



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 01:21 AM UTC

PDB ID : 1C51 / pdb_00001c51
Title : PHOTOSYNTHETIC REACTION CENTER AND CORE ANTENNA SYSTEM (TRIMERIC), ALPHA CARBON ONLY
Authors : Klukas, O.; Schubert, W.D.; Jordan, P.; Krauss, N.; Fromme, P.; Witt, H.T.; Saenger, W.
Deposited on : 1999-10-21
Resolution : 4.00 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

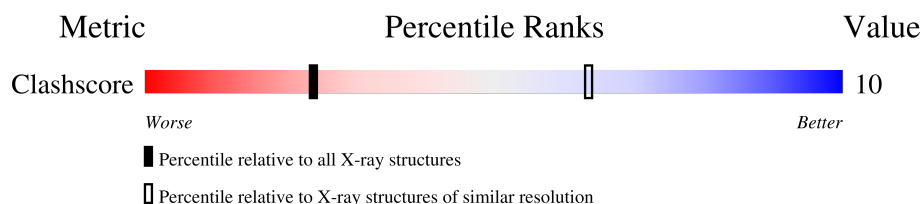
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.00 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	1129 (4.20-3.80)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	597	99% .
2	B	619	100%
3	C	77	95% 5%
4	D	125	97% .
5	E	75	97% .
6	F	153	100%
7	K	78	100%
8	L	120	96% .

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
9	CLA	A	598	X	-	-	-
9	CLA	A	599	X	-	-	-
9	CLA	A	600	X	-	-	-
9	CLA	A	603	X	-	-	-
9	CLA	A	604	X	-	-	-
9	CLA	A	605	X	-	-	-
9	CLA	A	606	X	-	-	-
9	CLA	A	607	X	-	-	-
9	CLA	A	608	X	-	-	-
9	CLA	A	609	X	-	-	-
9	CLA	A	610	X	-	-	-
9	CLA	A	611	X	-	-	-
9	CLA	A	612	X	-	-	-
9	CLA	A	613	X	-	-	-
9	CLA	A	616	X	-	-	-
9	CLA	A	619	X	-	-	-
9	CLA	A	620	X	-	-	-
9	CLA	A	621	X	-	-	-
9	CLA	A	622	X	-	-	-
9	CLA	A	623	X	-	-	-
9	CLA	A	624	X	-	-	-
9	CLA	A	625	X	-	-	-
9	CLA	A	626	X	-	-	-
9	CLA	A	627	X	-	-	-
9	CLA	A	628	X	-	-	-
9	CLA	A	629	X	-	-	-
9	CLA	B	620	X	-	-	-
9	CLA	B	621	X	-	-	-
9	CLA	B	622	X	-	-	-
9	CLA	B	624	X	-	-	-
9	CLA	B	625	X	-	-	-
9	CLA	B	626	X	-	-	-
9	CLA	B	627	X	-	-	-
9	CLA	B	628	X	-	-	-
9	CLA	B	629	X	-	-	-
9	CLA	B	630	X	-	-	-
9	CLA	B	631	X	-	-	-
9	CLA	B	632	X	-	-	-
9	CLA	B	633	X	-	-	-
9	CLA	B	634	X	-	-	-
9	CLA	B	635	X	-	-	-
9	CLA	B	636	X	-	-	-
9	CLA	B	637	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
9	CLA	B	638	X	-	-	-
9	CLA	B	639	X	-	-	-
9	CLA	B	640	X	-	-	-
9	CLA	B	641	X	-	-	-
9	CLA	B	642	X	-	-	-
9	CLA	B	643	X	-	-	-
9	CLA	B	644	X	-	-	-
9	CLA	B	645	X	-	-	-
9	CLA	B	646	X	-	-	-
9	CLA	B	647	X	-	-	-
9	CLA	B	648	X	-	-	-
9	CLA	B	649	X	-	-	-
9	CLA	B	650	X	-	-	-
9	CLA	B	651	X	-	-	-
9	CLA	B	652	X	-	-	-
9	CLA	B	653	X	-	-	-
9	CLA	F	154	X	-	-	-
9	CLA	F	155	X	-	-	-
9	CLA	F	156	X	-	-	-
9	CLA	F	157	X	-	-	-
9	CLA	K	135	X	-	-	-
9	CLA	L	147	X	-	-	-
9	CLA	L	149	X	-	-	-
9	CLA	L	163	X	-	-	-

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 3672 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 PROTEIN (PHOTOSYSTEM I: SUBUNIT PSAA).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
1	A	597	Total	C	0	0	597
			597	597			

- Molecule 2 is a protein called PROTEIN (PHOTOSYSTEM I: SUBUNIT PSAB).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
2	B	619	Total	C	0	0	619
			619	619			

- Molecule 3 is a protein called PROTEIN (PHOTOSYSTEM I: SUBUNIT PSAC).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
3	C	77	Total	C	0	0	77
			77	77			

- Molecule 4 is a protein called PROTEIN (PHOTOSYSTEM I: SUBUNIT PSAD).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
4	D	125	Total	C	0	0	125
			125	125			

- Molecule 5 is a protein called PROTEIN (PHOTOSYSTEM I: SUBUNIT PSAE).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
5	E	75	Total	C	0	0	75
			75	75			

- Molecule 6 is a protein called PROTEIN (PHOTOSYSTEM I: SUBUNIT PSAF).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
6	F	153	Total	C		0	0	153
			153	153				

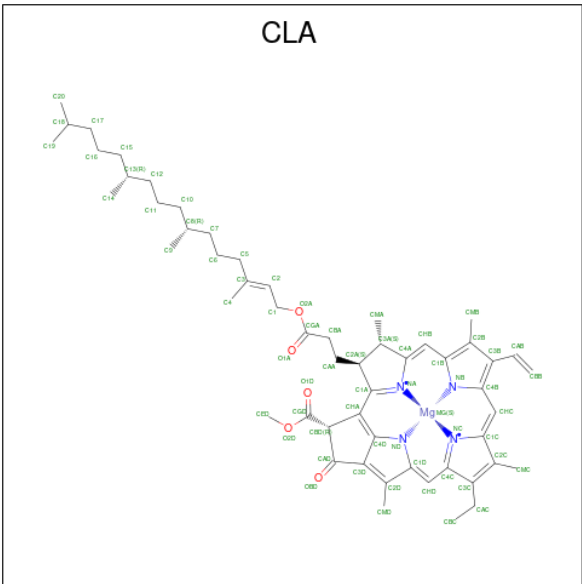
- Molecule 7 is a protein called PROTEIN (PHOTOSYSTEM I: SUBUNIT PSAK).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
7	K	78	Total	C		0	0	78
			78	78				

- Molecule 8 is a protein called PROTEIN (PHOTOSYSTEM I: SUBUNIT PSAL).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
8	L	120	Total	C		0	0	120
			120	120				

- Molecule 9 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅).



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

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

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

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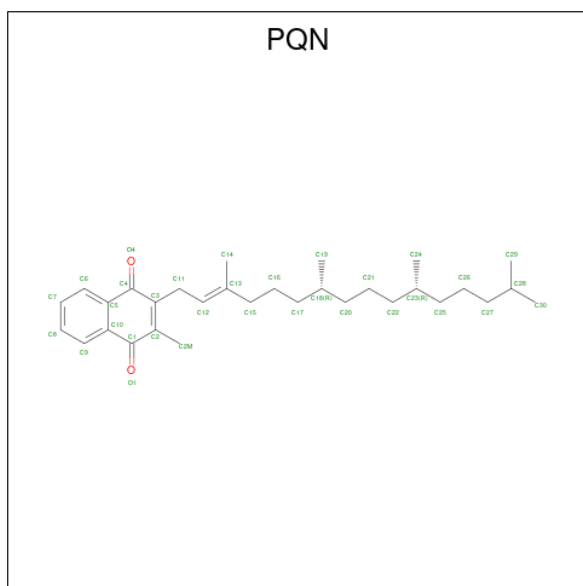
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	B	1	Total	C	Mg	N	0	0
			25	20	1	4		
9	B	1	Total	C	Mg	N	0	0
			25	20	1	4		
9	B	1	Total	C	Mg	N	0	0
			25	20	1	4		
9	B	1	Total	C	Mg	N	0	0
			25	20	1	4		
9	B	1	Total	C	Mg	N	0	0
			25	20	1	4		
9	B	1	Total	C	Mg	N	0	0
			25	20	1	4		
9	B	1	Total	C	Mg	N	0	0
			25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

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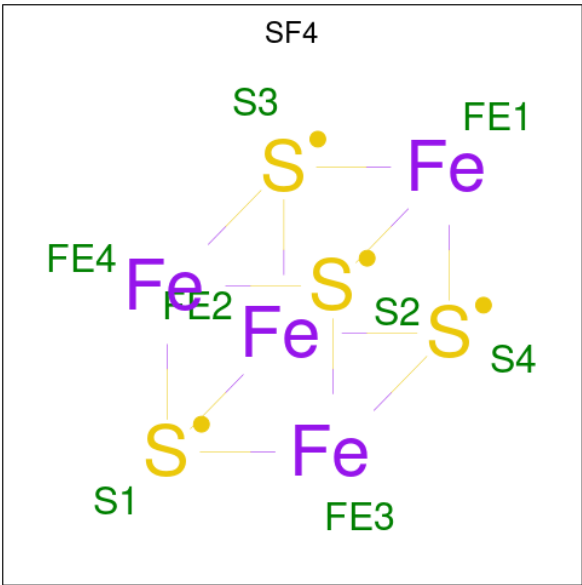
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	F	1	Total	C	Mg	N	0	0
			25	20	1	4		
9	K	1	Total	C	Mg	N	0	0
			25	20	1	4		
9	L	1	Total	C	Mg	N	0	0
			25	20	1	4		
9	L	1	Total	C	Mg	N	0	0
			25	20	1	4		
9	L	1	Total	C	Mg	N	0	0
			25	20	1	4		

- Molecule 10 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	1	Total	C	0	0
			2	2		
10	B	1	Total	C	0	0
			2	2		

- Molecule 11 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



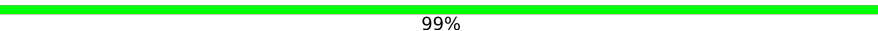
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	A	1	Total	Fe	S	0	0
			8	4	4		
11	C	1	Total	Fe	S	0	0
			8	4	4		
11	C	1	Total	Fe	S	0	0
			8	4	4		

3 Residue-property plots

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.

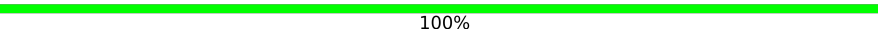
Note EDS was not executed.

- Molecule 1: PROTEIN (PHOTOSYSTEM I: SUBUNIT PSAA)

Chain A:  99%

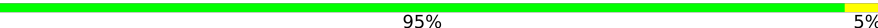


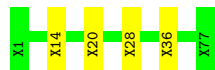
- Molecule 2: PROTEIN (PHOTOSYSTEM I: SUBUNIT PSAB)

Chain B:  100%

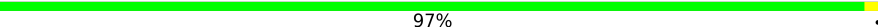


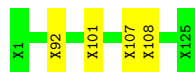
- Molecule 3: PROTEIN (PHOTOSYSTEM I: SUBUNIT PSAC)

Chain C:  95% 5%

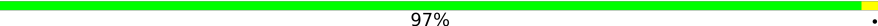


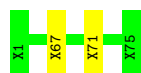
- Molecule 4: PROTEIN (PHOTOSYSTEM I: SUBUNIT PSAD)

Chain D:  97%



- Molecule 5: PROTEIN (PHOTOSYSTEM I: SUBUNIT PSAE)

Chain E:  97%



- Molecule 6: PROTEIN (PHOTOSYSTEM I: SUBUNIT PSAF)

Chain F:  100%

There are no outlier residues recorded for this chain.

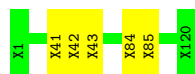
- Molecule 7: PROTEIN (PHOTOSYSTEM I: SUBUNIT PSAK)

Chain K:  100%

There are no outlier residues recorded for this chain.

- Molecule 8: PROTEIN (PHOTOSYSTEM I: SUBUNIT PSAL)

Chain L:  96%



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α , β , γ	286.00Å 286.00Å 167.00Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	60.00 – 4.00	Depositor
% Data completeness (in resolution range)	(Not available) (60.00-4.00)	Depositor
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
Refinement program		Depositor
R, R_{free}	(Not available) , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3672	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CLA, PQN, 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 [i](#)

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	597	0	0	4	0
2	B	619	0	0	6	0
3	C	77	0	0	3	0
4	D	125	0	0	2	0
5	E	75	0	0	1	0
6	F	153	0	0	0	0
7	K	78	0	0	0	0
8	L	120	0	0	0	4
9	A	750	0	90	8	0
9	B	825	0	99	22	0
9	F	125	0	15	0	0
9	K	25	0	3	13	0
9	L	75	0	9	0	0
10	A	2	0	0	0	0
10	B	2	0	0	0	0
11	A	8	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	C	16	0	0	2	0
All	All	3672	0	216	39	4

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 10.

The worst 5 of 39 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)
9:A:628:CLA:HHD	9:A:629:CLA:C2D	1.46	1.44
2:B:358:UNK:CA	9:B:627:CLA:C1A	2.28	1.10
9:A:628:CLA:C3C	9:A:629:CLA:C3D	2.33	1.06
9:A:628:CLA:CHD	9:A:629:CLA:C2D	2.33	1.06
9:B:641:CLA:HHC	9:K:135:CLA:C3D	1.95	0.95

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:L:42:UNK:CA	8:L:85:UNK:CA[3_665]	1.93	0.27
8:L:41:UNK:CA	8:L:85:UNK:CA[3_665]	2.08	0.12
8:L:42:UNK:CA	8:L:84:UNK:CA[3_665]	2.08	0.12
8:L:43:UNK:CA	8:L:84:UNK:CA[3_665]	2.09	0.11

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](#)

77 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$
11	SF4	A	602	1	0,12,12	-	-	-		
9	CLA	A	620	-	24,32,73	2.37	6 (25%)	31,54,113	1.92	4 (12%)
9	CLA	A	627	-	24,32,73	2.33	5 (20%)	31,54,113	1.95	5 (16%)
9	CLA	A	604	-	24,32,73	2.53	5 (20%)	31,54,113	1.91	4 (12%)
9	CLA	B	640	-	24,32,73	2.82	6 (25%)	31,54,113	2.93	11 (35%)
9	CLA	B	637	-	24,32,73	2.43	6 (25%)	31,54,113	2.03	5 (16%)
9	CLA	B	651	-	24,32,73	2.33	5 (20%)	31,54,113	2.04	4 (12%)
9	CLA	A	615	-	24,32,73	3.07	9 (37%)	31,54,113	2.39	8 (25%)
9	CLA	F	157	-	24,32,73	2.32	7 (29%)	31,54,113	1.89	4 (12%)
9	CLA	A	609	-	24,32,73	2.38	5 (20%)	31,54,113	1.99	5 (16%)
9	CLA	A	616	-	24,32,73	2.38	6 (25%)	31,54,113	1.95	4 (12%)
9	CLA	B	633	-	24,32,73	2.33	7 (29%)	31,54,113	1.88	4 (12%)
9	CLA	A	614	-	24,32,73	3.07	9 (37%)	31,54,113	2.39	8 (25%)
9	CLA	A	605	-	24,32,73	2.37	7 (29%)	31,54,113	1.93	5 (16%)
9	CLA	A	612	-	24,32,73	2.64	7 (29%)	31,54,113	3.25	12 (38%)
9	CLA	B	642	-	24,32,73	2.30	6 (25%)	31,54,113	1.97	4 (12%)
9	CLA	B	625	-	24,32,73	2.27	6 (25%)	31,54,113	2.01	5 (16%)
9	CLA	B	653	-	24,32,73	2.42	5 (20%)	31,54,113	2.04	4 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	CLA	B	626	-	24,32,73	2.40	5 (20%)	31,54,113	1.94	5 (16%)
9	CLA	B	650	-	24,32,73	2.36	5 (20%)	31,54,113	1.82	4 (12%)
9	CLA	K	135	-	24,32,73	2.54	6 (25%)	31,54,113	1.88	6 (19%)
9	CLA	A	622	-	24,32,73	2.43	5 (20%)	31,54,113	2.00	5 (16%)
9	CLA	A	610	-	24,32,73	2.35	5 (20%)	31,54,113	2.06	5 (16%)
9	CLA	B	631	-	24,32,73	2.25	5 (20%)	31,54,113	1.87	5 (16%)
9	CLA	B	622	-	24,32,73	2.34	7 (29%)	31,54,113	2.01	4 (12%)
9	CLA	B	636	-	24,32,73	2.37	5 (20%)	31,54,113	2.09	5 (16%)
9	CLA	L	163	-	24,32,73	2.39	5 (20%)	31,54,113	1.83	4 (12%)
9	CLA	B	652	-	24,32,73	2.30	5 (20%)	31,54,113	2.08	5 (16%)
9	CLA	A	599	-	24,32,73	2.32	7 (29%)	31,54,113	2.07	5 (16%)
9	CLA	B	624	-	24,32,73	2.29	5 (20%)	31,54,113	1.87	5 (16%)
9	CLA	A	607	-	24,32,73	2.34	6 (25%)	31,54,113	2.11	4 (12%)
9	CLA	A	624	-	24,32,73	2.34	6 (25%)	31,54,113	2.02	4 (12%)
9	CLA	A	603	-	24,32,73	2.38	5 (20%)	31,54,113	1.98	5 (16%)
9	CLA	A	608	-	24,32,73	2.43	6 (25%)	31,54,113	1.86	4 (12%)
9	CLA	B	629	-	24,32,73	2.29	5 (20%)	31,54,113	2.01	4 (12%)
9	CLA	B	645	-	24,32,73	2.47	6 (25%)	31,54,113	1.91	5 (16%)
9	CLA	B	632	-	24,32,73	2.44	6 (25%)	31,54,113	1.95	4 (12%)
11	SF4	C	79	-	0,12,12	-	-	-	-	-
9	CLA	B	634	-	24,32,73	2.45	5 (20%)	31,54,113	1.90	4 (12%)
9	CLA	A	628	-	24,32,73	2.36	6 (25%)	31,54,113	1.77	5 (16%)
9	CLA	A	629	-	24,32,73	2.27	6 (25%)	31,54,113	1.96	5 (16%)
9	CLA	B	635	-	24,32,73	2.63	7 (29%)	31,54,113	3.34	13 (41%)
9	CLA	F	154	-	24,32,73	2.44	7 (29%)	31,54,113	1.96	5 (16%)
9	CLA	A	613	-	24,32,73	2.32	5 (20%)	31,54,113	1.89	5 (16%)
9	CLA	F	156	-	24,32,73	2.47	6 (25%)	31,54,113	2.02	4 (12%)
9	CLA	B	641	-	24,32,73	2.40	7 (29%)	31,54,113	1.87	6 (19%)
9	CLA	A	598	-	24,32,73	2.33	6 (25%)	31,54,113	1.73	4 (12%)
9	CLA	A	619	-	24,32,73	2.39	5 (20%)	31,54,113	1.85	4 (12%)
9	CLA	A	606	-	24,32,73	2.30	6 (25%)	31,54,113	1.77	4 (12%)
9	CLA	B	630	-	24,32,73	2.26	7 (29%)	31,54,113	1.88	4 (12%)
9	CLA	B	620	-	24,32,73	2.60	6 (25%)	31,54,113	1.89	5 (16%)
9	CLA	B	643	-	24,32,73	2.29	5 (20%)	31,54,113	1.95	5 (16%)
9	CLA	A	618	-	24,32,73	3.07	9 (37%)	31,54,113	2.38	9 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	CLA	F	155	-	24,32,73	2.37	5 (20%)	31,54,113	1.91	4 (12%)
9	CLA	L	149	-	24,32,73	2.29	5 (20%)	31,54,113	2.16	5 (16%)
9	CLA	B	621	-	24,32,73	2.52	6 (25%)	31,54,113	1.85	4 (12%)
9	CLA	A	600	-	24,32,73	2.26	7 (29%)	31,54,113	2.07	4 (12%)
9	CLA	A	611	-	24,32,73	2.35	6 (25%)	31,54,113	1.94	4 (12%)
9	CLA	L	147	-	24,32,73	2.24	6 (25%)	31,54,113	1.88	4 (12%)
9	CLA	B	639	-	24,32,73	2.36	7 (29%)	31,54,113	1.96	5 (16%)
9	CLA	A	626	-	24,32,73	2.30	6 (25%)	31,54,113	1.98	4 (12%)
9	CLA	B	638	-	24,32,73	2.44	5 (20%)	31,54,113	1.72	5 (16%)
9	CLA	F	158	-	24,32,73	3.07	9 (37%)	31,54,113	2.36	8 (25%)
9	CLA	B	628	-	24,32,73	2.41	6 (25%)	31,54,113	2.13	5 (16%)
9	CLA	B	649	-	24,32,73	2.36	6 (25%)	31,54,113	1.86	4 (12%)
9	CLA	B	647	-	24,32,73	2.33	5 (20%)	31,54,113	1.84	5 (16%)
9	CLA	A	617	-	24,32,73	3.07	9 (37%)	31,54,113	2.38	8 (25%)
9	CLA	B	648	-	24,32,73	2.29	5 (20%)	31,54,113	1.78	4 (12%)
9	CLA	A	623	-	24,32,73	2.35	7 (29%)	31,54,113	1.91	4 (12%)
9	CLA	B	644	-	24,32,73	2.43	5 (20%)	31,54,113	1.87	5 (16%)
11	SF4	C	78	-	0,12,12	-	-	-	-	-
9	CLA	A	625	-	24,32,73	2.43	7 (29%)	31,54,113	1.96	4 (12%)
9	CLA	A	621	-	24,32,73	2.35	5 (20%)	31,54,113	1.92	5 (16%)
9	CLA	B	646	-	24,32,73	2.41	6 (25%)	31,54,113	2.04	4 (12%)
9	CLA	B	627	-	24,32,73	2.28	6 (25%)	31,54,113	1.86	5 (16%)

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
11	SF4	A	602	1	-	-	0/6/5/5
9	CLA	A	620	-	1/1/4/20	-	-
9	CLA	A	627	-	1/1/4/20	-	-
9	CLA	A	604	-	1/1/4/20	-	-
9	CLA	B	640	-	1/1/4/20	-	-
9	CLA	B	637	-	1/1/4/20	-	-
9	CLA	B	651	-	1/1/4/20	-	-
9	CLA	F	157	-	1/1/4/20	-	-
9	CLA	A	609	-	1/1/4/20	-	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	CLA	A	616	-	1/1/4/20	-	-
9	CLA	B	633	-	1/1/4/20	-	-
9	CLA	A	605	-	1/1/4/20	-	-
9	CLA	A	612	-	1/1/4/20	-	-
9	CLA	B	642	-	1/1/4/20	-	-
9	CLA	B	653	-	1/1/4/20	-	-
9	CLA	B	625	-	1/1/4/20	-	-
9	CLA	B	626	-	1/1/4/20	-	-
9	CLA	B	650	-	1/1/4/20	-	-
9	CLA	K	135	-	1/1/4/20	-	-
9	CLA	A	622	-	1/1/4/20	-	-
9	CLA	A	610	-	1/1/4/20	-	-
9	CLA	B	631	-	1/1/4/20	-	-
9	CLA	B	622	-	1/1/4/20	-	-
9	CLA	B	636	-	1/1/4/20	-	-
9	CLA	L	163	-	1/1/4/20	-	-
9	CLA	B	652	-	1/1/4/20	-	-
9	CLA	A	599	-	1/1/4/20	-	-
9	CLA	B	624	-	1/1/4/20	-	-
9	CLA	A	607	-	1/1/4/20	-	-
9	CLA	A	624	-	1/1/4/20	-	-
9	CLA	A	603	-	1/1/4/20	-	-
9	CLA	A	608	-	1/1/4/20	-	-
9	CLA	B	629	-	1/1/4/20	-	-
9	CLA	B	645	-	1/1/4/20	-	-
9	CLA	B	632	-	1/1/4/20	-	-
11	SF4	C	79	-	-	-	0/6/5/5
9	CLA	B	634	-	1/1/4/20	-	-
9	CLA	A	628	-	1/1/4/20	-	-
9	CLA	A	629	-	1/1/4/20	-	-
9	CLA	B	635	-	1/1/4/20	-	-
9	CLA	F	154	-	1/1/4/20	-	-
9	CLA	A	613	-	1/1/4/20	-	-
9	CLA	F	156	-	1/1/4/20	-	-
9	CLA	B	641	-	1/1/4/20	-	-
9	CLA	A	598	-	1/1/4/20	-	-
9	CLA	A	619	-	1/1/4/20	-	-
9	CLA	A	606	-	1/1/4/20	-	-
9	CLA	B	630	-	1/1/4/20	-	-
9	CLA	B	620	-	1/1/4/20	-	-
9	CLA	B	643	-	1/1/4/20	-	-
9	CLA	F	155	-	1/1/4/20	-	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	CLA	L	149	-	1/1/4/20	-	-
9	CLA	B	621	-	1/1/4/20	-	-
9	CLA	A	600	-	1/1/4/20	-	-
9	CLA	A	611	-	1/1/4/20	-	-
9	CLA	L	147	-	1/1/4/20	-	-
9	CLA	B	639	-	1/1/4/20	-	-
9	CLA	A	626	-	1/1/4/20	-	-
9	CLA	B	638	-	1/1/4/20	-	-
9	CLA	B	628	-	1/1/4/20	-	-
9	CLA	B	649	-	1/1/4/20	-	-
9	CLA	B	647	-	1/1/4/20	-	-
9	CLA	B	648	-	1/1/4/20	-	-
9	CLA	A	623	-	1/1/4/20	-	-
9	CLA	B	644	-	1/1/4/20	-	-
11	SF4	C	78	-	-	-	0/6/5/5
9	CLA	A	625	-	1/1/4/20	-	-
9	CLA	A	621	-	1/1/4/20	-	-
9	CLA	B	646	-	1/1/4/20	-	-
9	CLA	B	627	-	1/1/4/20	-	-

The worst 5 of 434 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	617	CLA	C3D-C2D	8.89	1.55	1.35
9	A	615	CLA	C3D-C2D	8.89	1.55	1.35
9	A	614	CLA	C3D-C2D	8.88	1.55	1.35
9	A	618	CLA	C3D-C2D	8.88	1.55	1.35
9	F	158	CLA	C3D-C2D	8.85	1.55	1.35

The worst 5 of 366 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B	635	CLA	C1C-NC-C4C	-11.97	101.22	106.68
9	B	640	CLA	C1C-NC-C4C	-10.62	101.83	106.68
9	A	612	CLA	C1C-NC-C4C	-10.59	101.85	106.68
9	B	628	CLA	C1C-NC-C4C	-7.80	103.12	106.68
9	A	600	CLA	C4A-NA-C1A	-7.67	103.18	106.68

5 of 67 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
9	A	598	CLA	ND

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Mol	Chain	Res	Type	Atom
9	A	599	CLA	ND
9	A	600	CLA	ND
9	A	603	CLA	ND
9	A	604	CLA	ND

There are no torsion outliers.

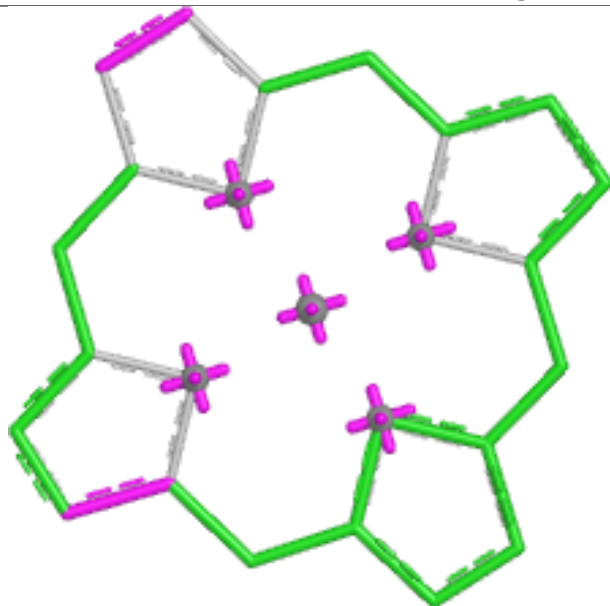
There are no ring outliers.

11 monomers are involved in 32 short contacts:

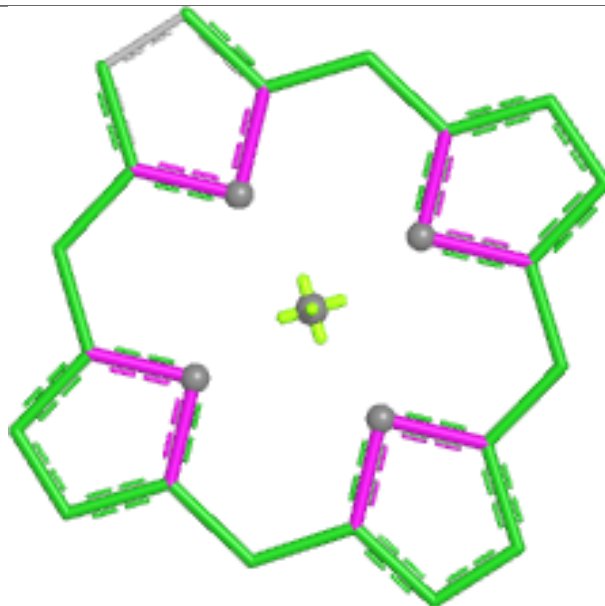
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	612	CLA	1	0
9	K	135	CLA	13	0
9	B	636	CLA	4	0
9	B	629	CLA	4	0
11	C	79	SF4	1	0
9	A	628	CLA	6	0
9	A	629	CLA	6	0
9	B	641	CLA	13	0
9	A	600	CLA	1	0
11	C	78	SF4	1	0
9	B	627	CLA	5	0

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 than 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.

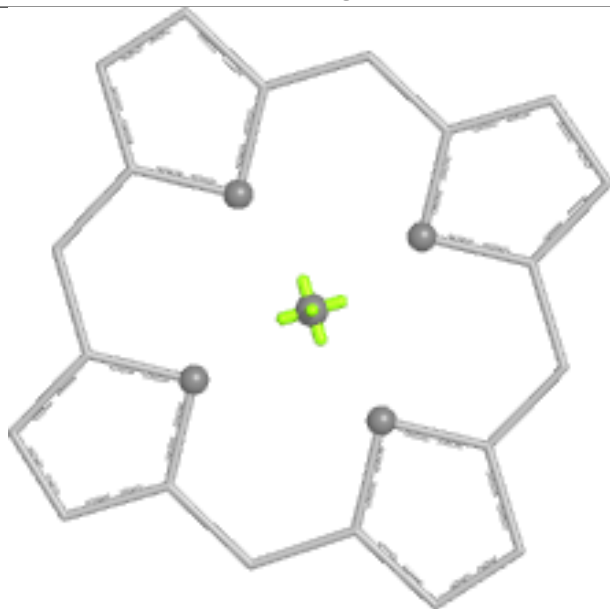
Ligand CLA A 620



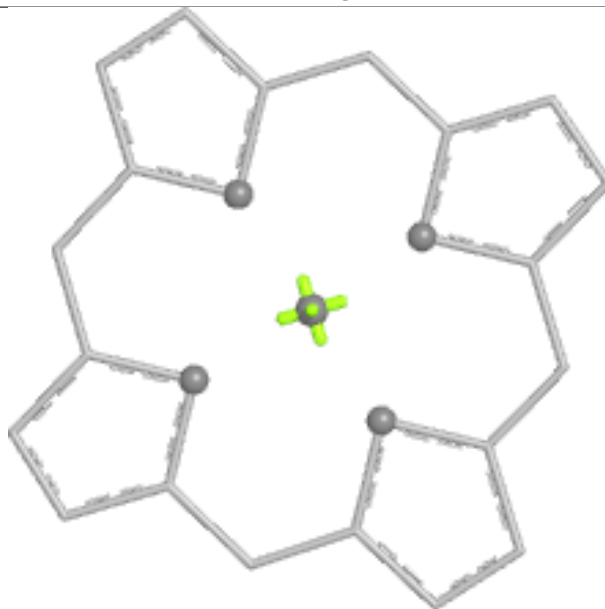
Bond lengths



Bond angles

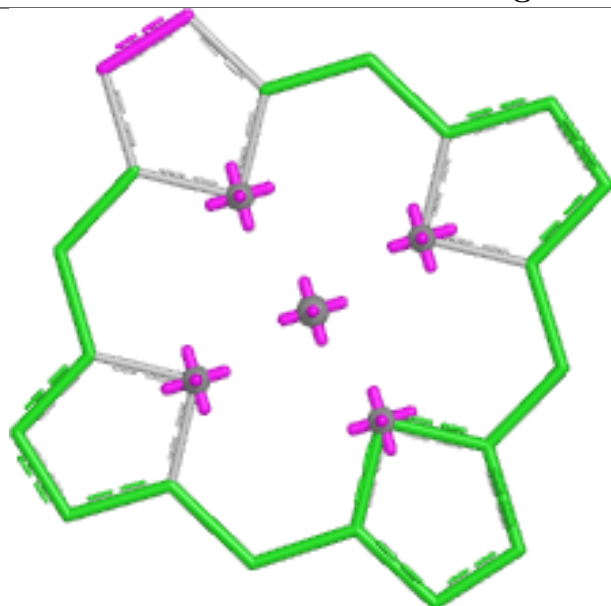


Torsions

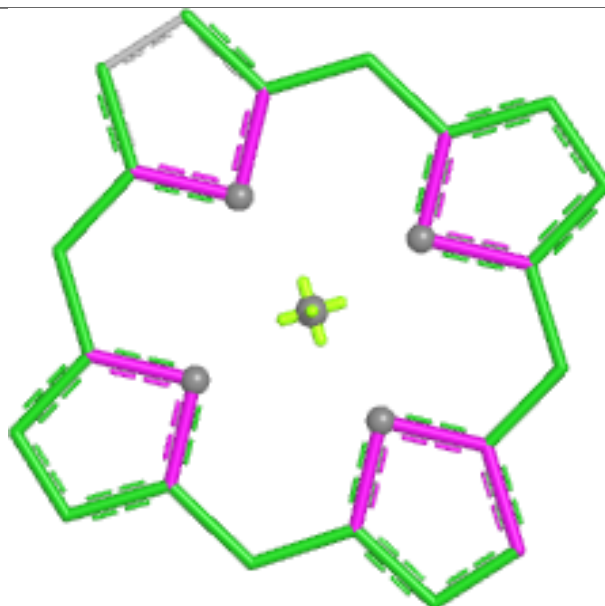


Rings

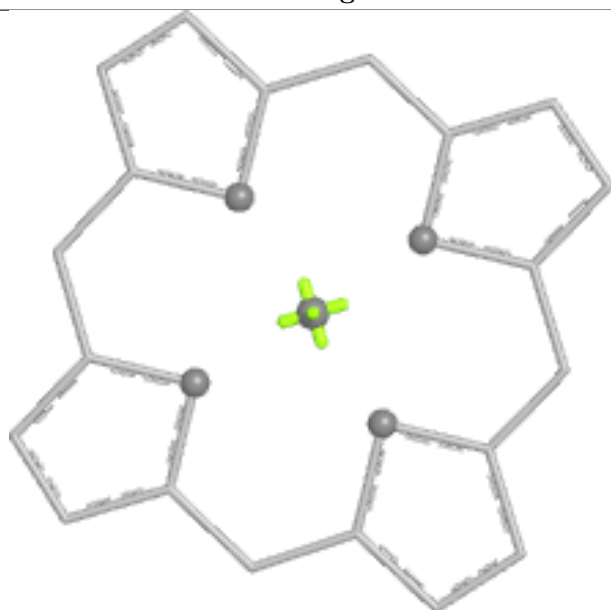
Ligand CLA A 627



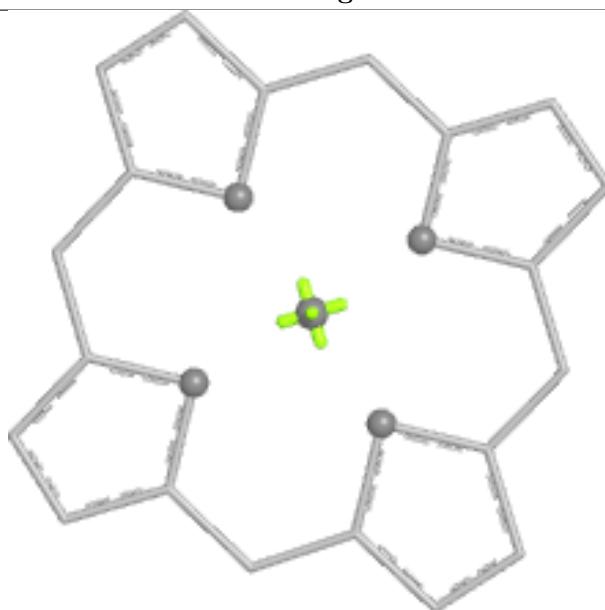
Bond lengths



Bond angles

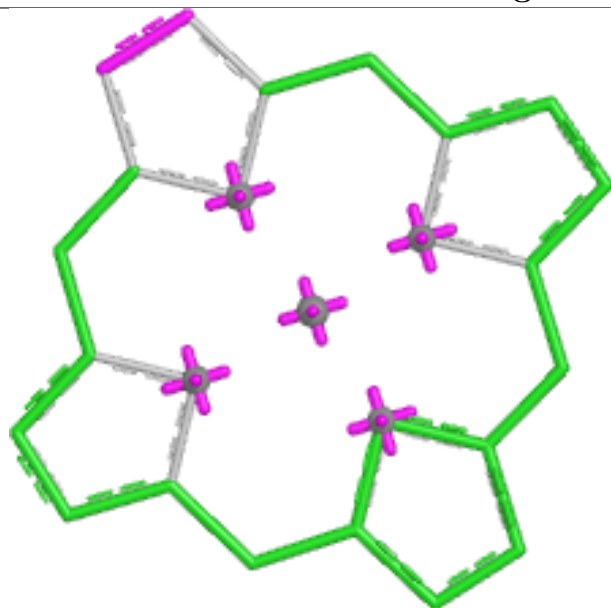


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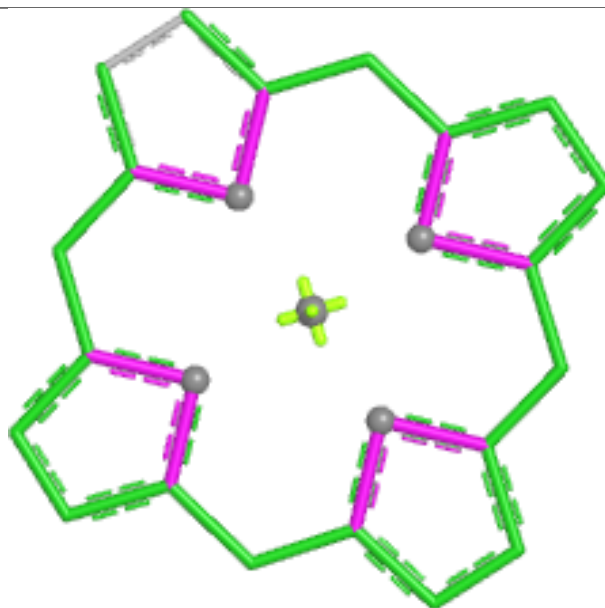


Rings

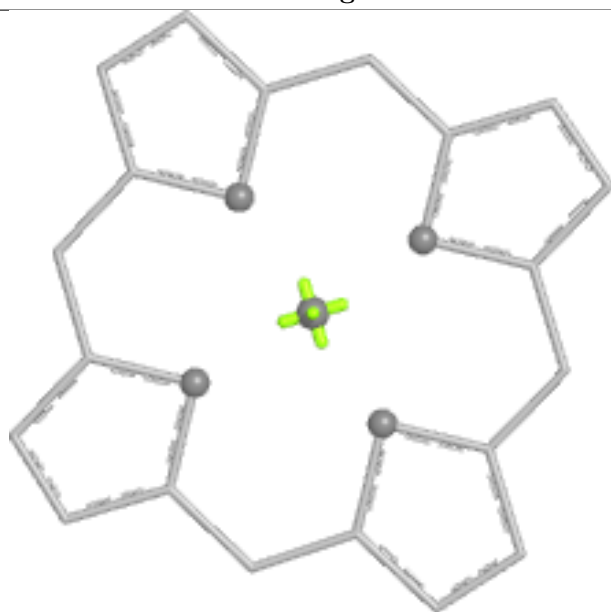
Ligand CLA A 604



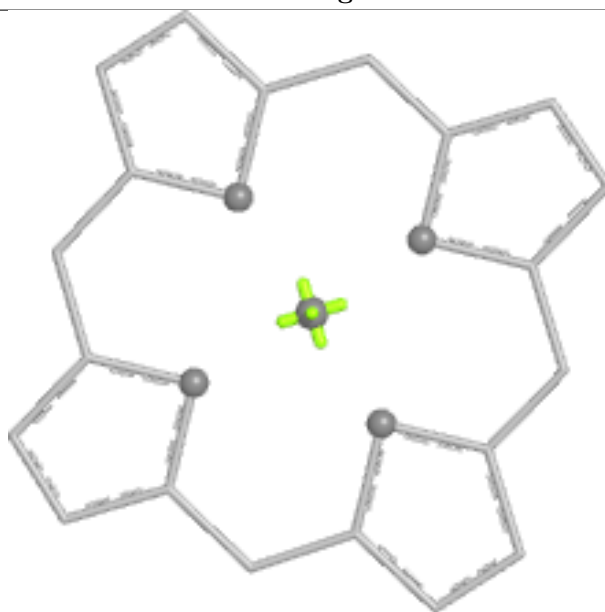
Bond lengths



Bond angles

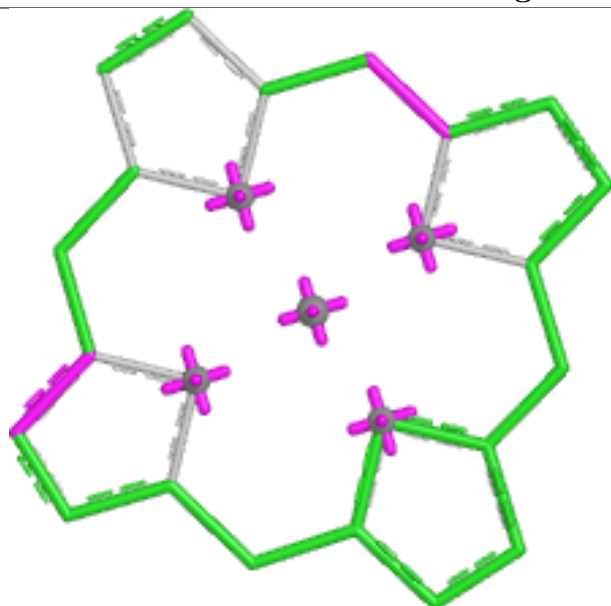


Torsions

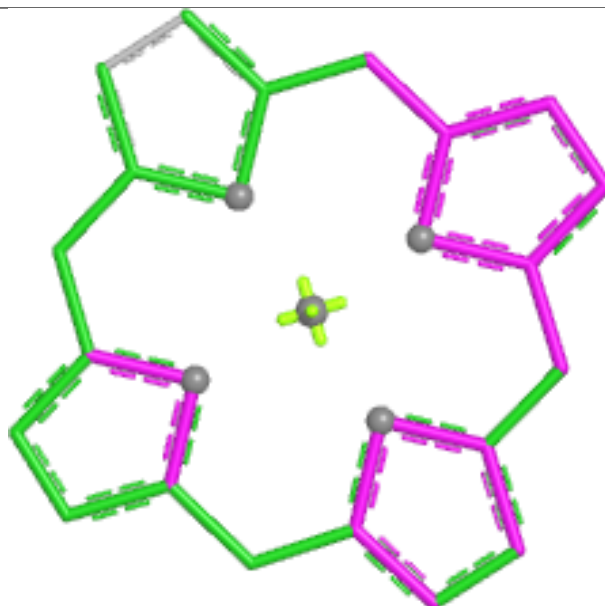


Rings

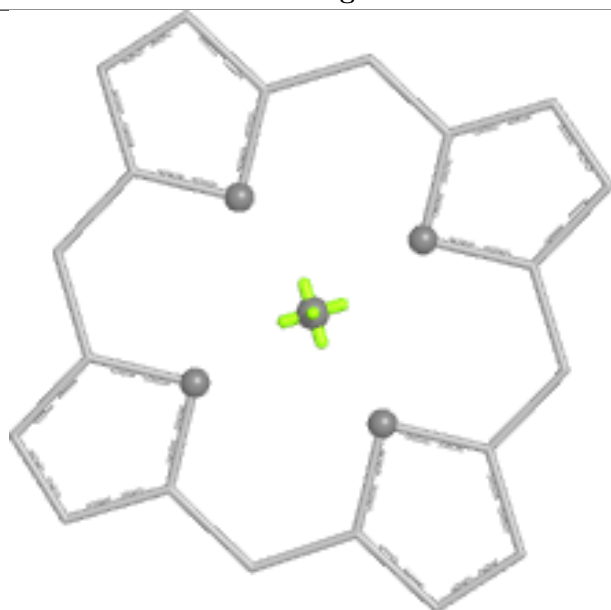
Ligand CLA B 640



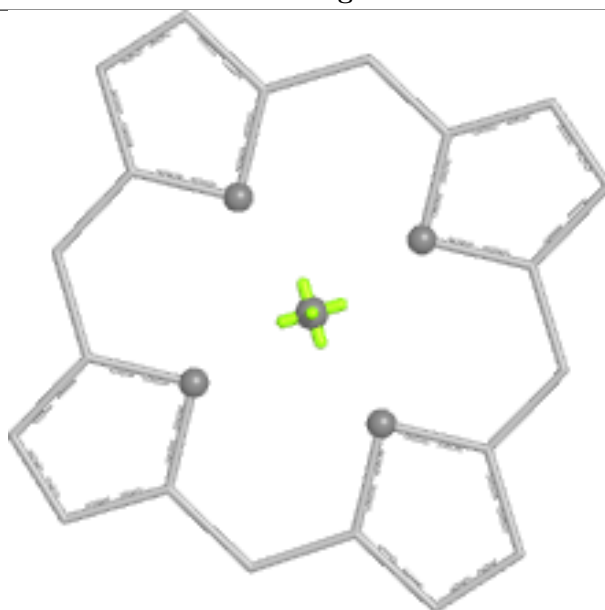
Bond lengths



Bond angles

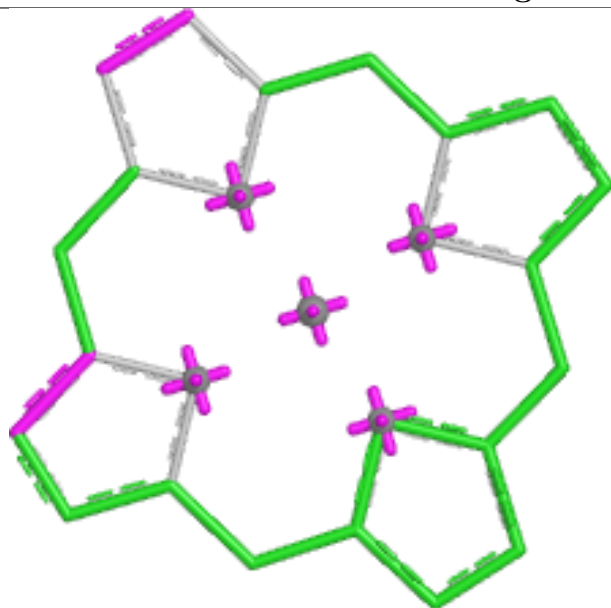


Torsions

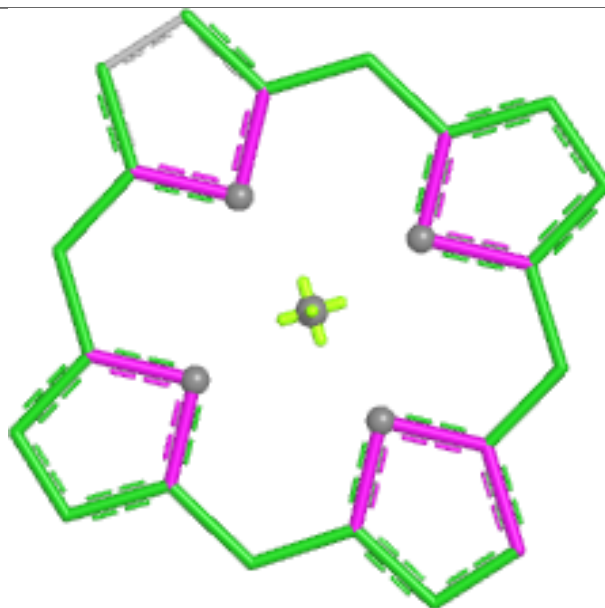


Rings

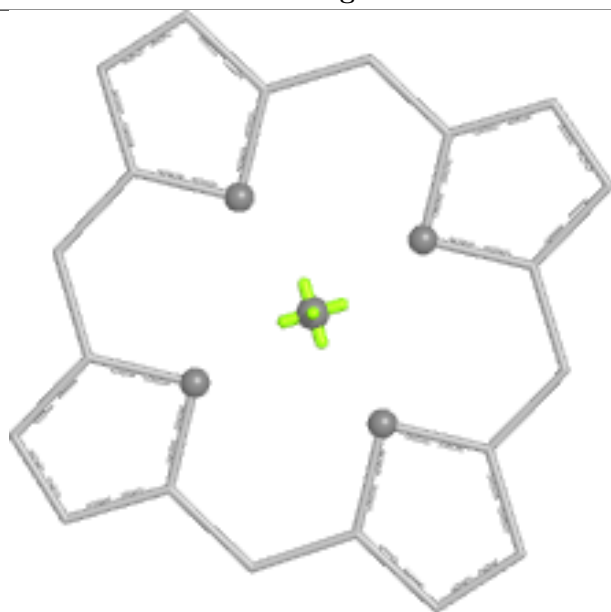
Ligand CLA B 637



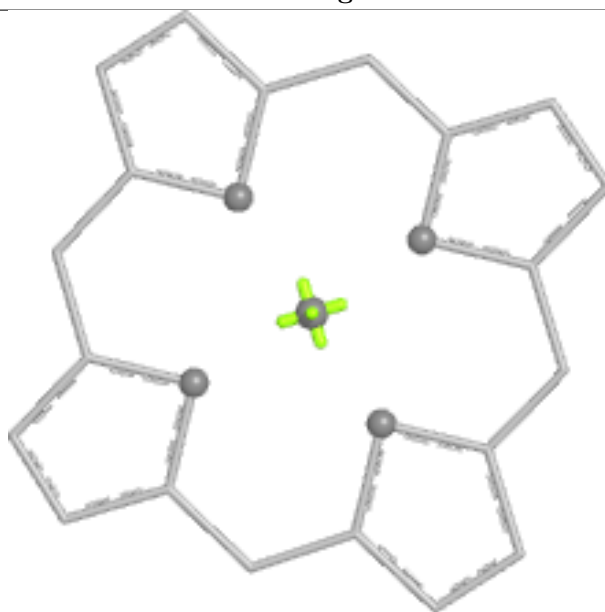
Bond lengths



Bond angles

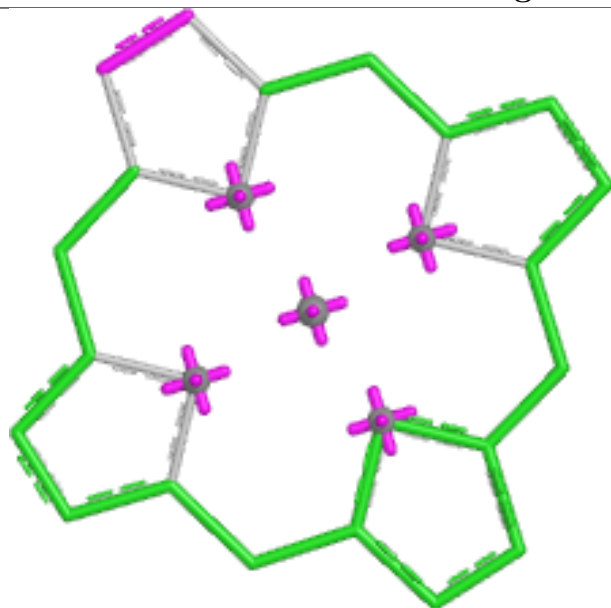


Torsions

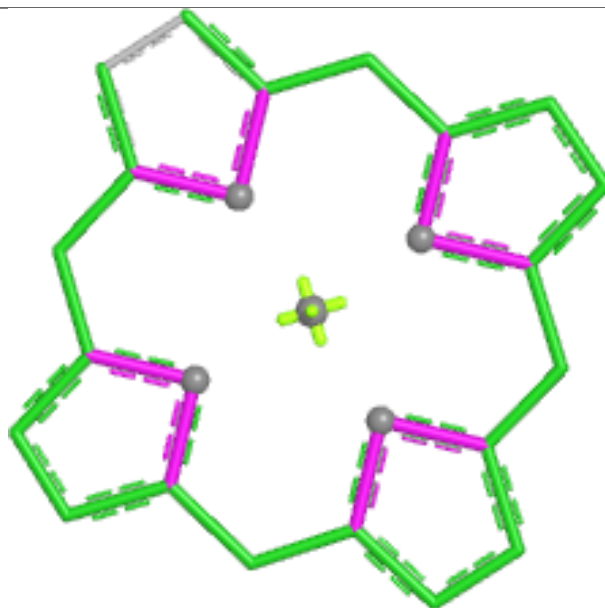


Rings

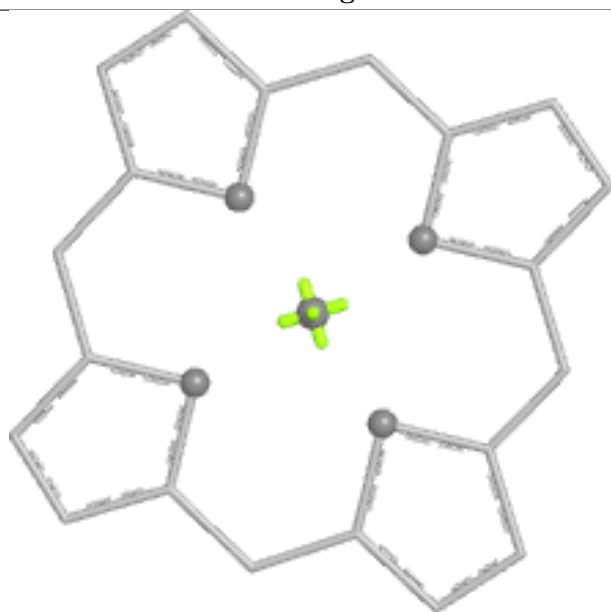
Ligand CLA B 651



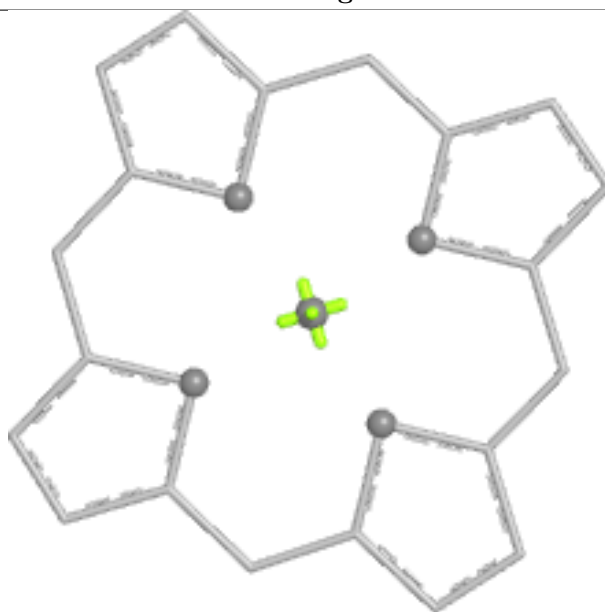
Bond lengths



Bond angles

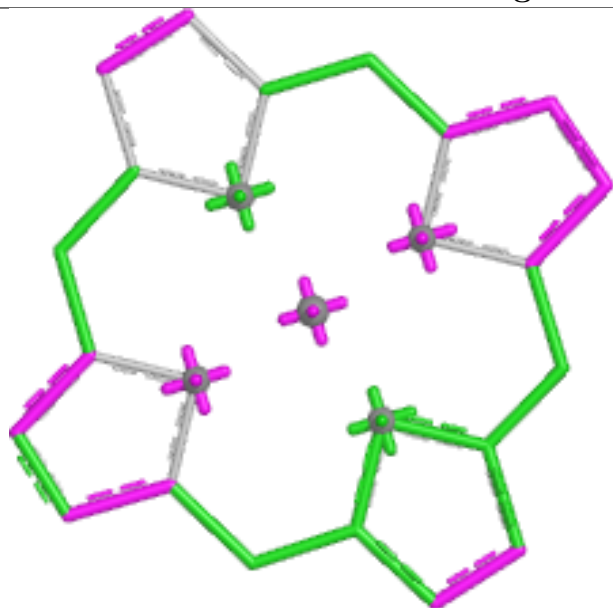


Torsions

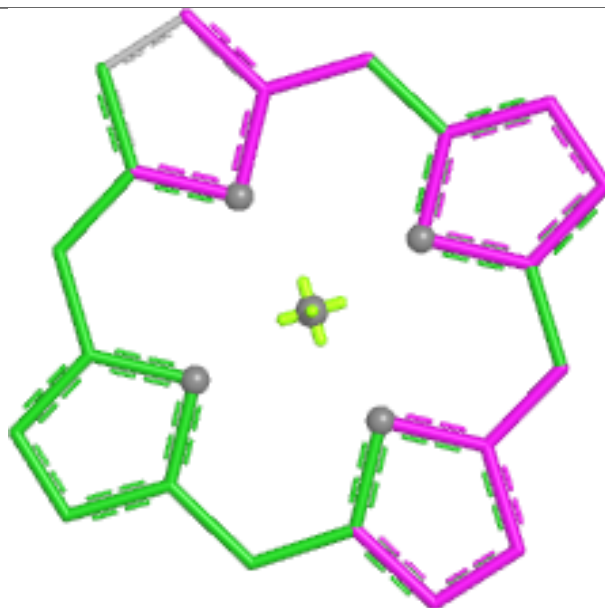


Rings

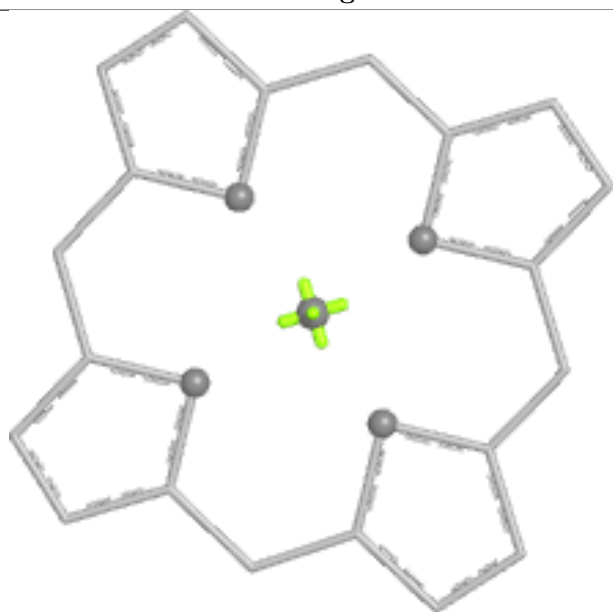
Ligand CLA A 615



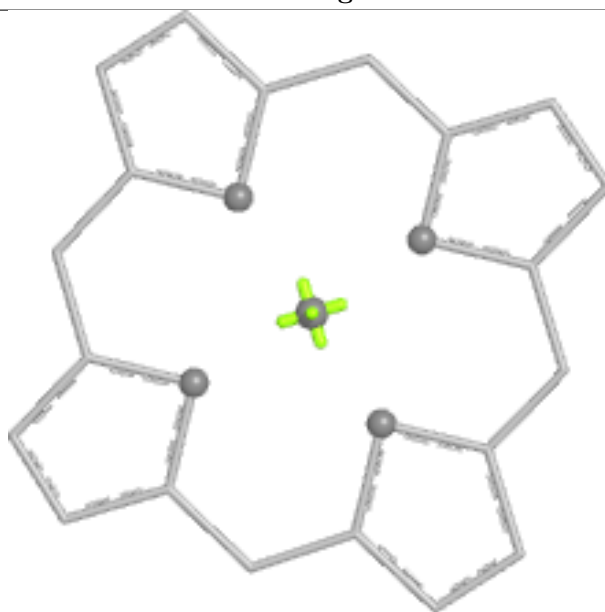
Bond lengths



Bond angles

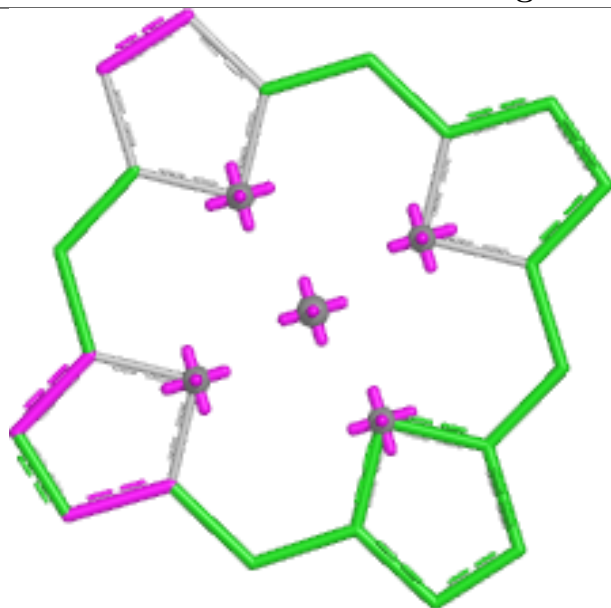


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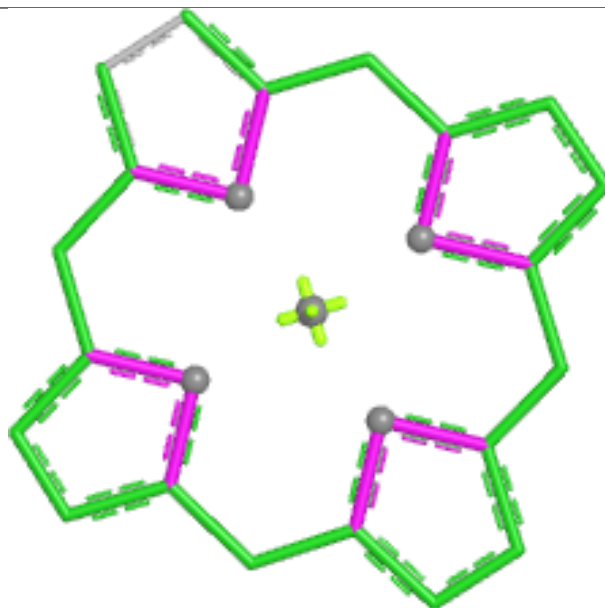


Rings

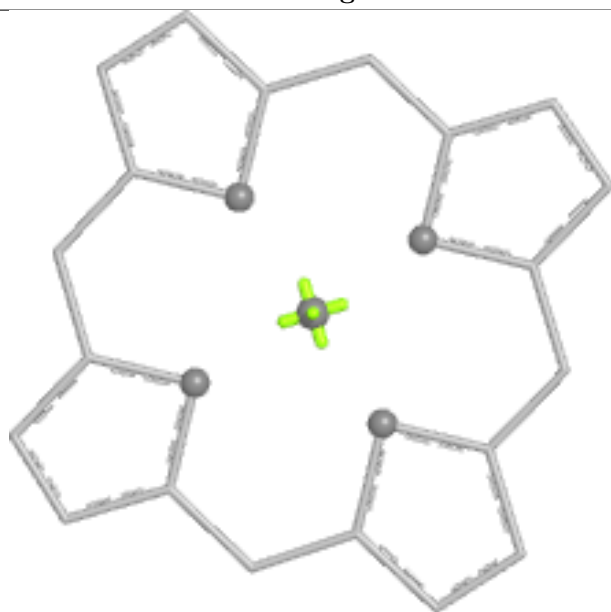
Ligand CLA F 157



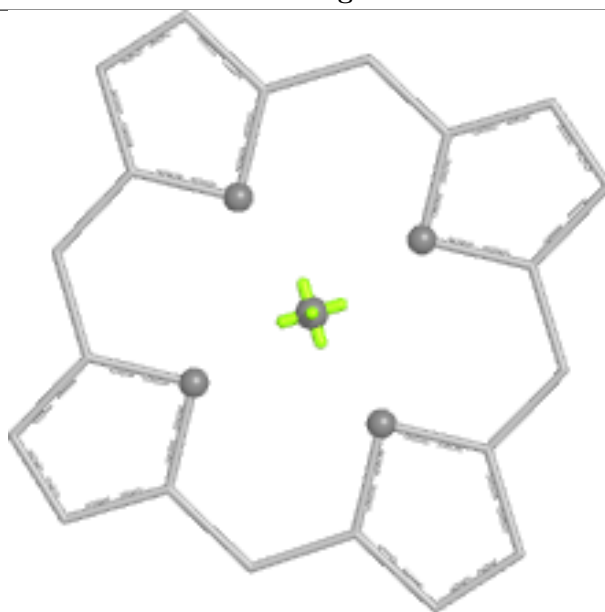
Bond lengths



Bond angles

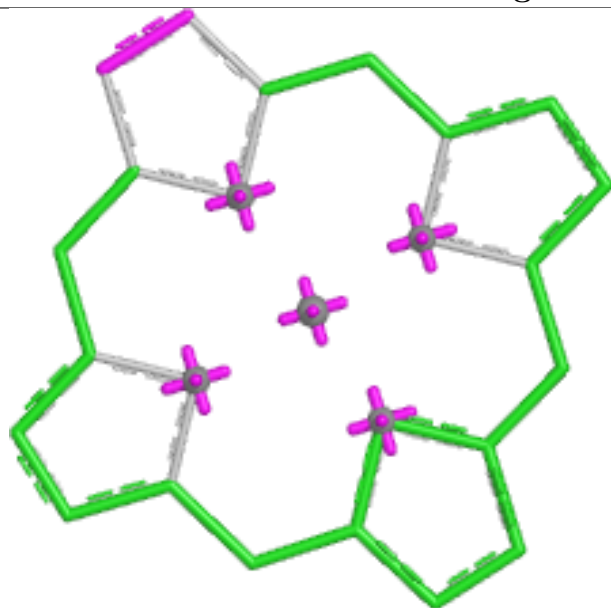


Torsions

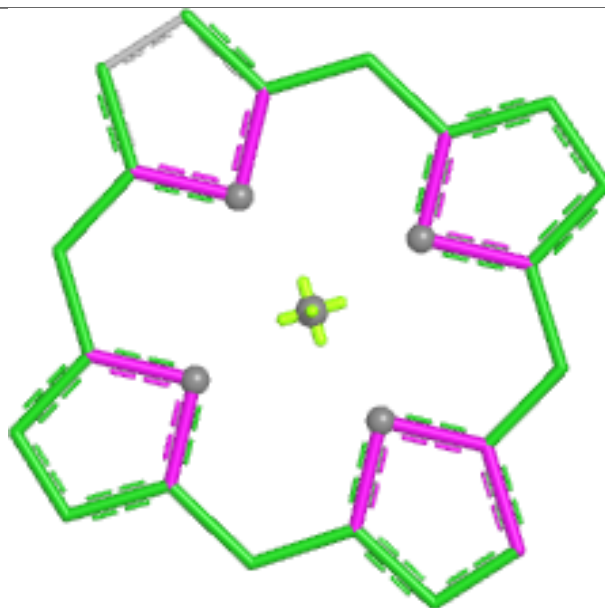


Rings

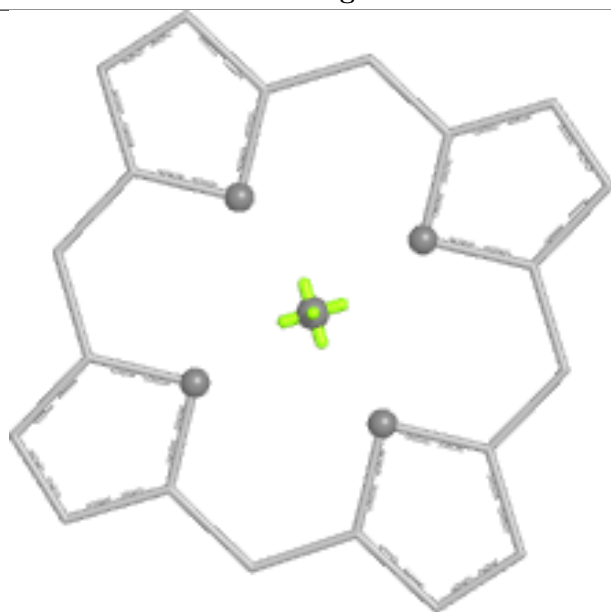
Ligand CLA A 609



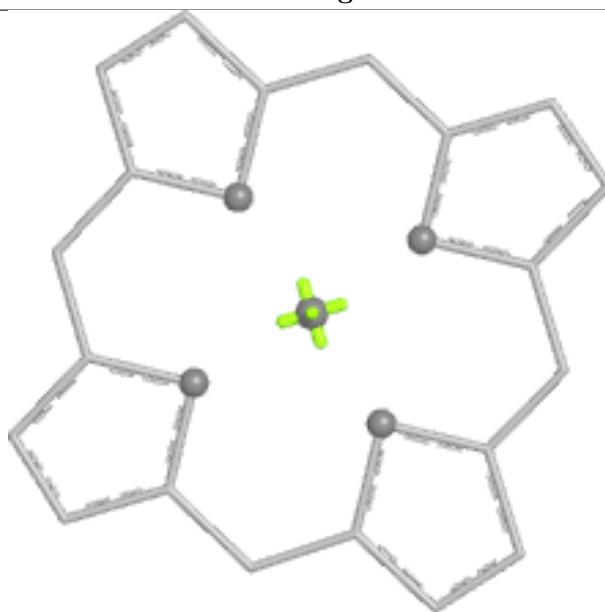
Bond lengths



Bond angles

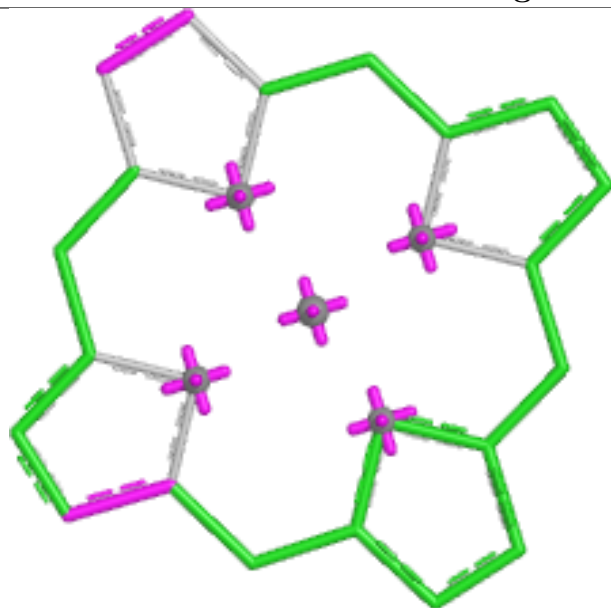


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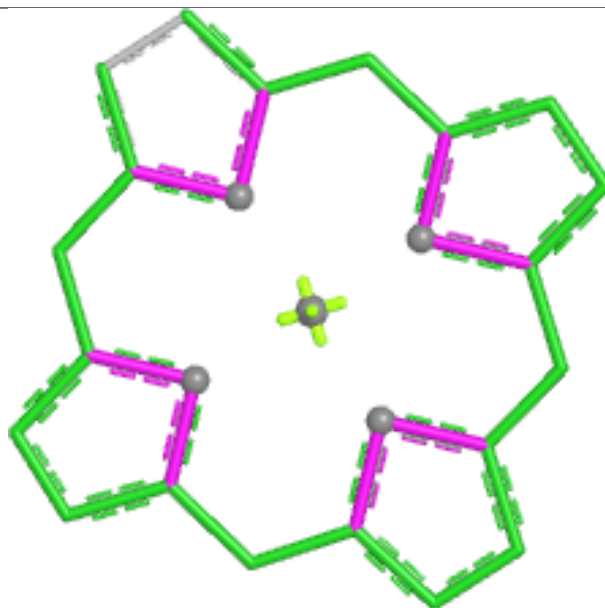


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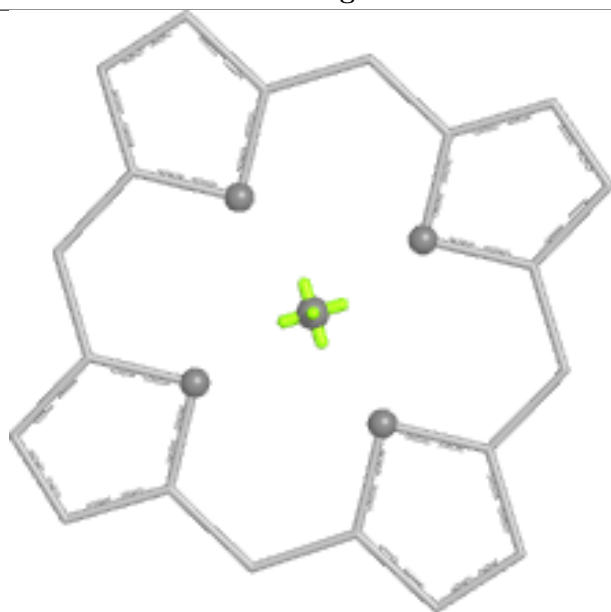
Ligand CLA A 616



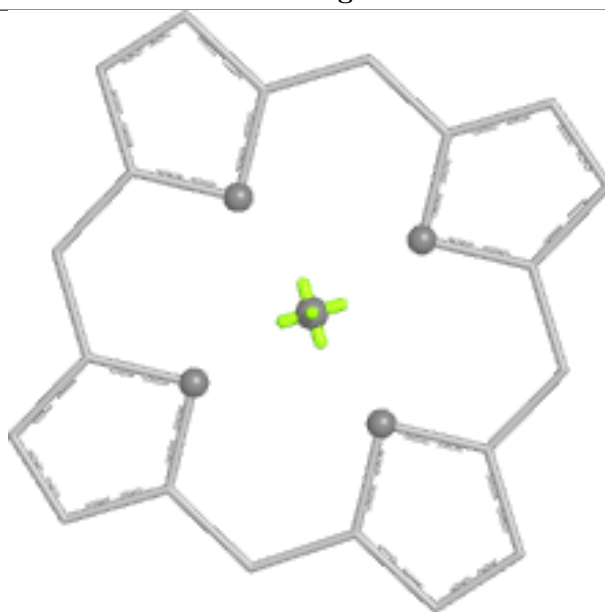
Bond lengths



Bond angles

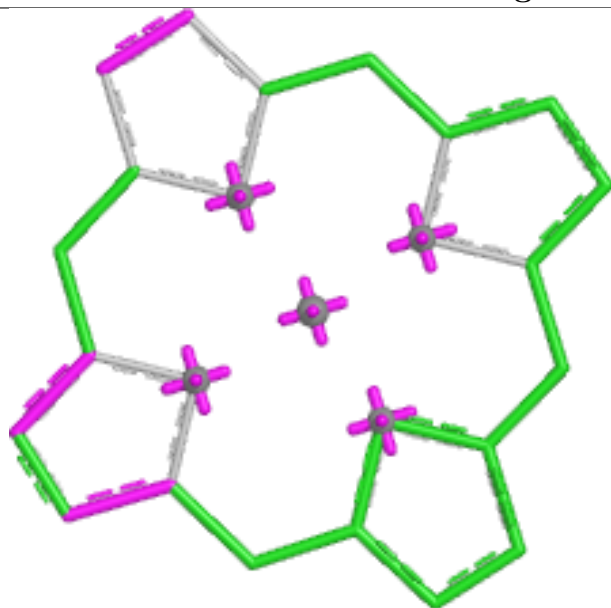


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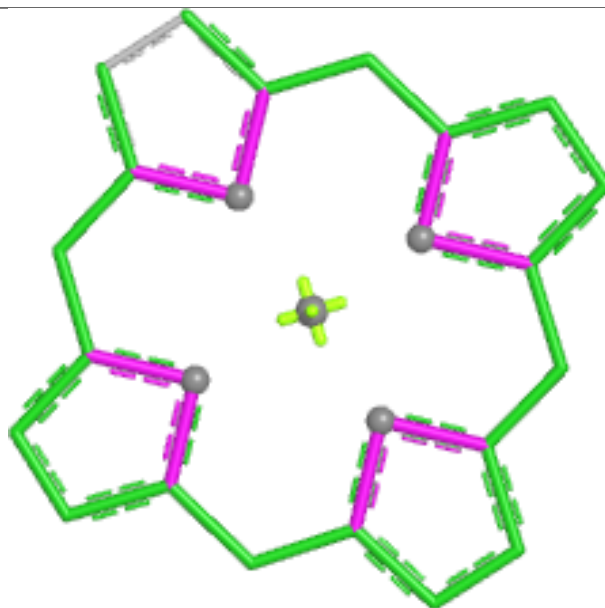


Rings

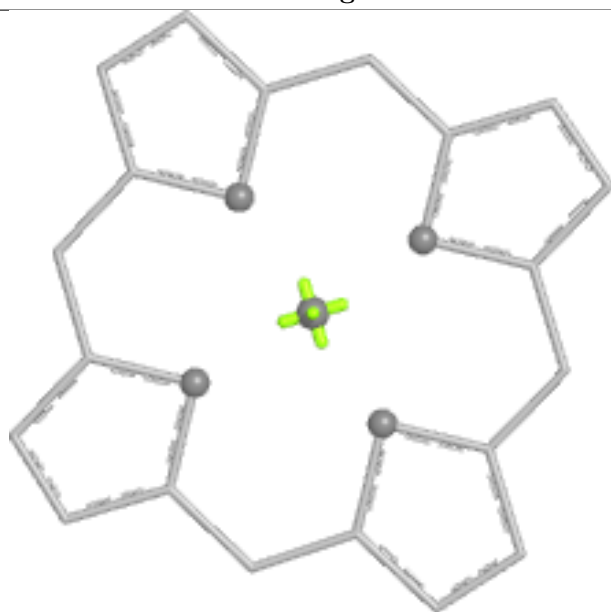
Ligand CLA B 633



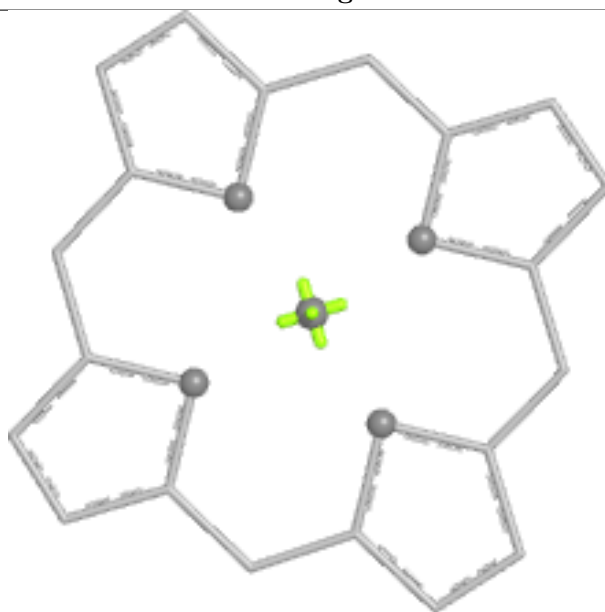
Bond lengths



Bond angles

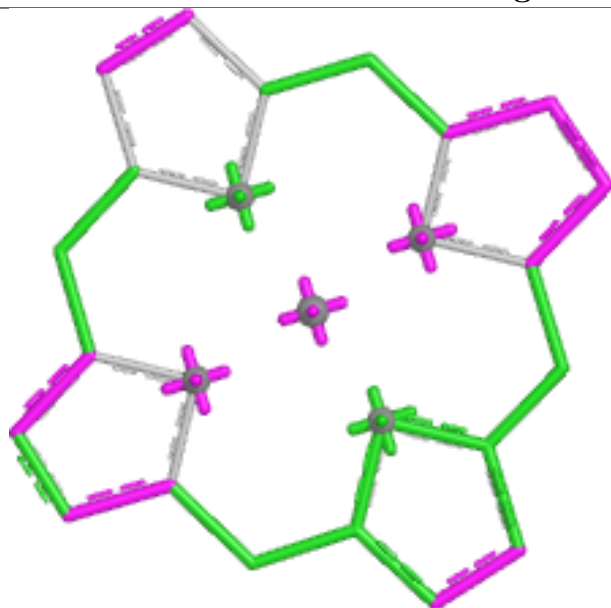


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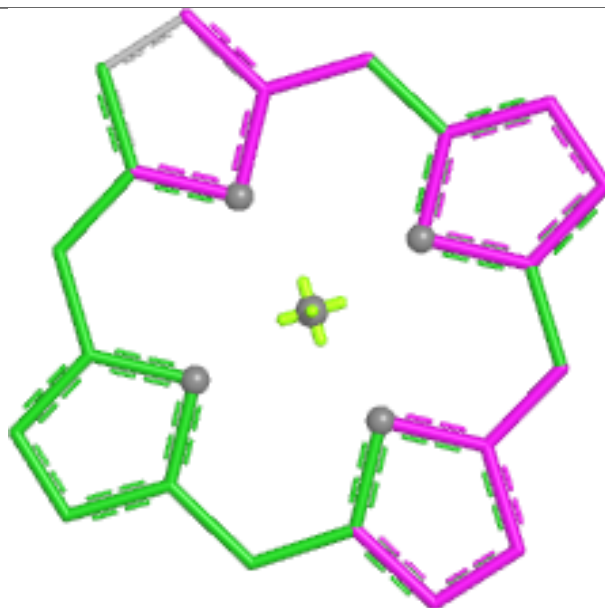


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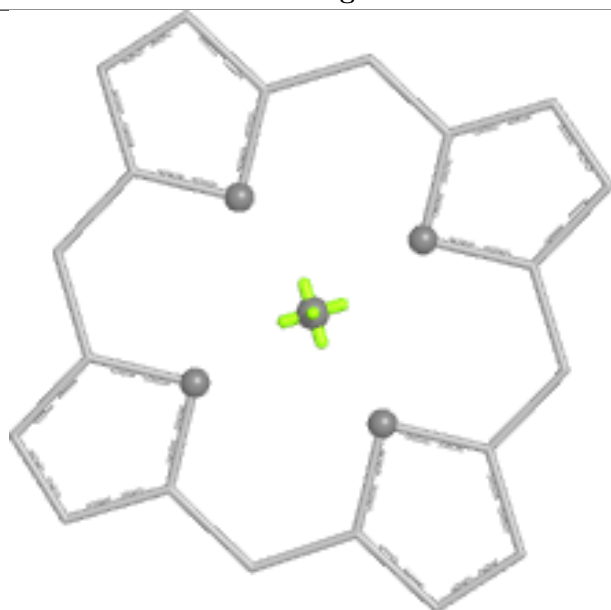
Ligand CLA A 614



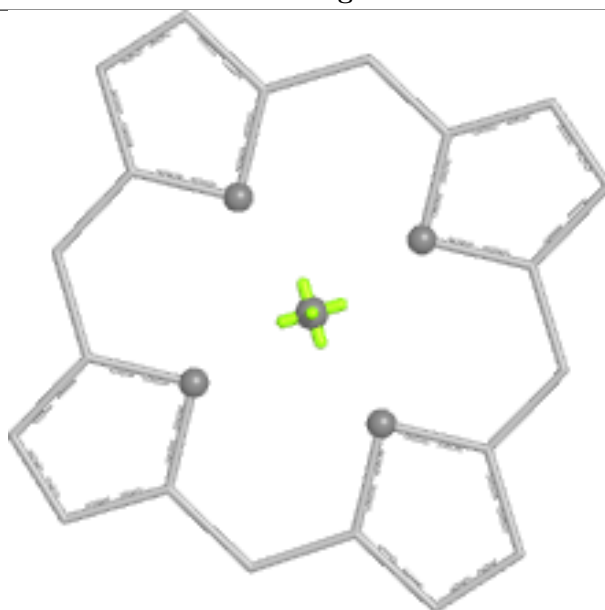
Bond lengths



Bond angles

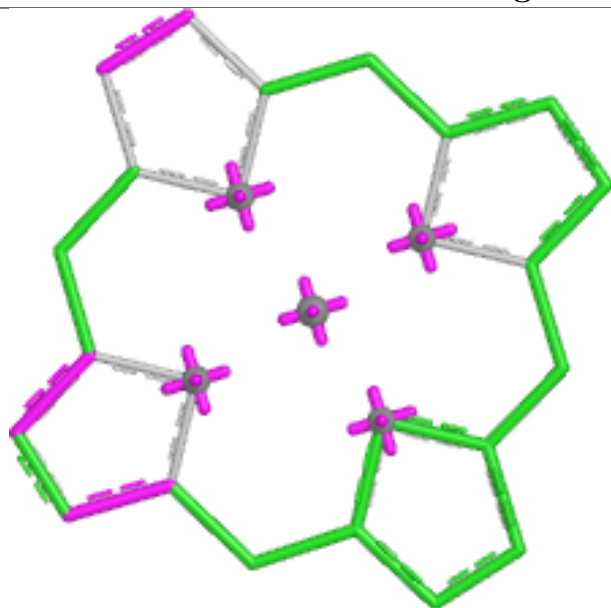


Torsions

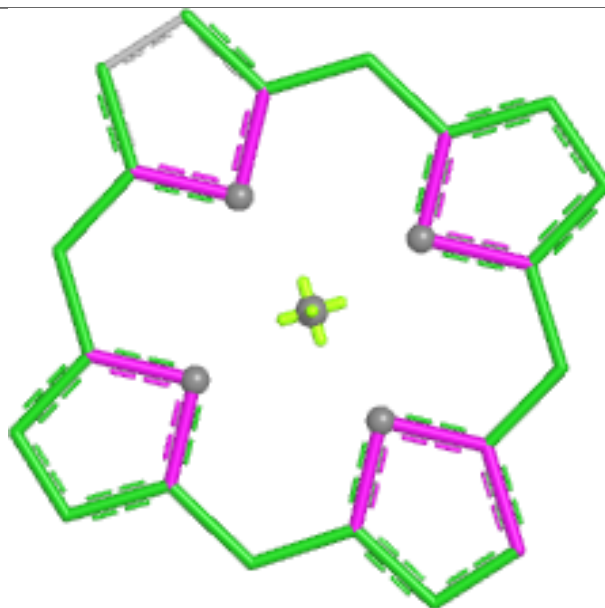


Rings

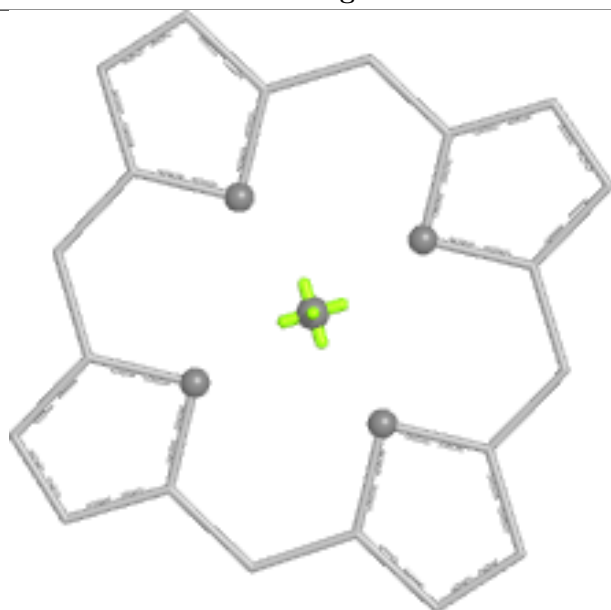
Ligand CLA A 605



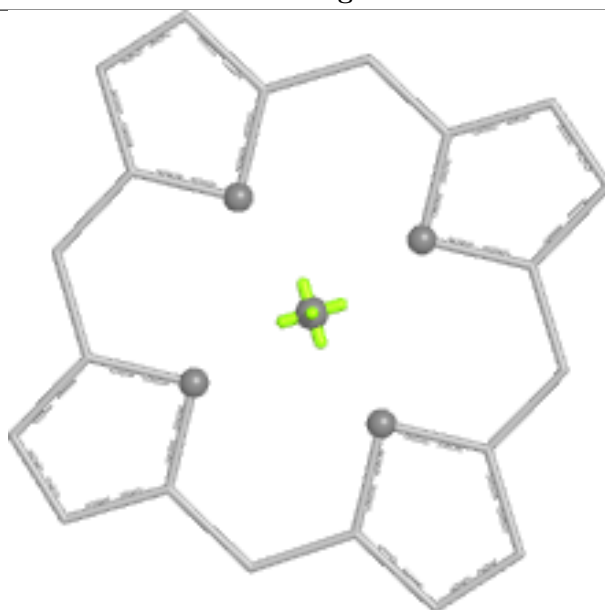
Bond lengths



Bond angles

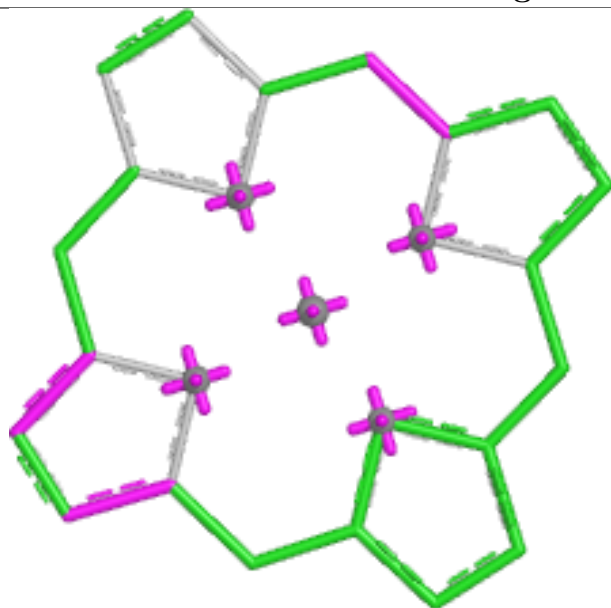


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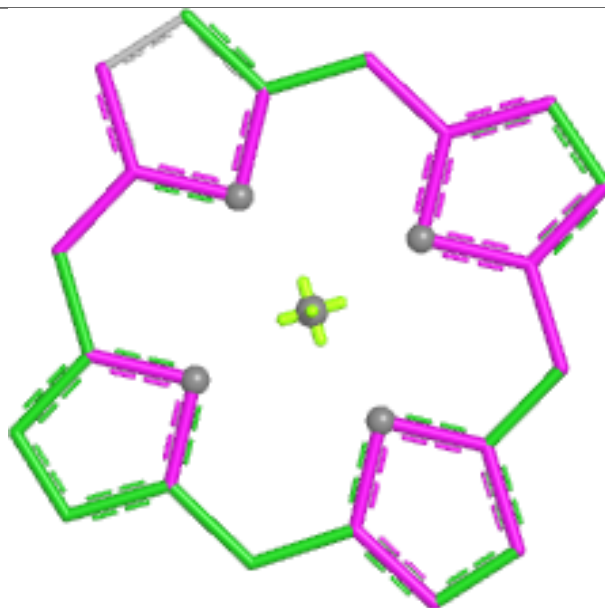


Rings

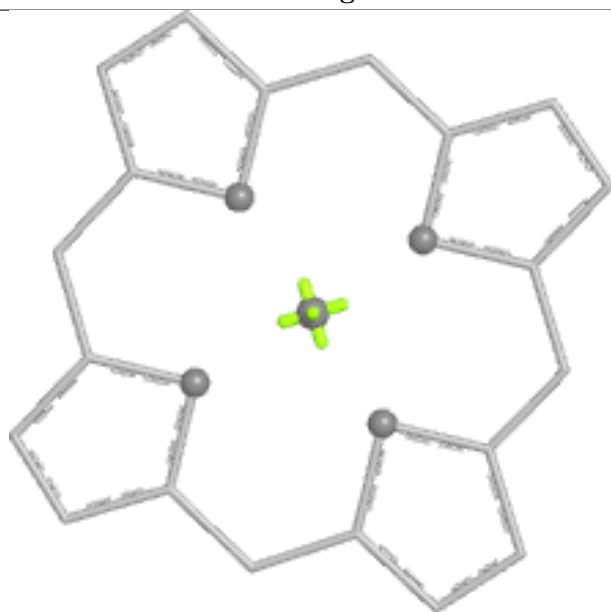
Ligand CLA A 612



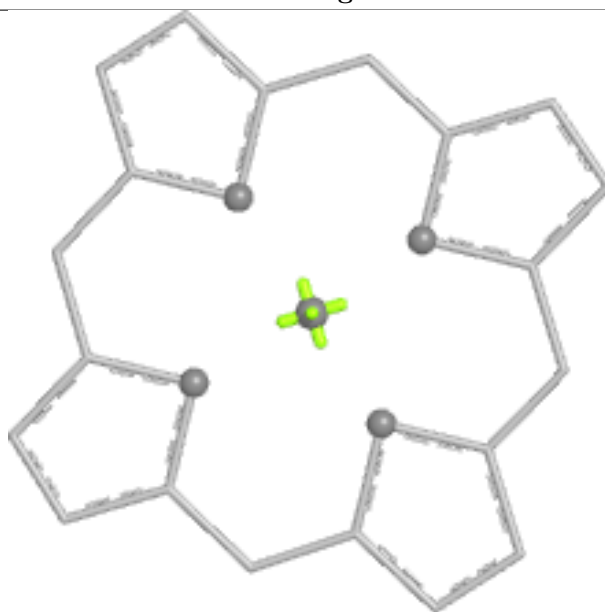
Bond lengths



Bond angles

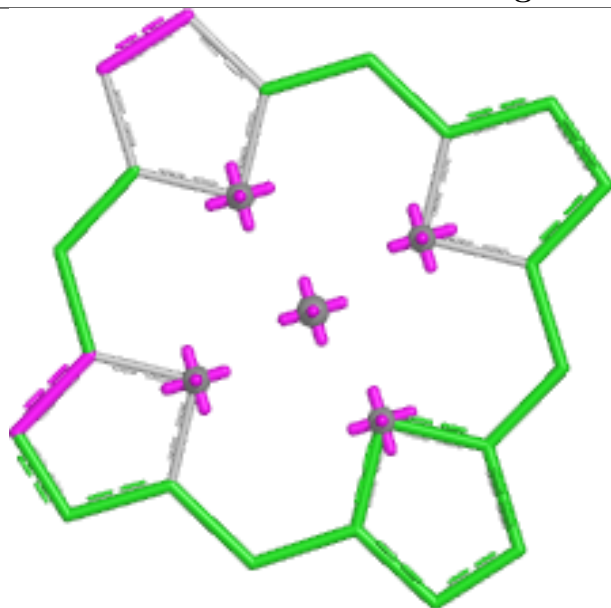


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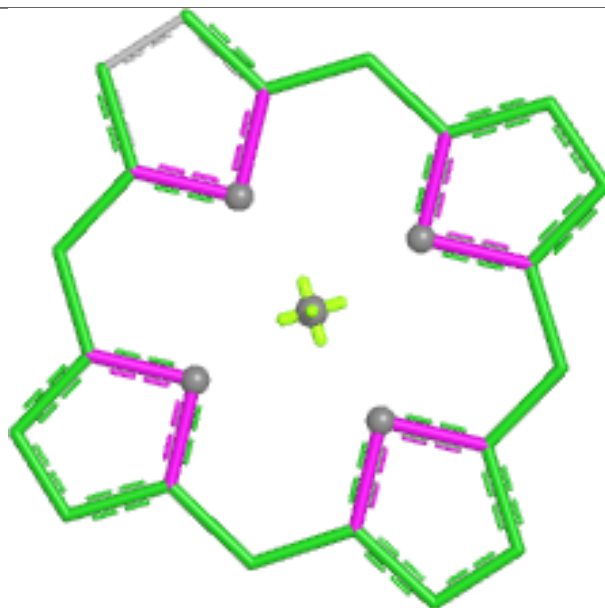


Rings

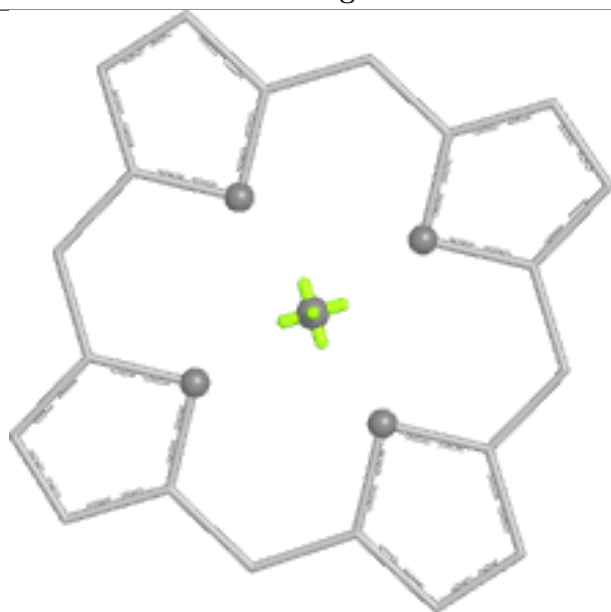
Ligand CLA B 642



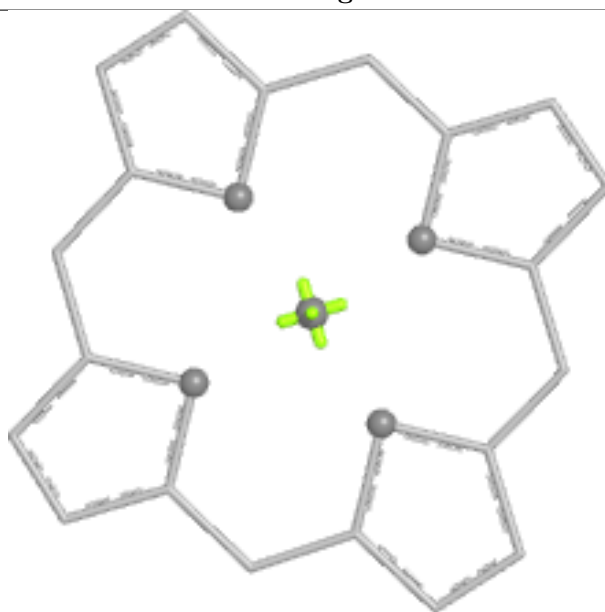
Bond lengths



Bond angles

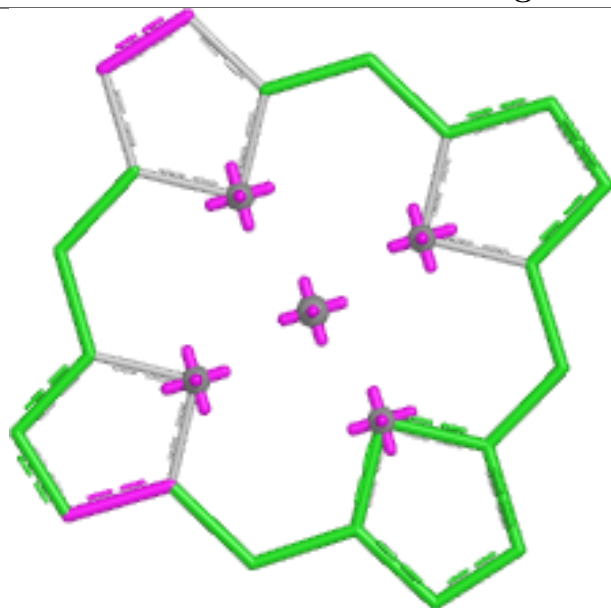


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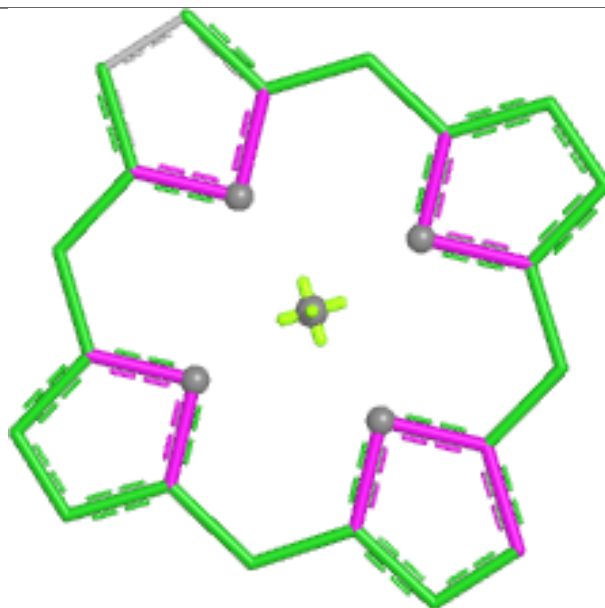


Rings

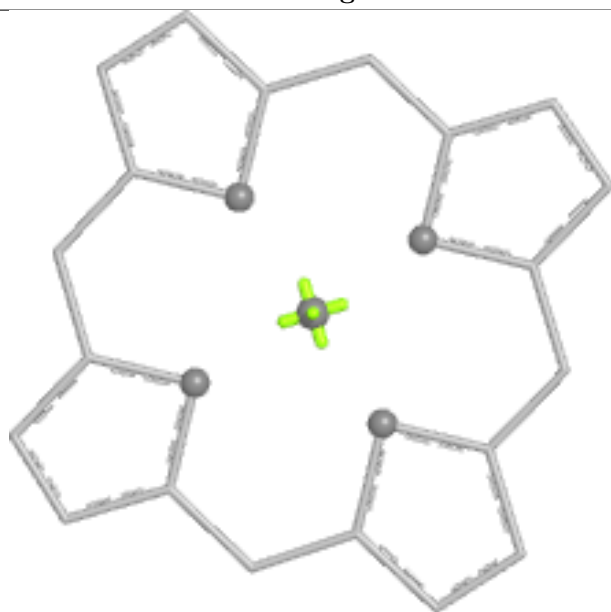
Ligand CLA B 625



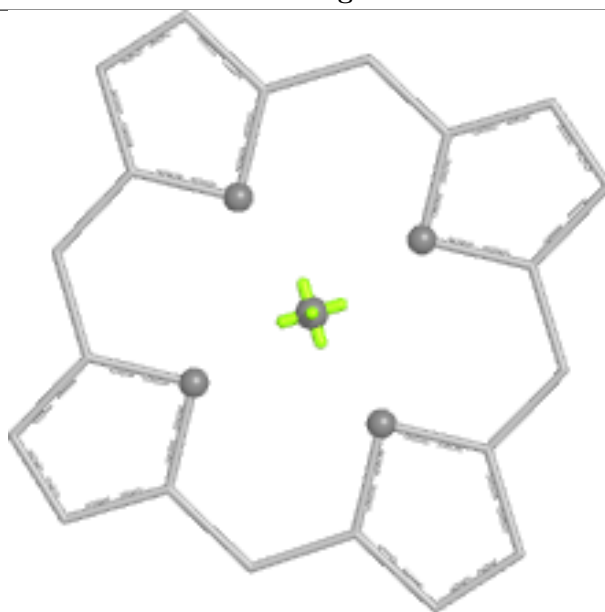
Bond lengths



Bond angles

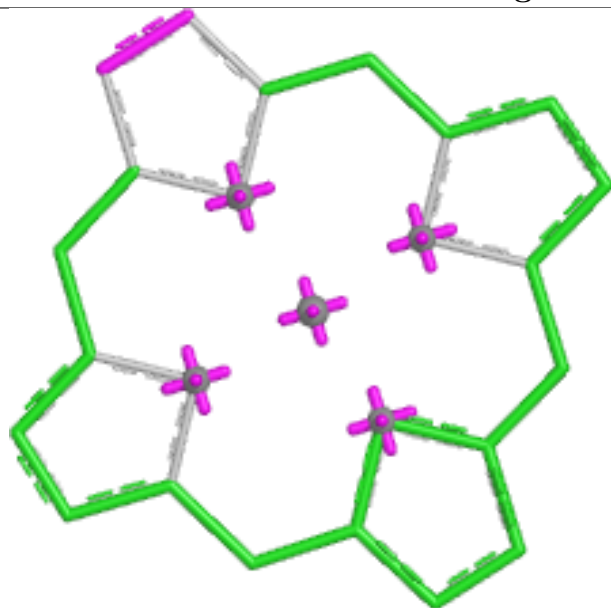


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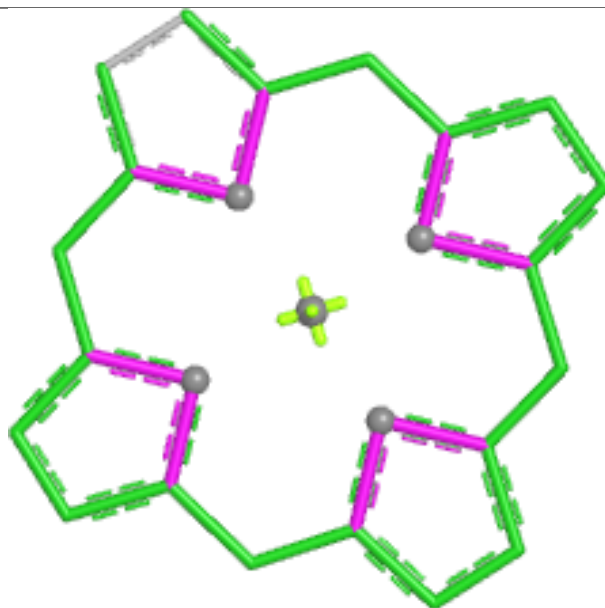


Rings

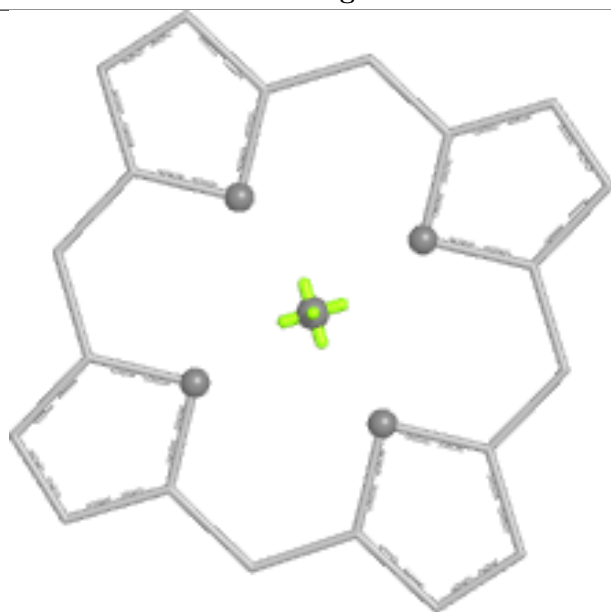
Ligand CLA B 653



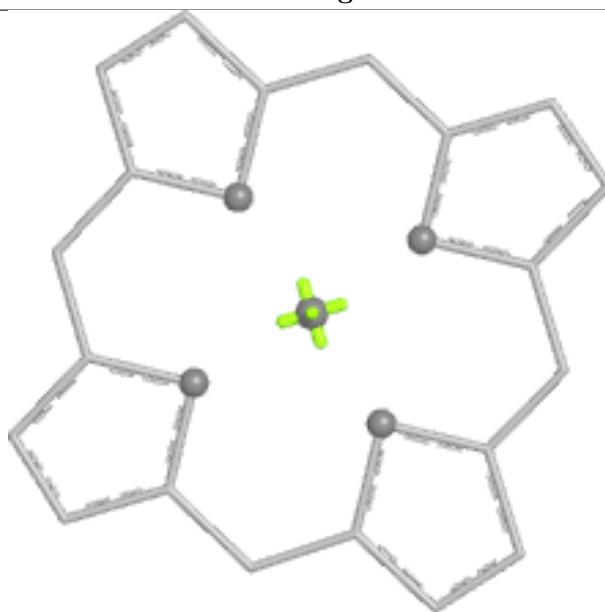
Bond lengths



Bond angles

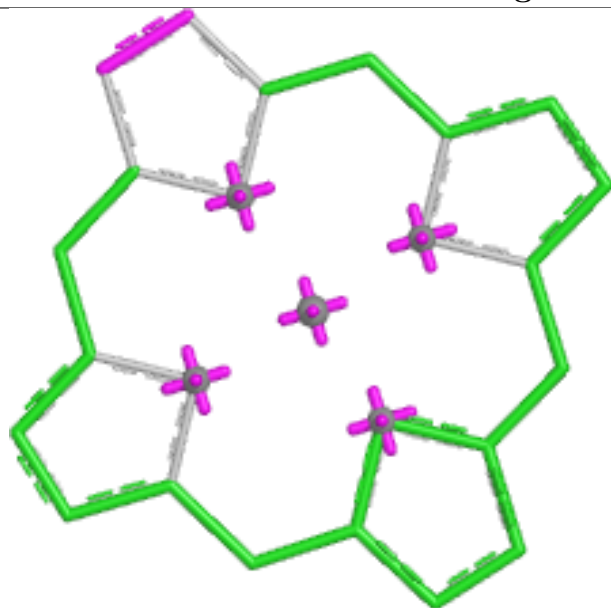


Torsions

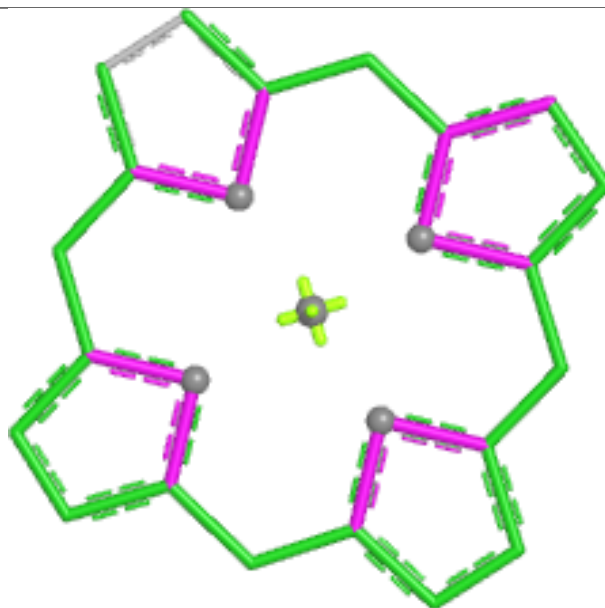


Rings

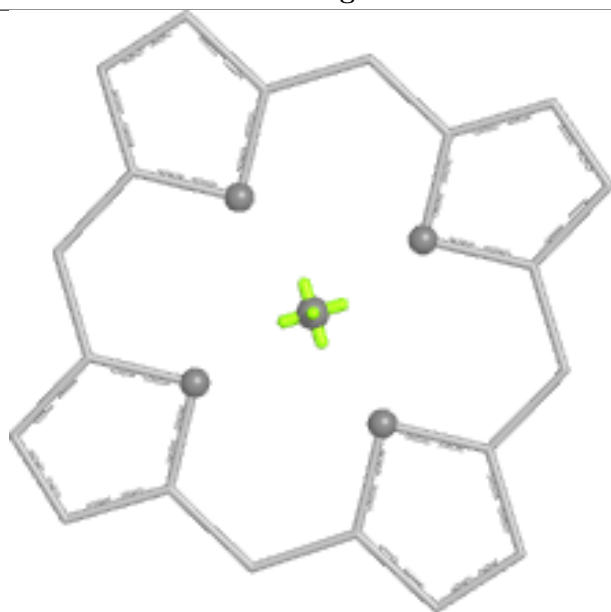
Ligand CLA B 626



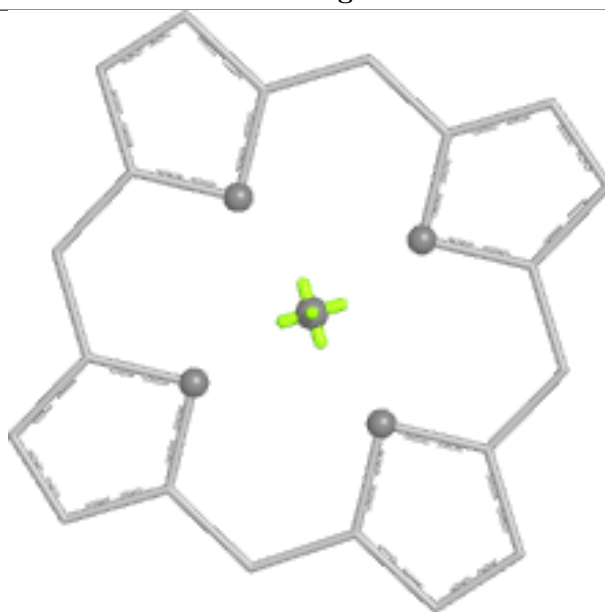
Bond lengths



Bond angles

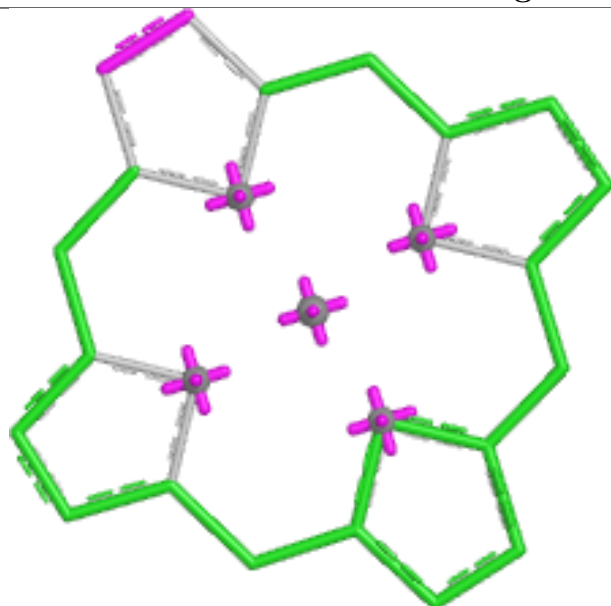


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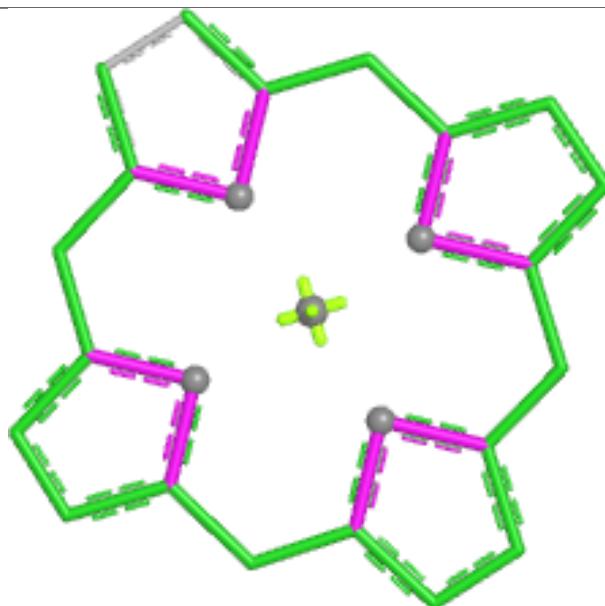


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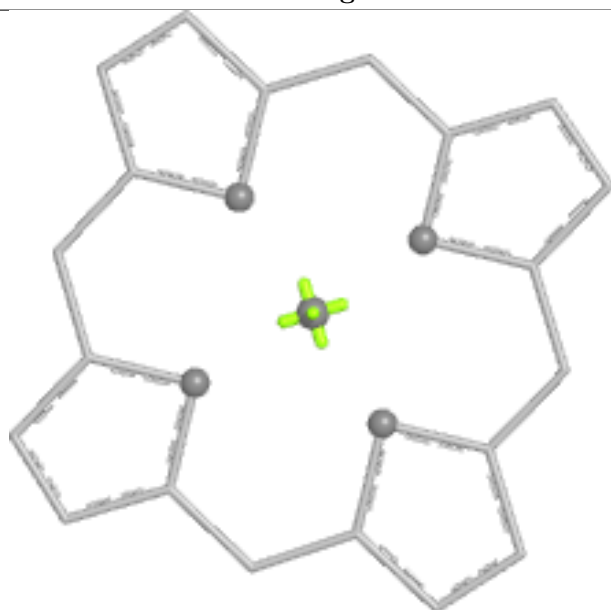
Ligand CLA B 650



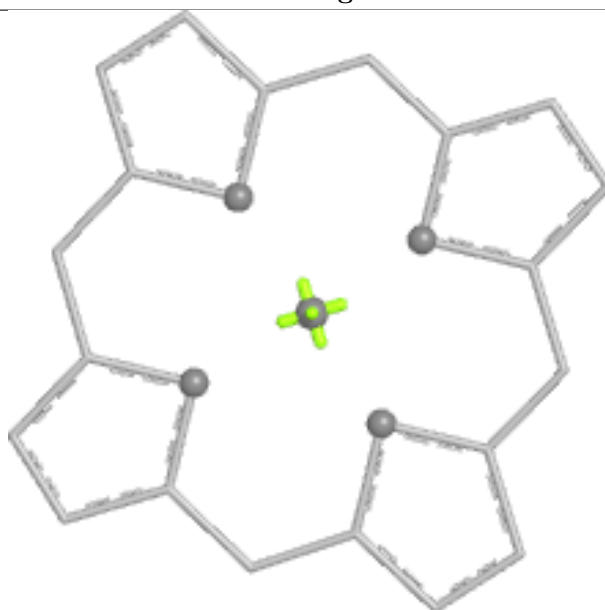
Bond lengths



Bond angles

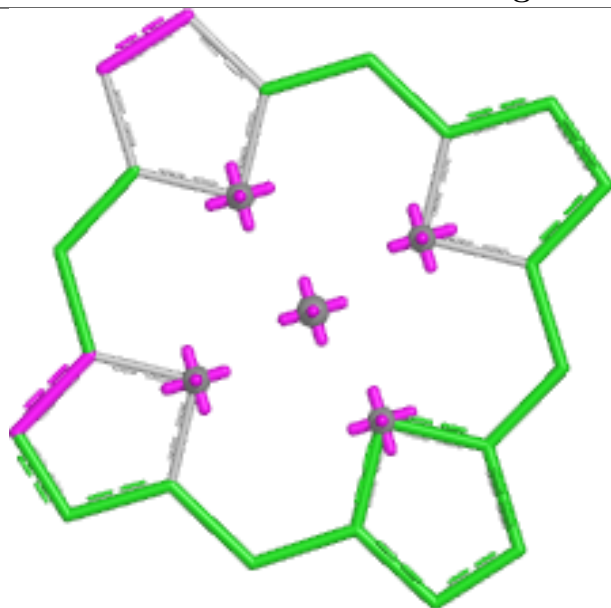


Torsions

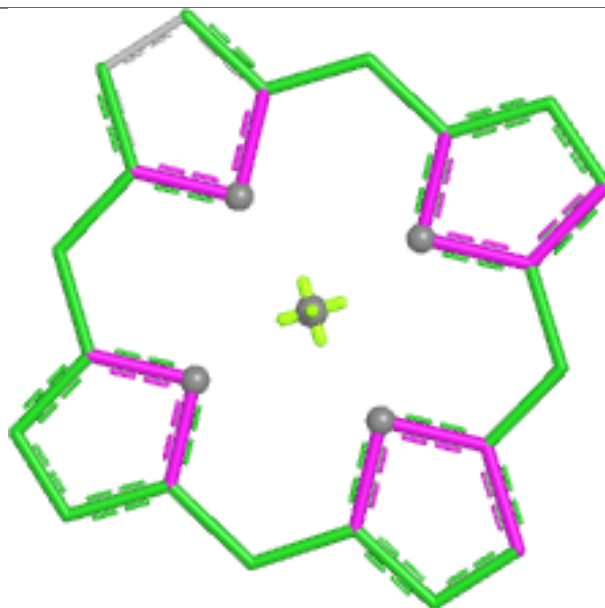


Rings

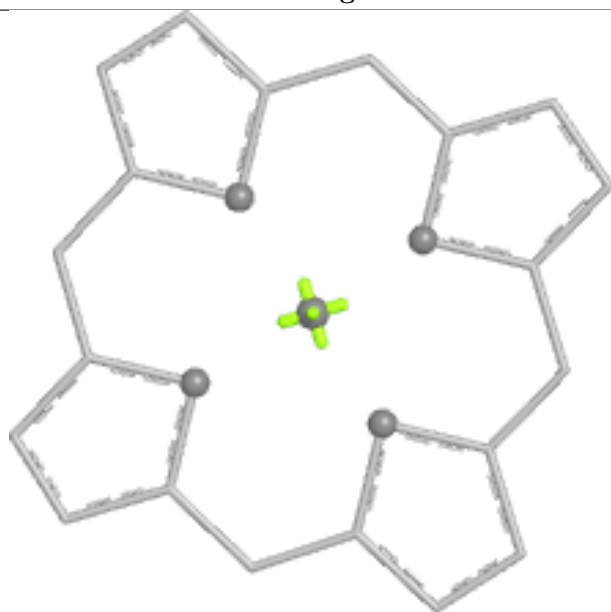
Ligand CLA K 135



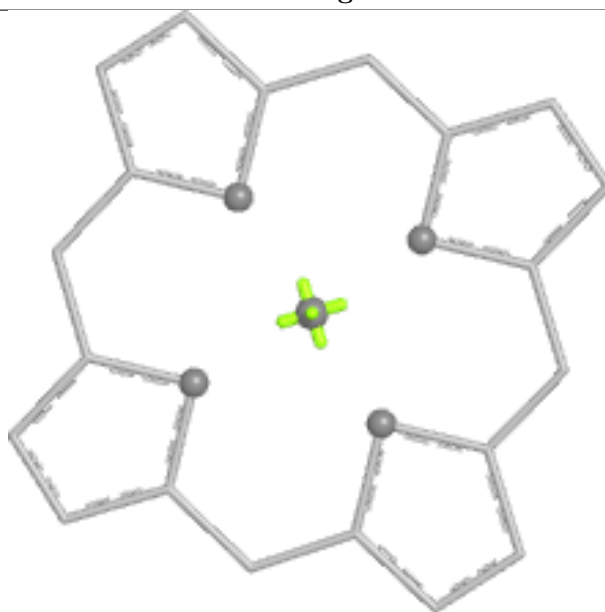
Bond lengths



Bond angles

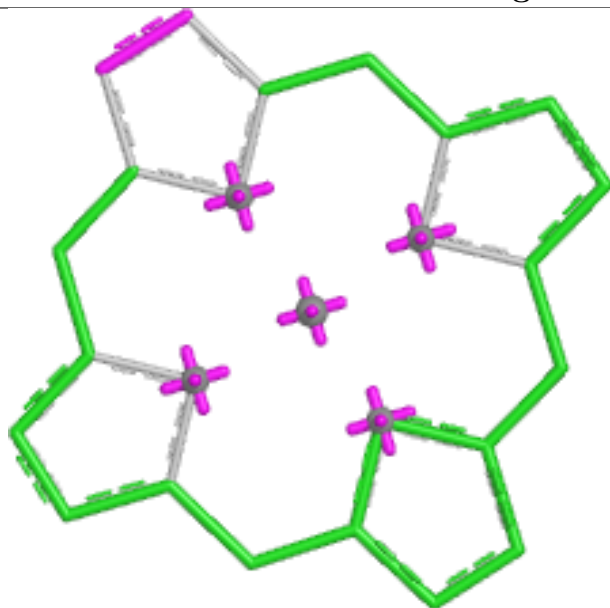


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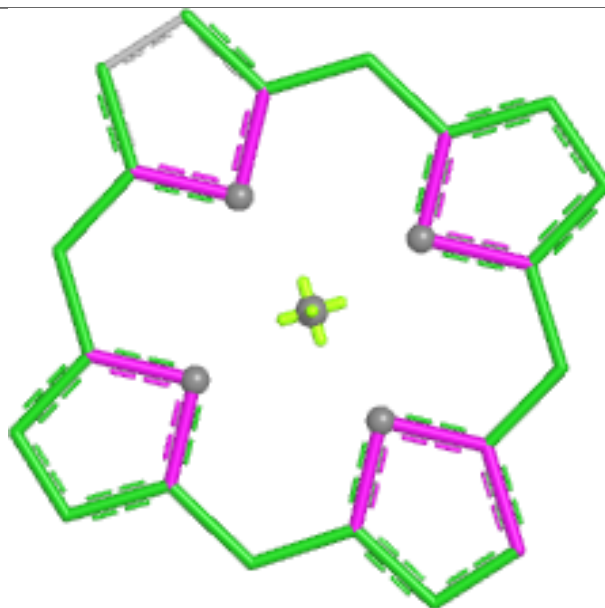


Rings

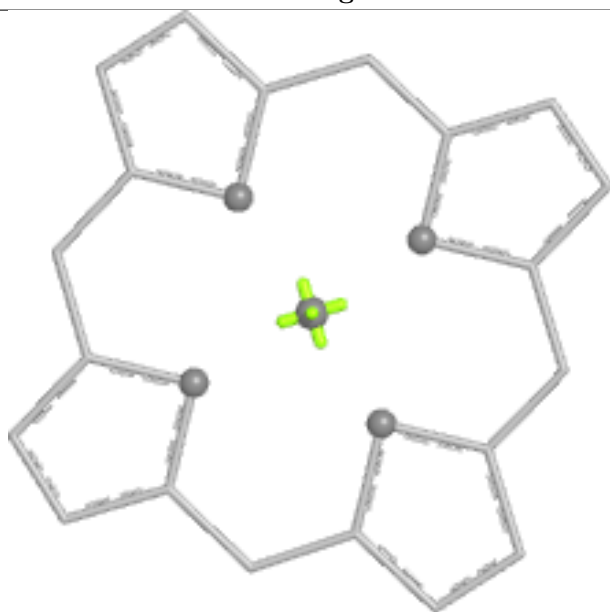
Ligand CLA A 622



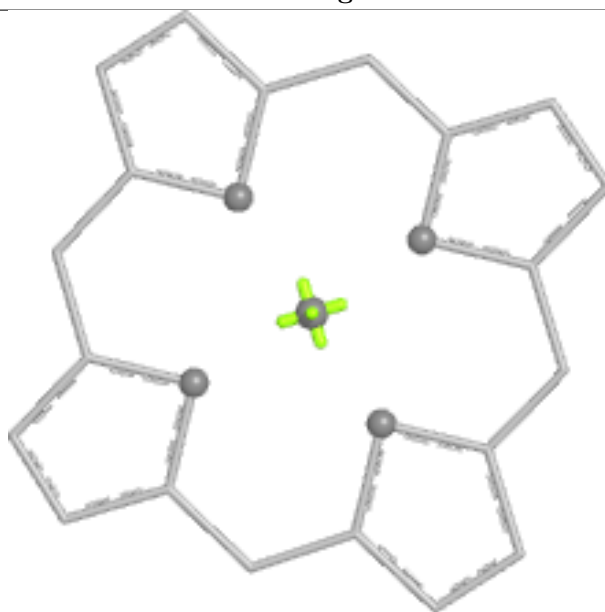
Bond lengths



Bond angles

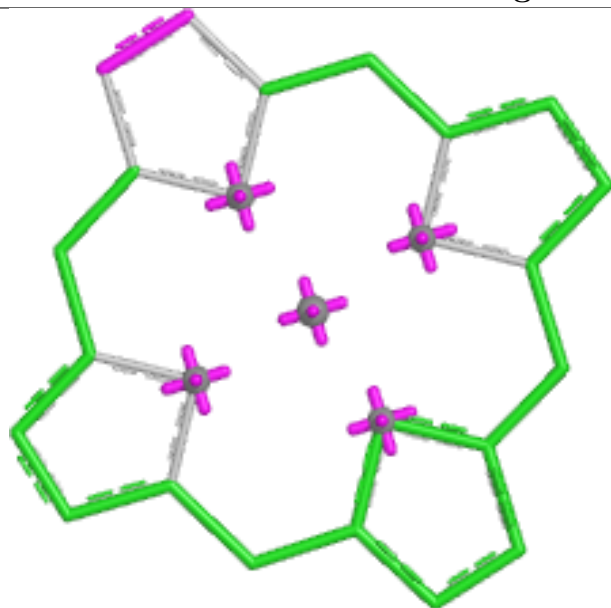


Torsions

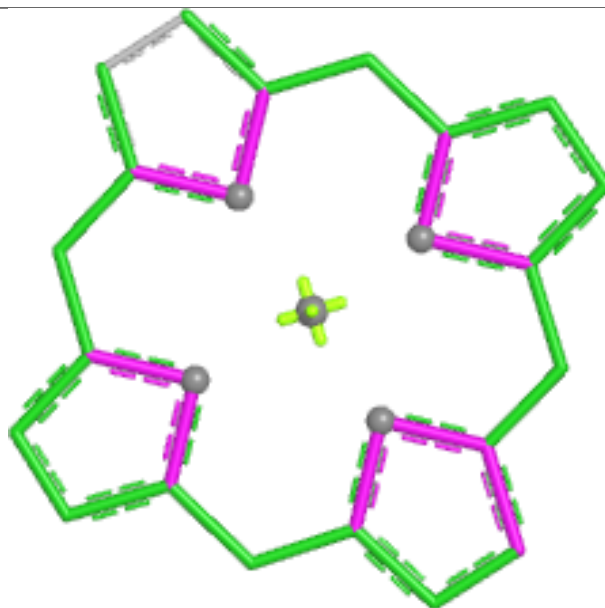


Rings

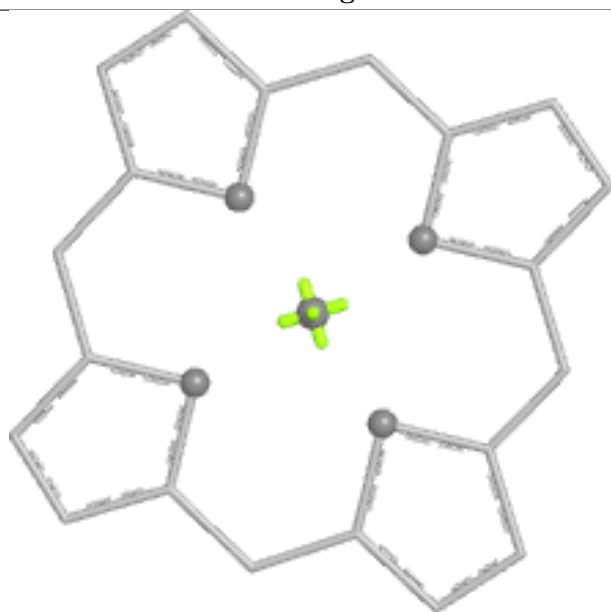
Ligand CLA A 610



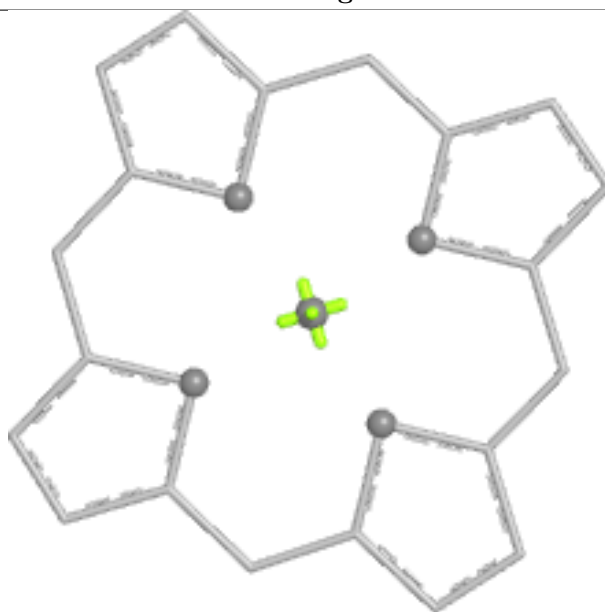
Bond lengths



Bond angles

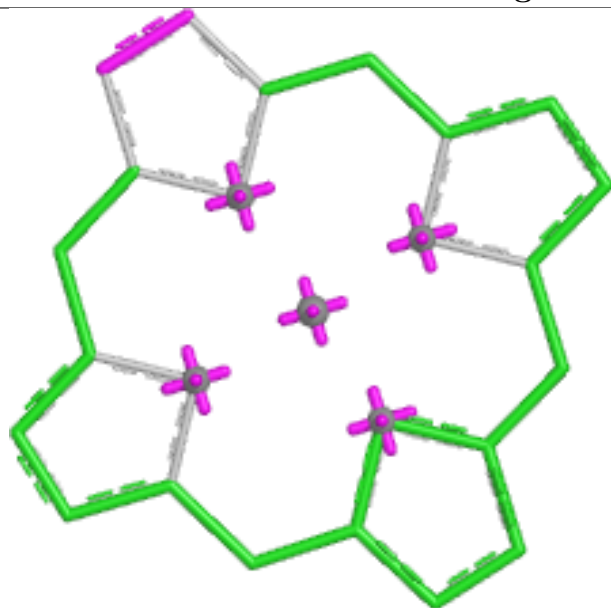


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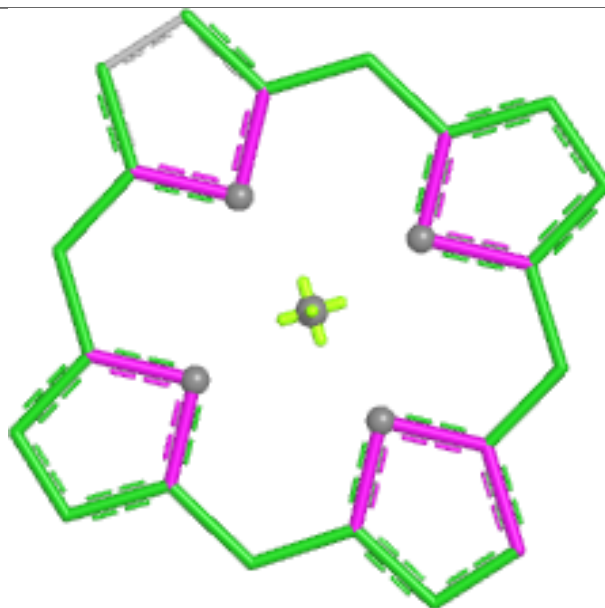


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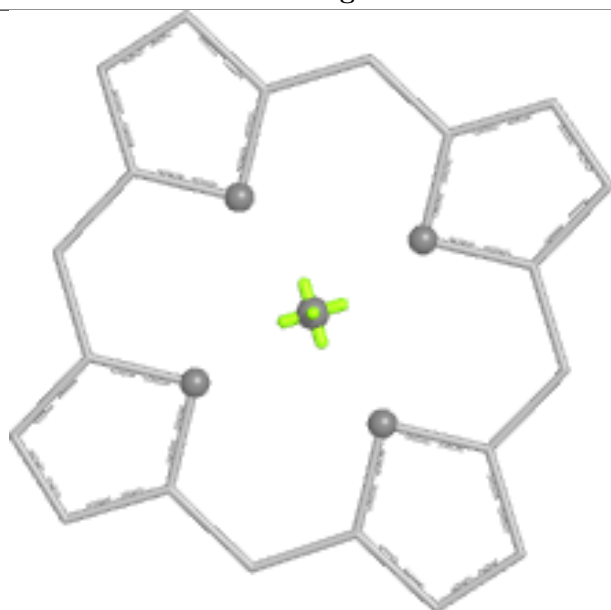
Ligand CLA B 631



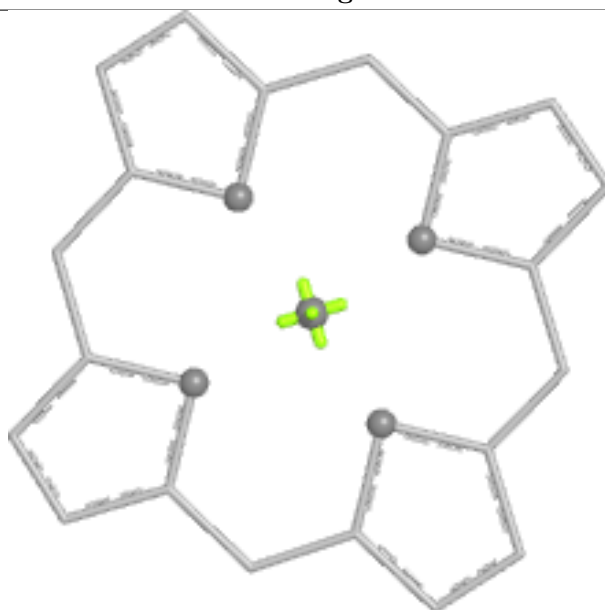
Bond lengths



Bond angles

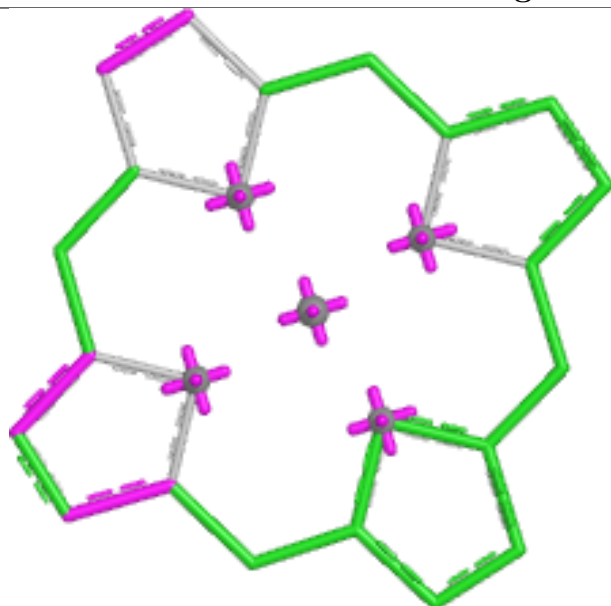


Torsions

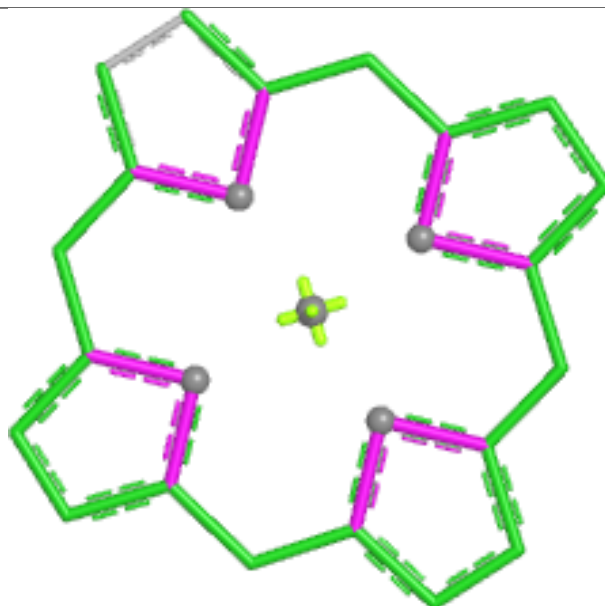


Rings

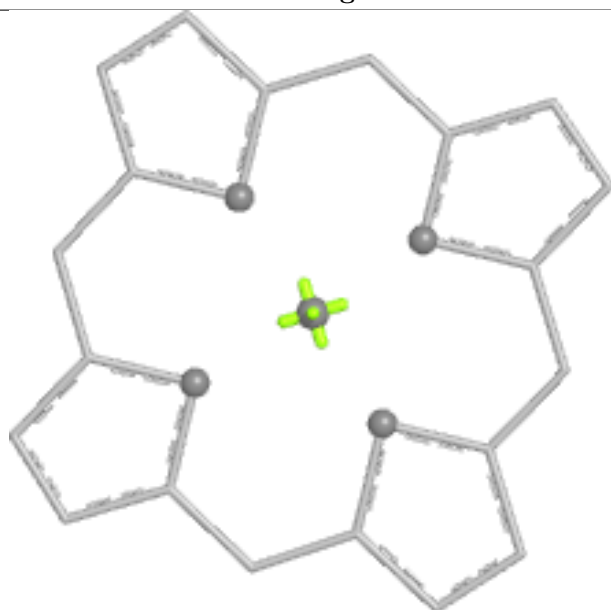
Ligand CLA B 622



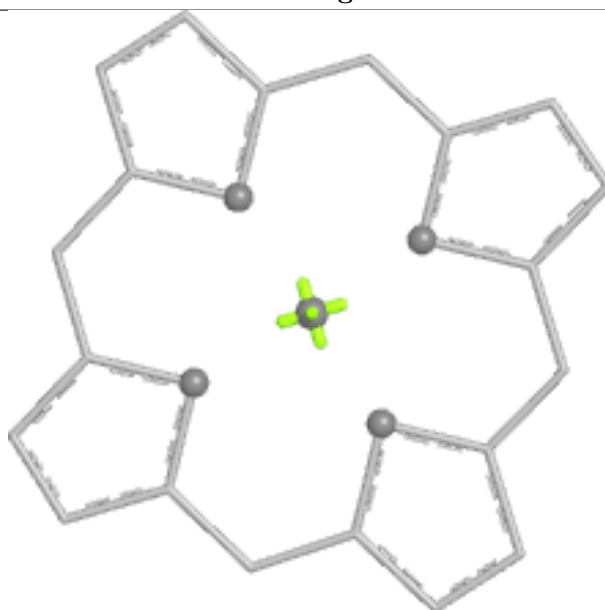
Bond lengths



Bond angles

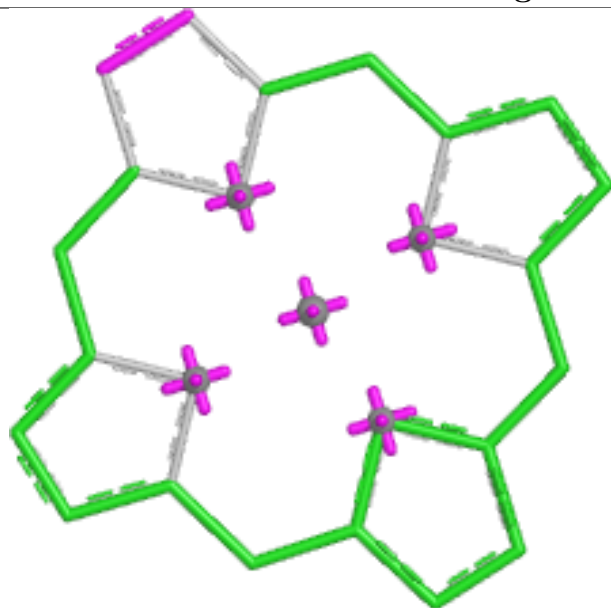


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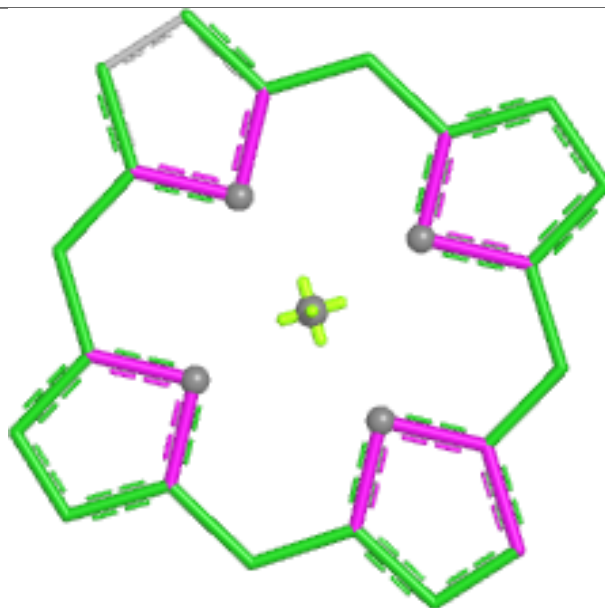


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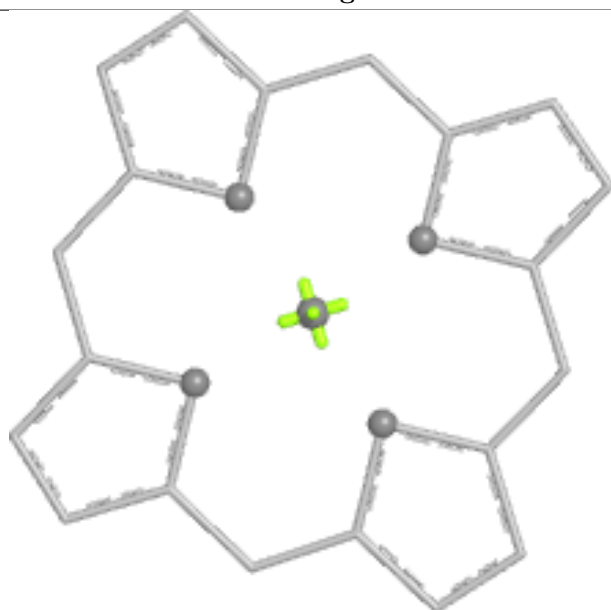
Ligand CLA B 636



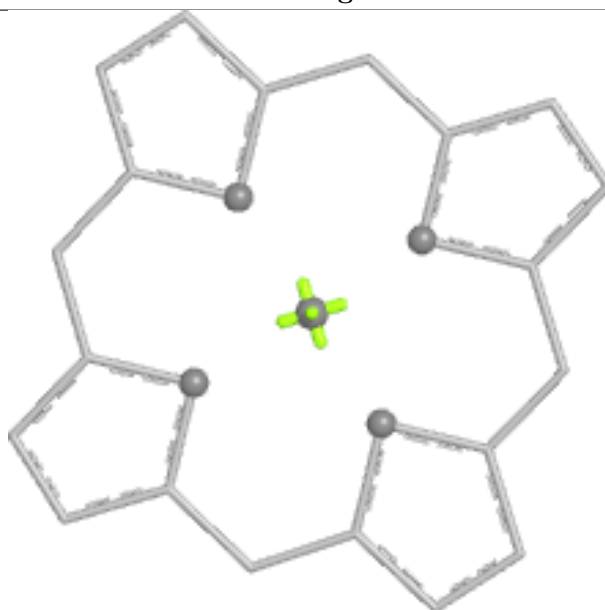
Bond lengths



Bond angles

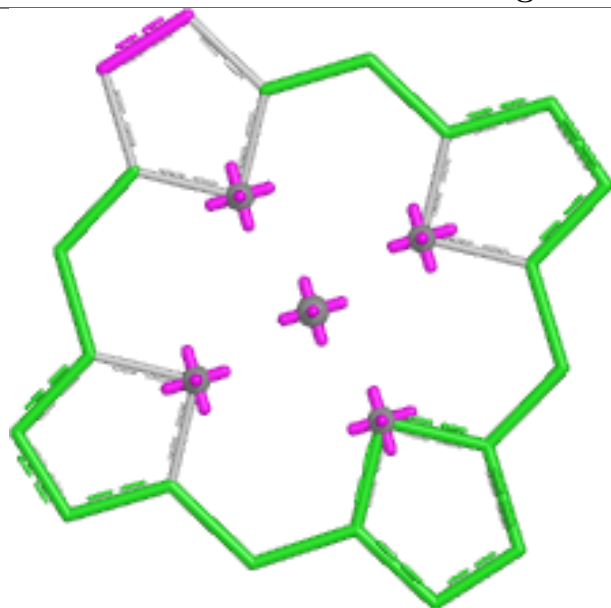


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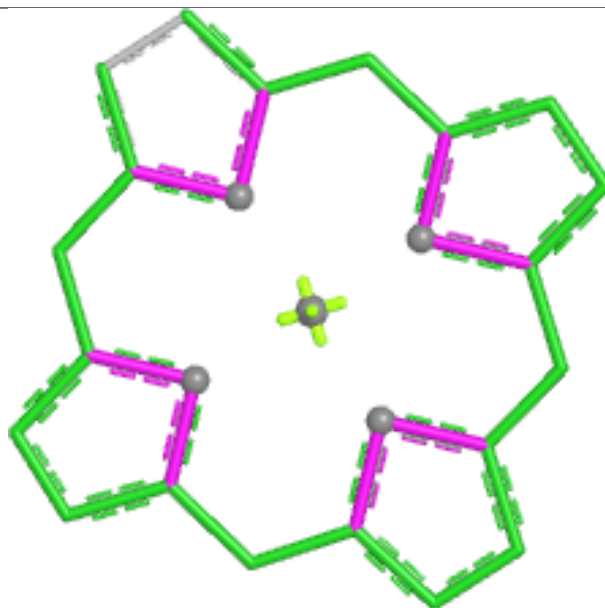


Rings

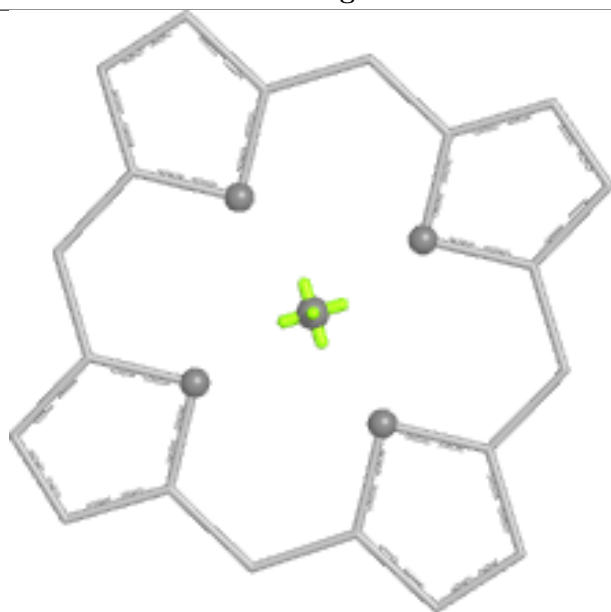
Ligand CLA L 163



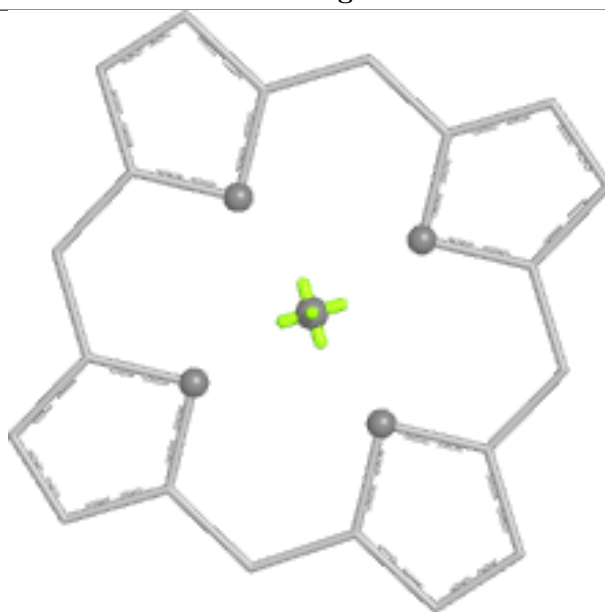
Bond lengths



Bond angles

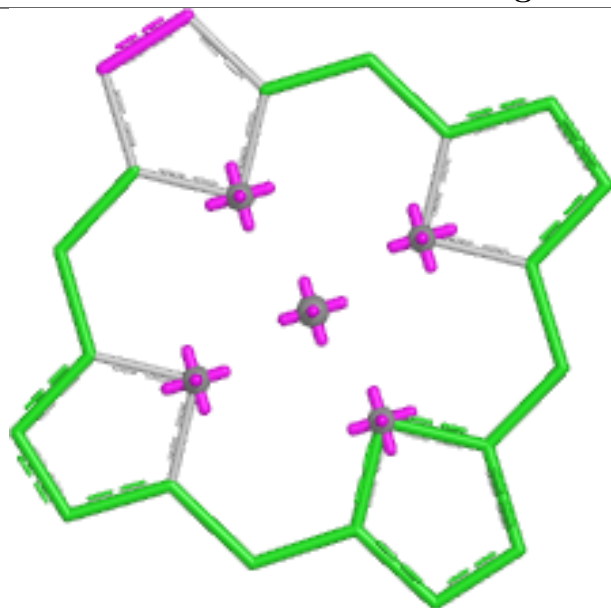


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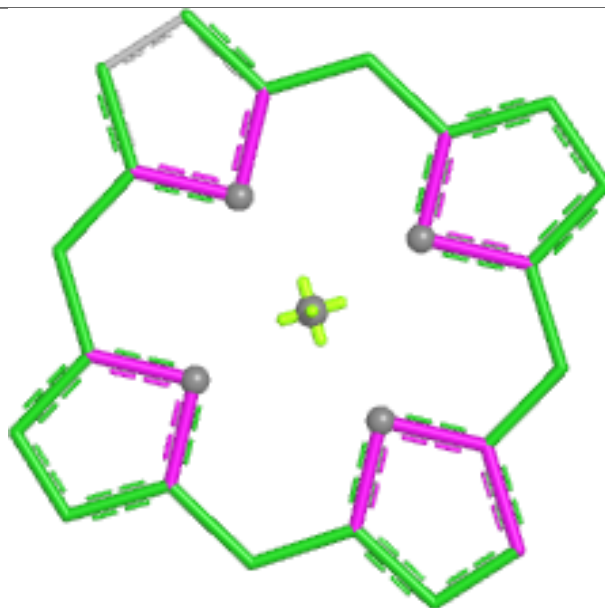


Rings

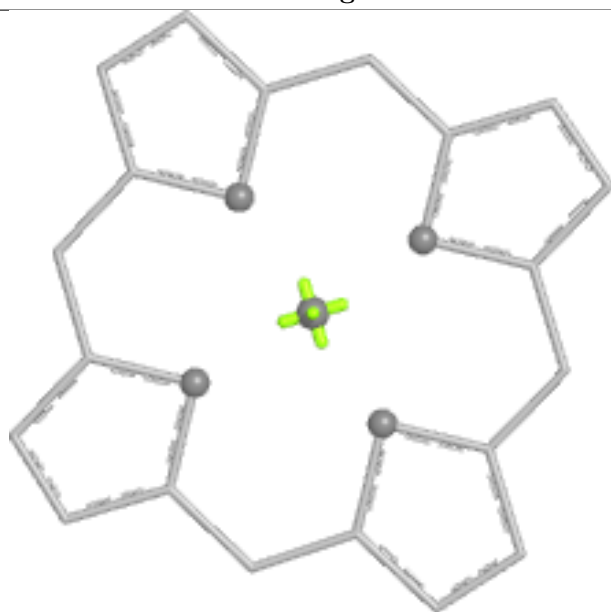
Ligand CLA B 652



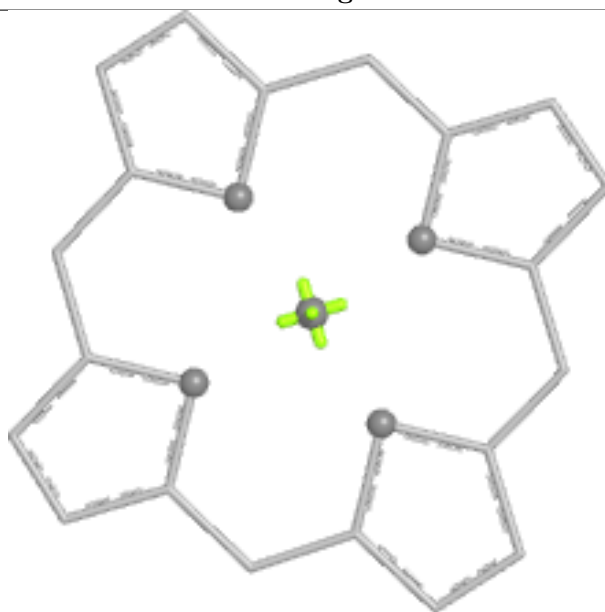
Bond lengths



Bond angles

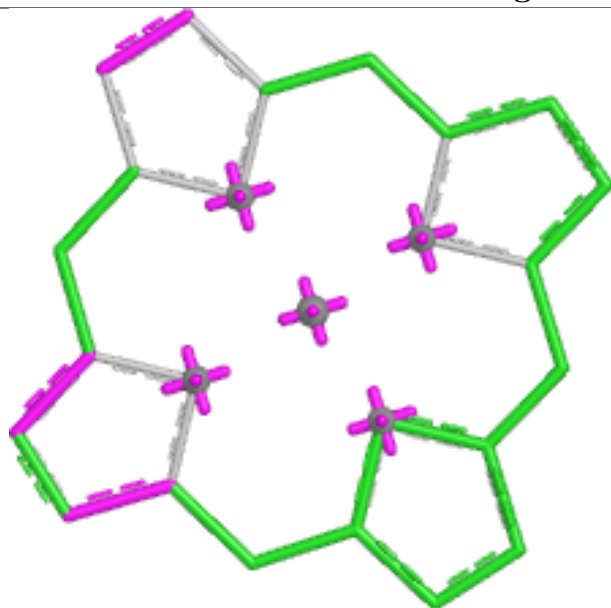


Torsions

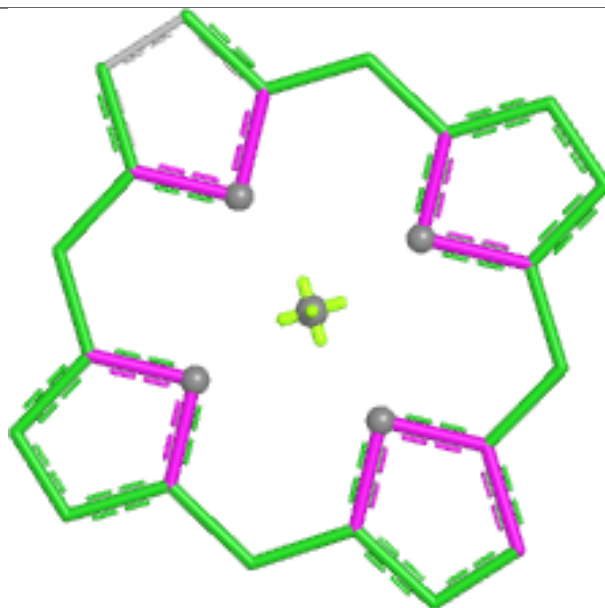


Rings

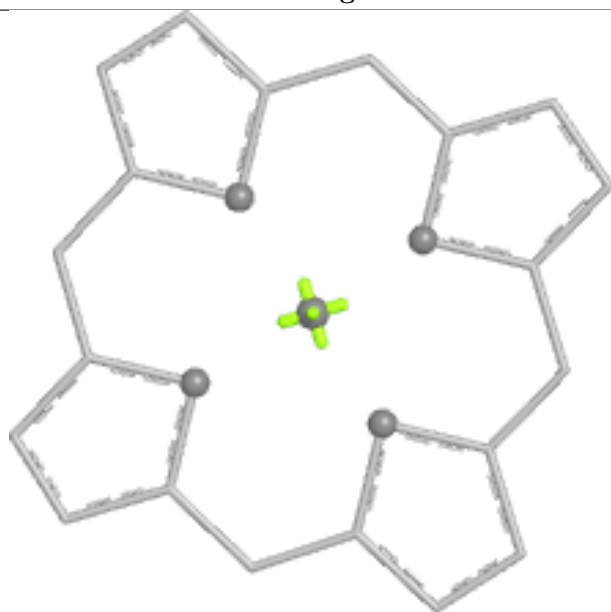
Ligand CLA A 599



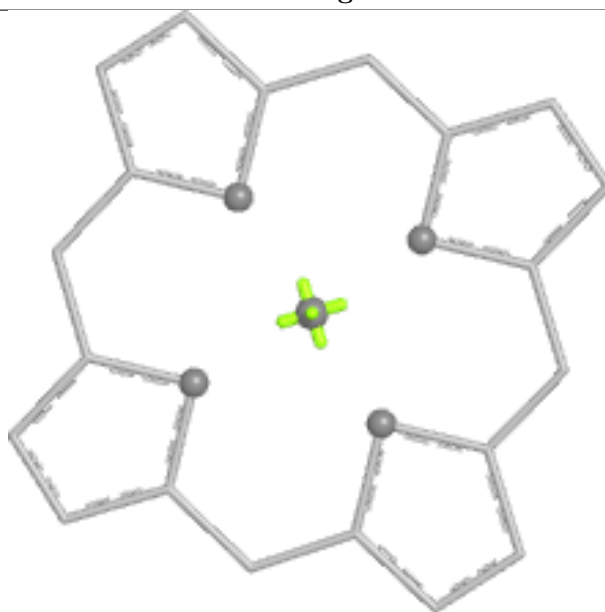
Bond lengths



Bond angles

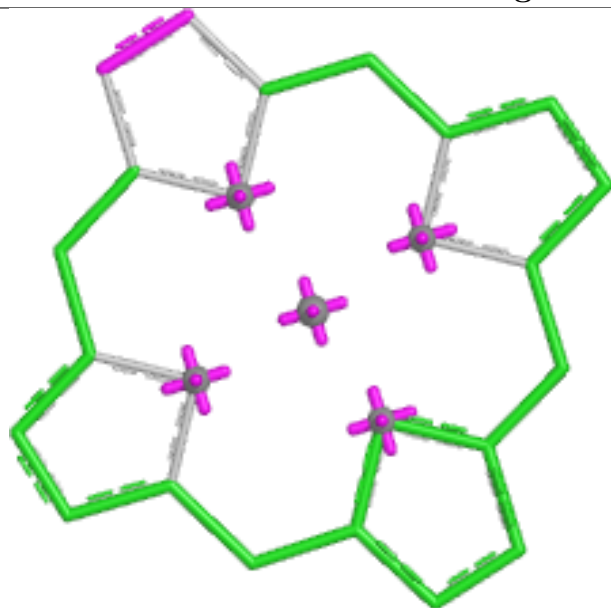


Torsions

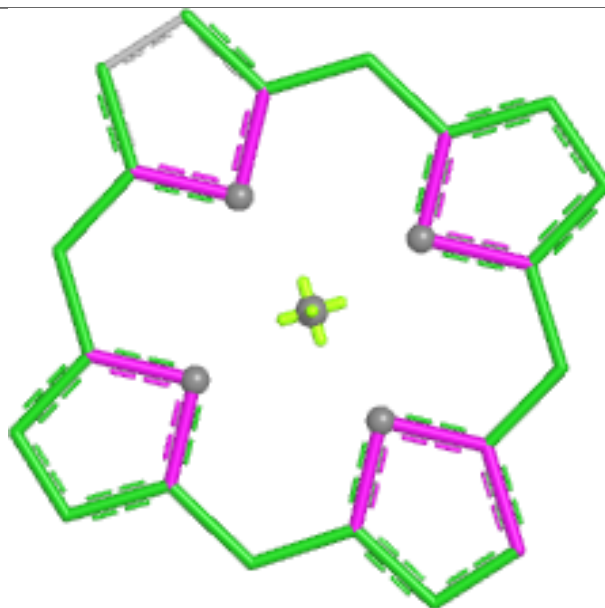


Rings

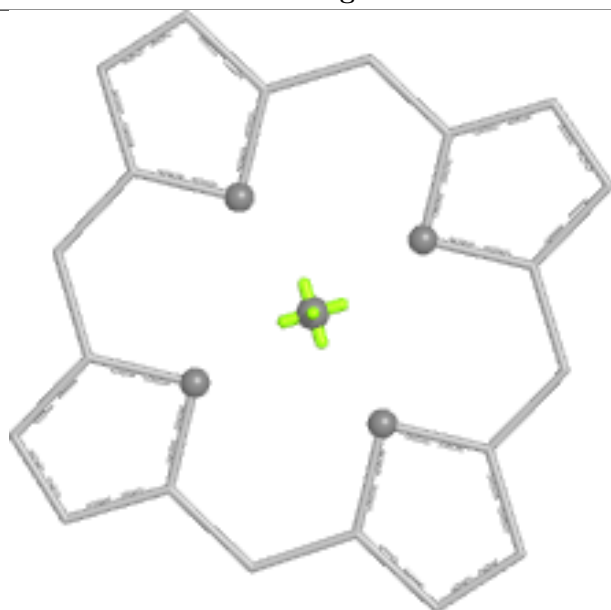
Ligand CLA B 624



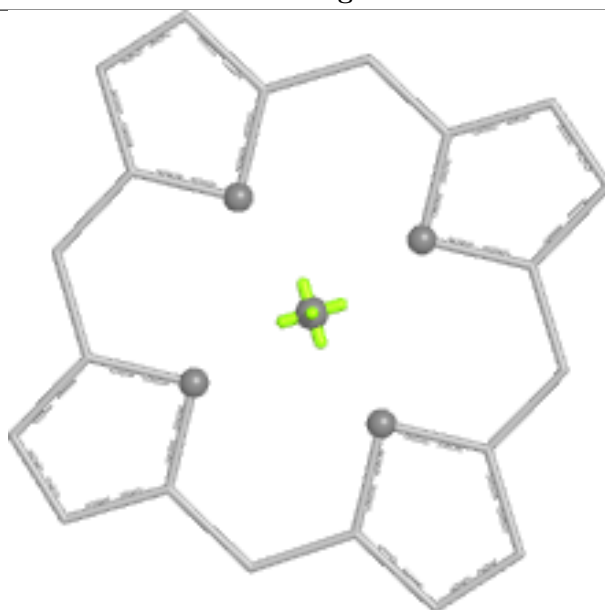
Bond lengths



Bond angles

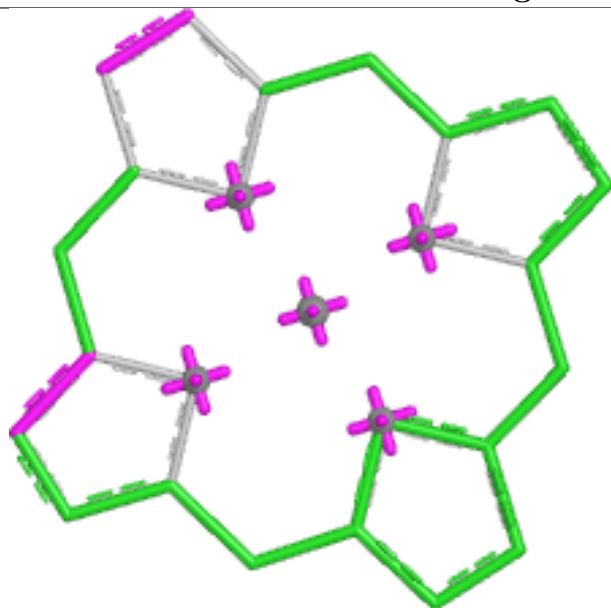


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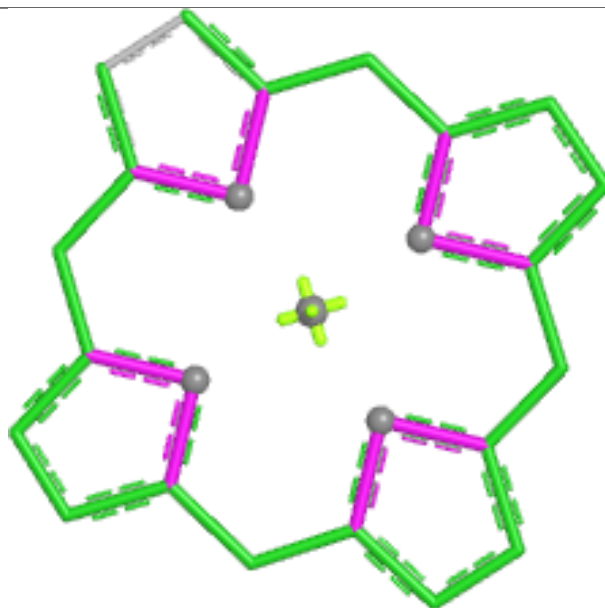


Rings

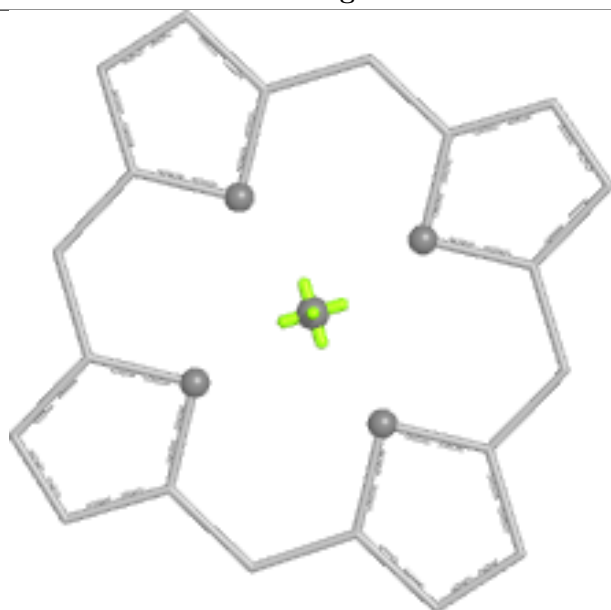
Ligand CLA A 607



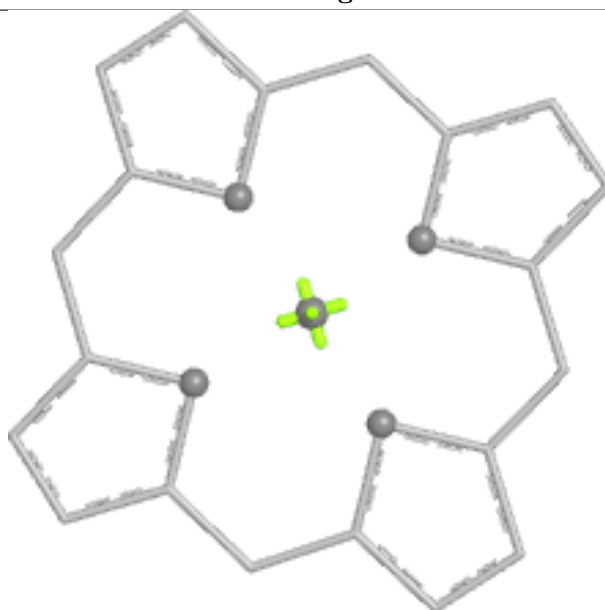
Bond lengths



Bond angles

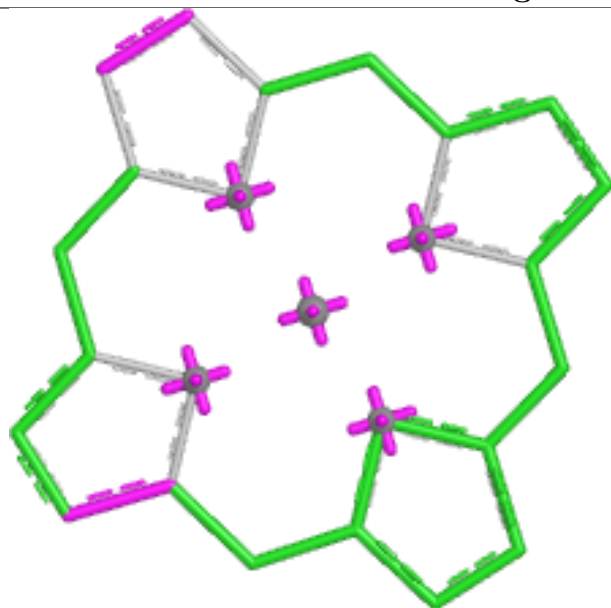


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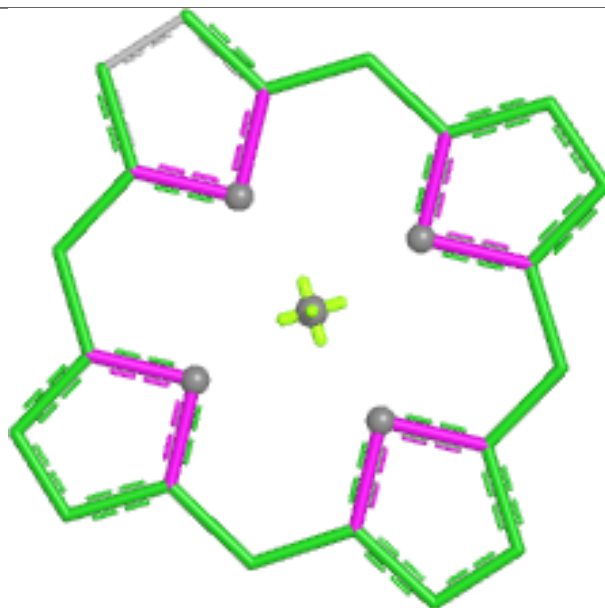


Rings

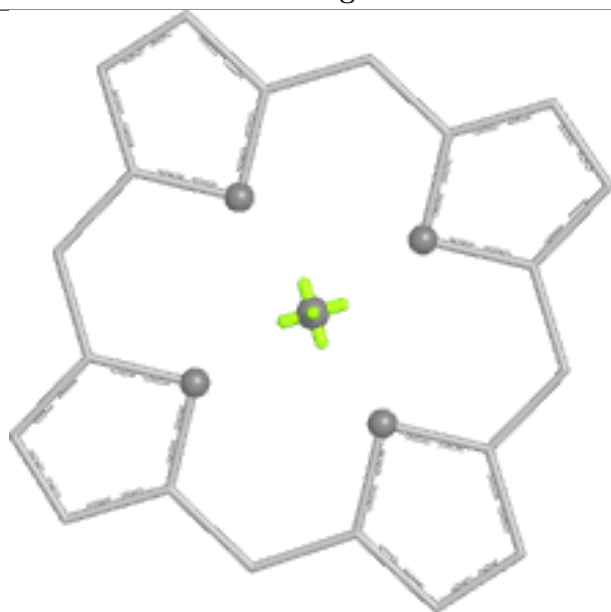
Ligand CLA A 624



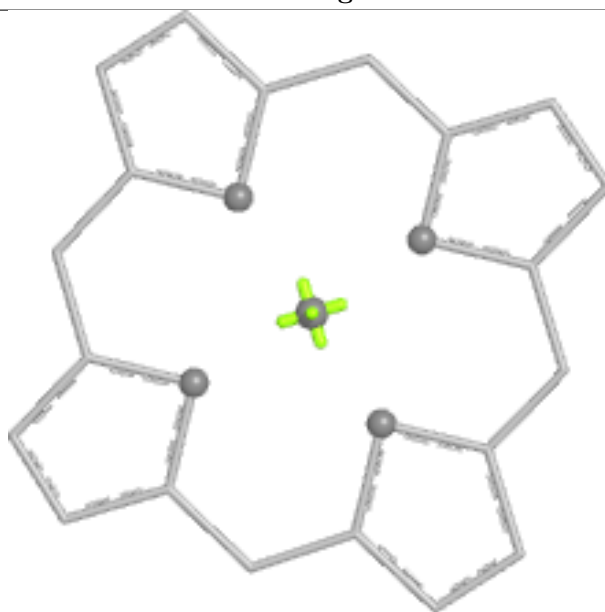
Bond lengths



Bond angles

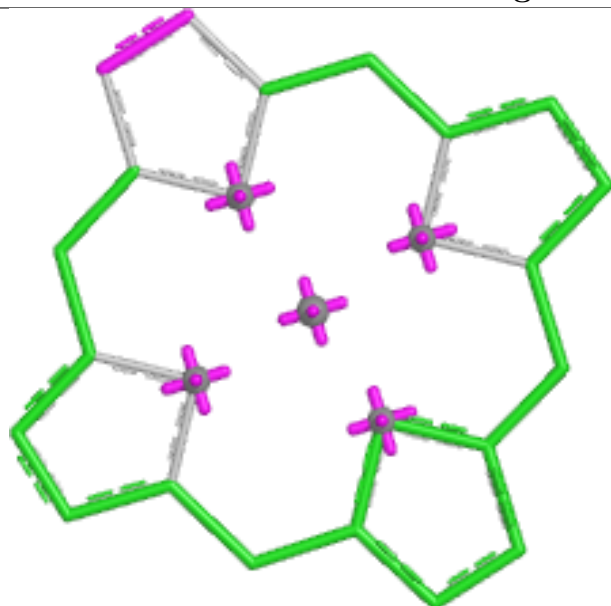


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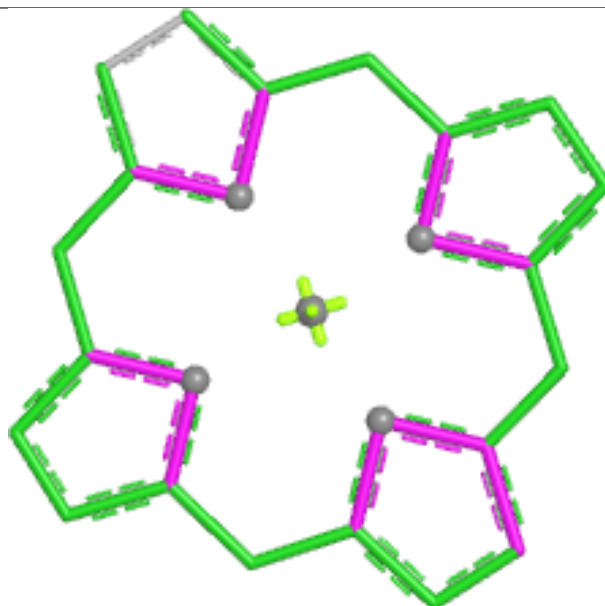


Rings

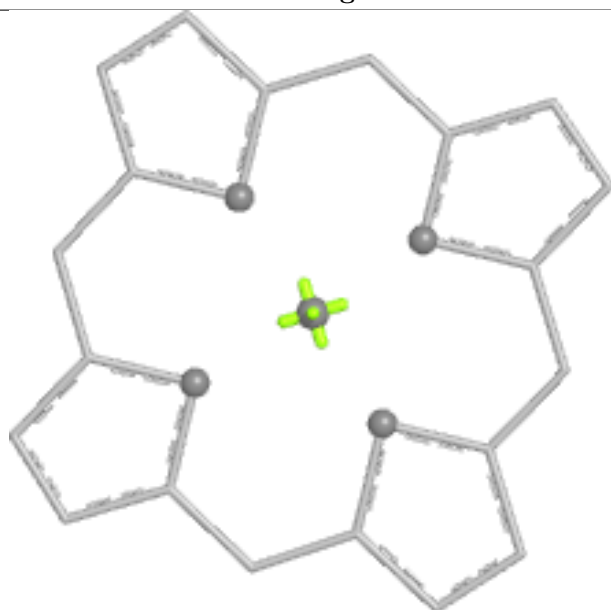
Ligand CLA A 603



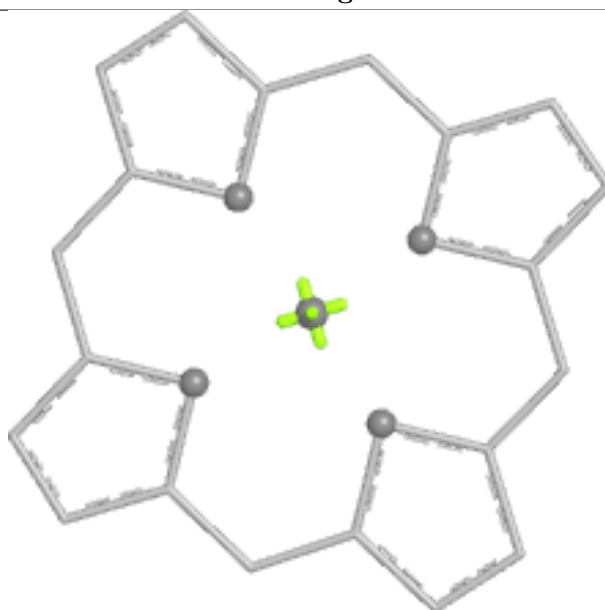
Bond lengths



Bond angles

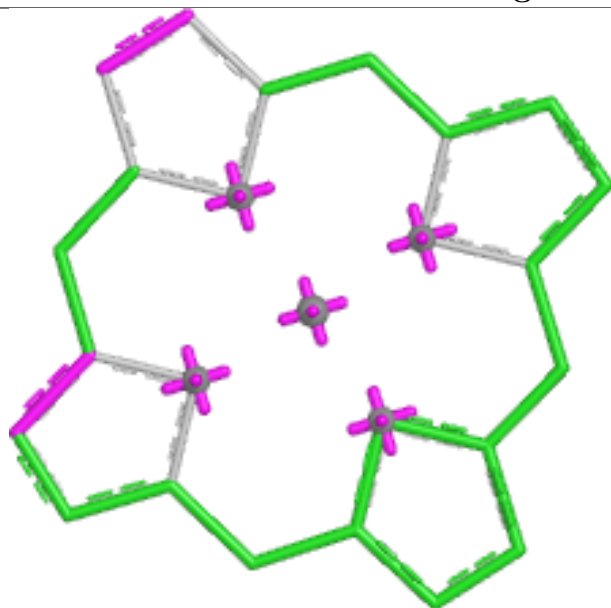


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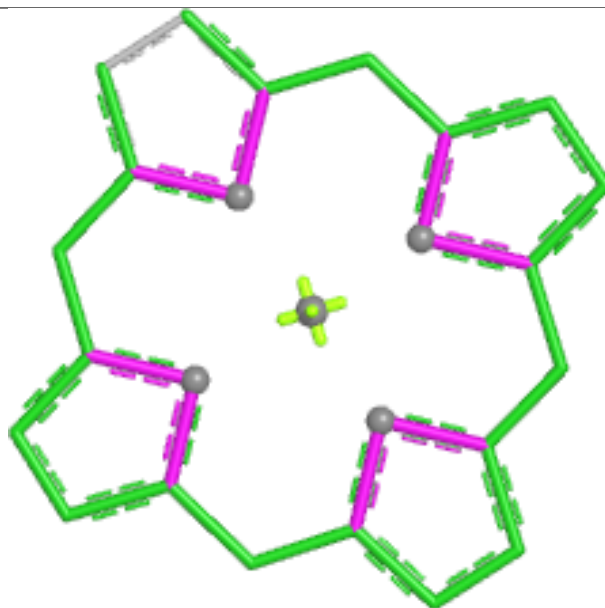


Rings

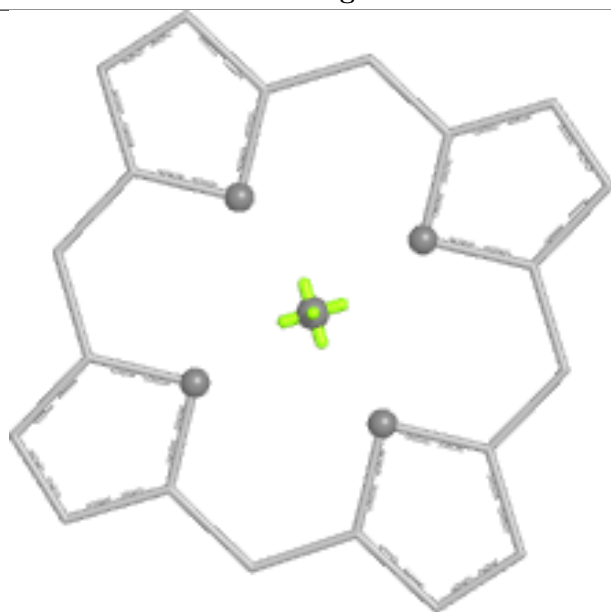
Ligand CLA A 608



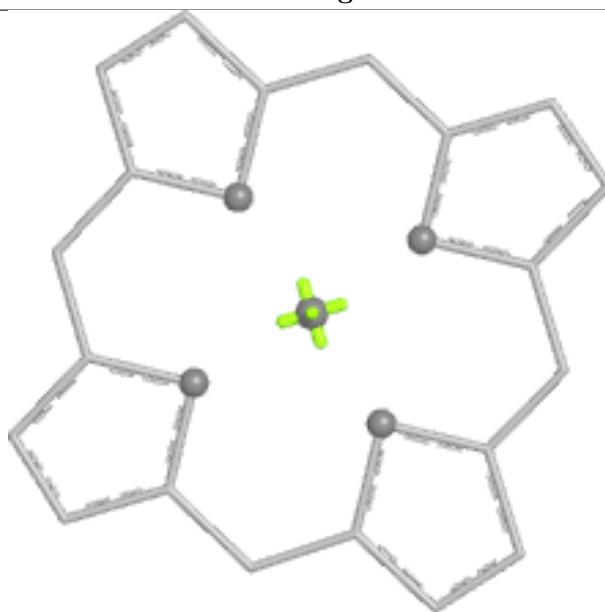
Bond lengths



Bond angles

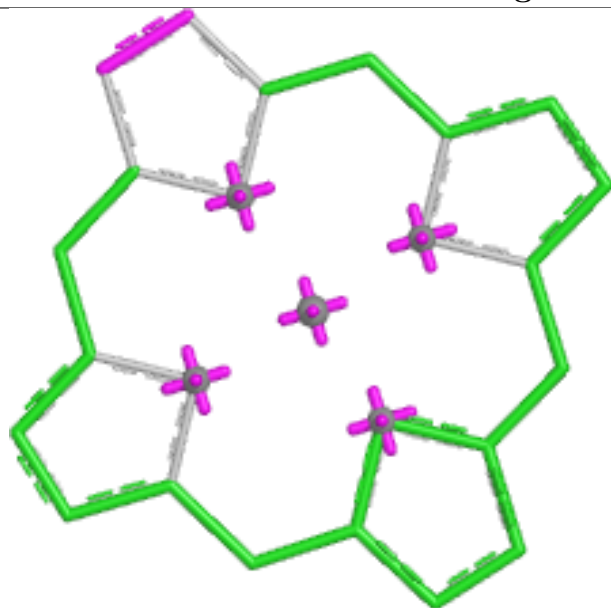


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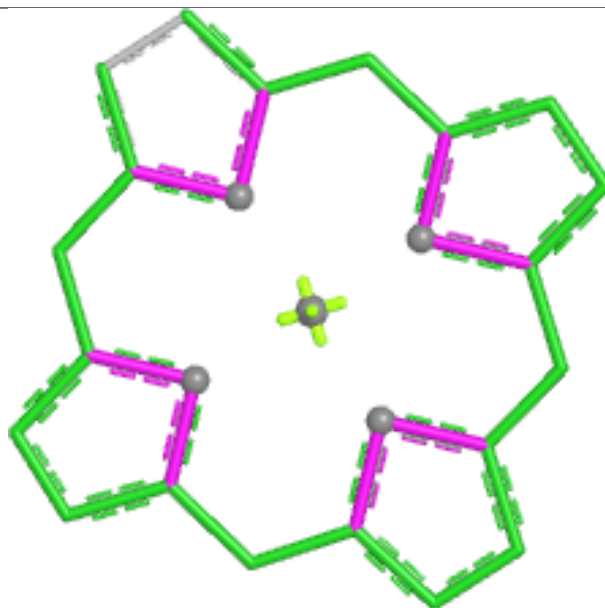


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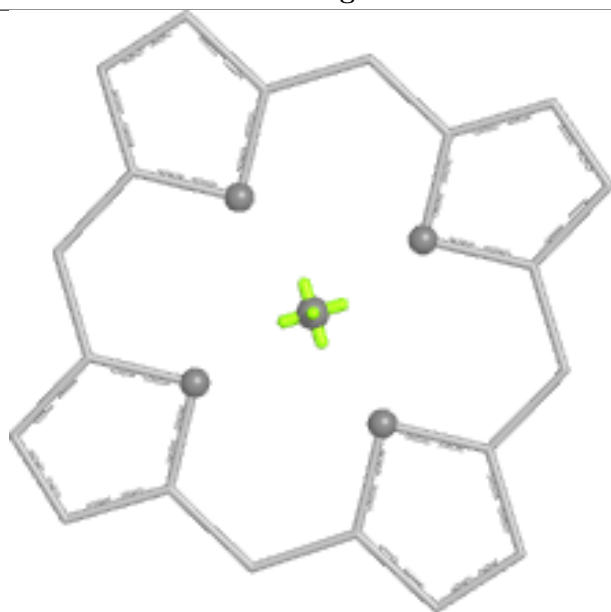
Ligand CLA B 629



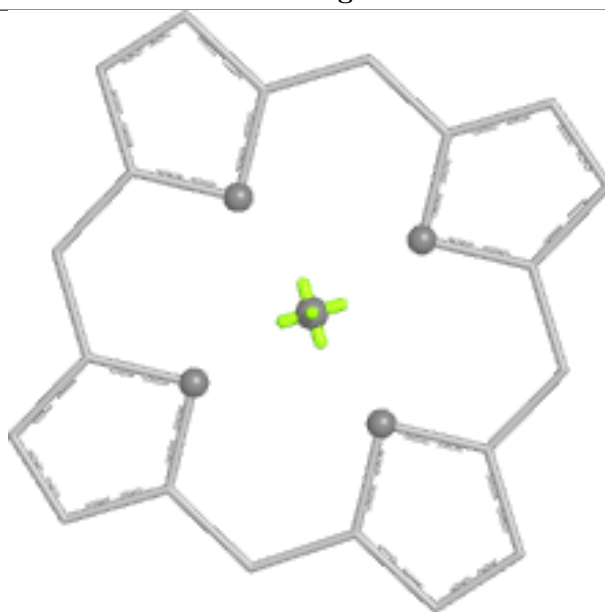
Bond lengths



Bond angles

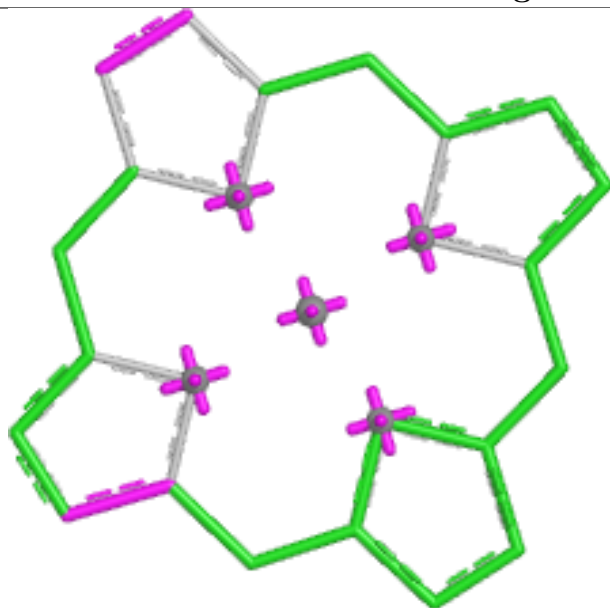


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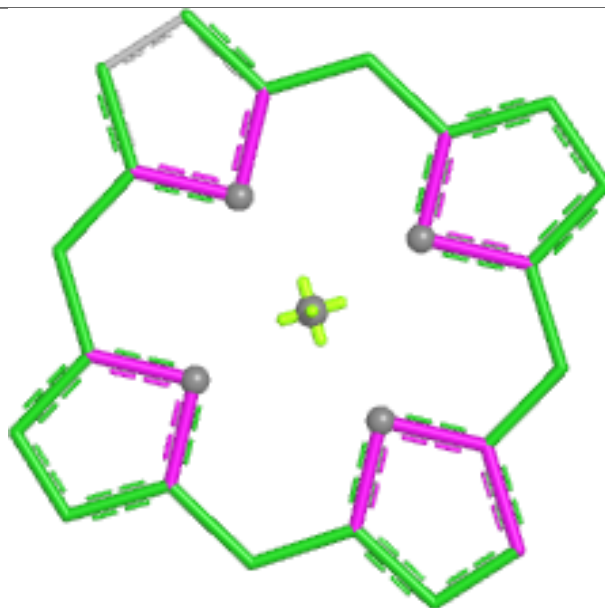


Rings

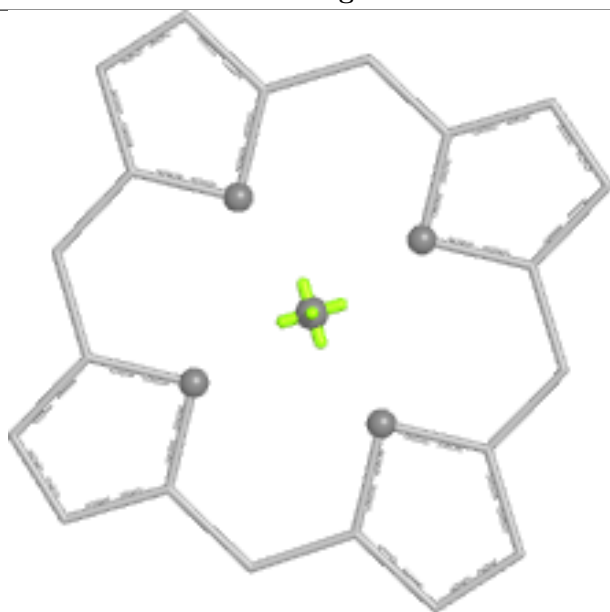
Ligand CLA B 645



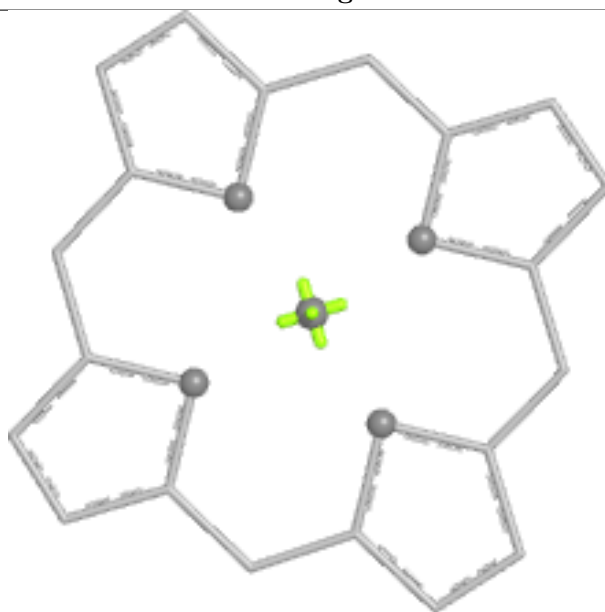
Bond lengths



Bond angles

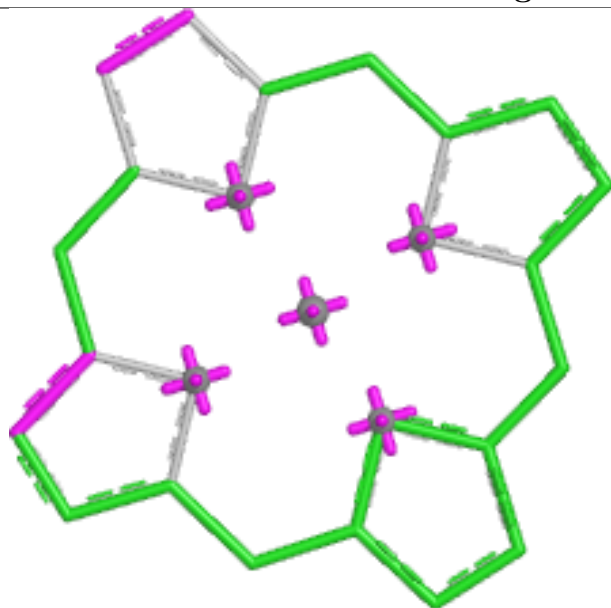


Torsions

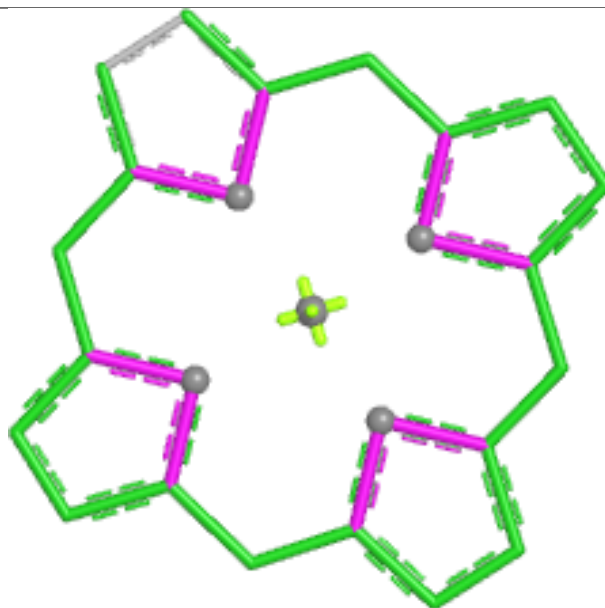


Rings

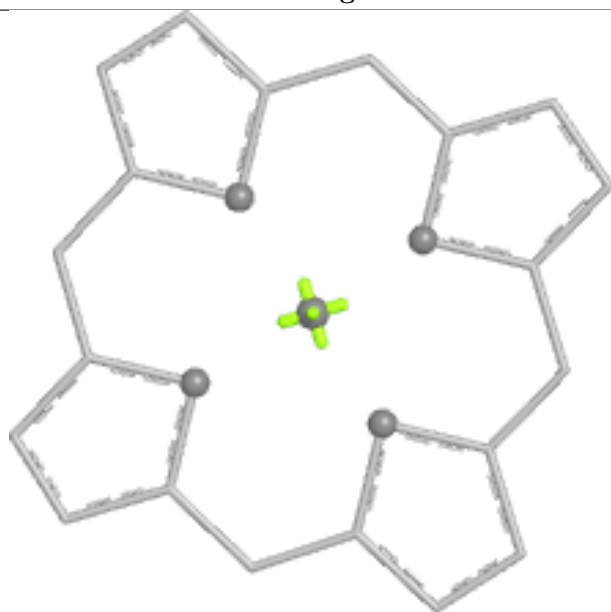
Ligand CLA B 632



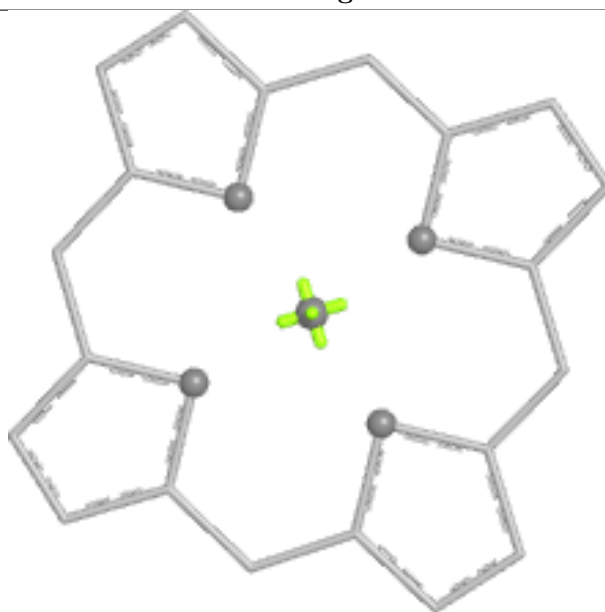
Bond lengths



Bond angles

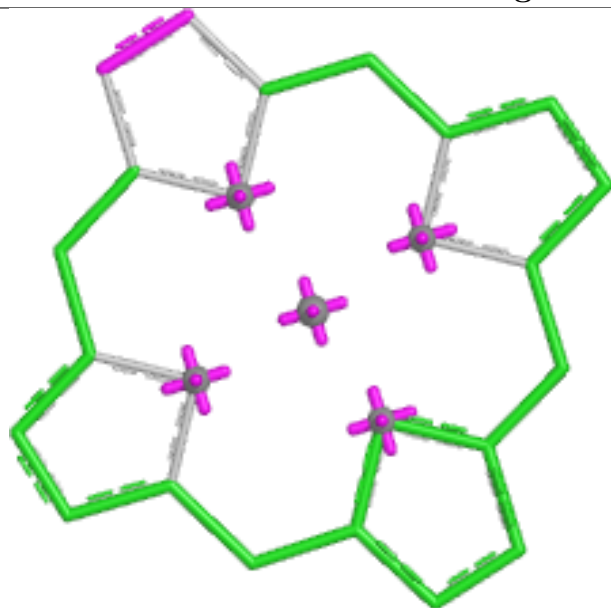


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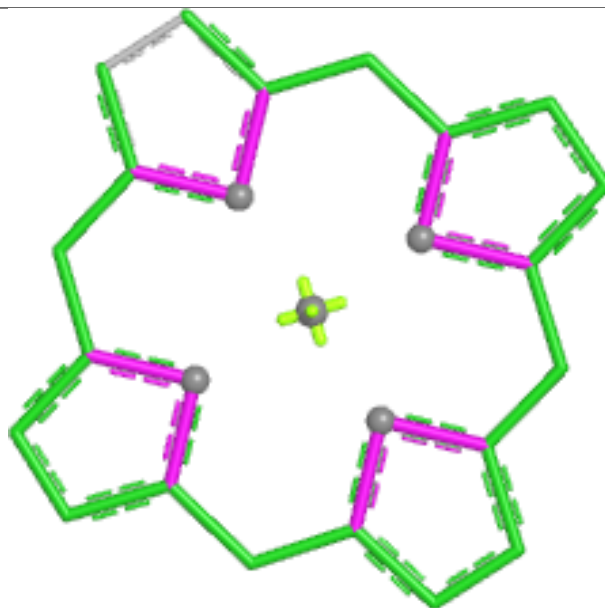


Rings

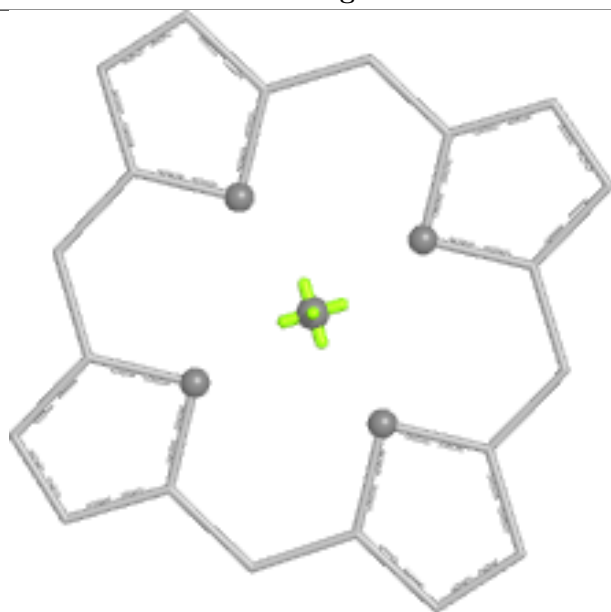
Ligand CLA B 634



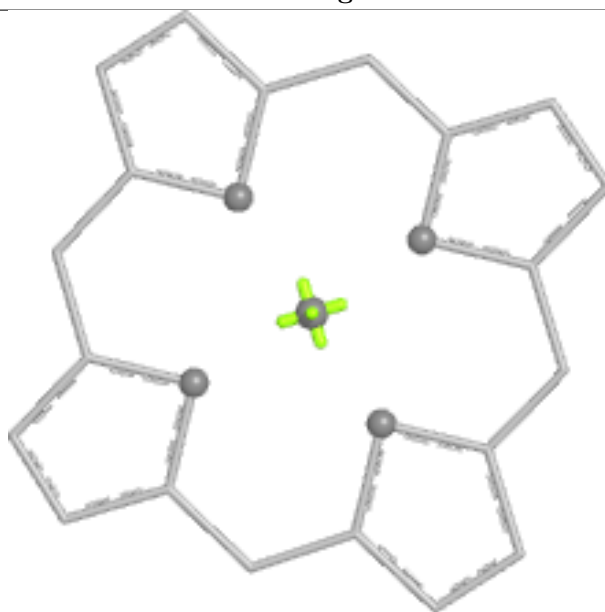
Bond lengths



Bond angles

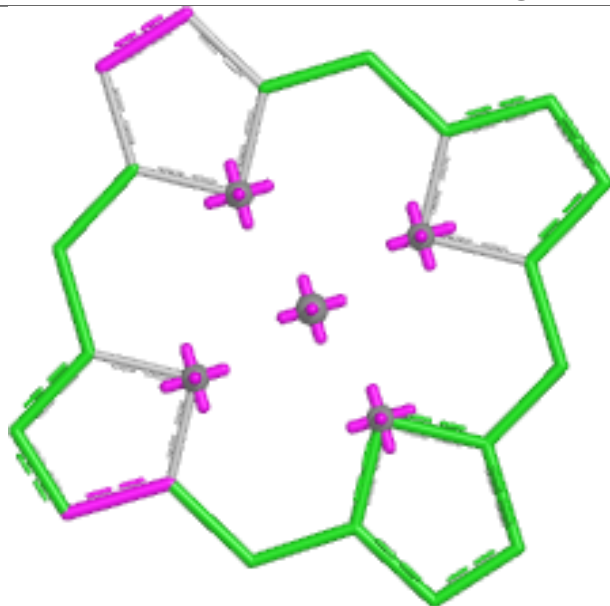


Torsions

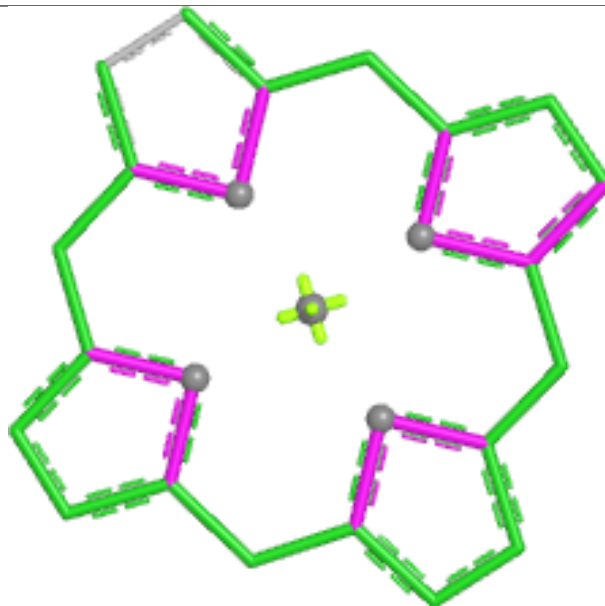


Rings

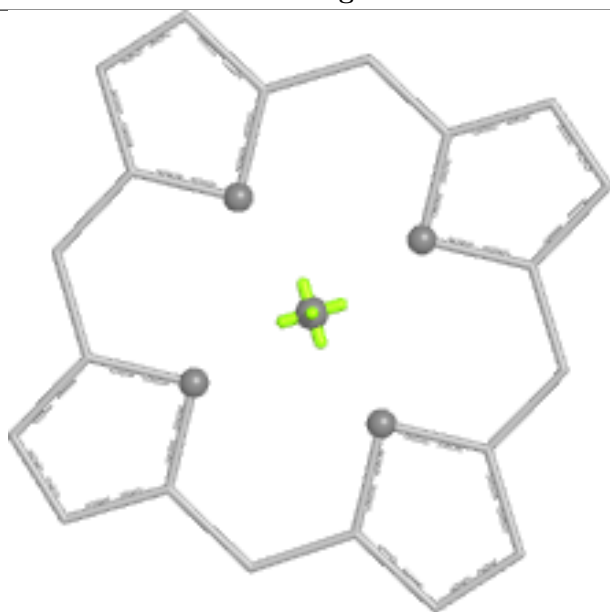
Ligand CLA A 628



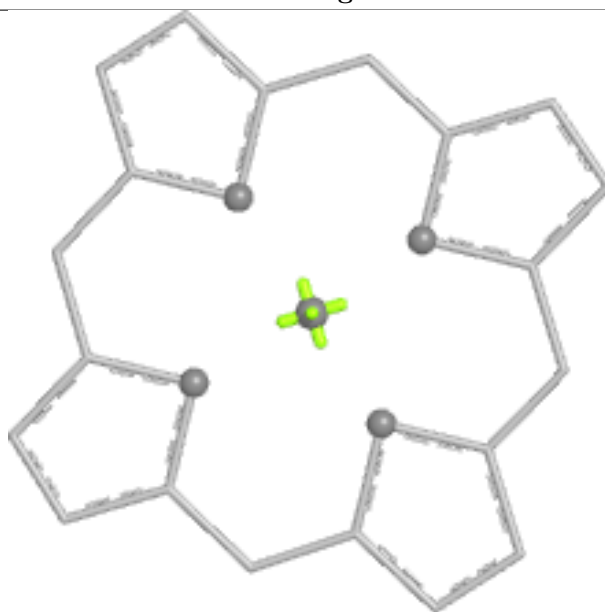
Bond lengths



Bond angles

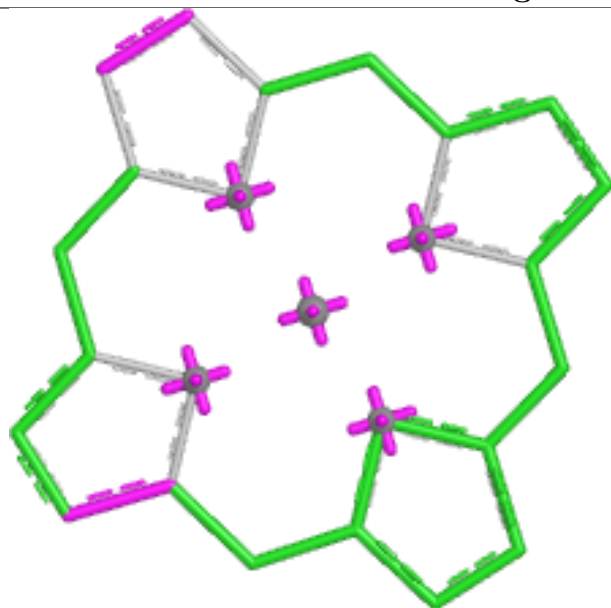


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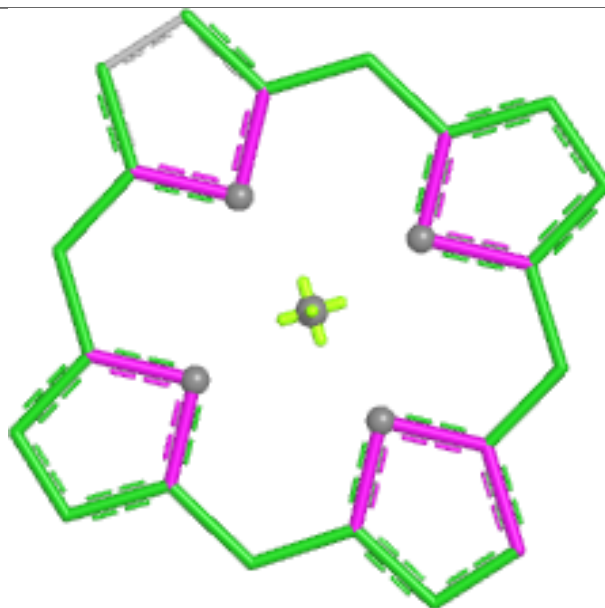


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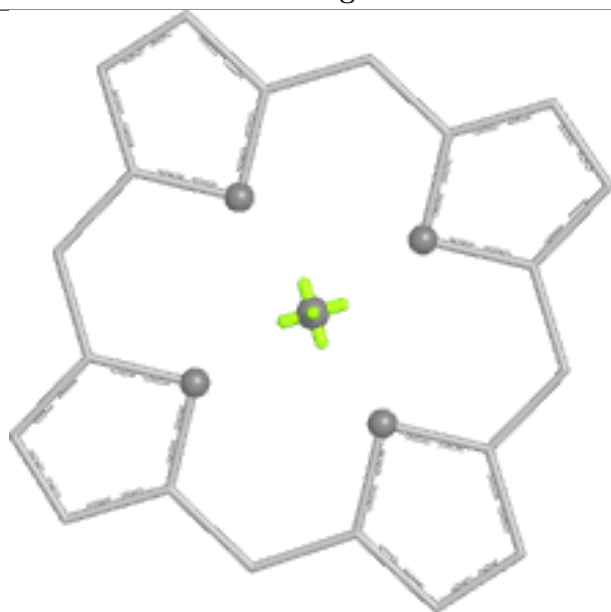
Ligand CLA A 629



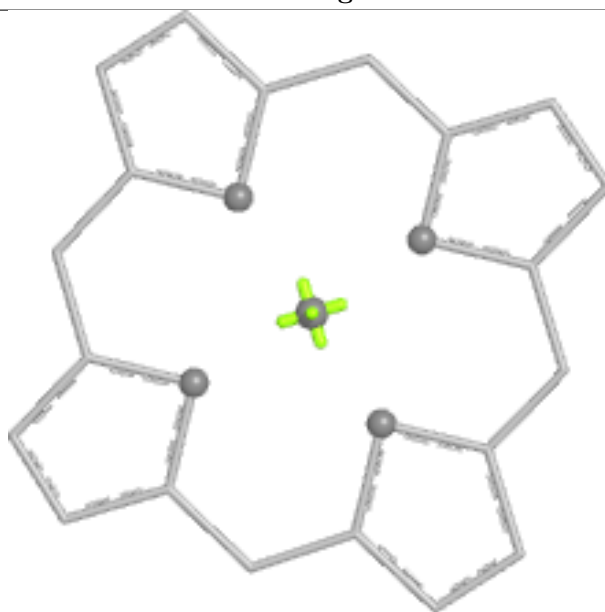
Bond lengths



Bond angles

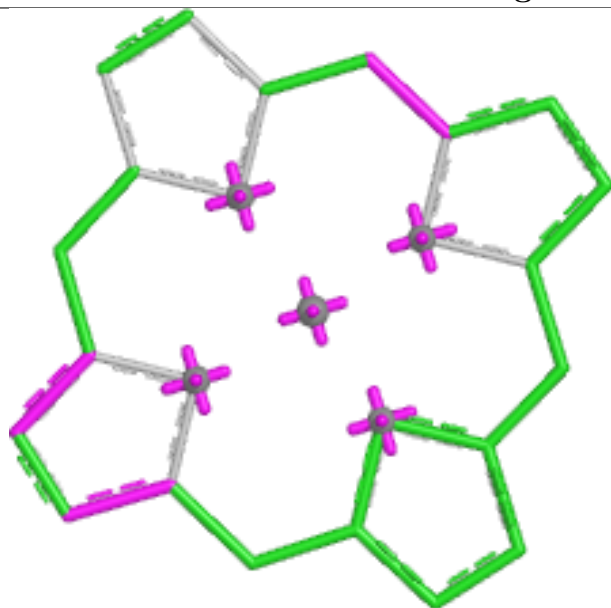


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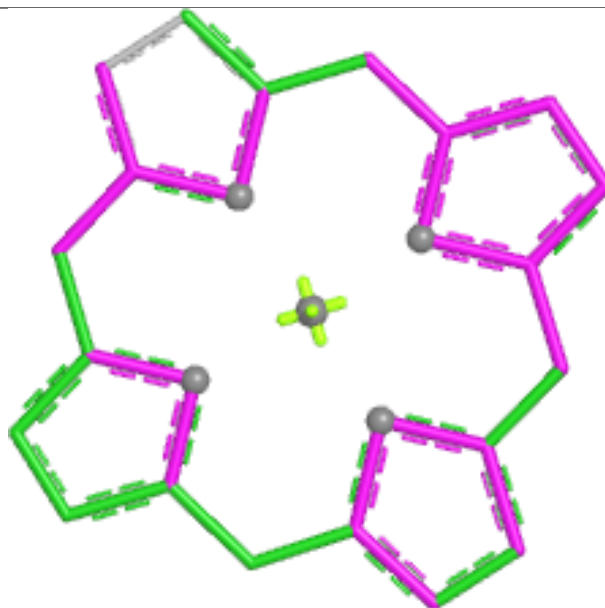


Rings

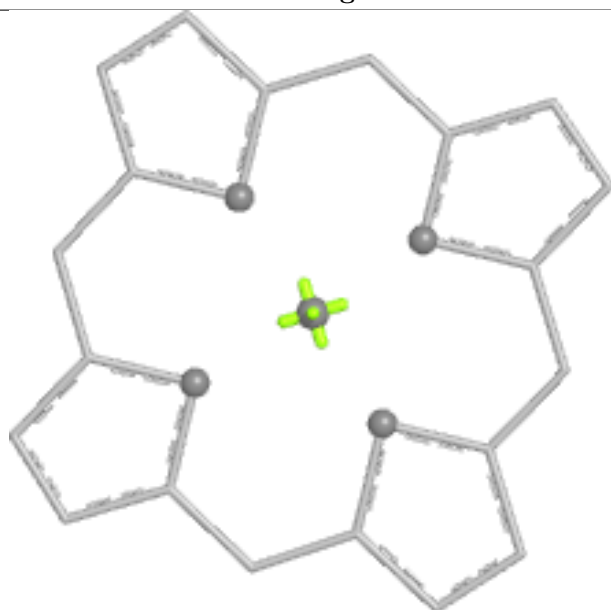
Ligand CLA B 635



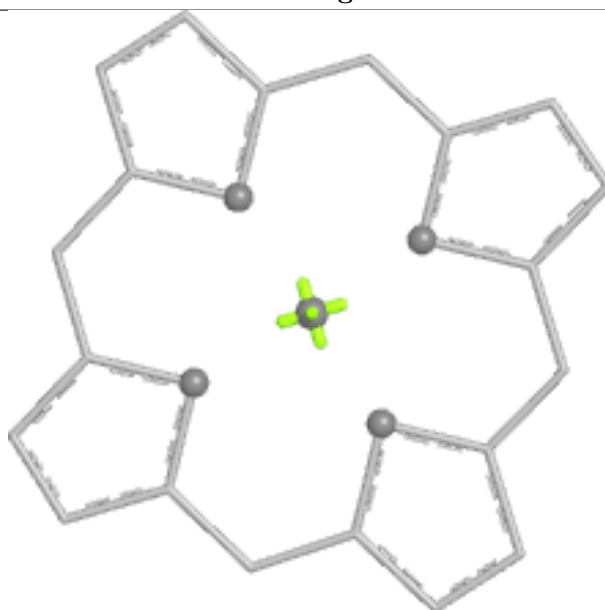
Bond lengths



Bond angles

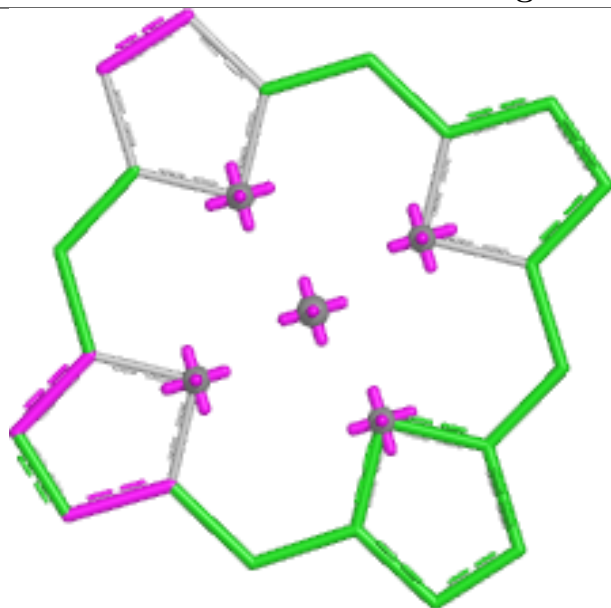


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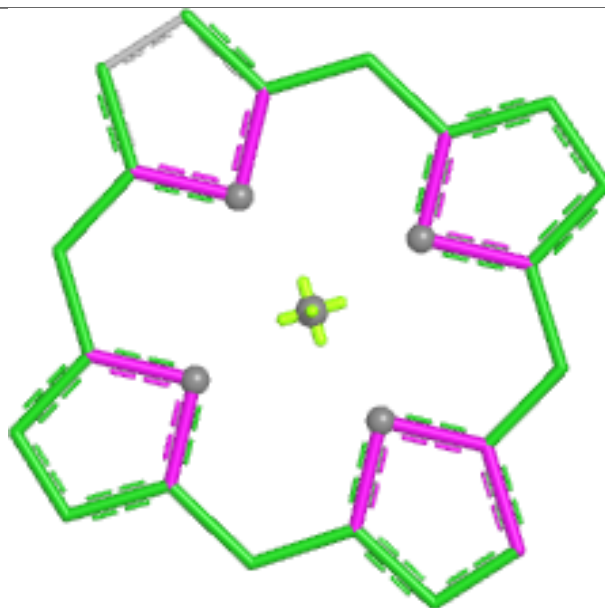


Rings

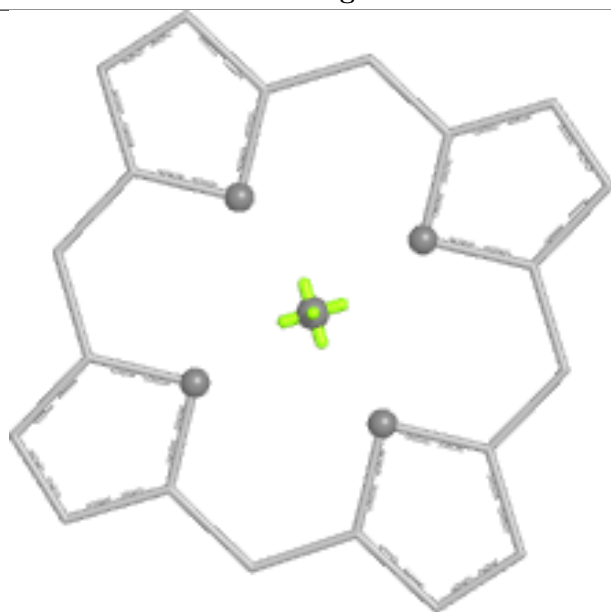
Ligand CLA F 154



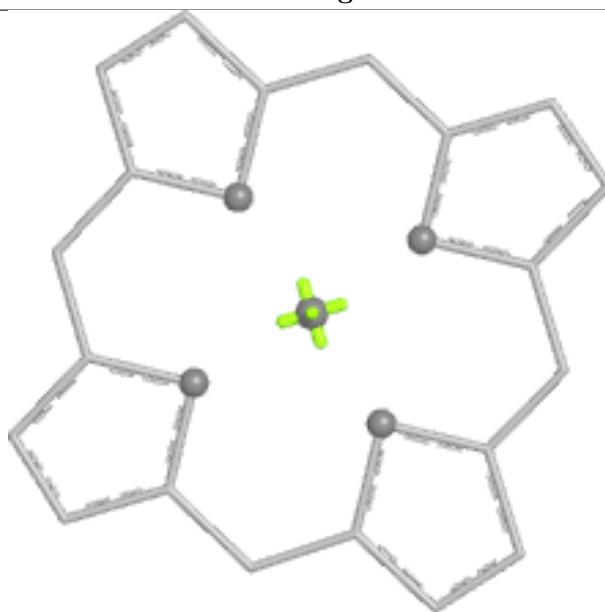
Bond lengths



Bond angles

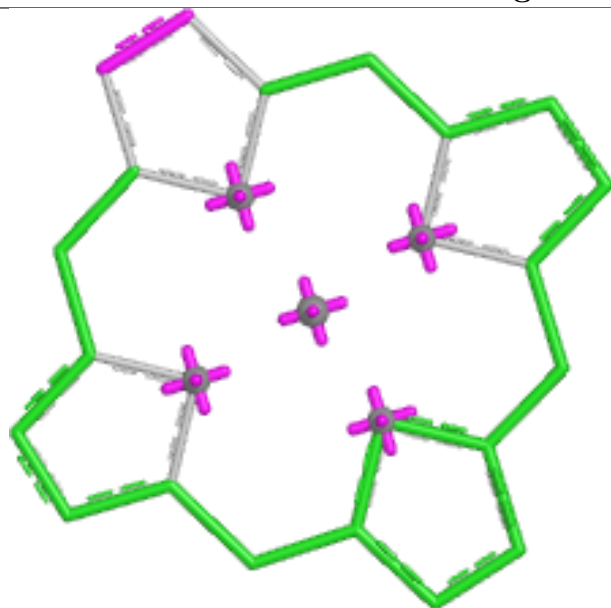


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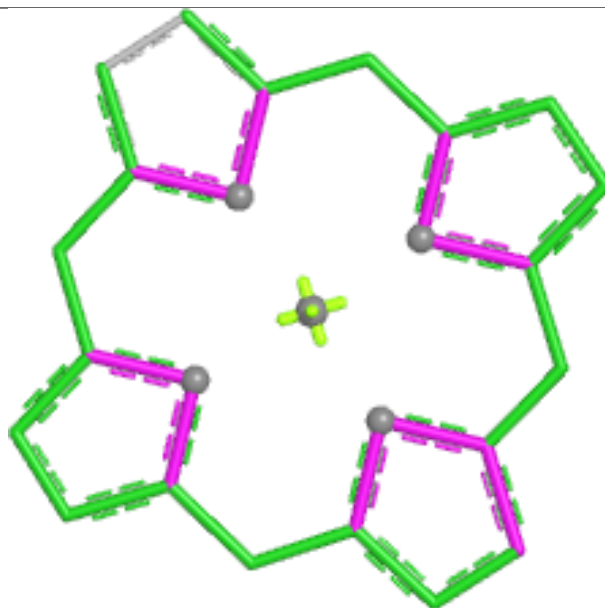


Rings

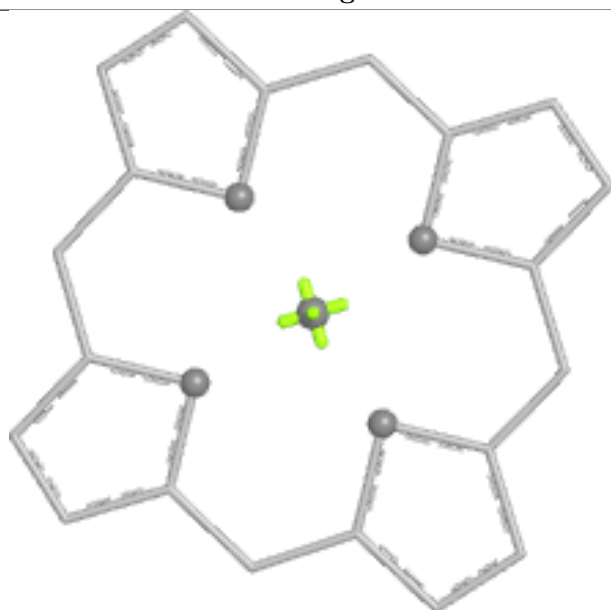
Ligand CLA A 613



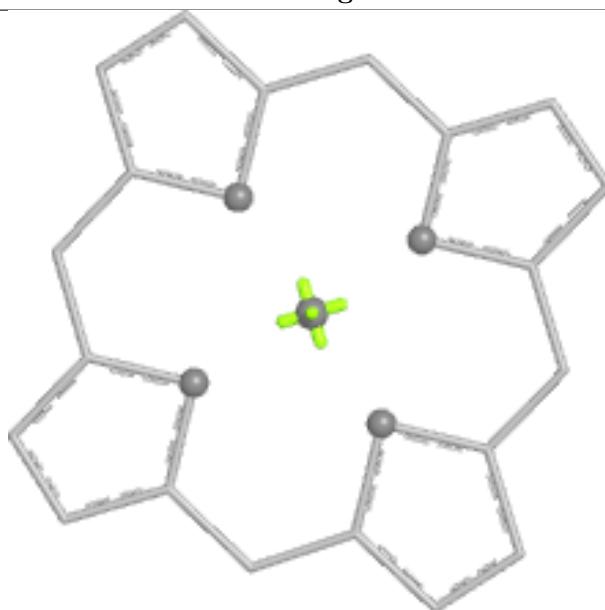
Bond lengths



Bond angles

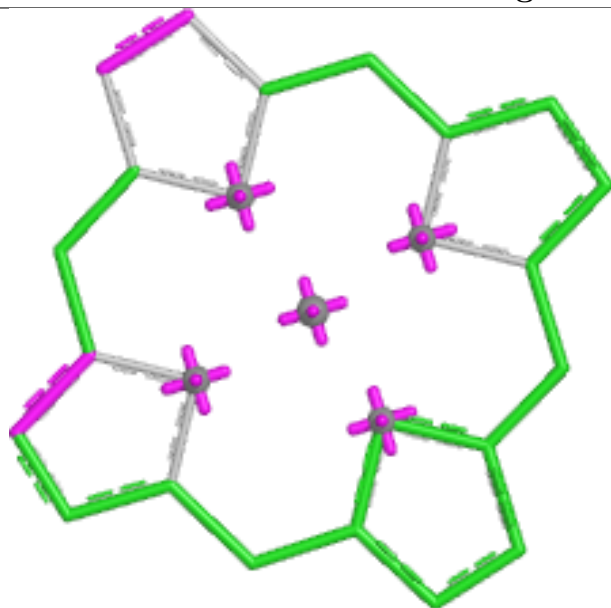


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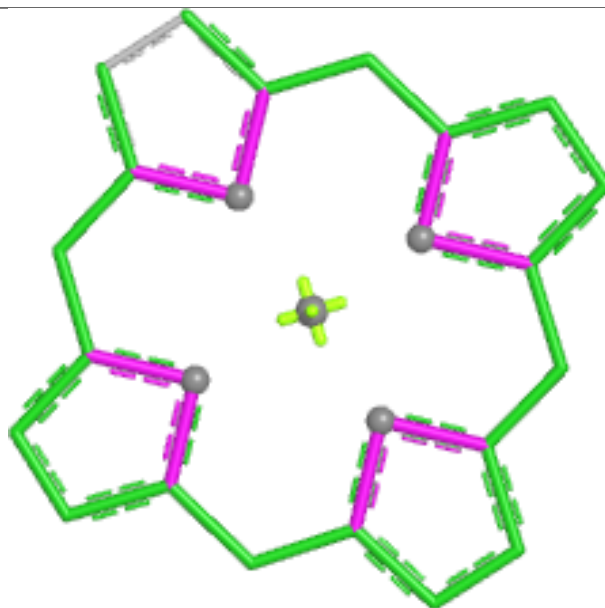


Rings

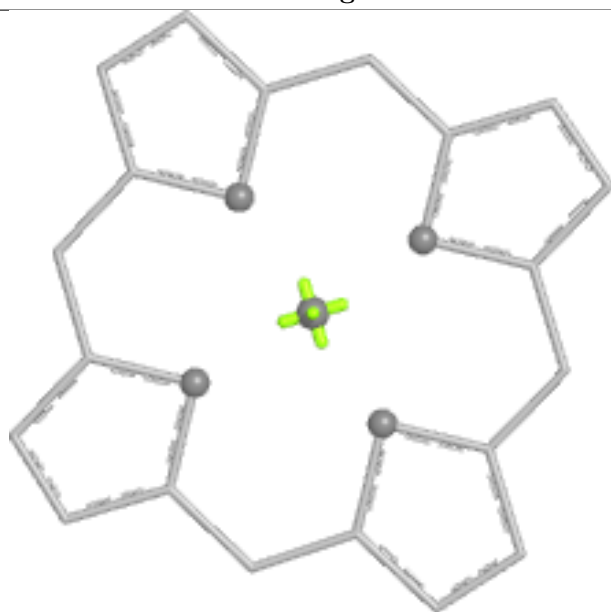
Ligand CLA F 156



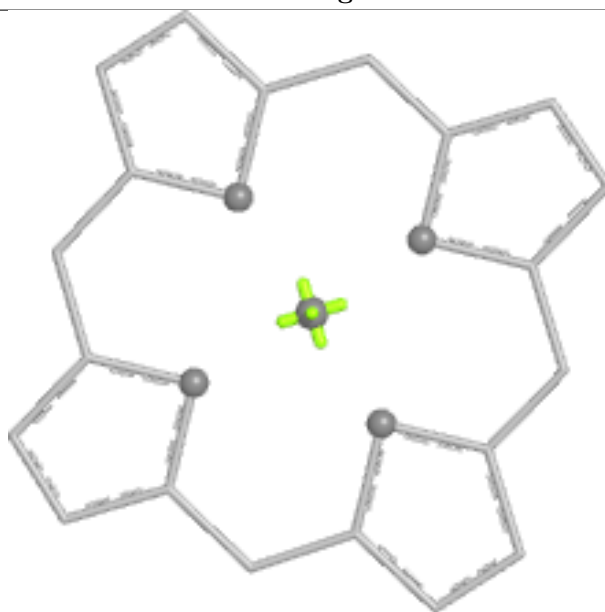
Bond lengths



Bond angles

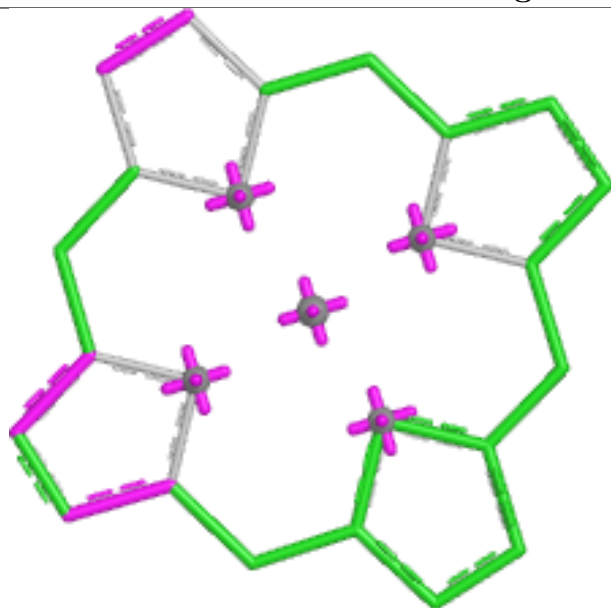


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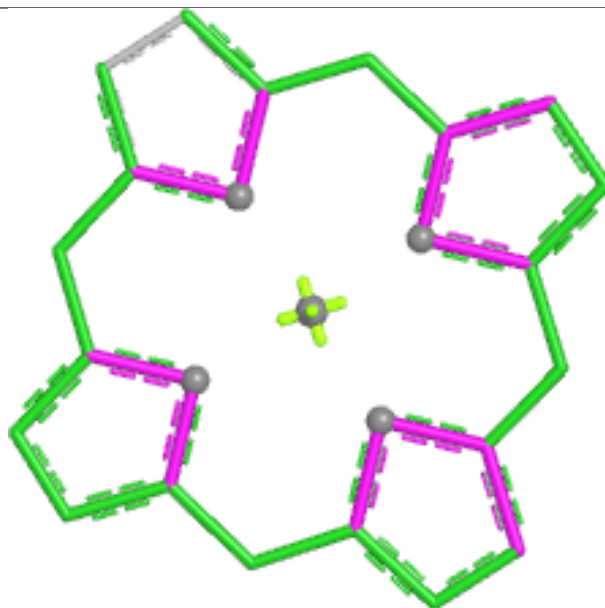


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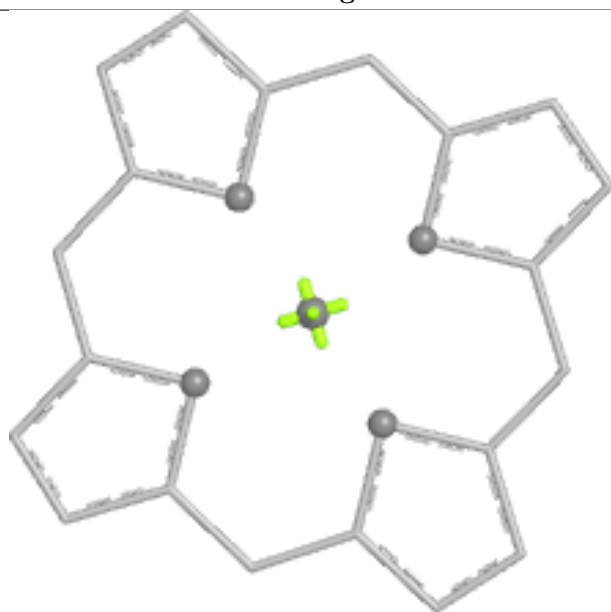
Ligand CLA B 641



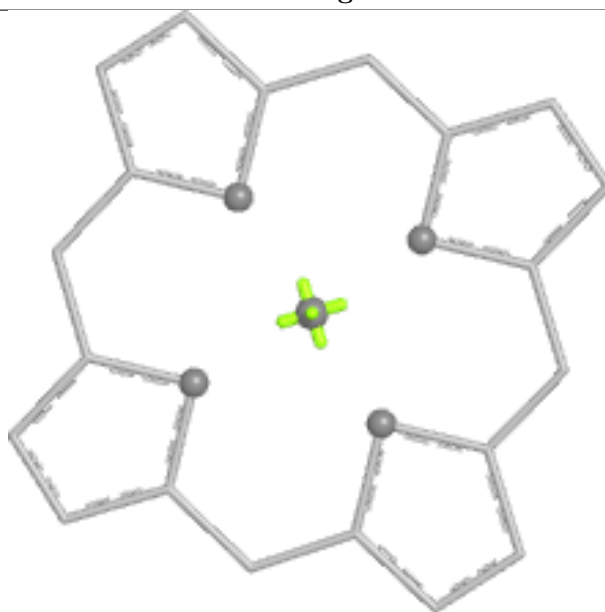
Bond lengths



Bond angles

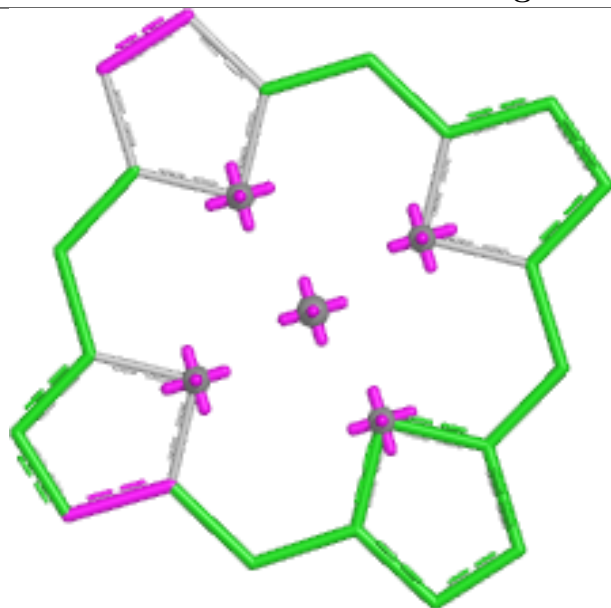


Torsions

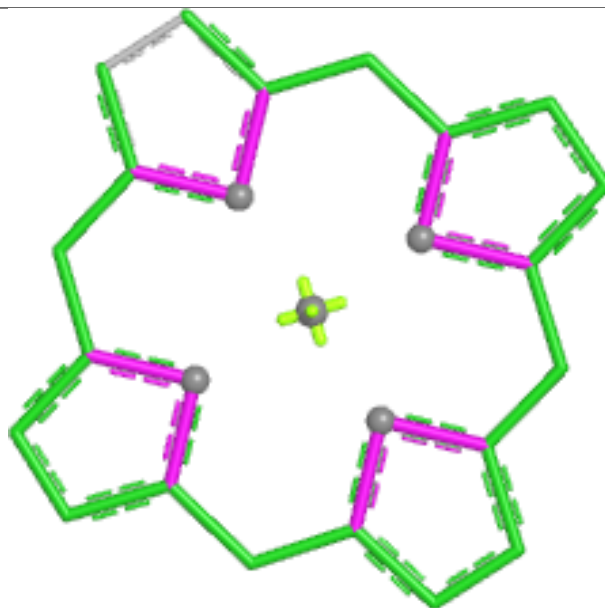


Rings

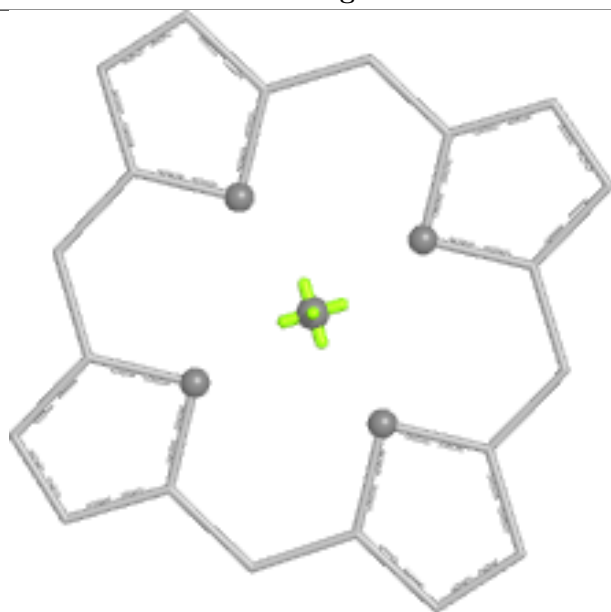
Ligand CLA A 598



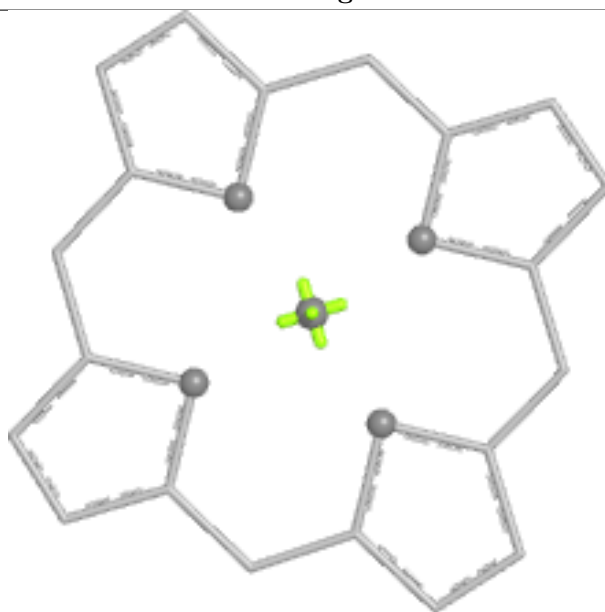
Bond lengths



Bond angles

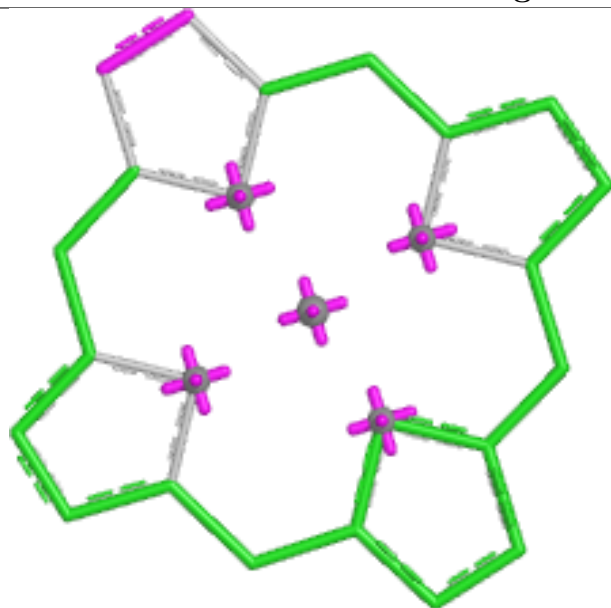


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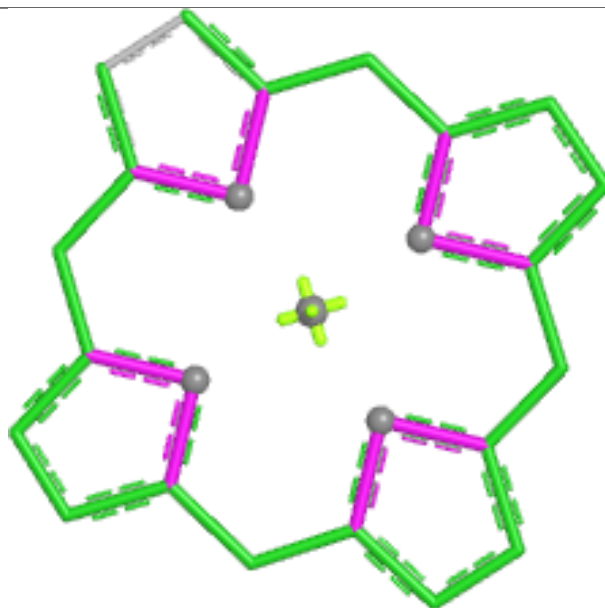


Rings

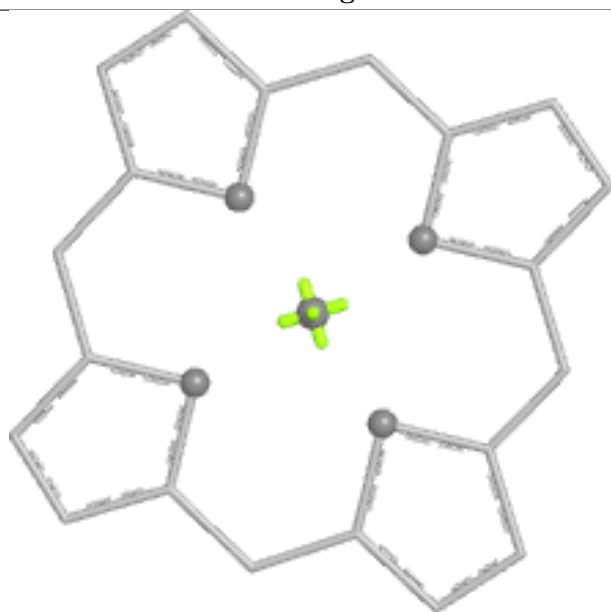
Ligand CLA A 619



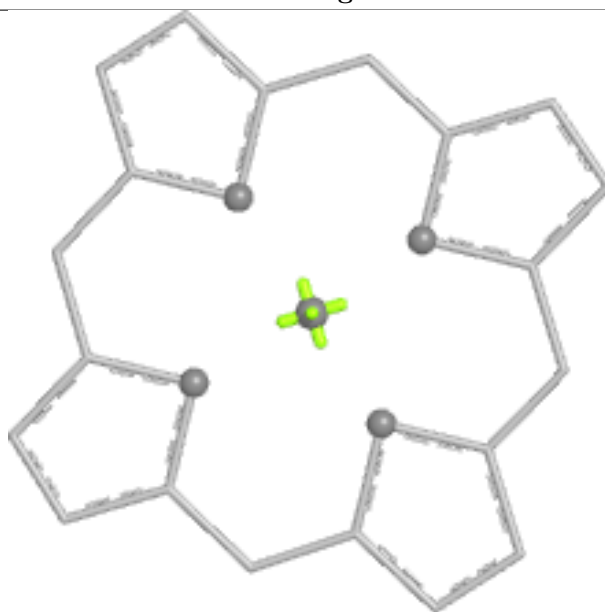
Bond lengths



Bond angles

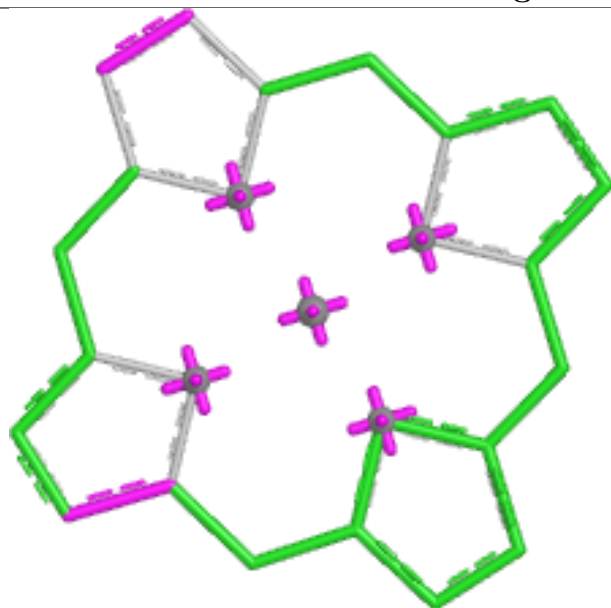


Torsions

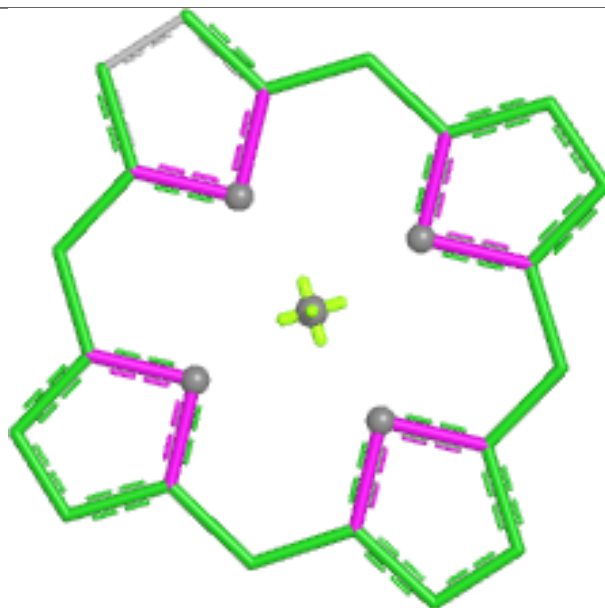


Rings

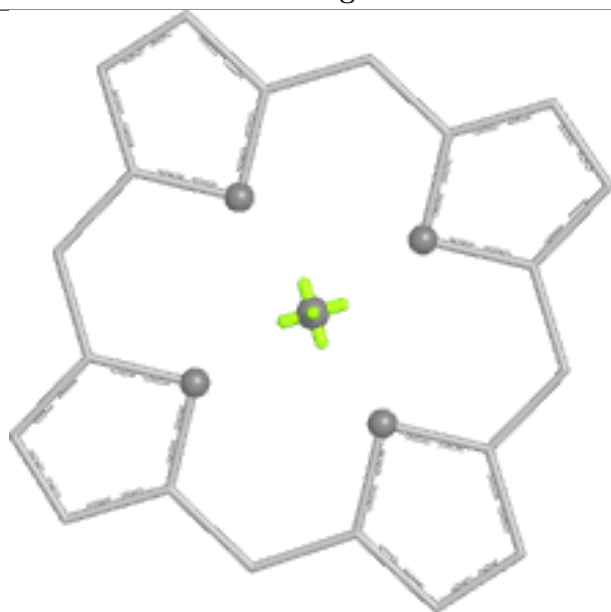
Ligand CLA A 606



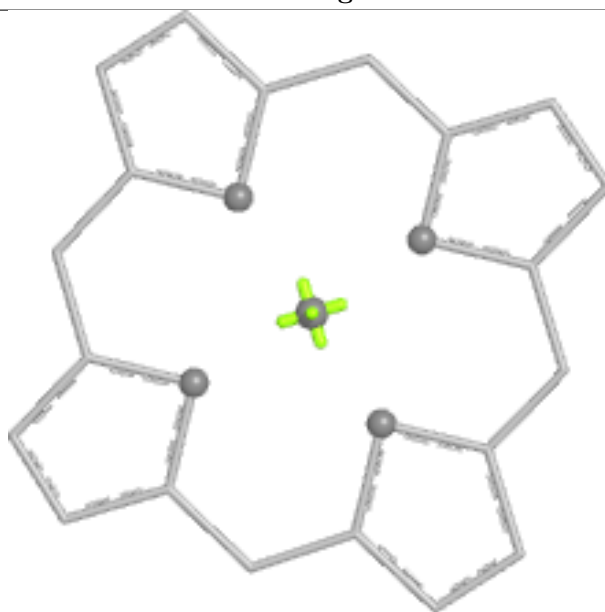
Bond lengths



Bond angles

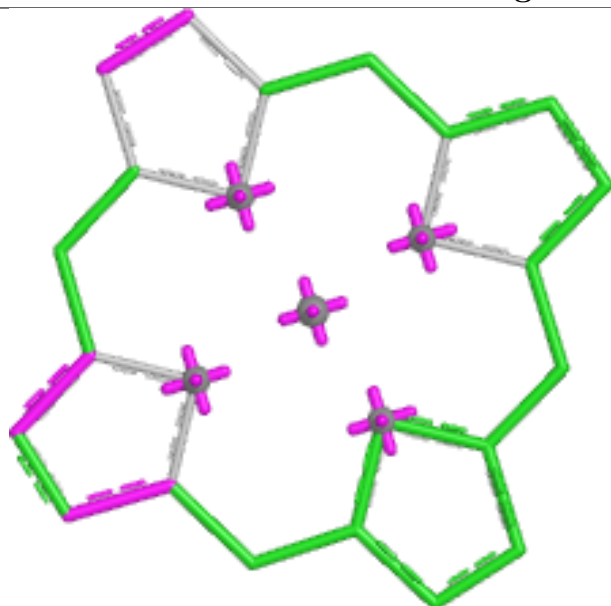


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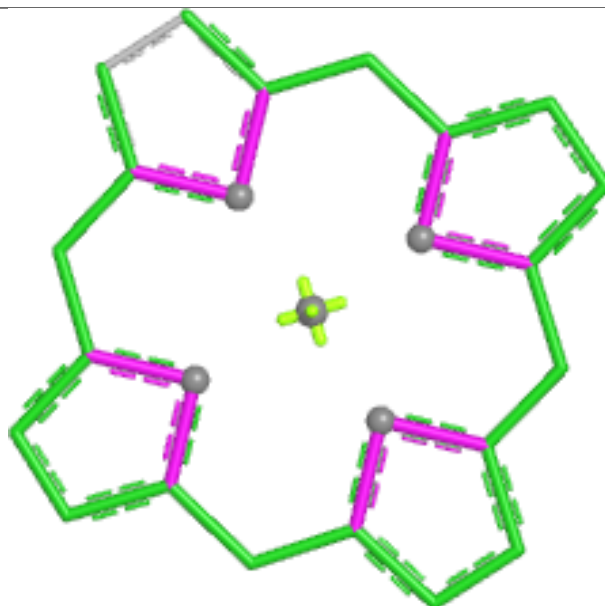


Rings

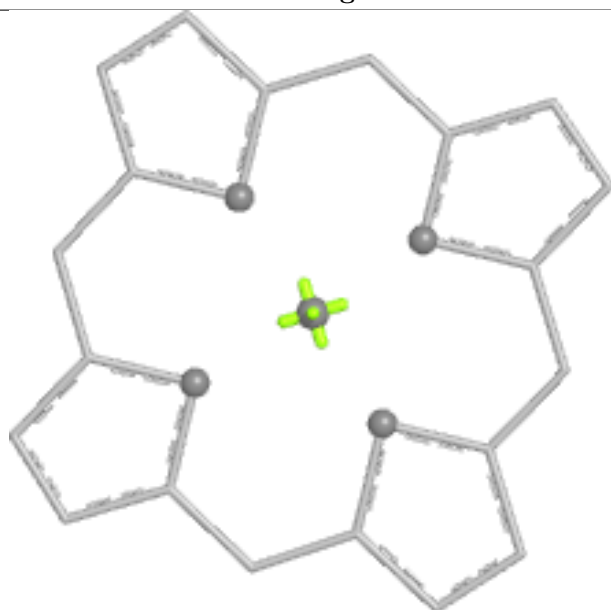
Ligand CLA B 630



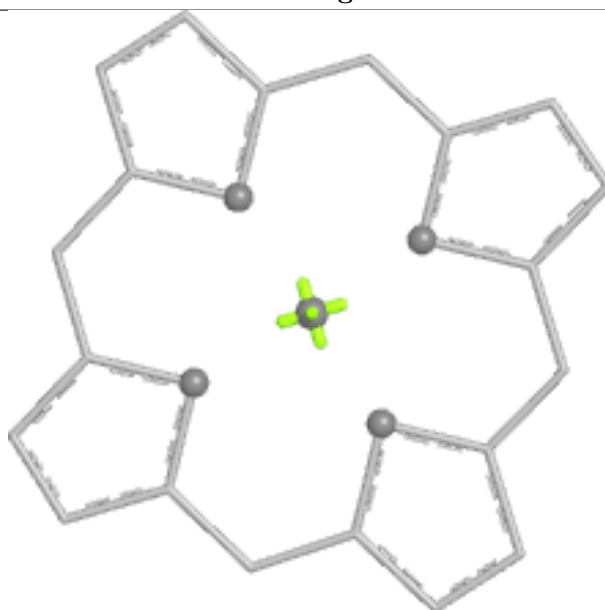
Bond lengths



Bond angles

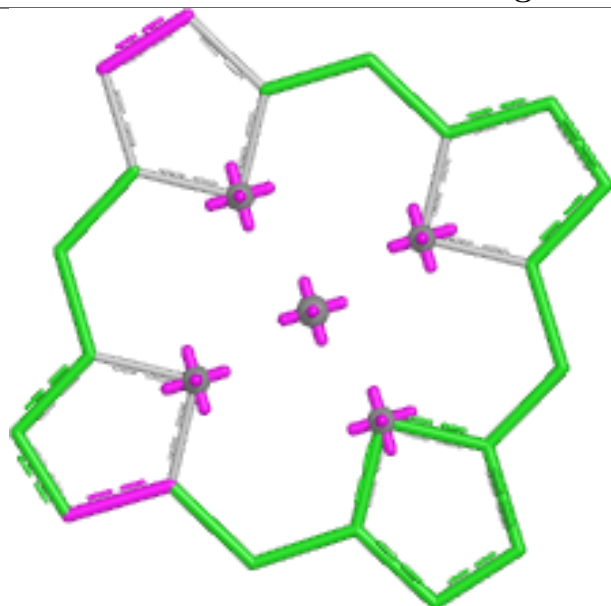


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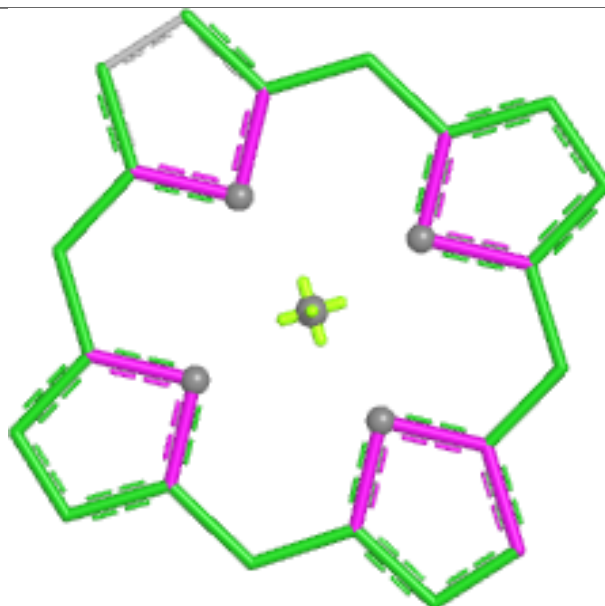


Rings

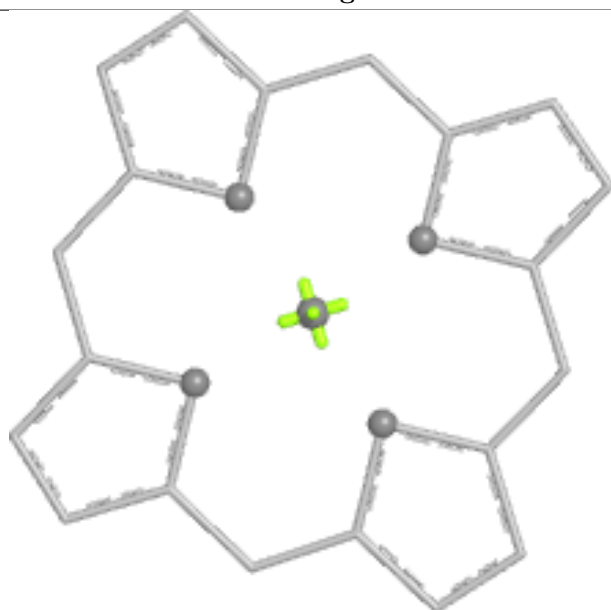
Ligand CLA B 620



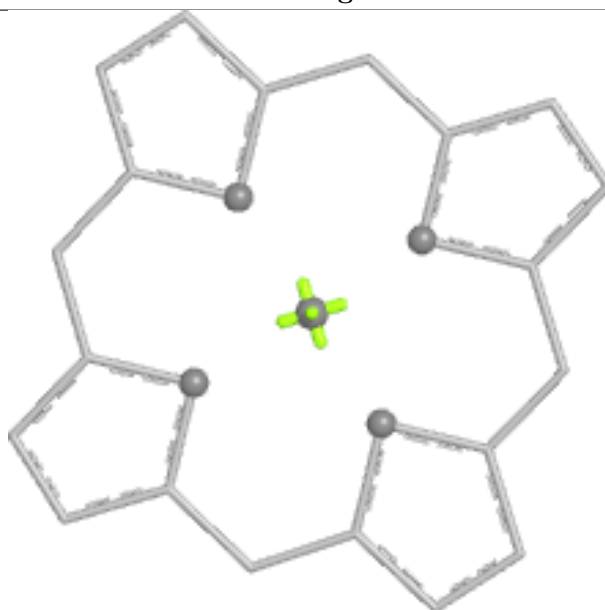
Bond lengths



Bond angles

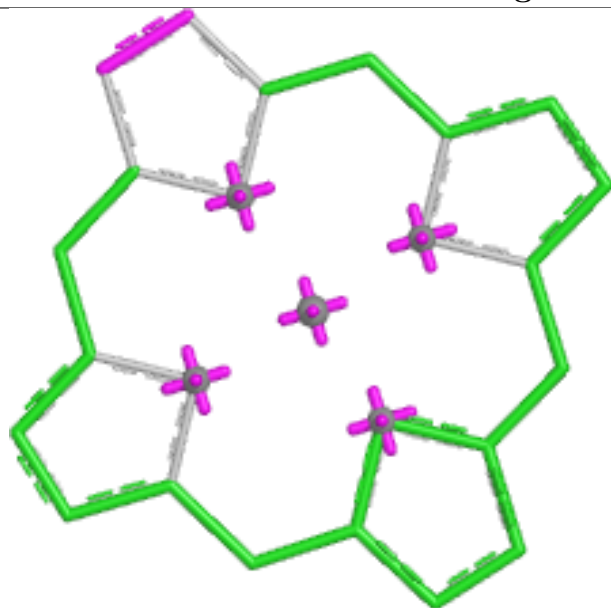


Torsions

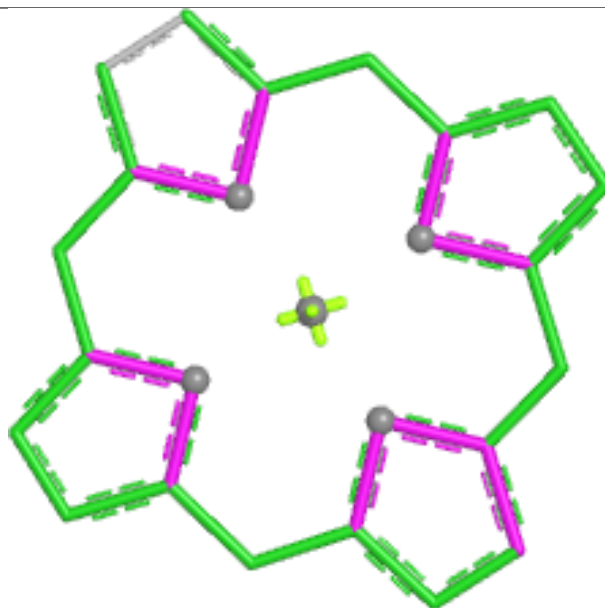


Rings

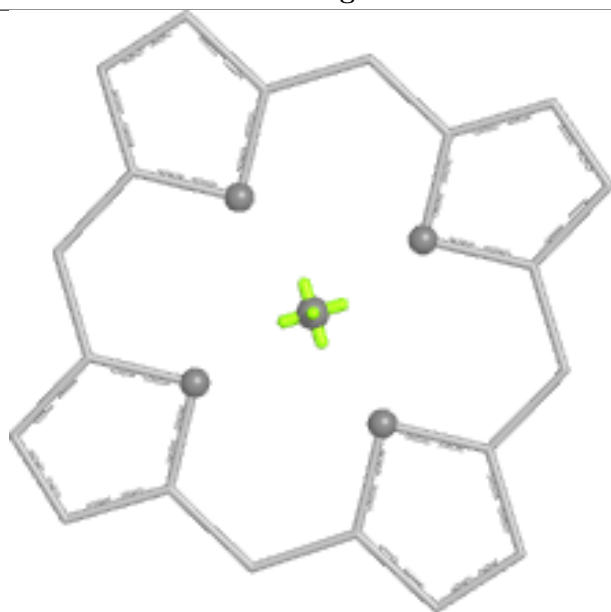
Ligand CLA B 643



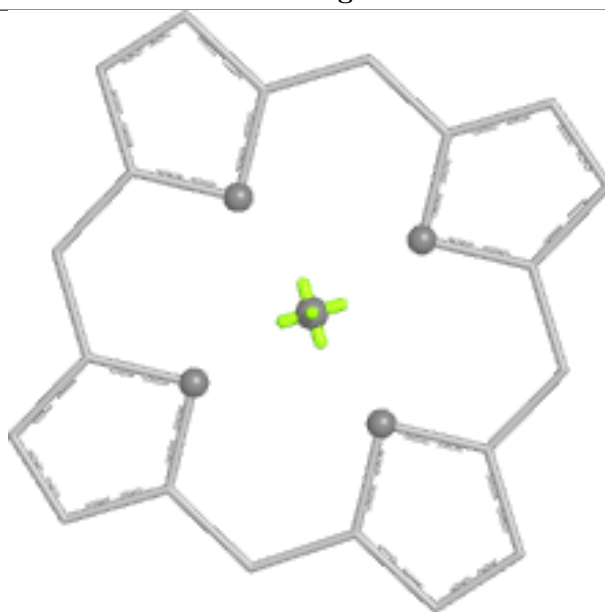
Bond lengths



Bond angles

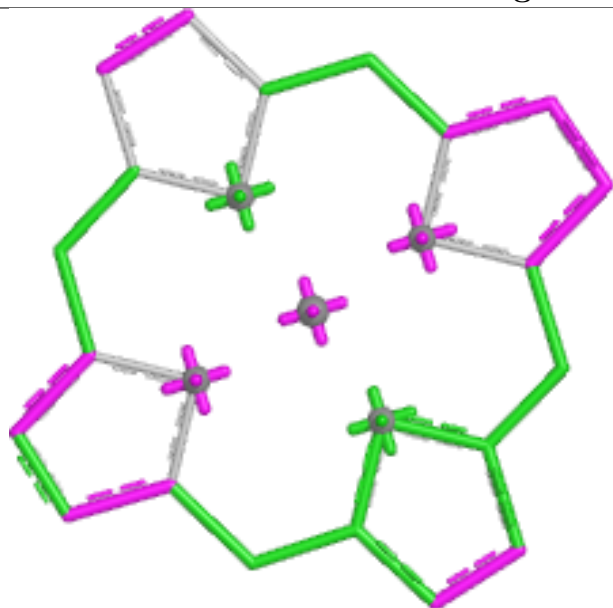


Torsions

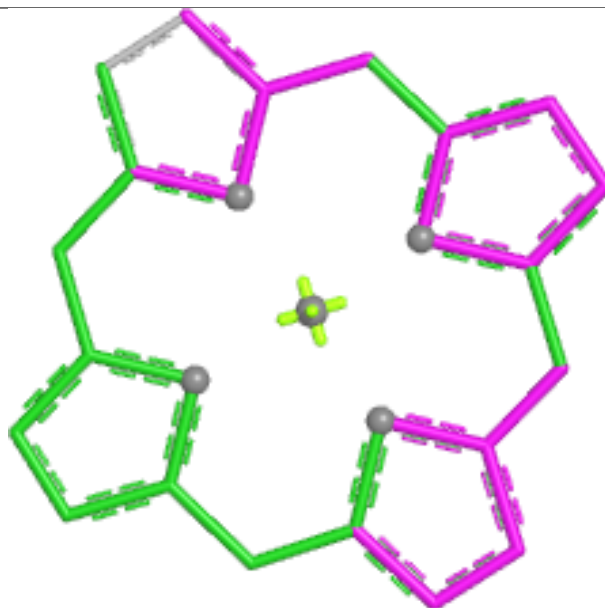


Rings

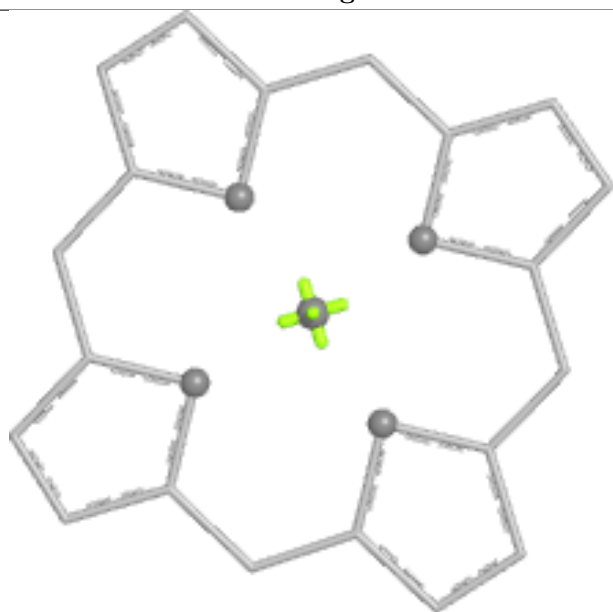
Ligand CLA A 618



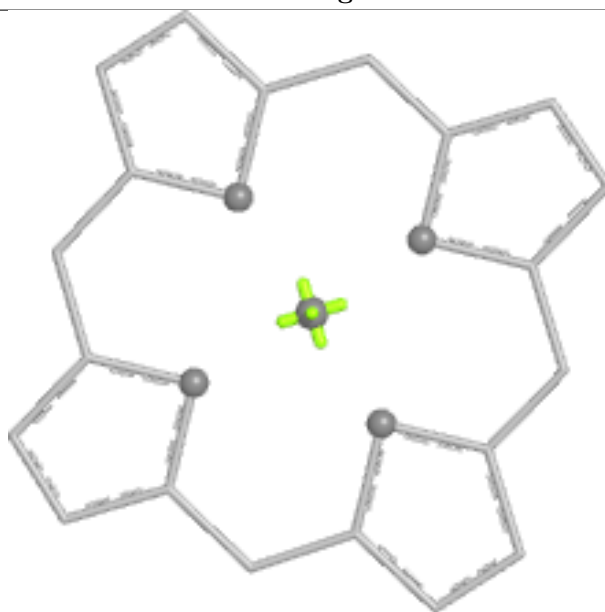
Bond lengths



Bond angles

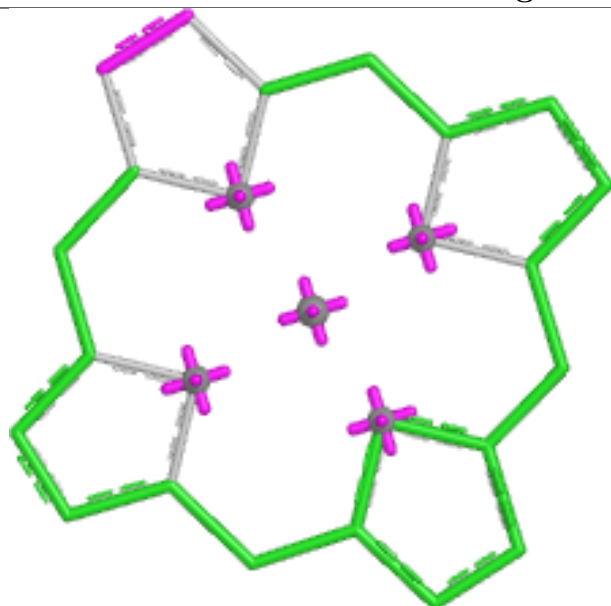


Torsions

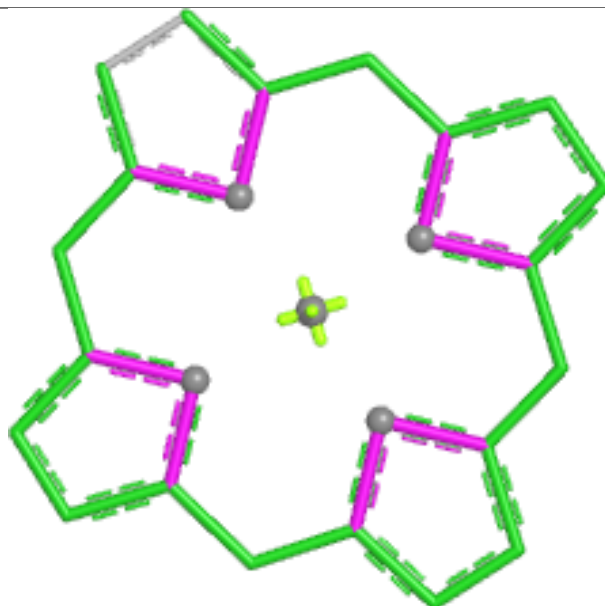


Rings

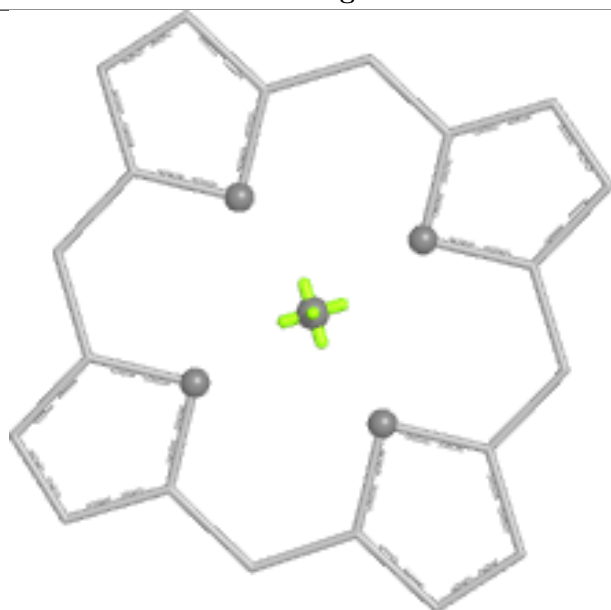
Ligand CLA F 155



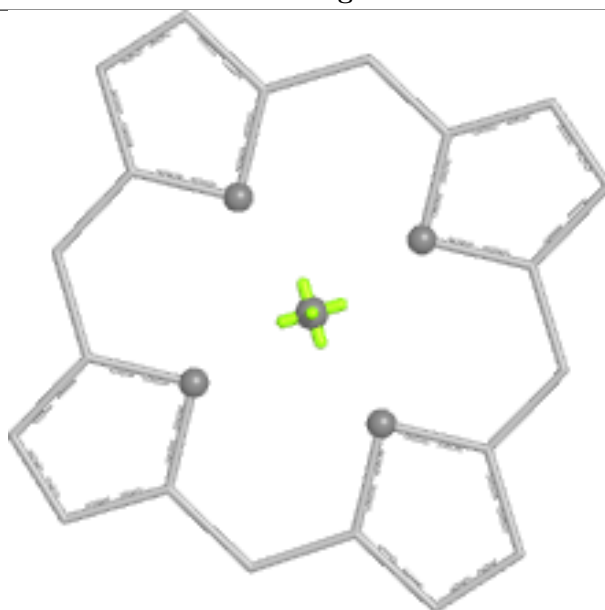
Bond lengths



Bond angles

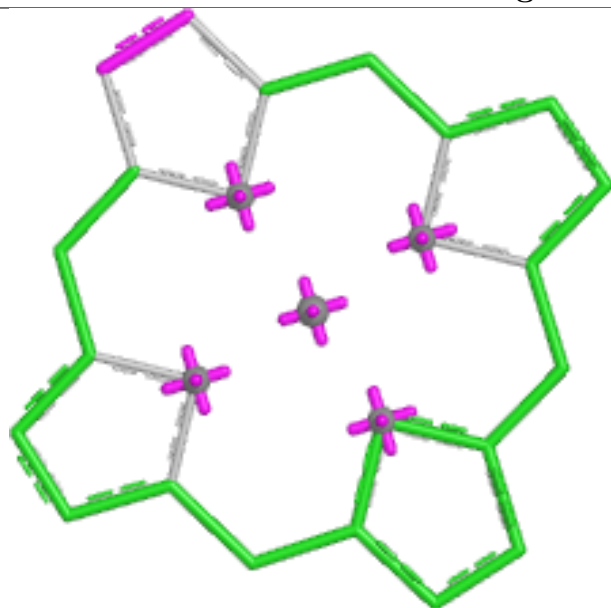


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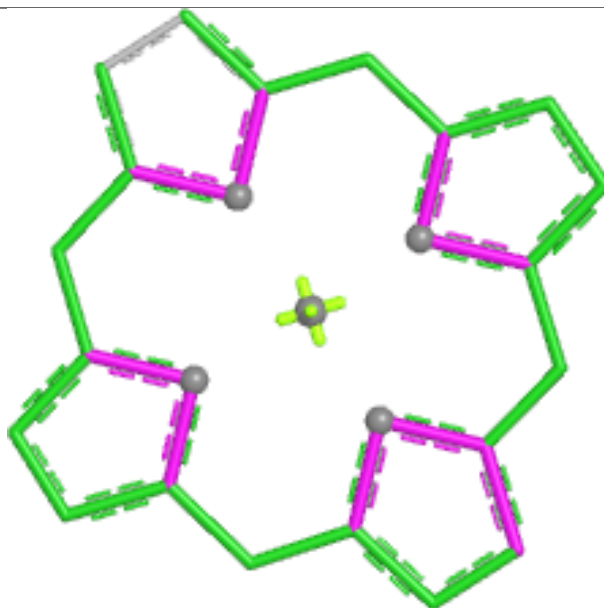


Rings

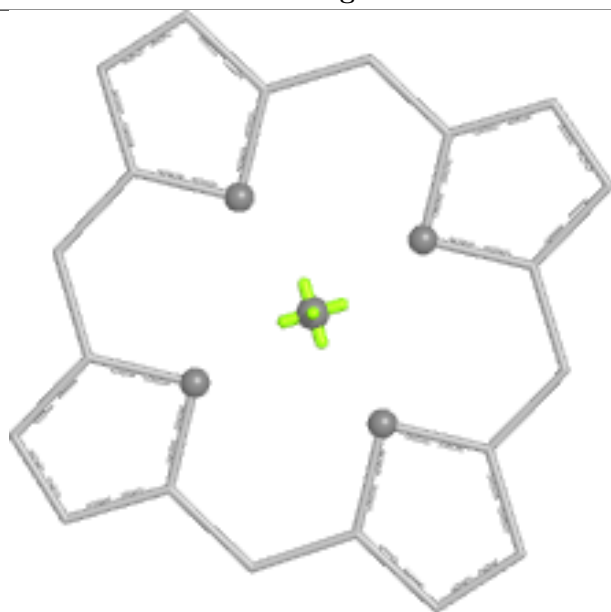
Ligand CLA L 149



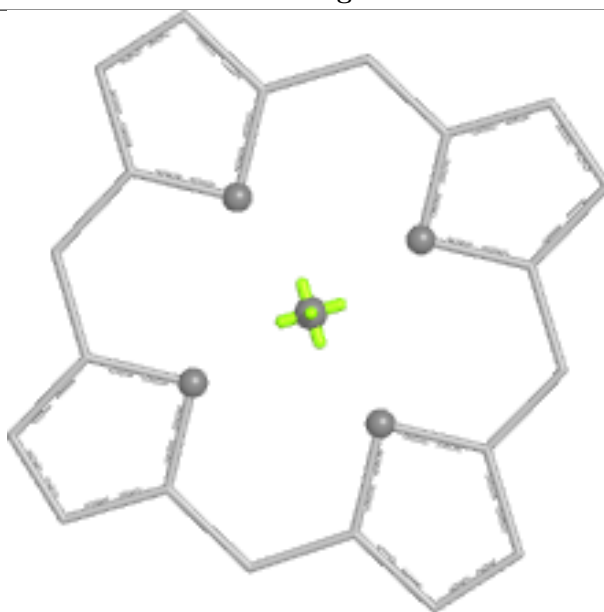
Bond lengths



Bond angles

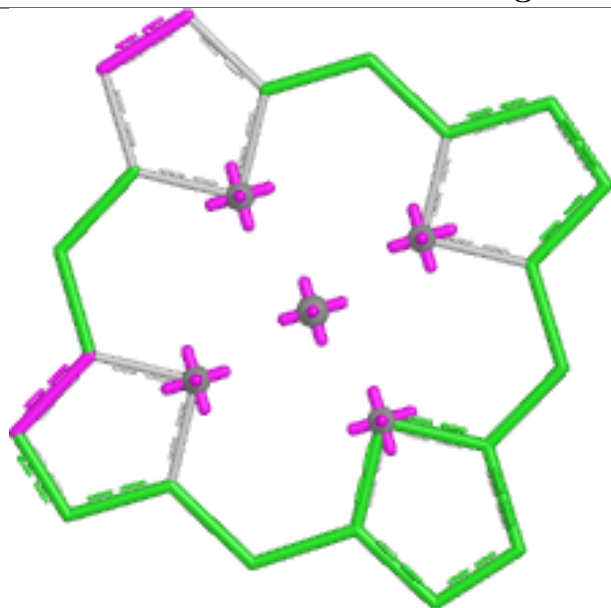


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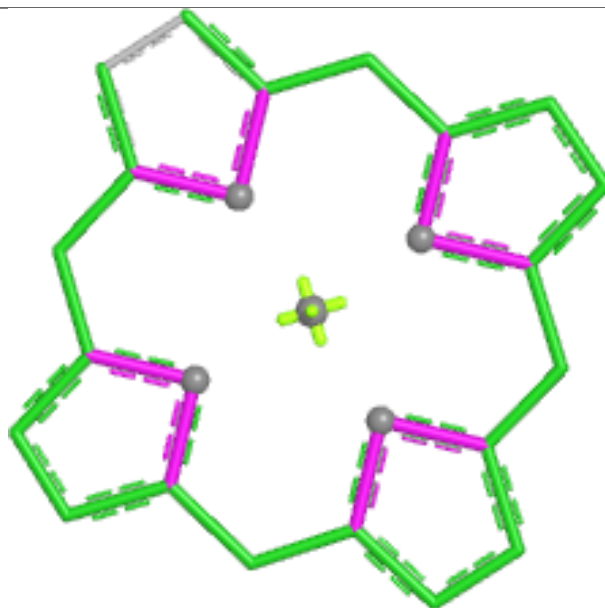


Rings

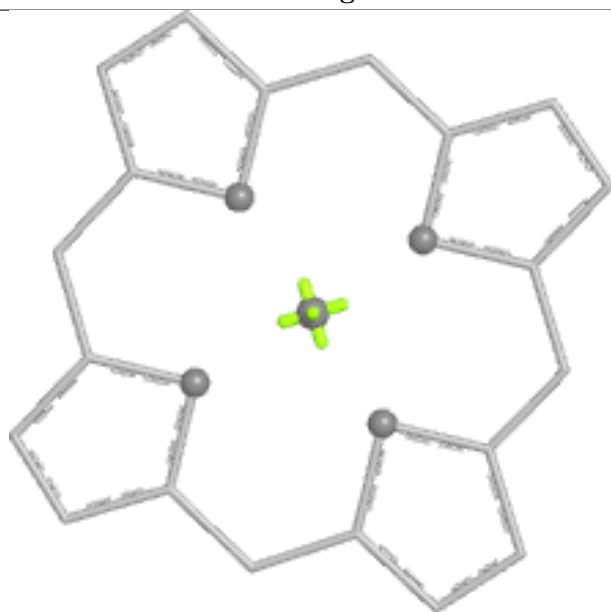
Ligand CLA B 621



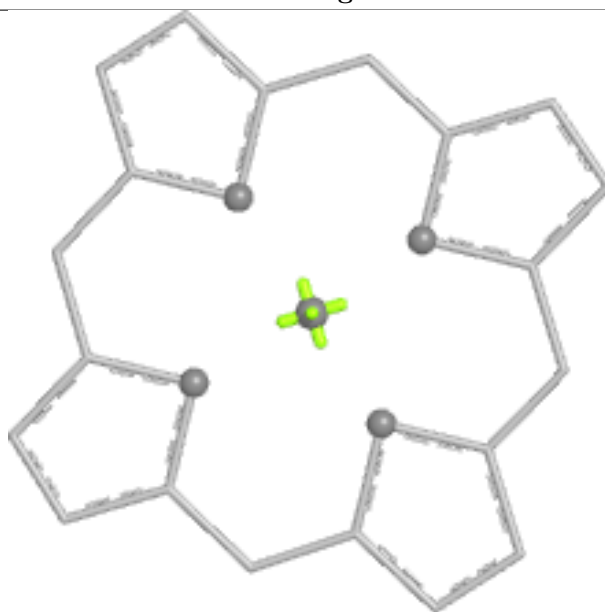
Bond lengths



Bond angles

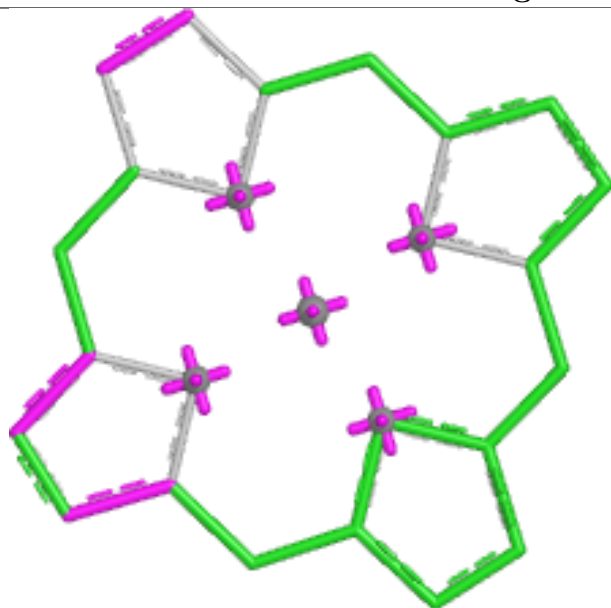


Torsions

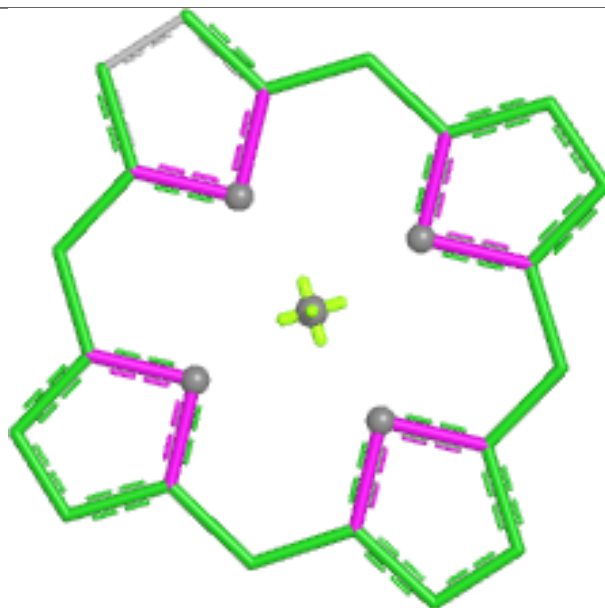


Rings

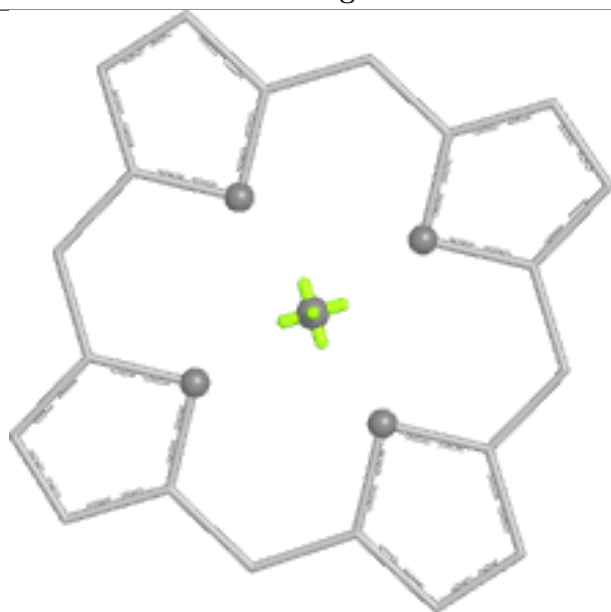
Ligand CLA A 600



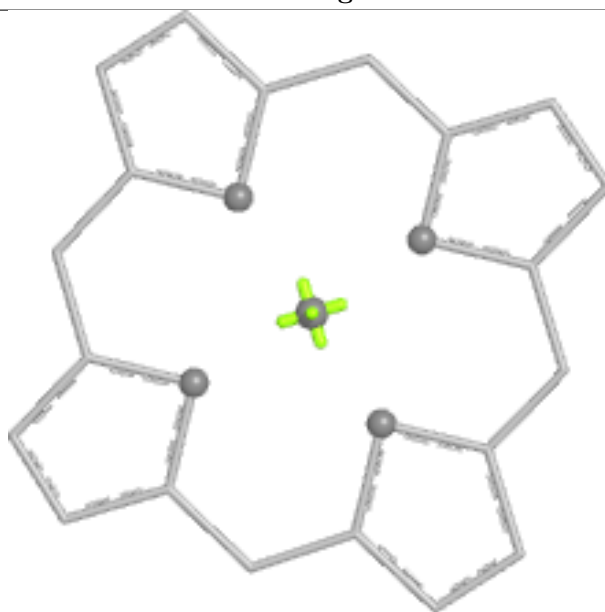
Bond lengths



Bond angles

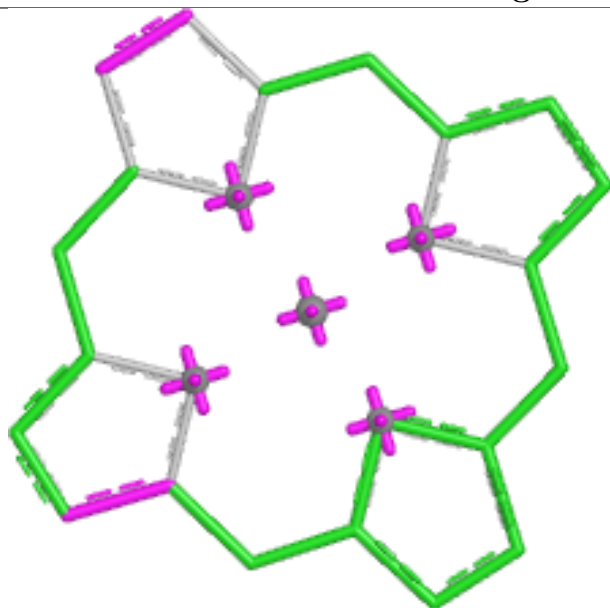


Torsions

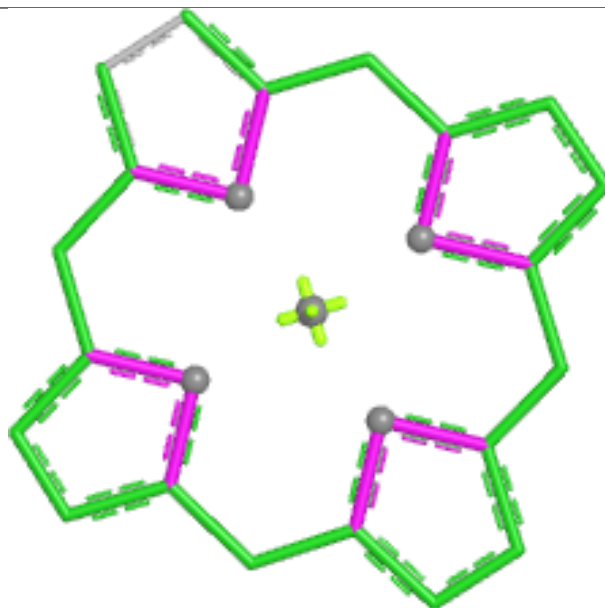


Rings

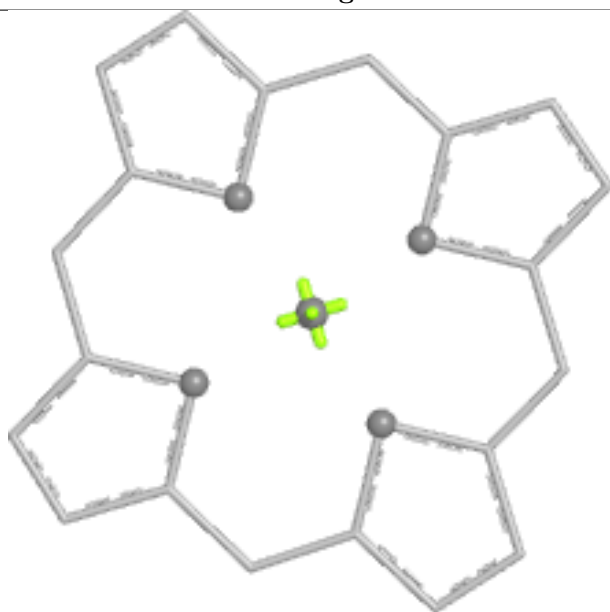
Ligand CLA A 611



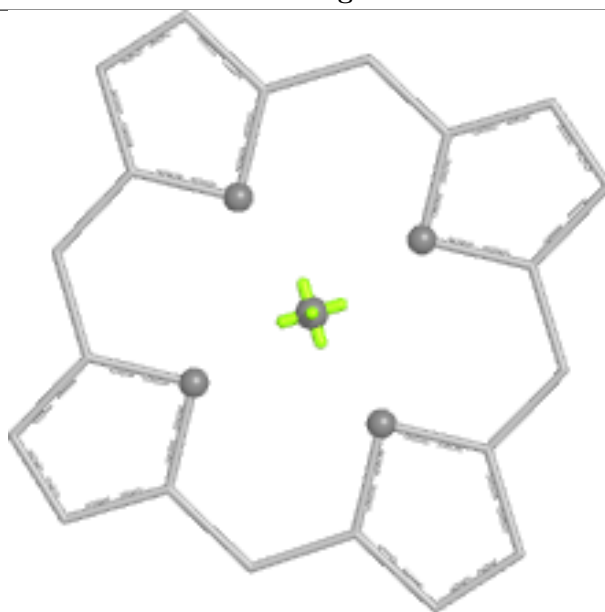
Bond lengths



Bond angles

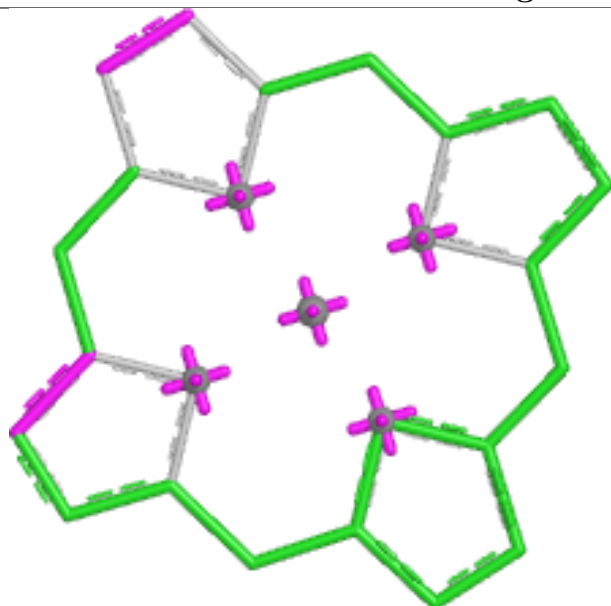


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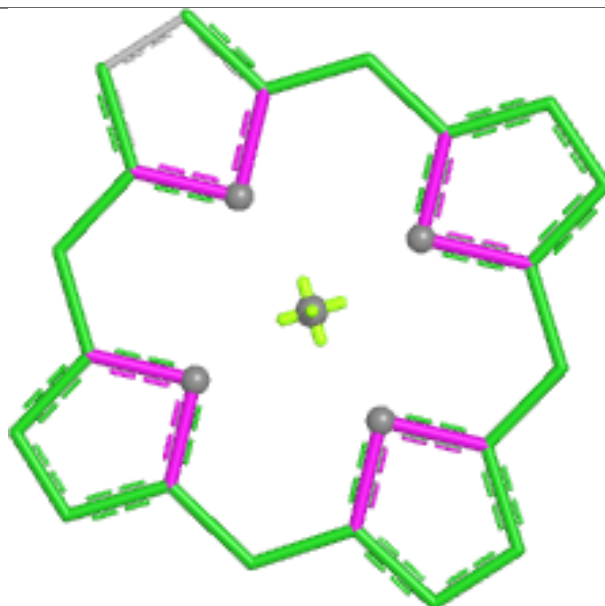


Rings

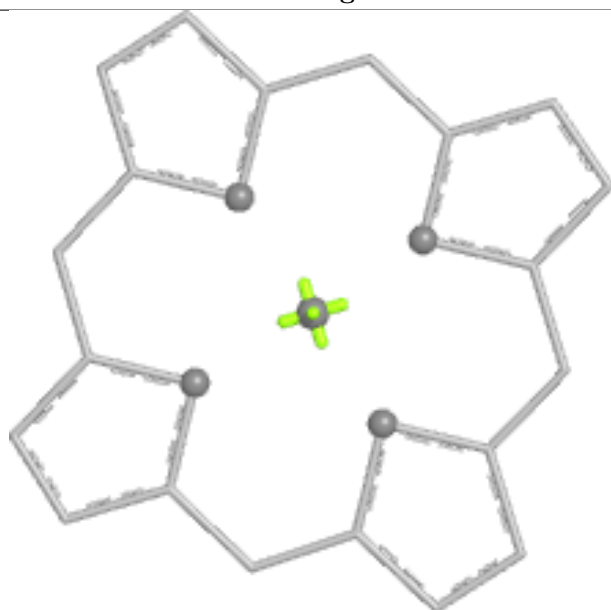
Ligand CLA L 147



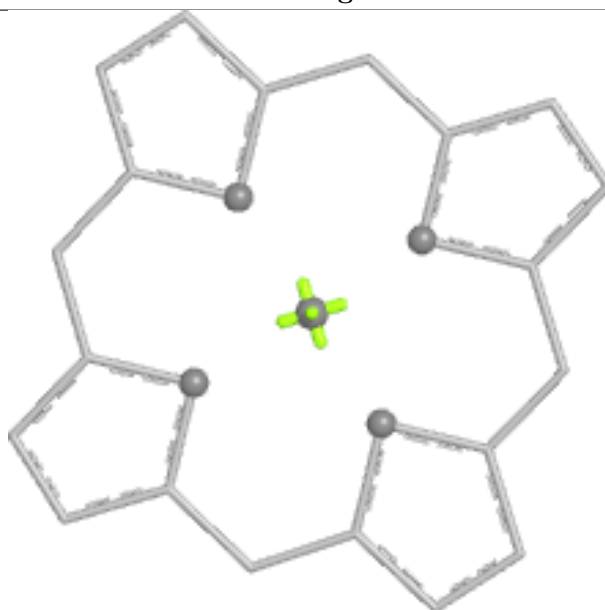
Bond lengths



Bond angles

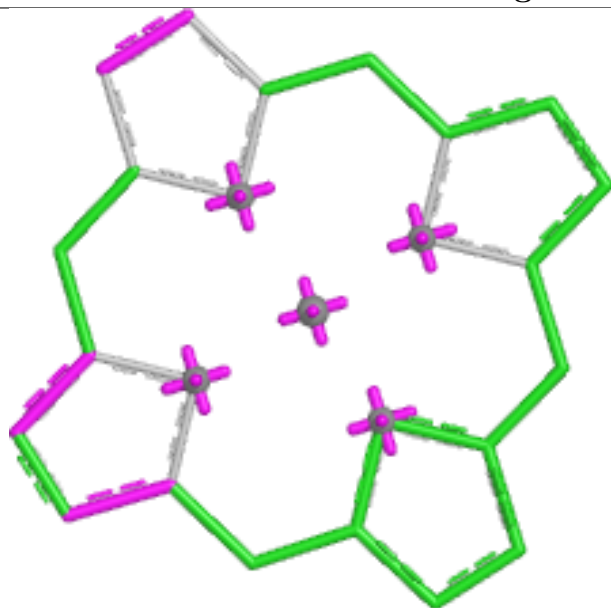


Torsions

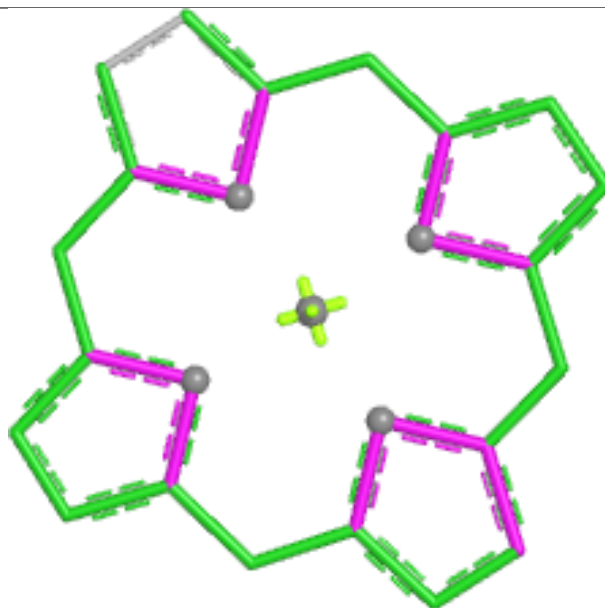


Rings

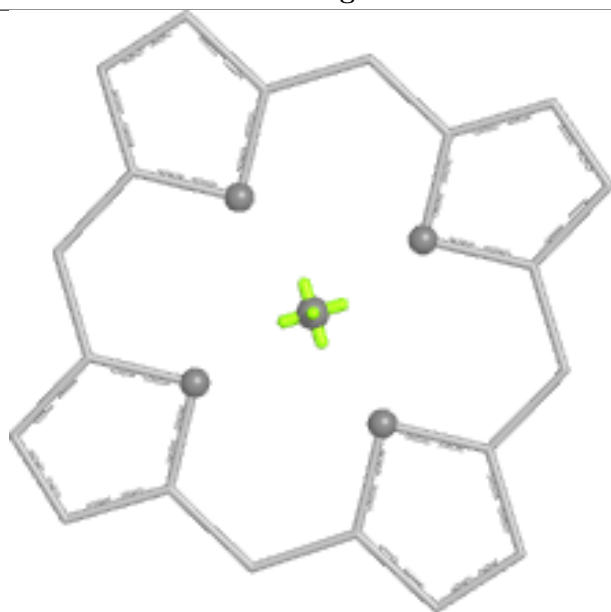
Ligand CLA B 639



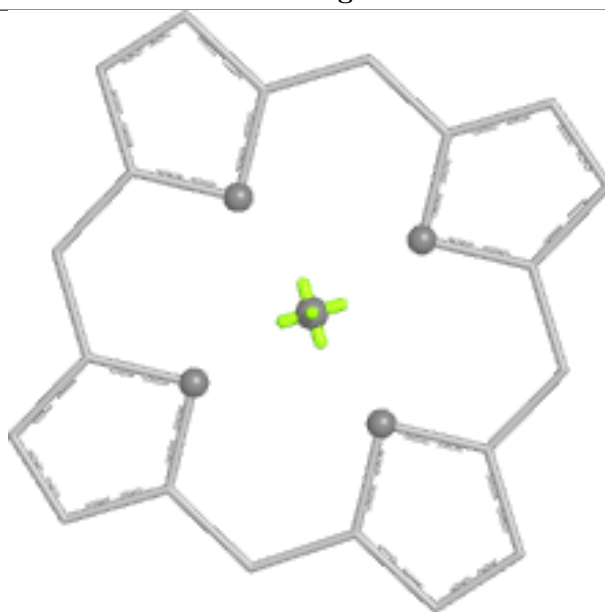
Bond lengths



Bond angles

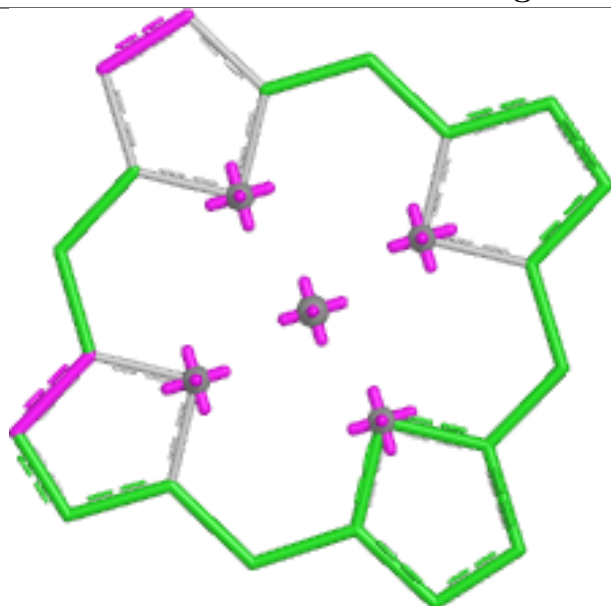


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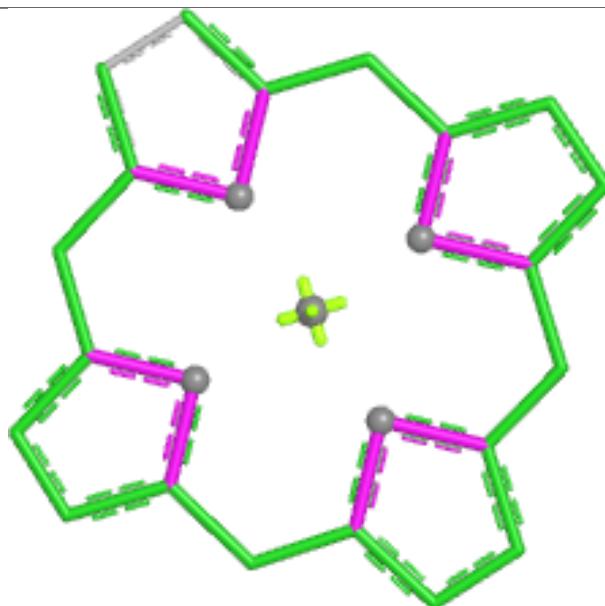


Rings

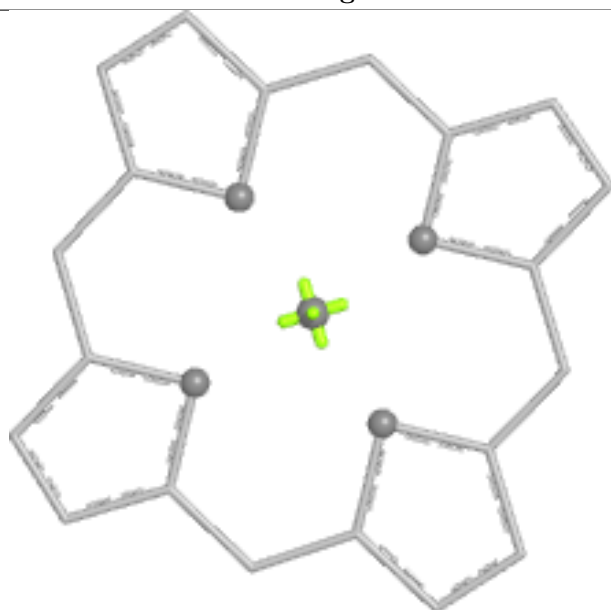
Ligand CLA A 626



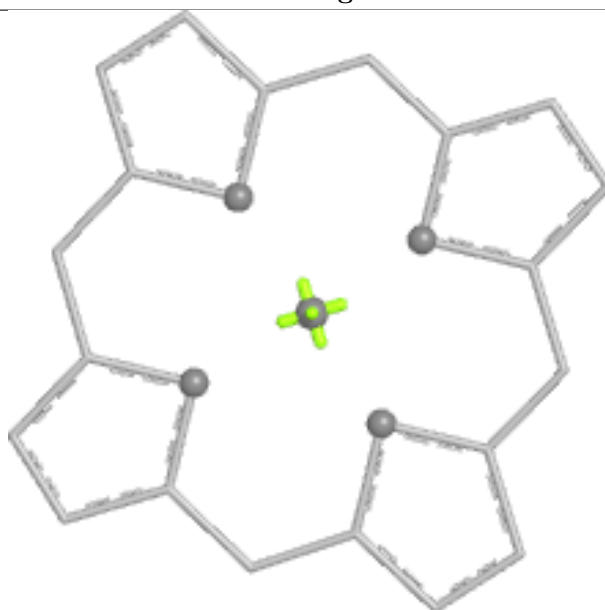
Bond lengths



Bond angles

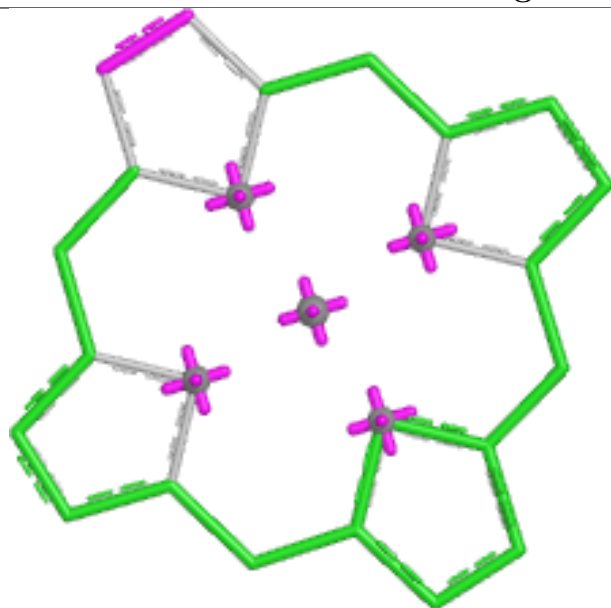


Torsions

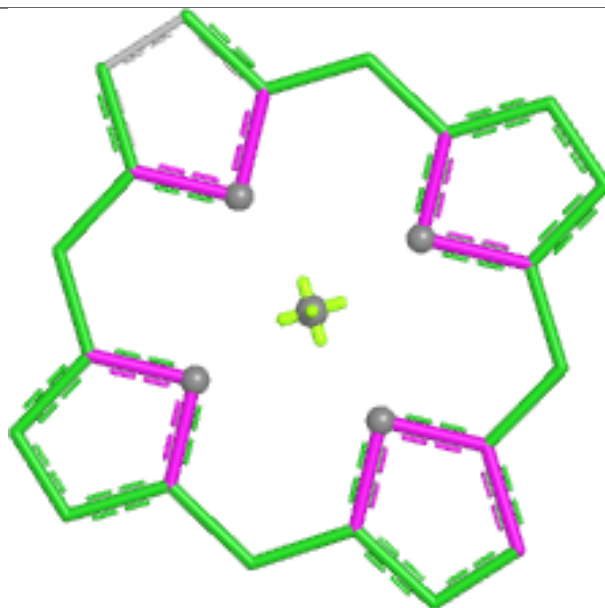


Rings

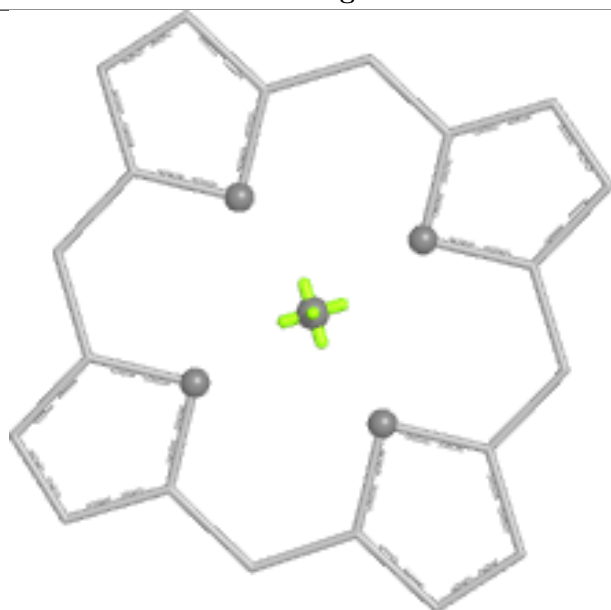
Ligand CLA B 638



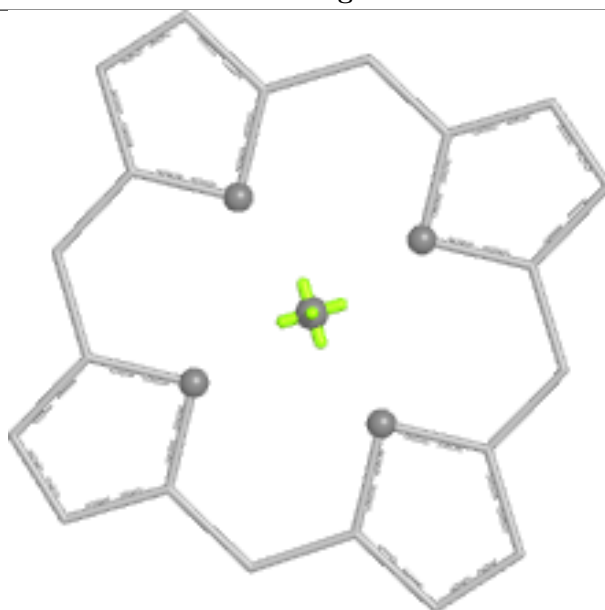
Bond lengths



Bond angles

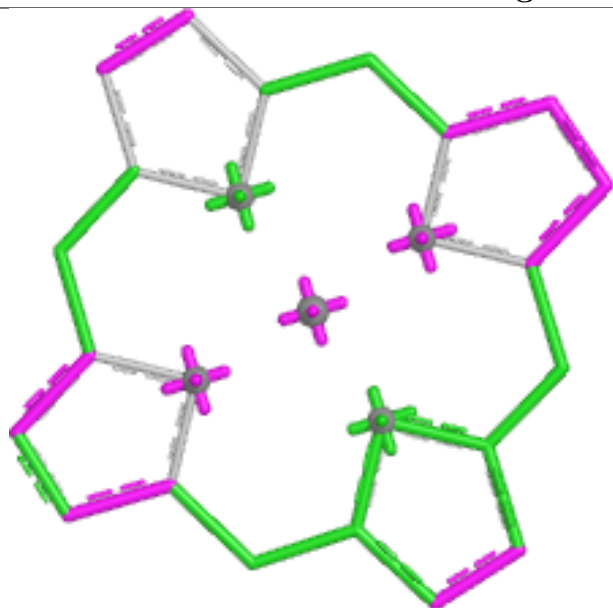


Torsions

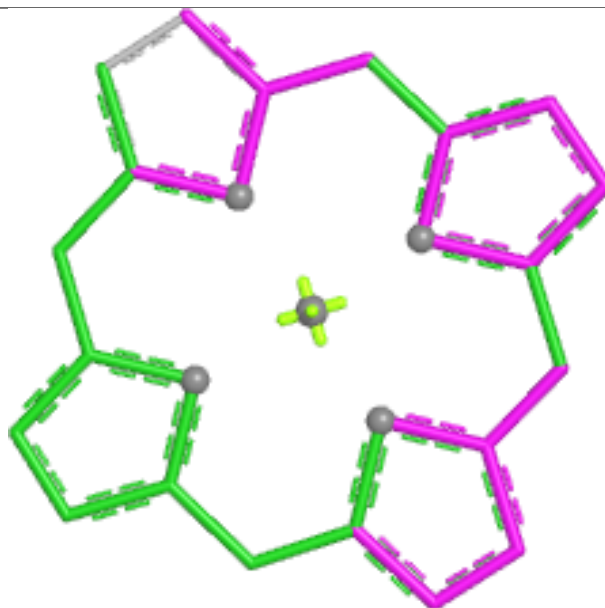


Rings

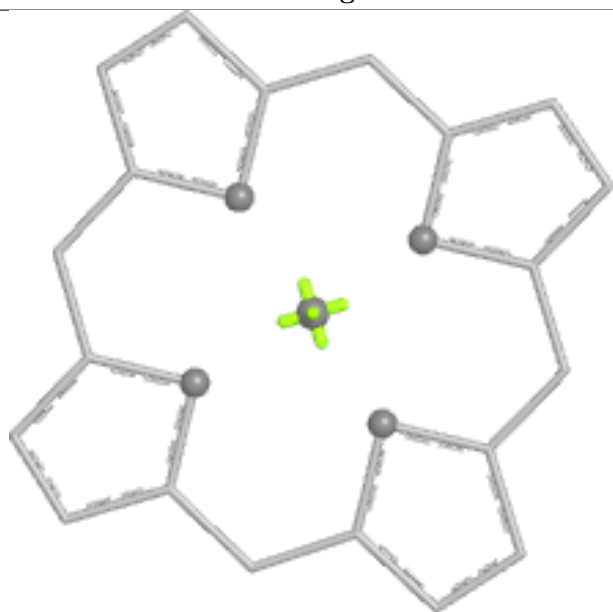
Ligand CLA F 158



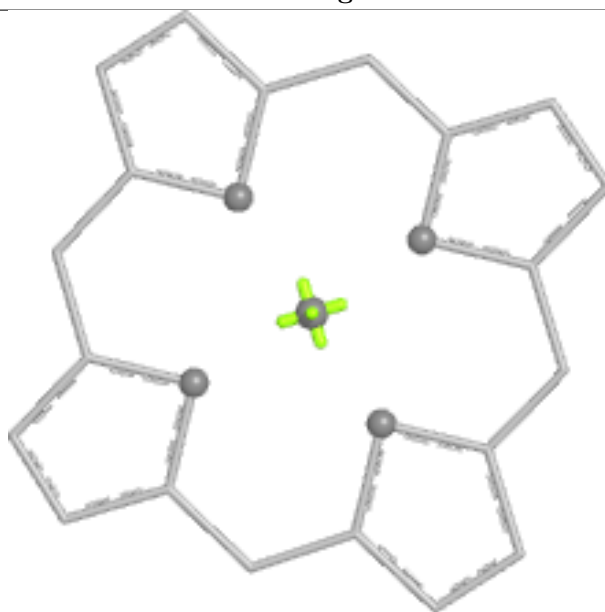
Bond lengths



Bond angles

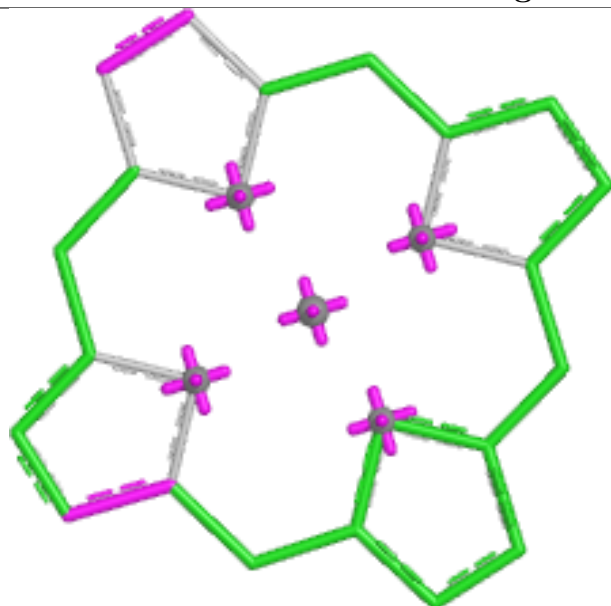


Torsions

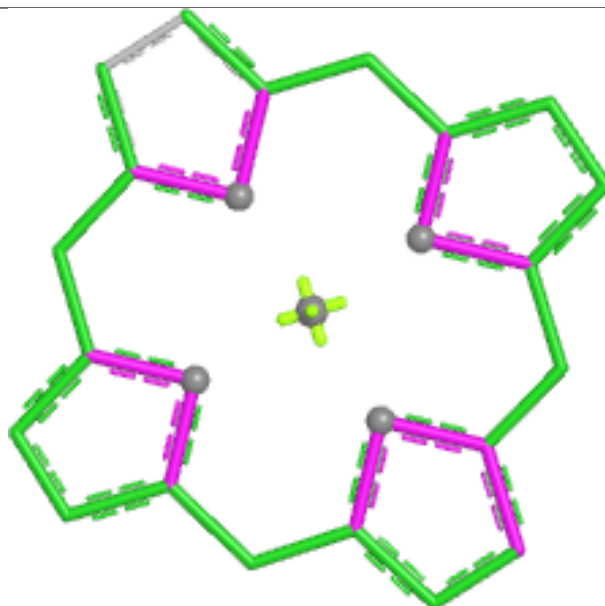


Rings

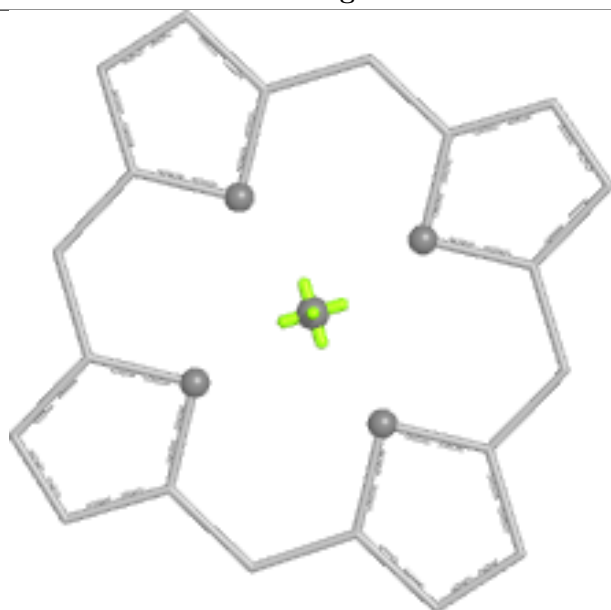
Ligand CLA B 628



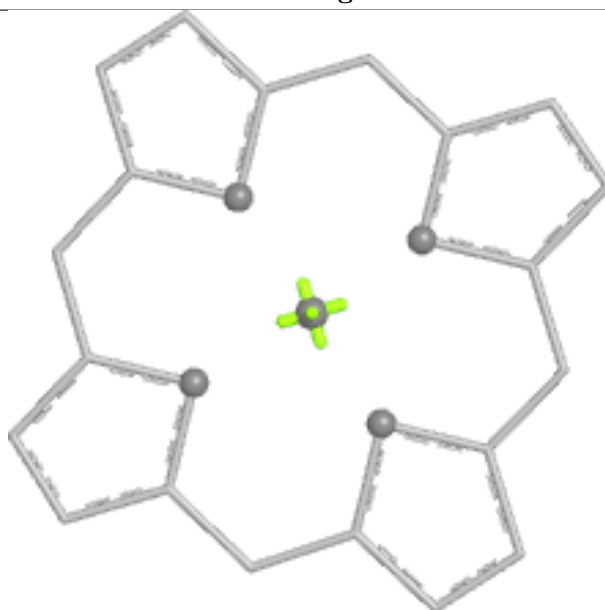
Bond lengths



Bond angles

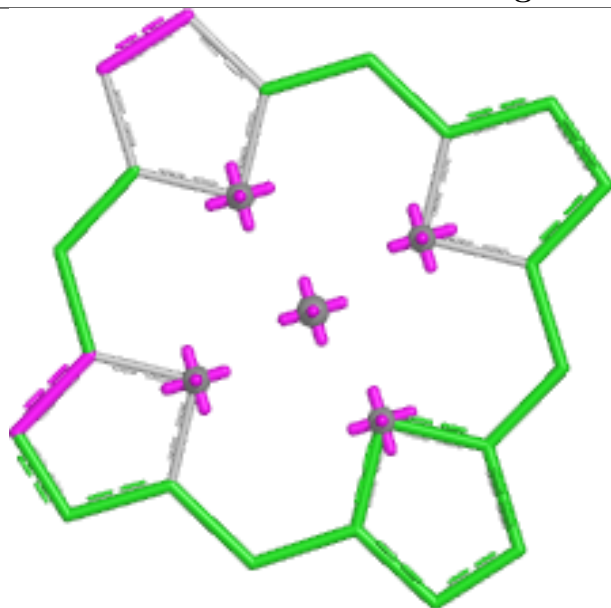


Torsions

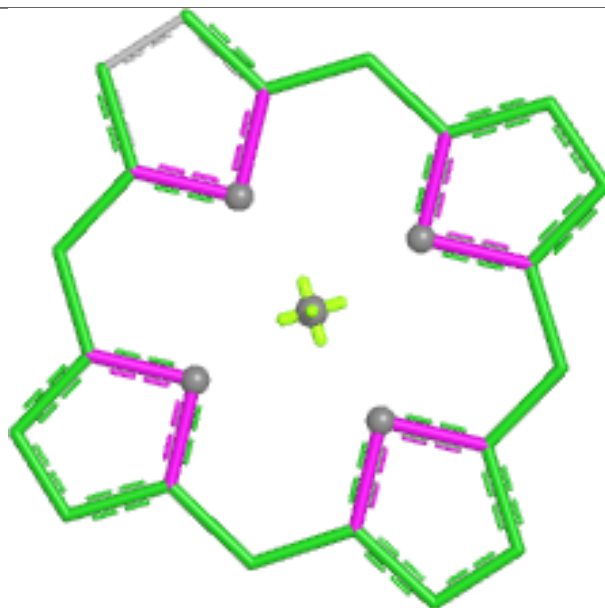


Rings

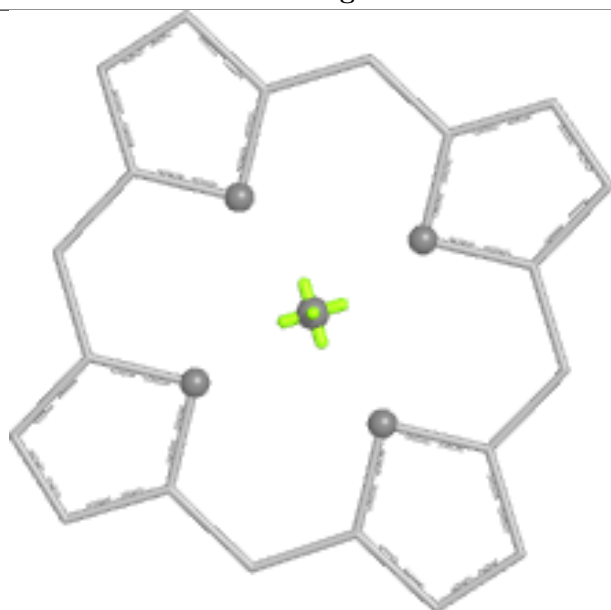
Ligand CLA B 649



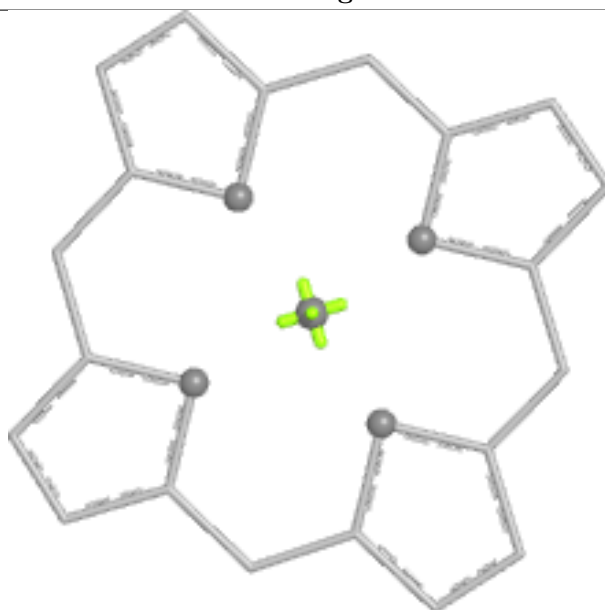
Bond lengths



Bond angles

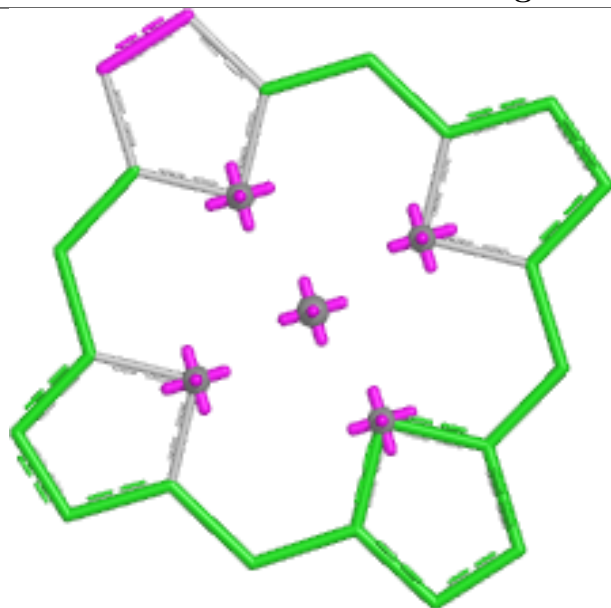


Torsions

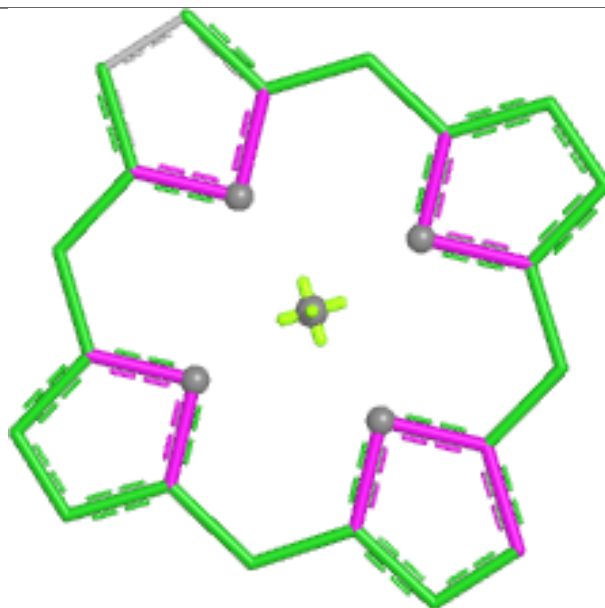


Rings

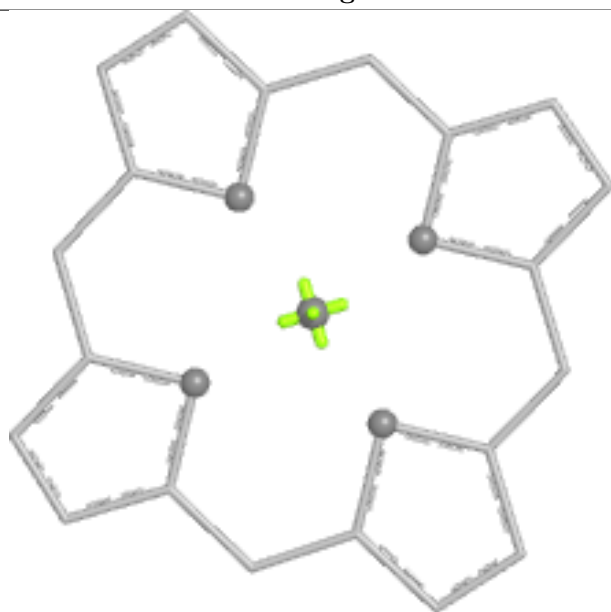
Ligand CLA B 647



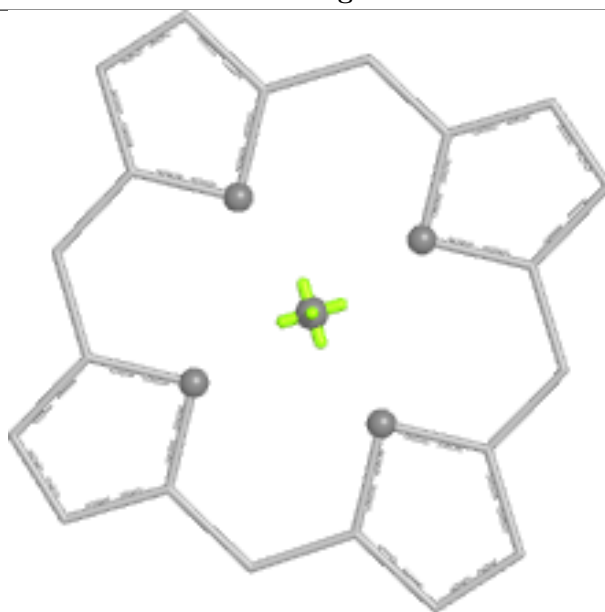
Bond lengths



Bond angles

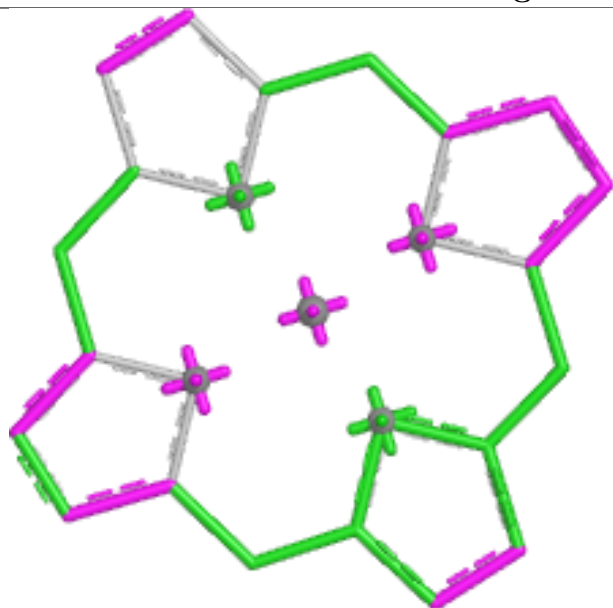


Torsions

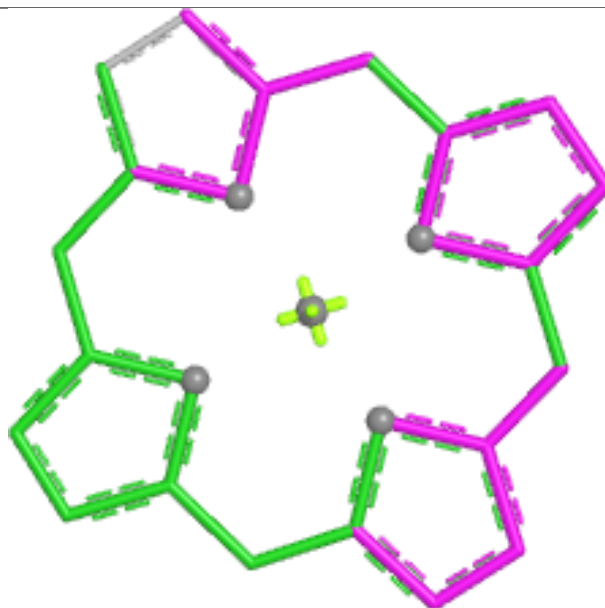


Rings

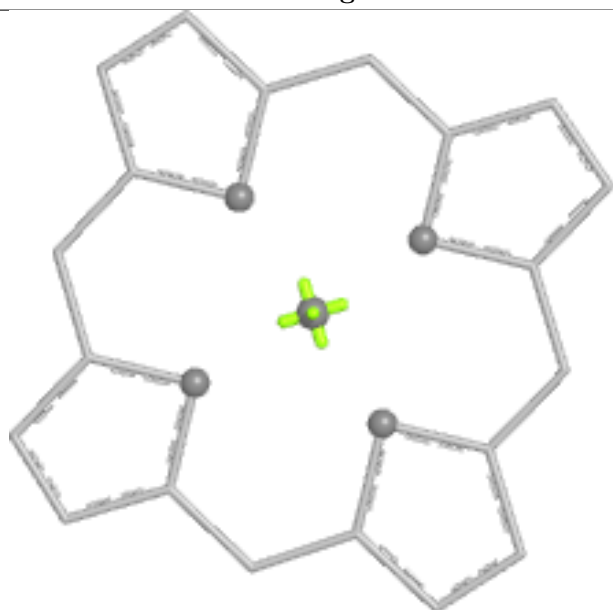
Ligand CLA A 617



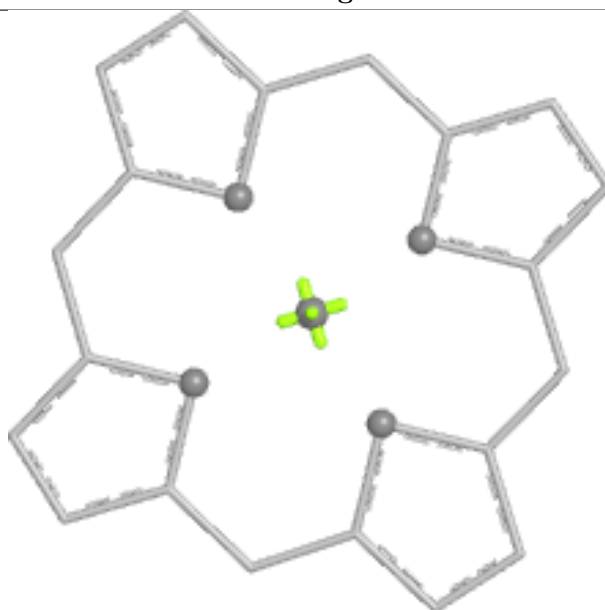
Bond lengths



Bond angles

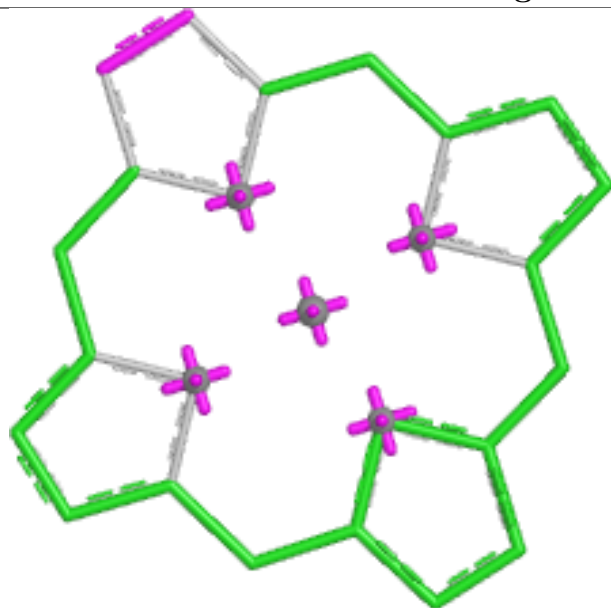


Torsions

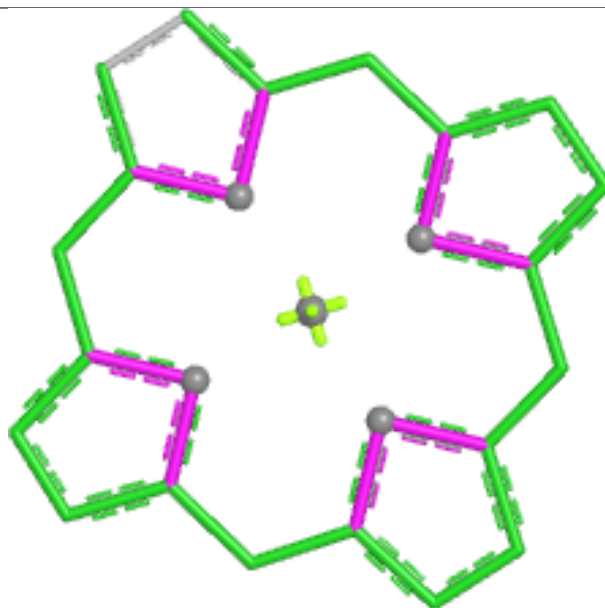


Rings

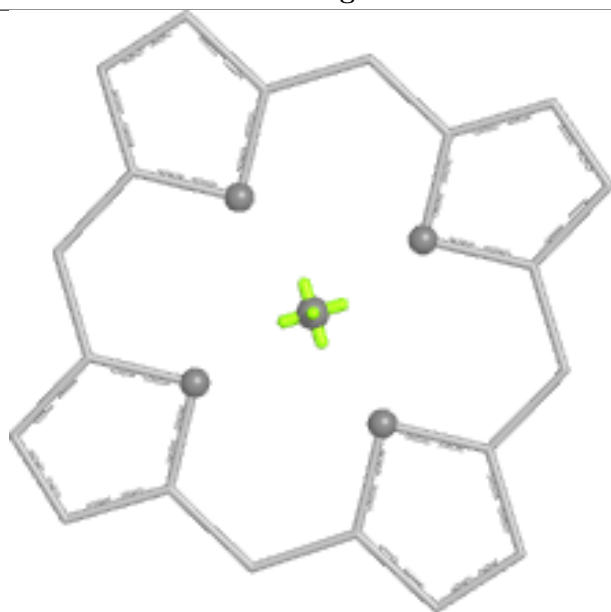
Ligand CLA B 648



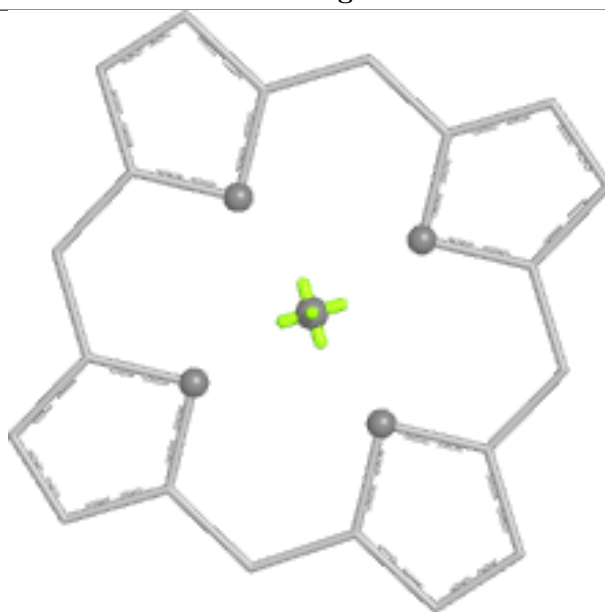
Bond lengths



Bond angles

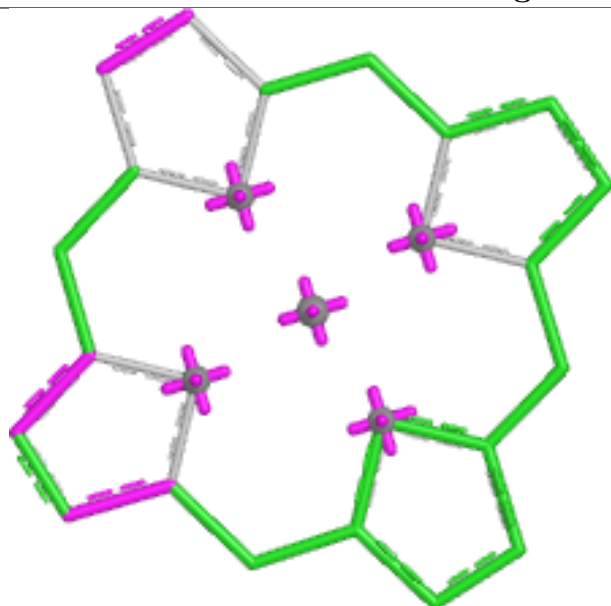


Torsions

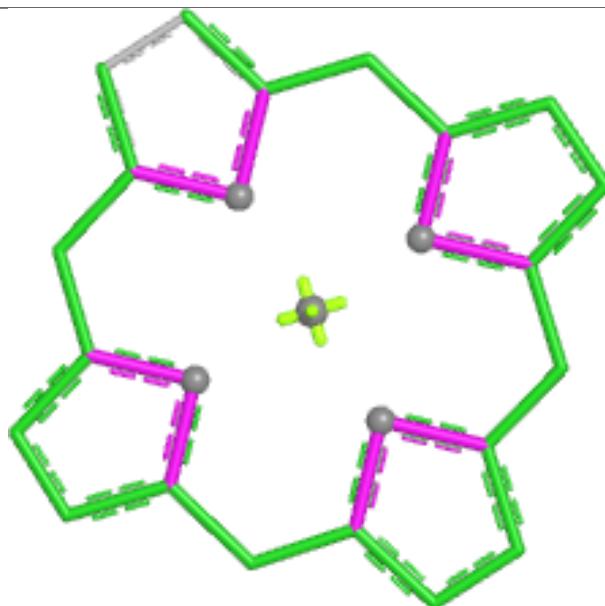


Rings

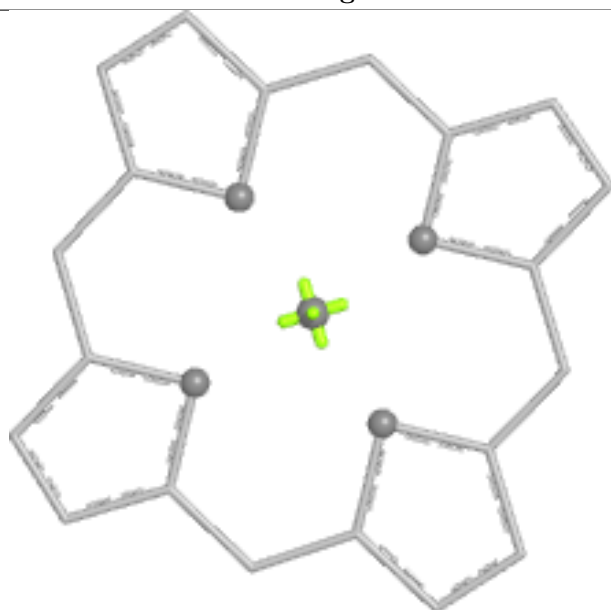
Ligand CLA A 623



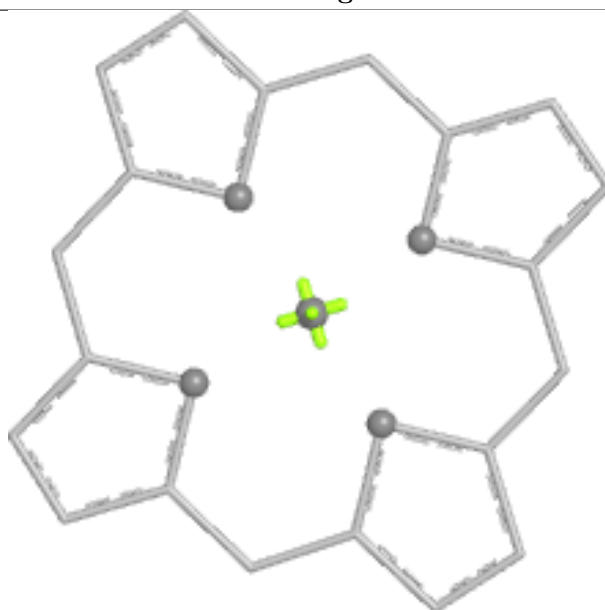
Bond lengths



Bond angles

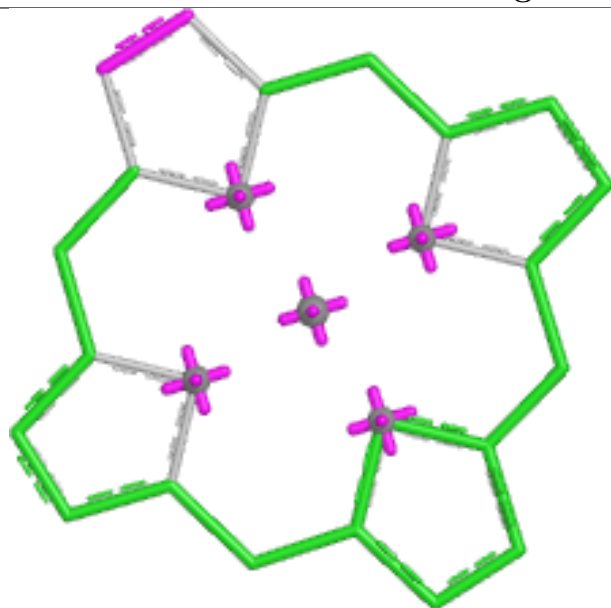


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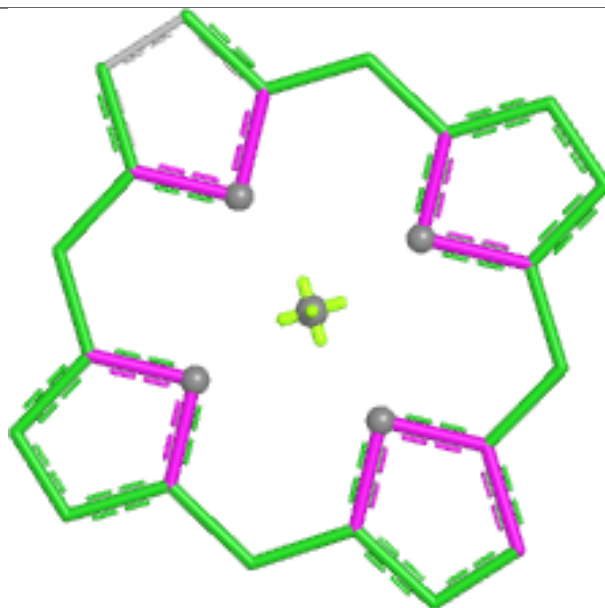


Rings

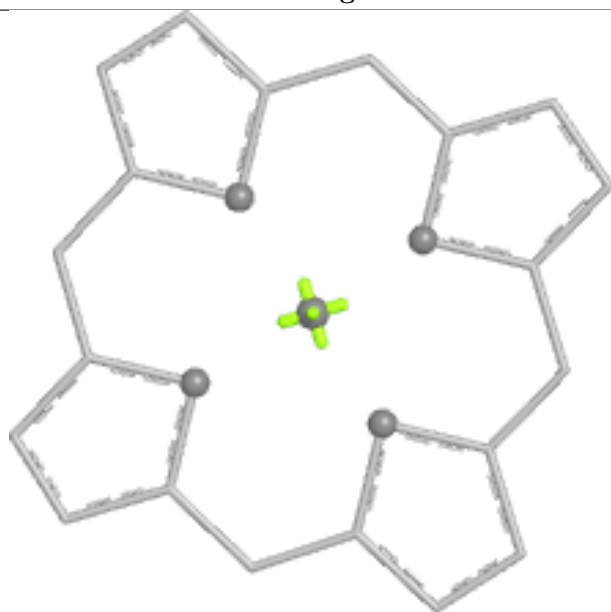
Ligand CLA B 644



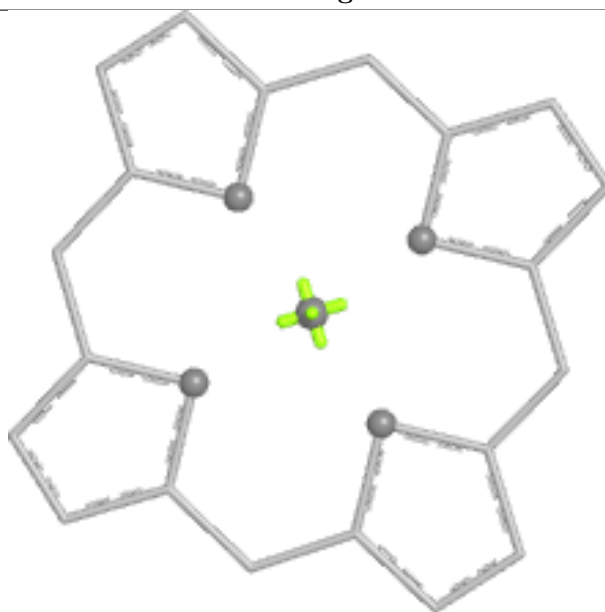
Bond lengths



Bond angles

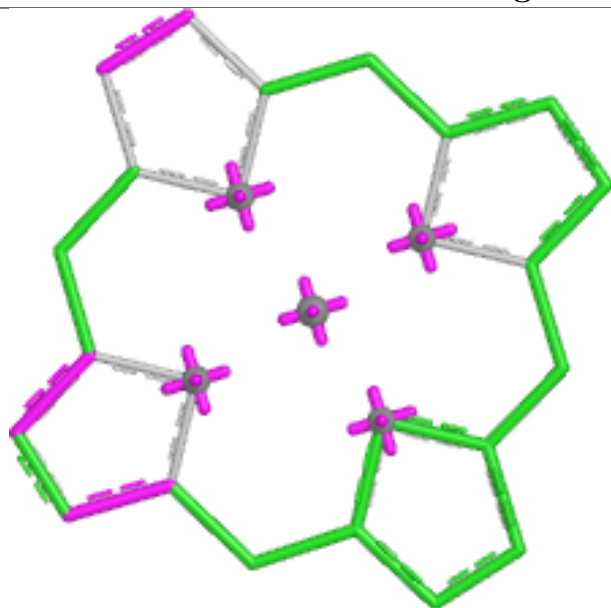


Torsions

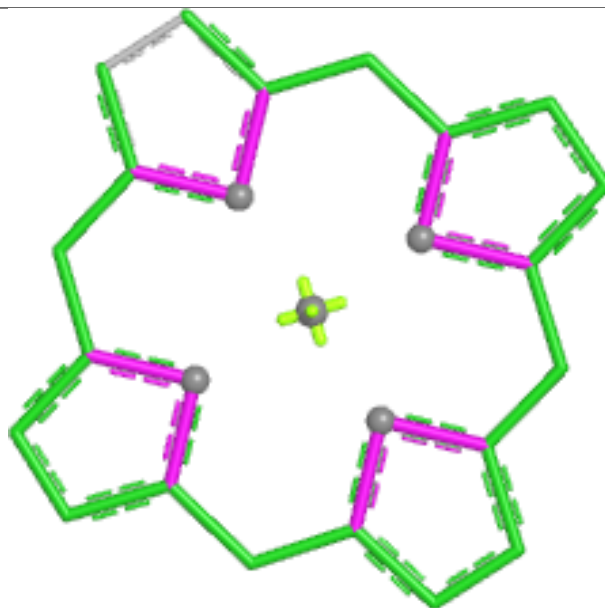


Rings

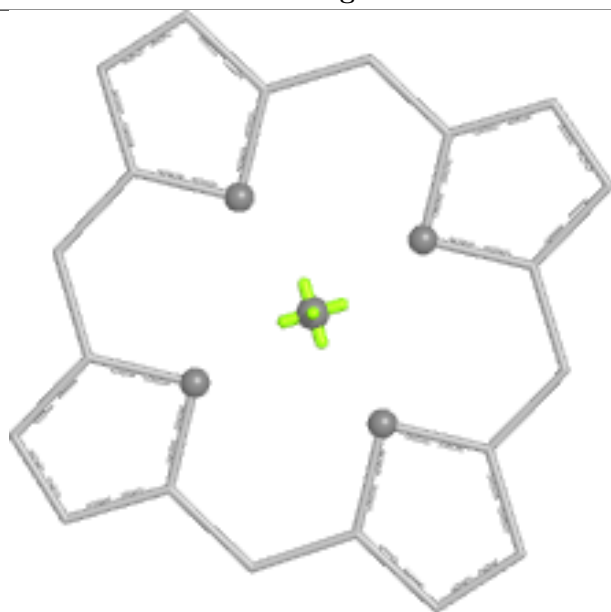
Ligand CLA A 625



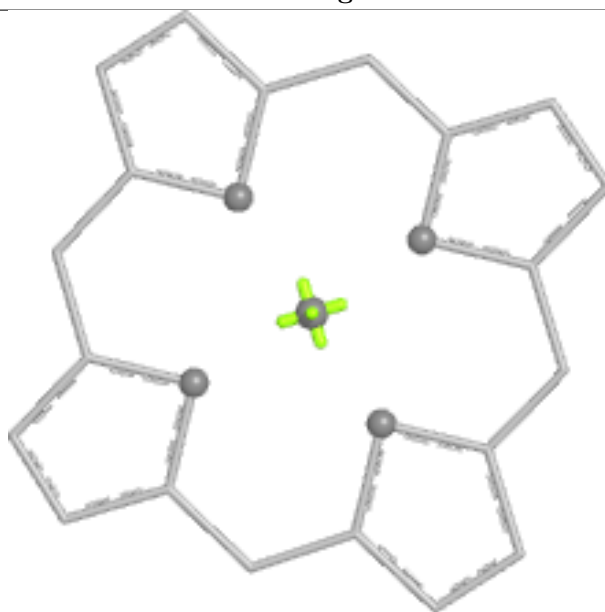
Bond lengths



Bond angles

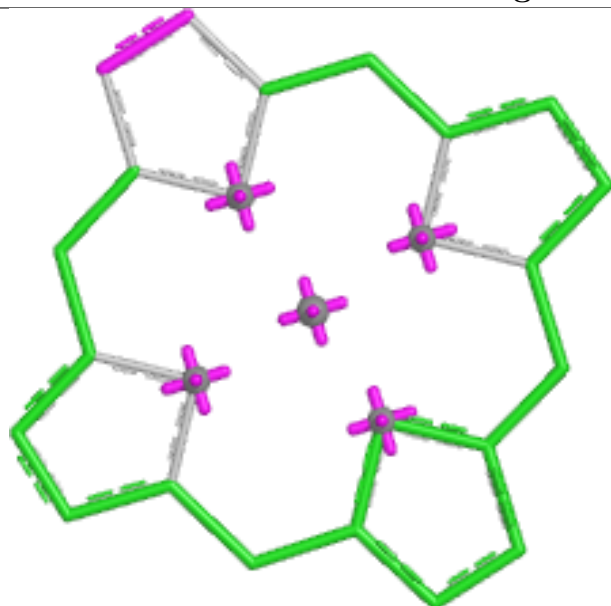


Torsions

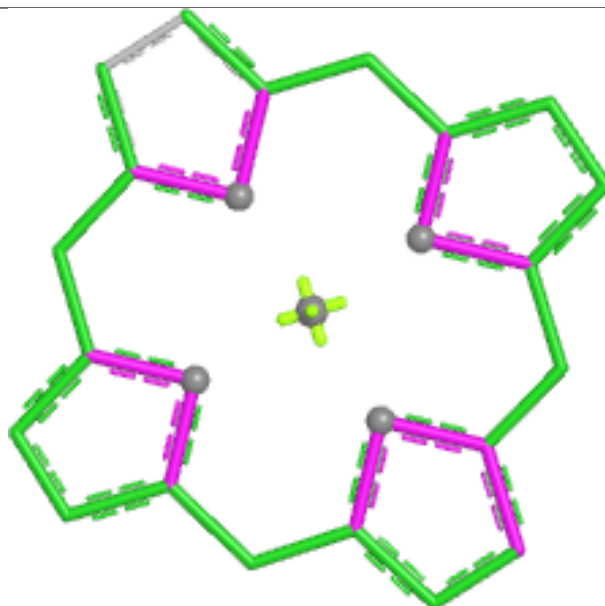


Rings

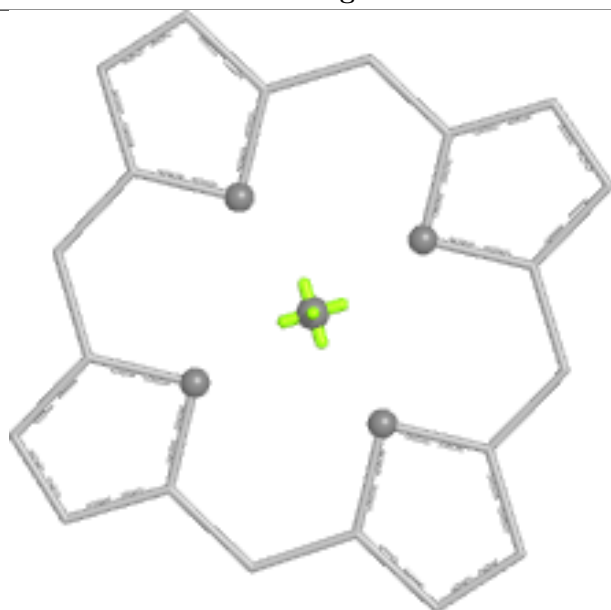
Ligand CLA A 621



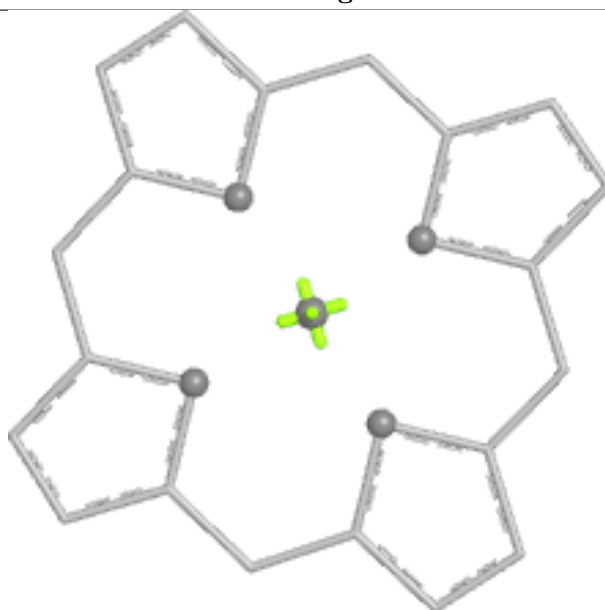
Bond lengths



Bond angles

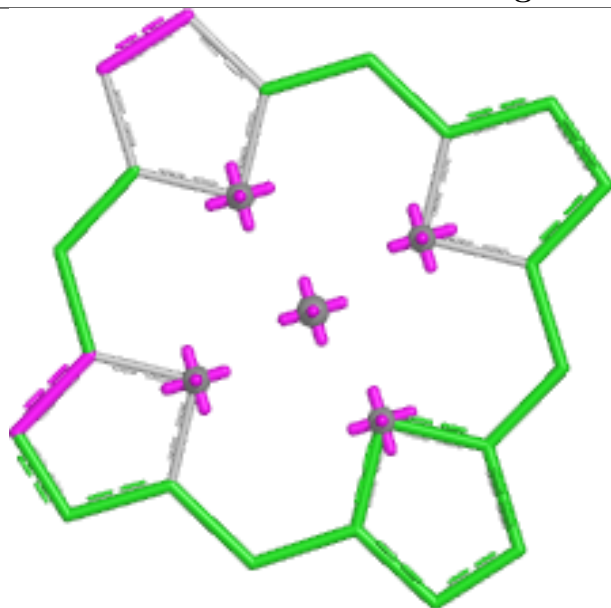


Torsions

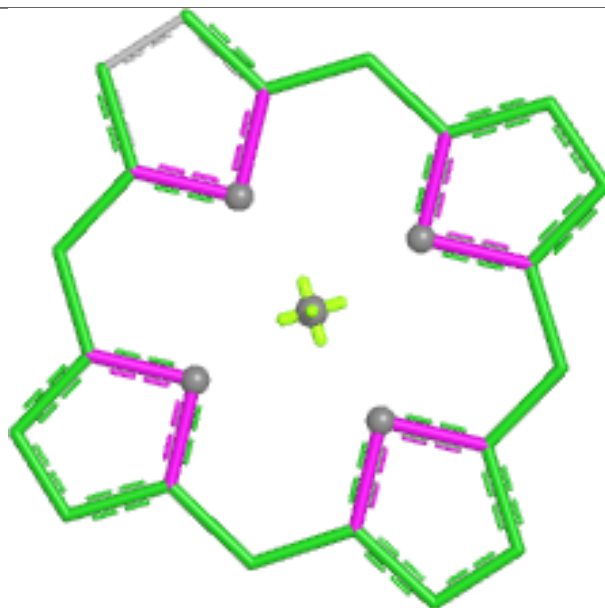


Rings

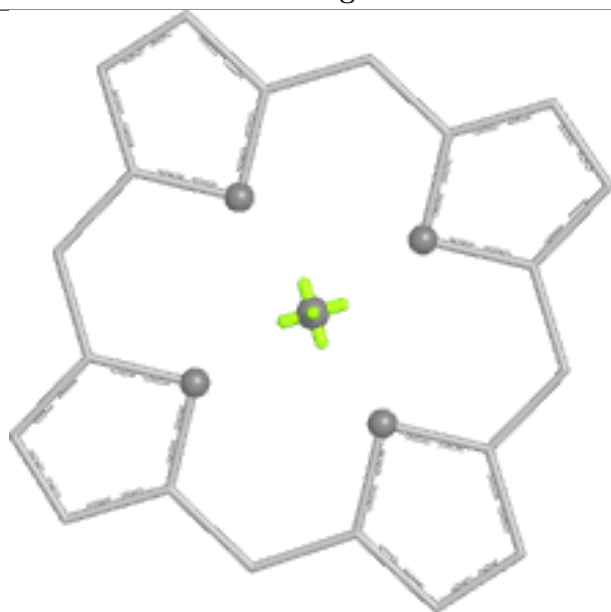
Ligand CLA B 646



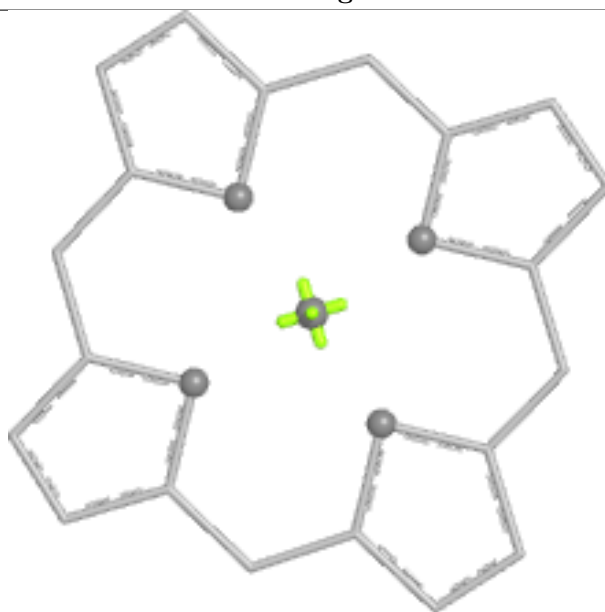
Bond lengths



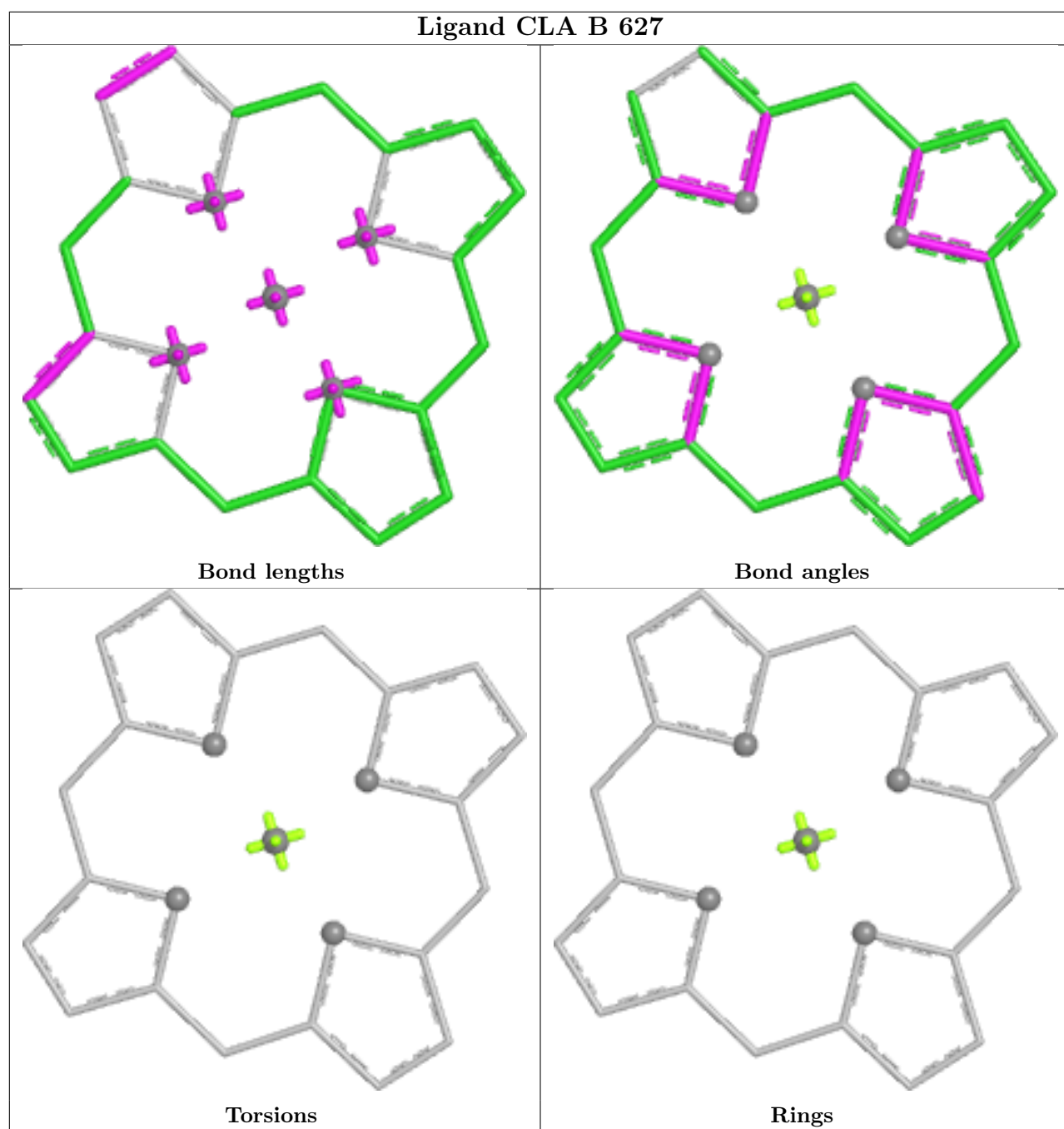
Bond angles



Torsions



Rings



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.