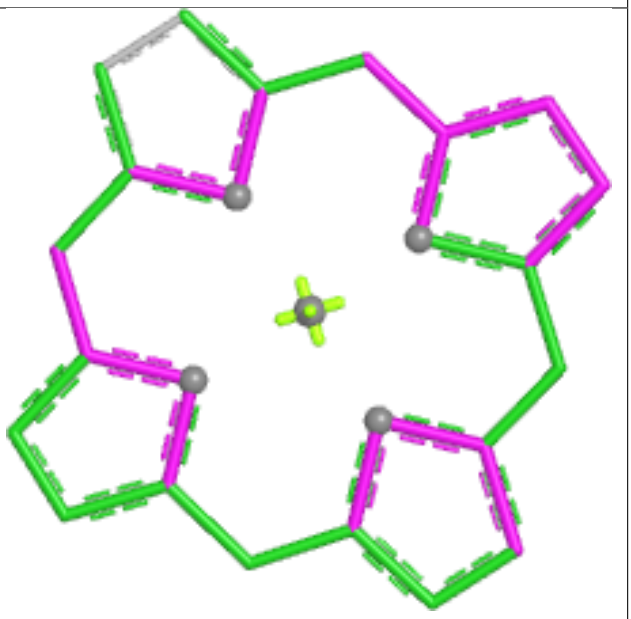


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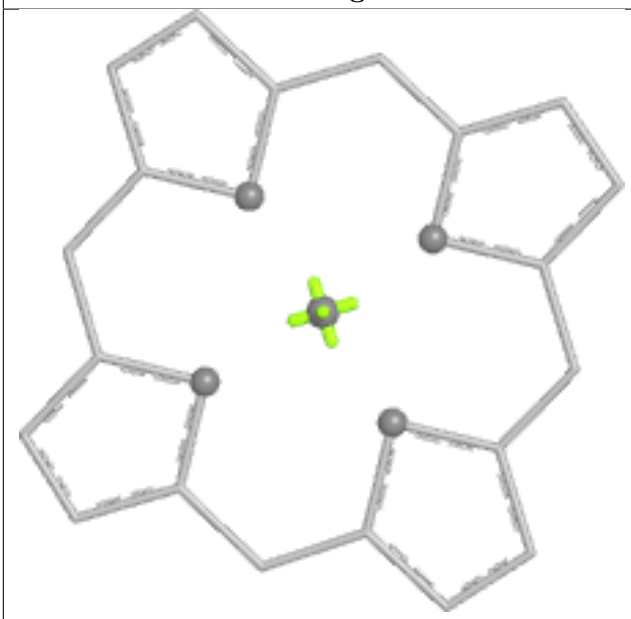
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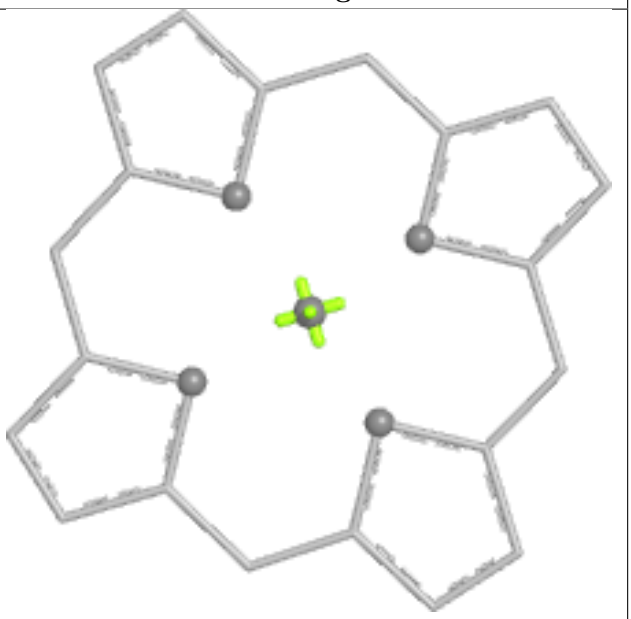
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Bond angles

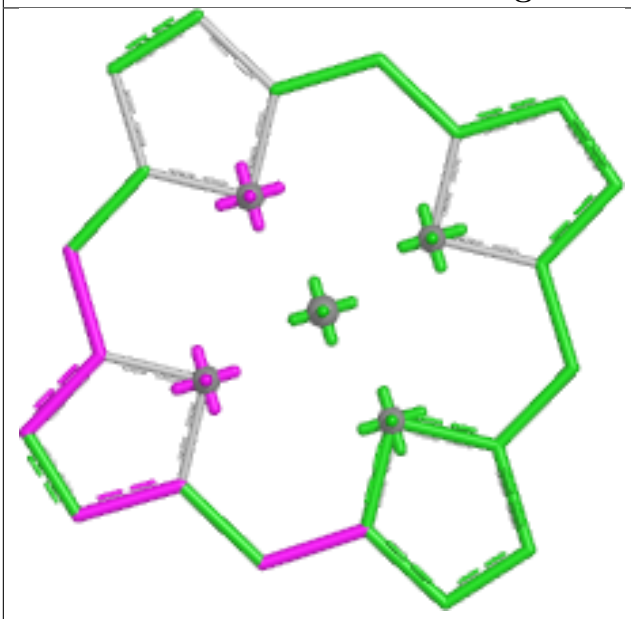


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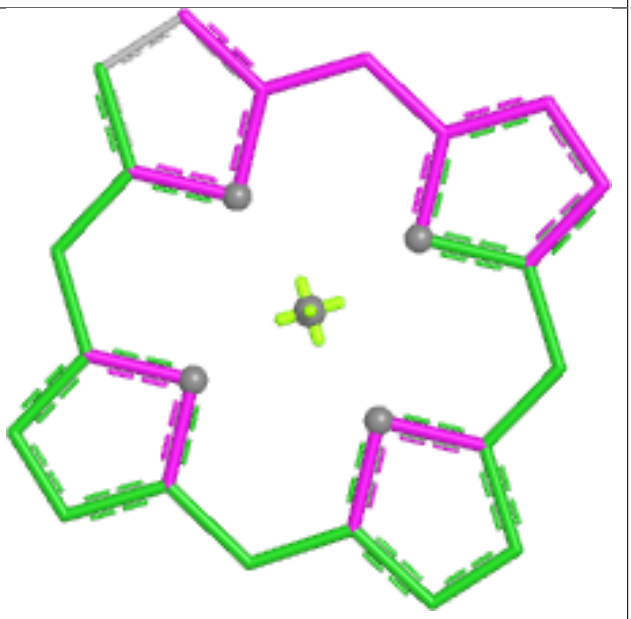


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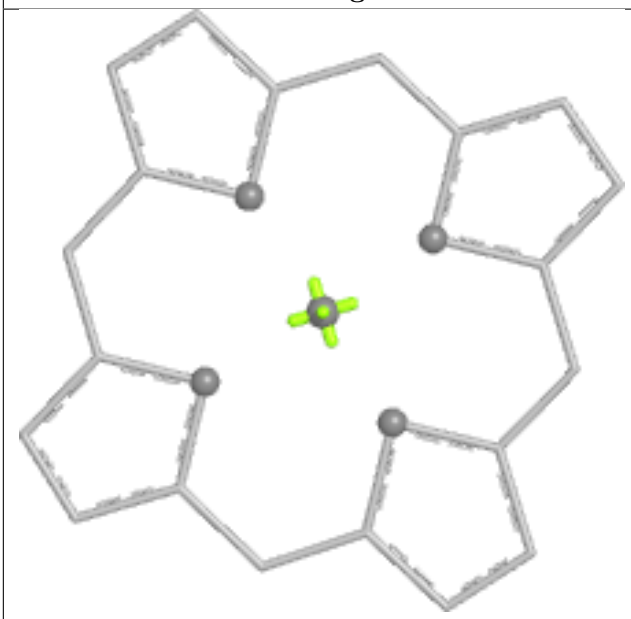
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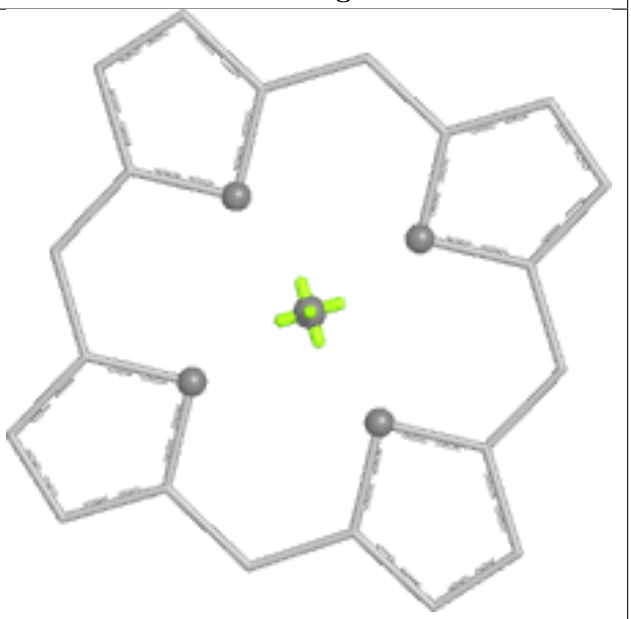
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Bond angles

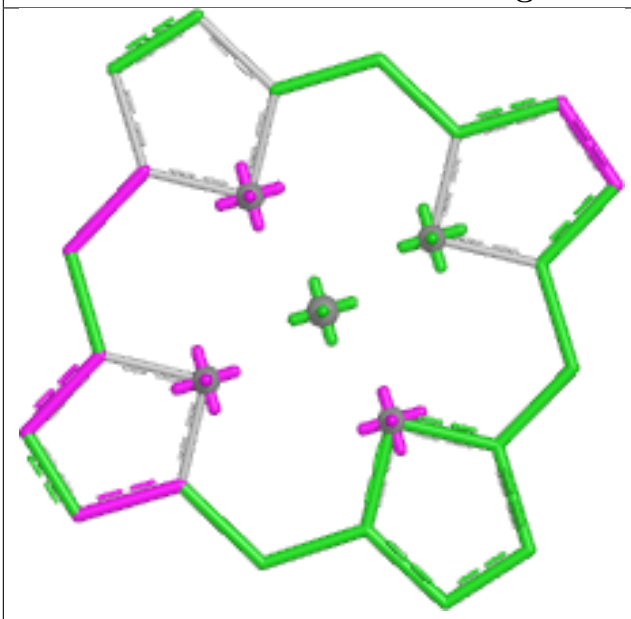


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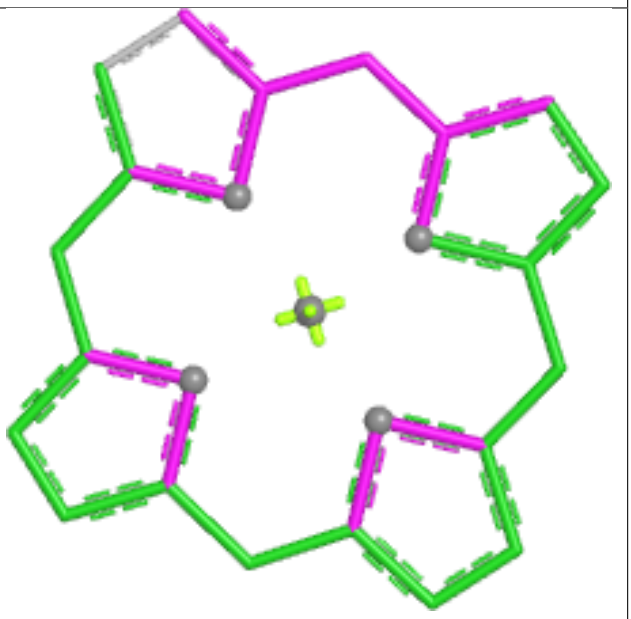


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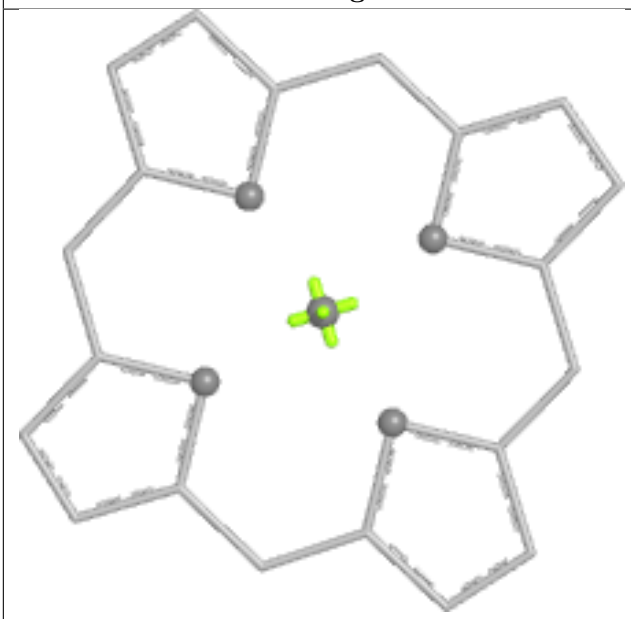
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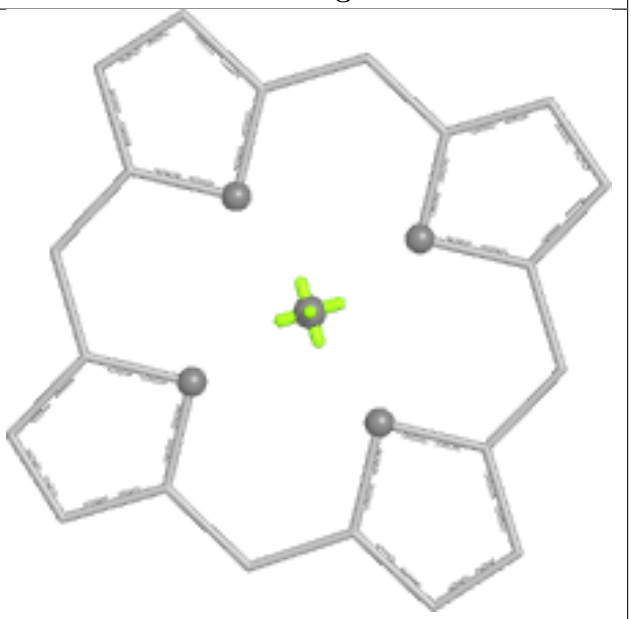
Bond lengths



Bond angles

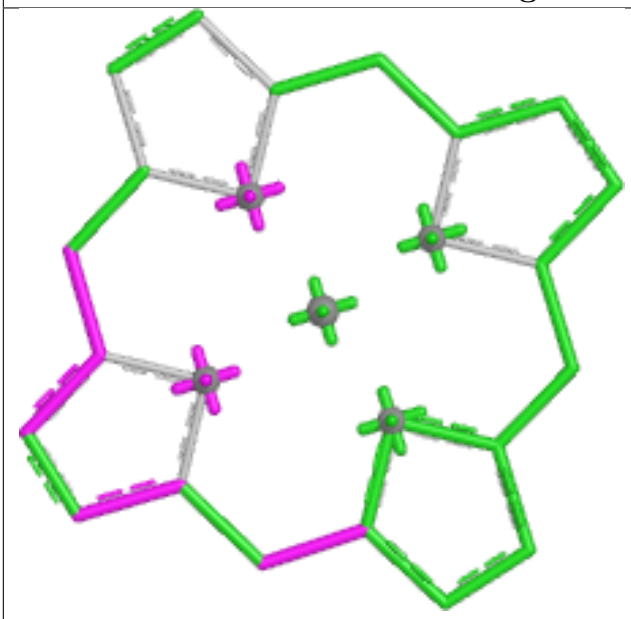


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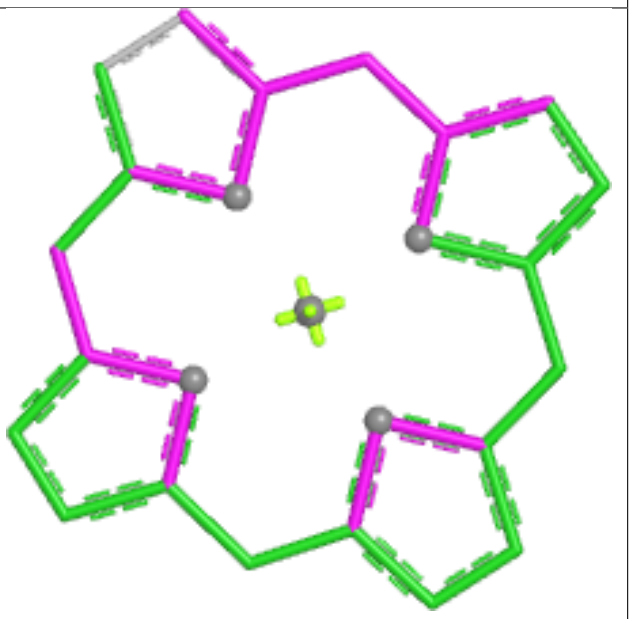


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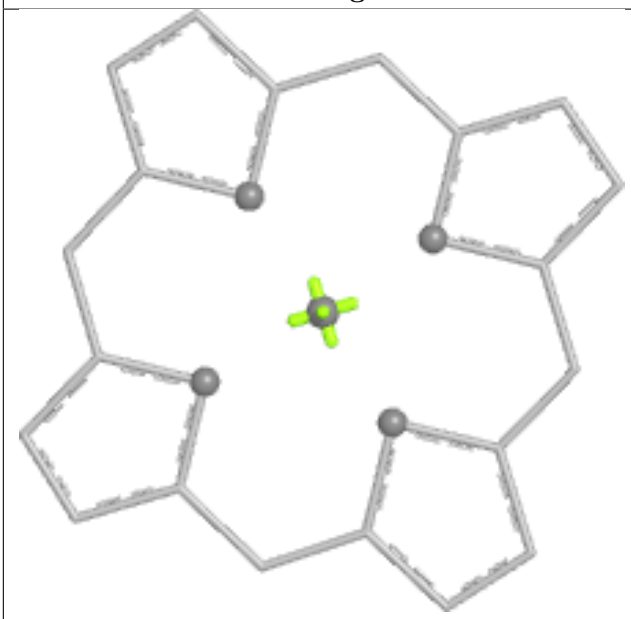
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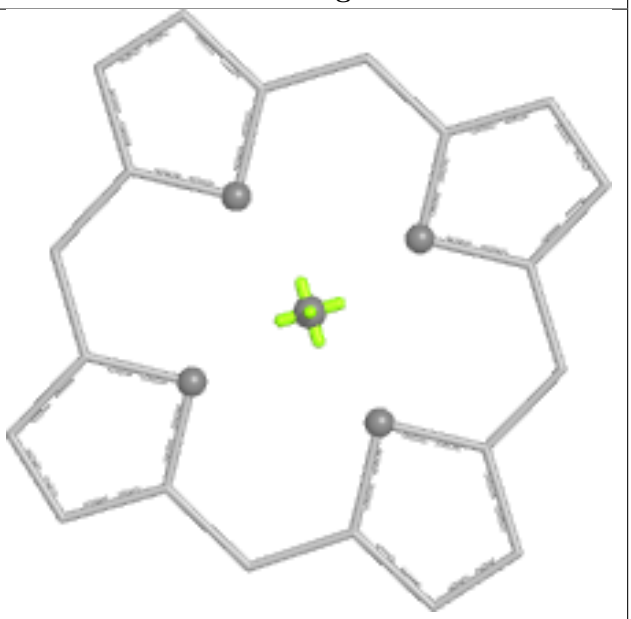
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Bond angles

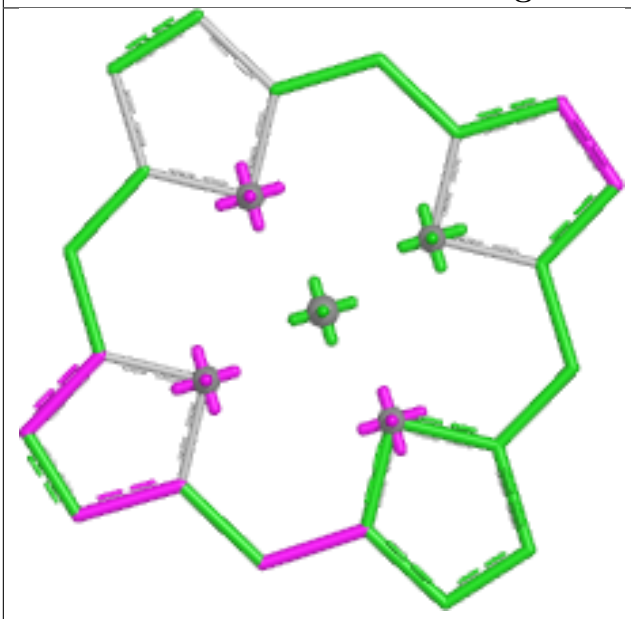


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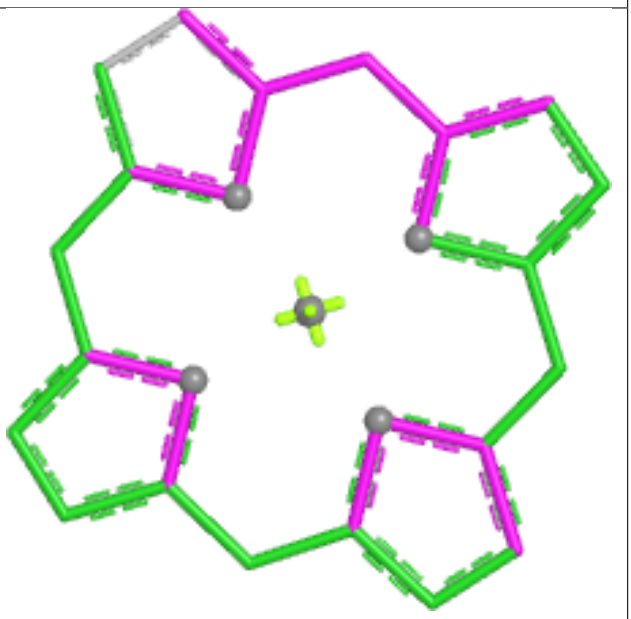


Rings

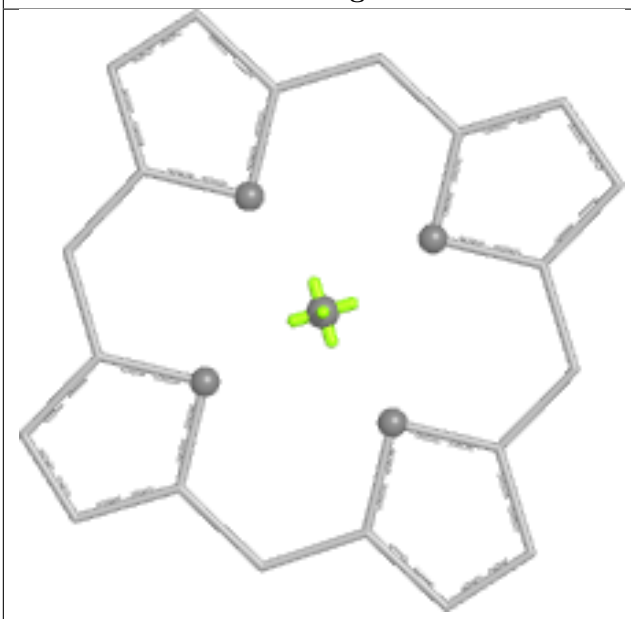
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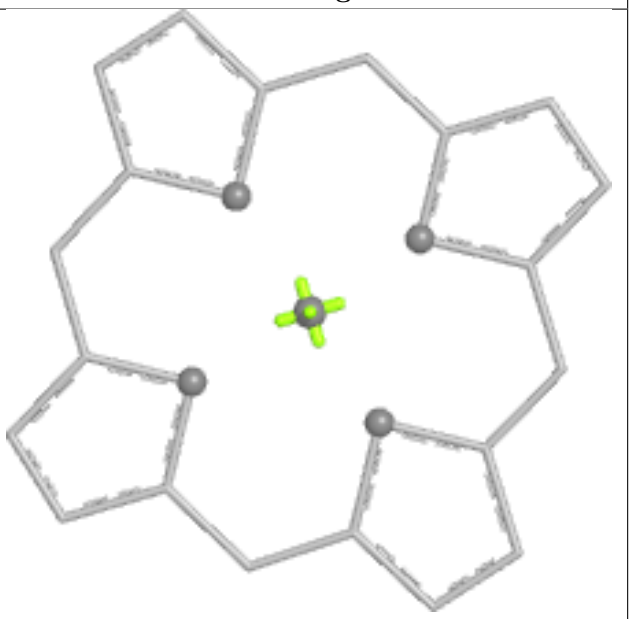
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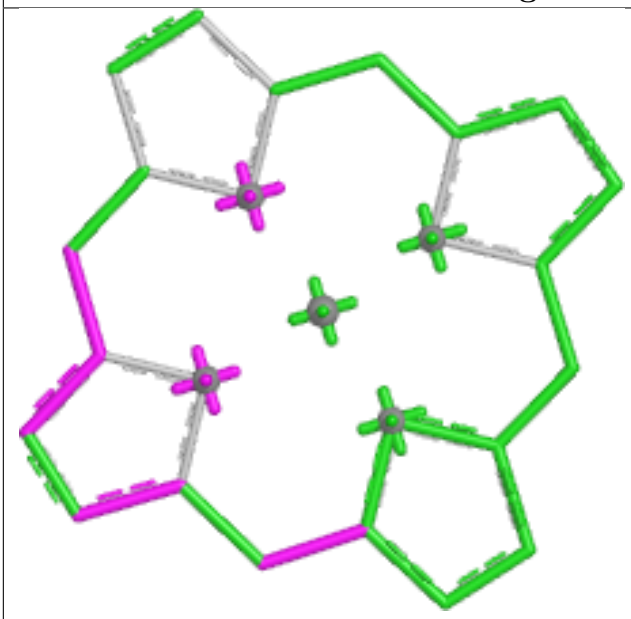


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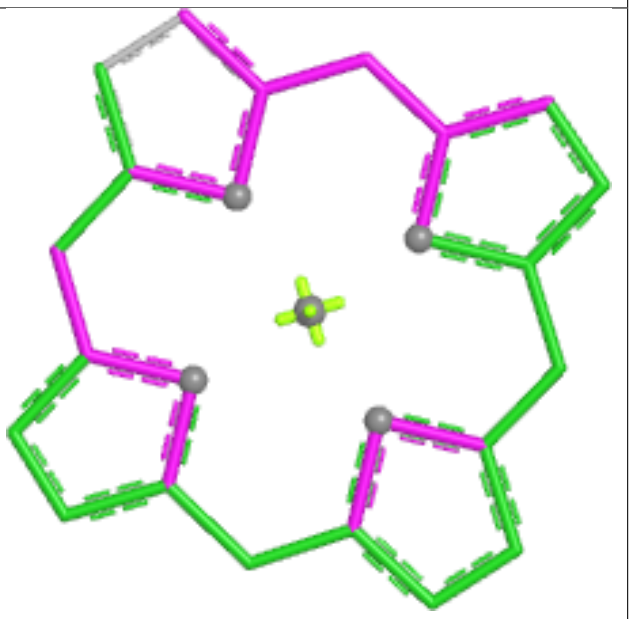


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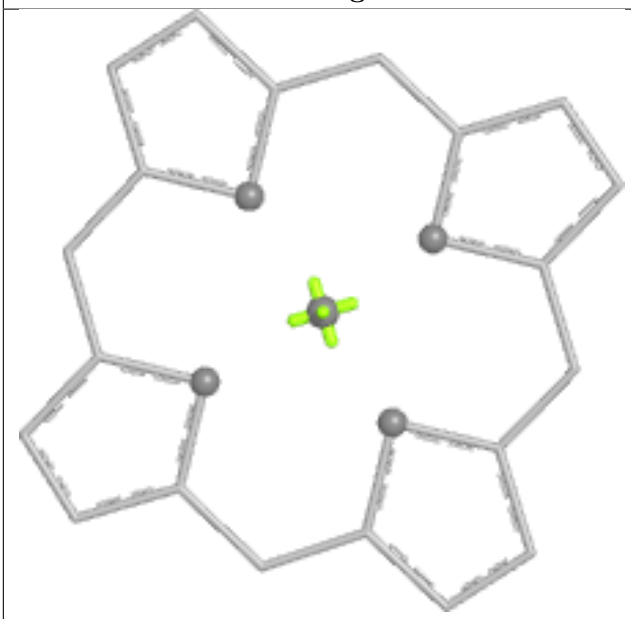
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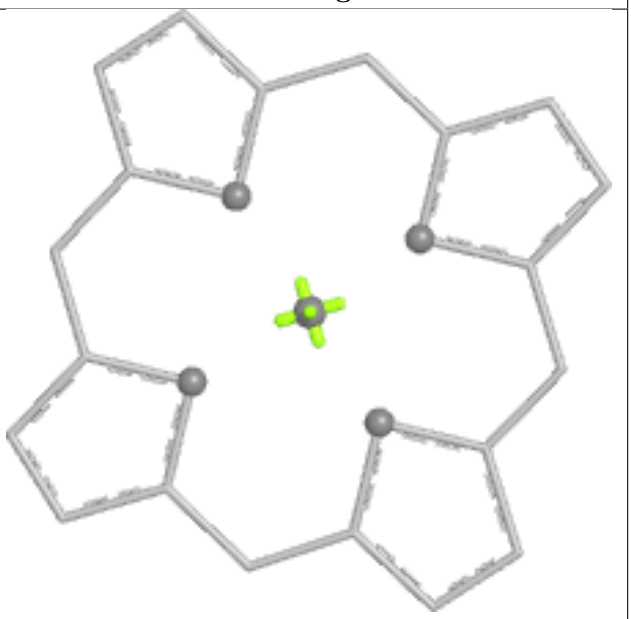
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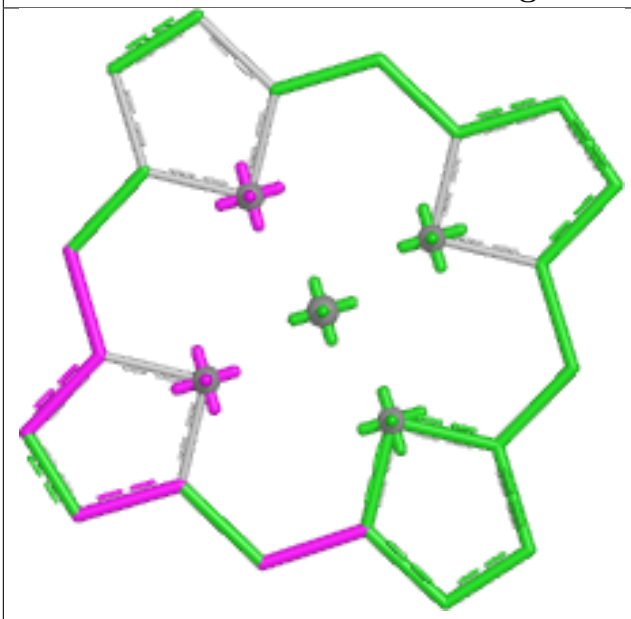


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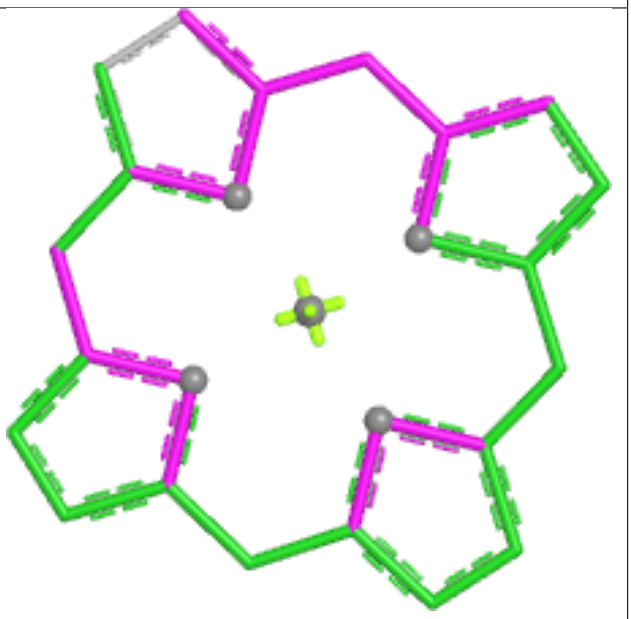


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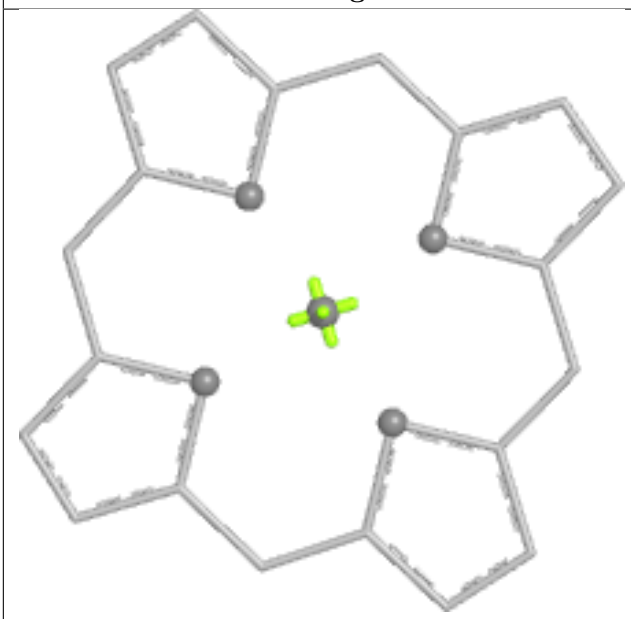
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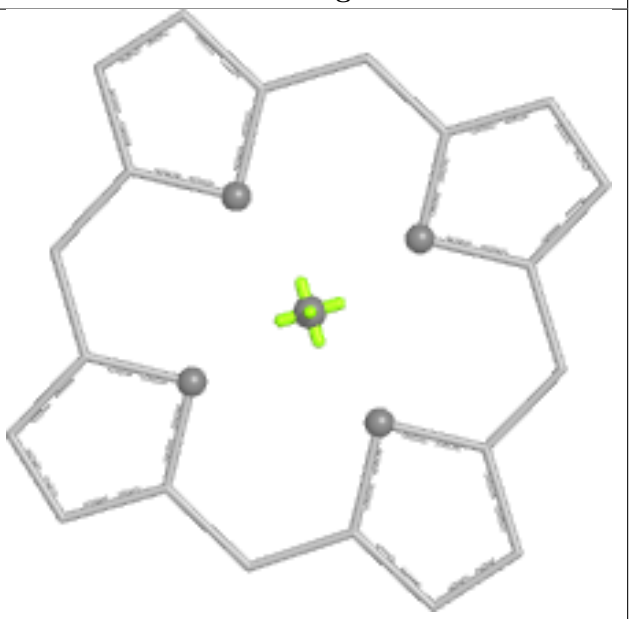
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Bond angles

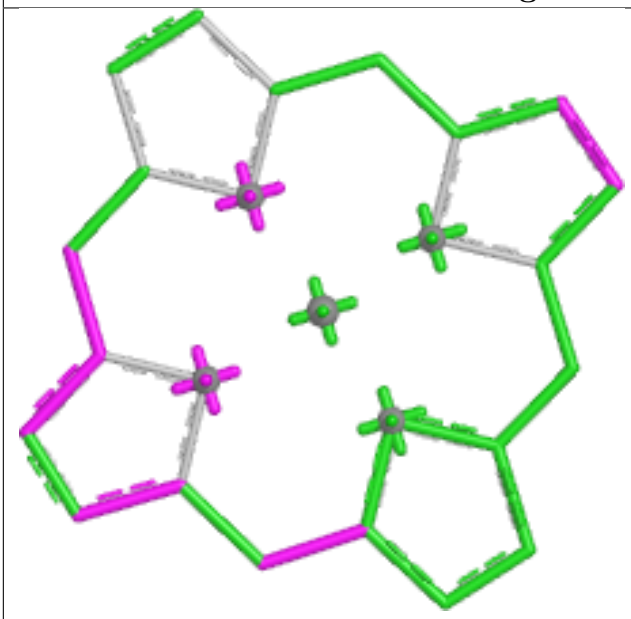


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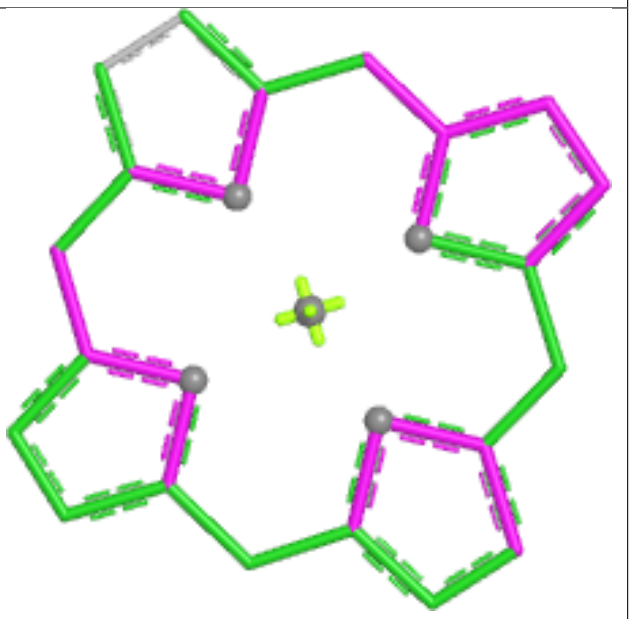


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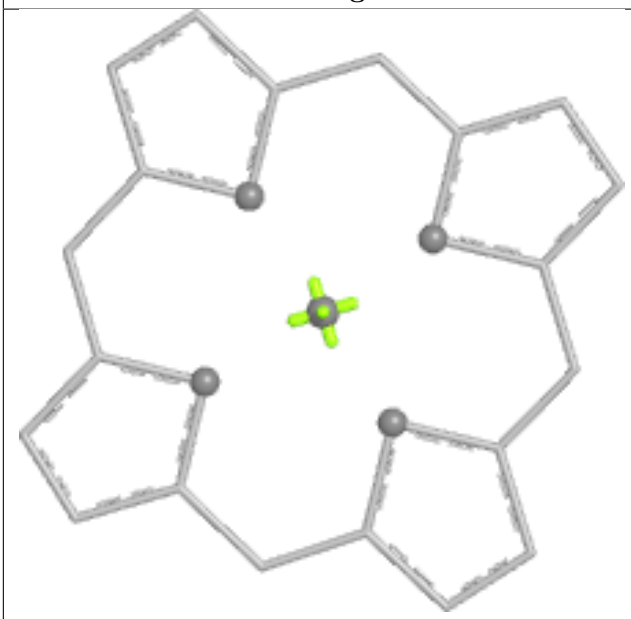
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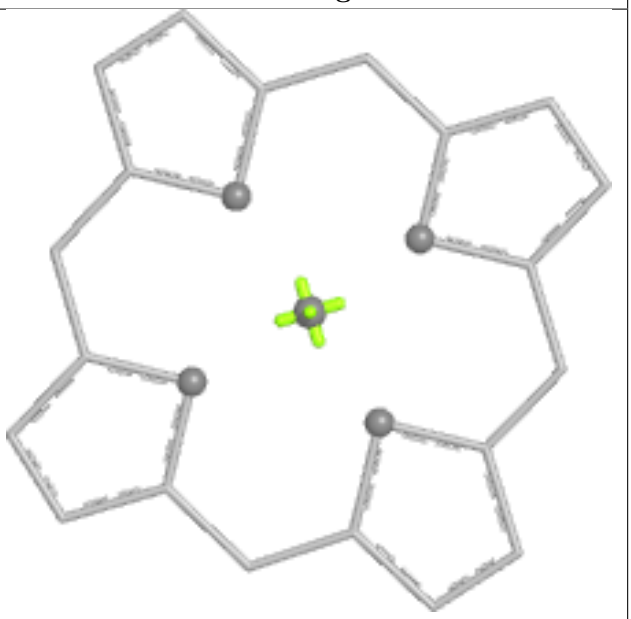
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Bond angles

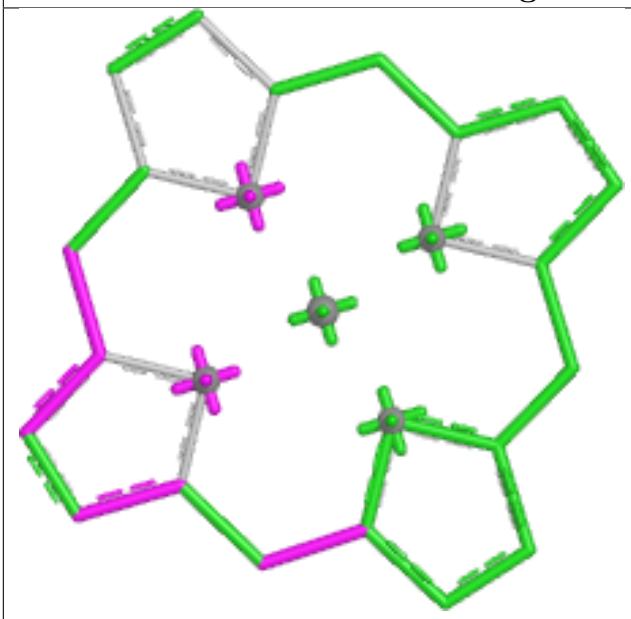


Torsions

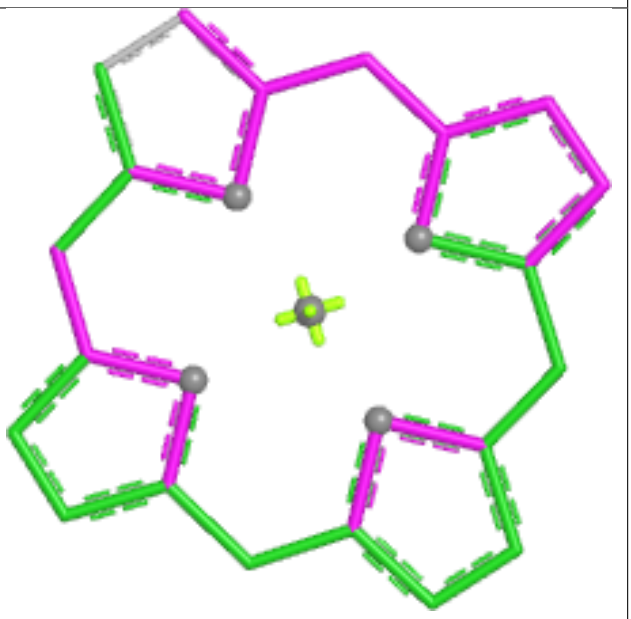


Rings

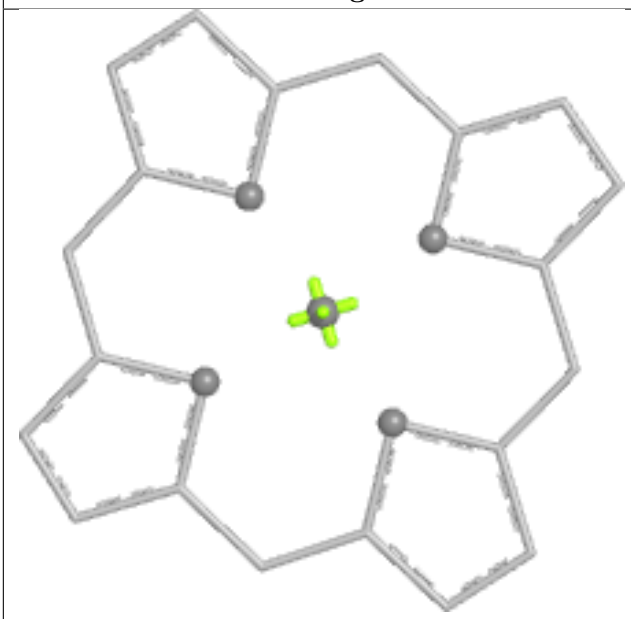
Ligand CLA 2 1014



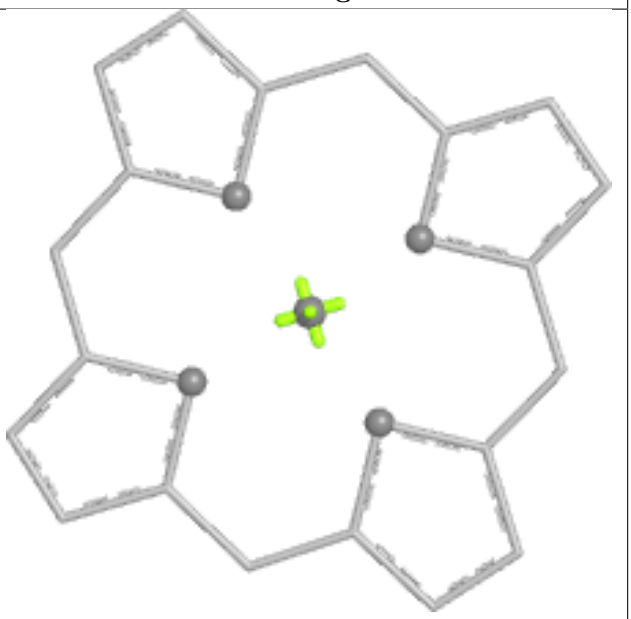
Bond lengths



Bond angles

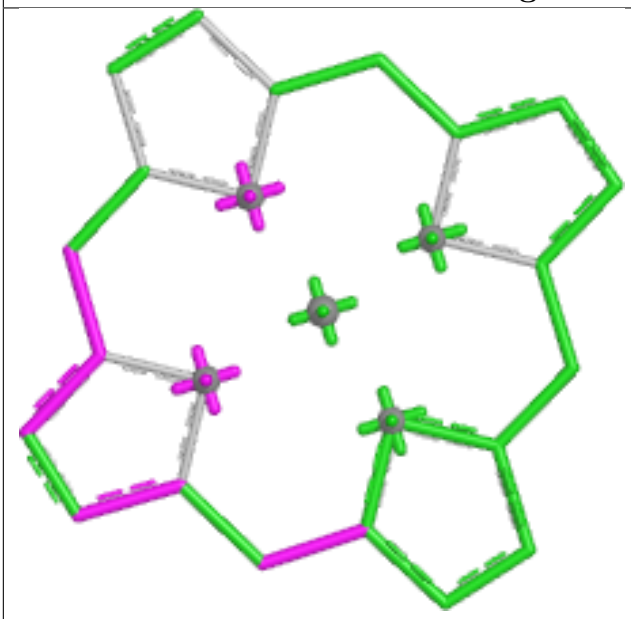


Torsions

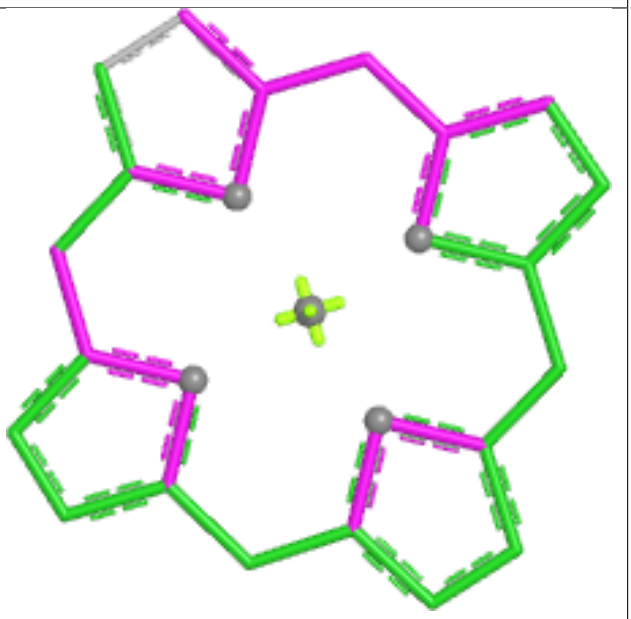


Rings

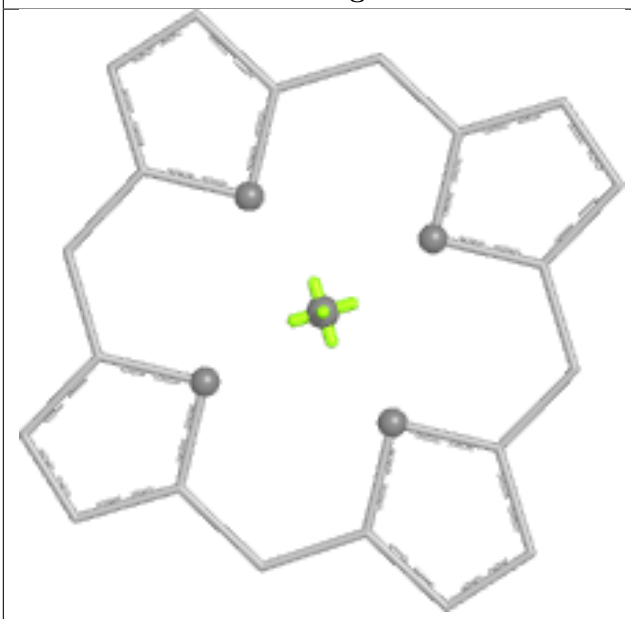
Ligand CLA 4 1014



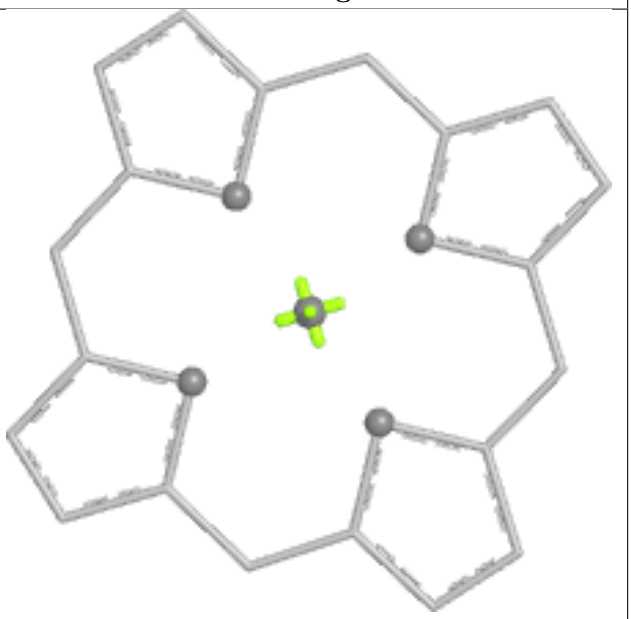
Bond lengths



Bond angles

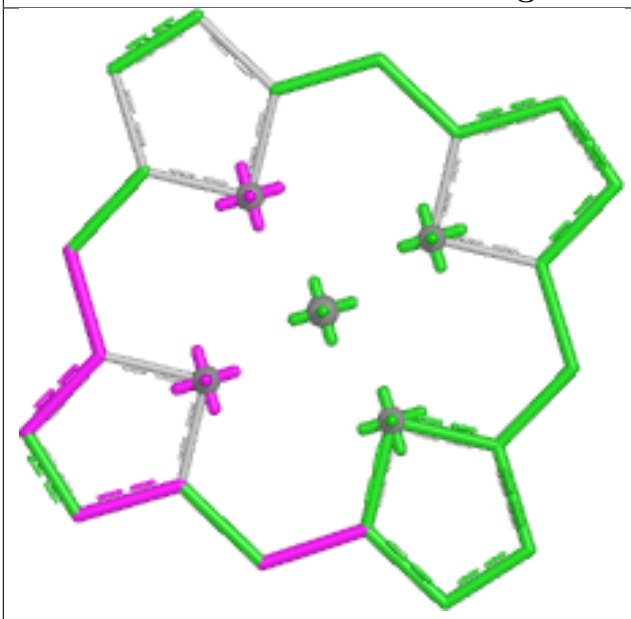


Torsions

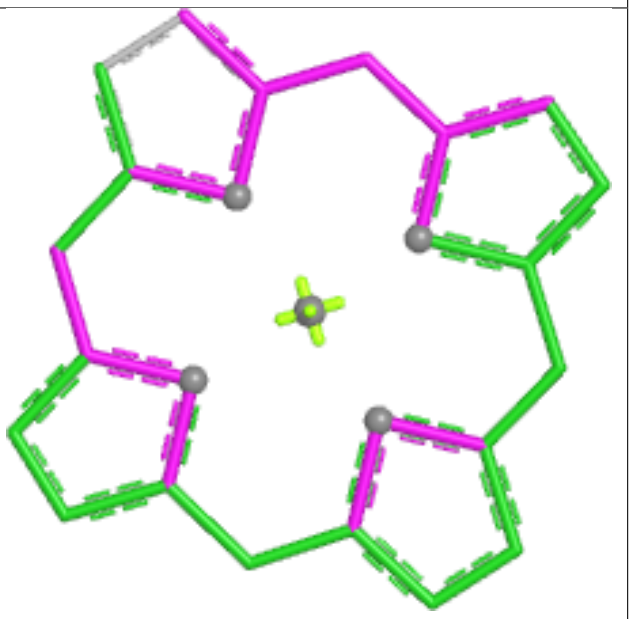


Rings

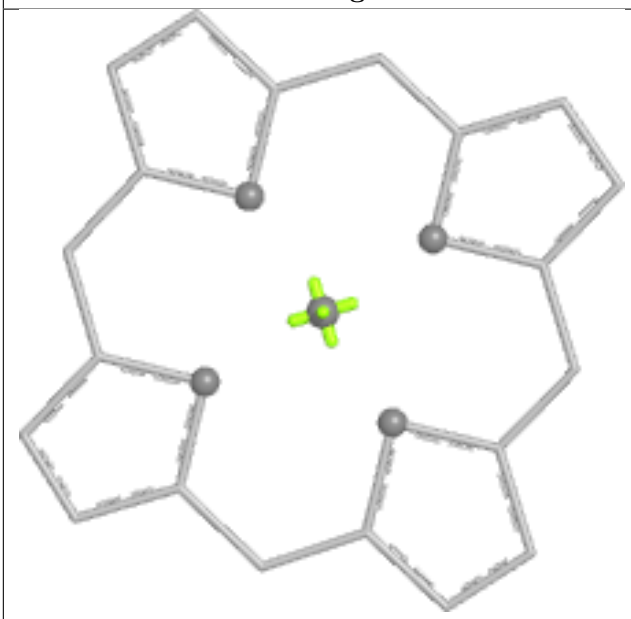
Ligand CLA L 1504



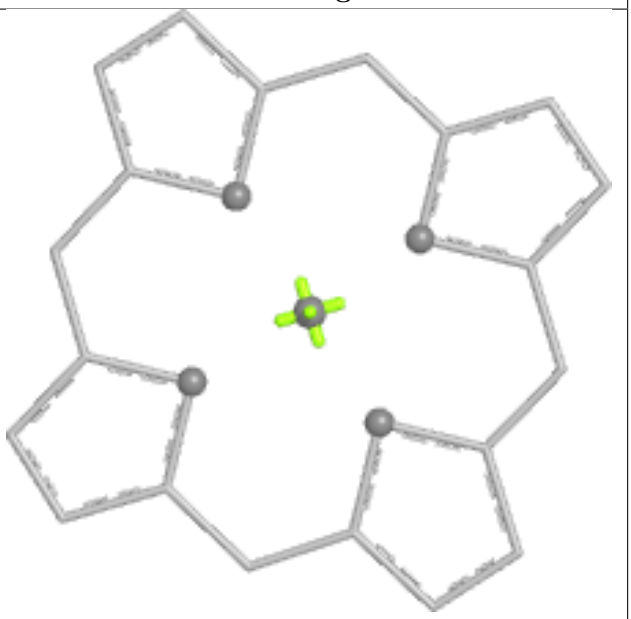
Bond lengths



Bond angles

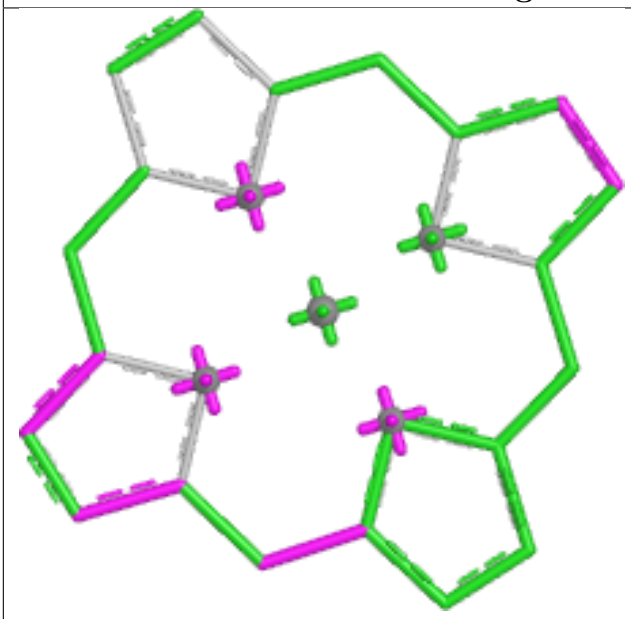


Torsions

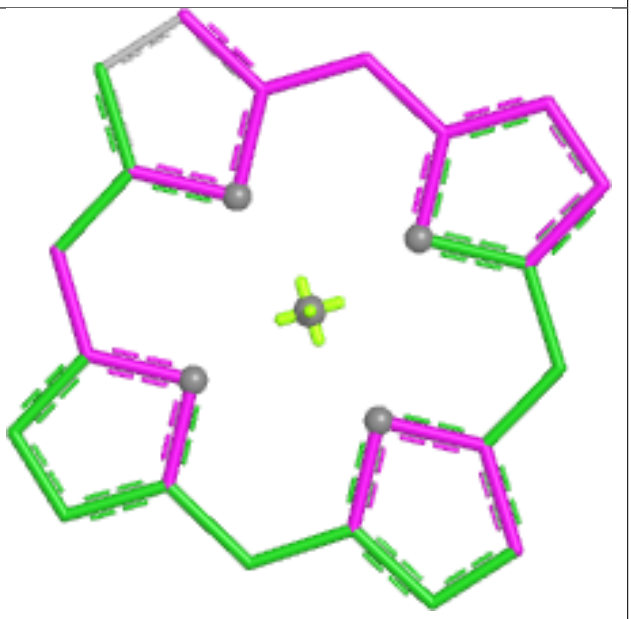


Rings

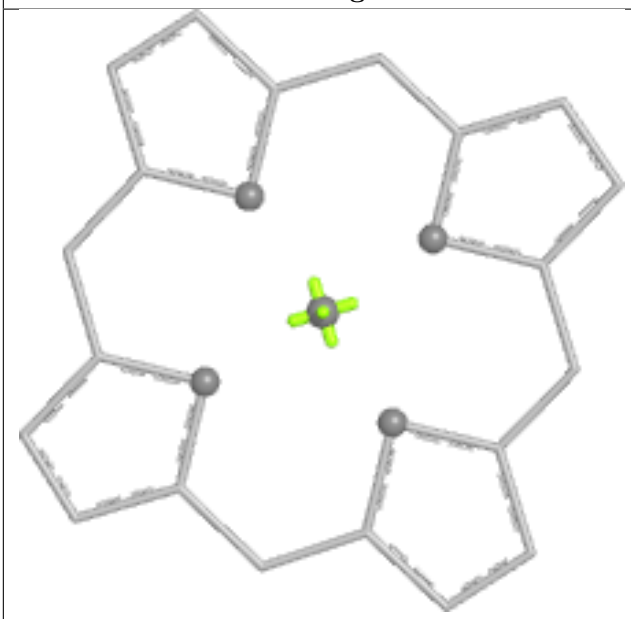
Ligand CLA B 1218



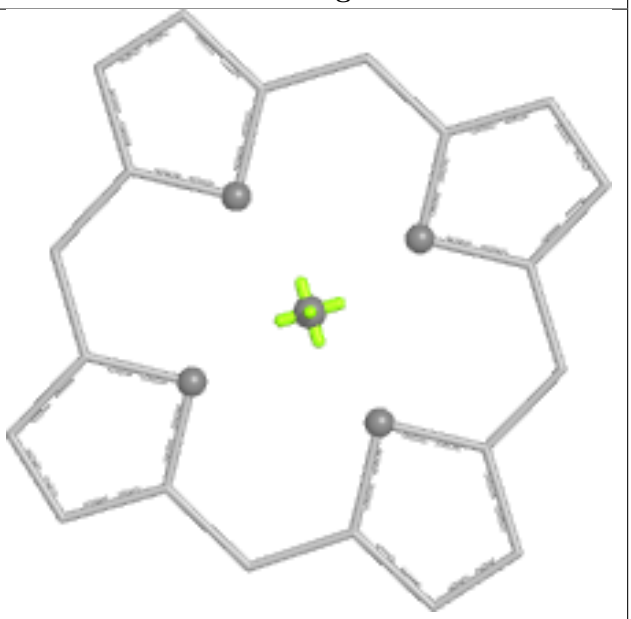
Bond lengths



Bond angles

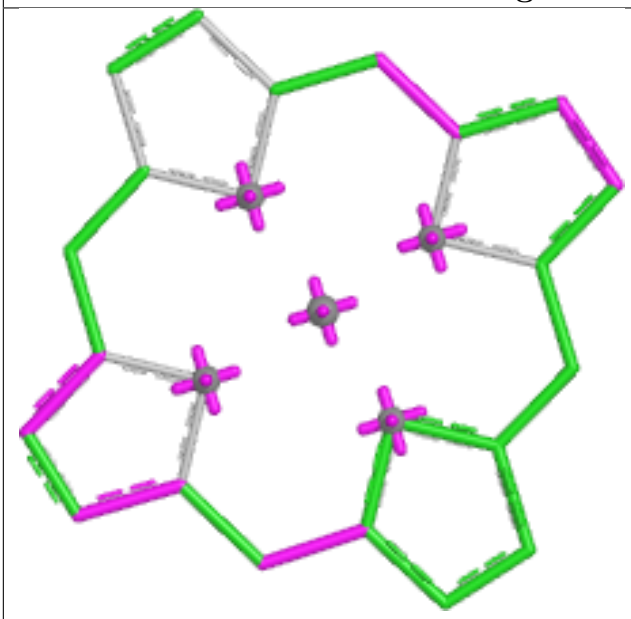


Torsions

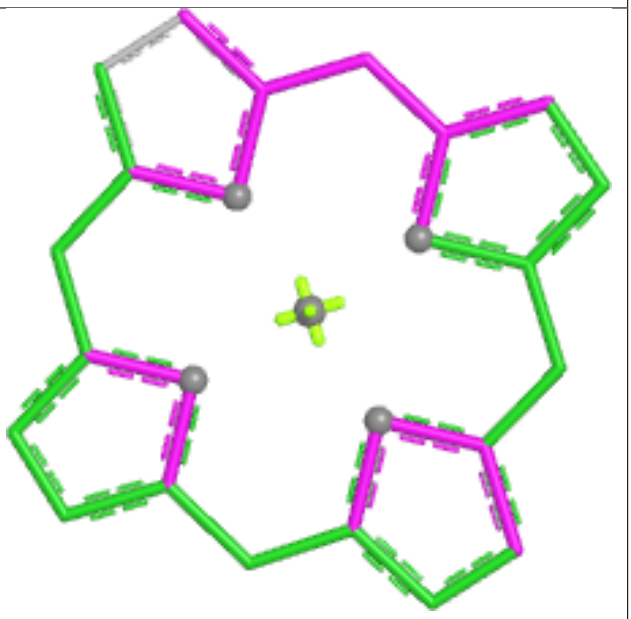


Rings

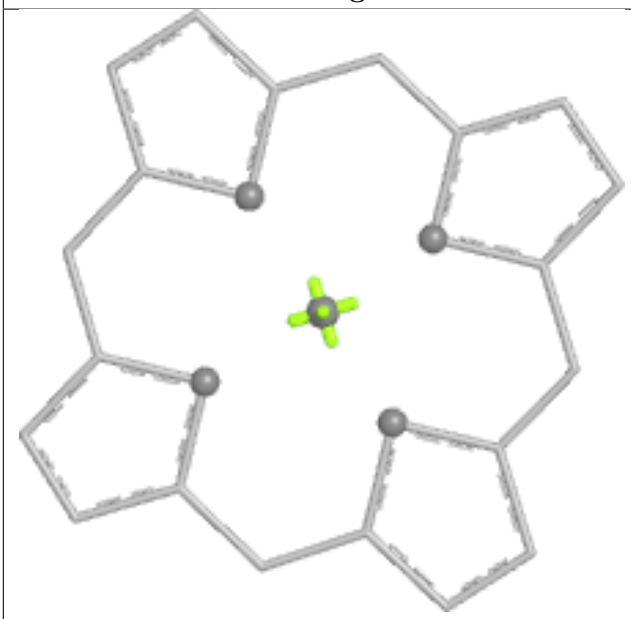
Ligand CLA P 5104



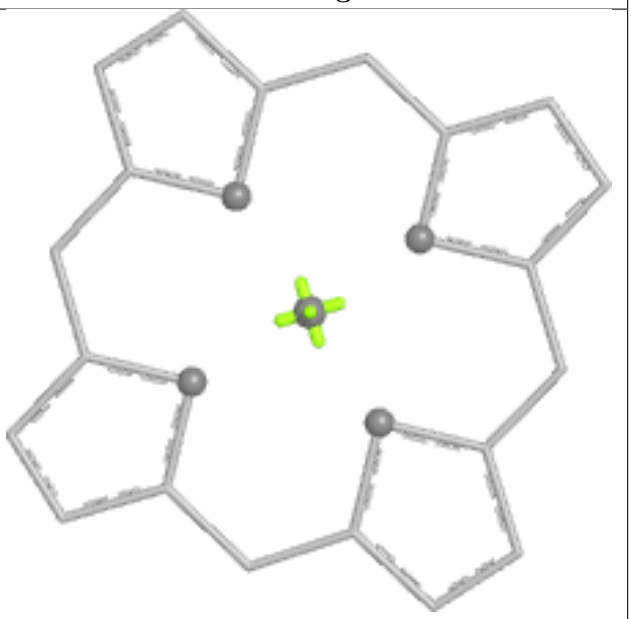
Bond lengths



Bond angles

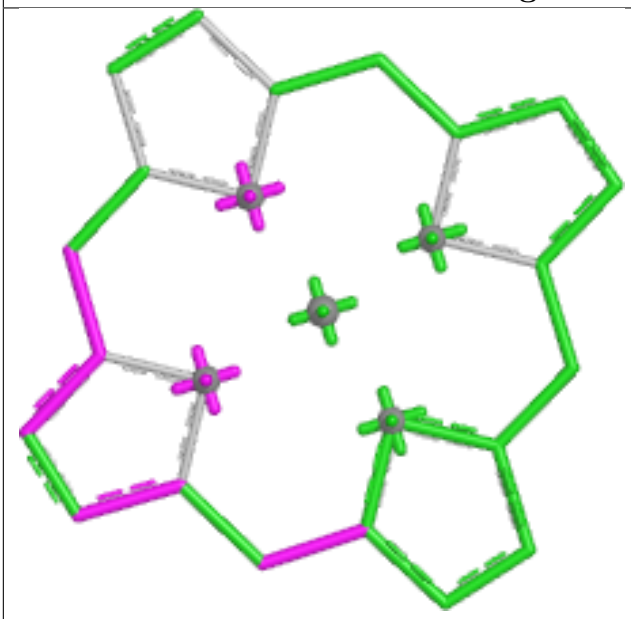


Torsions

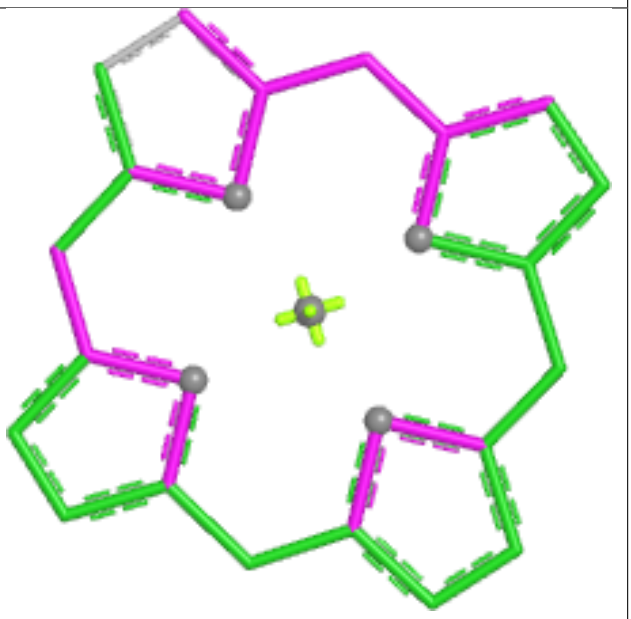


Rings

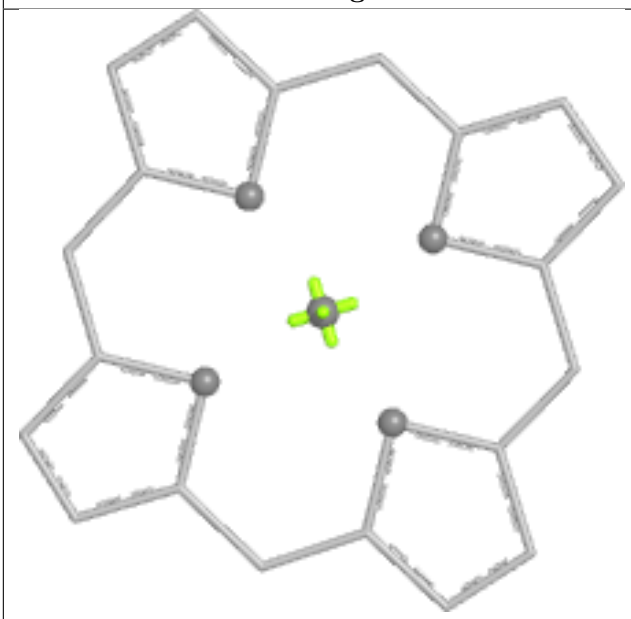
Ligand CLA 4 1033



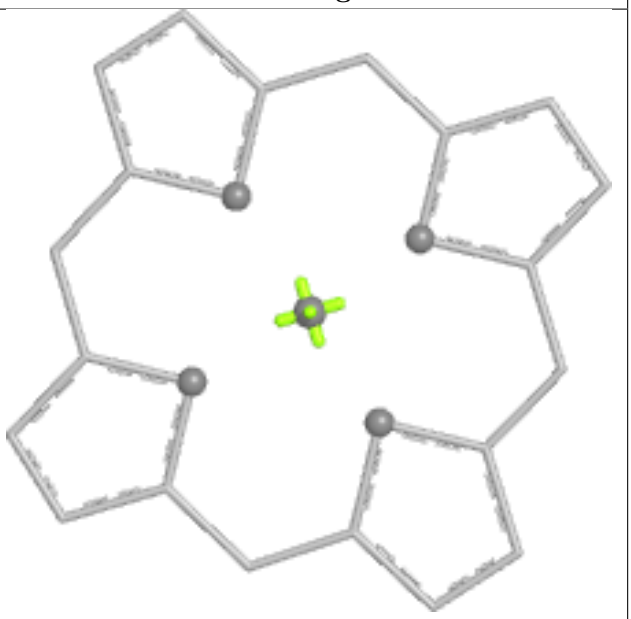
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.