



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 4, 2026 – 11:08 AM EDT

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 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)	:	2.50

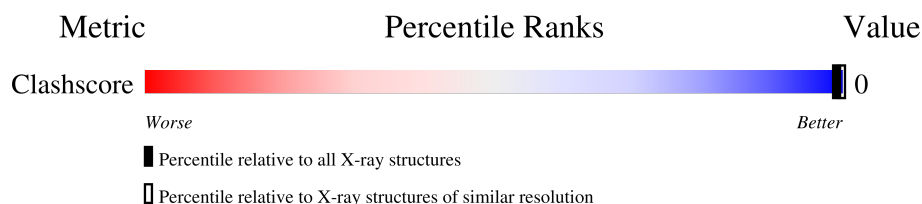
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.44 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)

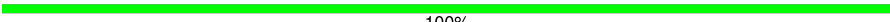
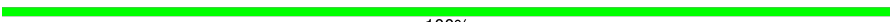
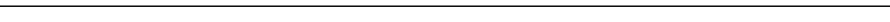
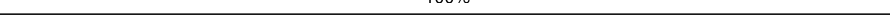
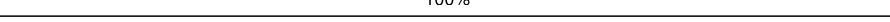
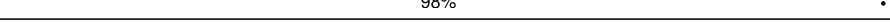
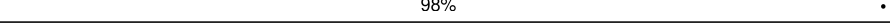
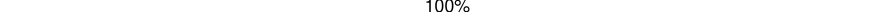
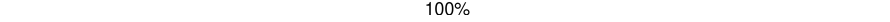
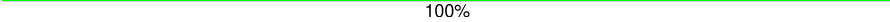
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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 $\leq 5\%$

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%

2 Entry composition

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	0	0	726
			726	726			
1	P	726	Total	C	0	0	726
			726	726			

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

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

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

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

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

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

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): SUB-UNIT 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): SUB-UNIT 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

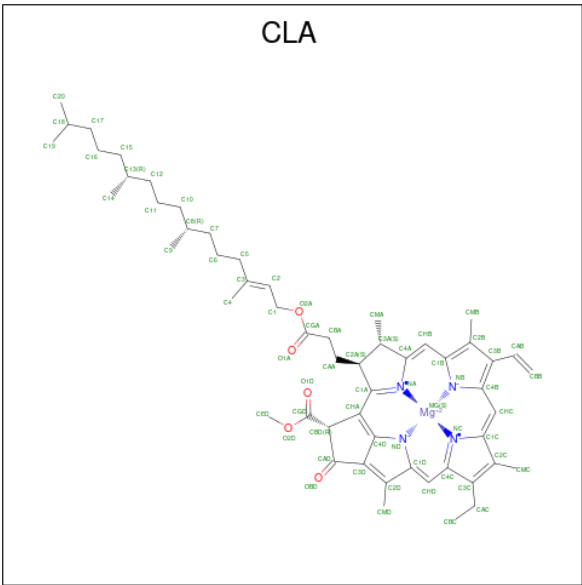
- Molecule 15 is a protein called PLANT LIGHT HARVESTING COMPLEX I(LHCI): SUB-UNIT LHCA3.

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

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

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

- Molecule 17 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅).



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		

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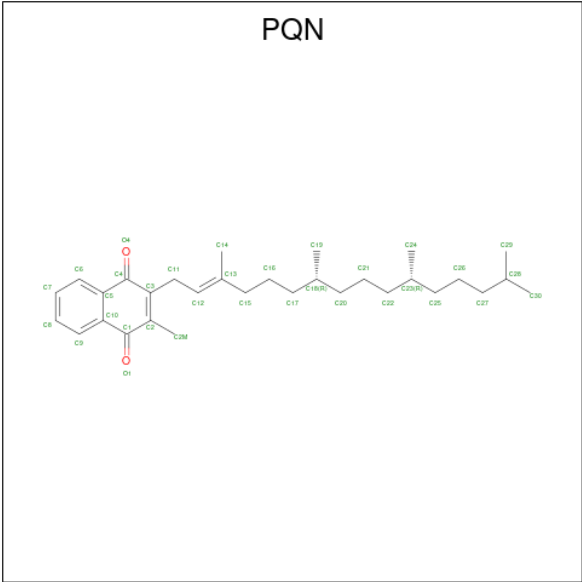
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
17	8	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	8	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	8	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	8	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	8	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	9	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	9	1	Total	C	Mg	N	0	0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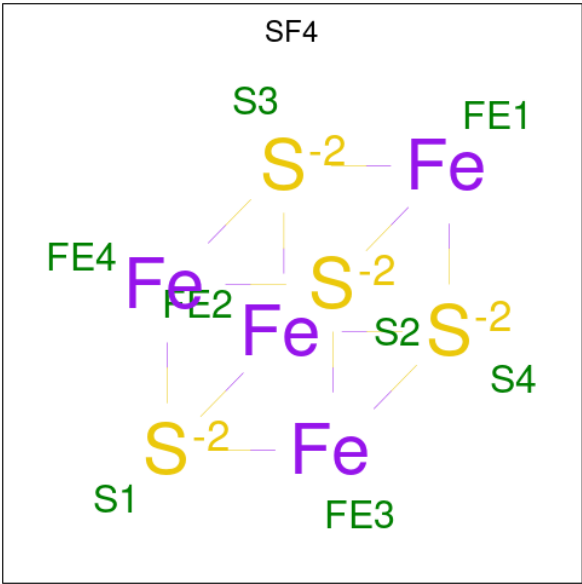
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
17	0	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	0	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	0	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	0	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	0	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	0	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	0	1	Total	C	Mg	N	0	0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

- 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	0	0
			13	11	2		
18	B	1	Total	C	O	0	0
			13	11	2		
18	P	1	Total	C	O	0	0
			13	11	2		
18	Q	1	Total	C	O	0	0
			13	11	2		

- Molecule 19 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



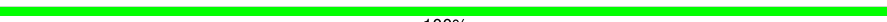
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
19	A	1	Total 8	Fe 4	S 4	0	0
19	C	1	Total 8	Fe 4	S 4	0	0
19	C	1	Total 8	Fe 4	S 4	0	0
19	P	1	Total 8	Fe 4	S 4	0	0
19	R	1	Total 8	Fe 4	S 4	0	0
19	R	1	Total 8	Fe 4	S 4	0	0

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.

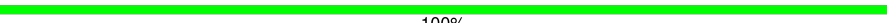
Note EDS was not executed.

- Molecule 1: PLANT PHOTOSYSTEM I: SUBUNIT PSAA

Chain A:  100%

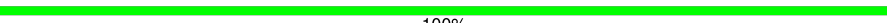
There are no outlier residues recorded for this chain.

- Molecule 1: PLANT PHOTOSYSTEM I: SUBUNIT PSAA

Chain P:  100%

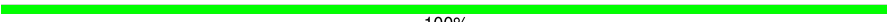
There are no outlier residues recorded for this chain.

- Molecule 2: PLANT PHOTOSYSTEM I: SUBUNIT PSAB

Chain B:  100%



- Molecule 2: PLANT PHOTOSYSTEM I: SUBUNIT PSAB

Chain Q:  100%

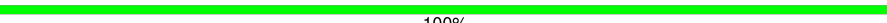


- Molecule 3: PLANT PHOTOSYSTEM I: SUBUNIT PSAC

Chain C:  100%

There are no outlier residues recorded for this chain.

- Molecule 3: PLANT PHOTOSYSTEM I: SUBUNIT PSAC

Chain R:  100%

There are no outlier residues recorded for this chain.

- Molecule 4: PLANT PHOTOSYSTEM I: SUBUNIT PSAD

Chain D:  100%

There are no outlier residues recorded for this chain.

- Molecule 4: PLANT PHOTOSYSTEM I: SUBUNIT PSAD

Chain S:  100%

There are no outlier residues recorded for this chain.

- Molecule 5: PLANT PHOTOSYSTEM I: SUBUNIT PSAE

Chain E:  100%

There are no outlier residues recorded for this chain.

- Molecule 5: PLANT PHOTOSYSTEM I: SUBUNIT PSAE

Chain T:  100%

There are no outlier residues recorded for this chain.

- Molecule 6: PLANT PHOTOSYSTEM I: SUBUNIT PSAF

Chain F:  100%

There are no outlier residues recorded for this chain.

- Molecule 6: PLANT PHOTOSYSTEM I: SUBUNIT PSAF

Chain U:  100%

There are no outlier residues recorded for this chain.

- Molecule 7: PLANT PHOTOSYSTEM I: SUBUNIT PSAG

Chain G:  100%

There are no outlier residues recorded for this chain.

- Molecule 7: PLANT PHOTOSYSTEM I: SUBUNIT PSAG

Chain V:  100%

There are no outlier residues recorded for this chain.

- Molecule 8: PLANT PHOTOSYSTEM I: SUBUNIT PSAH

Chain H:  100%

There are no outlier residues recorded for this chain.

- Molecule 8: PLANT PHOTOSYSTEM I: SUBUNIT PSAH

Chain W:  100%

There are no outlier residues recorded for this chain.

- Molecule 9: PLANT PHOTOSYSTEM I: SUBUNIT PSAI

Chain I:  100%

There are no outlier residues recorded for this chain.

- Molecule 9: PLANT PHOTOSYSTEM I: SUBUNIT PSAI

Chain Y:  100%

There are no outlier residues recorded for this chain.

- Molecule 10: PLANT PHOTOSYSTEM I: SUBUNIT PSAJ

Chain J:  100%

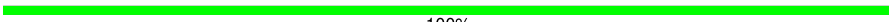
There are no outlier residues recorded for this chain.

- Molecule 10: PLANT PHOTOSYSTEM I: SUBUNIT PSAJ

Chain Z:  100%

There are no outlier residues recorded for this chain.

- Molecule 11: PLANT PHOTOSYSTEM I: SUBUNIT PSAK

Chain K:  100%

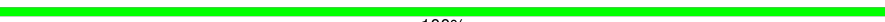
There are no outlier residues recorded for this chain.

- Molecule 11: PLANT PHOTOSYSTEM I: SUBUNIT PSAK

Chain 5:  100%

There are no outlier residues recorded for this chain.

- Molecule 12: PLANT PHOTOSYSTEM I: SUBUNIT PSAL

Chain L:  100%

There are no outlier residues recorded for this chain.

- Molecule 12: PLANT PHOTOSYSTEM I: SUBUNIT PSAL

Chain 6:  100%

There are no outlier residues recorded for this chain.

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

Chain 1:  100%

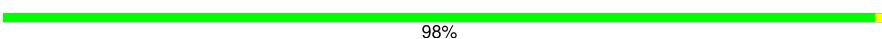
There are no outlier residues recorded for this chain.

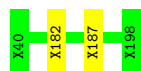
- Molecule 13: PLANT LIGHT HARVESTING COMPLEX I(LHCI): SUBUNIT LHCA1

Chain 7:  100%

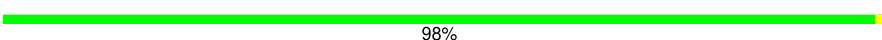
There are no outlier residues recorded for this chain.

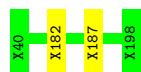
- Molecule 14: PLANT LIGHT HARVESTING COMPLEX I(LHCI): SUBUNIT LHCA2

Chain 2:  98%



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

Chain 8:  98%

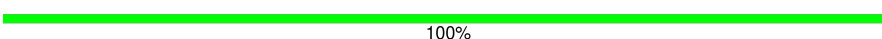


- Molecule 15: PLANT LIGHT HARVESTING COMPLEX I(LHCI): SUBUNIT LHCA3

Chain 3:  100%

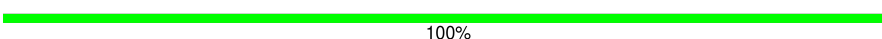
There are no outlier residues recorded for this chain.

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

Chain 9:  100%

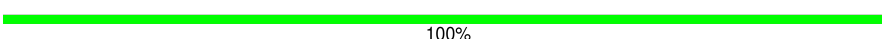
There are no outlier residues recorded for this chain.

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

Chain 4:  100%

There are no outlier residues recorded for this chain.

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

Chain 0:  100%

There are no outlier residues recorded for this chain.

4 Data and refinement statistics

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 [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	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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	P	5102	-	24,32,73	2.02	7 (29%)	31,54,113	2.94	7 (22%)
17	CLA	P	5131	-	24,32,73	1.97	5 (20%)	31,54,113	2.92	8 (25%)
18	PQN	Q	6002	-	14,14,34	4.40	13 (92%)	20,20,45	1.04	2 (10%)
17	CLA	P	5105	-	24,32,73	2.17	7 (29%)	31,54,113	2.74	7 (22%)
17	CLA	K	1403	-	24,32,73	2.08	6 (25%)	31,54,113	3.03	7 (22%)
17	CLA	B	1208	-	24,32,73	2.04	8 (33%)	31,54,113	2.80	7 (22%)
17	CLA	Q	5022	-	24,32,73	2.38	9 (37%)	31,54,113	3.04	8 (25%)
17	CLA	B	1215	-	24,32,73	1.91	6 (25%)	31,54,113	2.97	7 (22%)
17	CLA	B	1217	-	24,32,73	2.09	8 (33%)	31,54,113	3.05	7 (22%)
17	CLA	7	1021	-	24,32,73	2.86	7 (29%)	31,54,113	3.02	7 (22%)
17	CLA	Q	5214	-	24,32,73	2.06	8 (33%)	31,54,113	2.92	7 (22%)
17	CLA	P	5402	-	24,32,73	2.28	7 (29%)	31,54,113	3.06	6 (19%)
17	CLA	Q	5215	-	24,32,73	1.92	6 (25%)	31,54,113	2.98	7 (22%)
17	CLA	8	1033	-	24,32,73	2.09	6 (25%)	31,54,113	3.02	7 (22%)
17	CLA	Q	5206	-	24,32,73	1.97	4 (16%)	31,54,113	2.98	7 (22%)
17	CLA	9	1014	-	24,32,73	2.08	6 (25%)	31,54,113	3.05	7 (22%)
17	CLA	B	1230	-	24,32,73	1.97	8 (33%)	31,54,113	2.87	7 (22%)
17	CLA	A	1105	-	24,32,73	2.17	7 (29%)	31,54,113	2.75	7 (22%)
17	CLA	Q	5224	-	24,32,73	2.24	7 (29%)	31,54,113	2.94	8 (25%)
17	CLA	1	1026	-	24,32,73	2.08	6 (25%)	31,54,113	3.04	7 (22%)
17	CLA	4	1026	-	24,32,73	2.08	6 (25%)	31,54,113	3.04	7 (22%)
17	CLA	A	1107	-	24,32,73	1.94	7 (29%)	31,54,113	2.96	8 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	CLA	0	1022	-	24,32,73	2.09	6 (25%)	31,54,113	3.06	7 (22%)
17	CLA	Q	5237	-	24,32,73	1.85	8 (33%)	31,54,113	2.91	7 (22%)
17	CLA	B	1218	-	24,32,73	2.16	7 (29%)	31,54,113	3.04	9 (29%)
17	CLA	Q	5242	-	24,32,73	2.08	6 (25%)	31,54,113	3.01	7 (22%)
17	CLA	Q	5240	-	24,32,73	2.08	6 (25%)	31,54,113	3.02	7 (22%)
17	CLA	P	5119	-	24,32,73	2.00	7 (29%)	31,54,113	2.91	8 (25%)
17	CLA	W	5801	-	24,32,73	2.08	6 (25%)	31,54,113	3.03	7 (22%)
17	CLA	8	1022	-	24,32,73	2.08	6 (25%)	31,54,113	3.02	7 (22%)
17	CLA	4	1011	-	24,32,73	2.09	6 (25%)	31,54,113	3.05	7 (22%)
17	CLA	1	1025	-	24,32,73	2.08	6 (25%)	31,54,113	3.04	7 (22%)
17	CLA	B	1232	-	24,32,73	2.22	8 (33%)	31,54,113	2.90	7 (22%)
17	CLA	A	1116	-	24,32,73	2.16	7 (29%)	31,54,113	2.98	7 (22%)
17	CLA	4	1025	-	24,32,73	2.08	6 (25%)	31,54,113	3.02	7 (22%)
17	CLA	Q	5219	-	24,32,73	2.39	8 (33%)	31,54,113	3.98	9 (29%)
17	CLA	A	1111	-	24,32,73	2.06	8 (33%)	31,54,113	3.18	8 (25%)
17	CLA	6	5501	-	24,32,73	2.31	8 (33%)	31,54,113	2.72	8 (25%)
17	CLA	A	4010	-	24,32,73	2.08	6 (25%)	31,54,113	3.04	7 (22%)
17	CLA	1	1023	-	24,32,73	2.09	6 (25%)	31,54,113	3.03	7 (22%)
17	CLA	4	1023	-	24,32,73	2.07	6 (25%)	31,54,113	3.01	7 (22%)
17	CLA	7	1026	-	24,32,73	2.08	6 (25%)	31,54,113	3.05	7 (22%)
17	CLA	B	1225	-	24,32,73	2.13	7 (29%)	31,54,113	2.52	8 (25%)
17	CLA	A	1139	-	24,32,73	2.04	7 (29%)	31,54,113	2.79	6 (19%)
17	CLA	Q	5236	-	24,32,73	2.12	7 (29%)	31,54,113	2.80	7 (22%)
17	CLA	1	1014	-	24,32,73	2.08	6 (25%)	31,54,113	3.03	7 (22%)
17	CLA	4	1012	-	24,32,73	2.10	6 (25%)	31,54,113	3.05	7 (22%)
17	CLA	0	1016	-	24,32,73	2.08	6 (25%)	31,54,113	3.03	8 (25%)
17	CLA	B	4001	-	24,32,73	2.08	6 (25%)	31,54,113	3.04	7 (22%)
17	CLA	B	1234	-	24,32,73	2.25	8 (33%)	31,54,113	2.94	6 (19%)
17	CLA	6	5504	-	24,32,73	2.08	6 (25%)	31,54,113	3.03	7 (22%)
17	CLA	Q	5227	-	24,32,73	1.96	7 (29%)	31,54,113	3.00	9 (29%)
17	CLA	B	1209	-	24,32,73	2.10	8 (33%)	31,54,113	2.98	7 (22%)
17	CLA	H	1801	-	24,32,73	2.08	6 (25%)	31,54,113	3.03	7 (22%)
17	CLA	B	1221	-	24,32,73	2.43	9 (37%)	31,54,113	3.15	7 (22%)
17	CLA	A	1124	-	24,32,73	1.82	6 (25%)	31,54,113	2.81	7 (22%)
17	CLA	7	1012	-	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	0	1023	-	24,32,73	2.07	6 (25%)	31,54,113	3.01	8 (25%)
17	CLA	7	1025	-	24,32,73	2.07	6 (25%)	31,54,113	3.04	7 (22%)
17	CLA	8	1031	-	24,32,73	2.08	6 (25%)	31,54,113	3.02	7 (22%)
17	CLA	P	5108	-	24,32,73	2.45	5 (20%)	31,54,113	3.77	10 (32%)
17	CLA	F	4005	-	24,32,73	2.08	6 (25%)	31,54,113	3.04	7 (22%)
17	CLA	Q	5235	-	24,32,73	2.11	8 (33%)	31,54,113	2.90	7 (22%)
17	CLA	B	1212	-	24,32,73	2.13	7 (29%)	31,54,113	2.82	7 (22%)
17	CLA	2	1013	-	24,32,73	2.08	6 (25%)	31,54,113	3.03	7 (22%)
17	CLA	0	1017	-	24,32,73	2.07	6 (25%)	31,54,113	3.02	7 (22%)
17	CLA	3	1016	-	24,32,73	2.07	6 (25%)	31,54,113	3.01	7 (22%)
19	SF4	A	3001	-	0,12,12	-	-	-	-	-
17	CLA	Q	5211	-	24,32,73	1.97	7 (29%)	31,54,113	2.89	6 (19%)
17	CLA	B	1226	-	24,32,73	2.12	7 (29%)	31,54,113	2.77	8 (25%)
17	CLA	4	1021	-	24,32,73	2.07	6 (25%)	31,54,113	3.01	7 (22%)
17	CLA	8	1013	-	24,32,73	2.08	6 (25%)	31,54,113	3.04	7 (22%)
17	CLA	2	1025	-	24,32,73	2.09	6 (25%)	31,54,113	3.01	7 (22%)
17	CLA	L	1504	-	24,32,73	2.08	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	9	1022	-	24,32,73	2.09	6 (25%)	31,54,113	3.05	7 (22%)
17	CLA	0	1013	-	24,32,73	2.07	6 (25%)	31,54,113	3.01	7 (22%)
17	CLA	7	1023	-	24,32,73	2.08	6 (25%)	31,54,113	3.02	7 (22%)
17	CLA	B	1211	-	24,32,73	1.98	7 (29%)	31,54,113	2.88	6 (19%)
17	CLA	P	5114	-	24,32,73	2.02	8 (33%)	31,54,113	2.94	7 (22%)
17	CLA	U	8004	-	24,32,73	2.08	6 (25%)	31,54,113	3.03	7 (22%)
17	CLA	A	1901	-	24,32,73	2.41	8 (33%)	31,54,113	4.26	11 (35%)
17	CLA	L	1503	-	24,32,73	2.12	7 (29%)	31,54,113	2.78	6 (19%)
18	PQN	P	6001	-	14,14,34	4.54	13 (92%)	20,20,45	0.99	1 (5%)
17	CLA	1	1021	-	24,32,73	2.86	7 (29%)	31,54,113	3.03	7 (22%)
17	CLA	8	1017	-	24,32,73	2.09	6 (25%)	31,54,113	3.03	7 (22%)
17	CLA	F	1229	-	24,32,73	1.97	8 (33%)	31,54,113	2.92	7 (22%)
17	CLA	L	1501	-	24,32,73	2.31	8 (33%)	31,54,113	2.71	8 (25%)
17	CLA	0	1032	-	24,32,73	2.07	6 (25%)	31,54,113	3.06	7 (22%)
17	CLA	Q	5212	-	24,32,73	2.14	8 (33%)	31,54,113	2.84	7 (22%)
17	CLA	A	1013	-	24,32,73	2.11	8 (33%)	31,54,113	2.70	9 (29%)
17	CLA	P	5128	-	24,32,73	2.35	7 (29%)	31,54,113	2.71	8 (25%)

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	Q	5202	-	24,32,73	2.11	6 (25%)	31,54,113	2.98	6 (19%)
17	CLA	4	4002	-	24,32,73	2.08	6 (25%)	31,54,113	3.06	7 (22%)
17	CLA	P	5107	-	24,32,73	1.94	7 (29%)	31,54,113	2.95	8 (25%)
17	CLA	P	5136	-	24,32,73	2.20	8 (33%)	31,54,113	2.70	8 (25%)
17	CLA	Q	5021	-	24,32,73	2.15	8 (33%)	31,54,113	2.93	6 (19%)
17	CLA	P	5125	-	24,32,73	2.21	8 (33%)	31,54,113	3.14	8 (25%)
17	CLA	B	1235	-	24,32,73	2.12	8 (33%)	31,54,113	2.90	7 (22%)
17	CLA	3	1011	-	24,32,73	2.09	6 (25%)	31,54,113	3.04	7 (22%)
17	CLA	2	1017	-	24,32,73	2.09	6 (25%)	31,54,113	3.03	7 (22%)
17	CLA	Q	5213	-	24,32,73	2.12	7 (29%)	31,54,113	2.76	8 (25%)
17	CLA	0	8002	-	24,32,73	2.09	6 (25%)	31,54,113	3.08	8 (25%)
17	CLA	P	5138	-	24,32,73	2.01	7 (29%)	31,54,113	2.91	8 (25%)
17	CLA	Z	5101	-	24,32,73	2.08	6 (25%)	31,54,113	3.04	7 (22%)
17	CLA	7	1031	-	24,32,73	2.07	6 (25%)	31,54,113	3.02	7 (22%)
17	CLA	9	1021	-	24,32,73	2.08	6 (25%)	31,54,113	3.03	8 (25%)
17	CLA	A	1126	-	24,32,73	2.15	6 (25%)	31,54,113	2.91	7 (22%)
19	SF4	R	7003	-	0,12,12	-	-	-	-	-
17	CLA	P	5011	-	24,32,73	2.16	9 (37%)	31,54,113	2.96	5 (16%)
17	CLA	U	8006	-	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	5139	-	24,32,73	2.04	7 (29%)	31,54,113	2.79	6 (19%)
17	CLA	7	1017	-	24,32,73	2.09	6 (25%)	31,54,113	3.05	7 (22%)
17	CLA	A	1131	-	24,32,73	1.97	5 (20%)	31,54,113	2.92	8 (25%)
17	CLA	Q	5225	-	24,32,73	2.13	7 (29%)	31,54,113	2.53	8 (25%)
17	CLA	9	1017	-	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	0	1021	-	24,32,73	2.07	6 (25%)	31,54,113	3.00	7 (22%)
17	CLA	A	1122	-	24,32,73	1.93	8 (33%)	31,54,113	2.94	7 (22%)
17	CLA	Q	5220	-	24,32,73	2.19	7 (29%)	31,54,113	2.88	7 (22%)
17	CLA	2	1026	-	24,32,73	2.08	6 (25%)	31,54,113	3.05	7 (22%)
17	CLA	A	1125	-	24,32,73	2.20	8 (33%)	31,54,113	3.15	8 (25%)
17	CLA	1	1011	-	24,32,73	2.09	6 (25%)	31,54,113	3.05	7 (22%)
17	CLA	9	1016	-	24,32,73	2.08	6 (25%)	31,54,113	3.01	8 (25%)
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	Q	5226	-	24,32,73	2.13	7 (29%)	31,54,113	2.76	8 (25%)
17	CLA	P	5110	-	24,32,73	1.99	5 (20%)	31,54,113	3.11	8 (25%)
17	CLA	A	1114	-	24,32,73	2.01	8 (33%)	31,54,113	2.94	7 (22%)
18	PQN	B	2002	-	14,14,34	4.40	13 (92%)	20,20,45	1.04	2 (10%)
17	CLA	Q	5217	-	24,32,73	2.09	8 (33%)	31,54,113	3.05	7 (22%)
17	CLA	A	1109	-	24,32,73	2.00	8 (33%)	31,54,113	2.80	7 (22%)
17	CLA	Q	5221	-	24,32,73	2.42	9 (37%)	31,54,113	3.15	7 (22%)
17	CLA	B	1241	-	24,32,73	2.09	6 (25%)	31,54,113	3.03	7 (22%)
17	CLA	A	1011	-	24,32,73	2.15	9 (37%)	31,54,113	2.96	5 (16%)
17	CLA	J	1302	-	24,32,73	2.57	8 (33%)	31,54,113	4.24	9 (29%)
17	CLA	8	1014	-	24,32,73	2.08	6 (25%)	31,54,113	3.04	7 (22%)
19	SF4	R	7002	-	0,12,12	-	-	-	-	-
17	CLA	Q	5222	-	24,32,73	1.95	7 (29%)	31,54,113	2.93	6 (19%)
17	CLA	A	1134	-	24,32,73	2.04	8 (33%)	31,54,113	3.01	8 (25%)
17	CLA	2	1015	-	24,32,73	2.08	6 (25%)	31,54,113	3.03	7 (22%)
17	CLA	1	1012	-	24,32,73	2.08	6 (25%)	31,54,113	3.03	7 (22%)
17	CLA	9	1033	-	24,32,73	2.08	6 (25%)	31,54,113	3.05	7 (22%)
17	CLA	Q	5208	-	24,32,73	2.04	8 (33%)	31,54,113	2.80	7 (22%)
17	CLA	2	1023	-	24,32,73	2.08	6 (25%)	31,54,113	3.02	7 (22%)
19	SF4	P	7001	-	0,12,12	-	-	-	-	-
17	CLA	P	5104	-	24,32,73	2.24	9 (37%)	31,54,113	2.99	7 (22%)
17	CLA	1	1015	-	24,32,73	2.08	6 (25%)	31,54,113	3.04	7 (22%)
17	CLA	2	1012	-	24,32,73	2.08	6 (25%)	31,54,113	3.04	7 (22%)
17	CLA	P	5135	-	24,32,73	2.20	7 (29%)	31,54,113	3.05	7 (22%)
17	CLA	Q	5230	-	24,32,73	1.97	8 (33%)	31,54,113	2.87	7 (22%)
17	CLA	P	5140	-	24,32,73	1.90	6 (25%)	31,54,113	2.97	7 (22%)
17	CLA	P	5126	-	24,32,73	2.15	6 (25%)	31,54,113	2.91	7 (22%)
17	CLA	8	1026	-	24,32,73	2.08	6 (25%)	31,54,113	3.04	7 (22%)
17	CLA	K	1401	-	24,32,73	2.16	8 (33%)	31,54,113	2.84	8 (25%)
17	CLA	B	1220	-	24,32,73	2.19	7 (29%)	31,54,113	2.87	7 (22%)
17	CLA	A	1106	-	24,32,73	1.96	6 (25%)	31,54,113	2.90	7 (22%)
17	CLA	5	5404	-	24,32,73	2.09	6 (25%)	31,54,113	3.06	7 (22%)
17	CLA	P	5901	-	24,32,73	2.41	8 (33%)	31,54,113	4.25	11 (35%)
17	CLA	4	1017	-	24,32,73	2.08	6 (25%)	31,54,113	3.03	7 (22%)
17	CLA	A	1118	-	24,32,73	2.10	8 (33%)	31,54,113	3.18	8 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	CLA	5	5401	-	24,32,73	2.15	8 (33%)	31,54,113	2.84	8 (25%)
17	CLA	P	5116	-	24,32,73	2.16	7 (29%)	31,54,113	2.97	7 (22%)
17	CLA	A	1135	-	24,32,73	2.20	7 (29%)	31,54,113	3.07	7 (22%)
17	CLA	2	1033	-	24,32,73	2.09	6 (25%)	31,54,113	3.01	7 (22%)
17	CLA	4	1015	-	24,32,73	2.09	6 (25%)	31,54,113	3.04	7 (22%)
17	CLA	Q	5203	-	24,32,73	2.20	7 (29%)	31,54,113	2.94	7 (22%)
17	CLA	Q	5238	-	24,32,73	1.96	7 (29%)	31,54,113	2.80	8 (25%)
17	CLA	G	1701	-	24,32,73	2.08	6 (25%)	31,54,113	3.04	7 (22%)
17	CLA	P	5124	-	24,32,73	1.82	6 (25%)	31,54,113	2.82	7 (22%)
17	CLA	P	5115	-	24,32,73	2.17	8 (33%)	31,54,113	2.62	8 (25%)
17	CLA	3	1015	-	24,32,73	2.08	6 (25%)	31,54,113	3.04	7 (22%)
17	CLA	3	1021	-	24,32,73	2.09	6 (25%)	31,54,113	3.02	7 (22%)
17	CLA	B	1023	-	24,32,73	2.30	11 (45%)	31,54,113	2.99	9 (29%)
17	CLA	P	5122	-	24,32,73	1.93	8 (33%)	31,54,113	2.95	7 (22%)
17	CLA	0	1015	-	24,32,73	2.10	6 (25%)	31,54,113	3.04	7 (22%)
17	CLA	P	5113	-	24,32,73	2.39	8 (33%)	31,54,113	4.10	11 (35%)
17	CLA	B	1239	-	24,32,73	1.77	6 (25%)	31,54,113	2.93	6 (19%)
17	CLA	4	1016	-	24,32,73	2.07	6 (25%)	31,54,113	3.04	7 (22%)
17	CLA	A	1108	-	24,32,73	2.45	5 (20%)	31,54,113	3.78	10 (32%)
17	CLA	A	1103	-	24,32,73	1.99	7 (29%)	31,54,113	3.21	8 (25%)
17	CLA	B	1204	-	24,32,73	2.00	8 (33%)	31,54,113	3.21	8 (25%)
17	CLA	B	1021	-	24,32,73	2.16	8 (33%)	31,54,113	2.94	6 (19%)
17	CLA	J	4008	-	24,32,73	2.08	6 (25%)	31,54,113	3.04	7 (22%)
17	CLA	A	1133	-	24,32,73	1.87	8 (33%)	31,54,113	2.94	8 (25%)
17	CLA	4	1032	-	24,32,73	2.08	6 (25%)	31,54,113	3.04	7 (22%)
17	CLA	6	5502	-	24,32,73	2.12	7 (29%)	31,54,113	2.90	8 (25%)
17	CLA	6	5503	-	24,32,73	2.13	7 (29%)	31,54,113	2.78	6 (19%)
17	CLA	9	1041	-	24,32,73	2.09	6 (25%)	31,54,113	3.02	7 (22%)
17	CLA	U	8005	-	24,32,73	2.09	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	B	1206	-	24,32,73	1.97	4 (16%)	31,54,113	2.98	7 (22%)
17	CLA	2	1014	-	24,32,73	2.07	6 (25%)	31,54,113	3.03	8 (25%)
17	CLA	B	1231	-	24,32,73	2.12	9 (37%)	31,54,113	3.06	7 (22%)
17	CLA	8	1011	-	24,32,73	2.08	6 (25%)	31,54,113	3.03	7 (22%)
17	CLA	F	4004	-	24,32,73	2.08	6 (25%)	31,54,113	3.04	7 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	CLA	P	8010	-	24,32,73	2.09	6 (25%)	31,54,113	3.05	7 (22%)
17	CLA	0	1033	-	24,32,73	2.08	6 (25%)	31,54,113	3.04	7 (22%)
17	CLA	8	1023	-	24,32,73	2.08	6 (25%)	31,54,113	3.02	7 (22%)
17	CLA	Q	5232	-	24,32,73	2.21	8 (33%)	31,54,113	2.89	7 (22%)
17	CLA	9	1032	-	24,32,73	2.09	6 (25%)	31,54,113	3.06	7 (22%)
17	CLA	P	5123	-	24,32,73	2.34	7 (29%)	31,54,113	3.09	8 (25%)
17	CLA	P	5117	-	24,32,73	1.92	6 (25%)	31,54,113	2.82	9 (29%)
17	CLA	V	5233	-	24,32,73	2.08	8 (33%)	31,54,113	2.98	6 (19%)
17	CLA	9	1015	-	24,32,73	2.08	6 (25%)	31,54,113	3.03	7 (22%)
17	CLA	3	1031	-	24,32,73	2.08	6 (25%)	31,54,113	3.03	7 (22%)
17	CLA	A	1110	-	24,32,73	1.99	5 (20%)	31,54,113	3.09	8 (25%)
17	CLA	A	1128	-	24,32,73	2.34	7 (29%)	31,54,113	2.69	8 (25%)
17	CLA	B	1242	-	24,32,73	2.09	6 (25%)	31,54,113	3.02	7 (22%)
17	CLA	P	5013	-	24,32,73	2.11	8 (33%)	31,54,113	2.69	8 (25%)
17	CLA	B	1210	-	24,32,73	2.39	8 (33%)	31,54,113	3.03	8 (25%)
17	CLA	B	1203	-	24,32,73	2.19	7 (29%)	31,54,113	2.92	7 (22%)
17	CLA	A	1121	-	24,32,73	2.16	8 (33%)	31,54,113	2.72	6 (19%)
17	CLA	B	1202	-	24,32,73	2.11	6 (25%)	31,54,113	2.98	6 (19%)
17	CLA	A	1138	-	24,32,73	2.01	7 (29%)	31,54,113	2.91	8 (25%)
18	PQN	A	2001	-	14,14,34	4.55	13 (92%)	20,20,45	0.99	1 (5%)
17	CLA	Q	5201	-	24,32,73	1.96	7 (29%)	31,54,113	2.95	8 (25%)
17	CLA	4	1033	-	24,32,73	2.08	6 (25%)	31,54,113	3.04	7 (22%)
17	CLA	U	8003	-	24,32,73	2.07	6 (25%)	31,54,113	3.03	7 (22%)
17	CLA	3	1022	-	24,32,73	2.09	6 (25%)	31,54,113	3.06	7 (22%)
17	CLA	Q	5223	-	24,32,73	2.31	8 (33%)	31,54,113	3.13	8 (25%)
17	CLA	Q	5210	-	24,32,73	2.39	8 (33%)	31,54,113	3.03	8 (25%)
17	CLA	8	8007	-	24,32,73	2.09	6 (25%)	31,54,113	3.04	7 (22%)
17	CLA	7	1016	-	24,32,73	2.08	6 (25%)	31,54,113	3.02	7 (22%)
17	CLA	P	5012	-	24,32,73	2.33	7 (29%)	31,54,113	3.09	8 (25%)
17	CLA	8	1021	-	24,32,73	2.08	6 (25%)	31,54,113	3.01	7 (22%)
17	CLA	Q	5231	-	24,32,73	2.11	9 (37%)	31,54,113	3.03	7 (22%)
17	CLA	B	1201	-	24,32,73	1.97	7 (29%)	31,54,113	2.94	8 (25%)
17	CLA	7	1015	-	24,32,73	2.09	7 (29%)	31,54,113	3.05	7 (22%)
17	CLA	B	1224	-	24,32,73	2.24	8 (33%)	31,54,113	2.95	8 (25%)
17	CLA	0	1031	-	24,32,73	2.09	7 (29%)	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	A	1132	-	24,32,73	1.82	7 (29%)	31,54,113	2.83	7 (22%)
17	CLA	B	1236	-	24,32,73	2.12	7 (29%)	31,54,113	2.79	7 (22%)
17	CLA	2	1031	-	24,32,73	2.08	6 (25%)	31,54,113	3.02	7 (22%)
17	CLA	2	1021	-	24,32,73	2.07	6 (25%)	31,54,113	3.00	7 (22%)
17	CLA	B	1237	-	24,32,73	1.85	8 (33%)	31,54,113	2.90	7 (22%)
17	CLA	3	1025	-	24,32,73	2.08	6 (25%)	31,54,113	3.04	7 (22%)
17	CLA	P	5133	-	24,32,73	1.87	8 (33%)	31,54,113	2.94	8 (25%)
17	CLA	0	1011	-	24,32,73	2.09	6 (25%)	31,54,113	3.04	7 (22%)
17	CLA	B	1240	-	24,32,73	2.08	6 (25%)	31,54,113	3.03	7 (22%)
17	CLA	B	1223	-	24,32,73	2.31	8 (33%)	31,54,113	3.13	8 (25%)
17	CLA	4	1031	-	24,32,73	2.08	7 (29%)	31,54,113	3.06	7 (22%)
17	CLA	Q	5228	-	24,32,73	2.05	8 (33%)	31,54,113	3.04	9 (29%)
17	CLA	P	5111	-	24,32,73	2.07	8 (33%)	31,54,113	3.19	8 (25%)
17	CLA	P	5127	-	24,32,73	2.10	7 (29%)	31,54,113	2.86	6 (19%)
17	CLA	F	4003	-	24,32,73	2.08	6 (25%)	31,54,113	3.04	7 (22%)
17	CLA	A	1112	-	24,32,73	2.24	8 (33%)	31,54,113	2.85	8 (25%)
17	CLA	B	1216	-	24,32,73	2.03	8 (33%)	31,54,113	2.76	7 (22%)
17	CLA	P	8009	-	24,32,73	2.09	6 (25%)	31,54,113	3.03	7 (22%)
17	CLA	V	5701	-	24,32,73	2.08	6 (25%)	31,54,113	3.04	7 (22%)
17	CLA	A	1127	-	24,32,73	2.11	7 (29%)	31,54,113	2.84	6 (19%)
17	CLA	B	1214	-	24,32,73	2.05	8 (33%)	31,54,113	2.91	7 (22%)
17	CLA	3	1017	-	24,32,73	2.08	6 (25%)	31,54,113	3.03	7 (22%)
17	CLA	7	1011	-	24,32,73	2.09	6 (25%)	31,54,113	3.05	7 (22%)
17	CLA	B	1205	-	24,32,73	2.09	7 (29%)	31,54,113	2.64	6 (19%)
17	CLA	2	4007	-	24,32,73	2.09	6 (25%)	31,54,113	3.03	7 (22%)
17	CLA	P	5121	-	24,32,73	2.15	8 (33%)	31,54,113	2.73	6 (19%)
17	CLA	9	1031	-	24,32,73	2.08	6 (25%)	31,54,113	3.03	7 (22%)
17	CLA	Q	5239	-	24,32,73	1.77	6 (25%)	31,54,113	2.93	6 (19%)
17	CLA	7	1022	-	24,32,73	2.08	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	B	1022	-	24,32,73	2.38	9 (37%)	31,54,113	3.05	8 (25%)
17	CLA	4	1022	-	24,32,73	2.09	6 (25%)	31,54,113	3.05	7 (22%)
17	CLA	3	1032	-	24,32,73	2.09	6 (25%)	31,54,113	3.06	7 (22%)
17	CLA	3	1012	-	24,32,73	2.08	6 (25%)	31,54,113	3.05	7 (22%)
17	CLA	9	1011	-	24,32,73	2.09	6 (25%)	31,54,113	3.05	7 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	CLA	A	1137	-	24,32,73	2.57	8 (33%)	31,54,113	3.85	9 (29%)
17	CLA	2	1011	-	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	P	5106	-	24,32,73	1.96	6 (25%)	31,54,113	2.91	7 (22%)
17	CLA	Q	5209	-	24,32,73	2.10	8 (33%)	31,54,113	2.97	7 (22%)
17	CLA	1	1013	-	24,32,73	2.08	6 (25%)	31,54,113	3.03	7 (22%)
17	CLA	4	1013	-	24,32,73	2.07	6 (25%)	31,54,113	3.03	7 (22%)
17	CLA	3	1014	-	24,32,73	2.09	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	Q	5207	-	24,32,73	2.35	8 (33%)	31,54,113	3.03	6 (19%)
17	CLA	A	1102	-	24,32,73	2.02	7 (29%)	31,54,113	2.95	7 (22%)
17	CLA	2	1022	-	24,32,73	2.08	6 (25%)	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	0	1025	-	24,32,73	2.07	6 (25%)	31,54,113	3.01	7 (22%)
17	CLA	B	1130	-	24,32,73	1.99	7 (29%)	31,54,113	3.09	7 (22%)
17	CLA	3	1033	-	24,32,73	2.08	6 (25%)	31,54,113	3.05	7 (22%)
17	CLA	Q	5234	-	24,32,73	2.25	8 (33%)	31,54,113	2.94	6 (19%)
17	CLA	9	1012	-	24,32,73	2.08	6 (25%)	31,54,113	3.05	7 (22%)
17	CLA	Q	5023	-	24,32,73	2.30	11 (45%)	31,54,113	3.00	9 (29%)
17	CLA	P	5129	-	24,32,73	1.91	8 (33%)	31,54,113	3.05	9 (29%)
17	CLA	Z	5302	-	24,32,73	2.57	8 (33%)	31,54,113	4.24	9 (29%)
17	CLA	A	1113	-	24,32,73	2.38	8 (33%)	31,54,113	4.10	11 (35%)
17	CLA	3	1026	-	24,32,73	2.08	6 (25%)	31,54,113	3.04	7 (22%)
17	CLA	B	1219	-	24,32,73	2.40	8 (33%)	31,54,113	3.99	9 (29%)
17	CLA	0	1012	-	24,32,73	2.10	6 (25%)	31,54,113	3.05	7 (22%)
17	CLA	P	5118	-	24,32,73	2.10	8 (33%)	31,54,113	3.18	9 (29%)
17	CLA	B	1238	-	24,32,73	1.97	7 (29%)	31,54,113	2.79	8 (25%)
17	CLA	A	1115	-	24,32,73	2.17	8 (33%)	31,54,113	2.61	8 (25%)
17	CLA	F	4006	-	24,32,73	2.08	6 (25%)	31,54,113	3.04	7 (22%)
17	CLA	Q	5241	-	24,32,73	2.09	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	B	1227	-	24,32,73	1.96	7 (29%)	31,54,113	3.00	9 (29%)
17	CLA	8	1025	-	24,32,73	2.09	6 (25%)	31,54,113	3.01	7 (22%)
17	CLA	F	1301	-	24,32,73	2.23	7 (29%)	31,54,113	2.87	6 (19%)
17	CLA	0	1014	-	24,32,73	2.07	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	A	1104	-	24,32,73	2.24	9 (37%)	31,54,113	2.99	7 (22%)
17	CLA	A	1140	-	24,32,73	1.90	6 (25%)	31,54,113	2.97	7 (22%)
17	CLA	P	5120	-	24,32,73	2.02	8 (33%)	31,54,113	2.95	7 (22%)
17	CLA	9	1026	-	24,32,73	2.08	6 (25%)	31,54,113	3.04	7 (22%)
17	CLA	7	1014	-	24,32,73	2.07	6 (25%)	31,54,113	3.01	7 (22%)
17	CLA	5	5403	-	24,32,73	2.09	6 (25%)	31,54,113	3.03	7 (22%)
19	SF4	C	3002	-	0,12,12	-	-	-	-	-
17	CLA	B	1213	-	24,32,73	2.12	7 (29%)	31,54,113	2.77	8 (25%)
17	CLA	A	1012	-	24,32,73	2.33	7 (29%)	31,54,113	3.10	8 (25%)
17	CLA	B	1222	-	24,32,73	1.94	6 (25%)	31,54,113	2.93	6 (19%)
17	CLA	1	1031	-	24,32,73	2.07	6 (25%)	31,54,113	3.03	7 (22%)
17	CLA	G	1233	-	24,32,73	2.09	8 (33%)	31,54,113	3.00	6 (19%)
17	CLA	8	1012	-	24,32,73	2.09	6 (25%)	31,54,113	3.05	7 (22%)
17	CLA	A	1117	-	24,32,73	1.92	6 (25%)	31,54,113	2.83	9 (29%)
17	CLA	P	5103	-	24,32,73	1.99	7 (29%)	31,54,113	3.22	8 (25%)
17	CLA	7	1013	-	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	B	1228	-	24,32,73	2.04	8 (33%)	31,54,113	3.03	9 (29%)
17	CLA	A	1119	-	24,32,73	1.99	7 (29%)	31,54,113	2.92	8 (25%)
17	CLA	Q	5130	-	24,32,73	2.00	7 (29%)	31,54,113	3.10	7 (22%)
17	CLA	P	5137	-	24,32,73	2.57	7 (29%)	31,54,113	3.86	9 (29%)
17	CLA	Z	8008	-	24,32,73	2.08	6 (25%)	31,54,113	3.04	7 (22%)
17	CLA	Q	5218	-	24,32,73	2.16	7 (29%)	31,54,113	3.02	9 (29%)
17	CLA	8	1015	-	24,32,73	2.08	6 (25%)	31,54,113	3.03	8 (25%)
17	CLA	P	5134	-	24,32,73	2.04	8 (33%)	31,54,113	3.00	8 (25%)
17	CLA	K	1404	-	24,32,73	2.09	6 (25%)	31,54,113	3.05	7 (22%)
17	CLA	Q	8001	-	24,32,73	2.08	6 (25%)	31,54,113	3.04	7 (22%)
17	CLA	Q	5216	-	24,32,73	2.03	8 (33%)	31,54,113	2.76	7 (22%)
19	SF4	C	3003	-	0,12,12	-	-	-	-	-
17	CLA	U	5229	-	24,32,73	1.98	8 (33%)	31,54,113	2.94	7 (22%)
17	CLA	3	1041	-	24,32,73	2.08	6 (25%)	31,54,113	3.04	7 (22%)
17	CLA	P	5112	-	24,32,73	2.24	8 (33%)	31,54,113	2.84	8 (25%)
17	CLA	Q	5205	-	24,32,73	2.09	7 (29%)	31,54,113	2.64	6 (19%)
17	CLA	A	4009	-	24,32,73	2.09	6 (25%)	31,54,113	3.04	7 (22%)
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	J	1101	-	24,32,73	2.08	6 (25%)	31,54,113	3.04	7 (22%)
17	CLA	1	1022	-	24,32,73	2.08	6 (25%)	31,54,113	3.05	7 (22%)
17	CLA	A	1402	-	24,32,73	2.28	7 (29%)	31,54,113	3.07	6 (19%)
17	CLA	8	1016	-	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	U	5301	-	24,32,73	2.23	7 (29%)	31,54,113	2.88	6 (19%)
17	CLA	4	1014	-	24,32,73	2.07	6 (25%)	31,54,113	3.03	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
19	SF4	C	3003	-	-	-	0/6/5/5
18	PQN	A	2001	-	-	-	0/2/2/2
19	SF4	R	7003	-	-	-	0/6/5/5
19	SF4	A	3001	-	-	-	0/6/5/5
19	SF4	C	3002	-	-	-	0/6/5/5
18	PQN	B	2002	-	-	-	0/2/2/2
19	SF4	P	7001	-	-	-	0/6/5/5
18	PQN	P	6001	-	-	-	0/2/2/2
18	PQN	Q	6002	-	-	-	0/2/2/2
19	SF4	R	7002	-	-	-	0/6/5/5

The worst 5 of 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

The worst 5 of 2439 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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(°)	Ideal(°)
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

There are no chirality outliers.

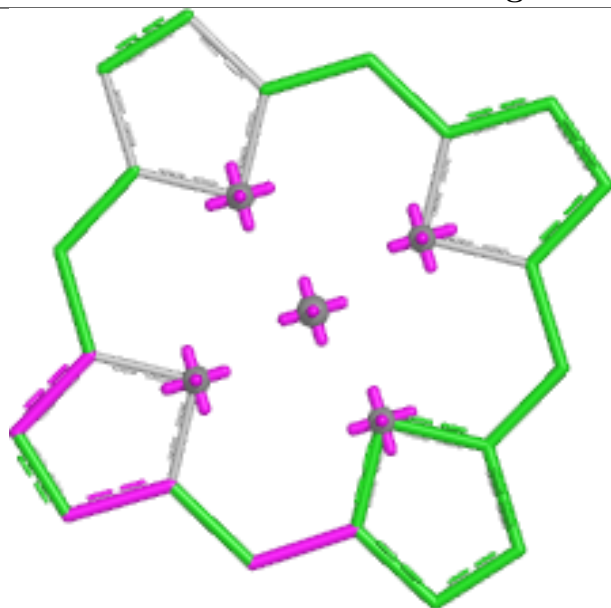
There are no torsion outliers.

There are no ring outliers.

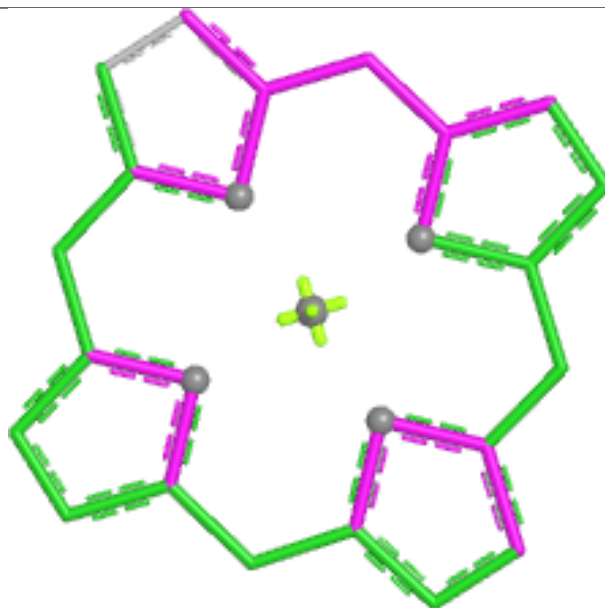
No monomer is involved in short contacts.

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 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.

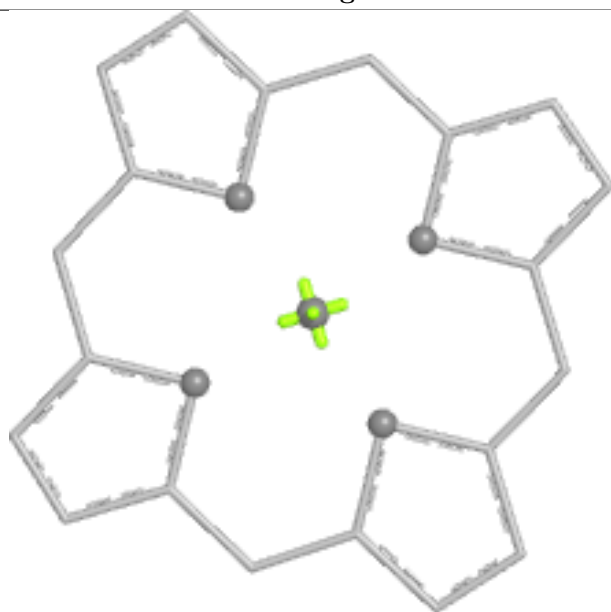
Ligand CLA P 5102



Bond lengths



Bond angles

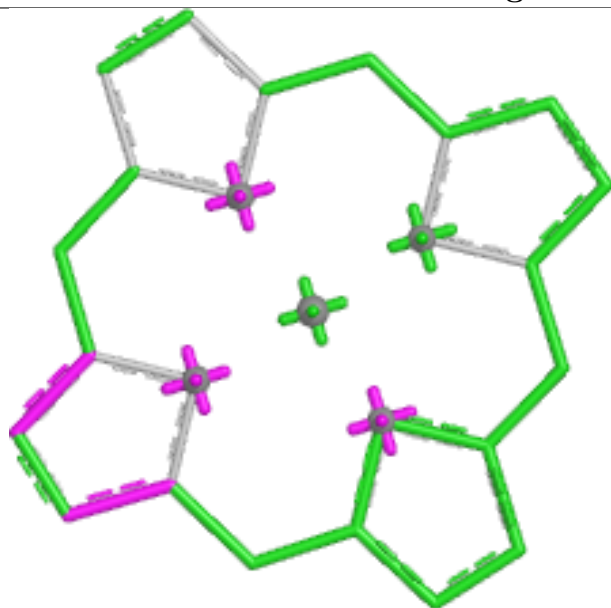


Torsions

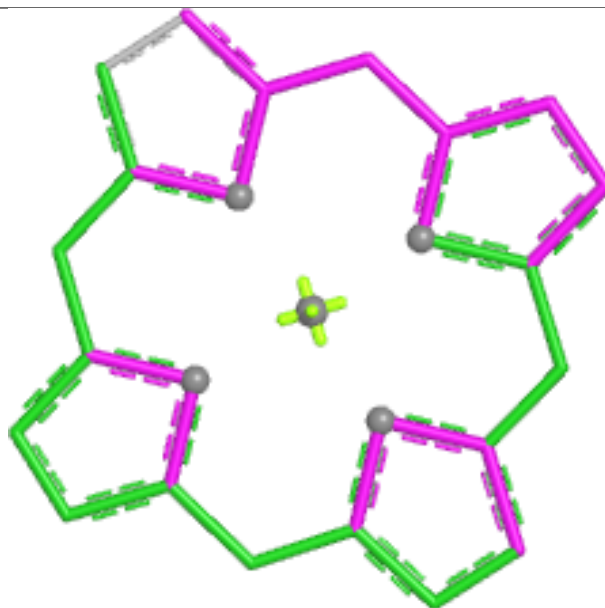


Rings

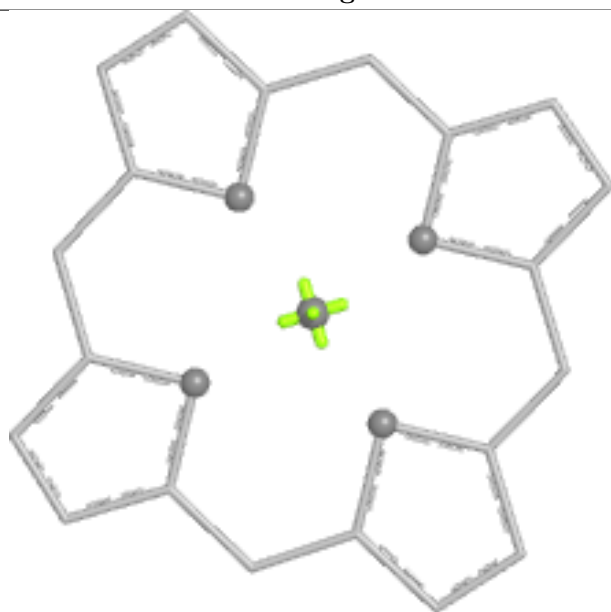
Ligand CLA P 5131



Bond lengths



Bond angles

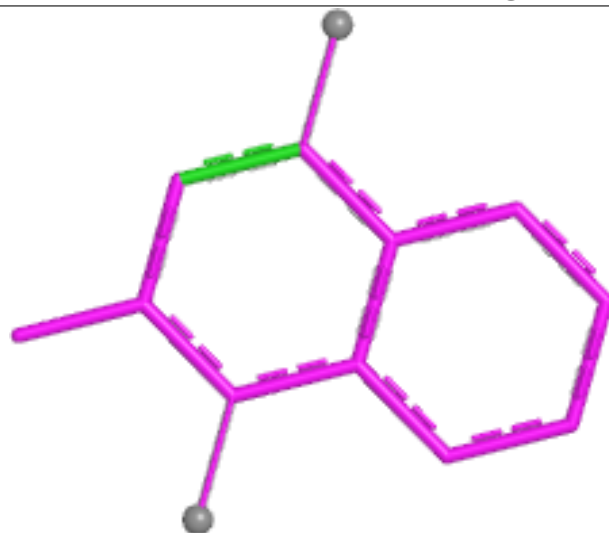


Torsions

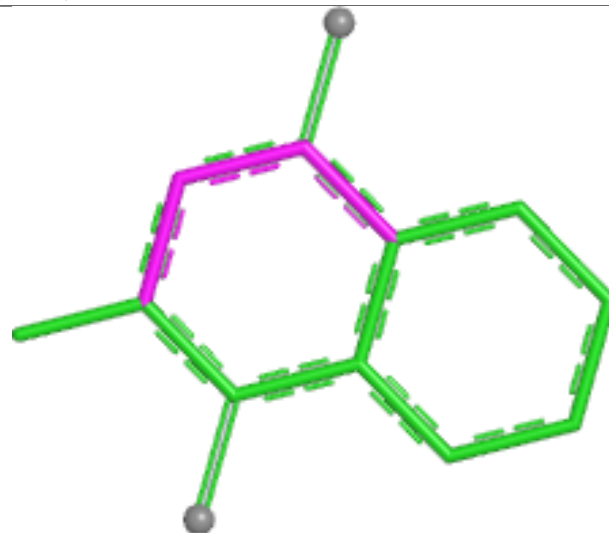


Rings

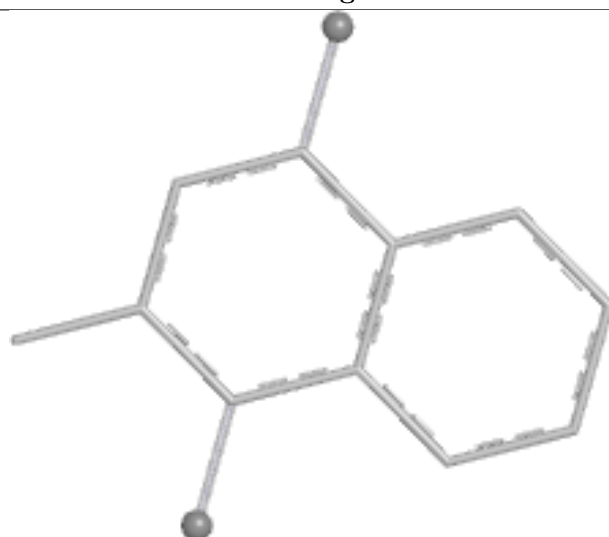
Ligand PQN Q 6002



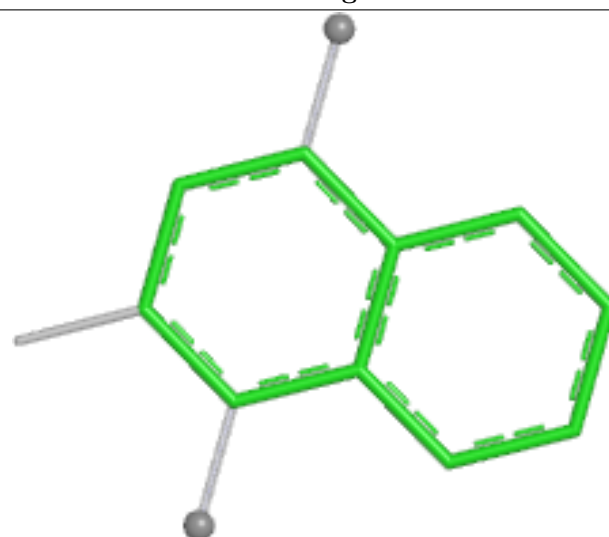
Bond lengths



Bond angles

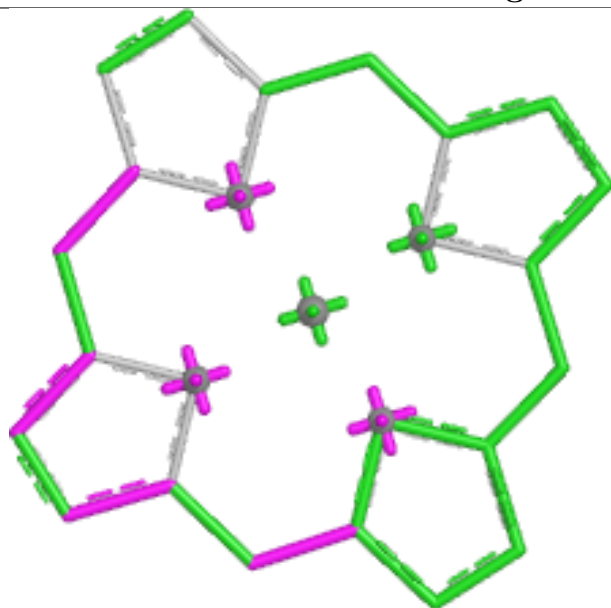


Torsions

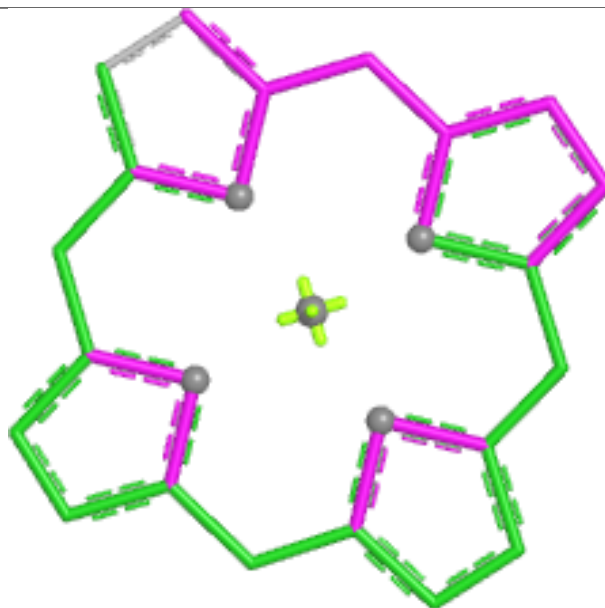


Rings

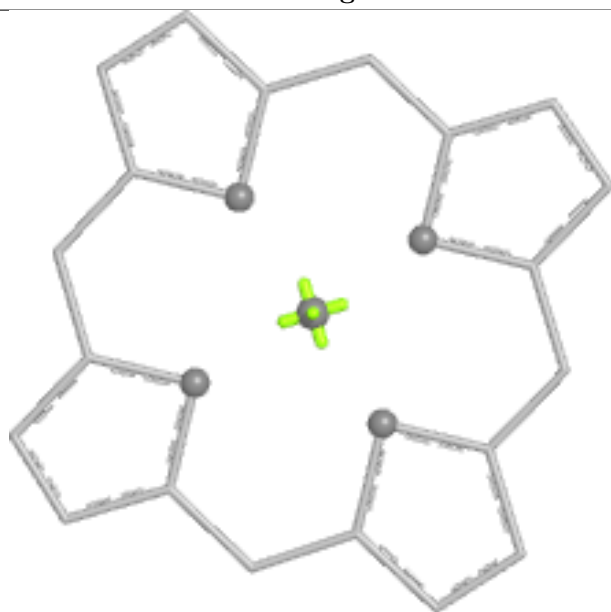
Ligand CLA P 5105



Bond lengths



Bond angles

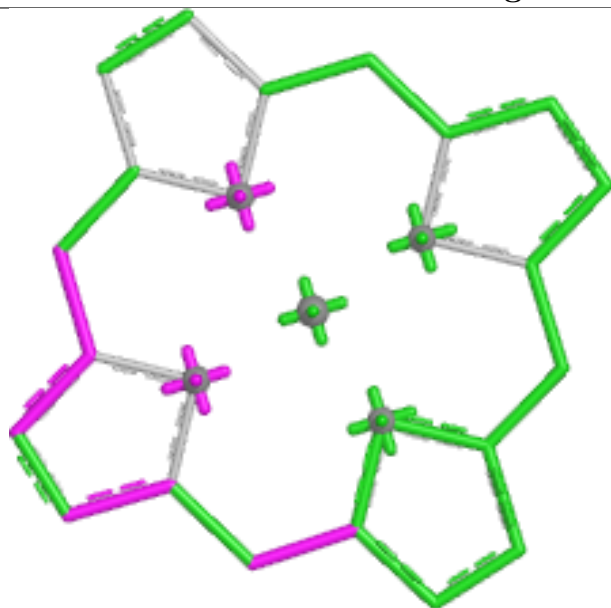


Torsions

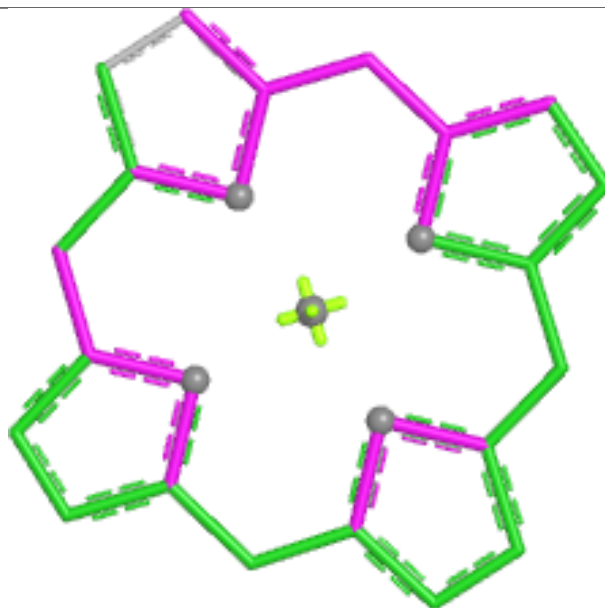


Rings

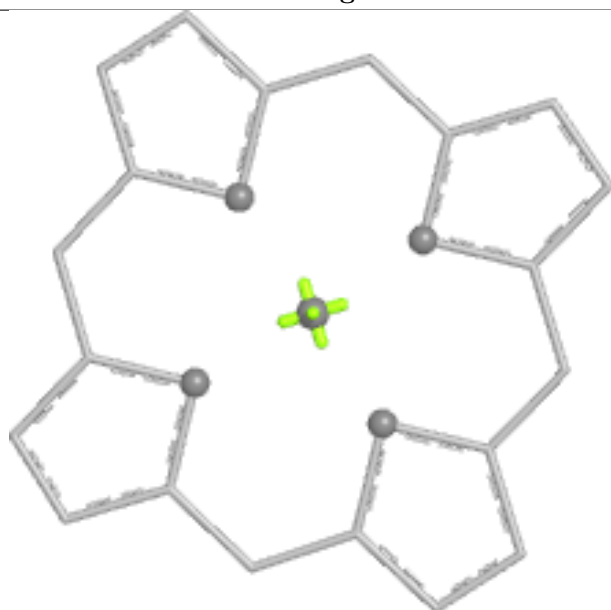
Ligand CLA K 1403



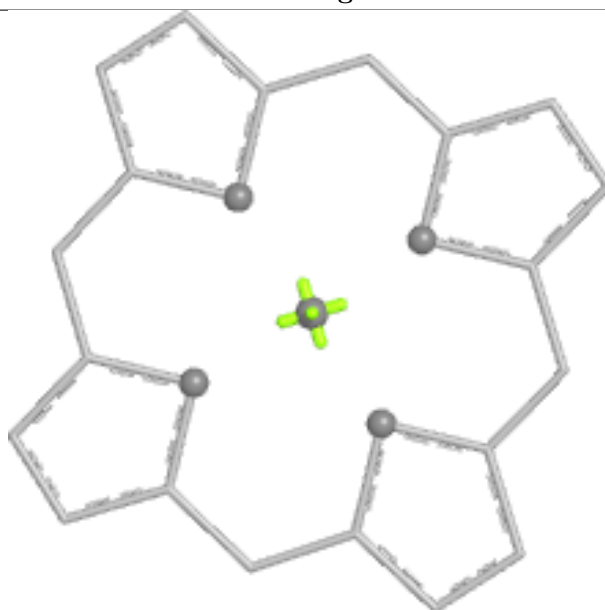
Bond lengths



Bond angles

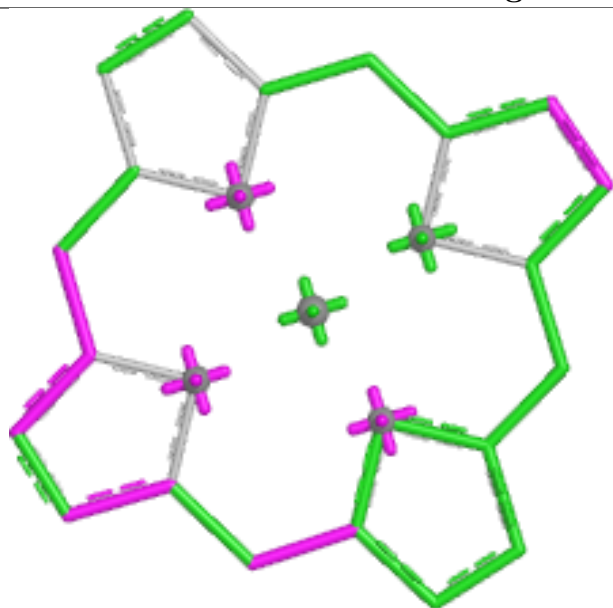


Torsions

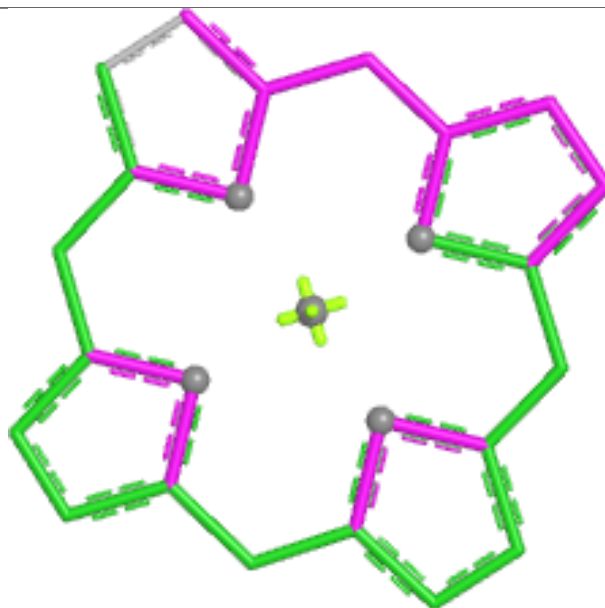


Rings

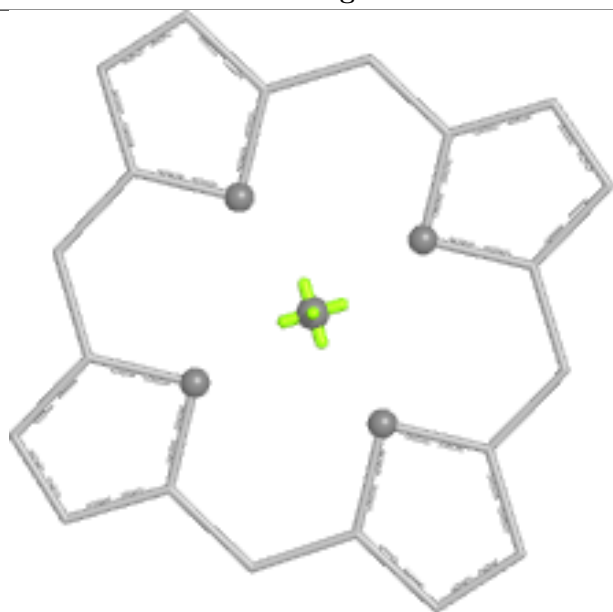
Ligand CLA B 1208



Bond lengths



Bond angles

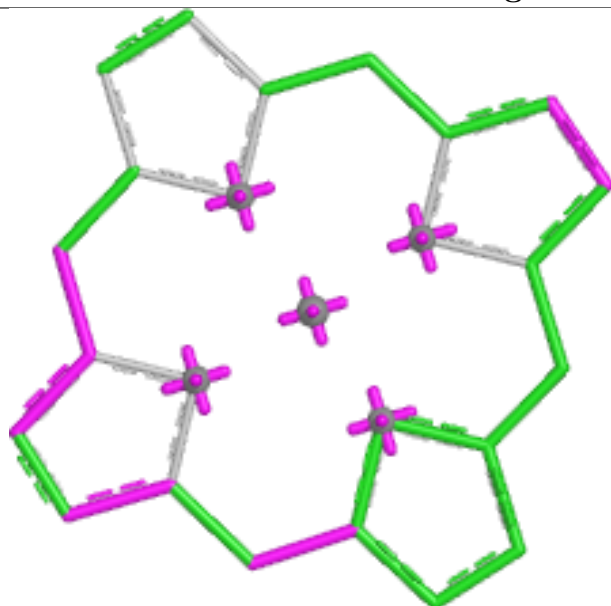


Torsions

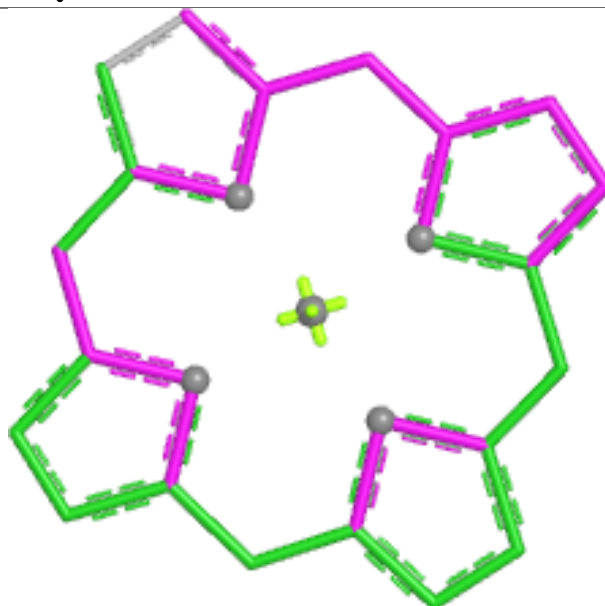


Rings

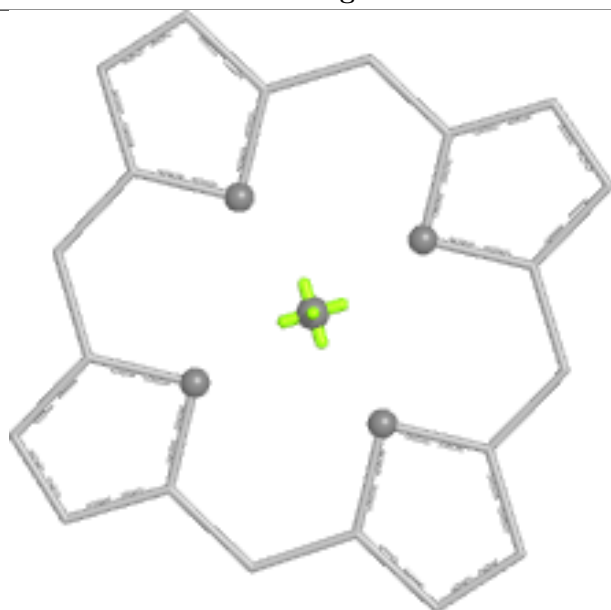
Ligand CLA Q 5022



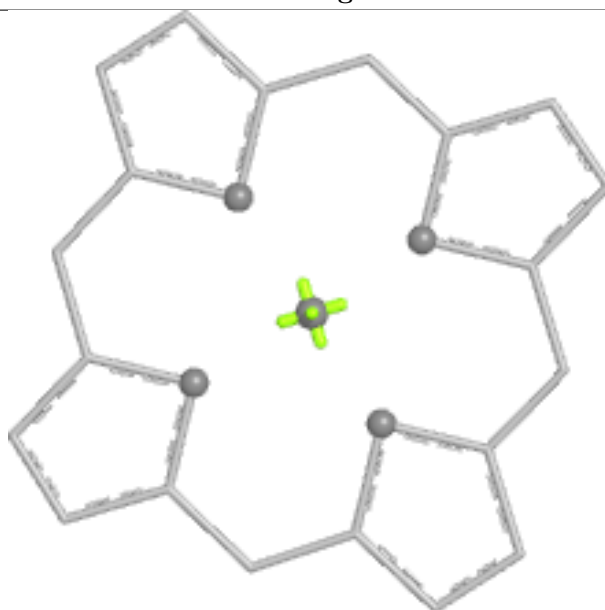
Bond lengths



Bond angles

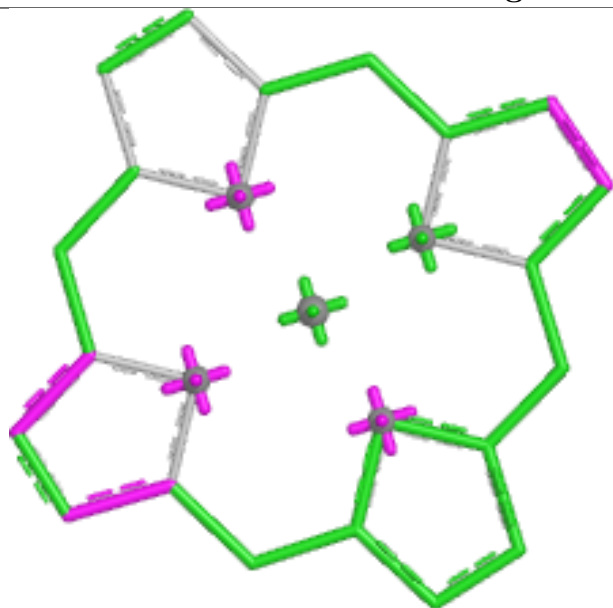


Torsions

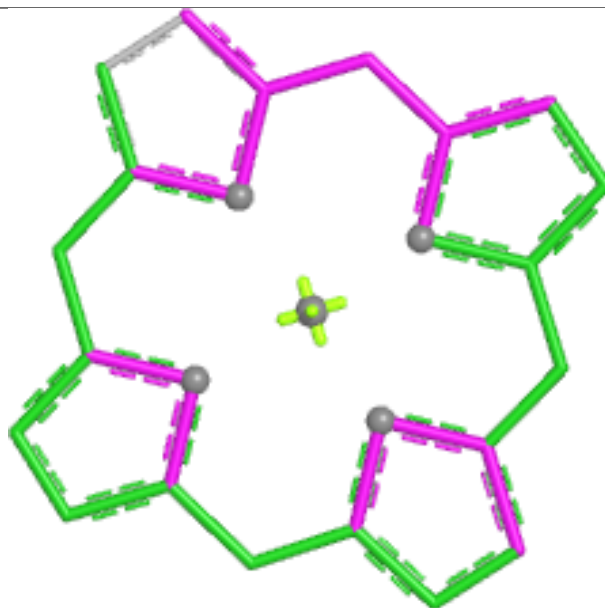


Rings

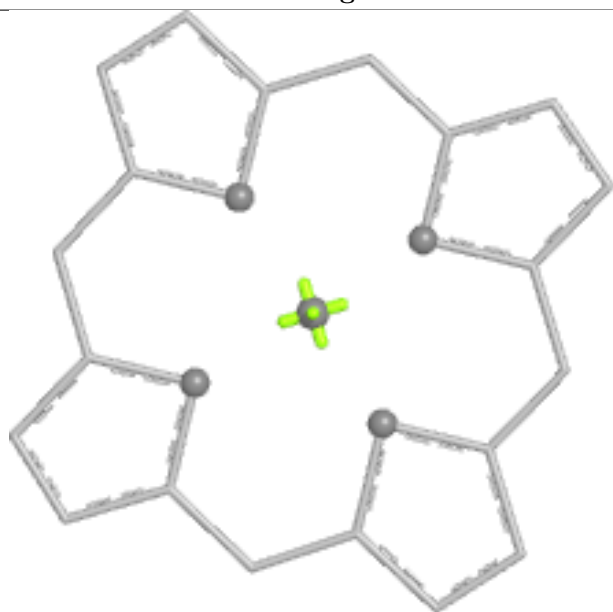
Ligand CLA B 1215



Bond lengths



Bond angles

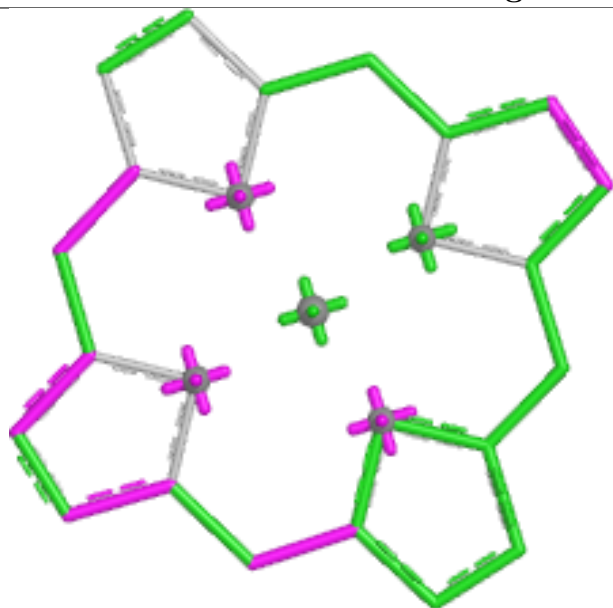


Torsions

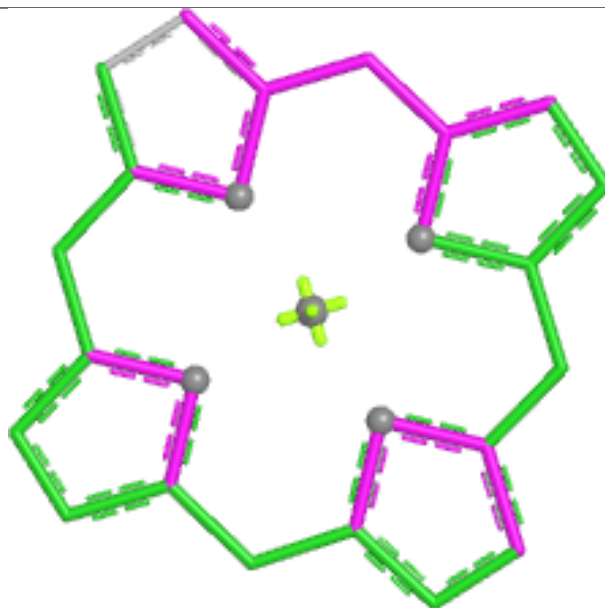


Rings

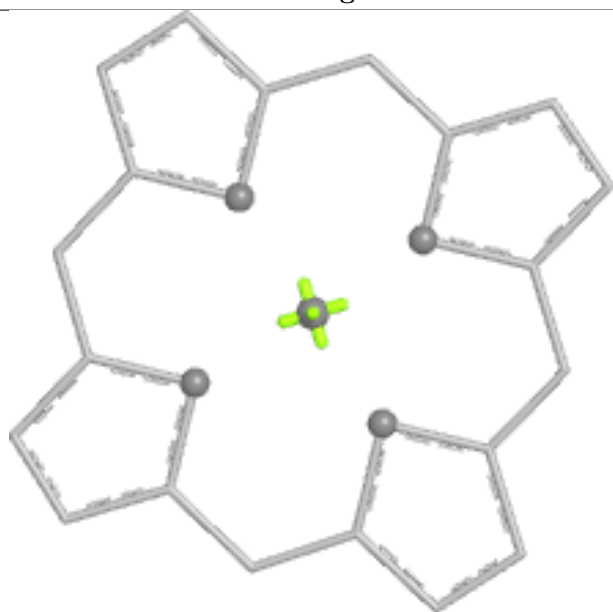
Ligand CLA B 1217



Bond lengths



Bond angles

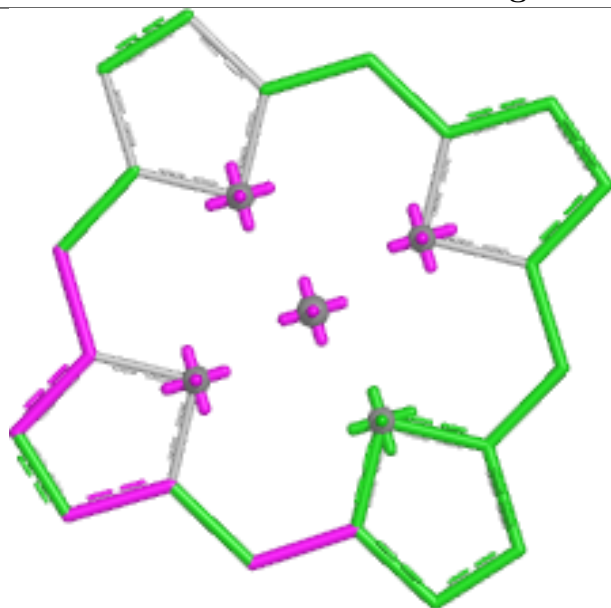


Torsions

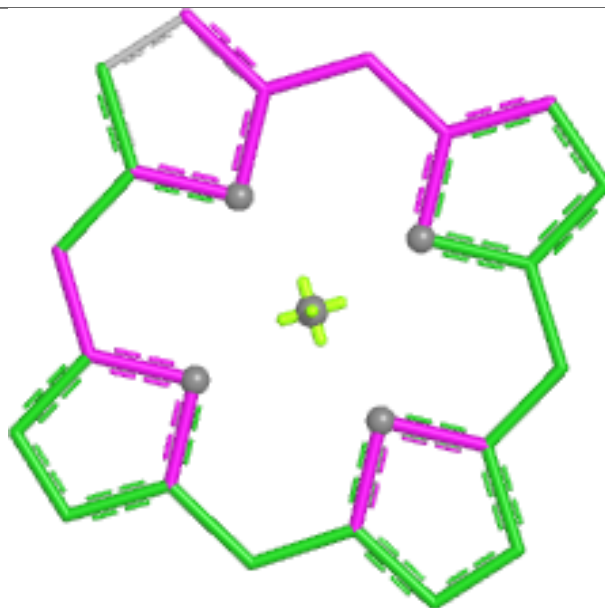


Rings

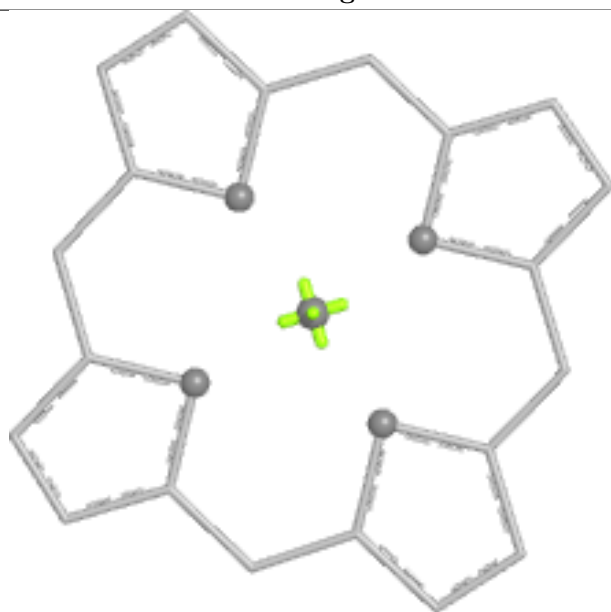
Ligand CLA 7 1021



Bond lengths



Bond angles

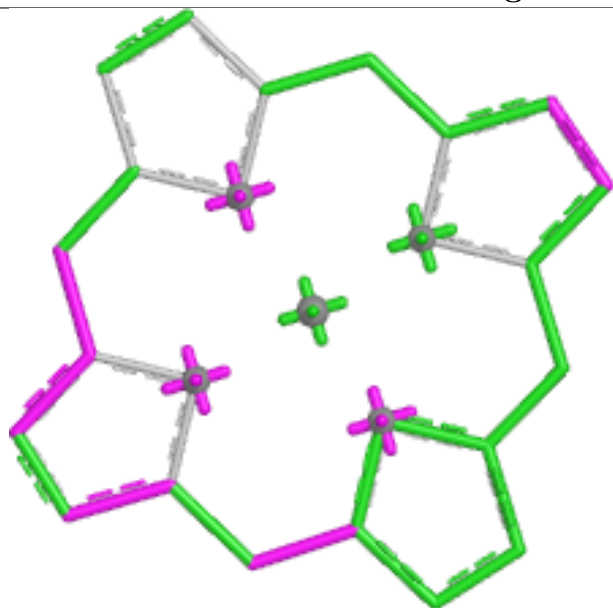


Torsions

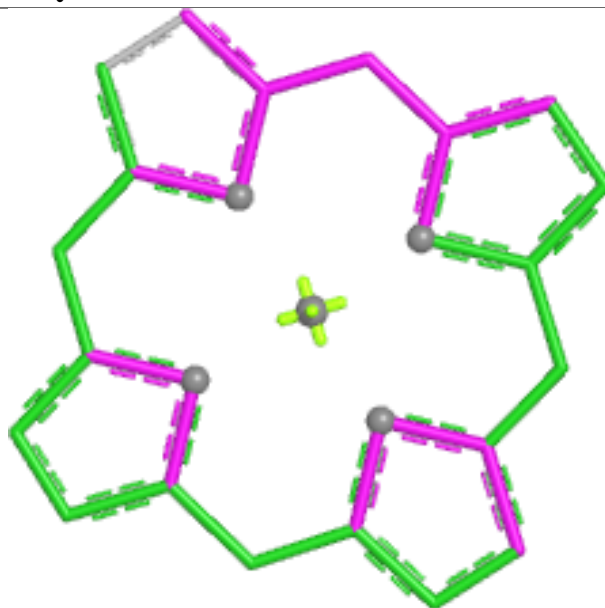


Rings

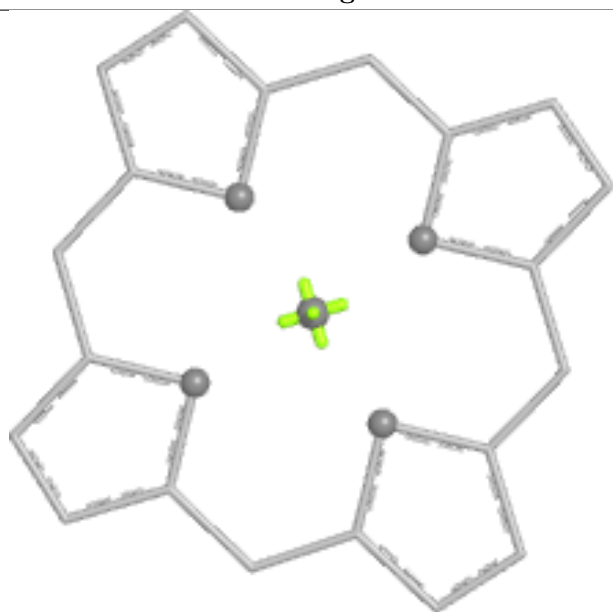
Ligand CLA Q 5214



Bond lengths



Bond angles

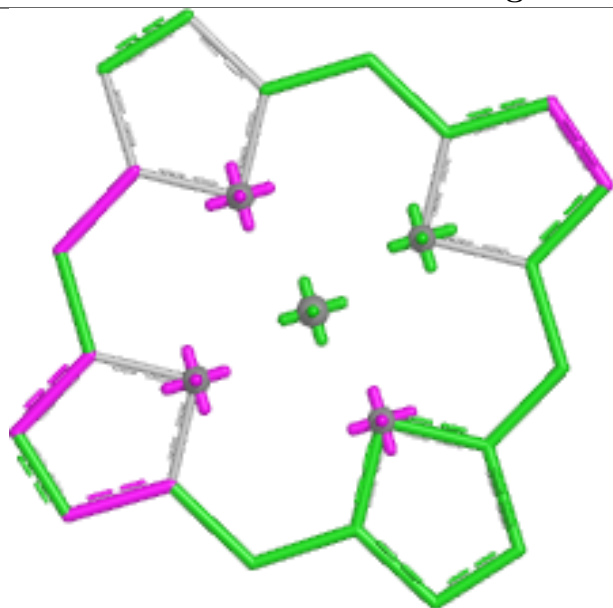


Torsions

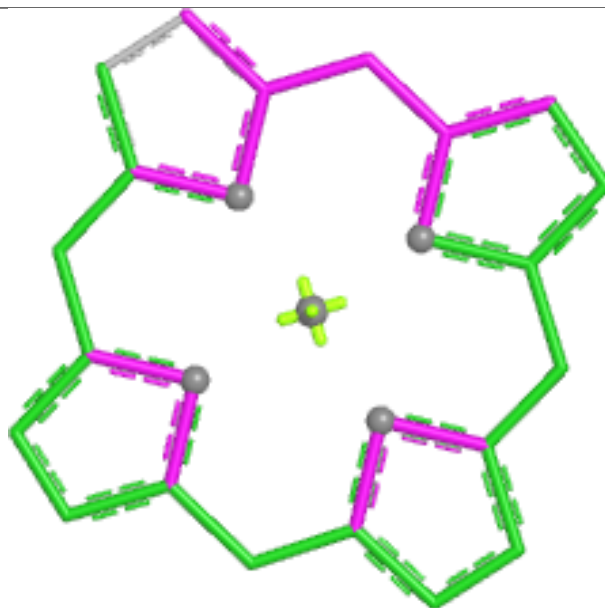


Rings

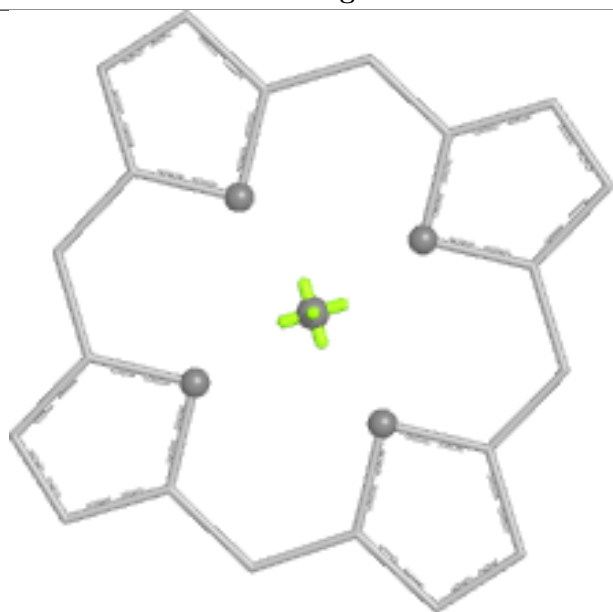
Ligand CLA P 5402



Bond lengths



Bond angles

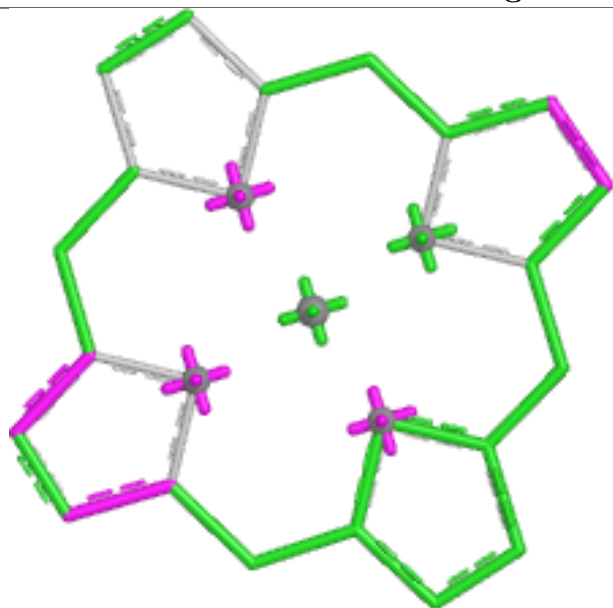


Torsions

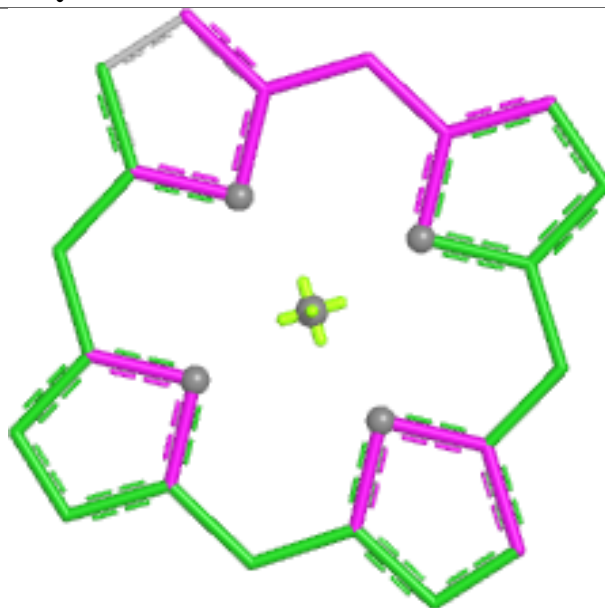


Rings

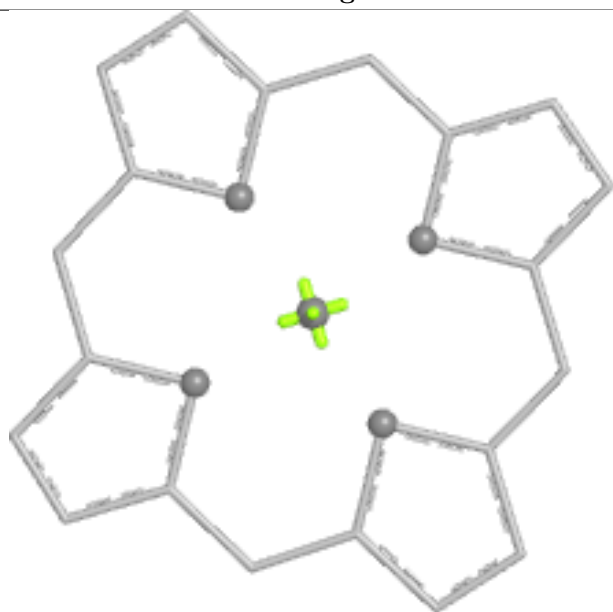
Ligand CLA Q 5215



Bond lengths



Bond angles

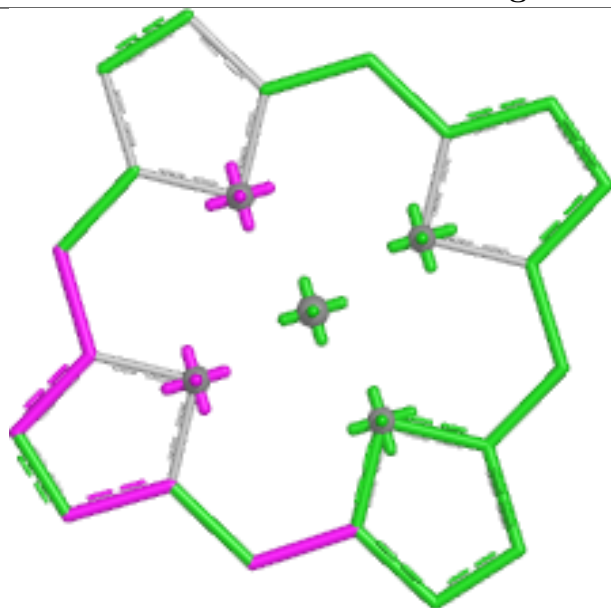


Torsions

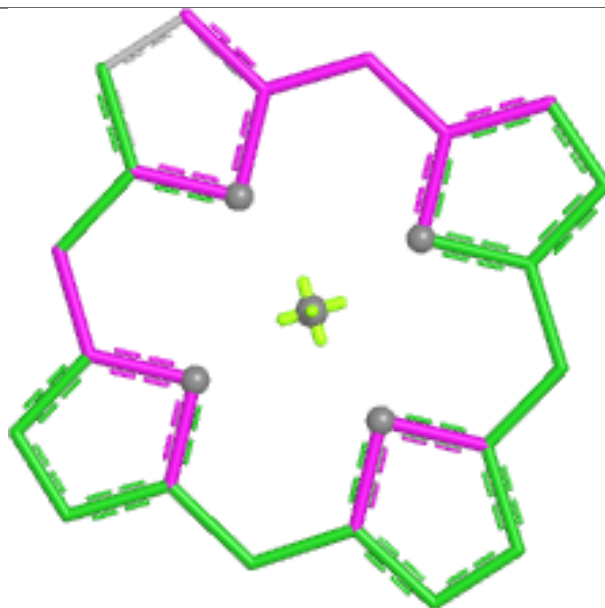


Rings

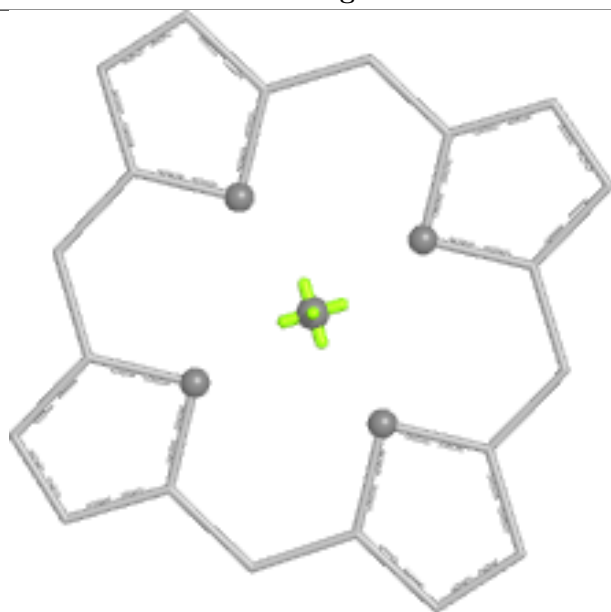
Ligand CLA 8 1033



Bond lengths



Bond angles

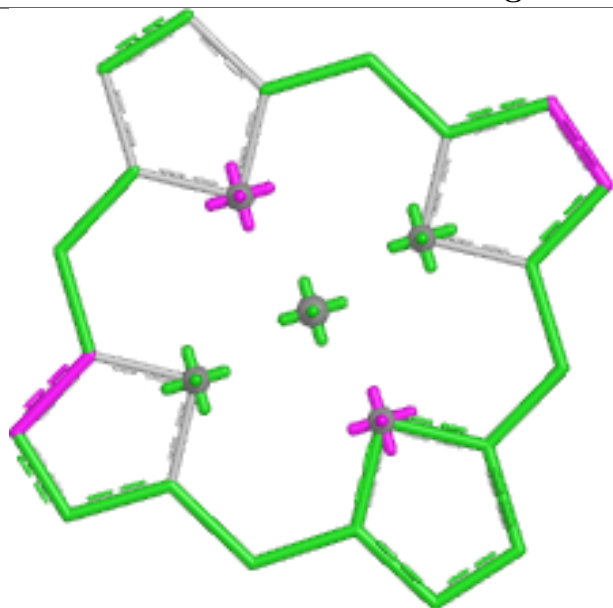


Torsions

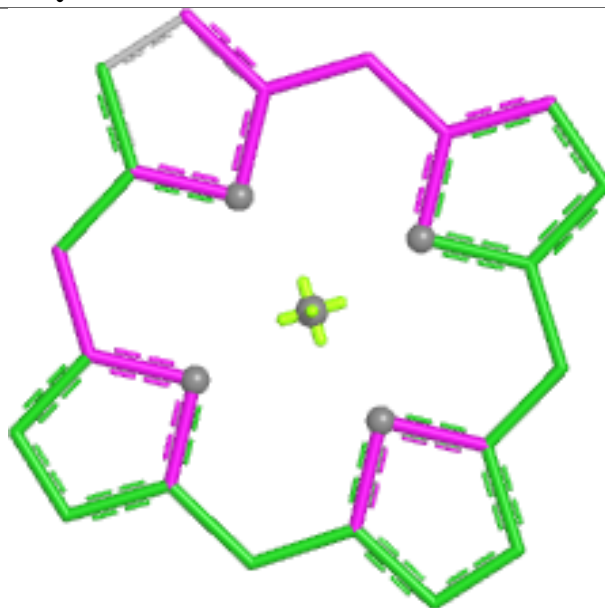


Rings

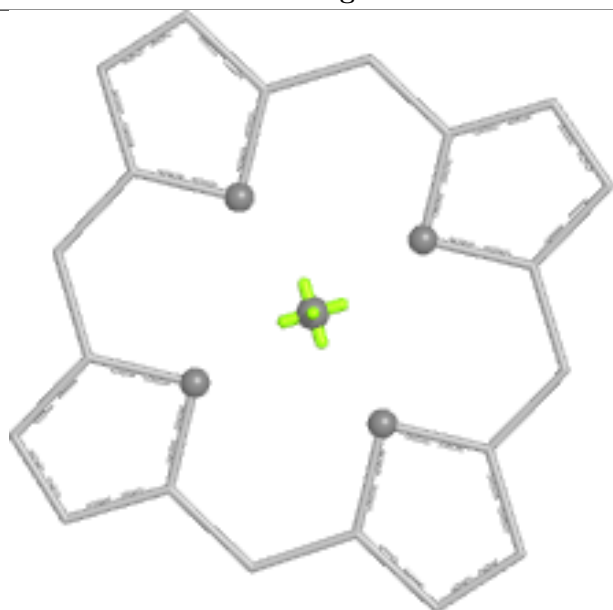
Ligand CLA Q 5206



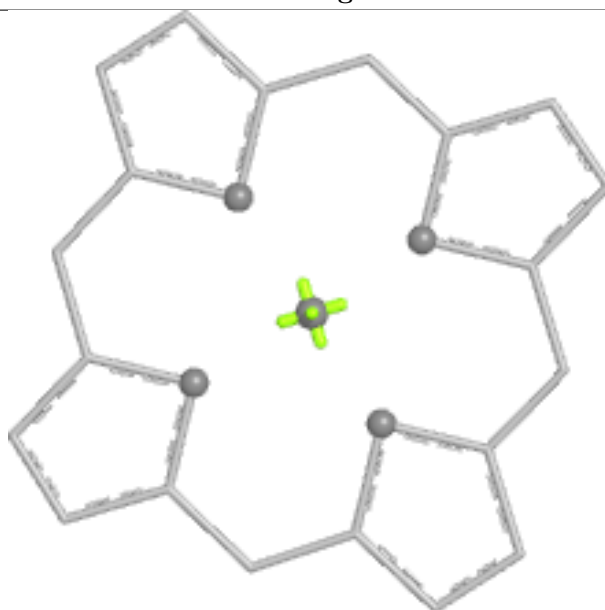
Bond lengths



Bond angles

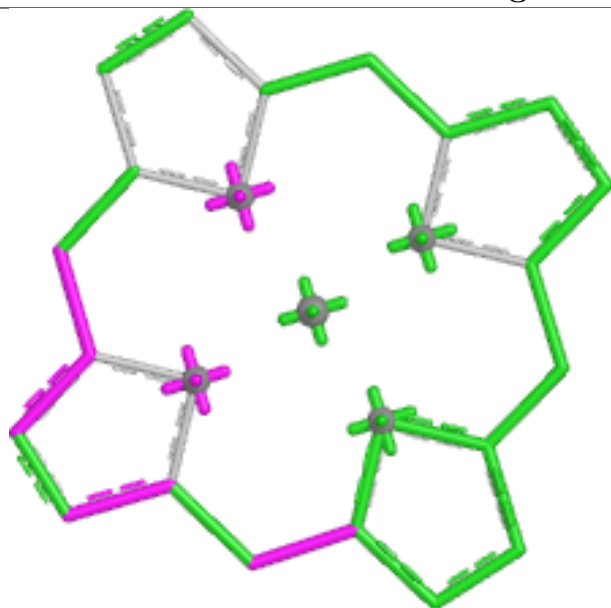


Torsions

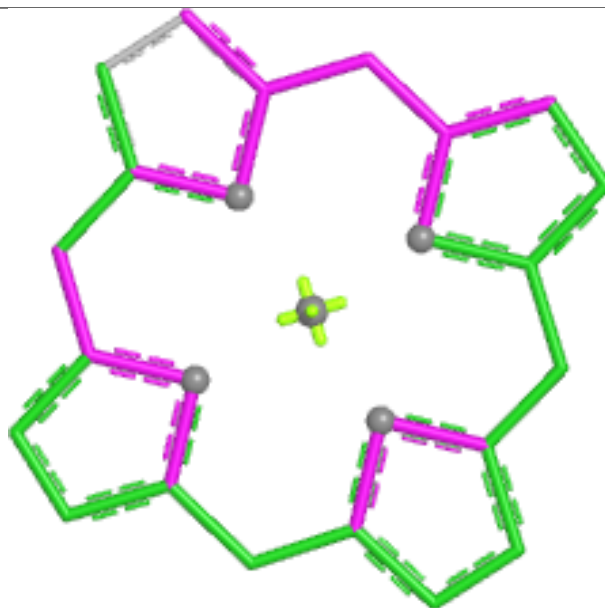


Rings

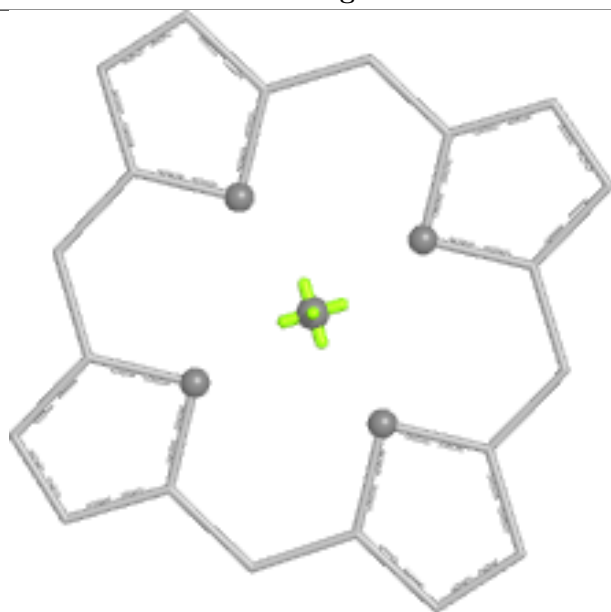
Ligand CLA 9 1014



Bond lengths



Bond angles

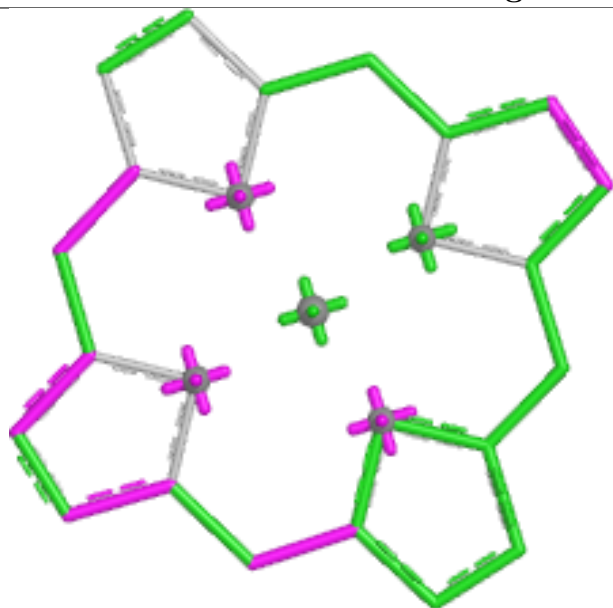


Torsions

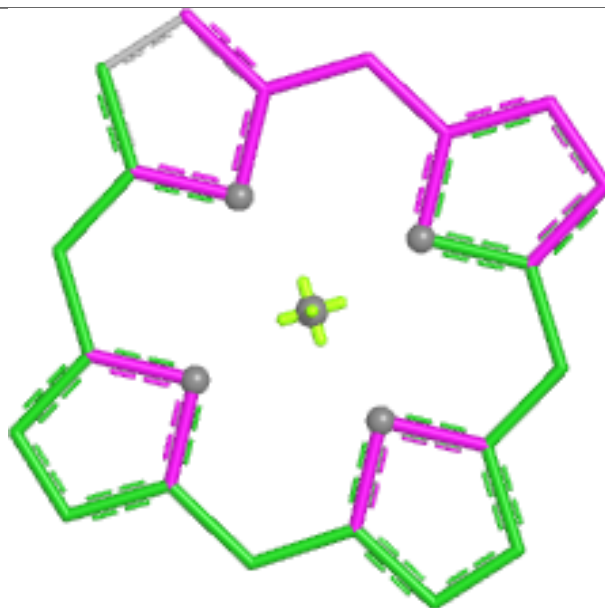


Rings

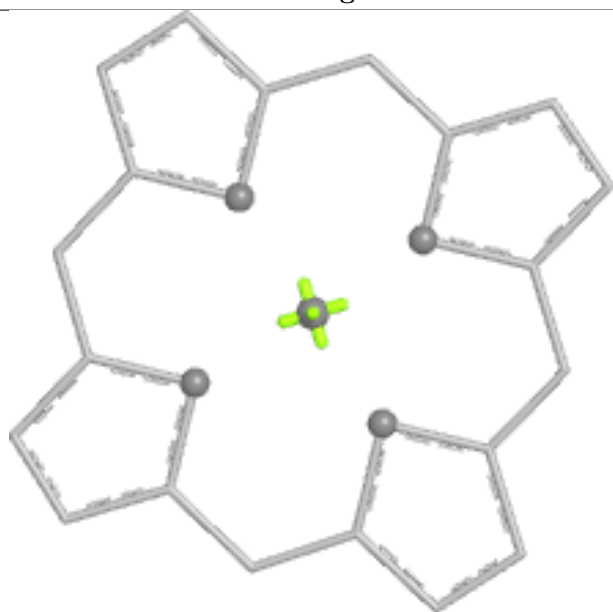
Ligand CLA B 1230



Bond lengths



Bond angles

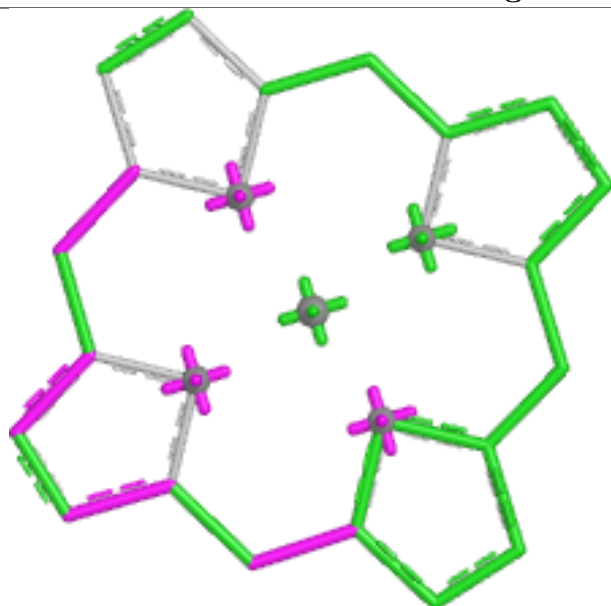


Torsions

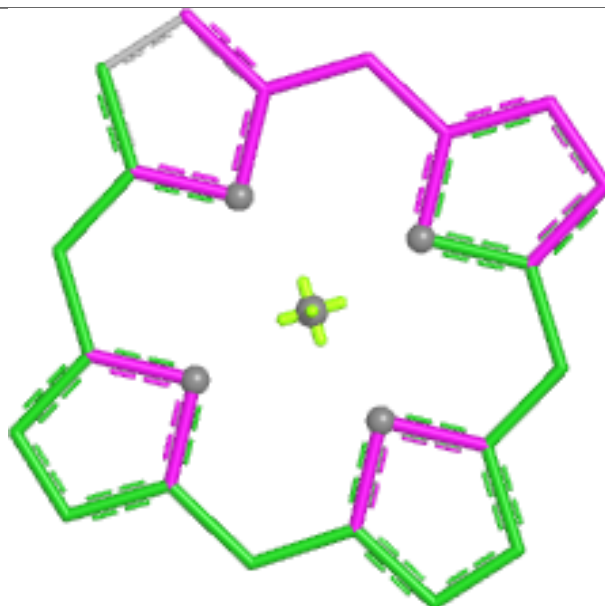


Rings

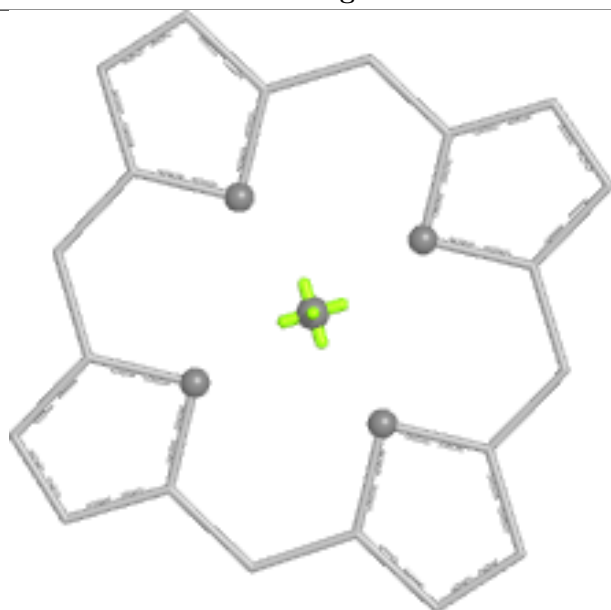
Ligand CLA A 1105



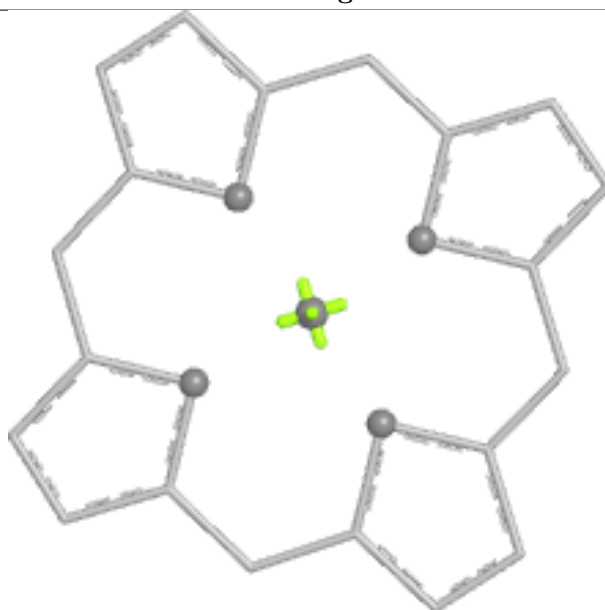
Bond lengths



Bond angles

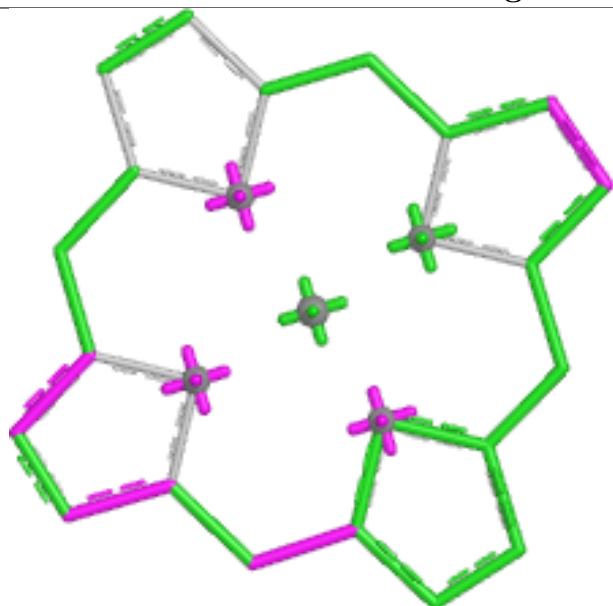


Torsions

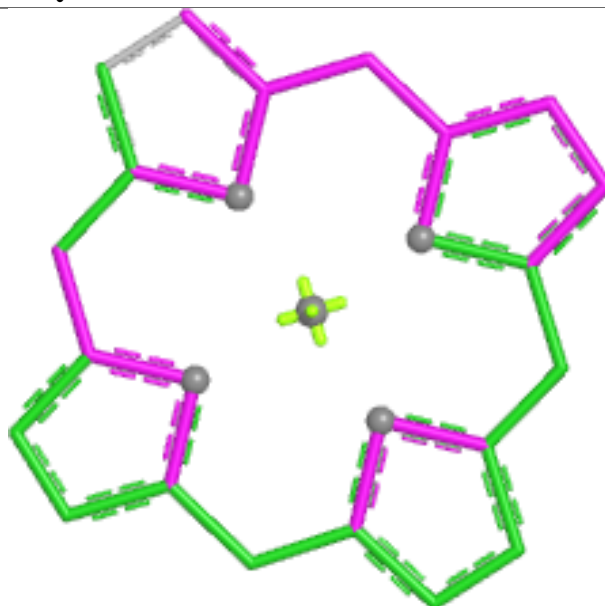


Rings

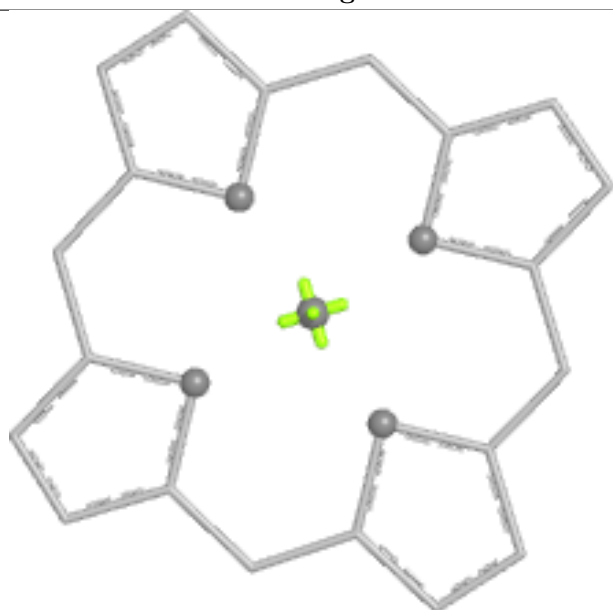
Ligand CLA Q 5224



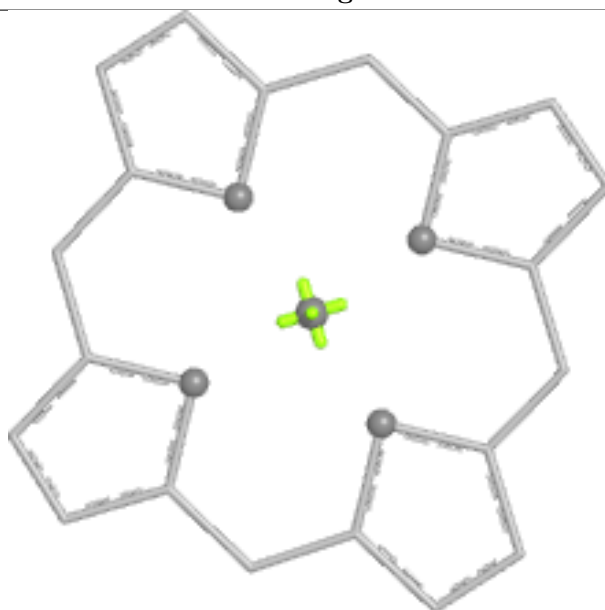
Bond lengths



Bond angles

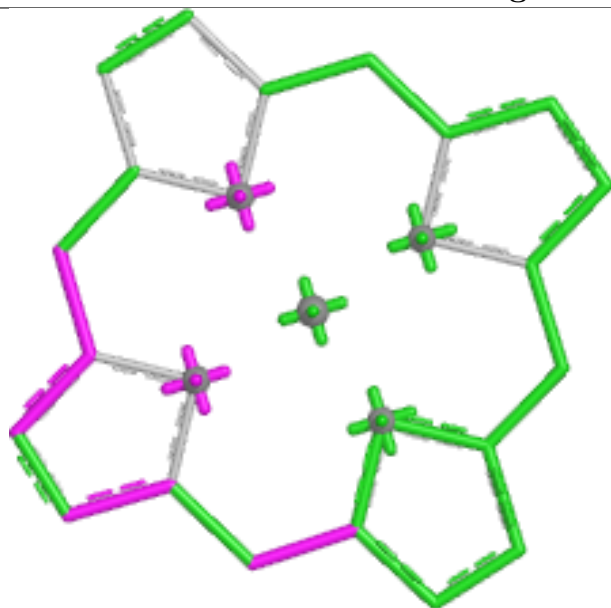


Torsions

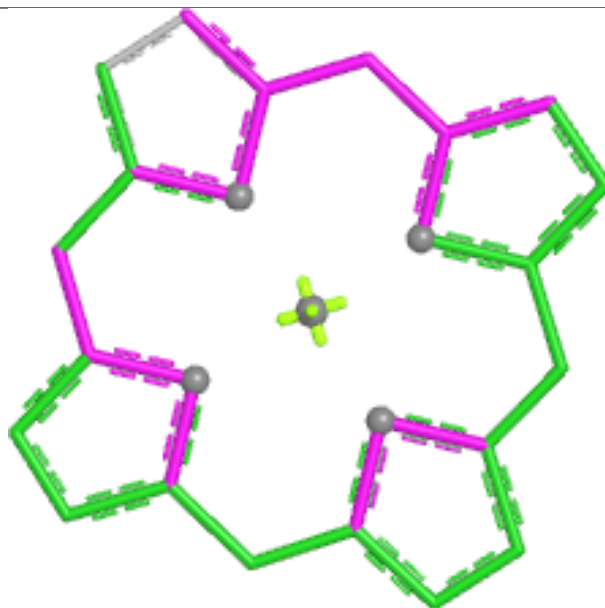


Rings

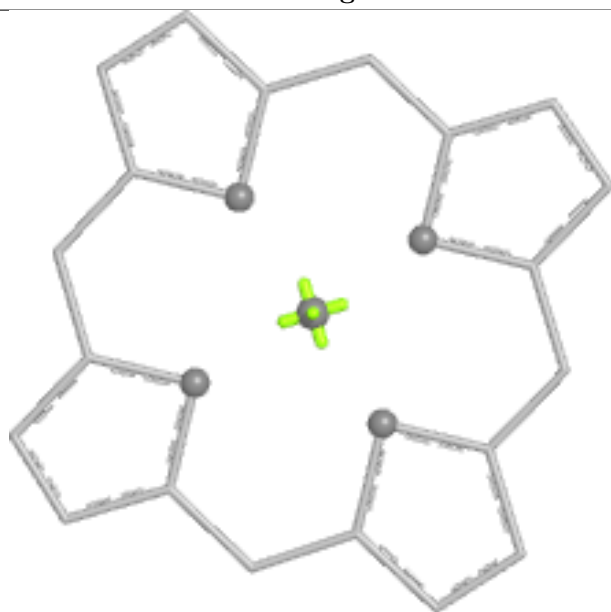
Ligand CLA 1 1026



Bond lengths



Bond angles

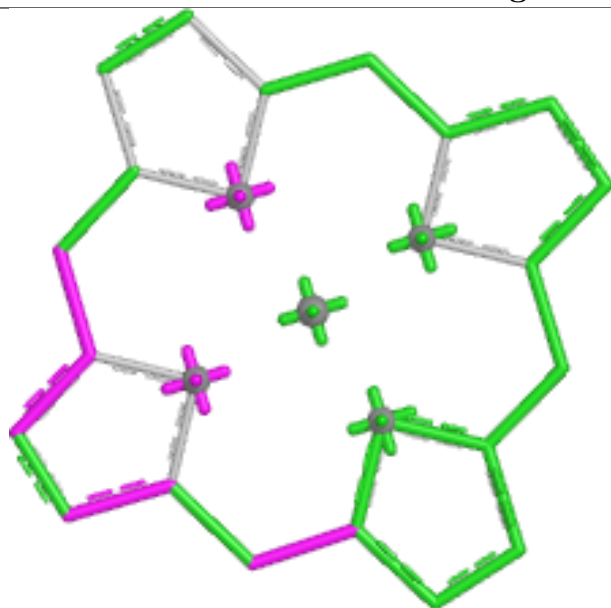


Torsions

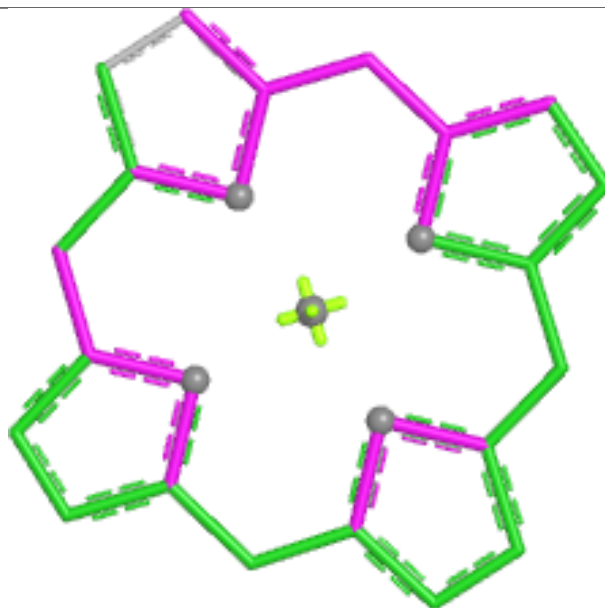


Rings

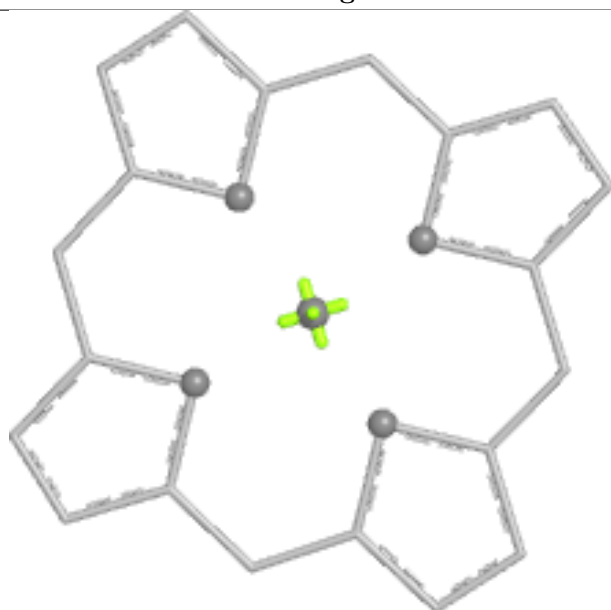
Ligand CLA 4 1026



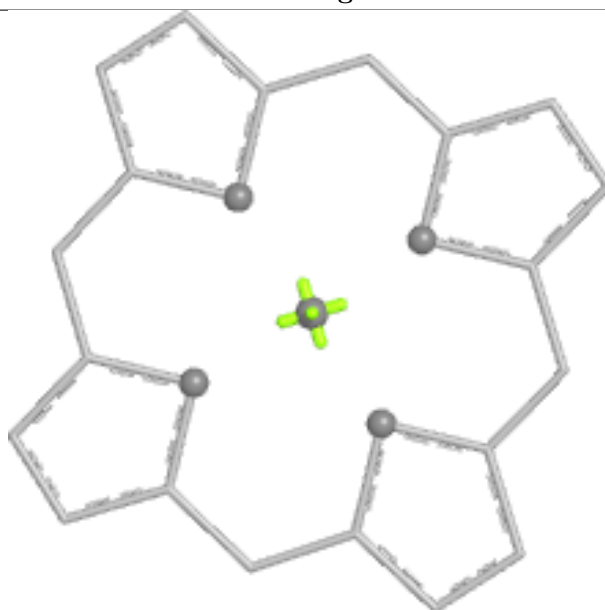
Bond lengths



Bond angles

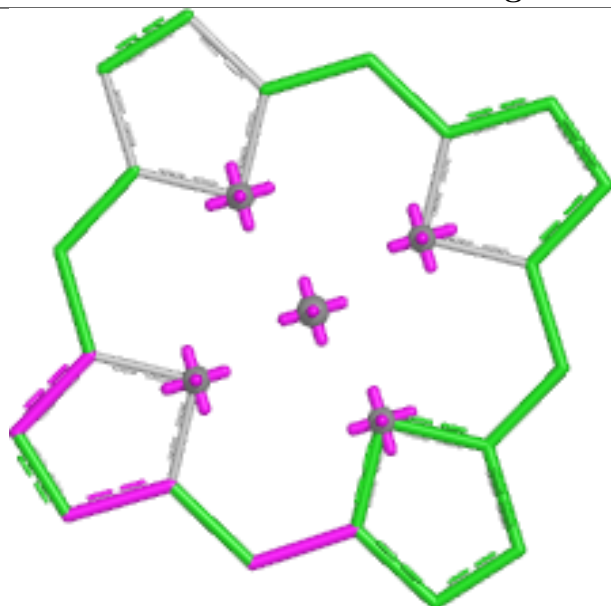


Torsions

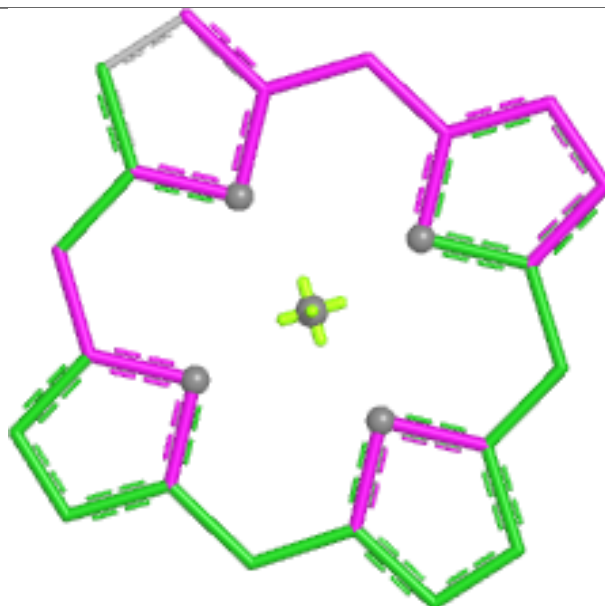


Rings

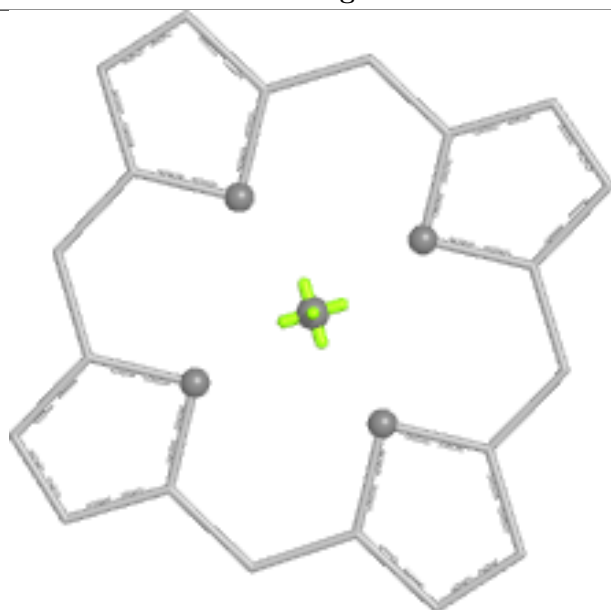
Ligand CLA A 1107



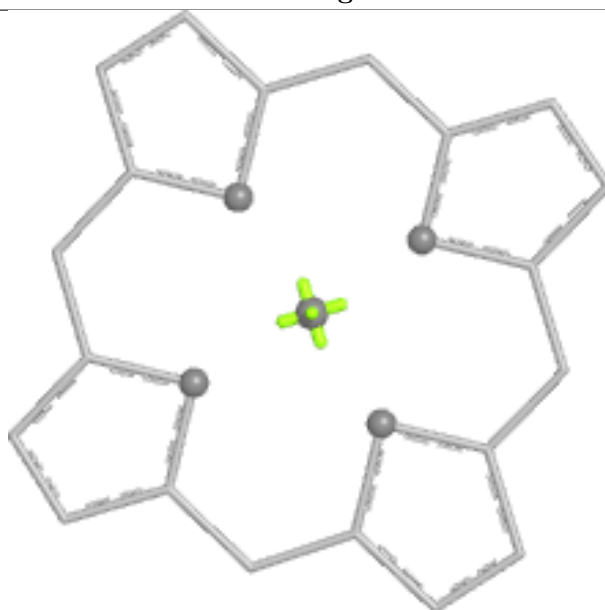
Bond lengths



Bond angles

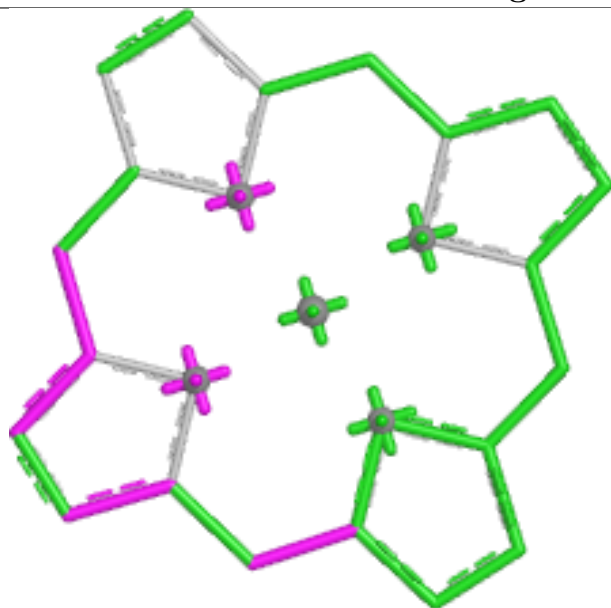


Torsions



Rings

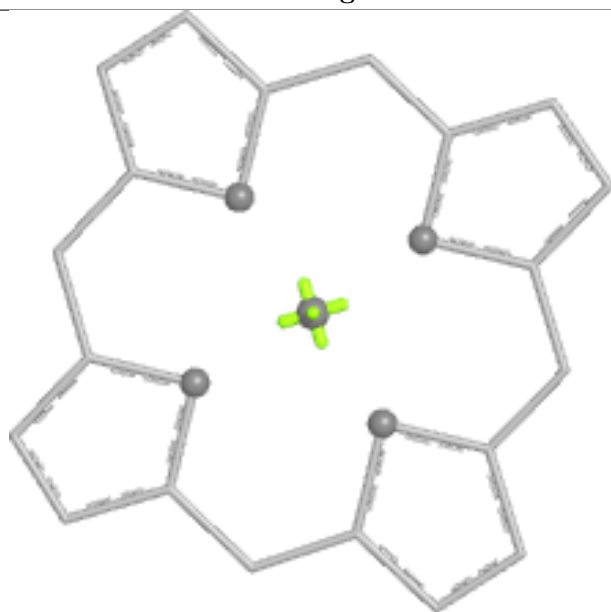
Ligand CLA 0 1022



Bond lengths



Bond angles

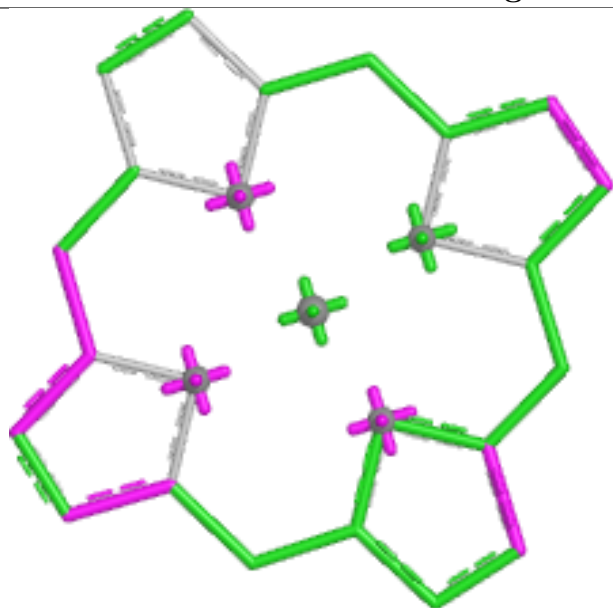


Torsions

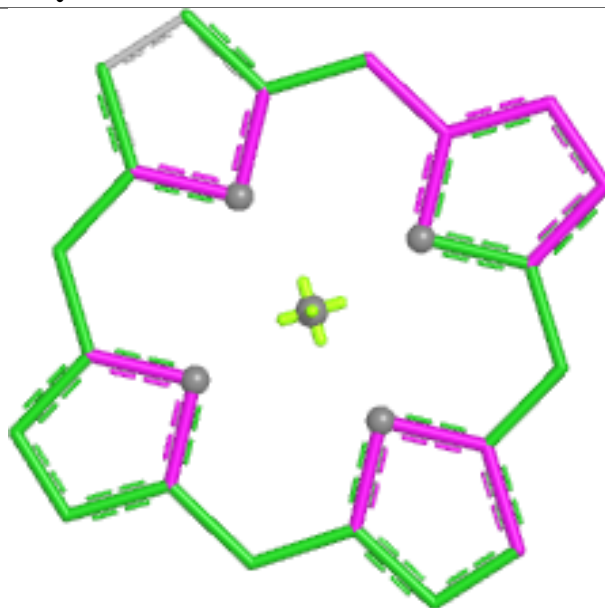


Rings

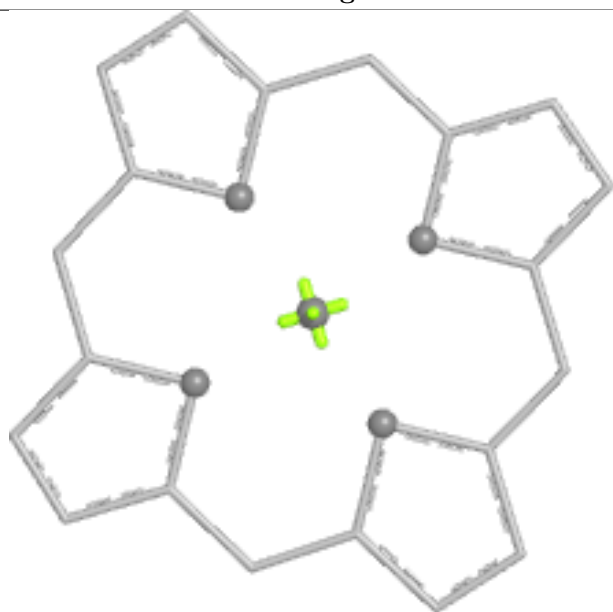
Ligand CLA Q 5237



Bond lengths



Bond angles

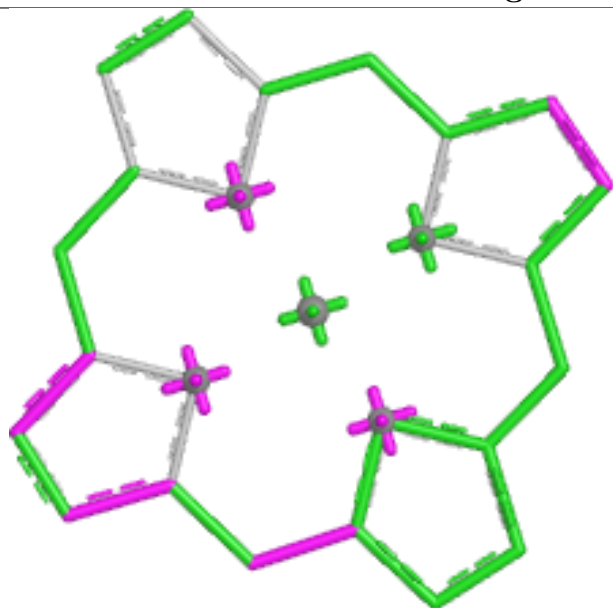


Torsions

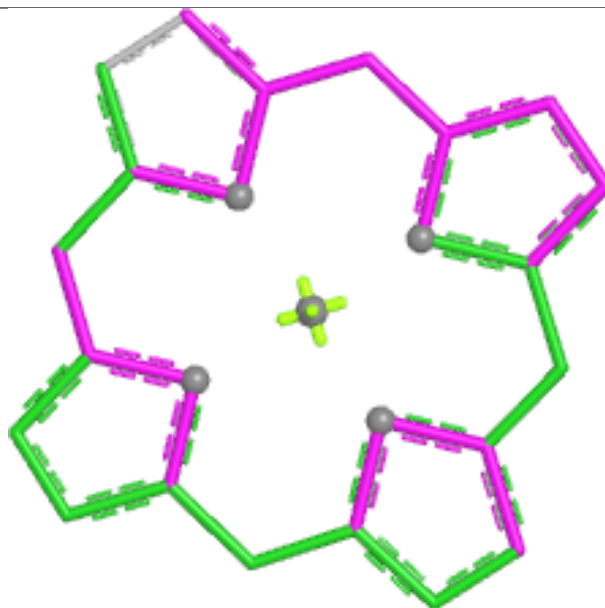


Rings

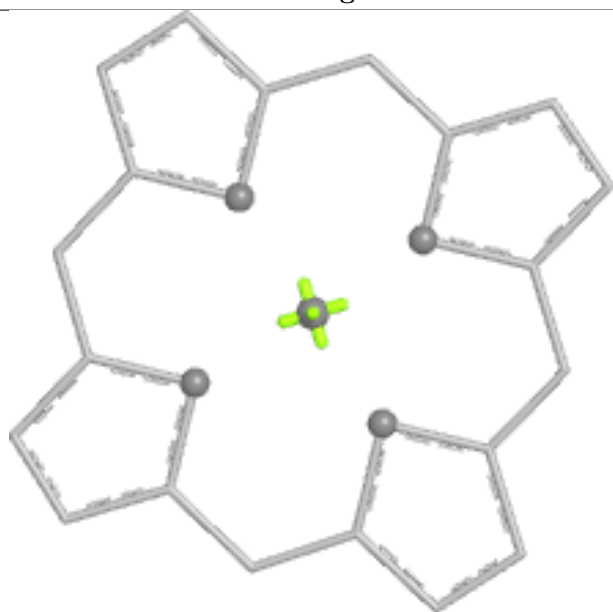
Ligand CLA B 1218



Bond lengths



Bond angles

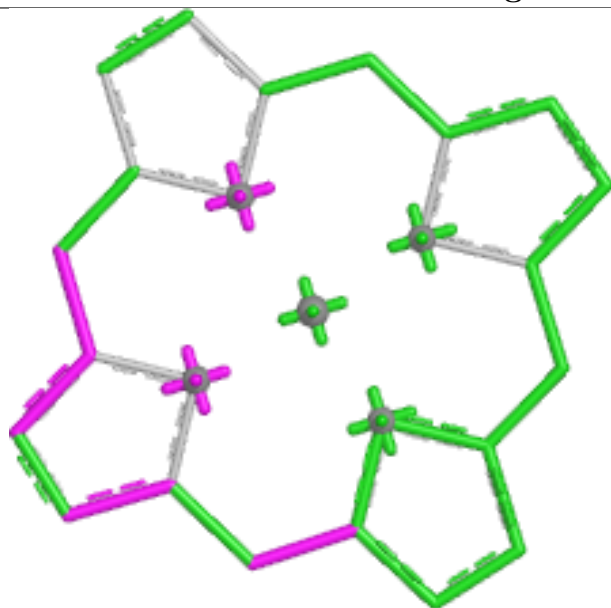


Torsions

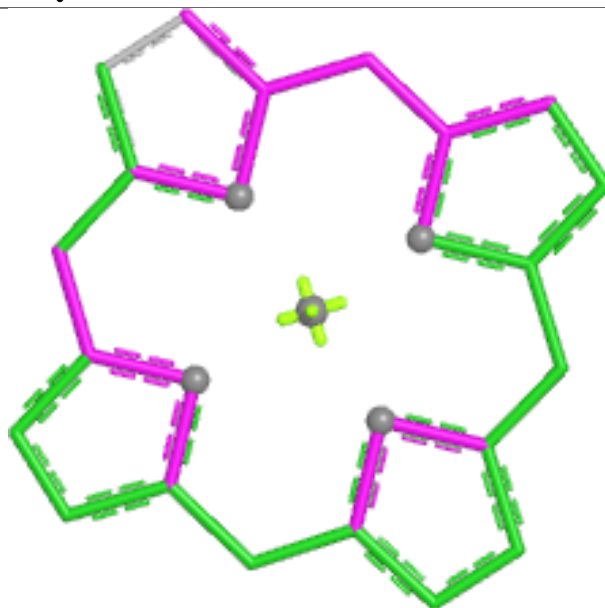


Rings

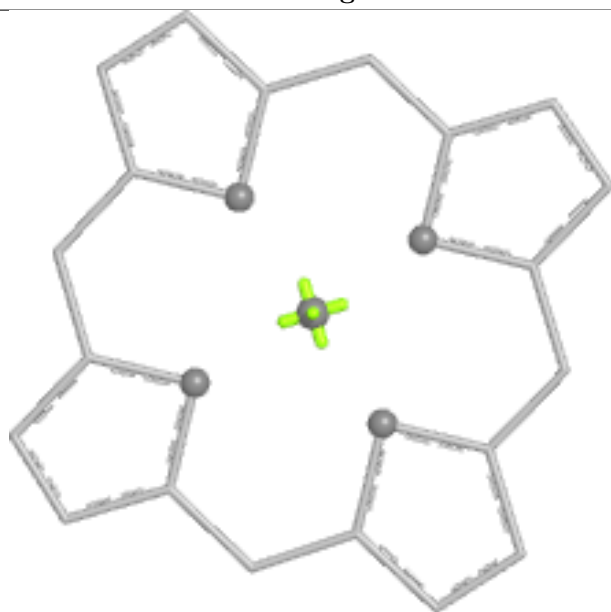
Ligand CLA Q 5242



Bond lengths



Bond angles

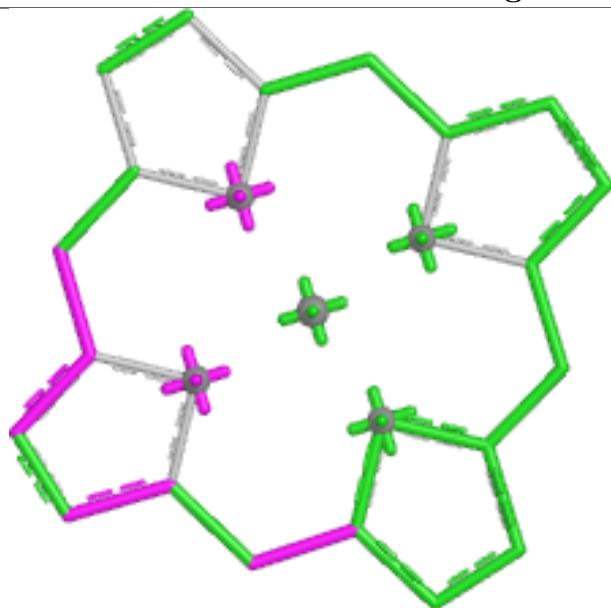


Torsions

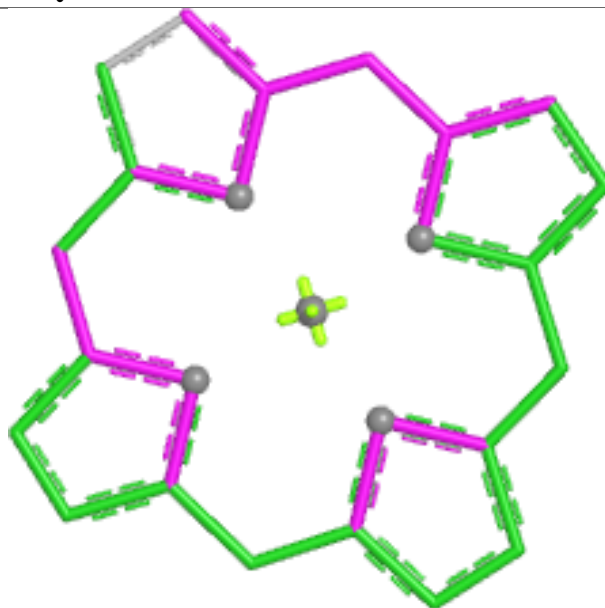


Rings

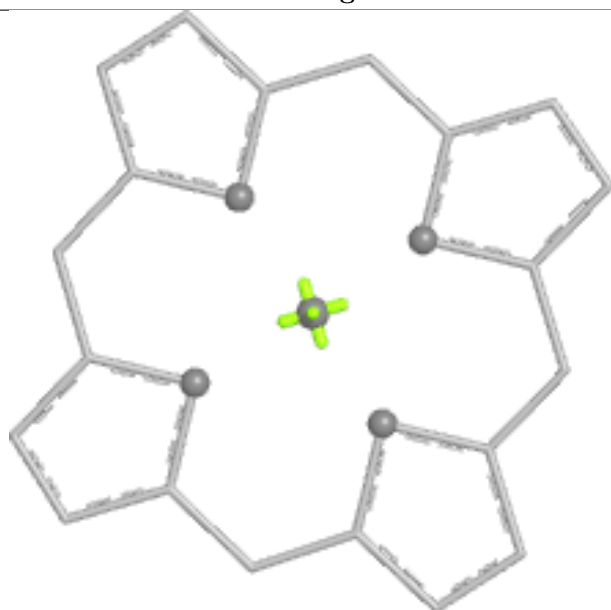
Ligand CLA Q 5240



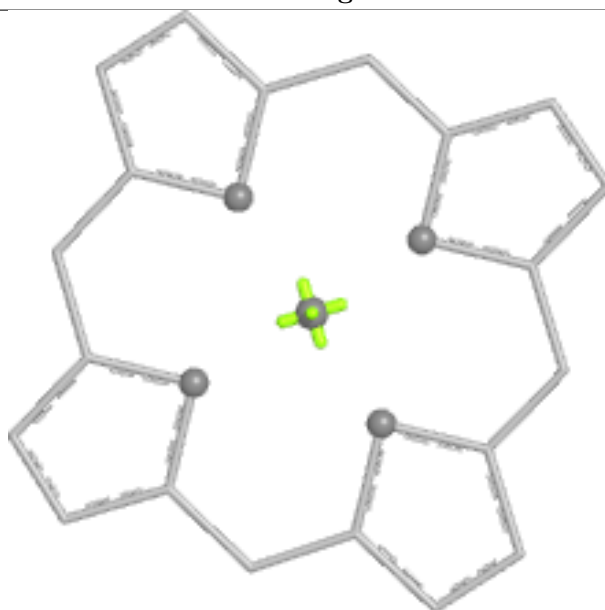
Bond lengths



Bond angles

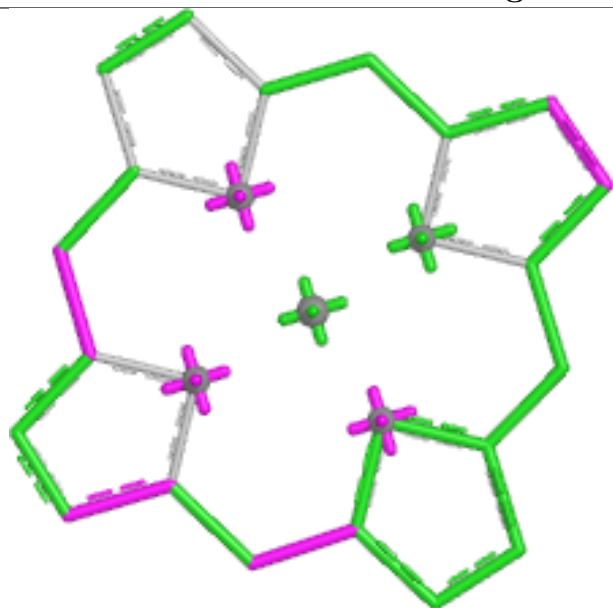


Torsions

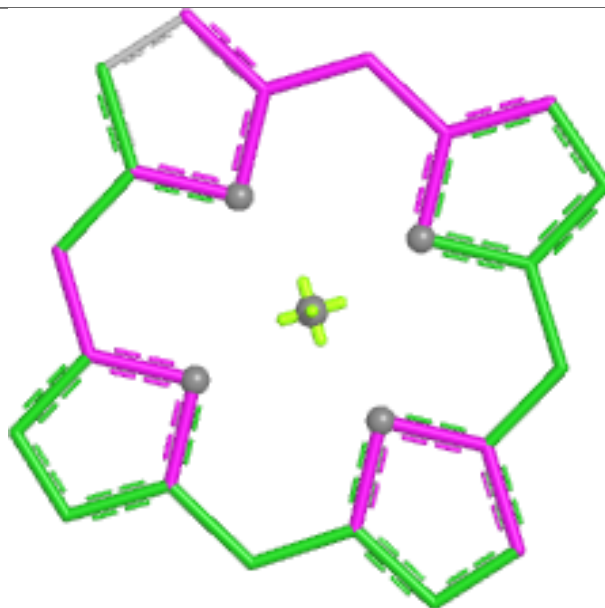


Rings

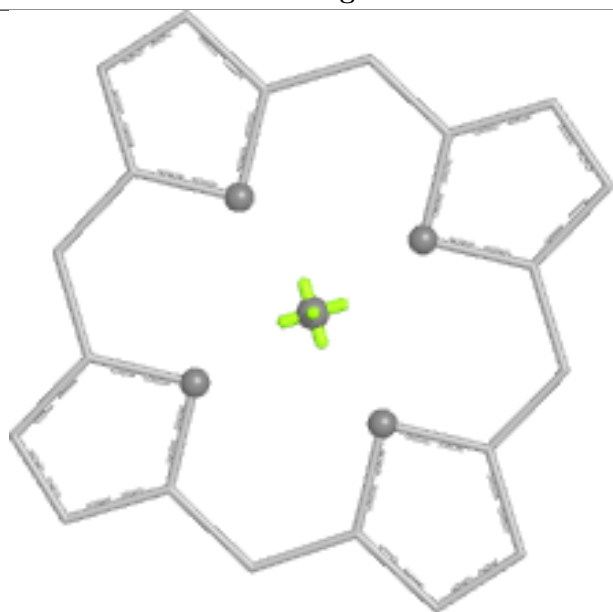
Ligand CLA P 5119



Bond lengths



Bond angles

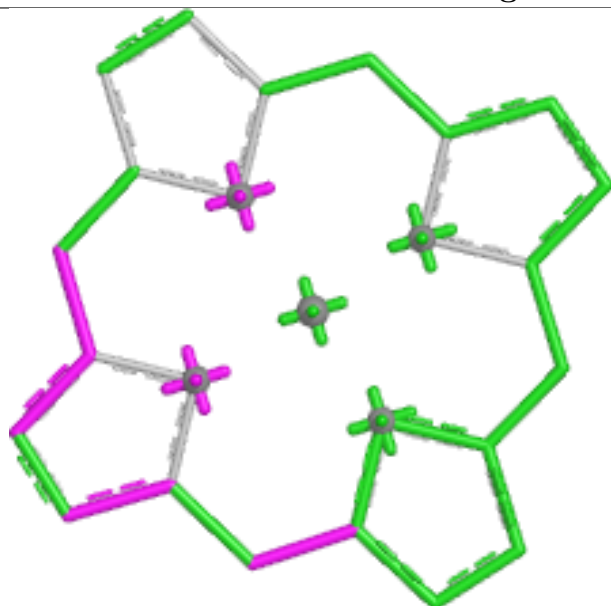


Torsions

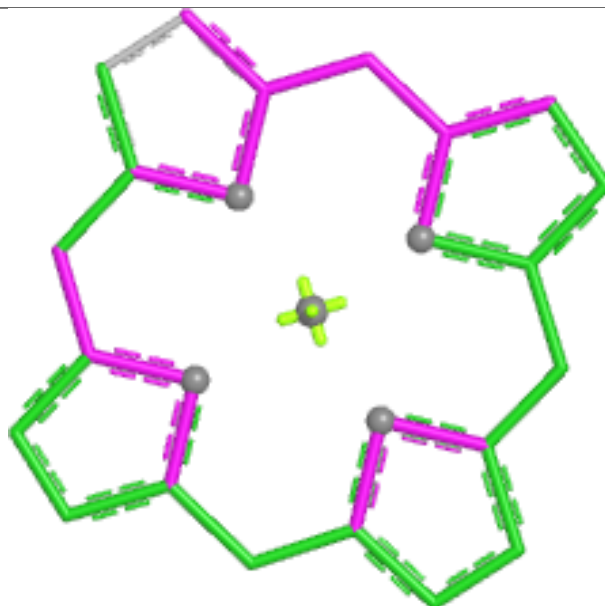


Rings

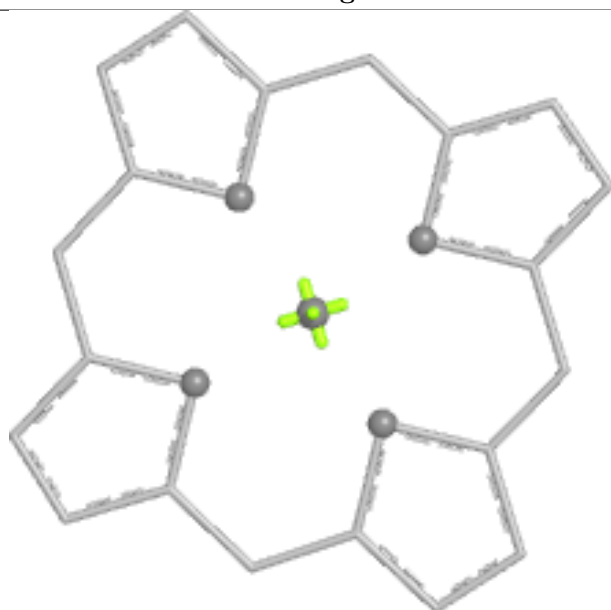
Ligand CLA W 5801



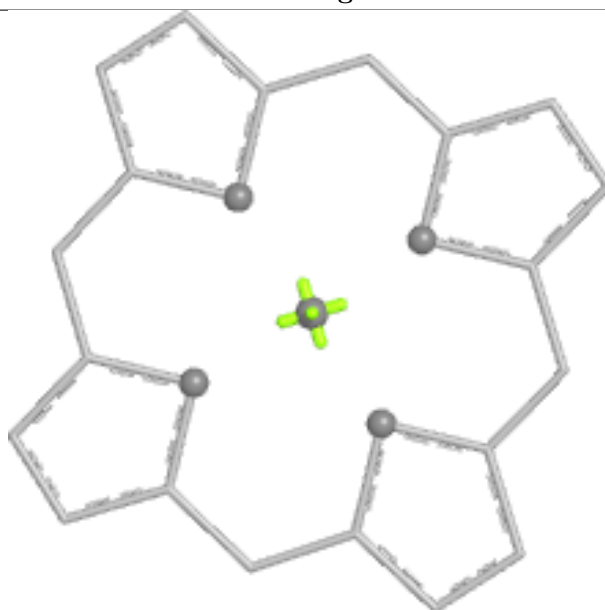
Bond lengths



Bond angles

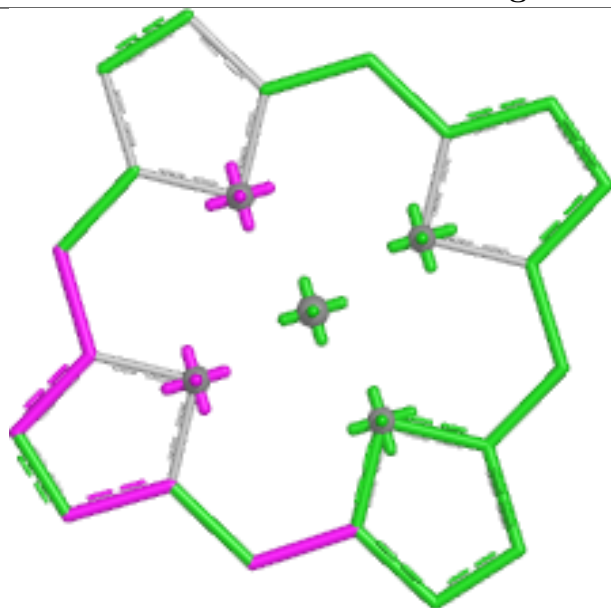


Torsions

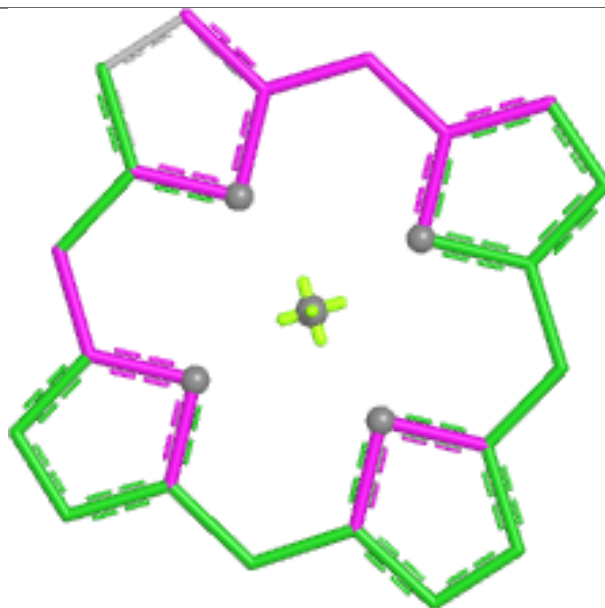


Rings

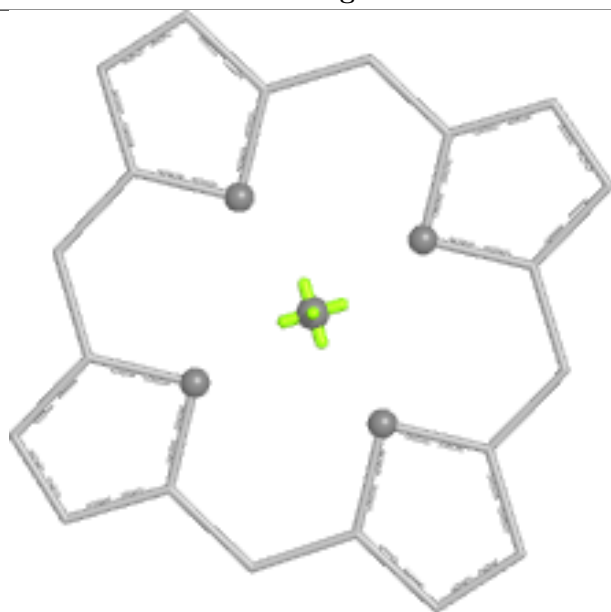
Ligand CLA 8 1022



Bond lengths



Bond angles

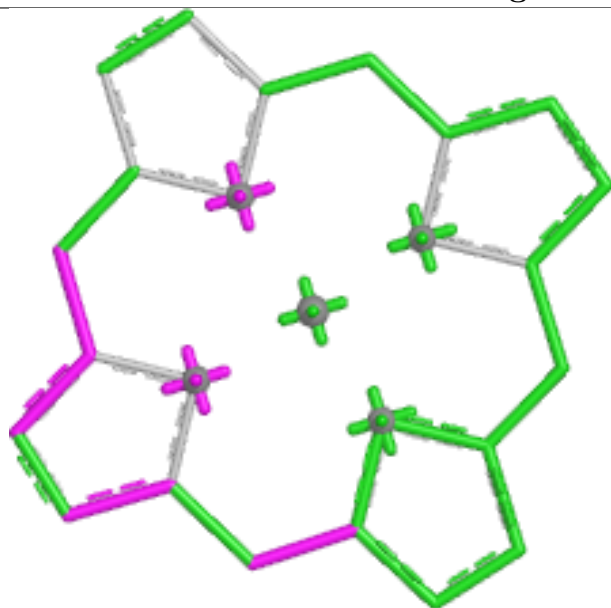


Torsions



Rings

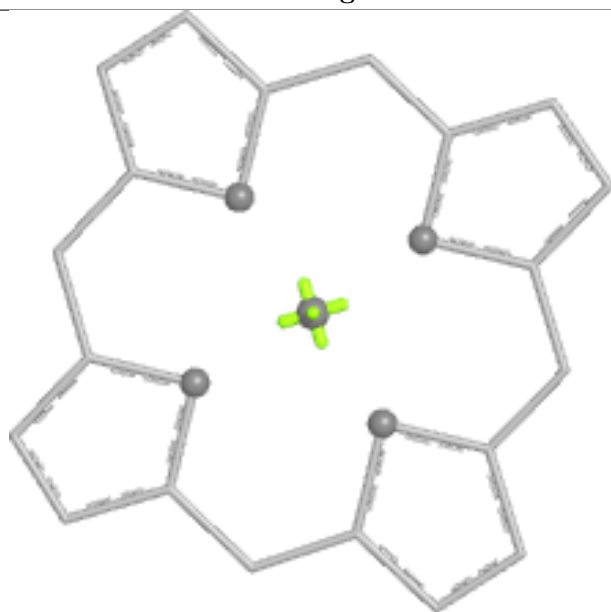
Ligand CLA 4 1011



Bond lengths



Bond angles

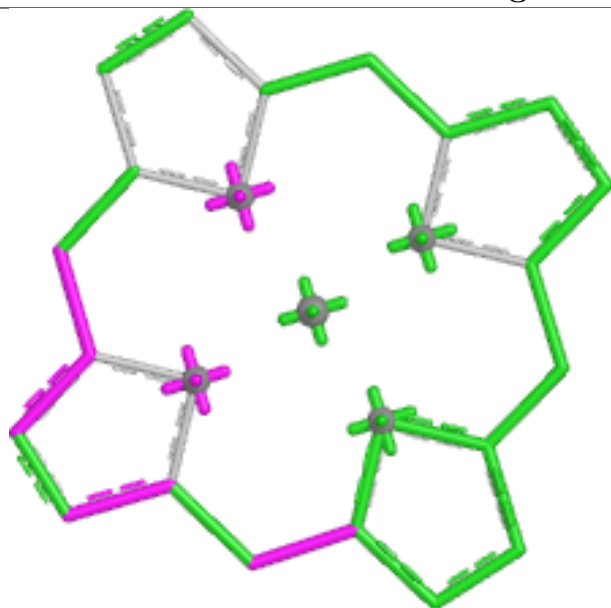


Torsions

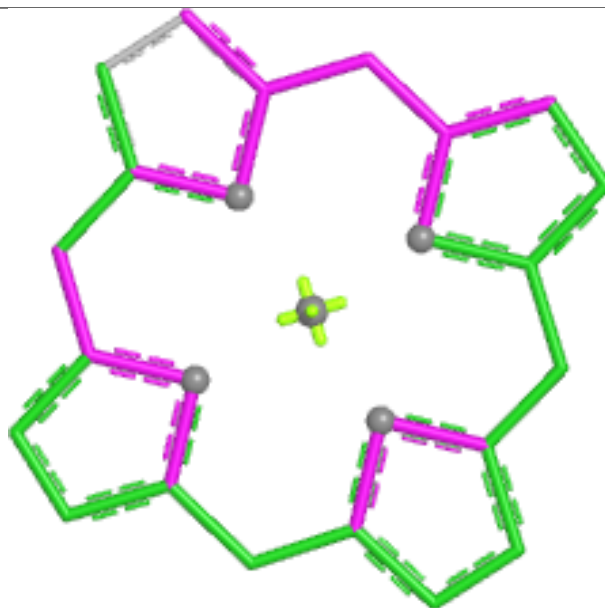


Rings

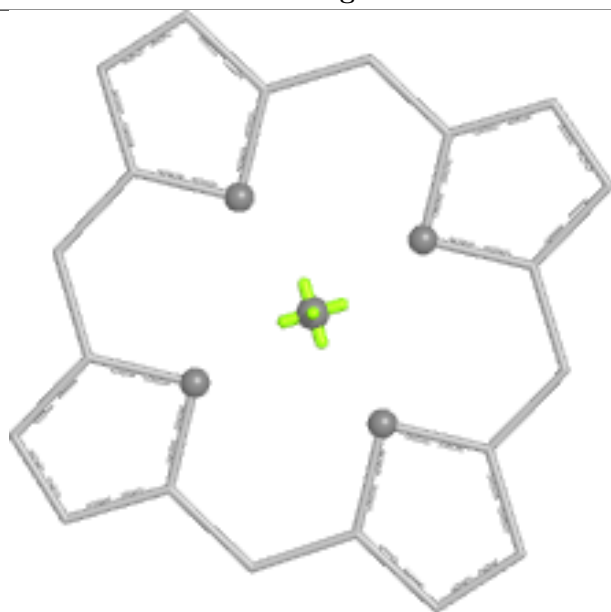
Ligand CLA 1 1025



Bond lengths



Bond angles

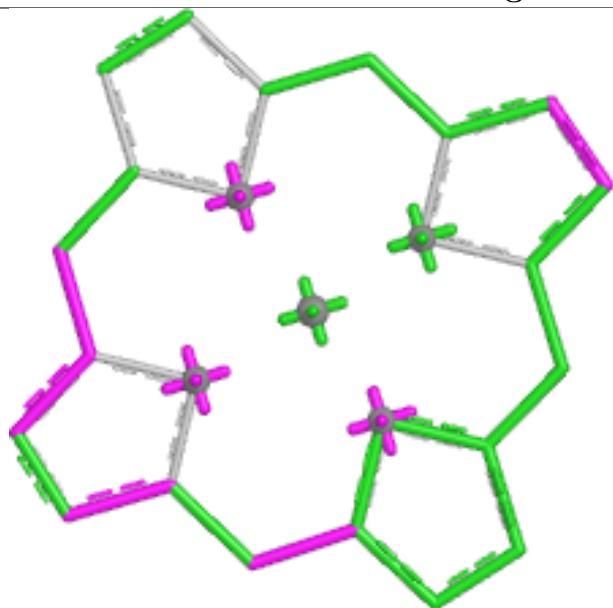


Torsions

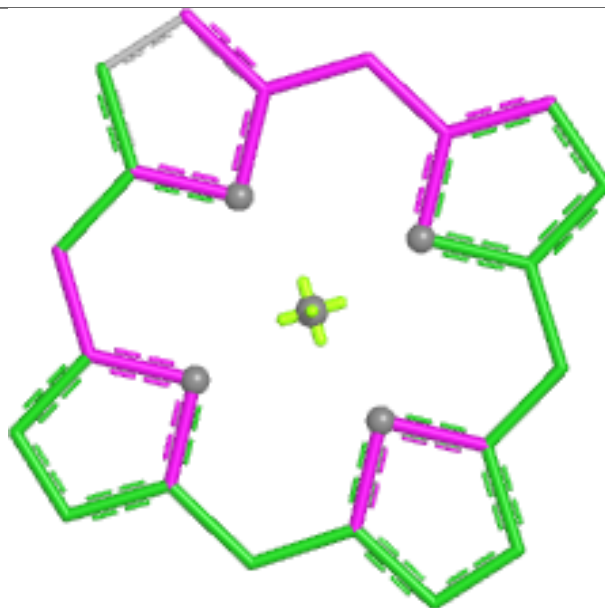


Rings

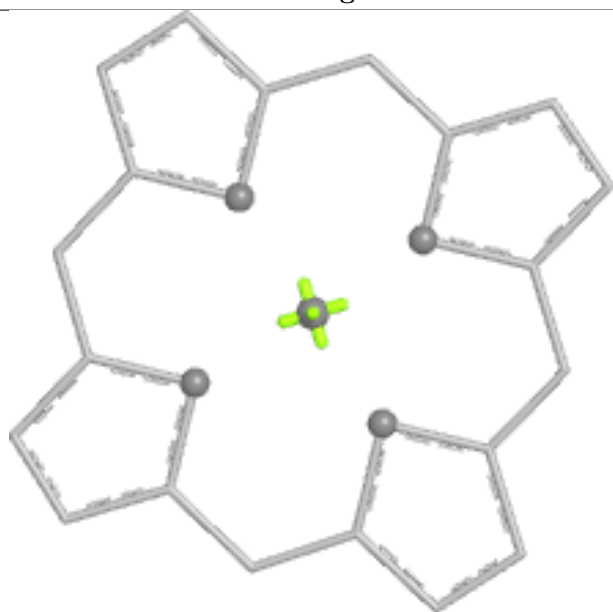
Ligand CLA B 1232



Bond lengths



Bond angles

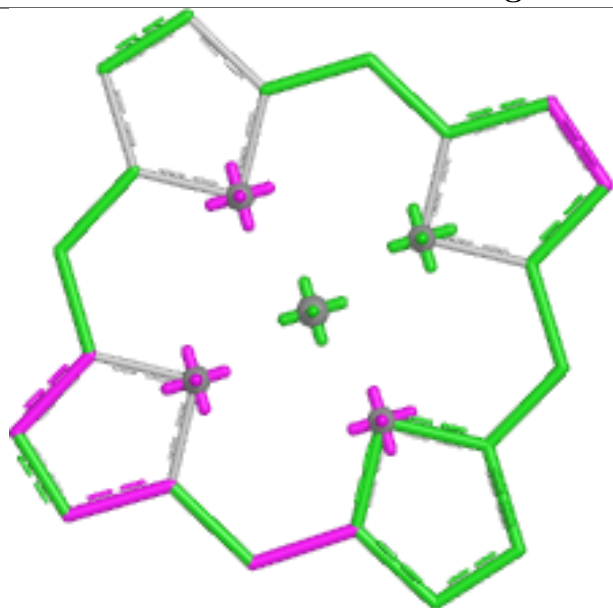


Torsions

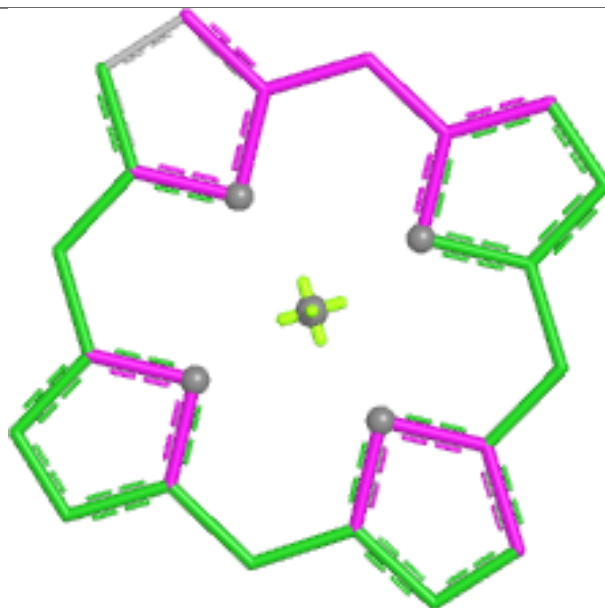


Rings

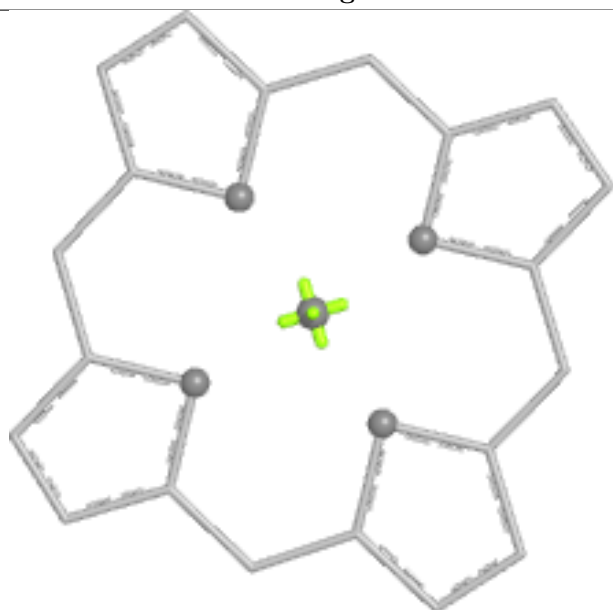
Ligand CLA A 1116



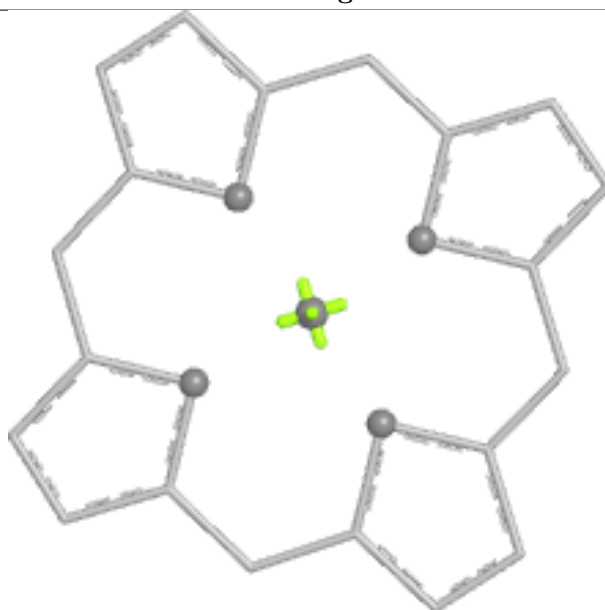
Bond lengths



Bond angles

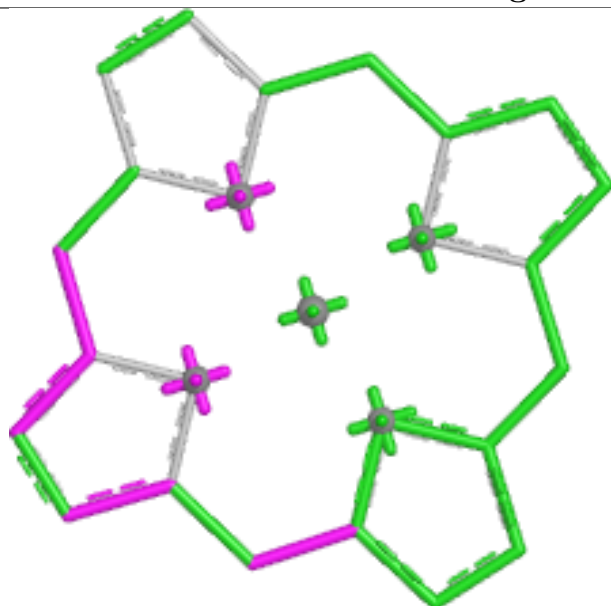


Torsions

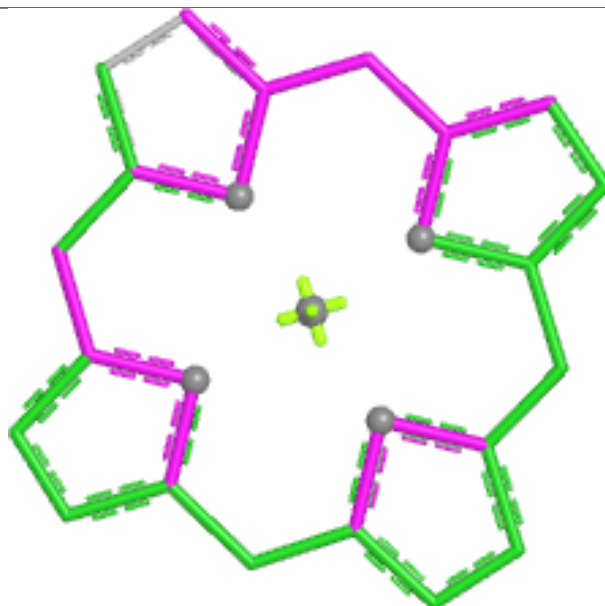


Rings

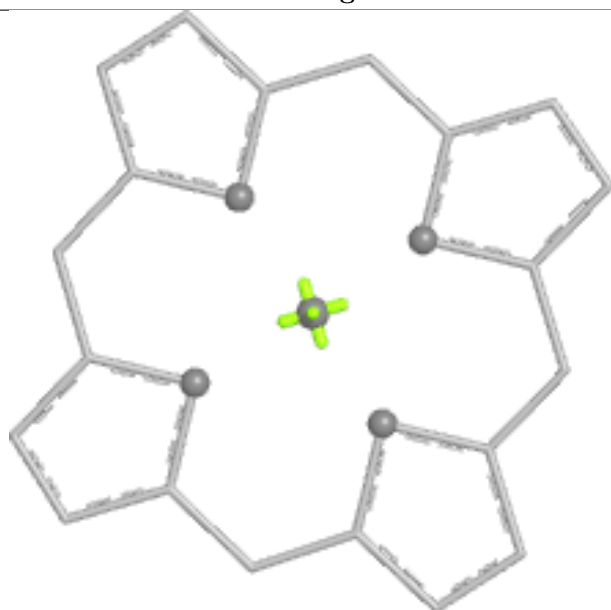
Ligand CLA 4 1025



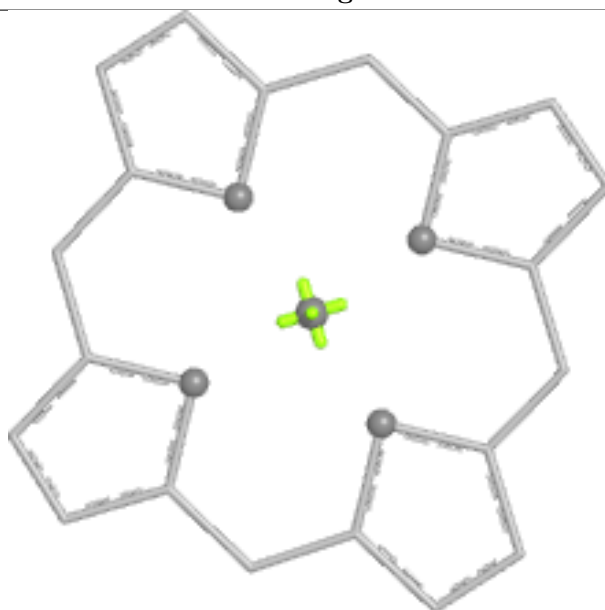
Bond lengths



Bond angles

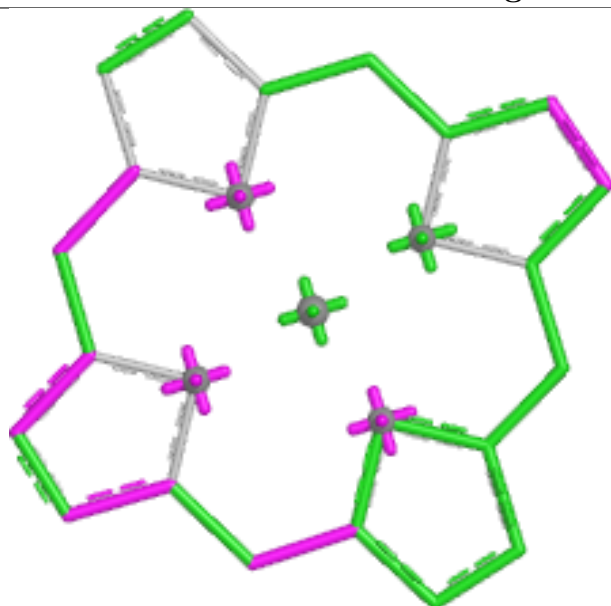


Torsions

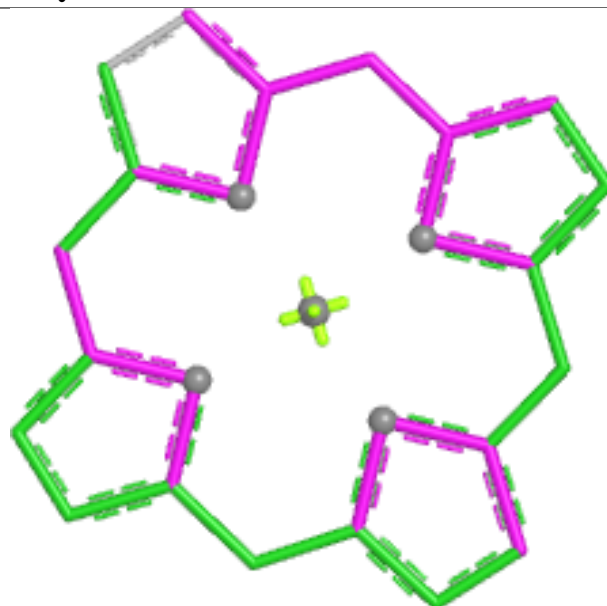


Rings

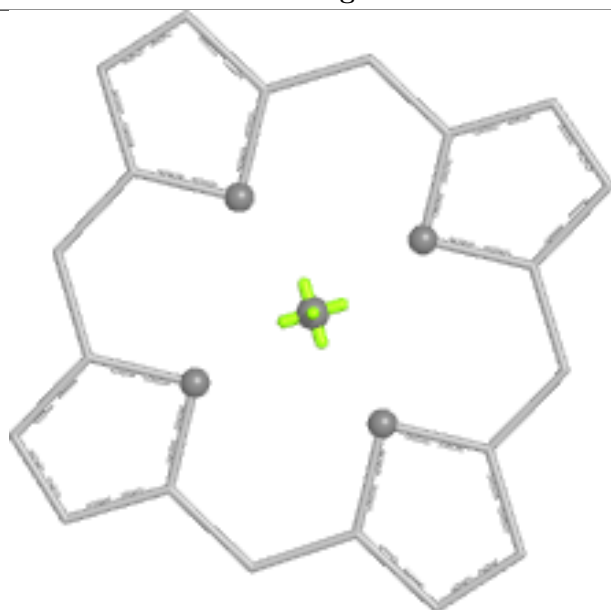
Ligand CLA Q 5219



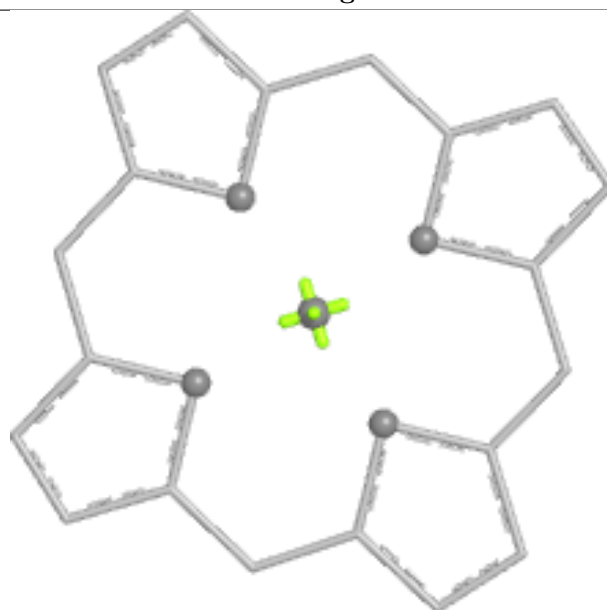
Bond lengths



Bond angles

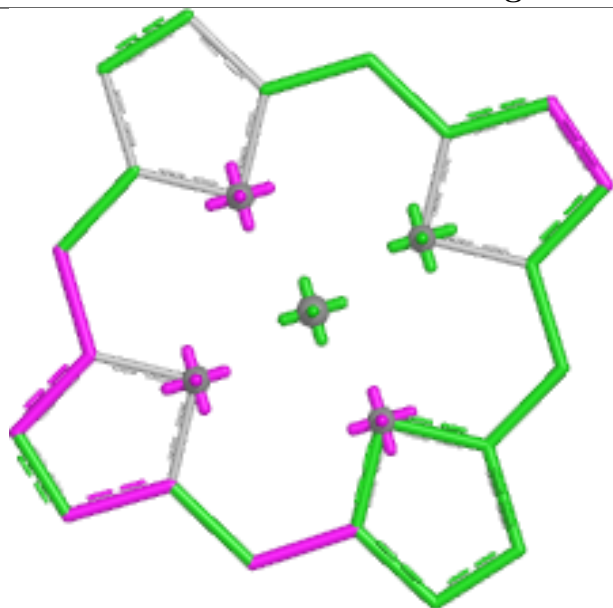


Torsions

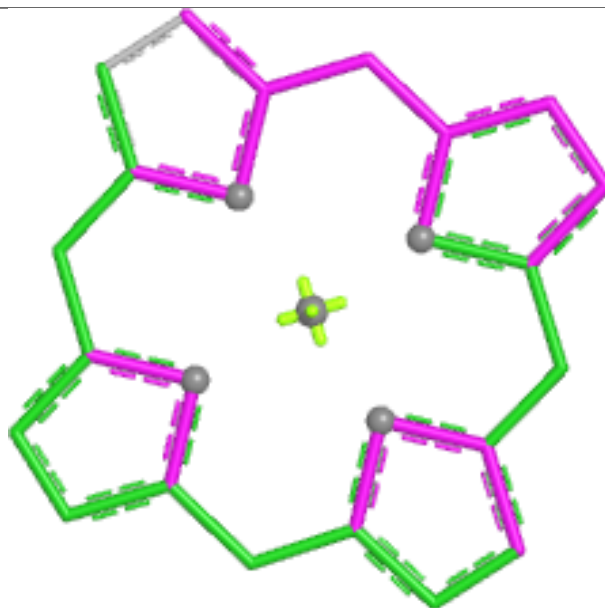


Rings

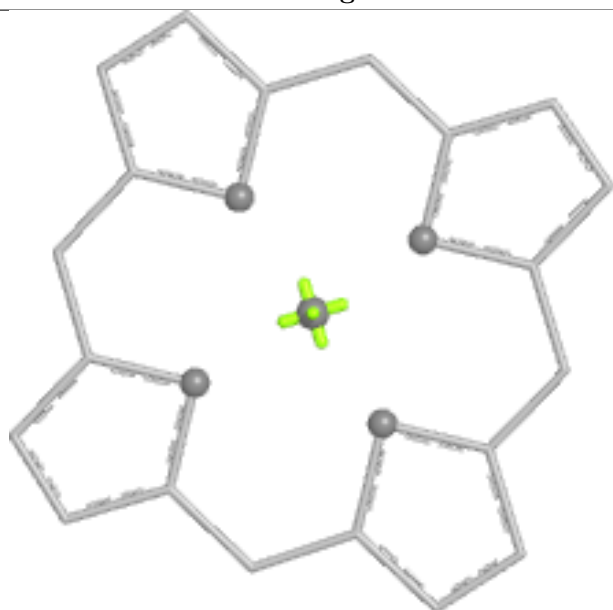
Ligand CLA A 1111



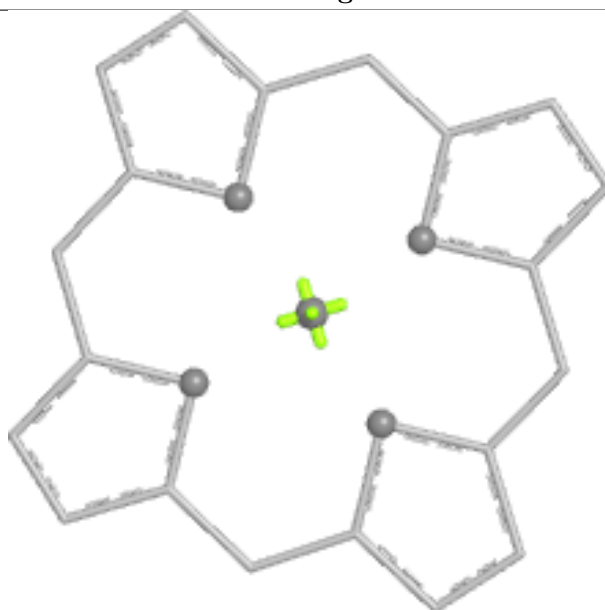
Bond lengths



Bond angles

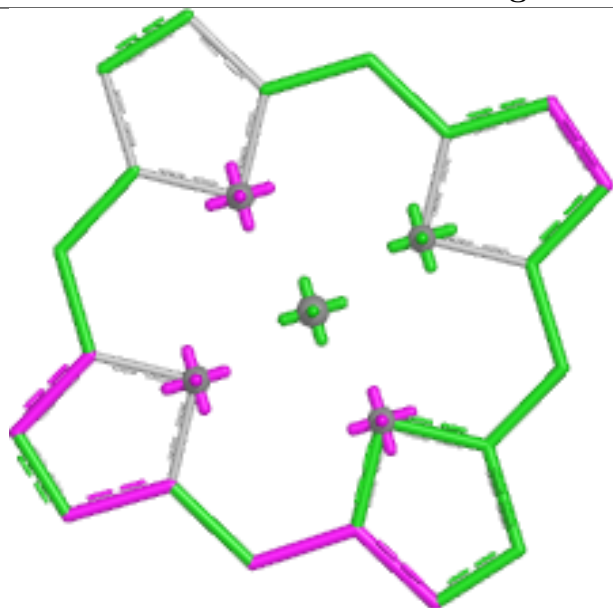


Torsions

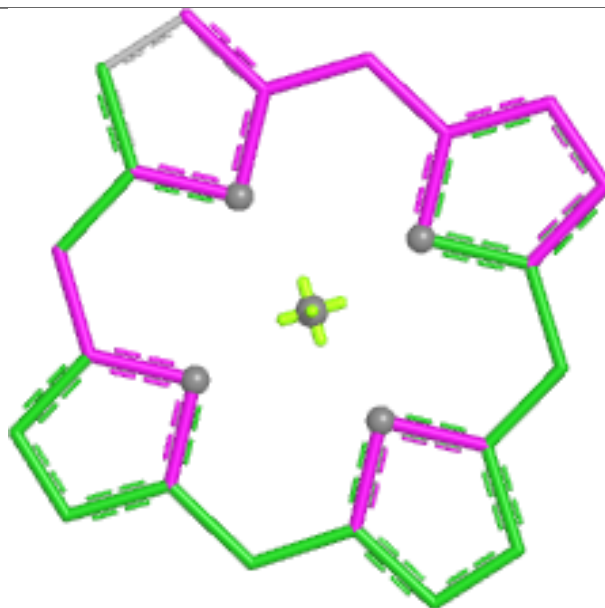


Rings

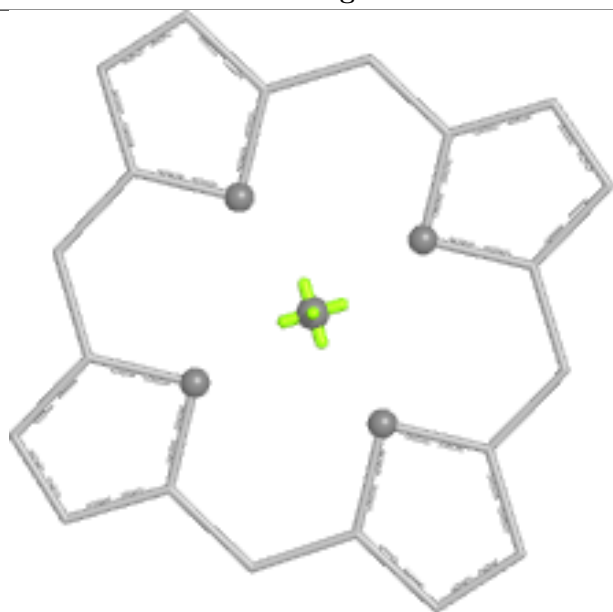
Ligand CLA 6 5501



Bond lengths



Bond angles

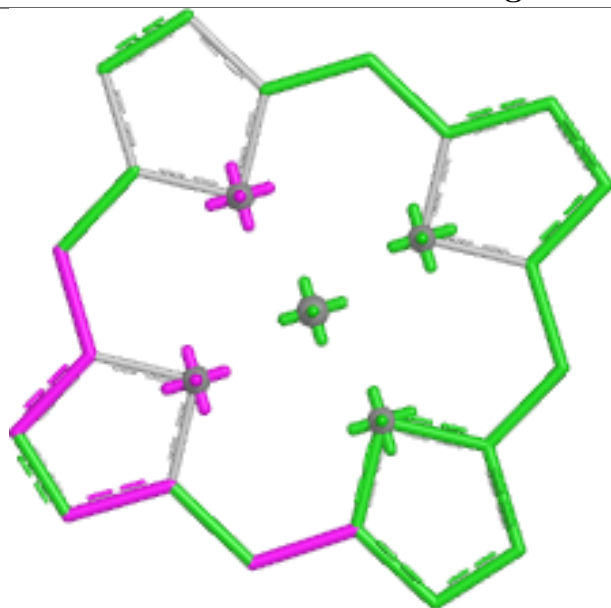


Torsions



Rings

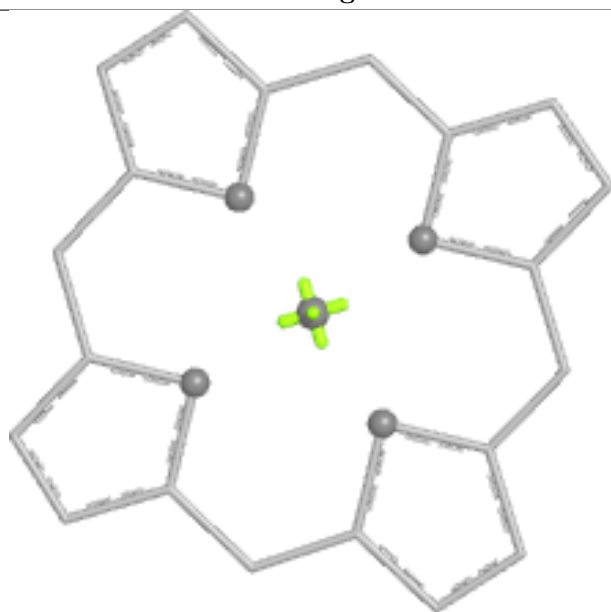
Ligand CLA A 4010



Bond lengths



Bond angles

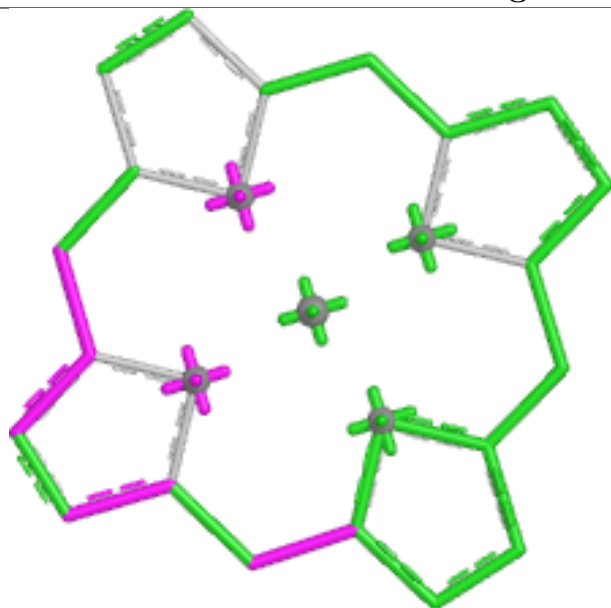


Torsions

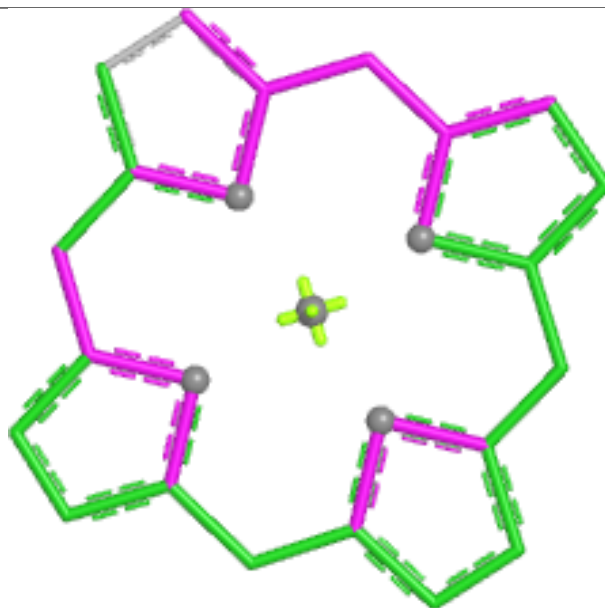


Rings

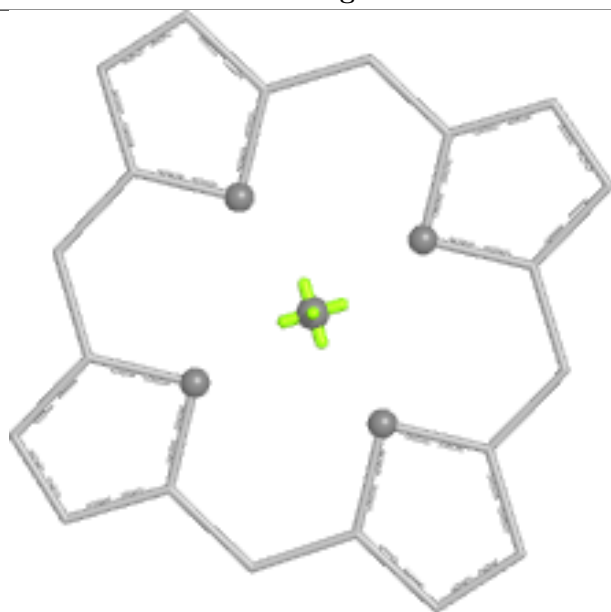
Ligand CLA 1 1023



Bond lengths



Bond angles

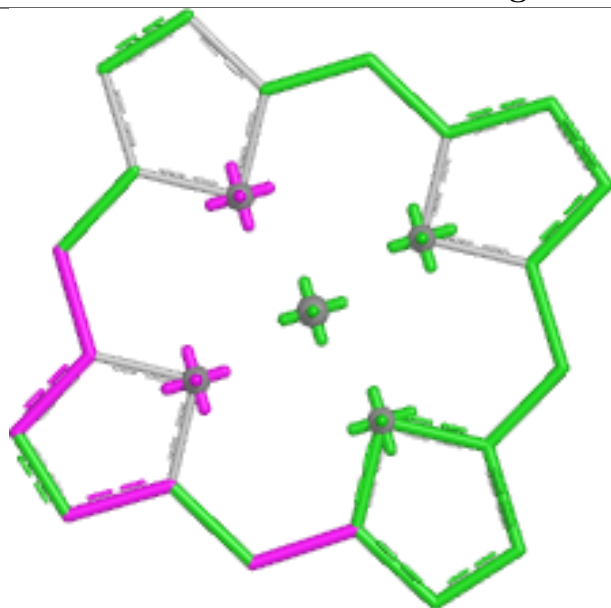


Torsions

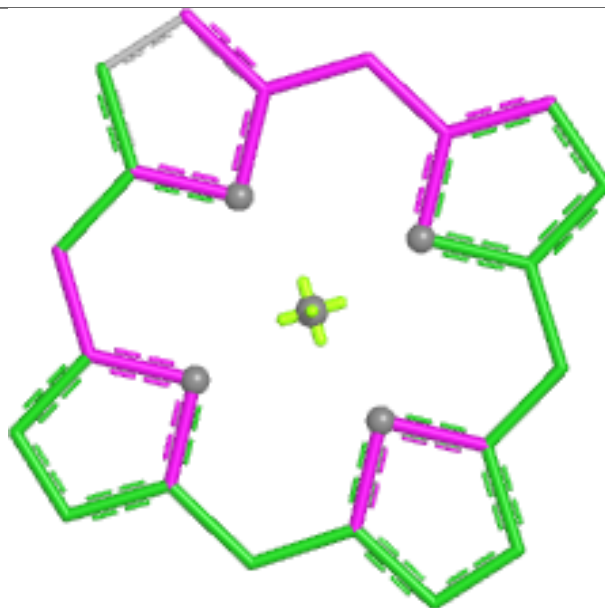


Rings

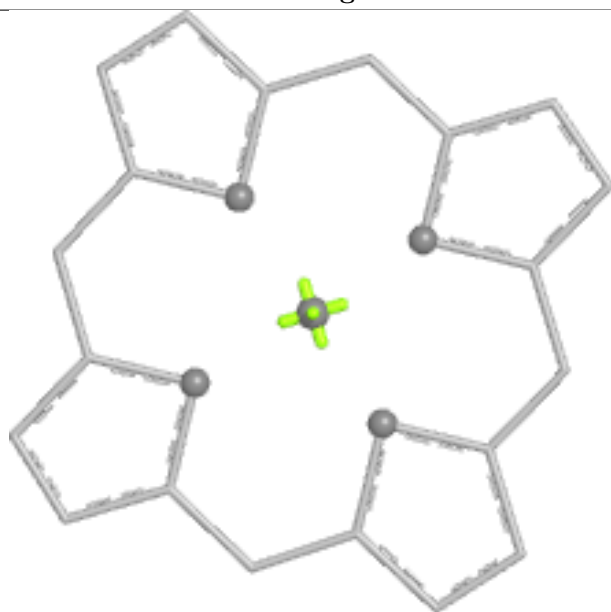
Ligand CLA 4 1023



Bond lengths



Bond angles

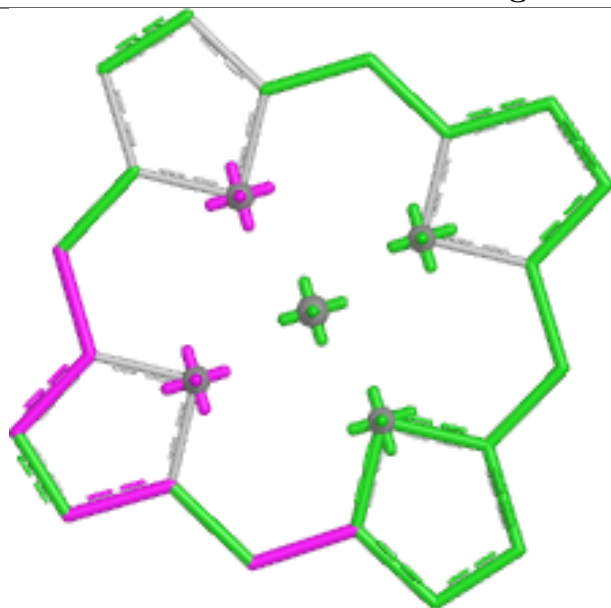


Torsions

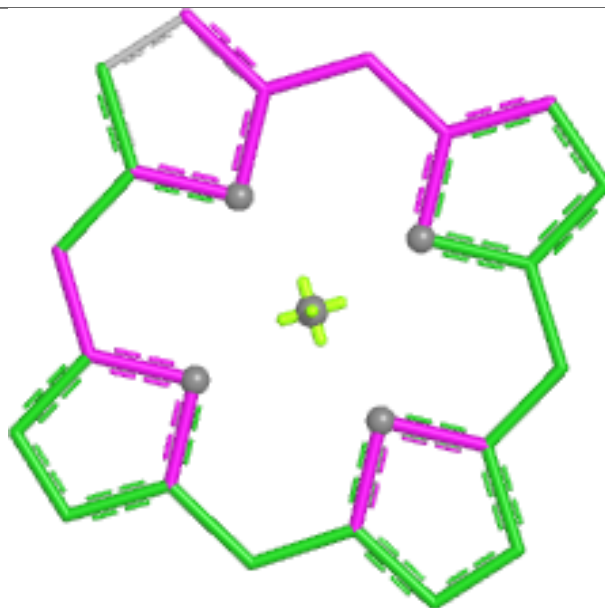


Rings

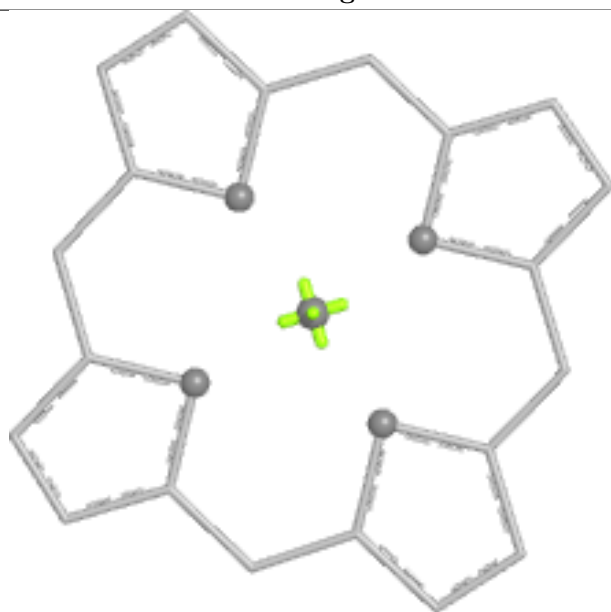
Ligand CLA 7 1026



Bond lengths



Bond angles

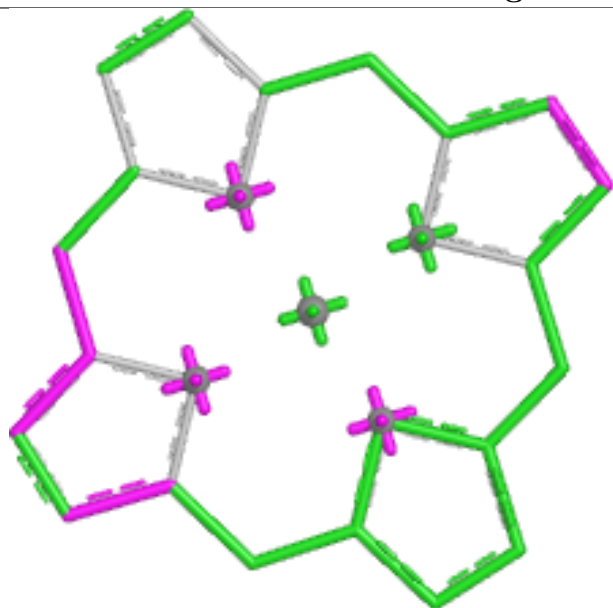


Torsions

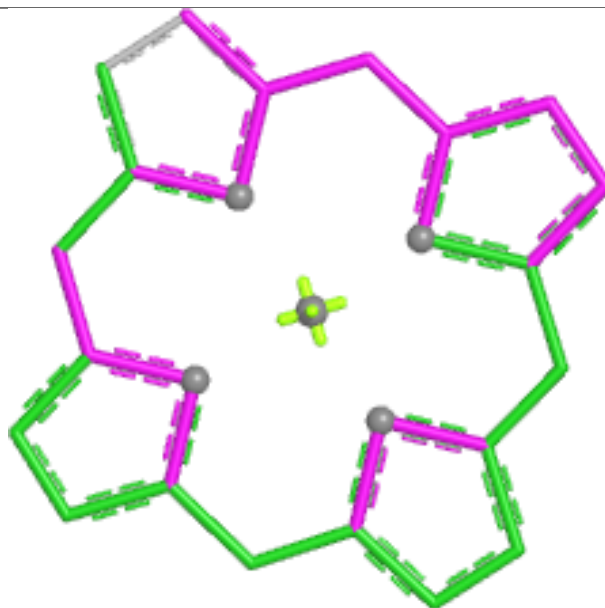


Rings

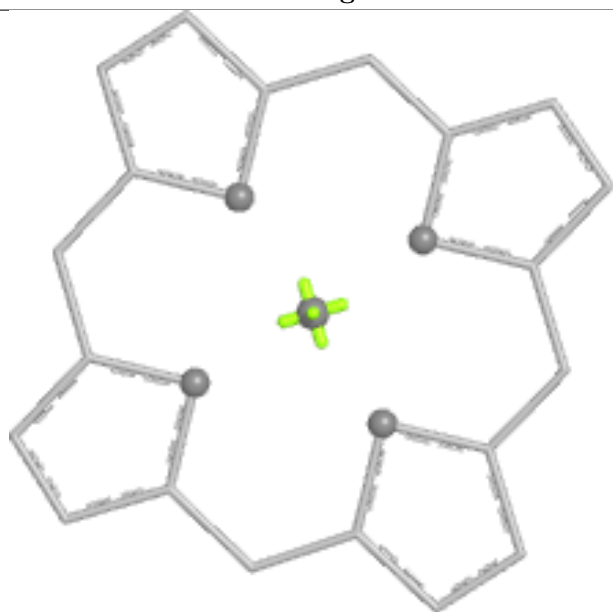
Ligand CLA B 1225



Bond lengths



Bond angles

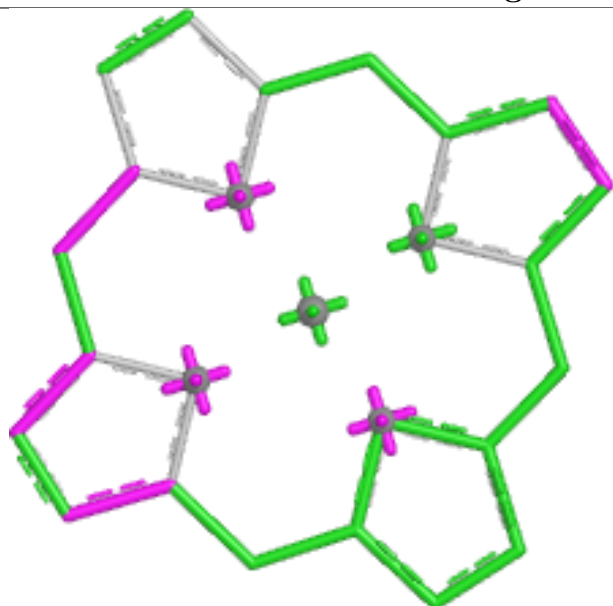


Torsions

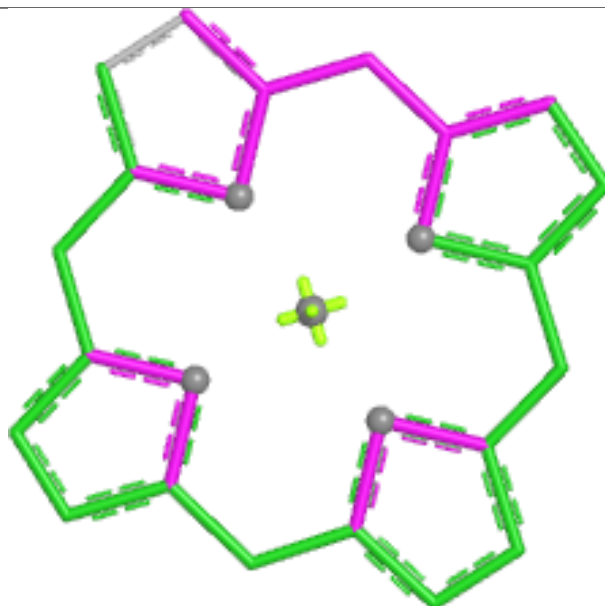


Rings

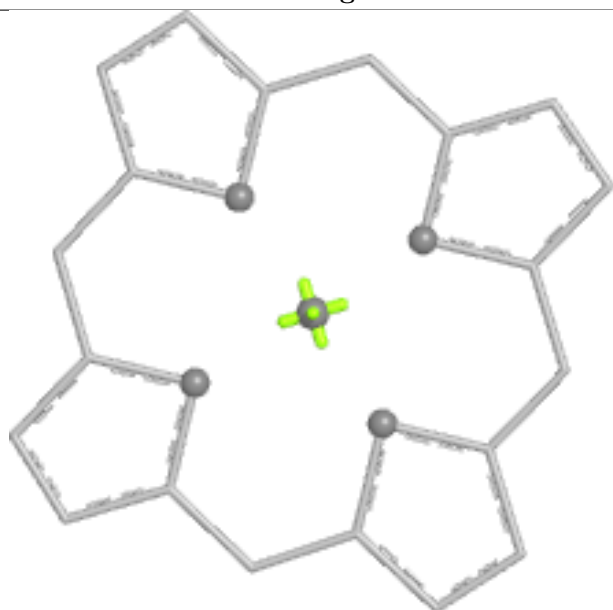
Ligand CLA A 1139



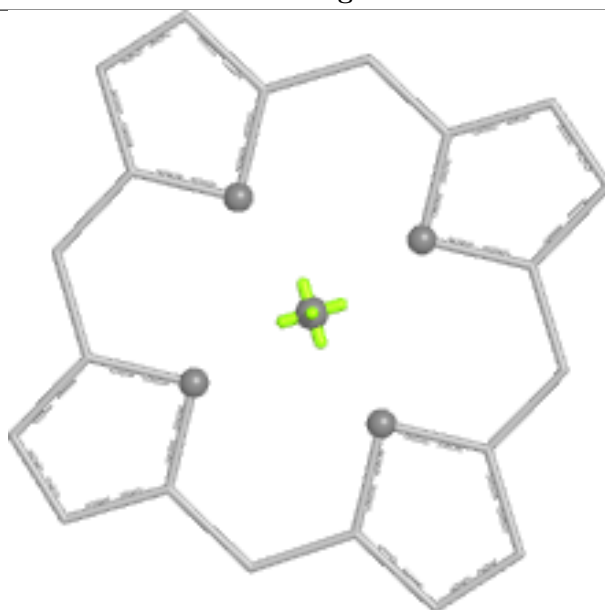
Bond lengths



Bond angles

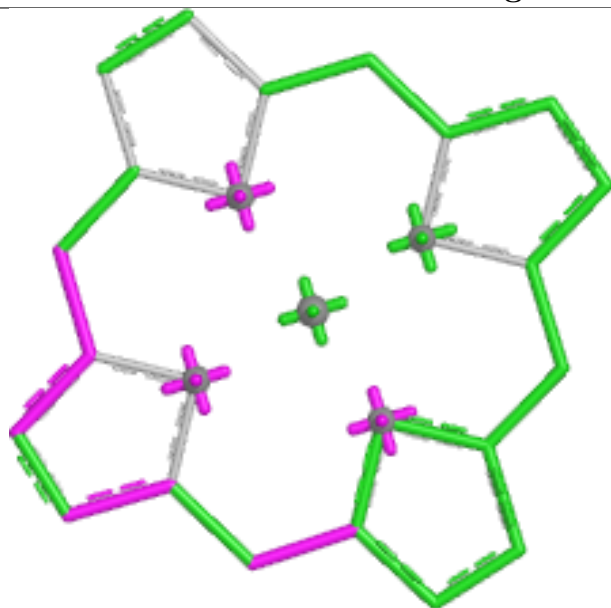


Torsions

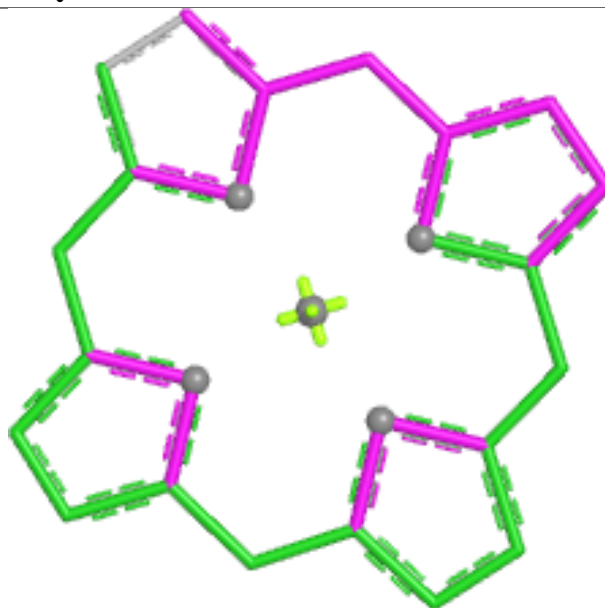


Rings

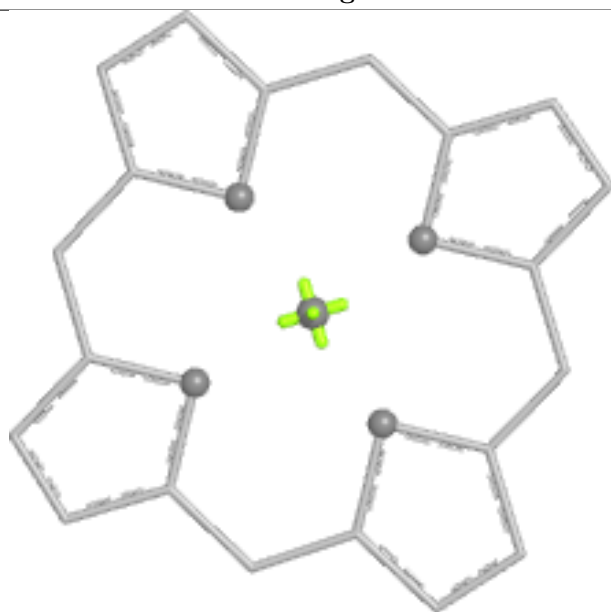
Ligand CLA Q 5236



Bond lengths



Bond angles

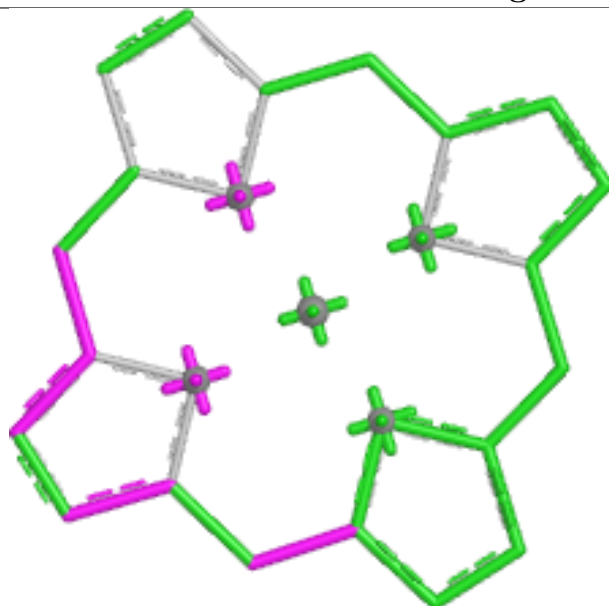


Torsions

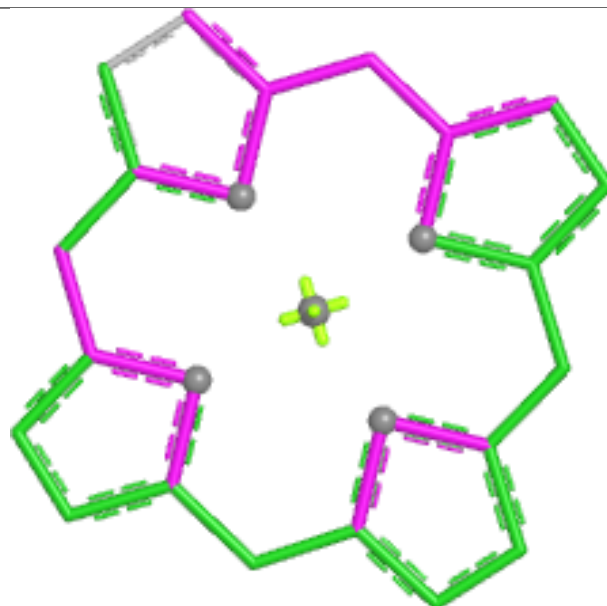


Rings

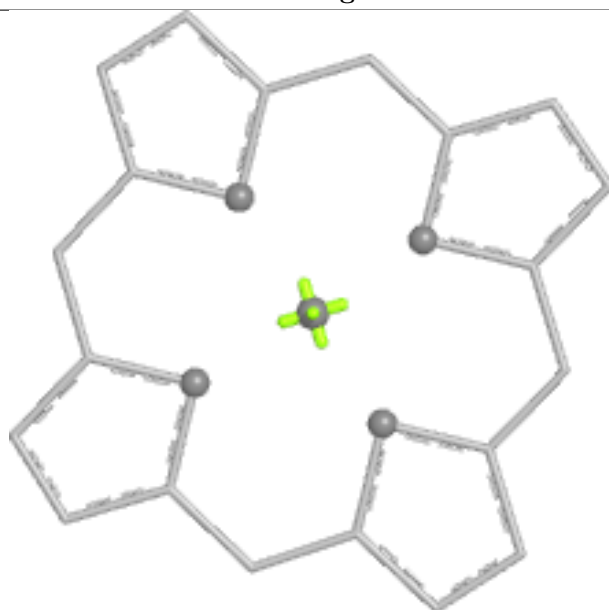
Ligand CLA 1 1014



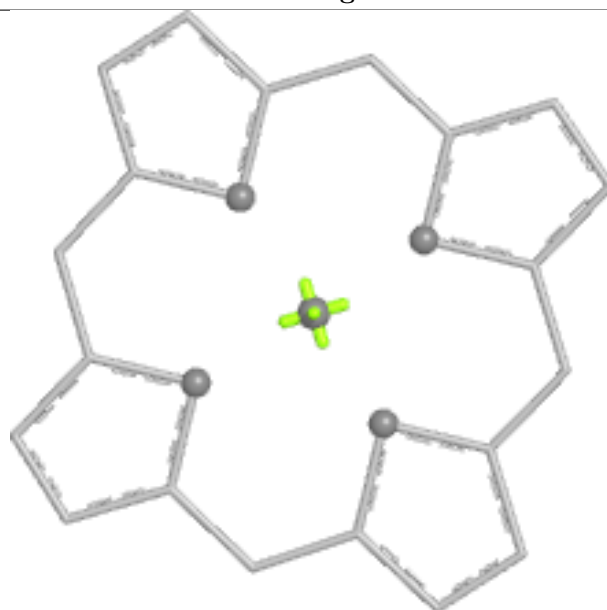
Bond lengths



Bond angles

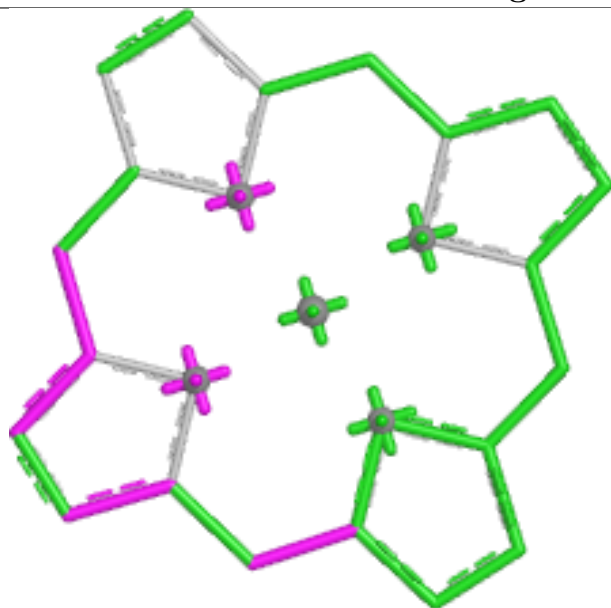


Torsions



Rings

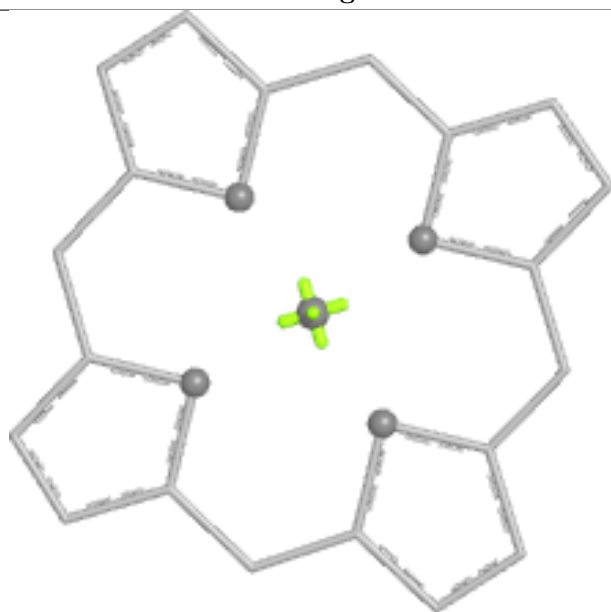
Ligand CLA 4 1012



Bond lengths



Bond angles

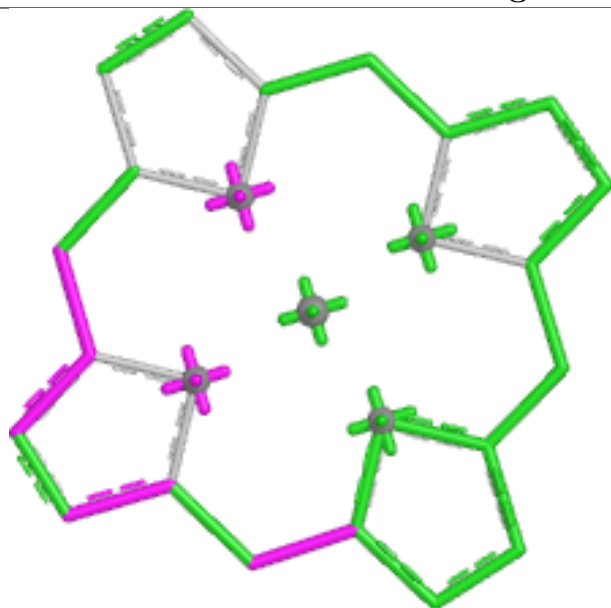


Torsions

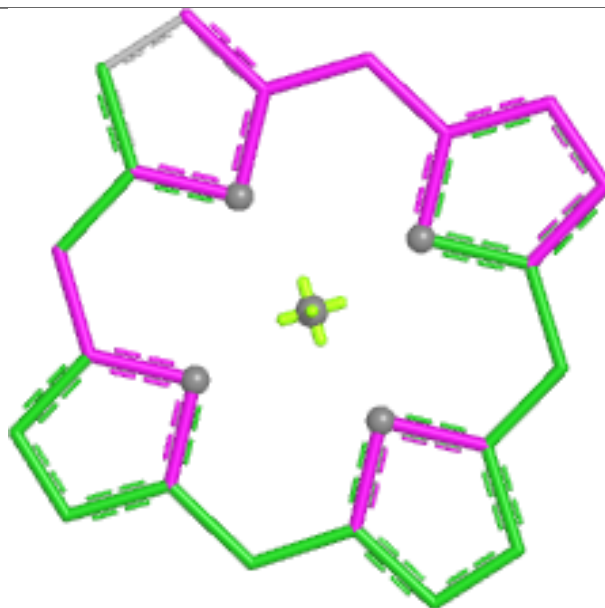


Rings

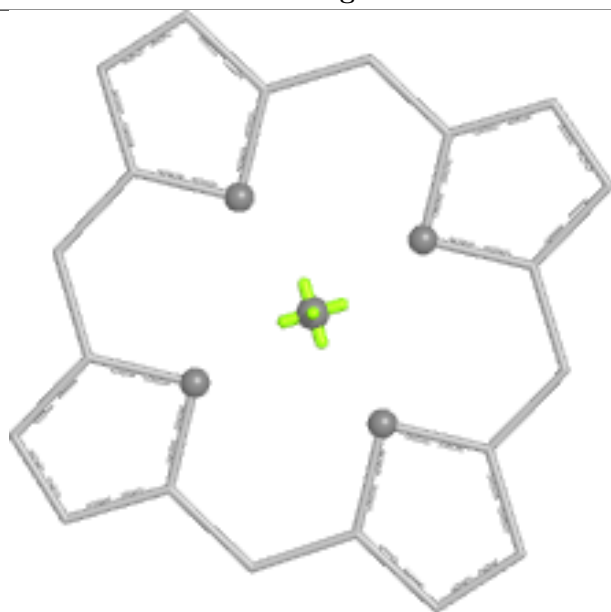
Ligand CLA 0 1016



Bond lengths



Bond angles

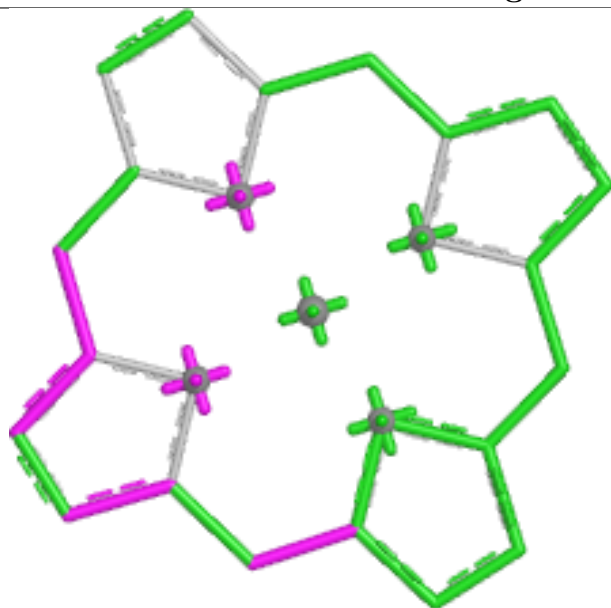


Torsions

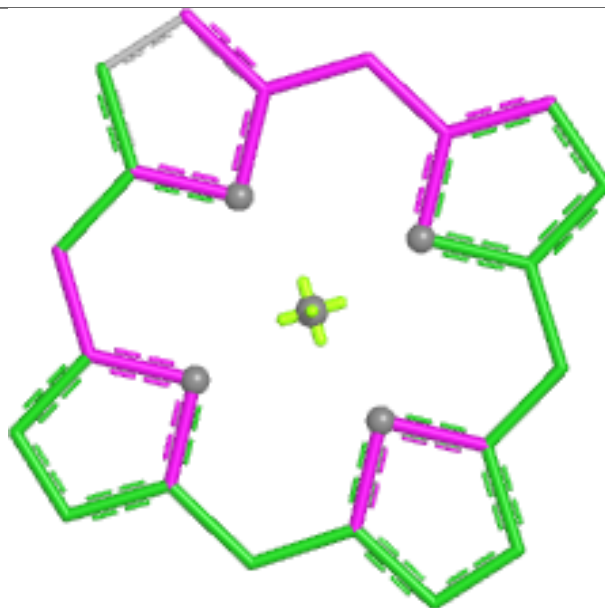


Rings

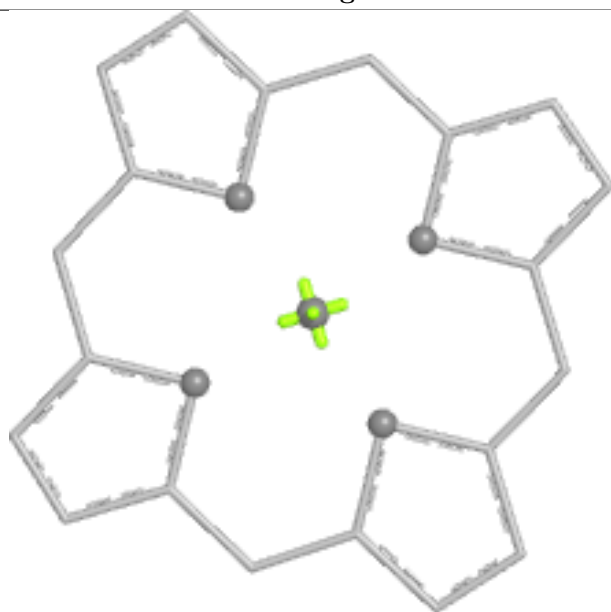
Ligand CLA B 4001



Bond lengths



Bond angles

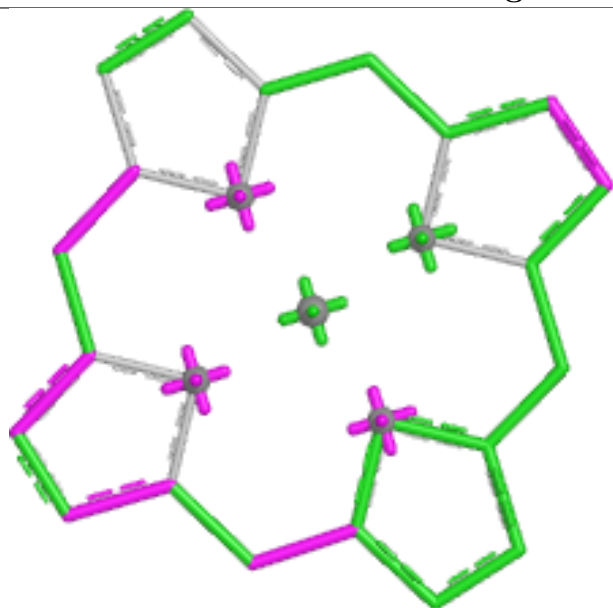


Torsions

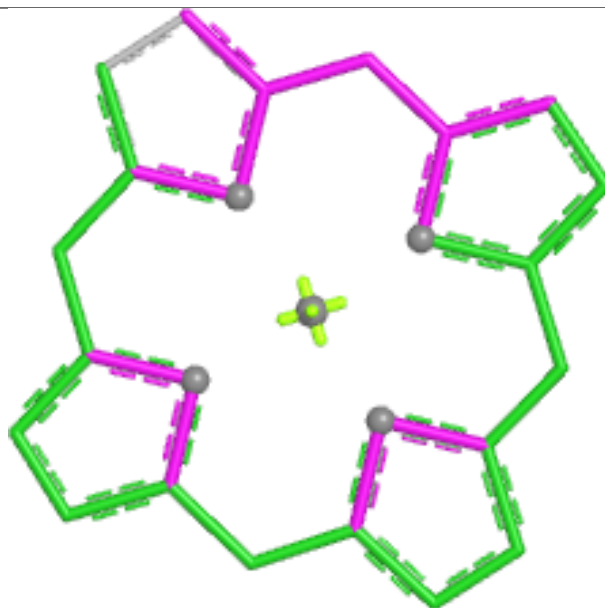


Rings

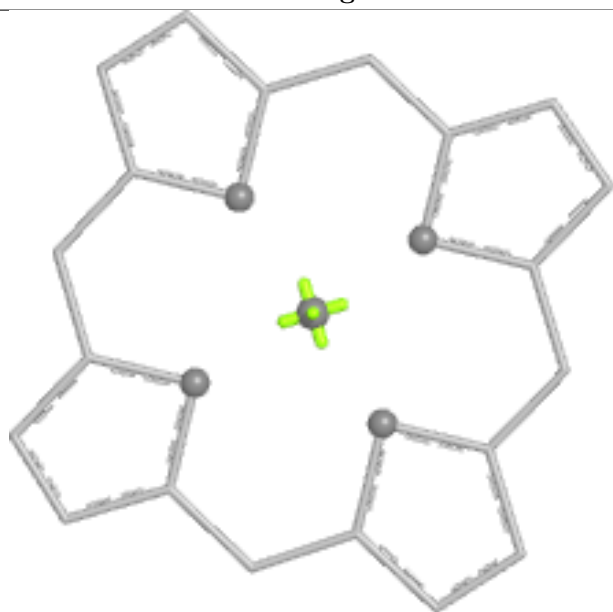
Ligand CLA B 1234



Bond lengths



Bond angles

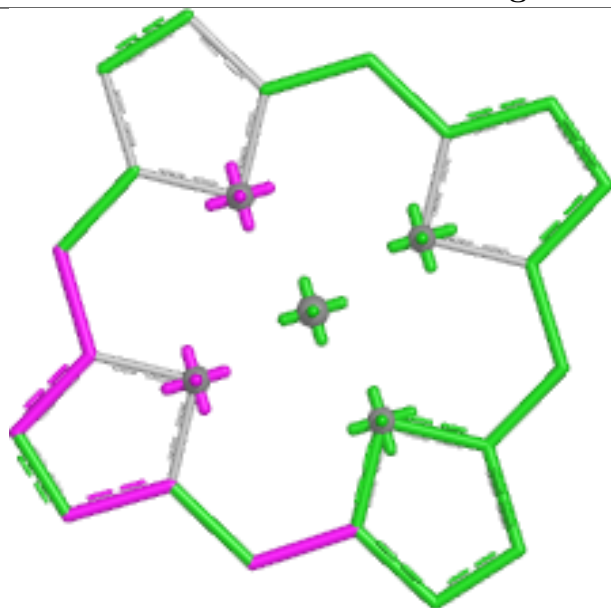


Torsions

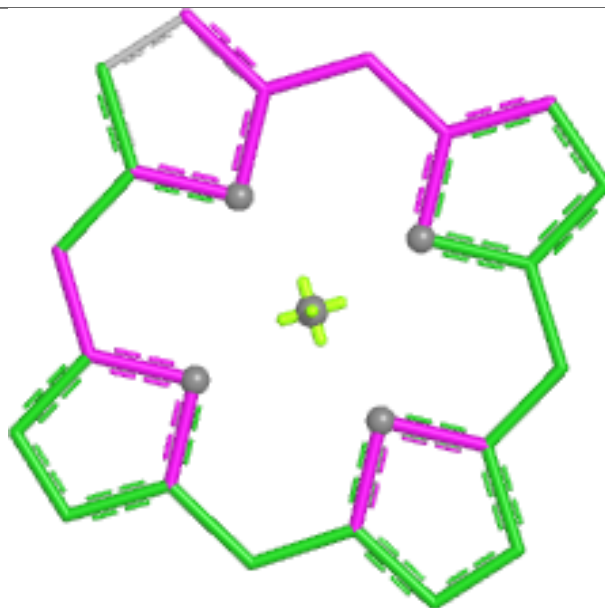


Rings

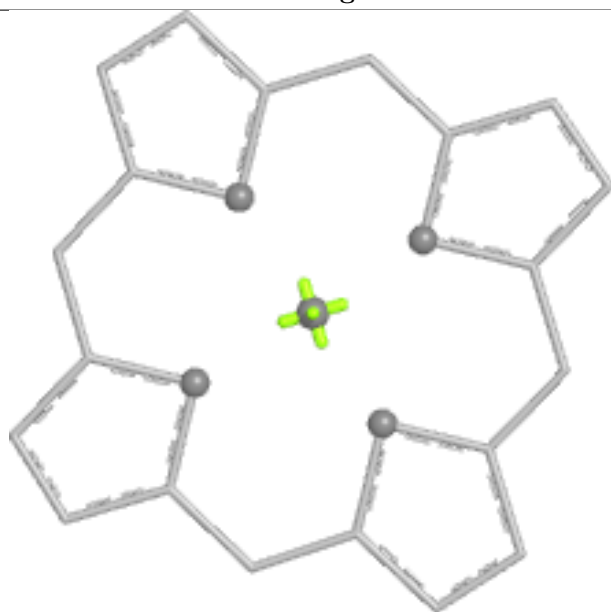
Ligand CLA 6 5504



Bond lengths



Bond angles

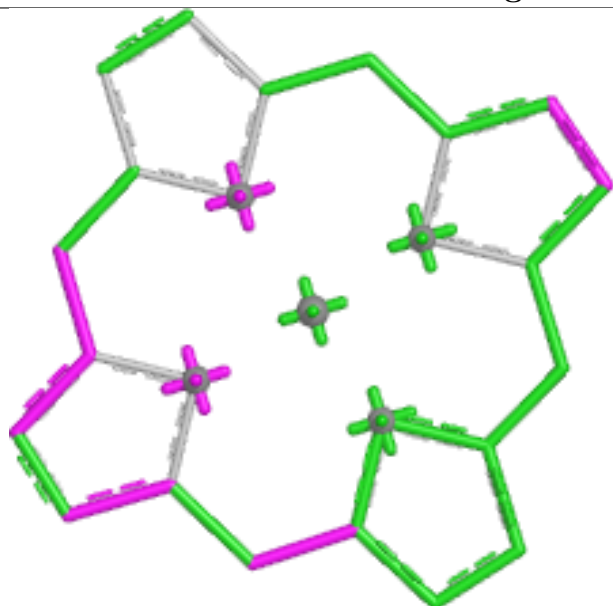


Torsions

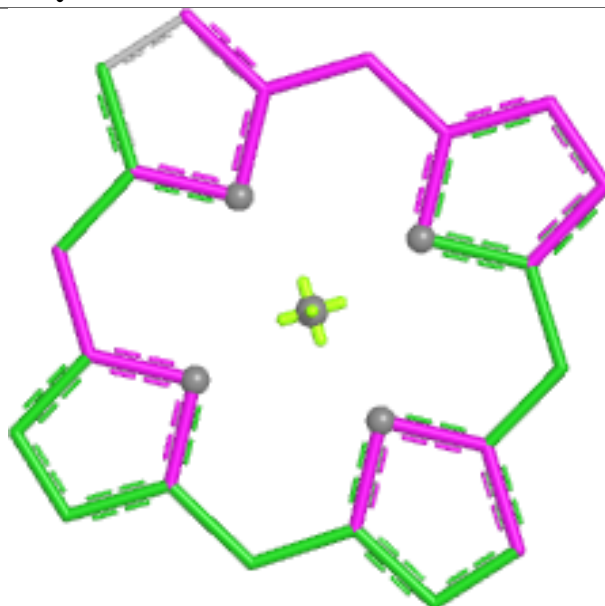


Rings

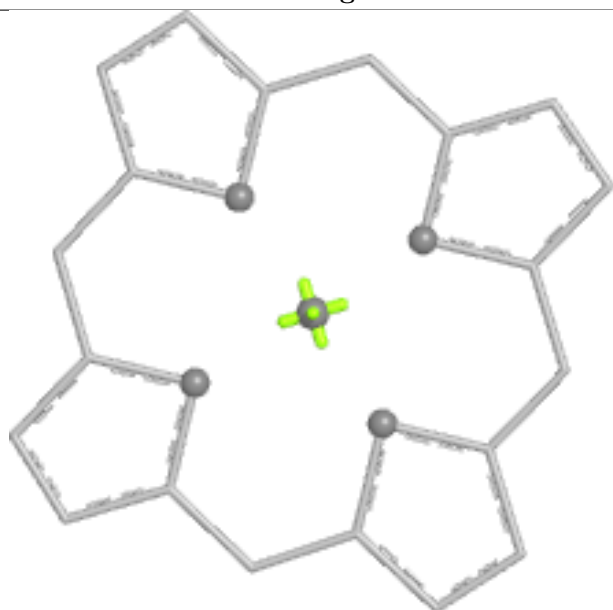
Ligand CLA Q 5227



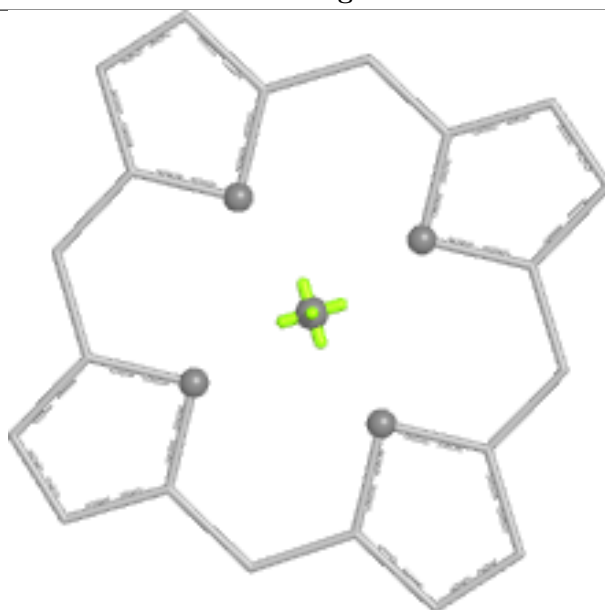
Bond lengths



Bond angles

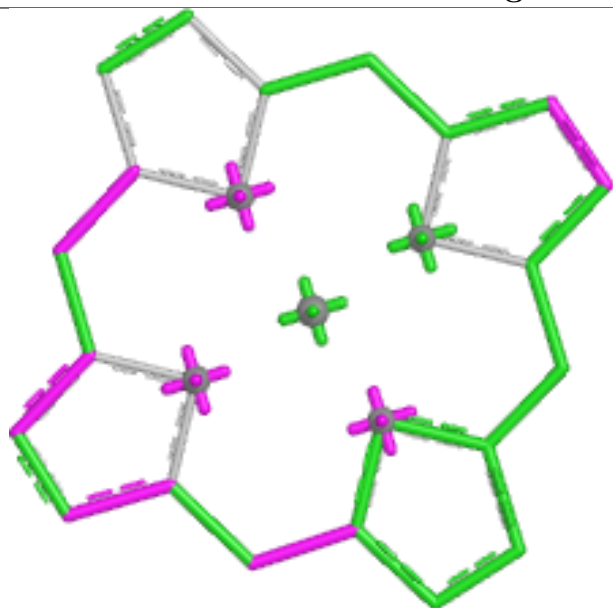


Torsions

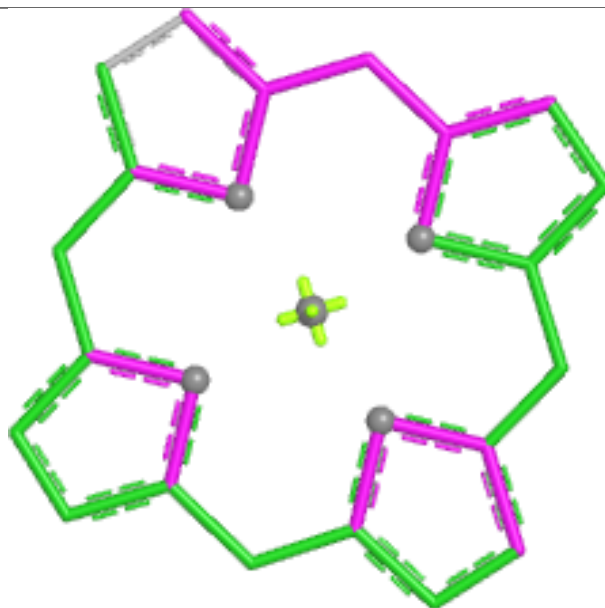


Rings

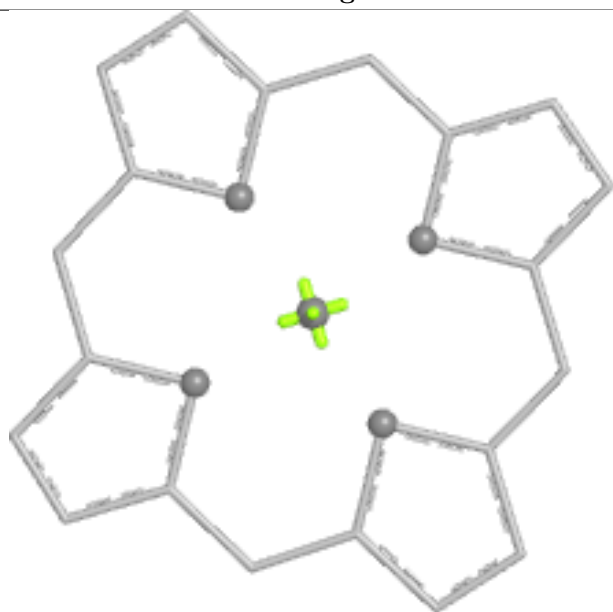
Ligand CLA B 1209



Bond lengths



Bond angles

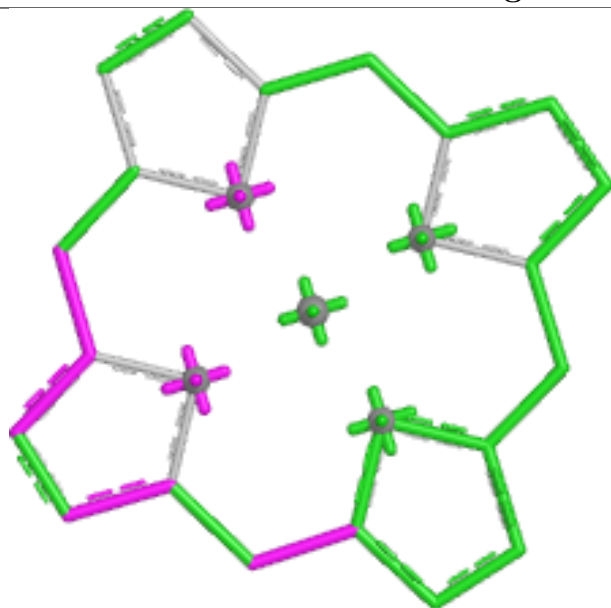


Torsions

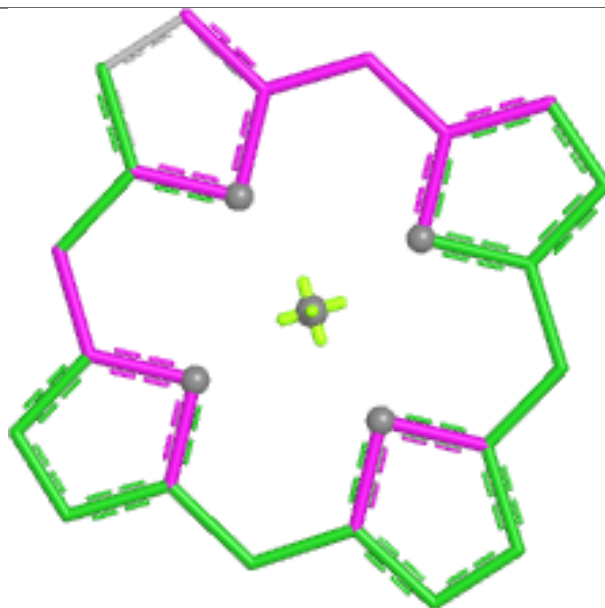


Rings

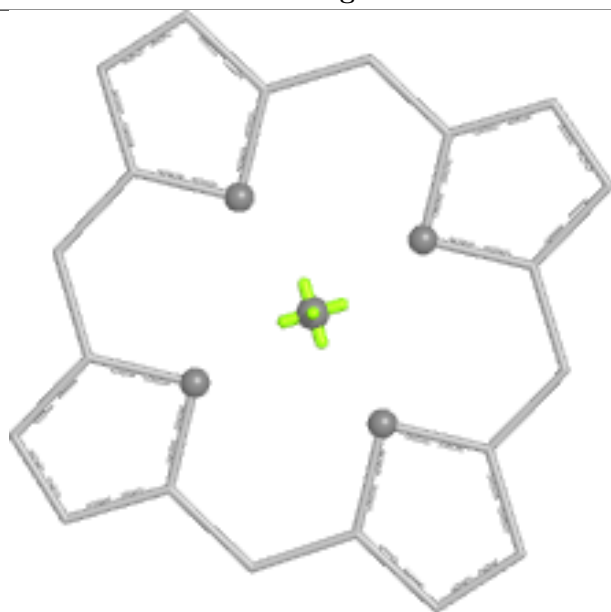
Ligand CLA H 1801



Bond lengths



Bond angles

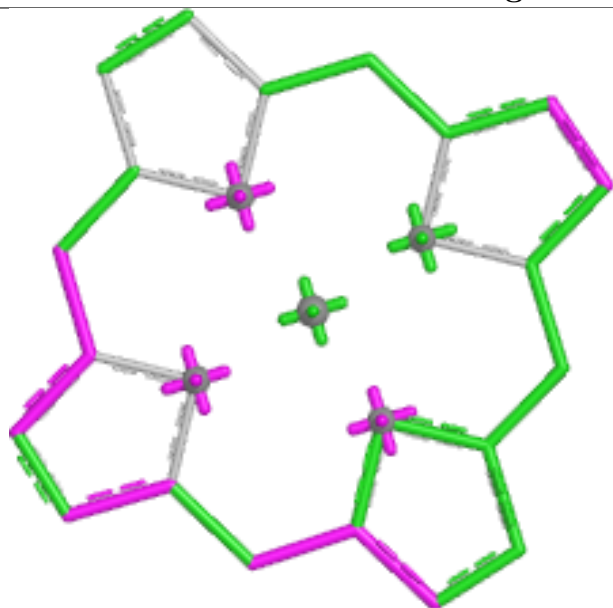


Torsions



Rings

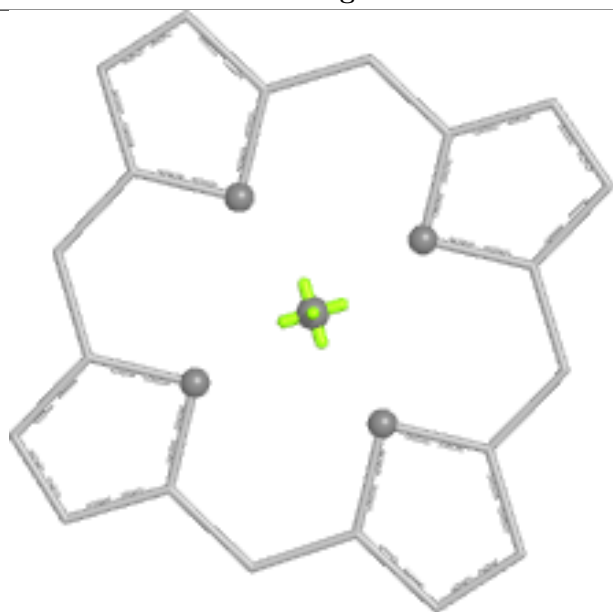
Ligand CLA B 1221



Bond lengths



Bond angles

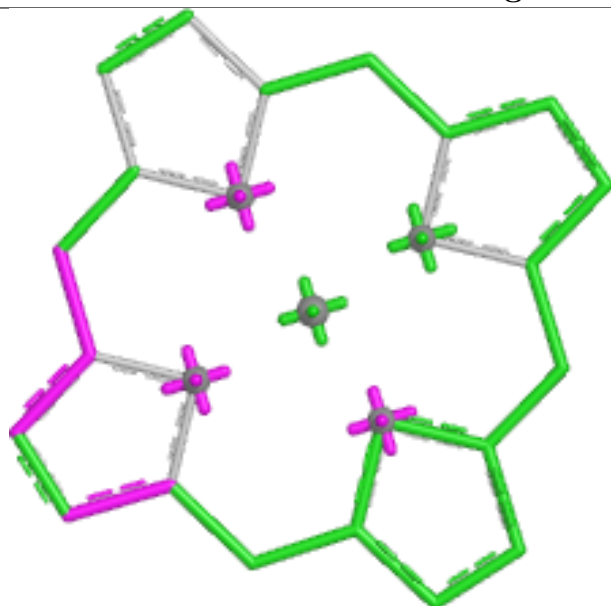


Torsions

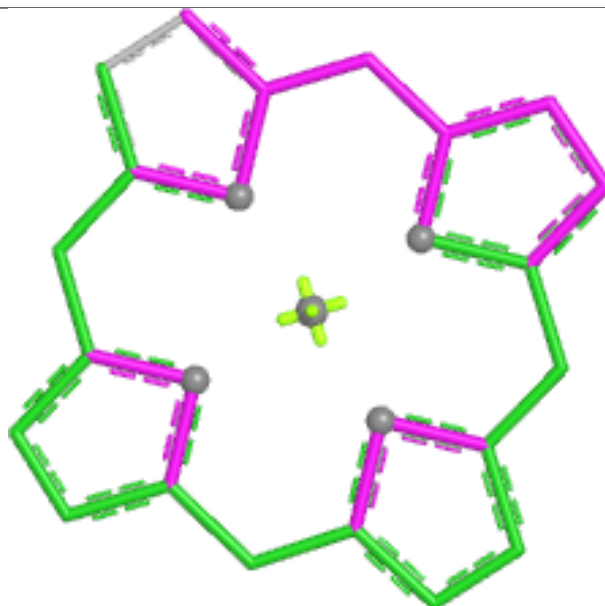


Rings

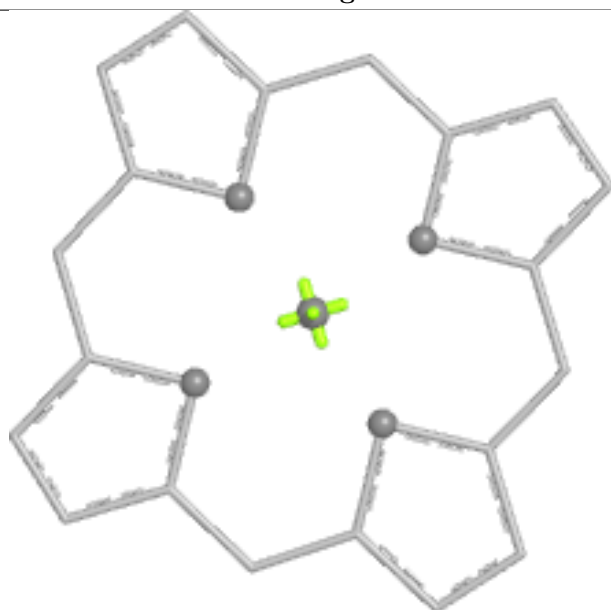
Ligand CLA A 1124



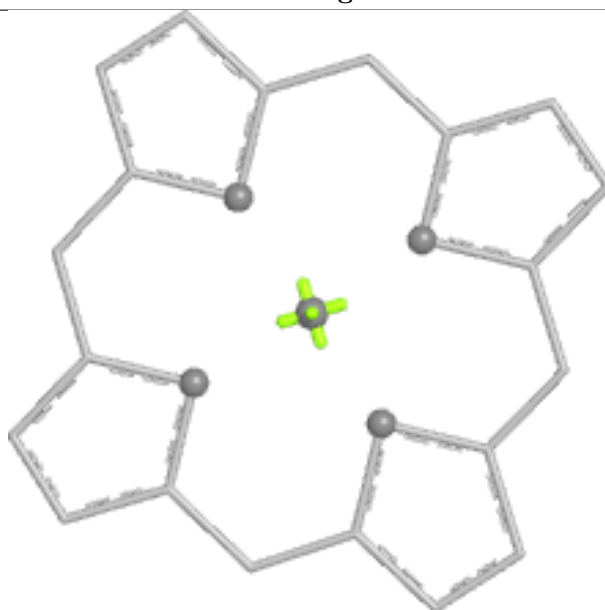
Bond lengths



Bond angles

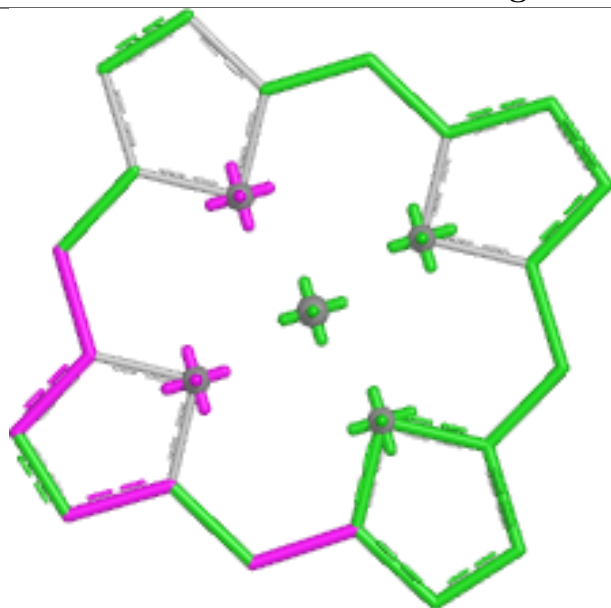


Torsions

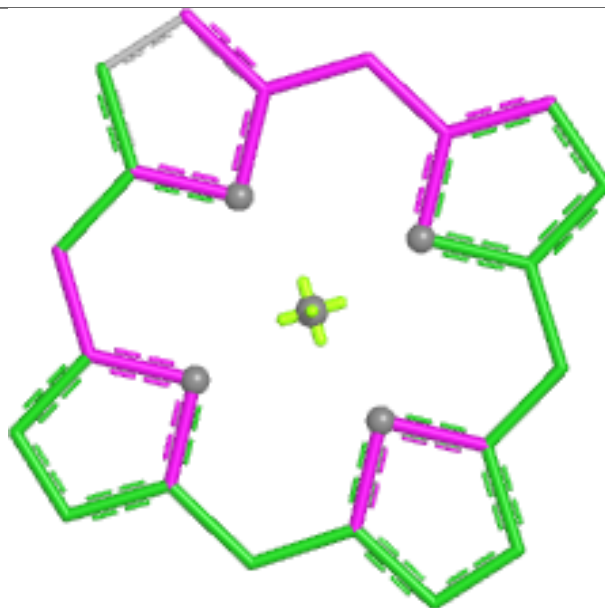


Rings

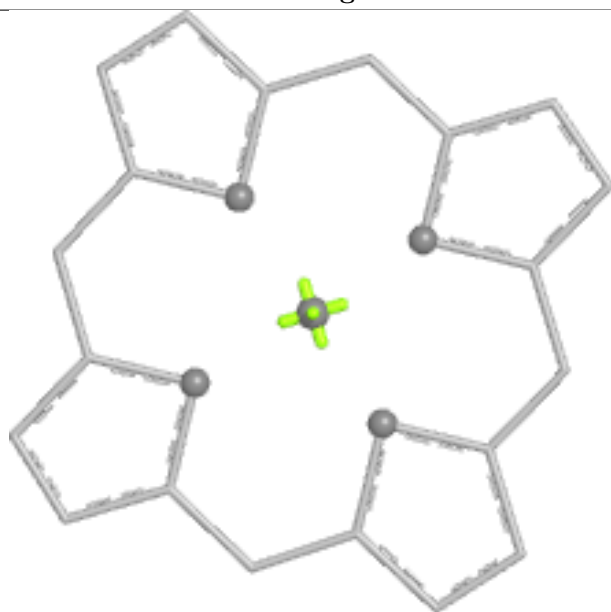
Ligand CLA 7 1012



Bond lengths



Bond angles

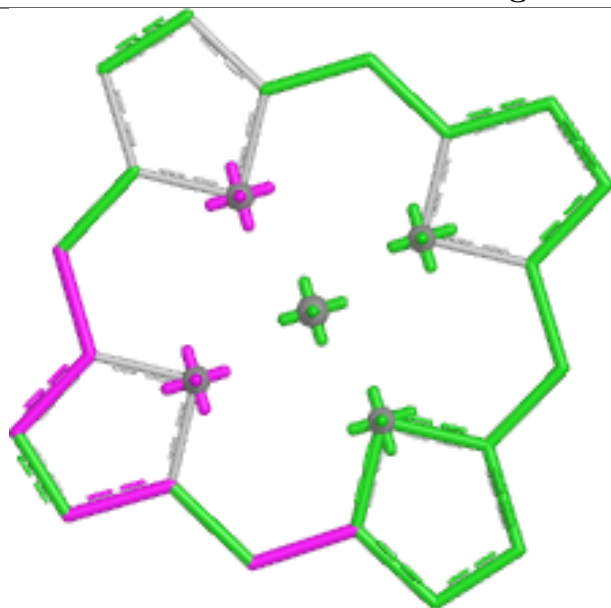


Torsions

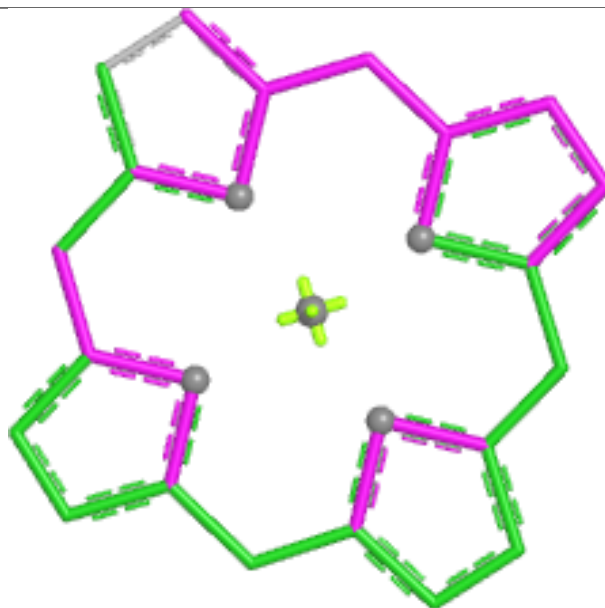


Rings

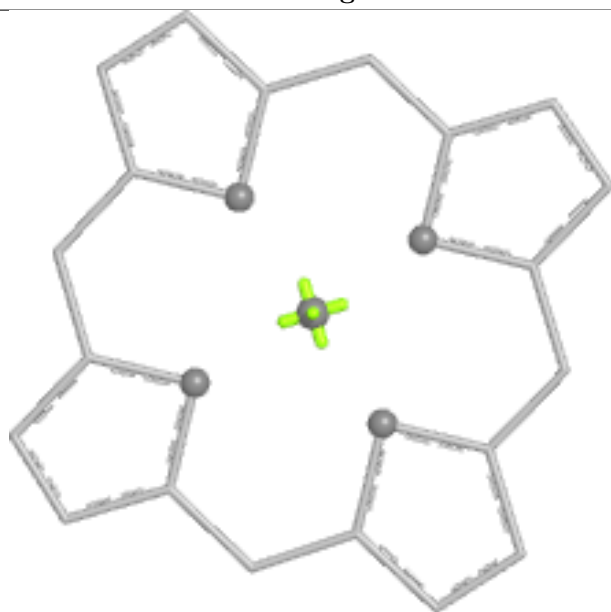
Ligand CLA 0 1023



Bond lengths



Bond angles

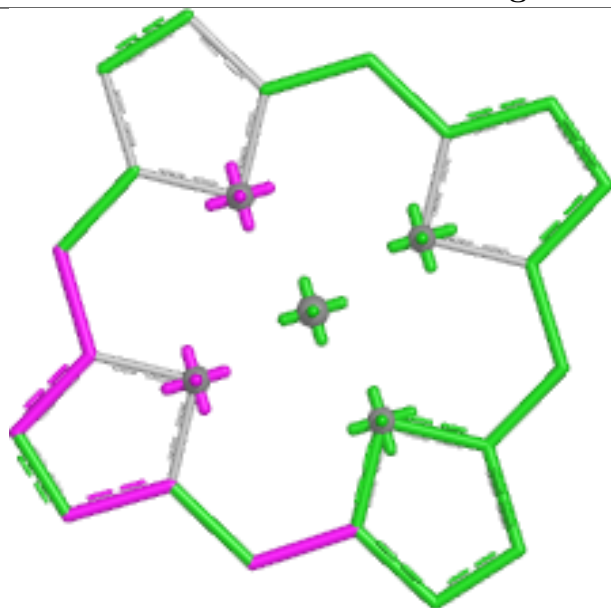


Torsions

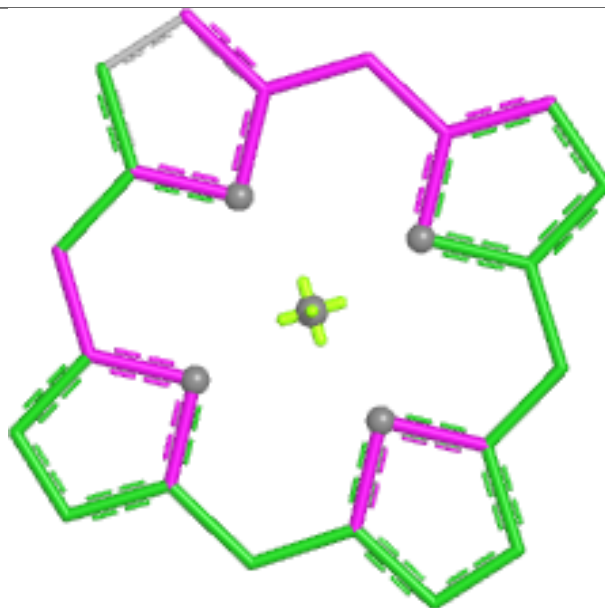


Rings

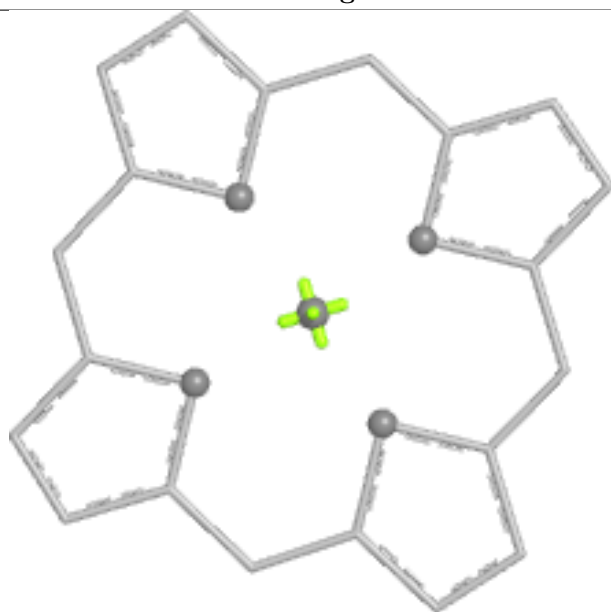
Ligand CLA 7 1025



Bond lengths



Bond angles

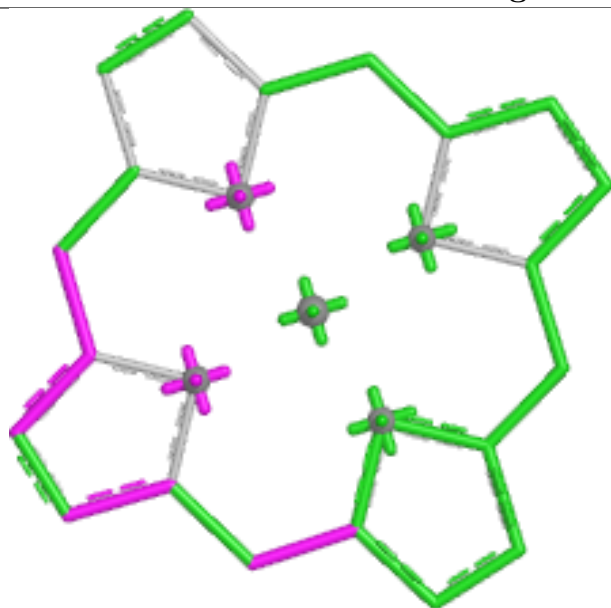


Torsions

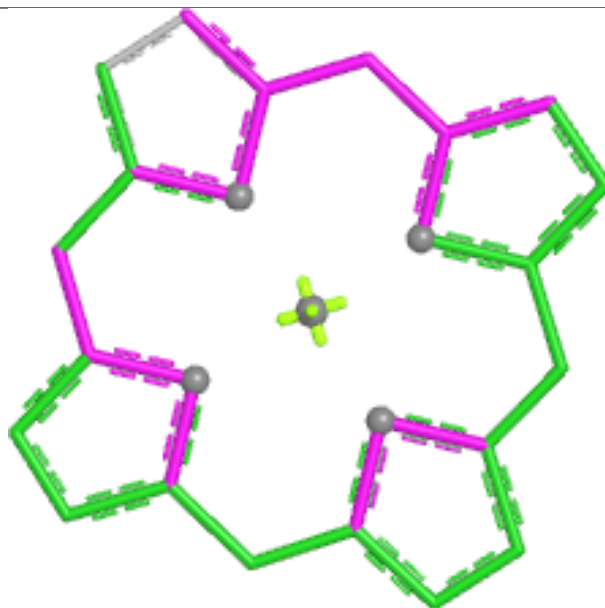


Rings

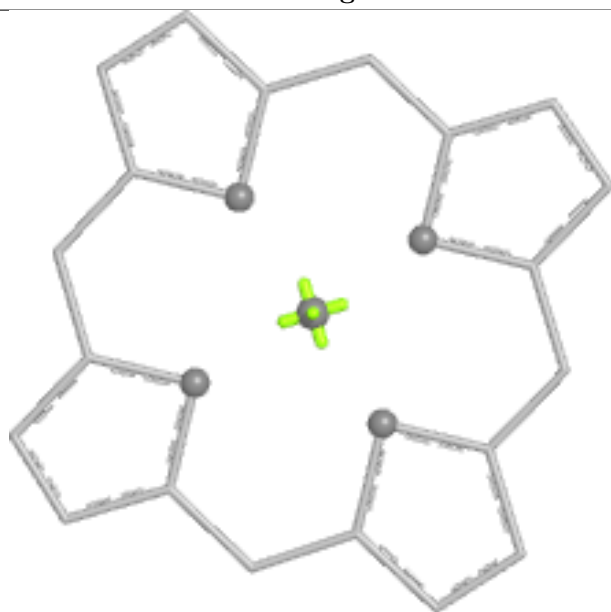
Ligand CLA 8 1031



Bond lengths



Bond angles

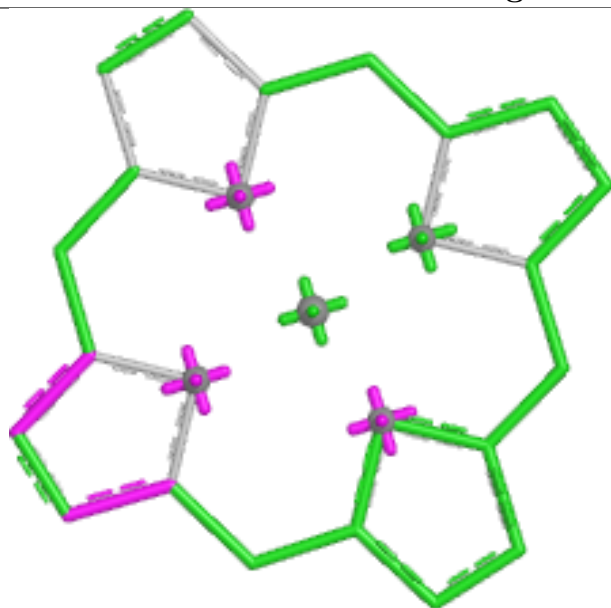


Torsions

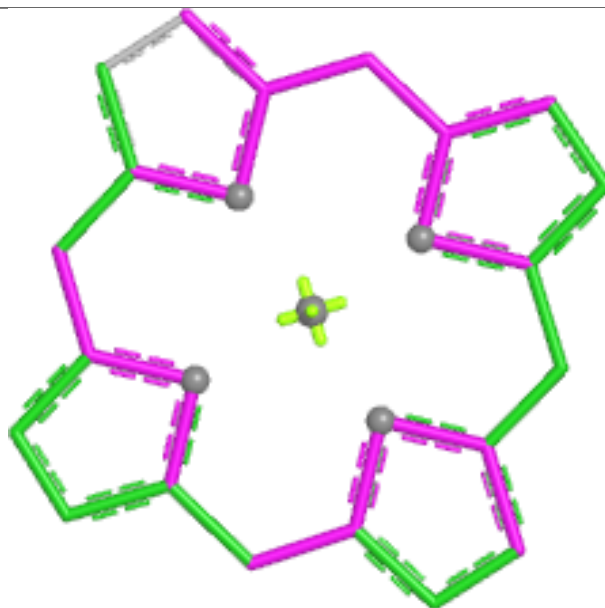


Rings

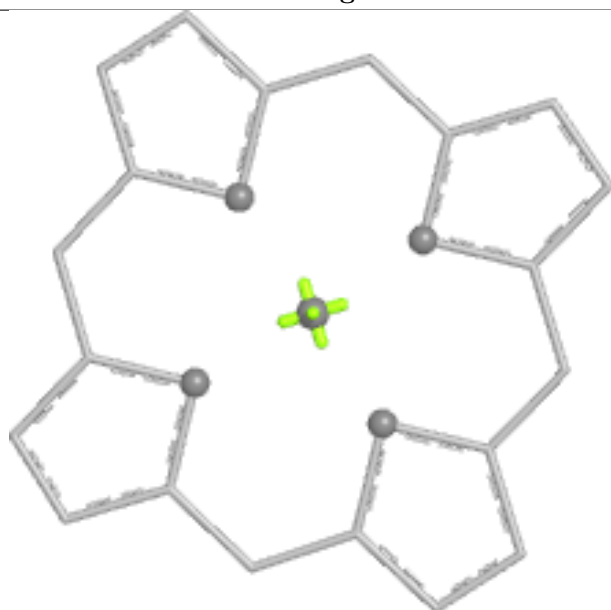
Ligand CLA P 5108



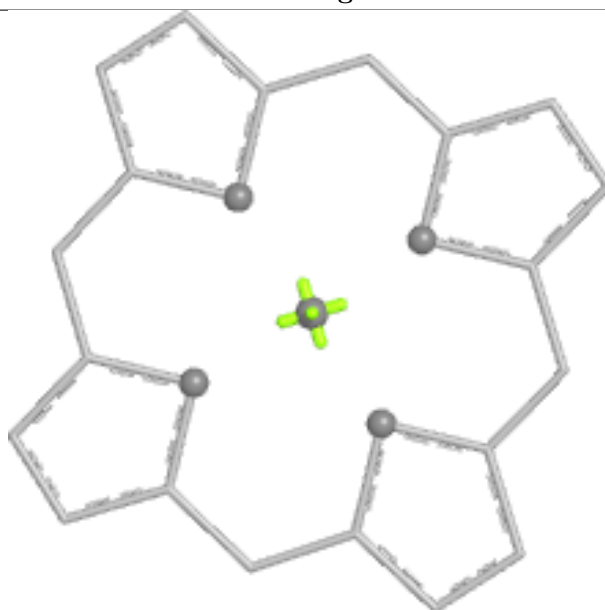
Bond lengths



Bond angles

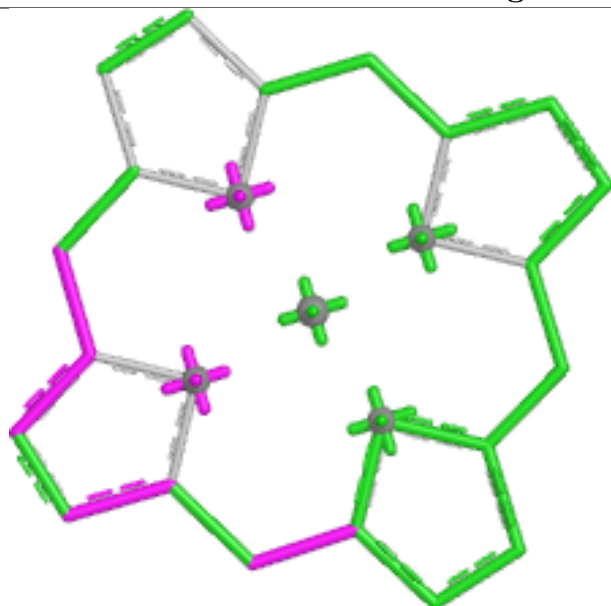


Torsions

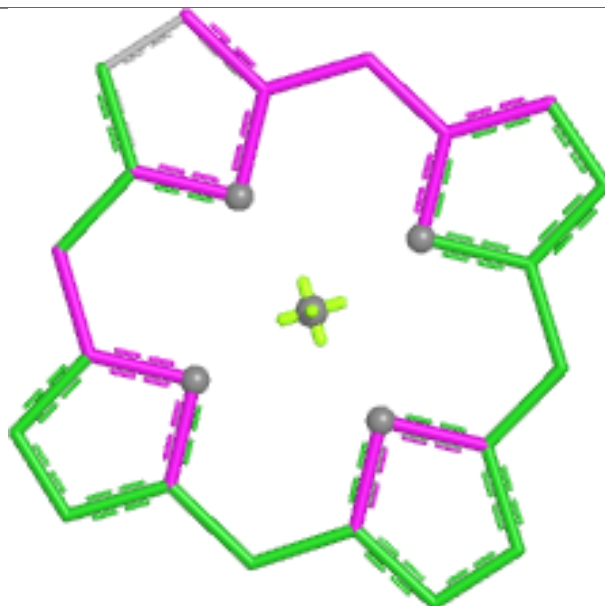


Rings

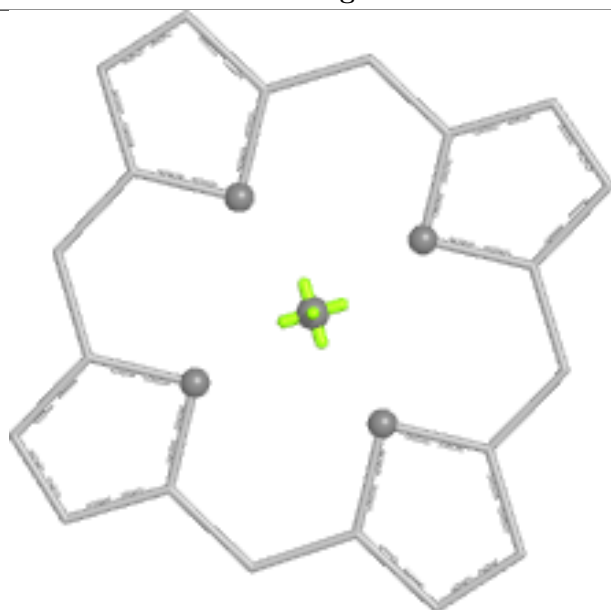
Ligand CLA F 4005



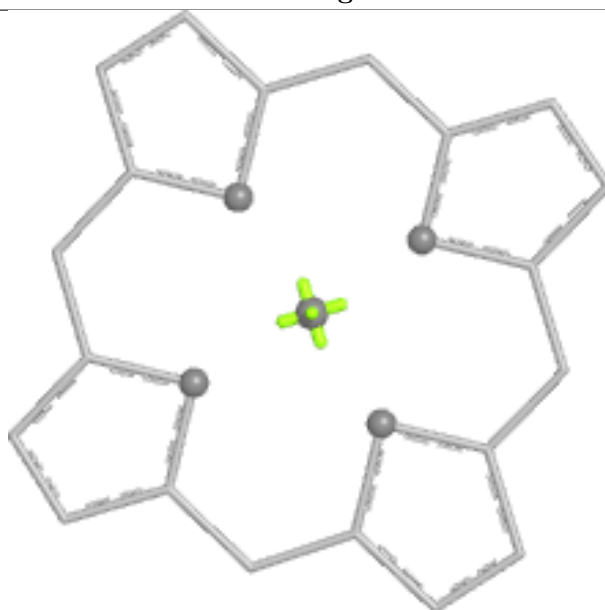
Bond lengths



Bond angles

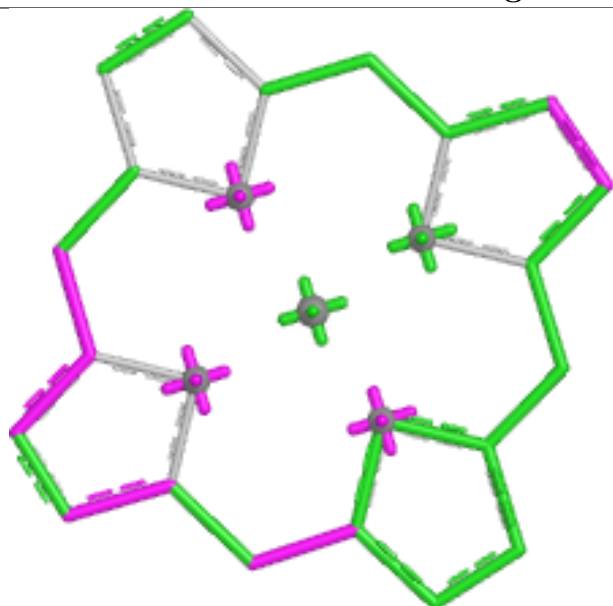


Torsions

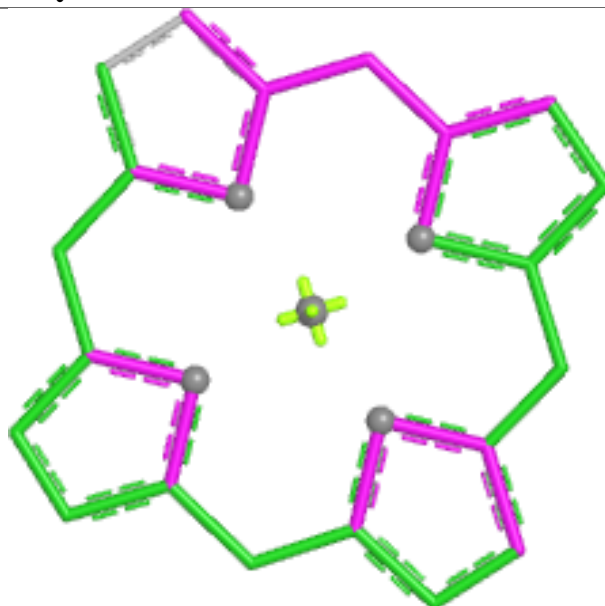


Rings

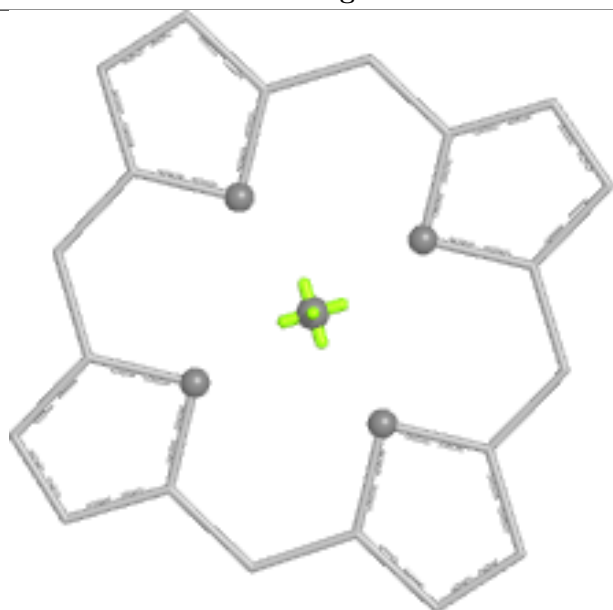
Ligand CLA Q 5235



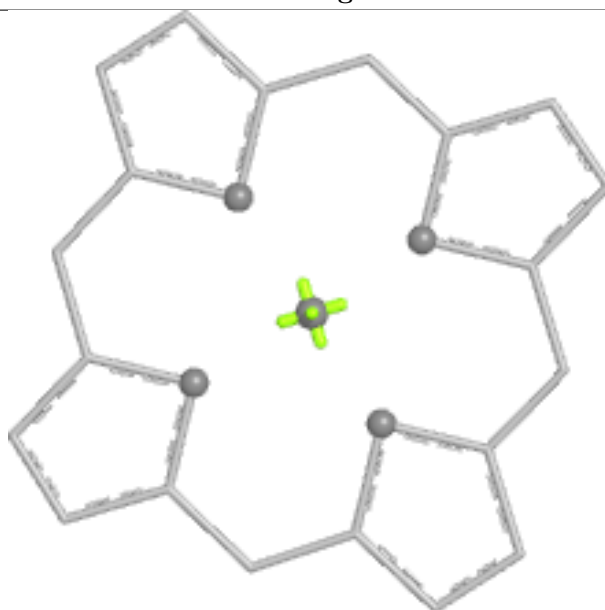
Bond lengths



Bond angles

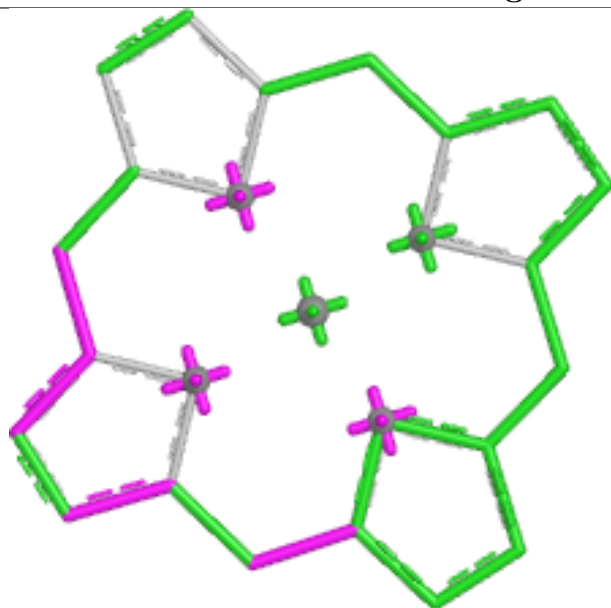


Torsions

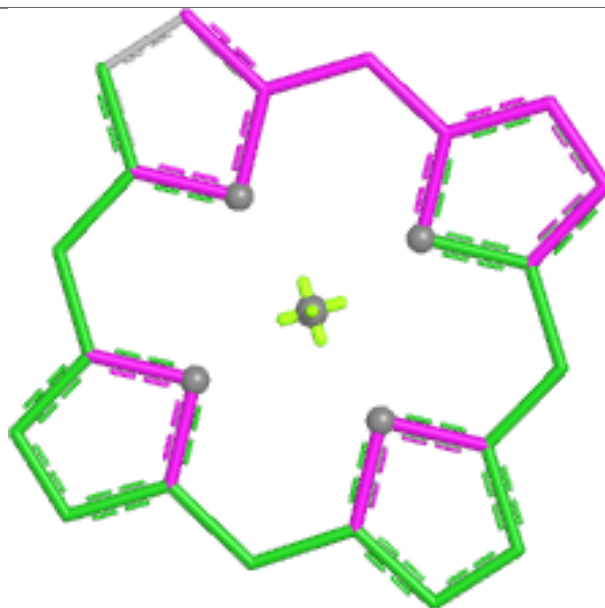


Rings

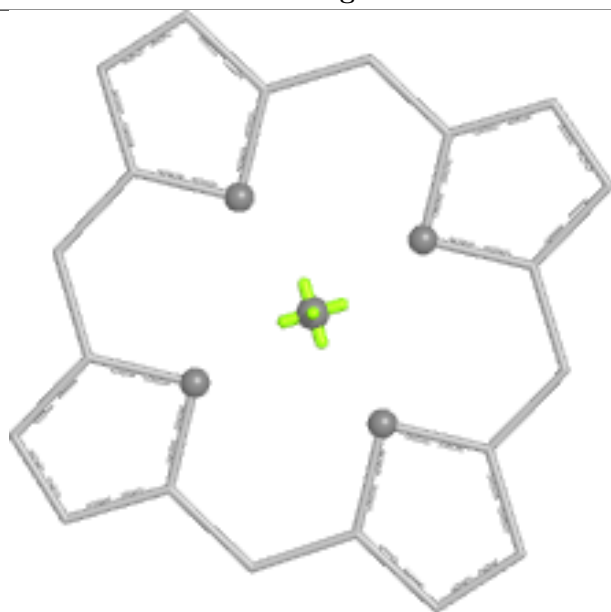
Ligand CLA B 1212



Bond lengths



Bond angles

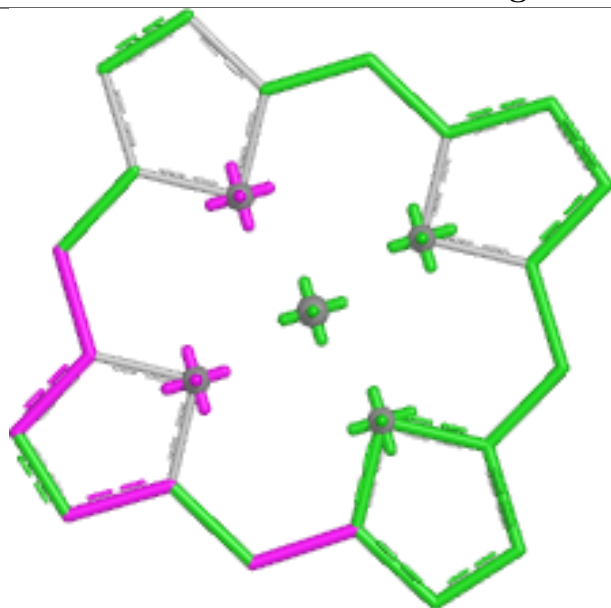


Torsions

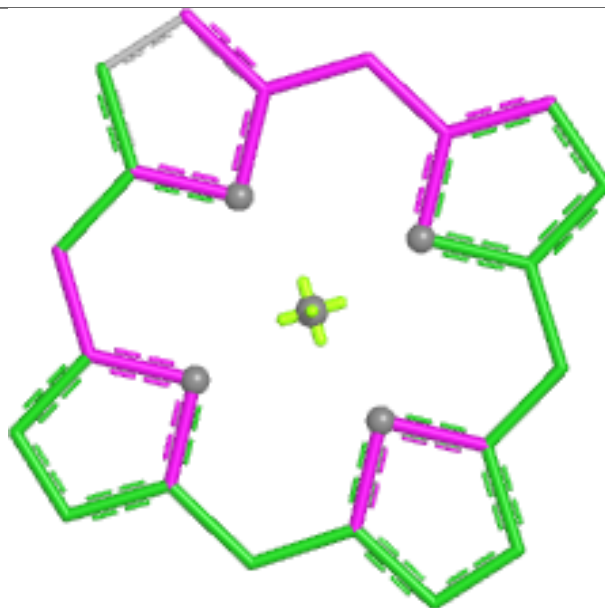


Rings

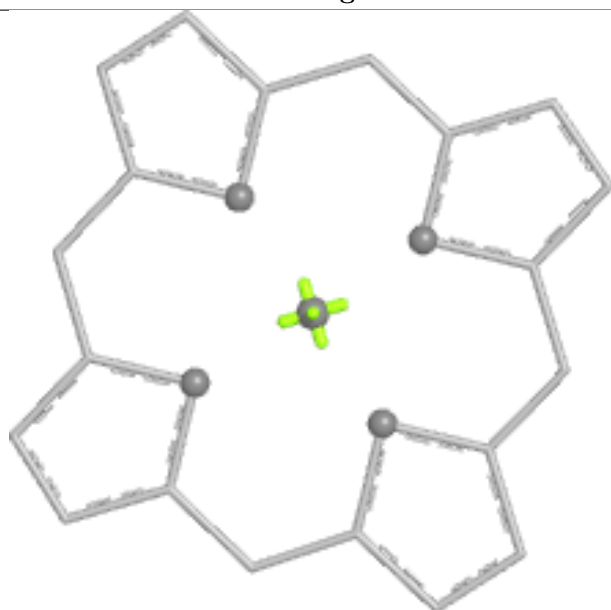
Ligand CLA 2 1013



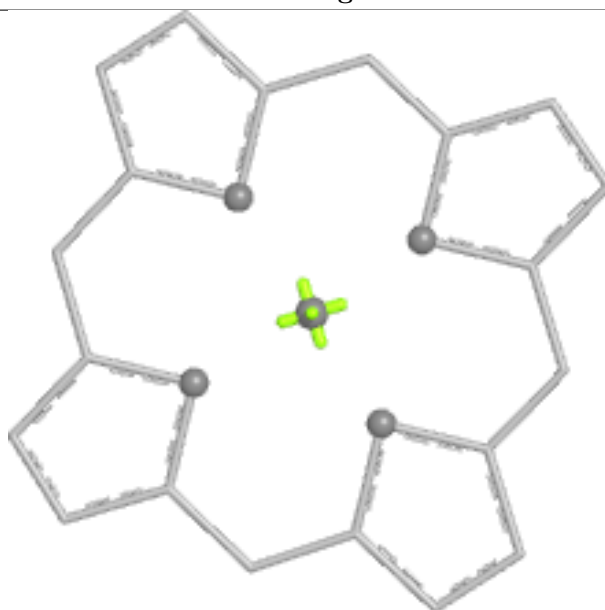
Bond lengths



Bond angles

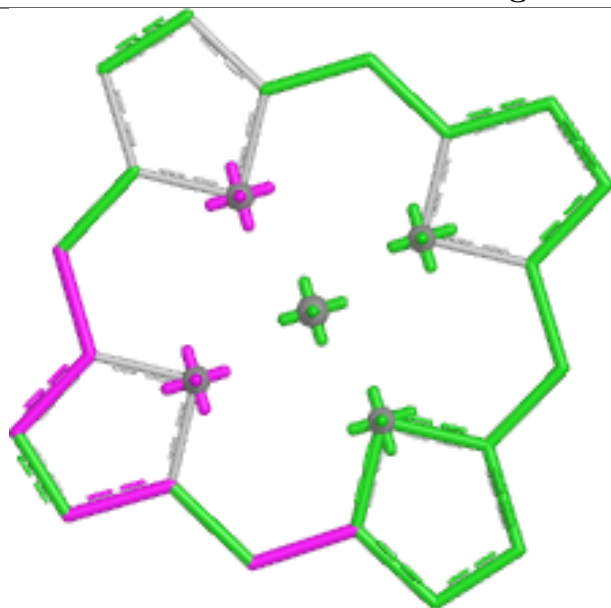


Torsions

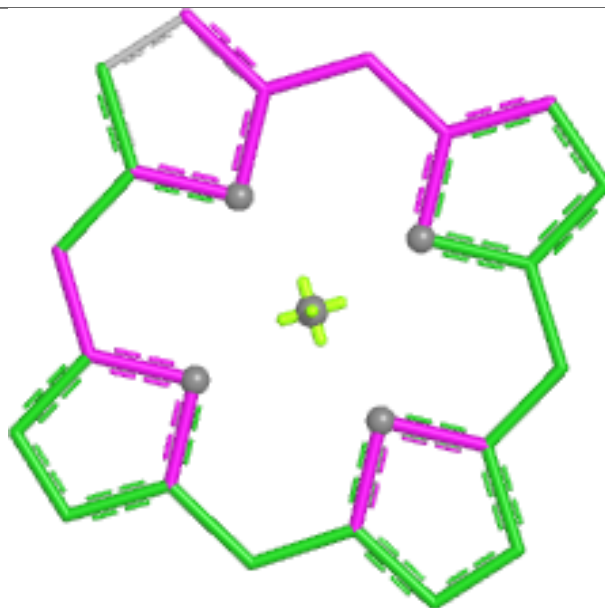


Rings

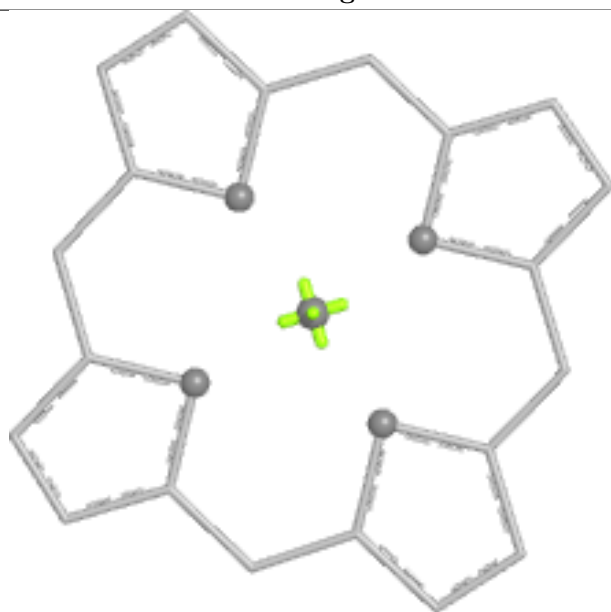
Ligand CLA 0 1017



Bond lengths



Bond angles

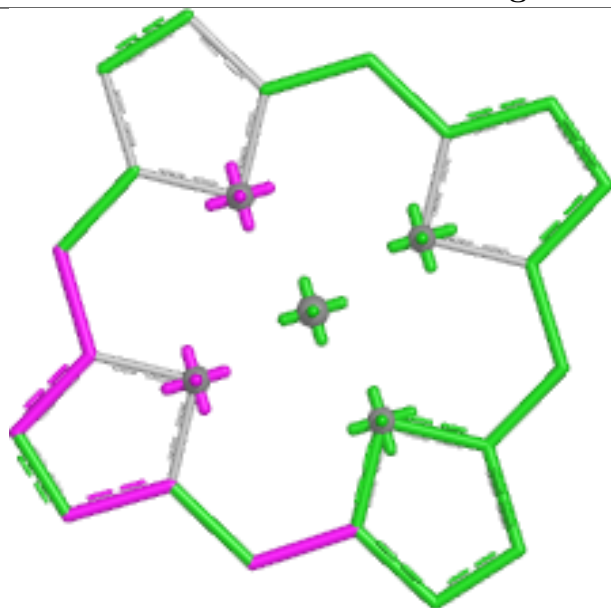


Torsions

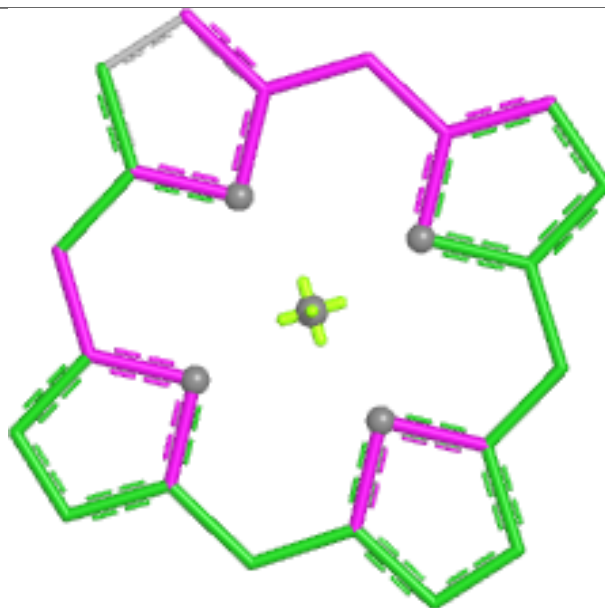


Rings

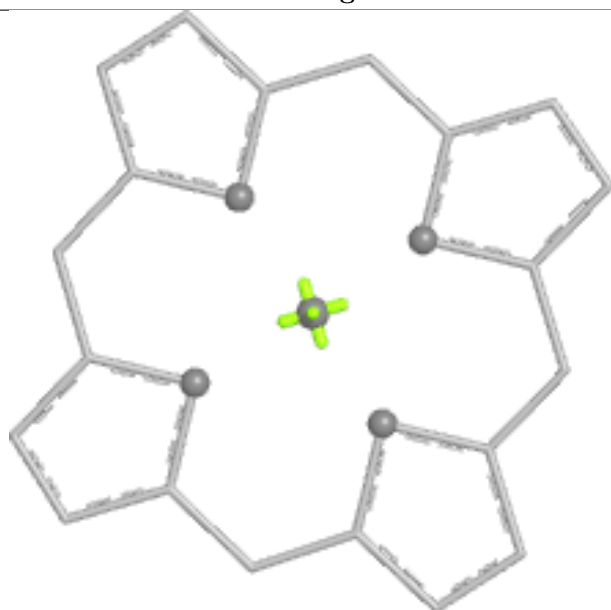
Ligand CLA 3 1016



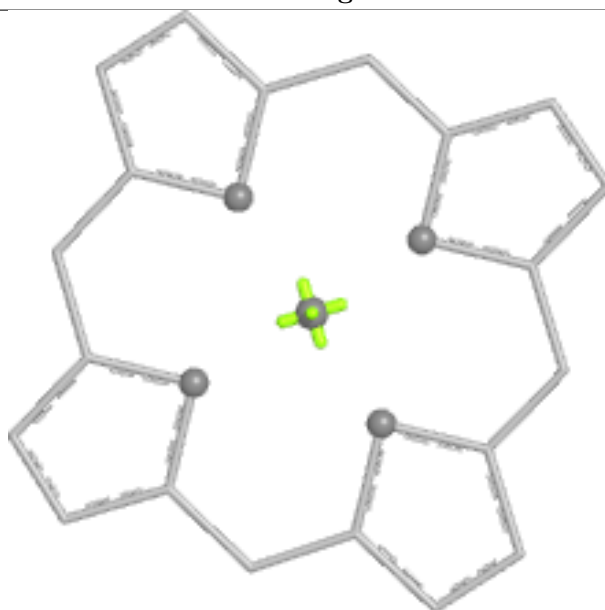
Bond lengths



Bond angles

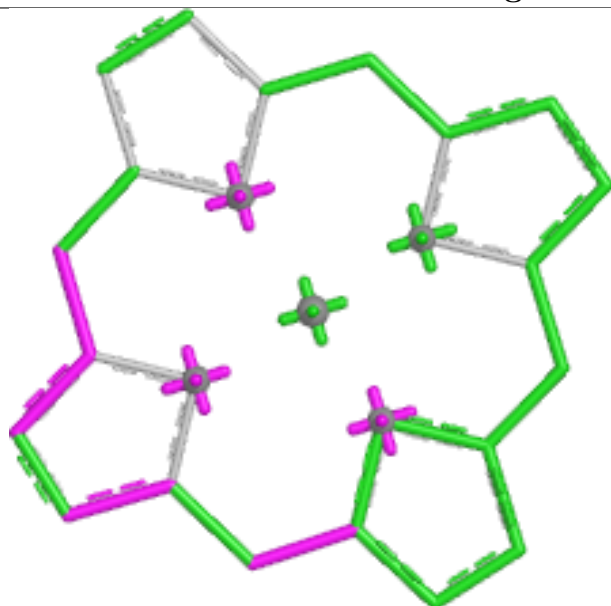


Torsions

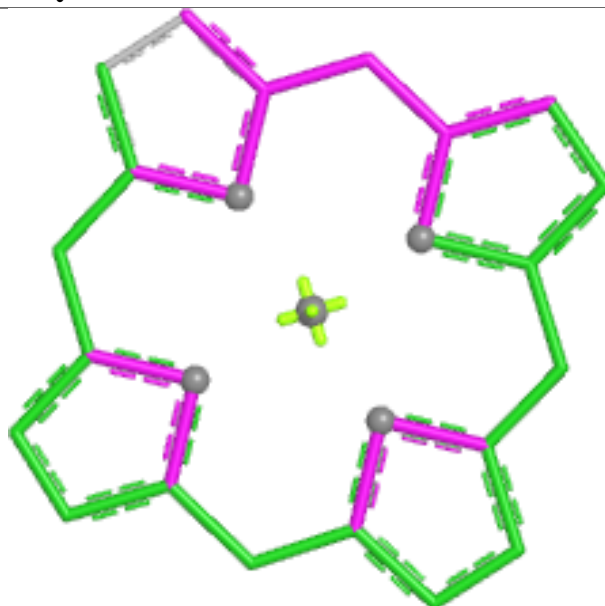


Rings

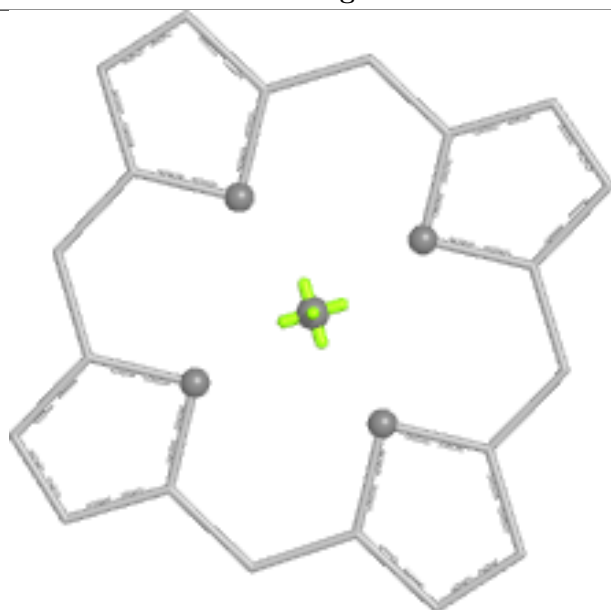
Ligand CLA Q 5211



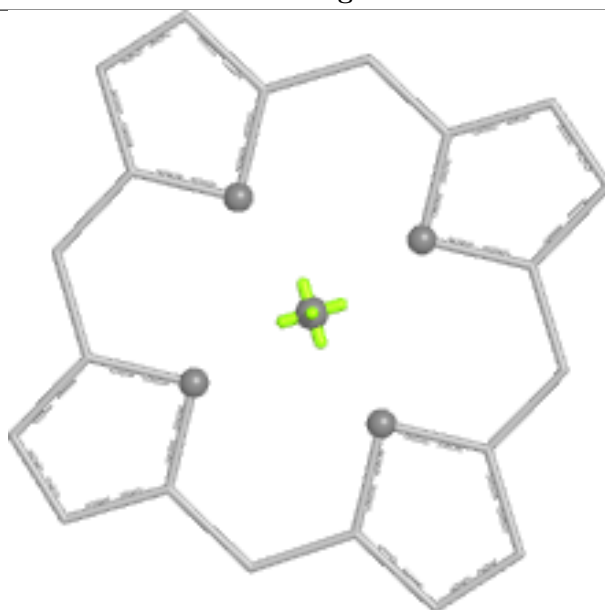
Bond lengths



Bond angles

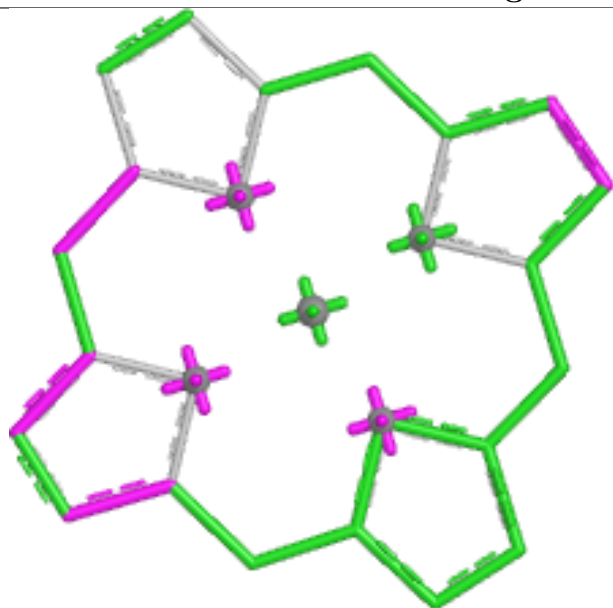


Torsions

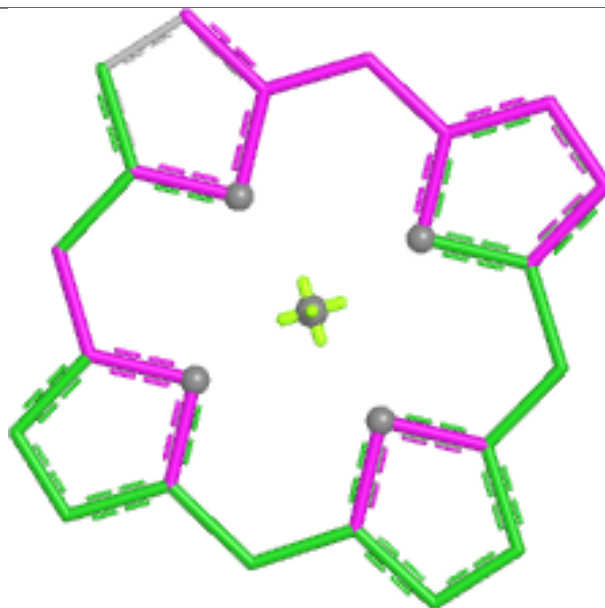


Rings

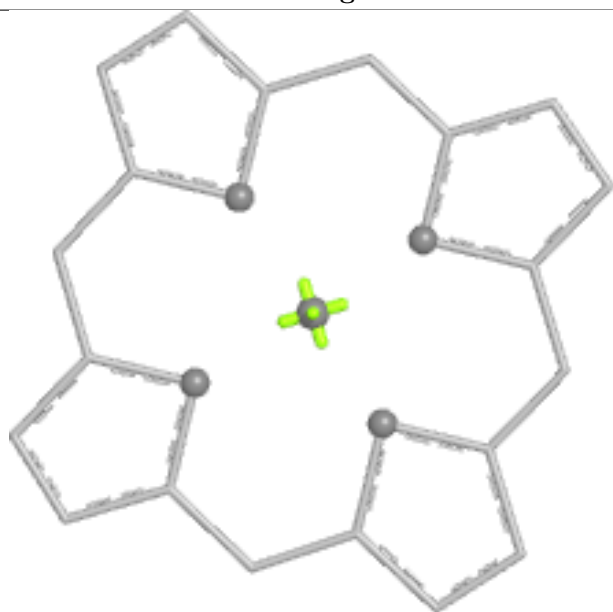
Ligand CLA B 1226



Bond lengths



Bond angles

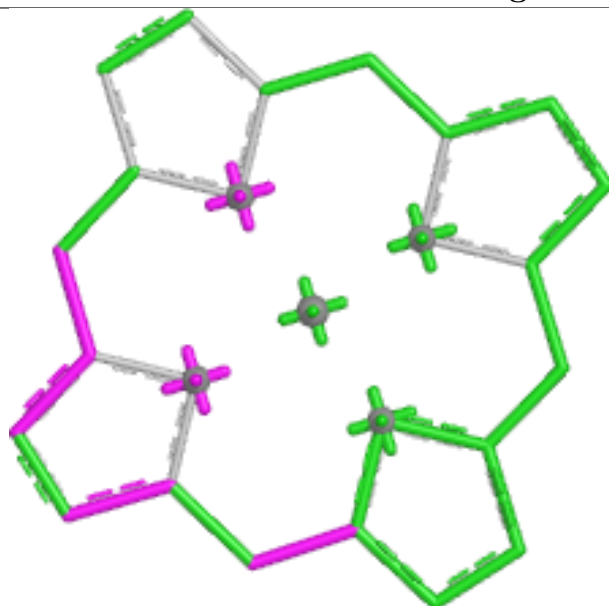


Torsions

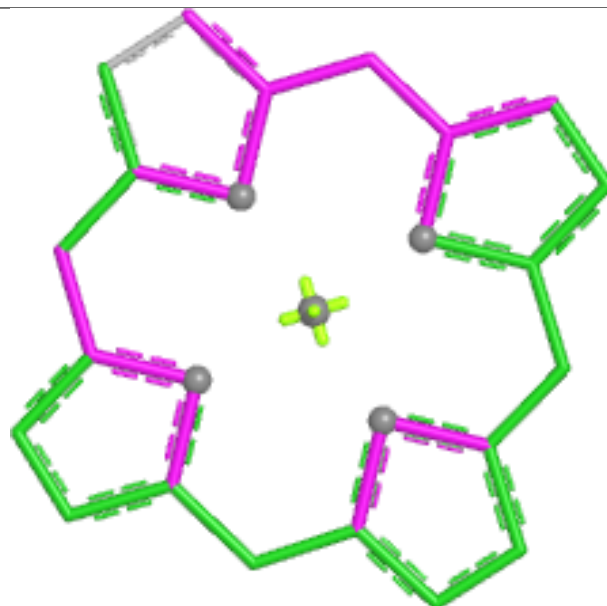


Rings

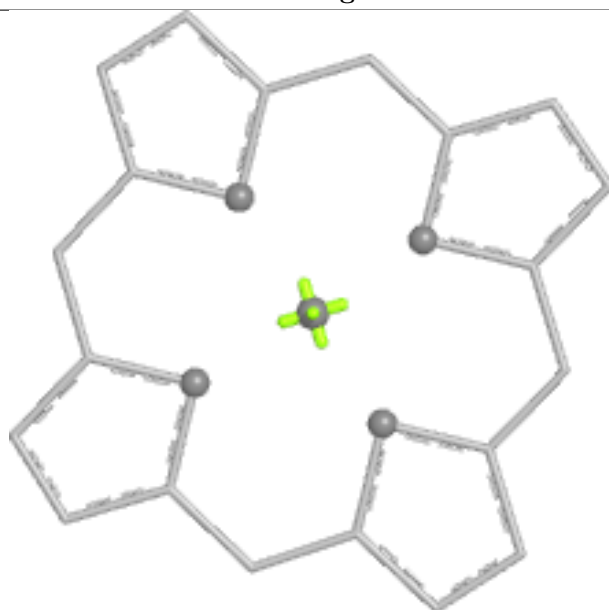
Ligand CLA 4 1021



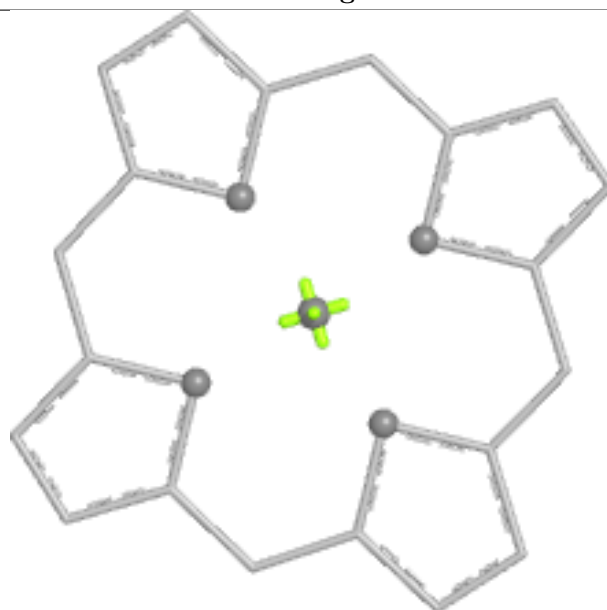
Bond lengths



Bond angles

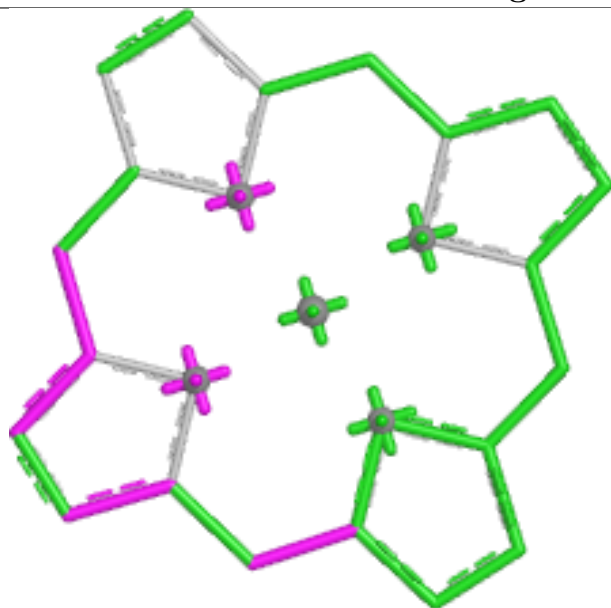


Torsions



Rings

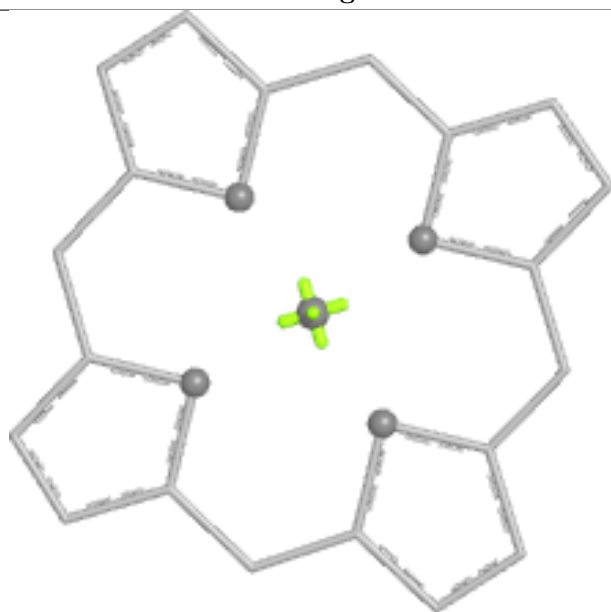
Ligand CLA 8 1013



Bond lengths



Bond angles

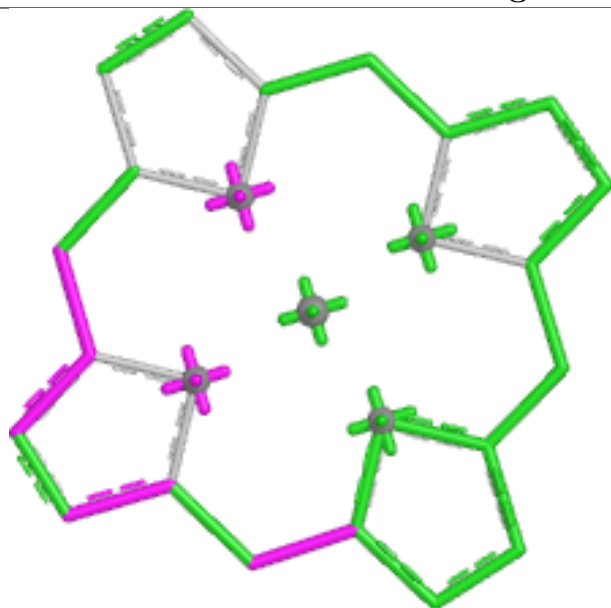


Torsions

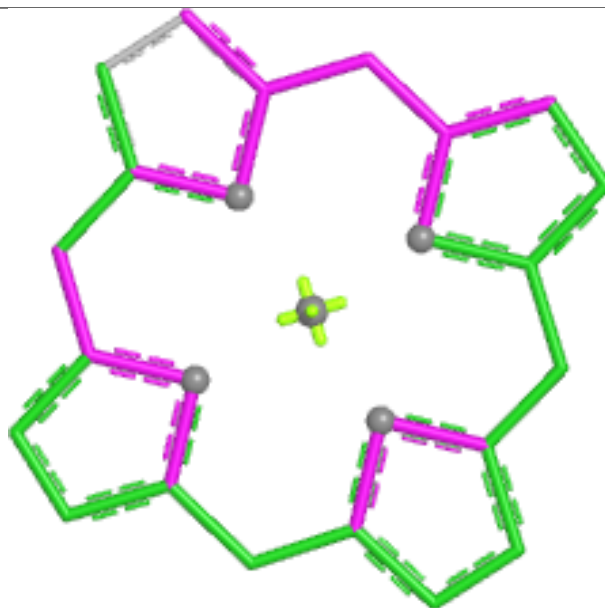


Rings

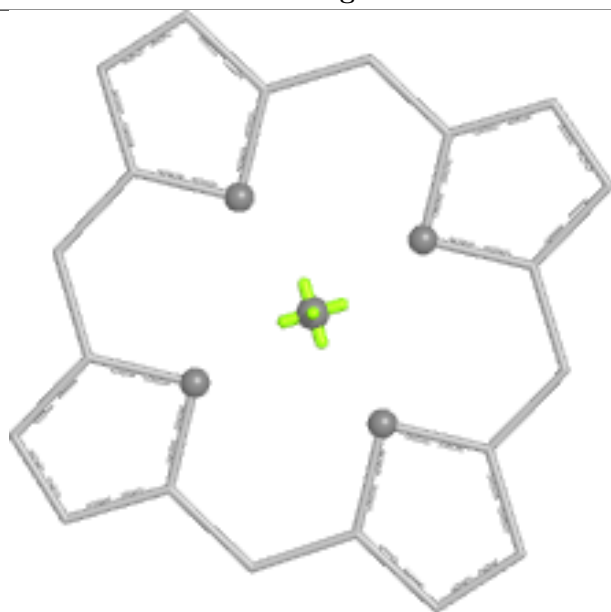
Ligand CLA 2 1025



Bond lengths



Bond angles

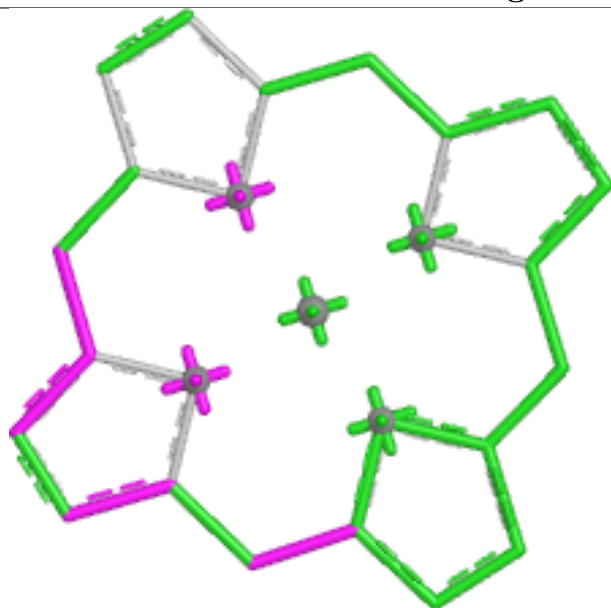


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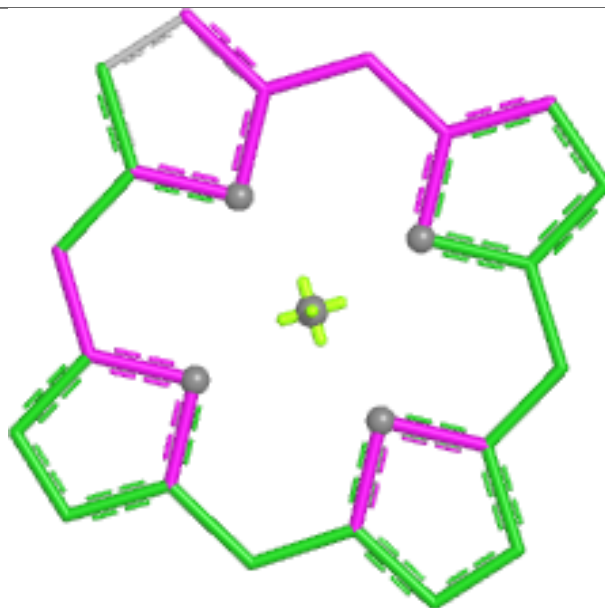


Rings

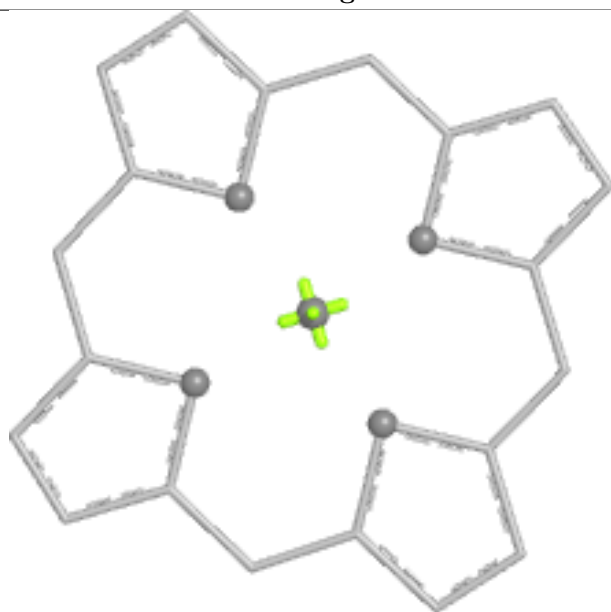
Ligand CLA L 1504



Bond lengths



Bond angles

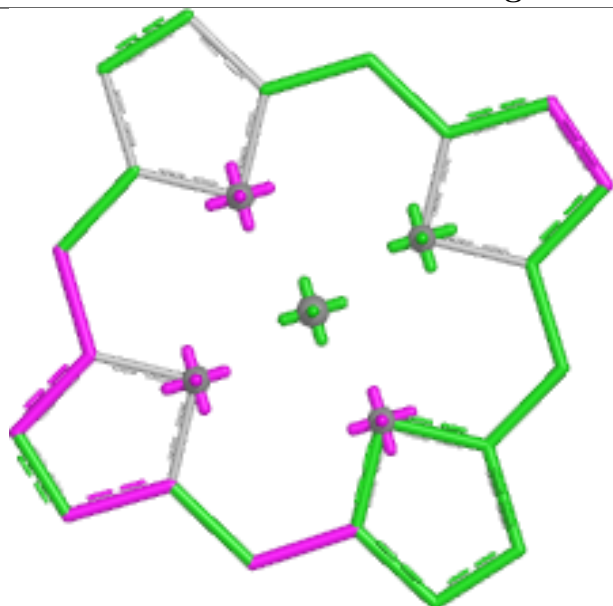


Torsions

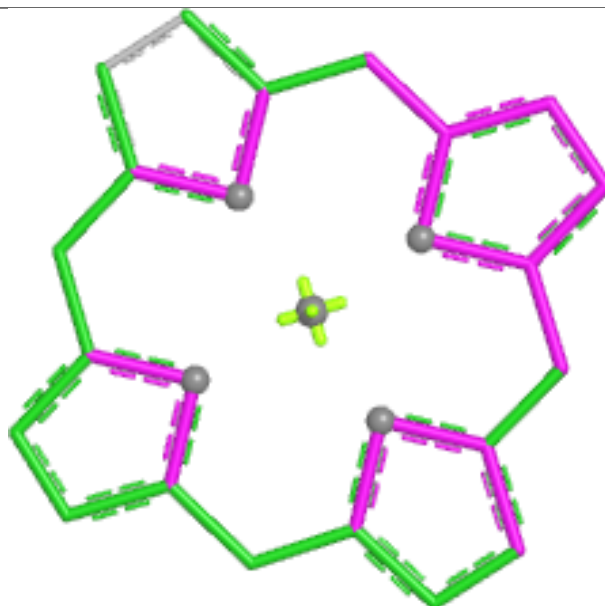


Rings

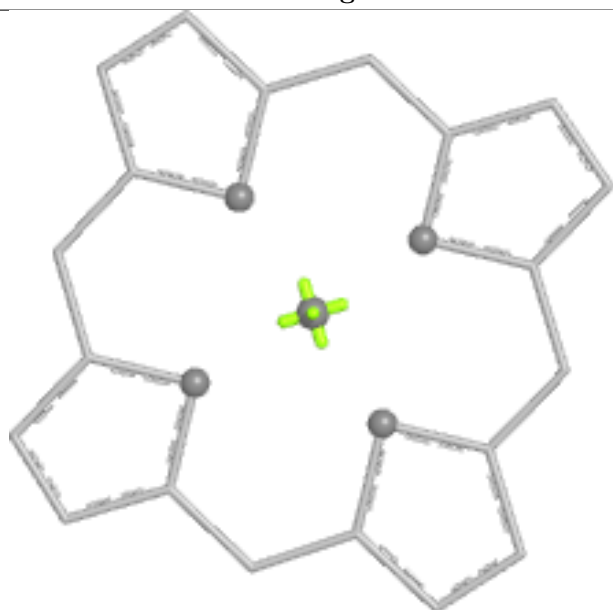
Ligand CLA A 1136



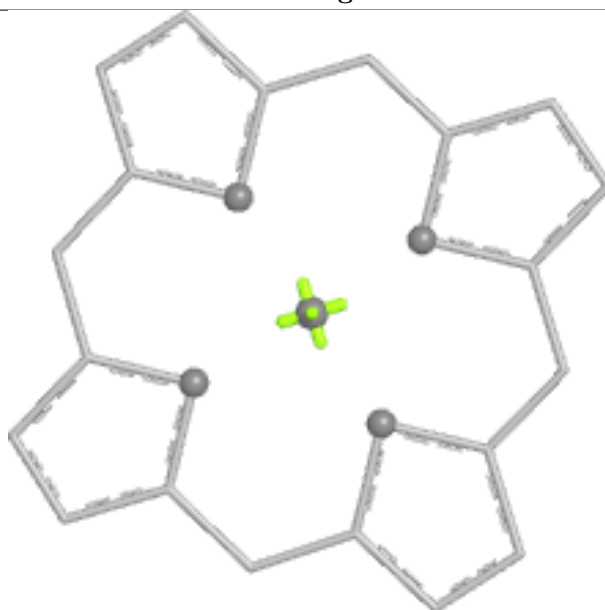
Bond lengths



Bond angles

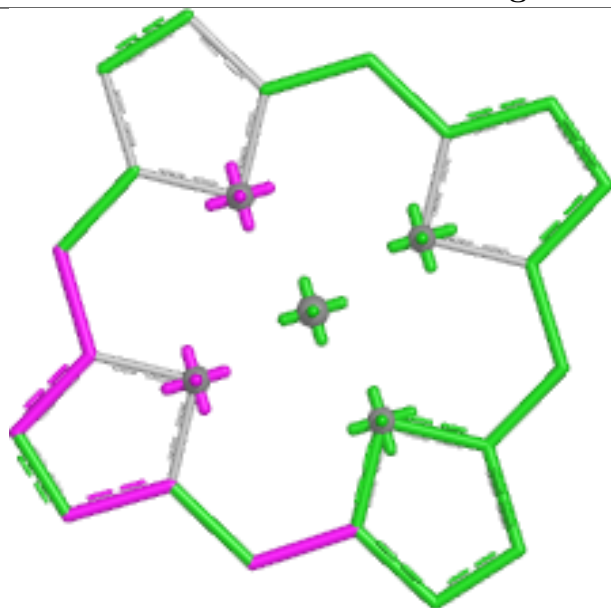


Torsions

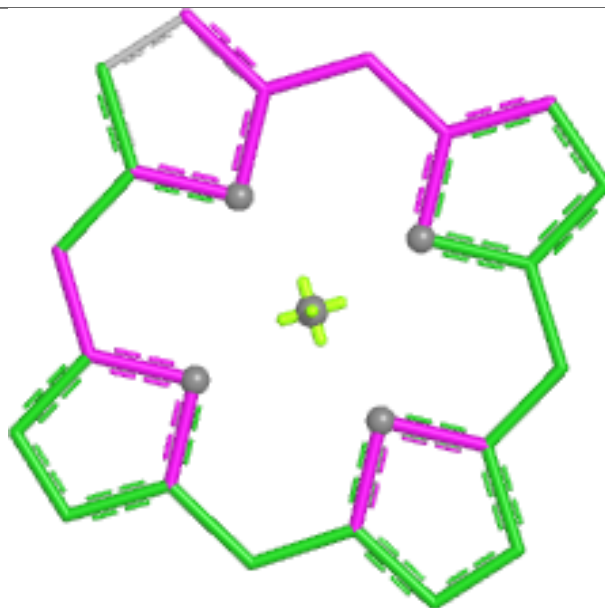


Rings

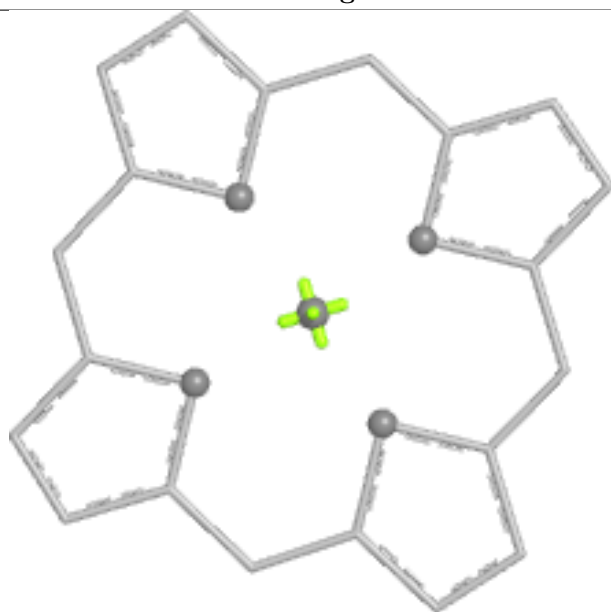
Ligand CLA 9 1022



Bond lengths



Bond angles

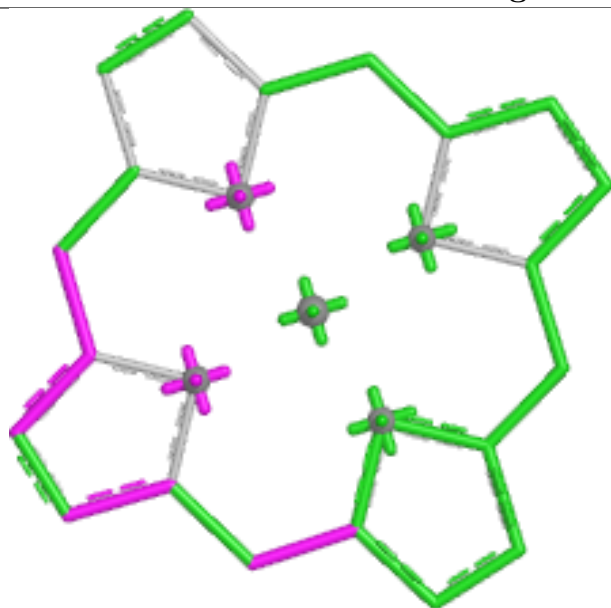


Torsions

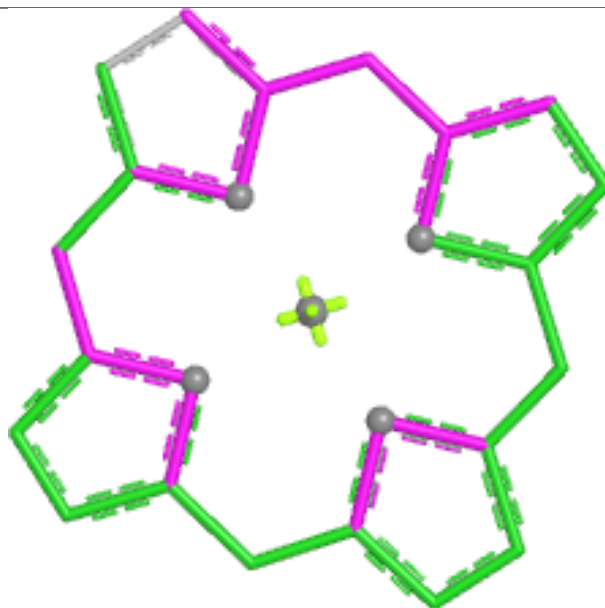


Rings

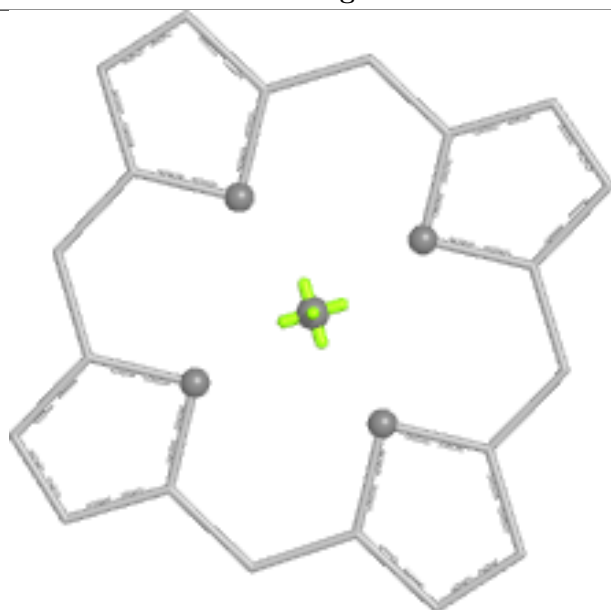
Ligand CLA 0 1013



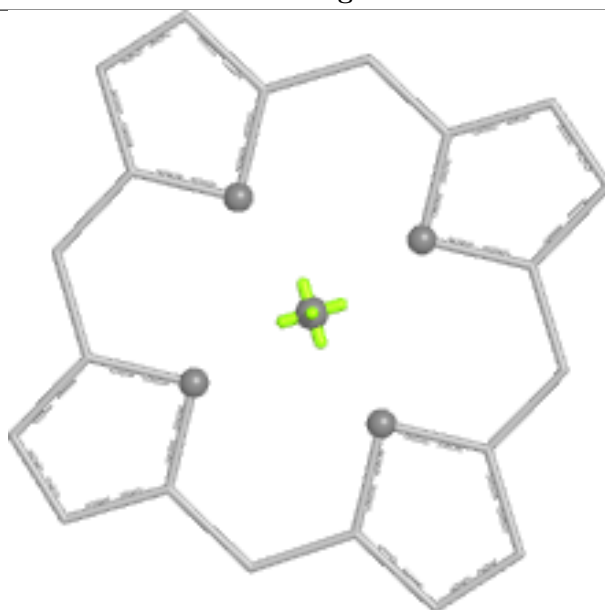
Bond lengths



Bond angles

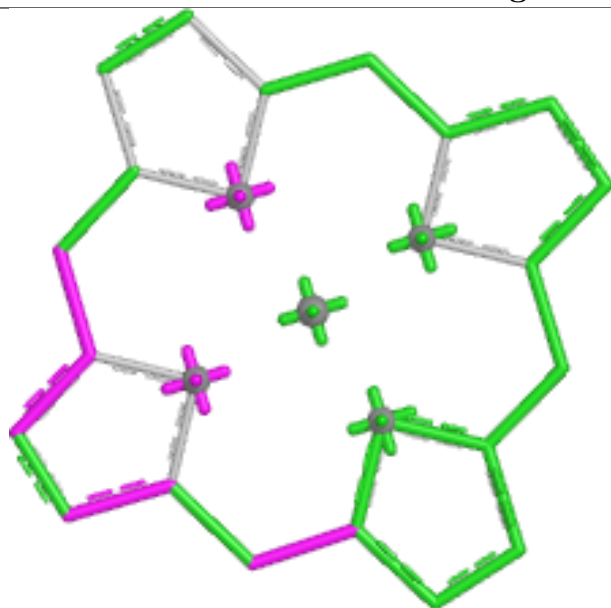


Torsions

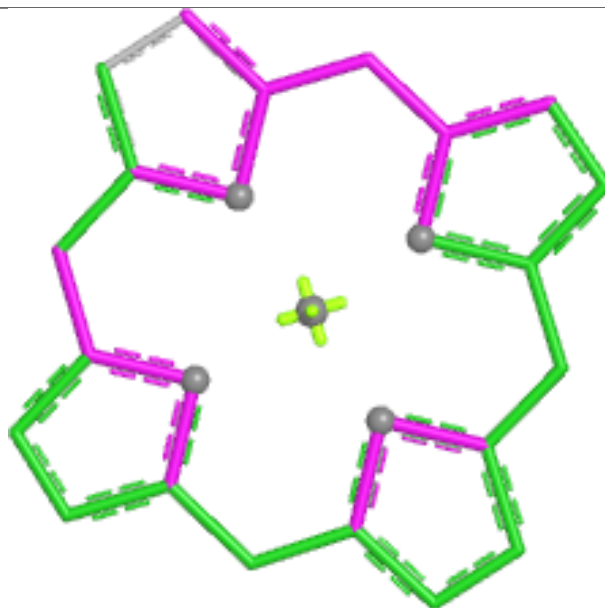


Rings

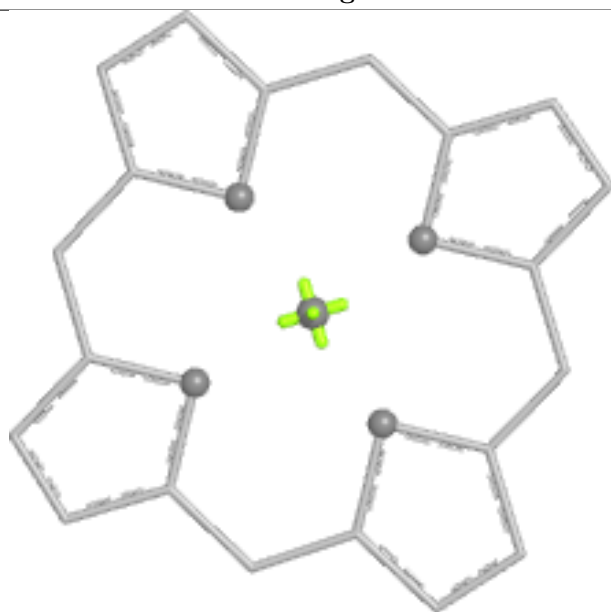
Ligand CLA 7 1023



Bond lengths



Bond angles

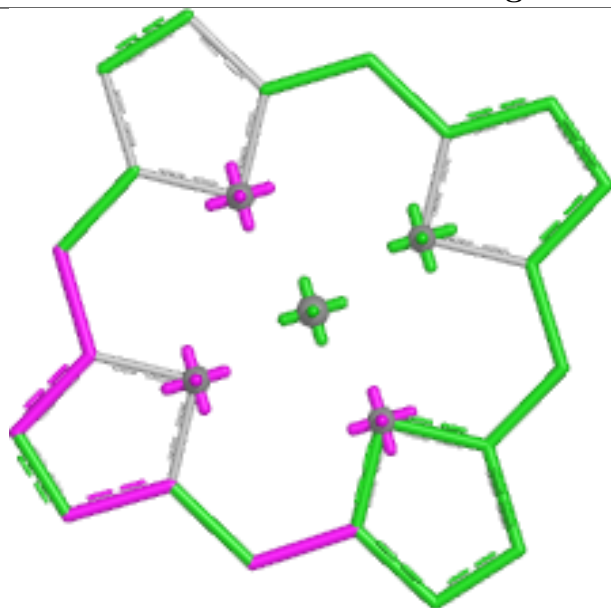


Torsions

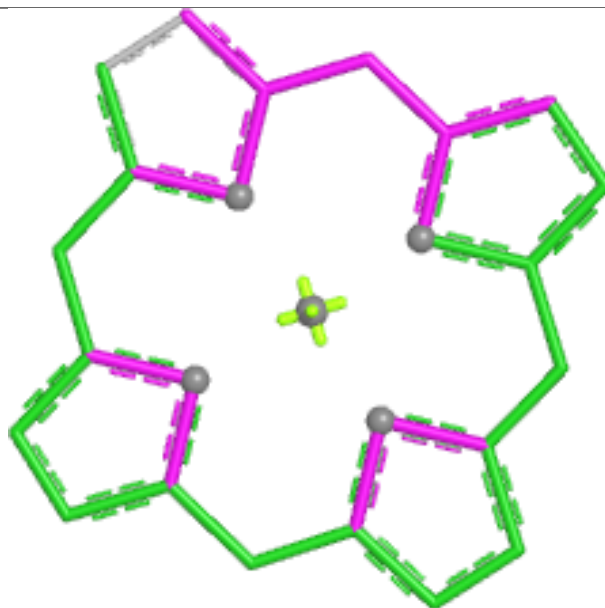


Rings

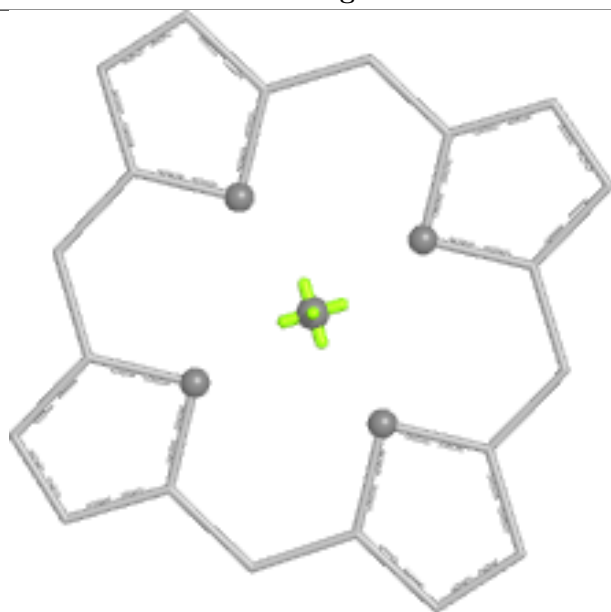
Ligand CLA B 1211



Bond lengths



Bond angles

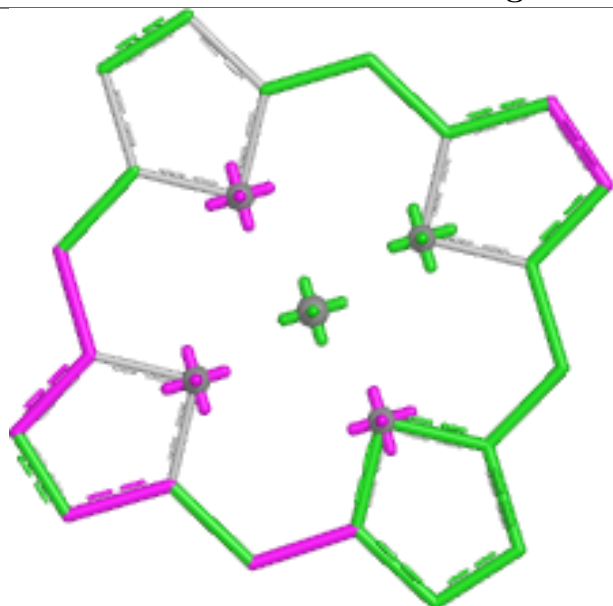


Torsions

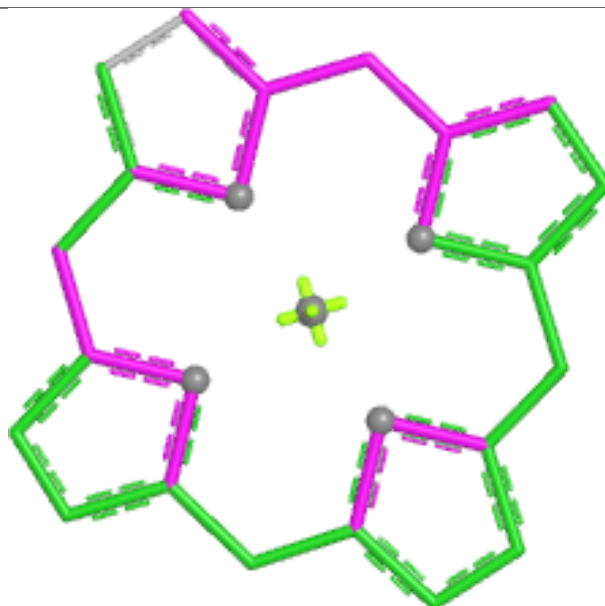


Rings

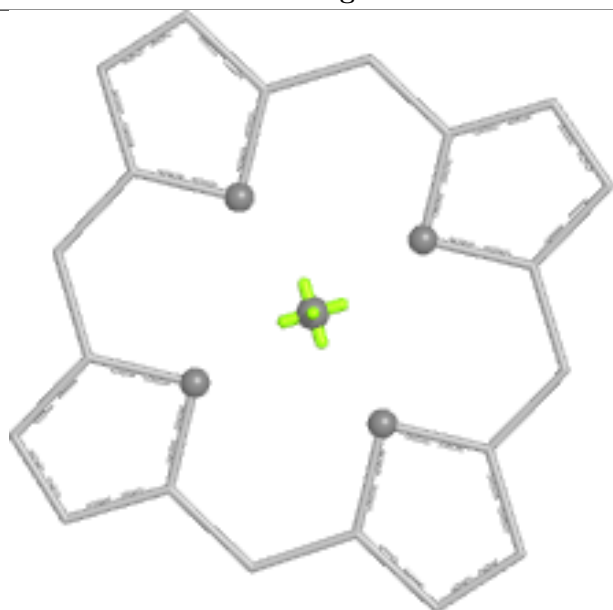
Ligand CLA P 5114



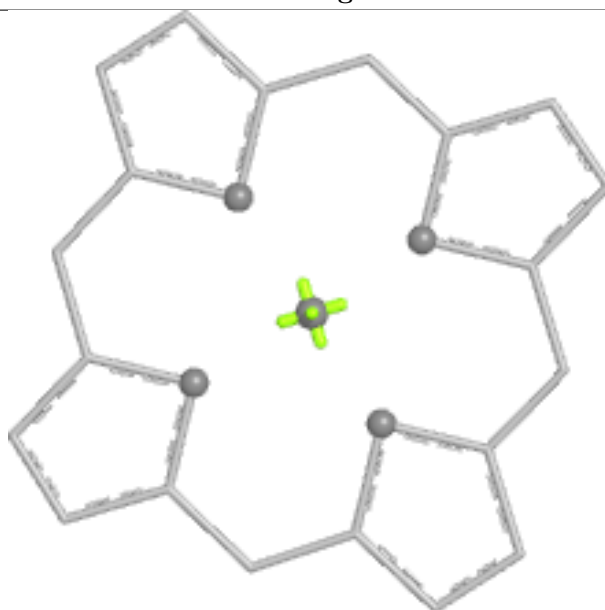
Bond lengths



Bond angles

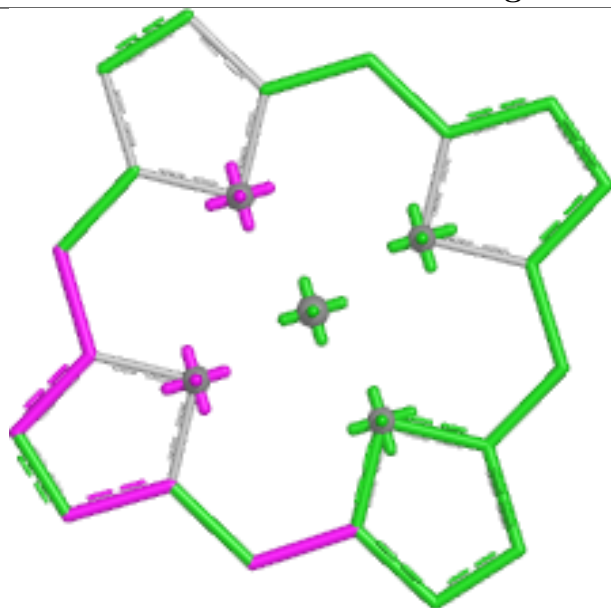


Torsions

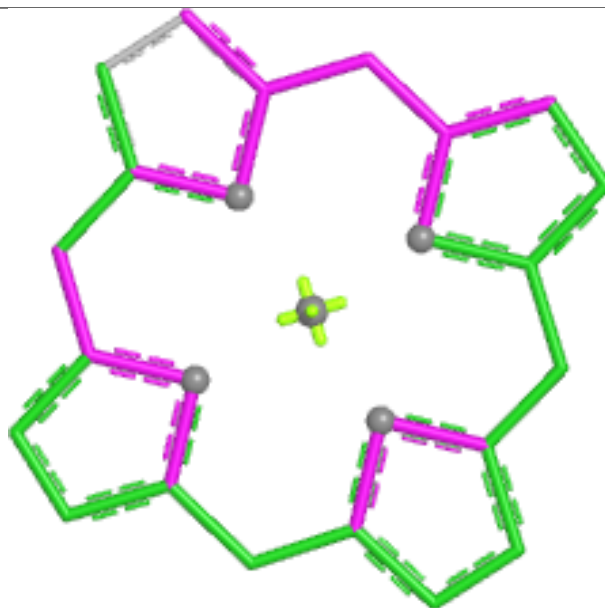


Rings

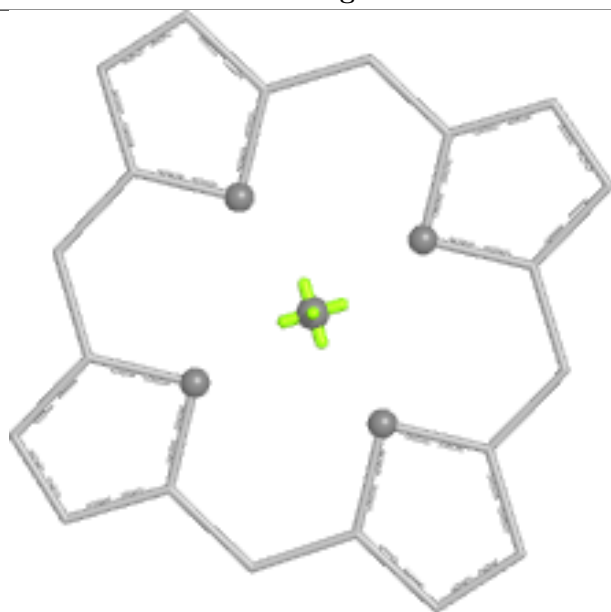
Ligand CLA U 8004



Bond lengths



Bond angles

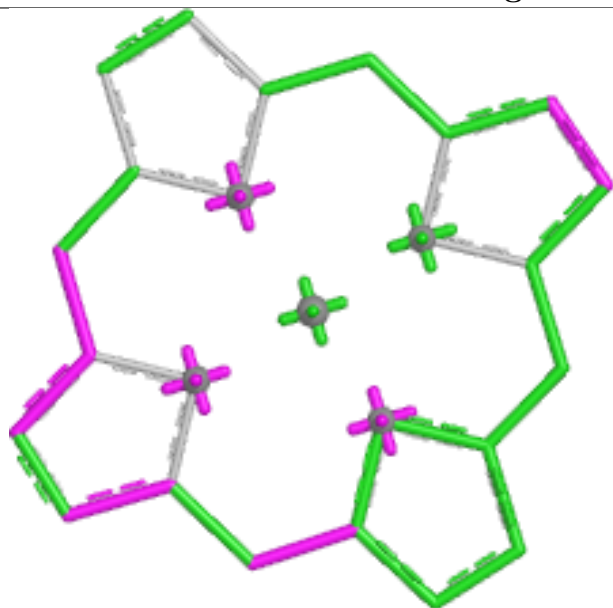


Torsions

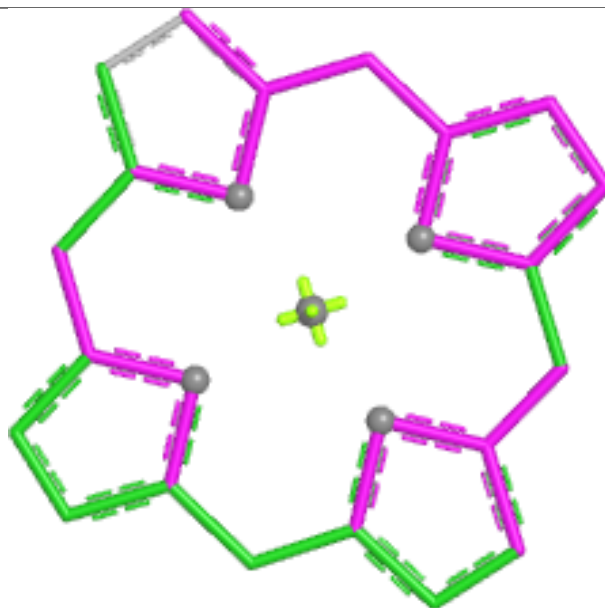


Rings

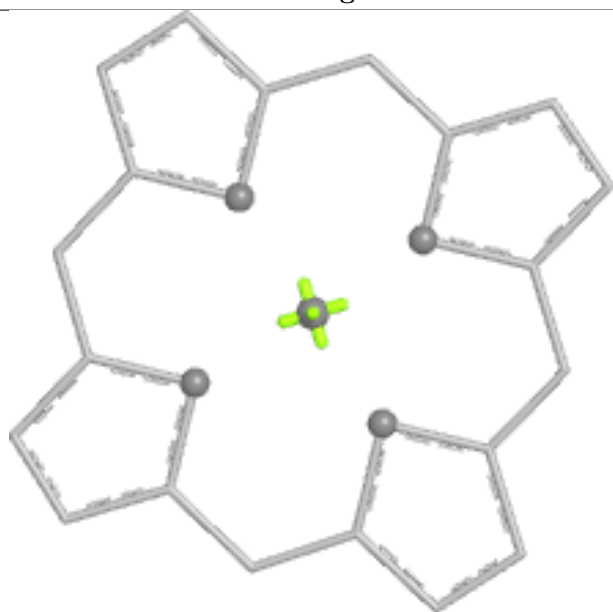
Ligand CLA A 1901



Bond lengths



Bond angles

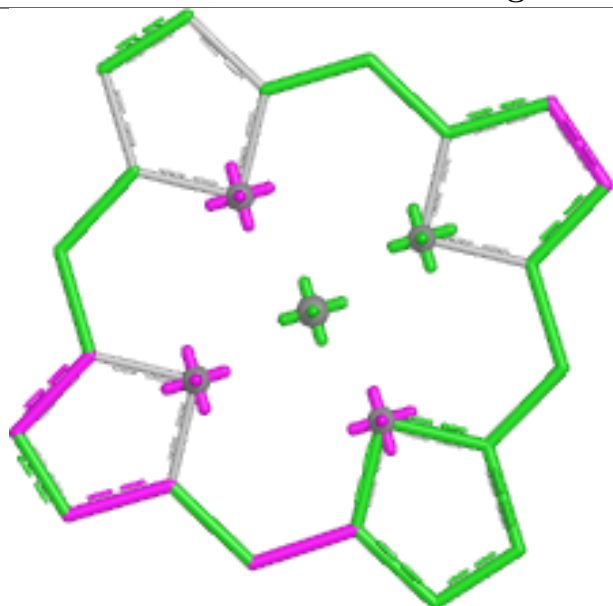


Torsions

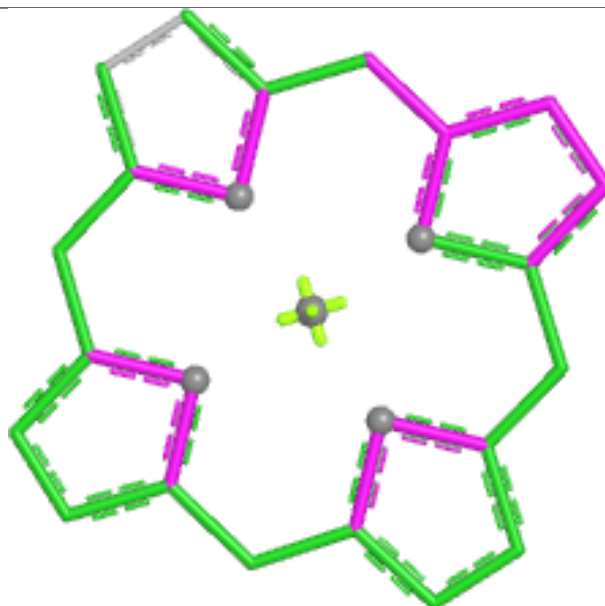


Rings

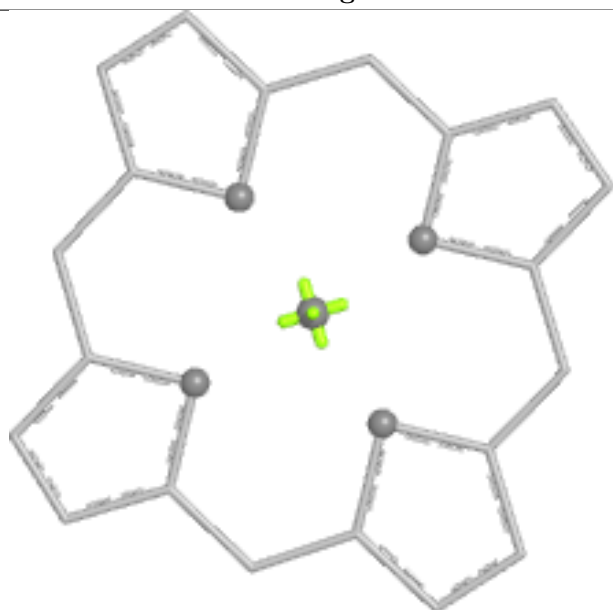
Ligand CLA L 1503



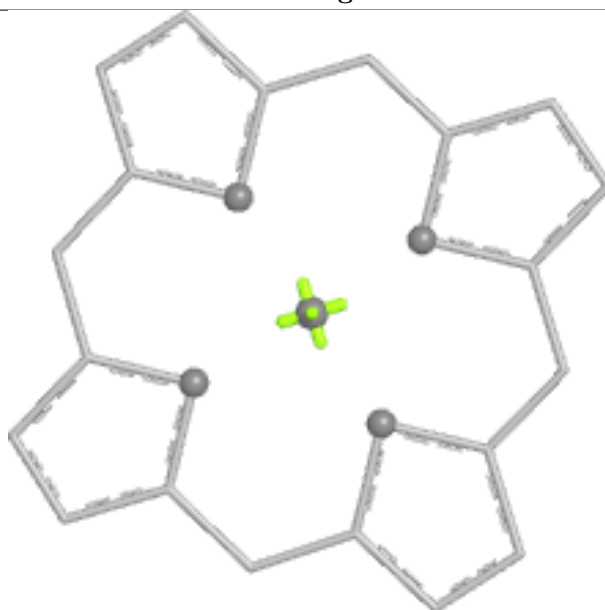
Bond lengths



Bond angles

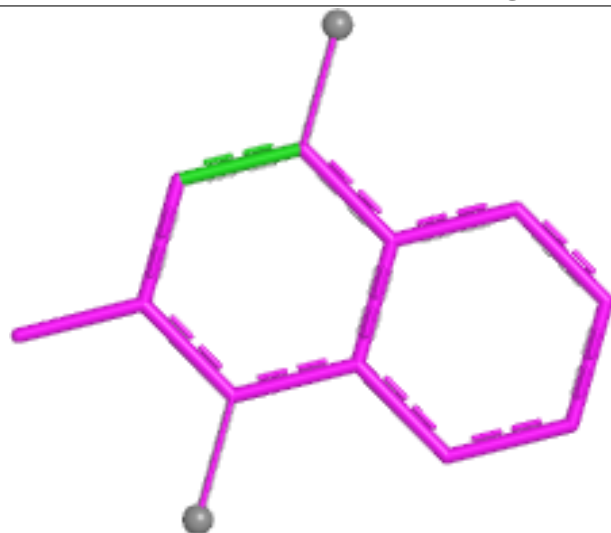


Torsions

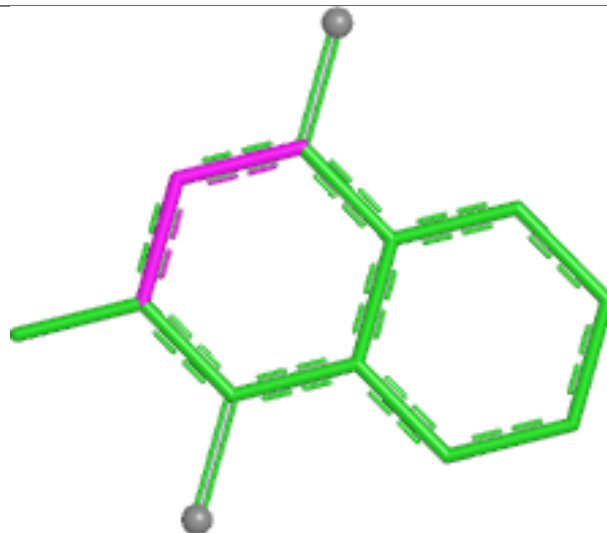


Rings

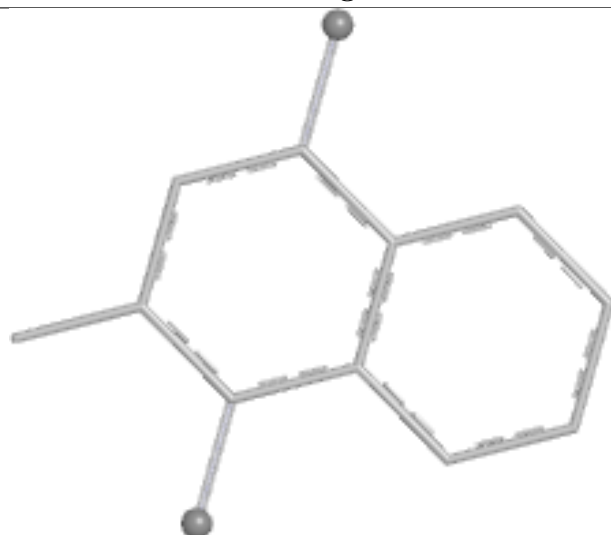
Ligand PQN P 6001



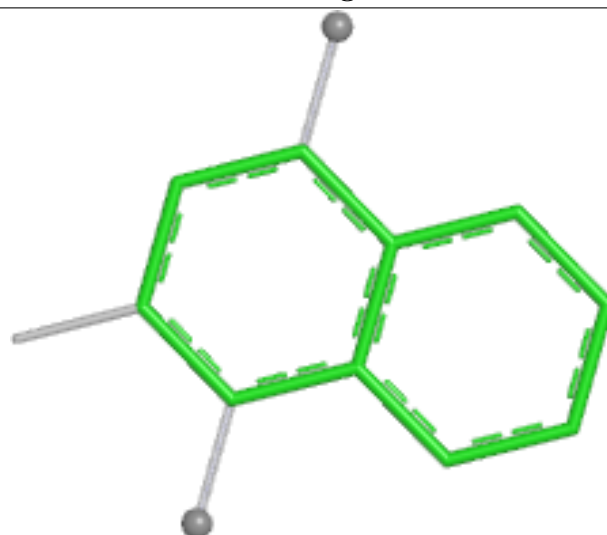
Bond lengths



Bond angles

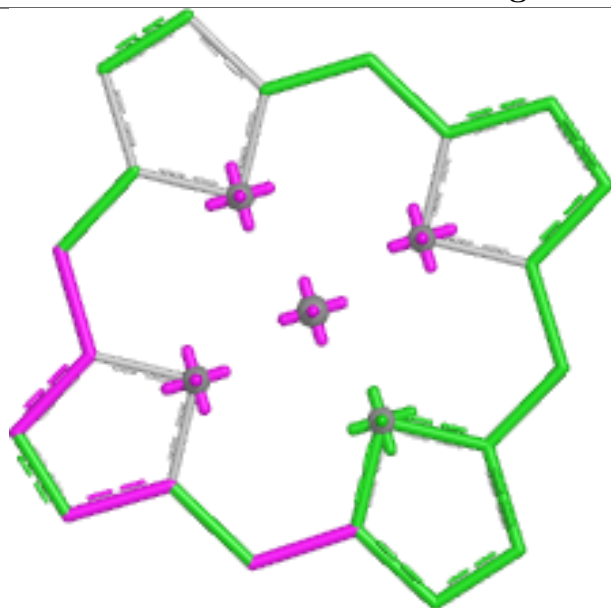


Torsions

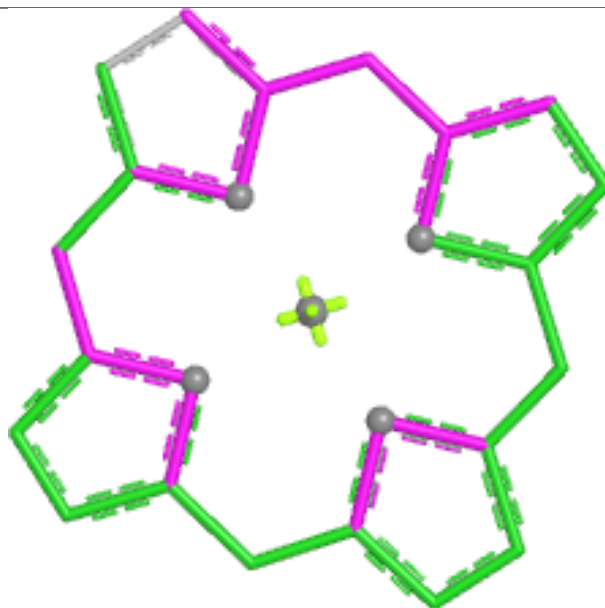


Rings

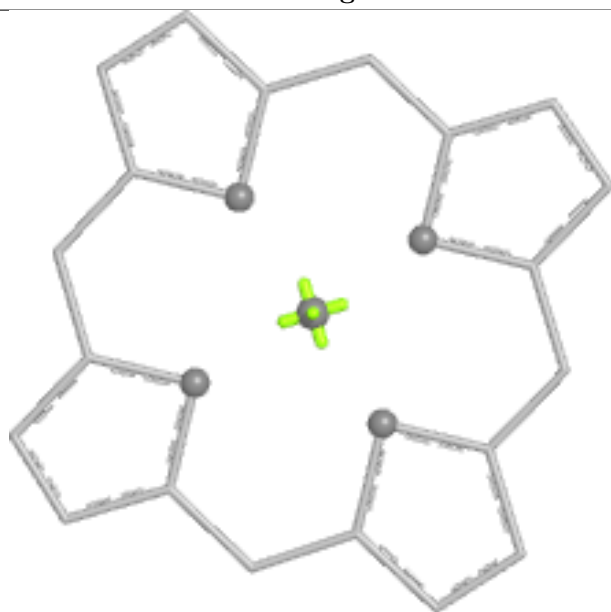
Ligand CLA 1 1021



Bond lengths



Bond angles

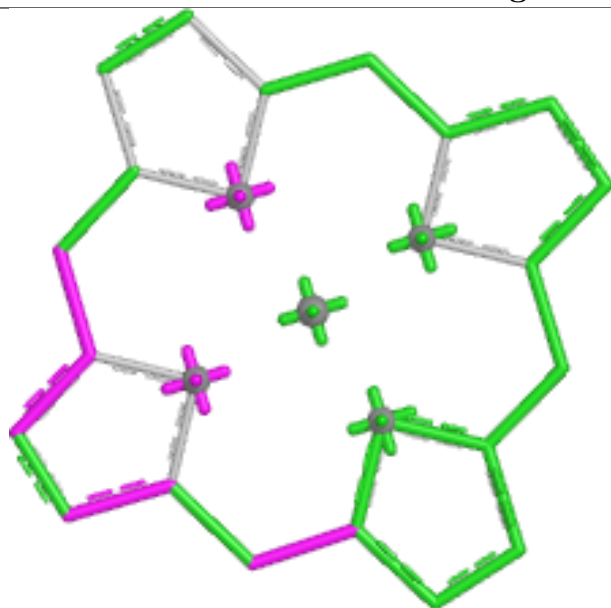


Torsions

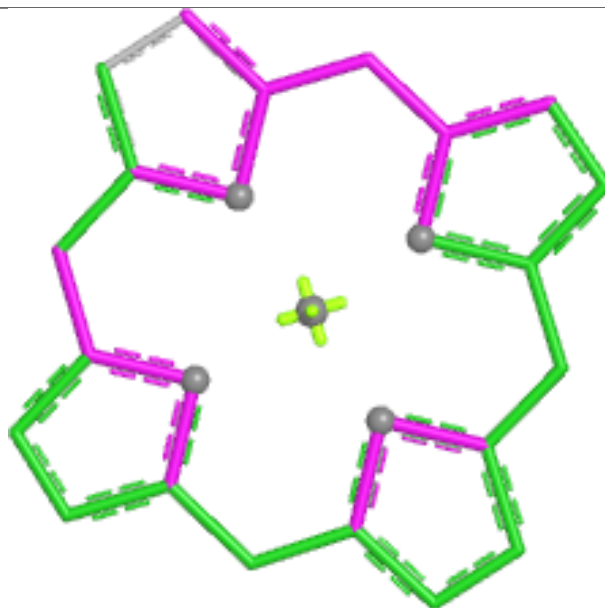


Rings

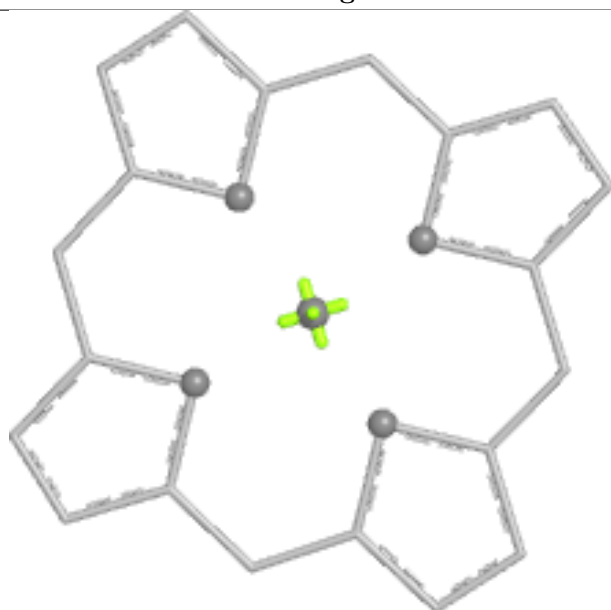
Ligand CLA 8 1017



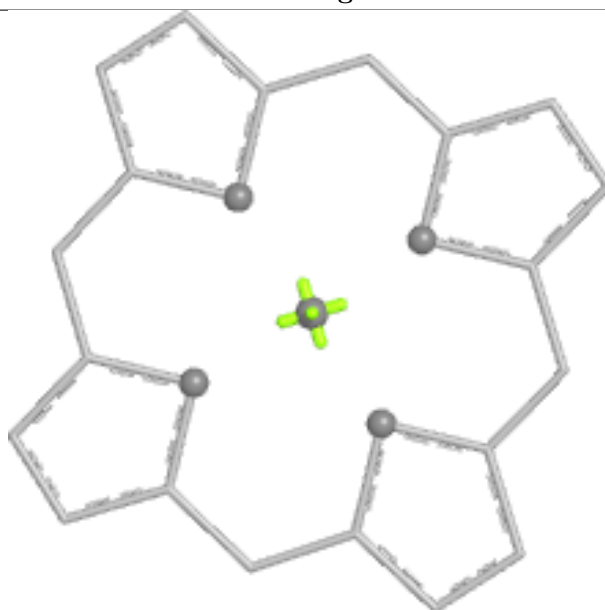
Bond lengths



Bond angles

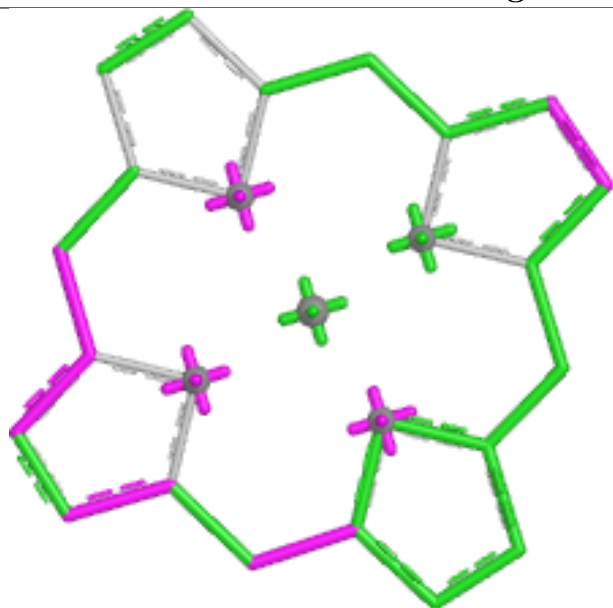


Torsions

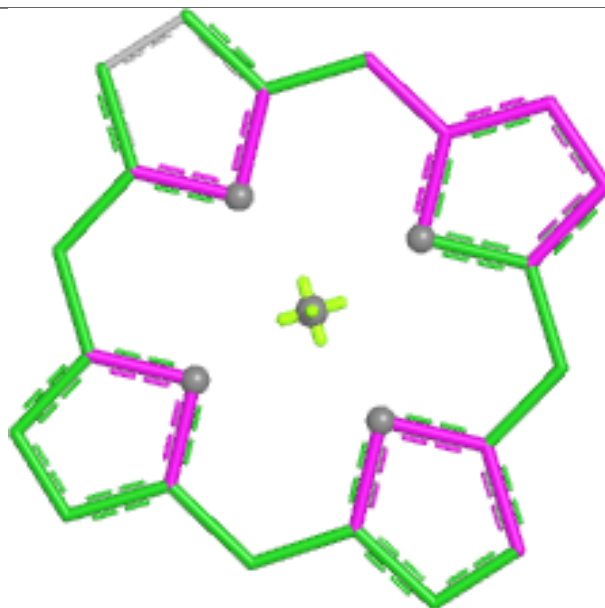


Rings

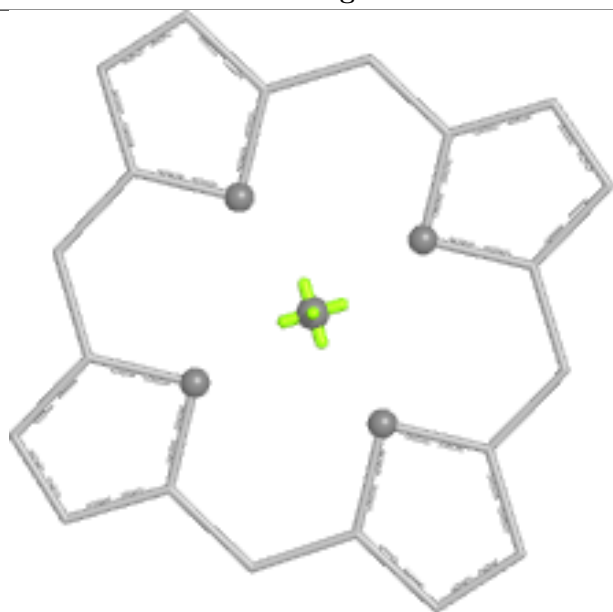
Ligand CLA F 1229



Bond lengths



Bond angles

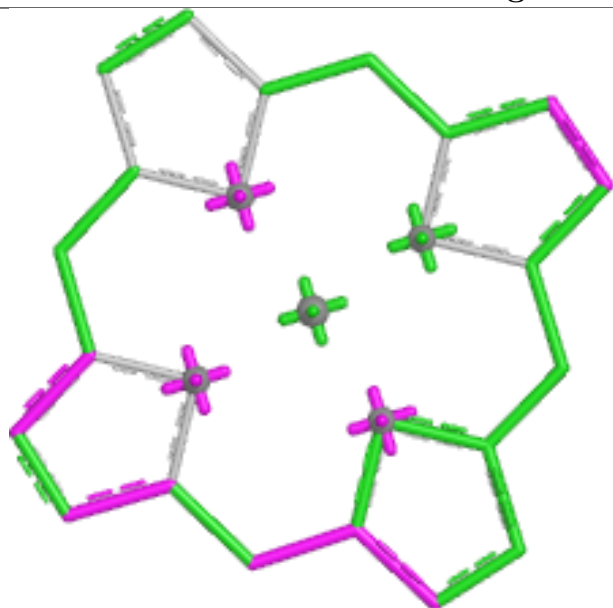


Torsions

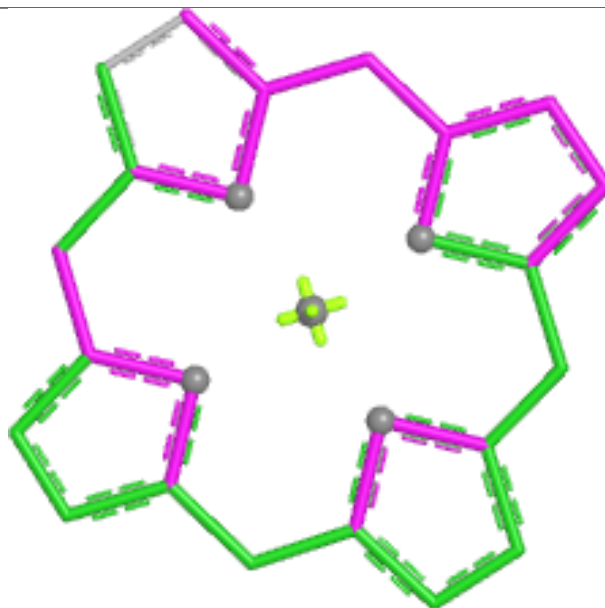


Rings

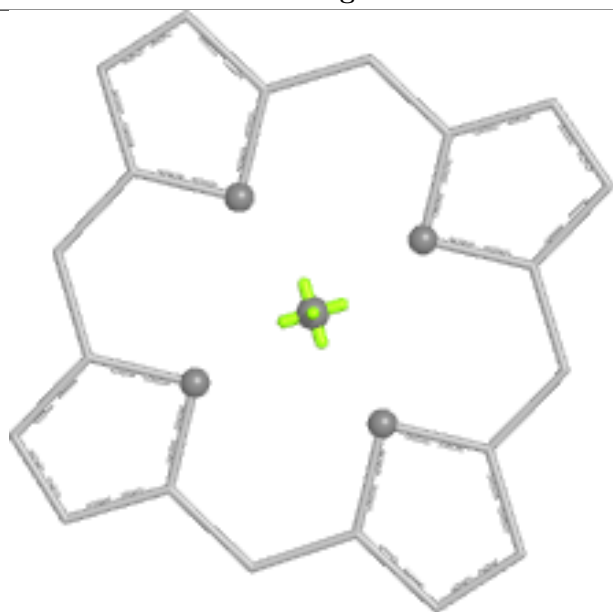
Ligand CLA L 1501



Bond lengths



Bond angles

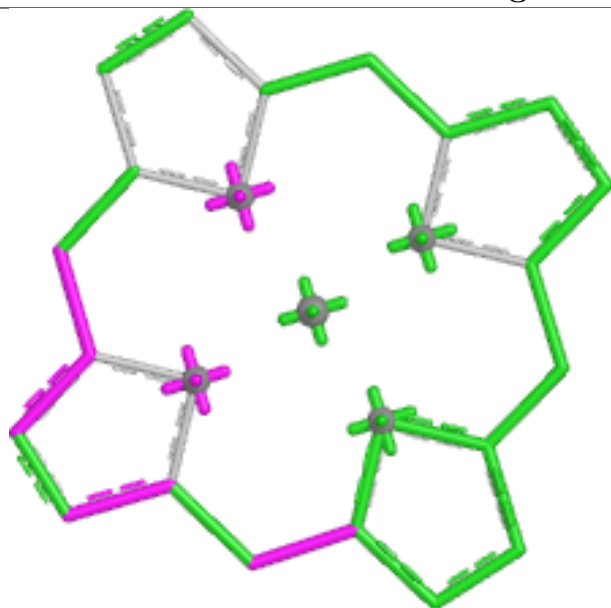


Torsions

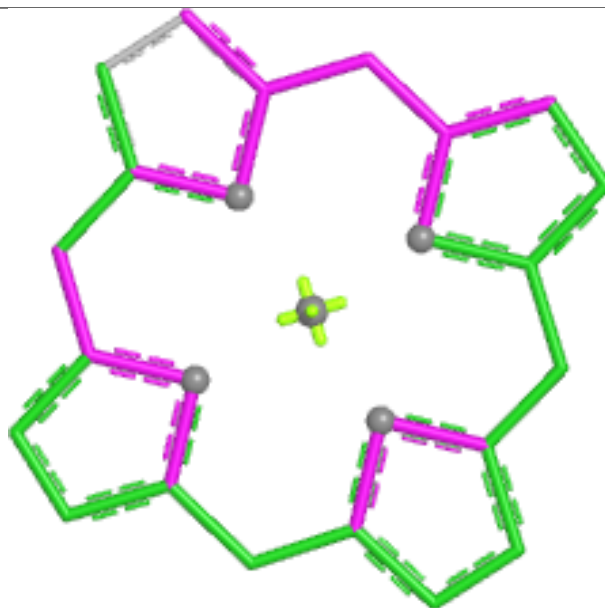


Rings

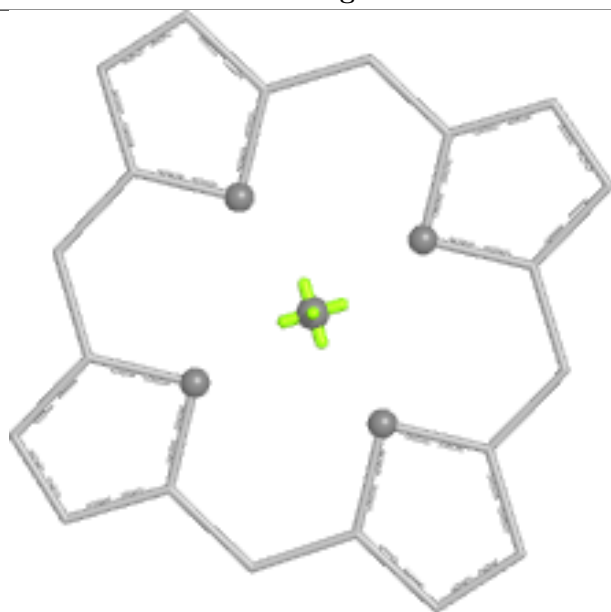
Ligand CLA 0 1032



Bond lengths



Bond angles

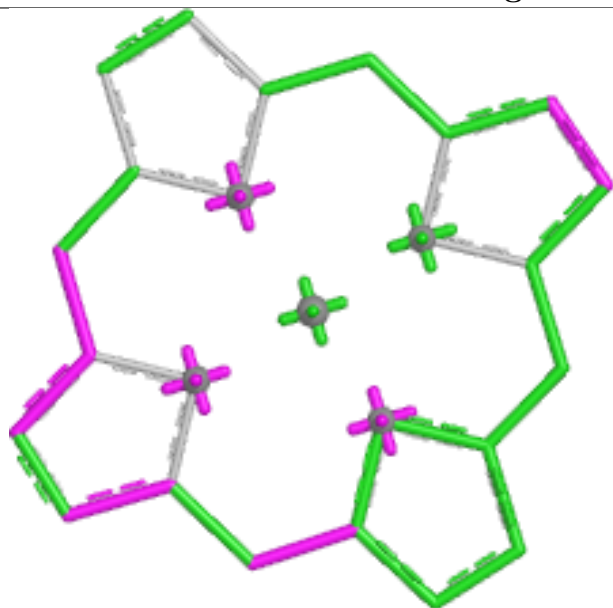


Torsions

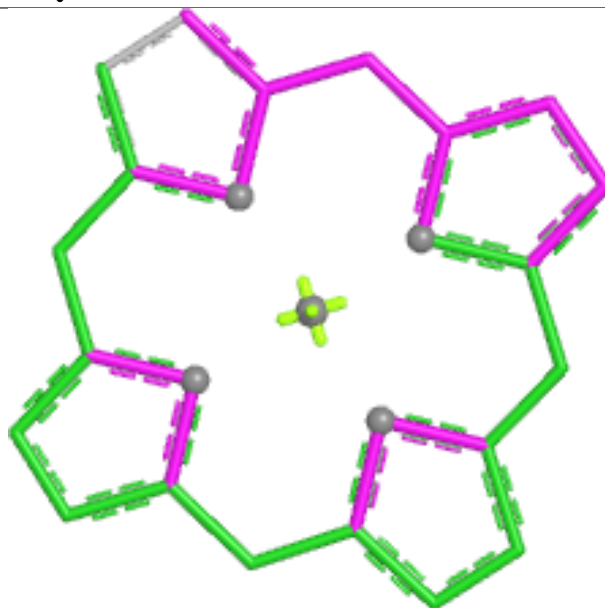


Rings

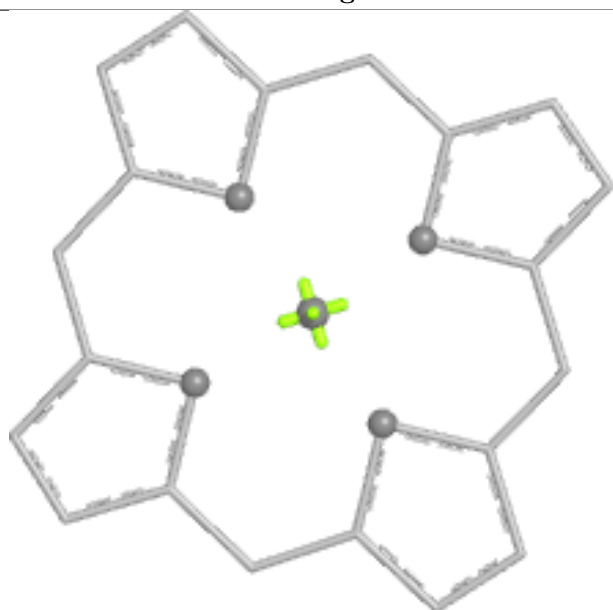
Ligand CLA Q 5212



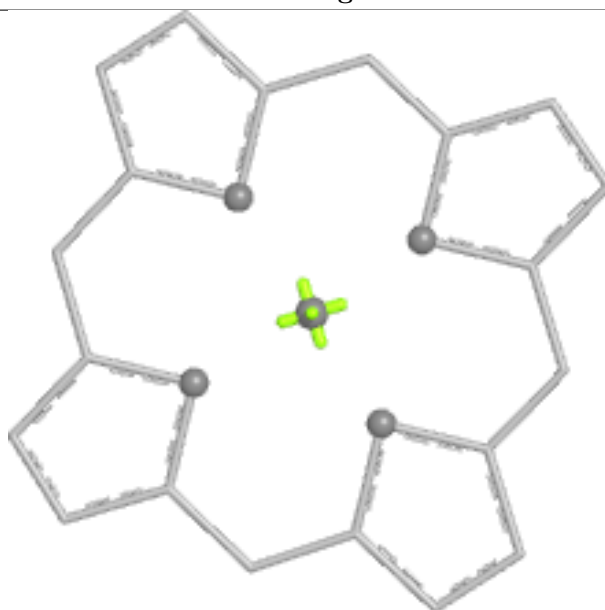
Bond lengths



Bond angles

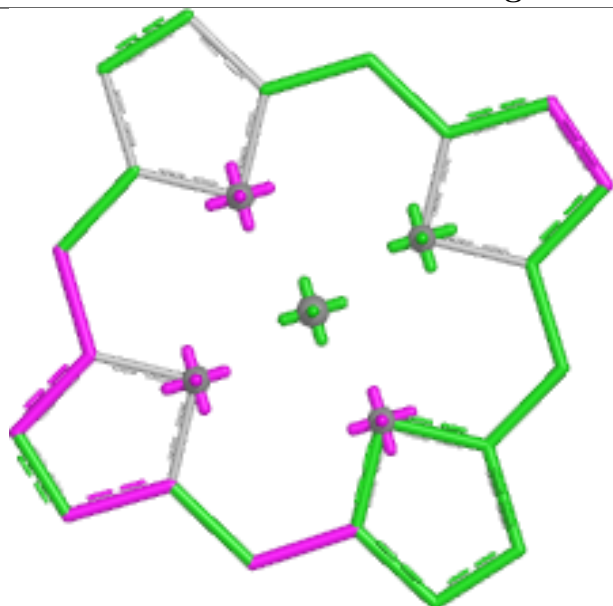


Torsions

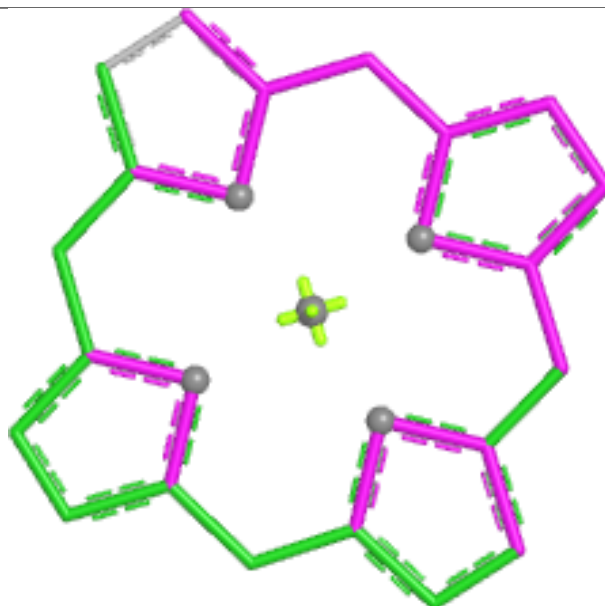


Rings

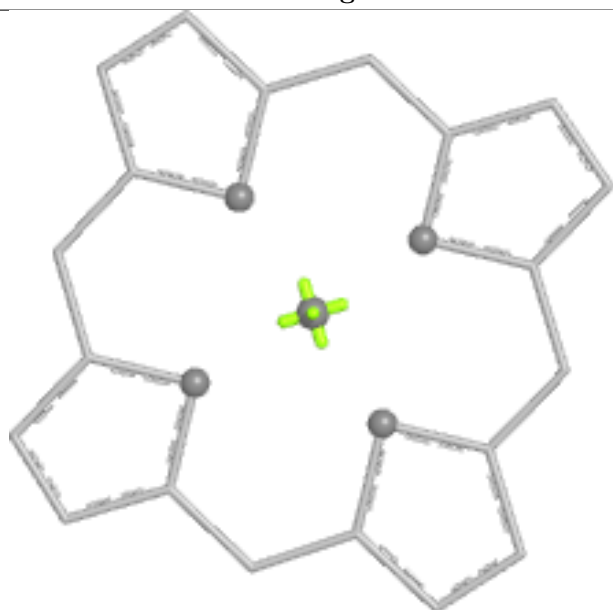
Ligand CLA A 1013



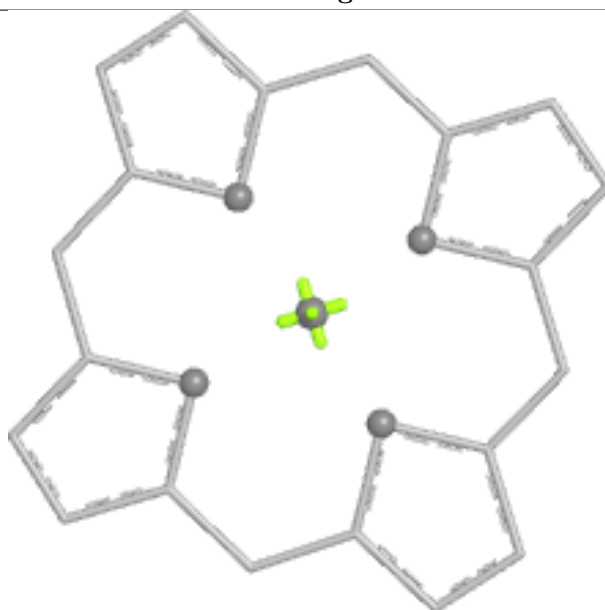
Bond lengths



Bond angles

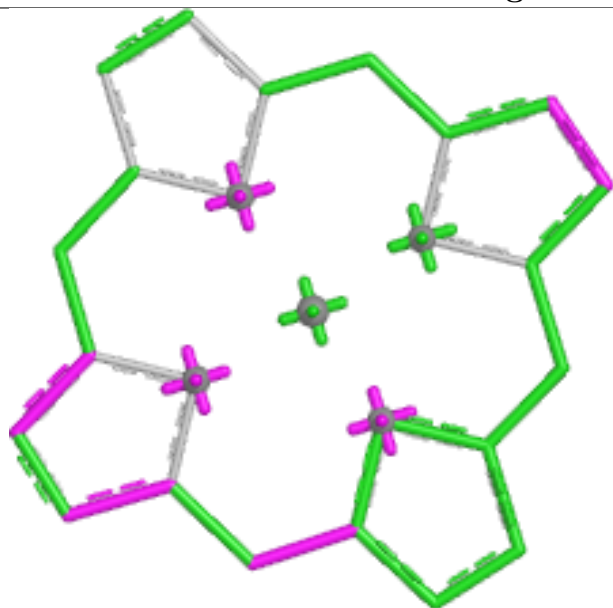


Torsions

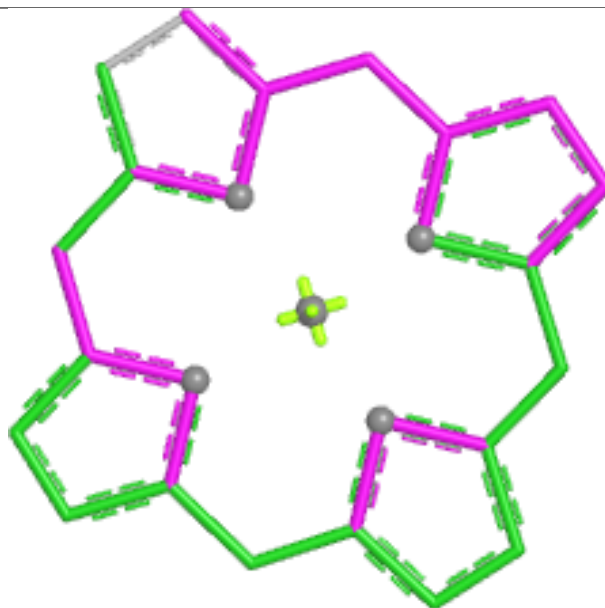


Rings

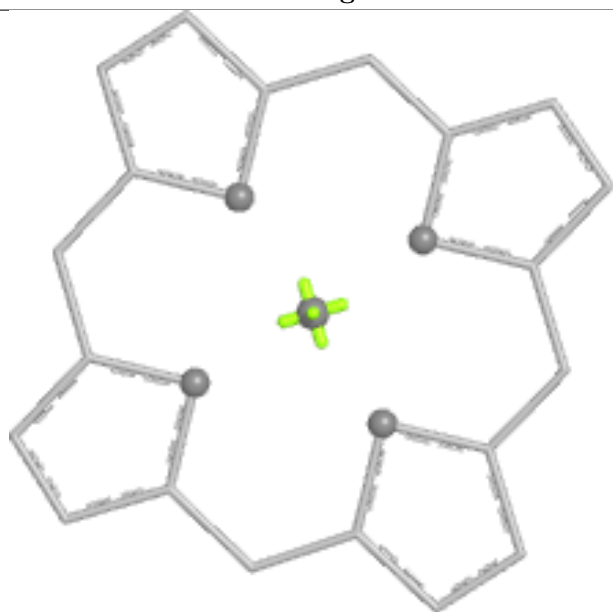
Ligand CLA P 5128



Bond lengths



Bond angles

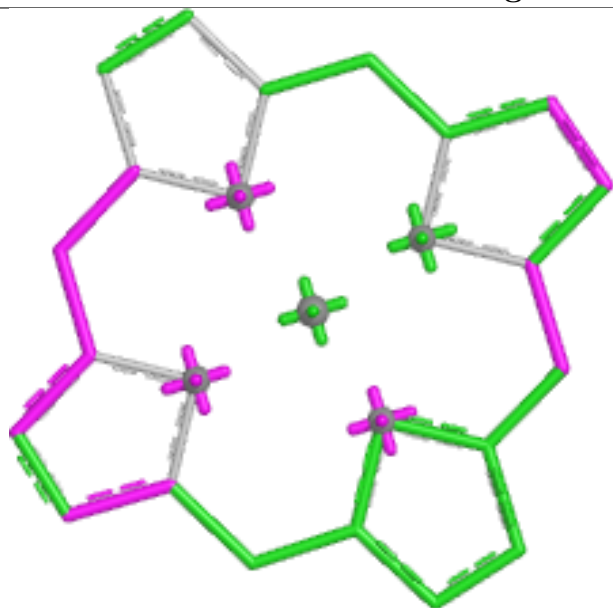


Torsions

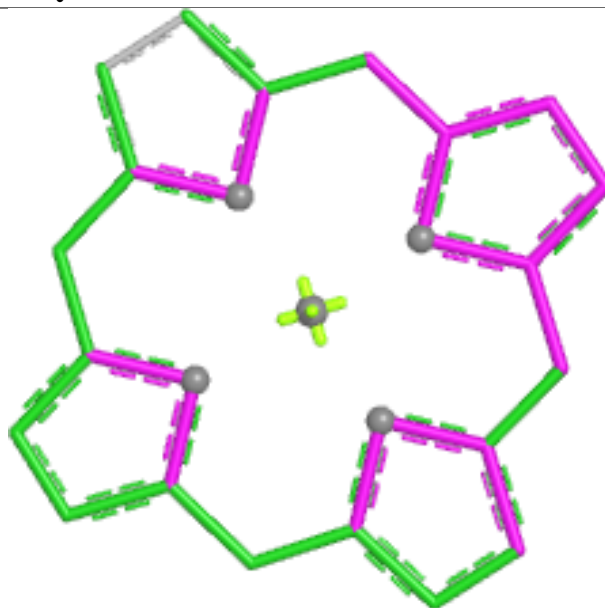


Rings

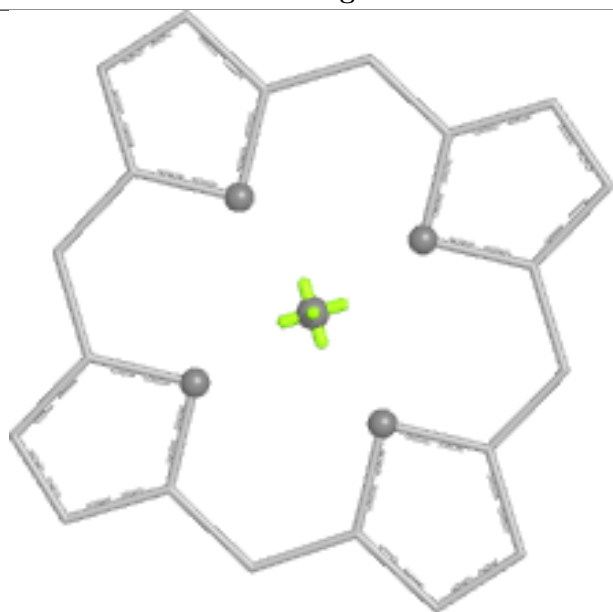
Ligand CLA Q 5204



Bond lengths



Bond angles

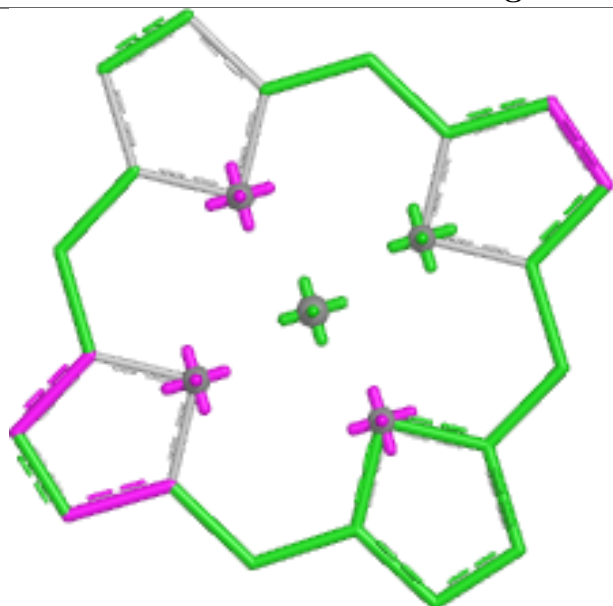


Torsions

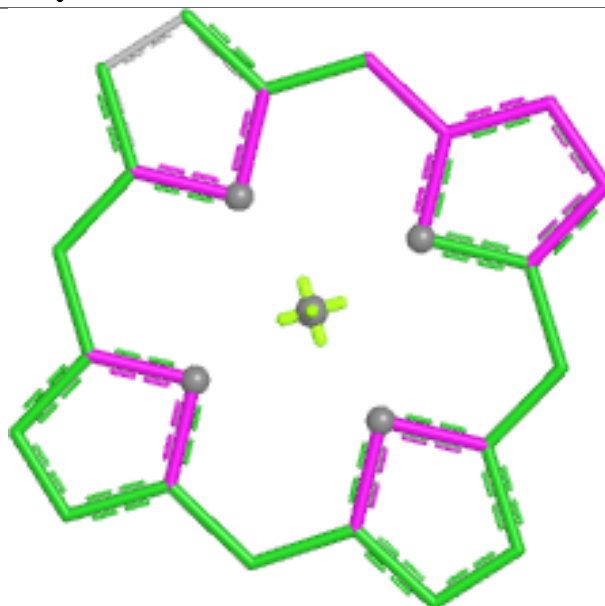


Rings

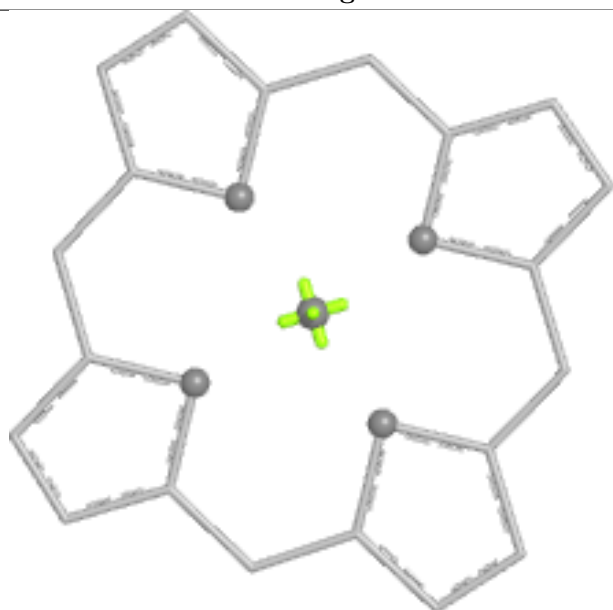
Ligand CLA Q 5202



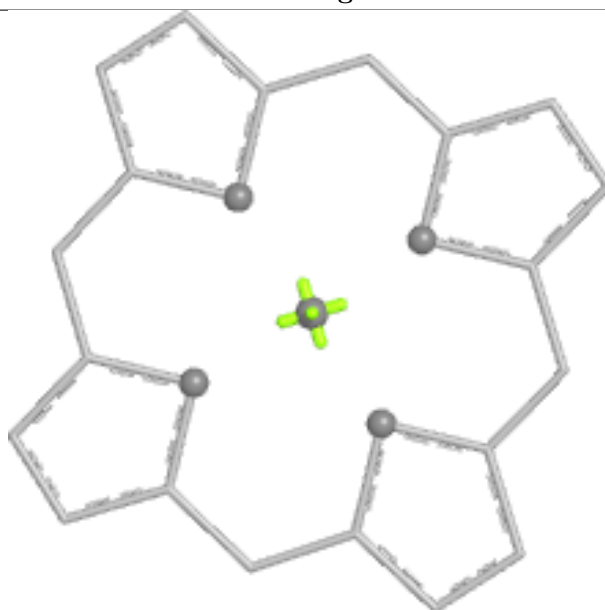
Bond lengths



Bond angles

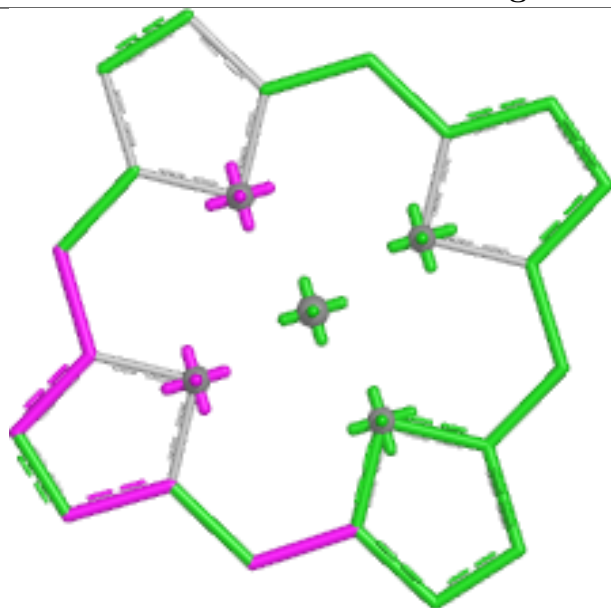


Torsions

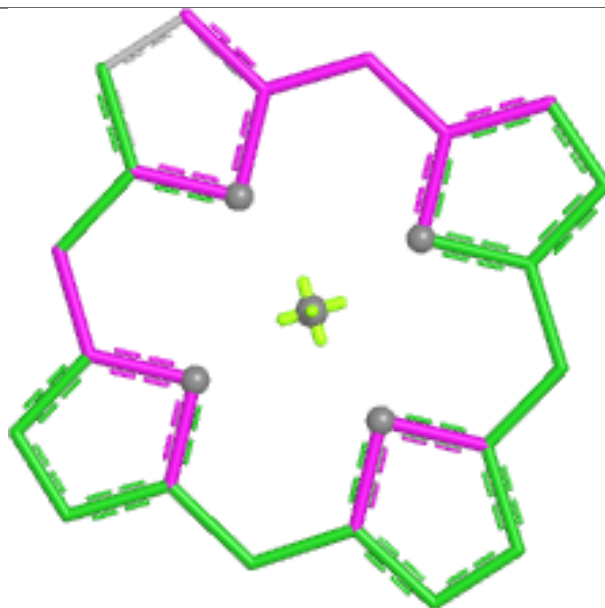


Rings

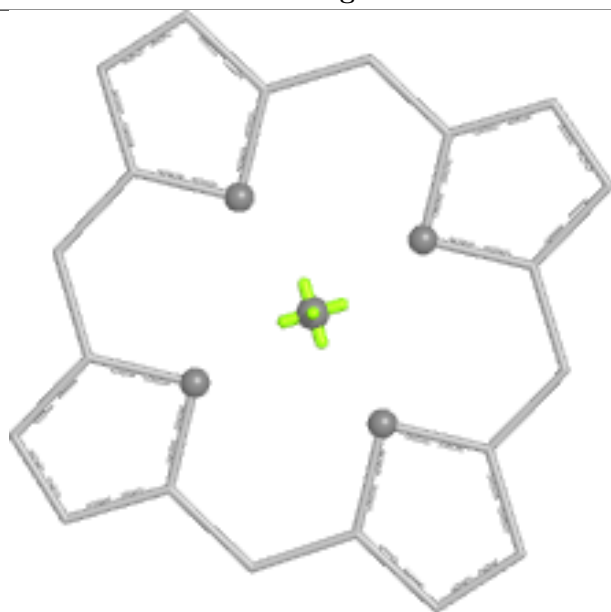
Ligand CLA 4 4002



Bond lengths



Bond angles

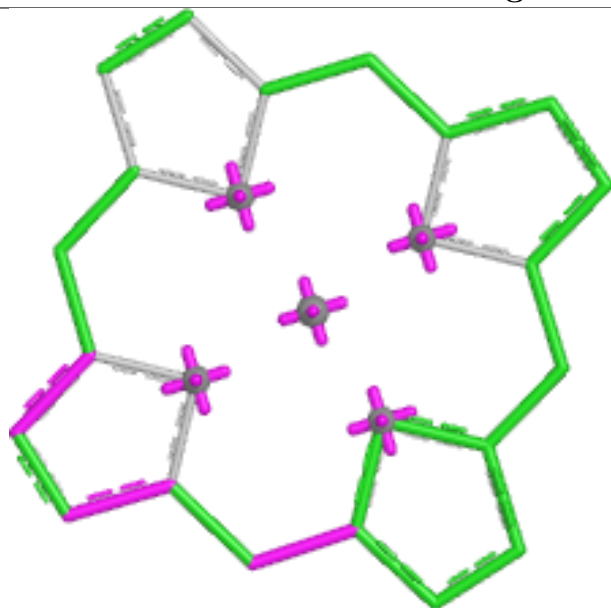


Torsions

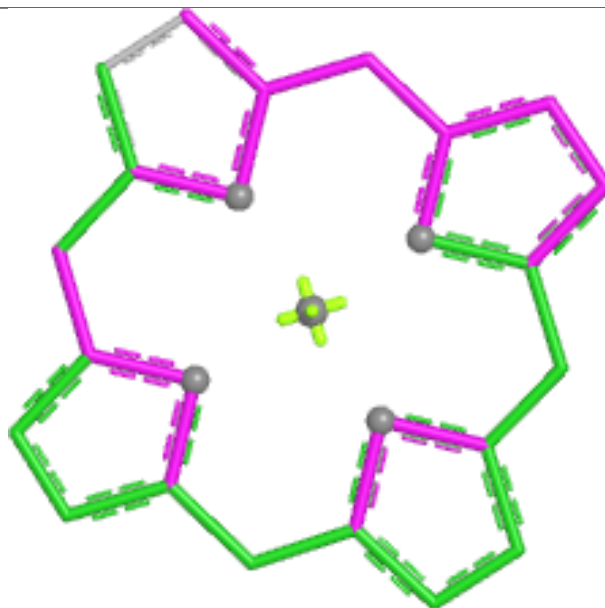


Rings

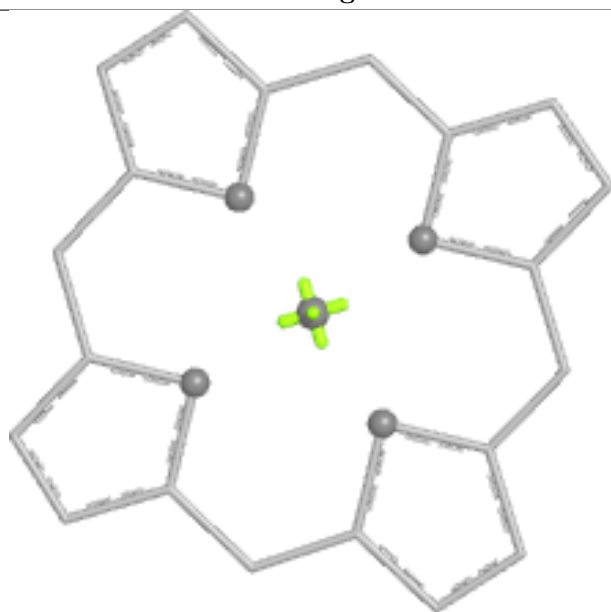
Ligand CLA P 5107



Bond lengths



Bond angles

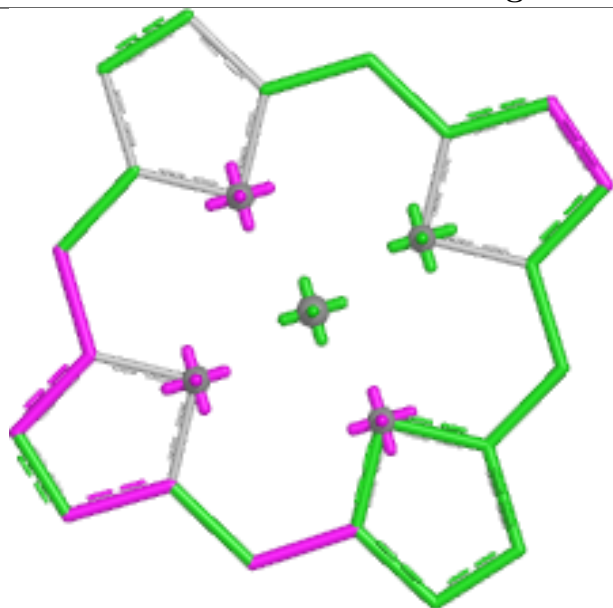


Torsions

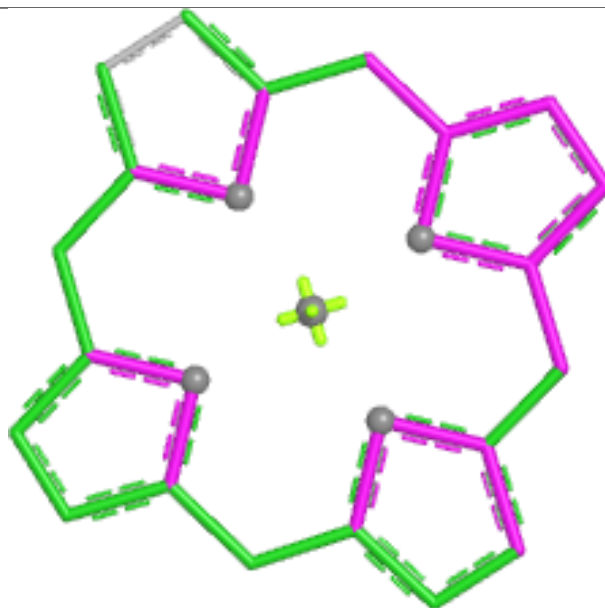


Rings

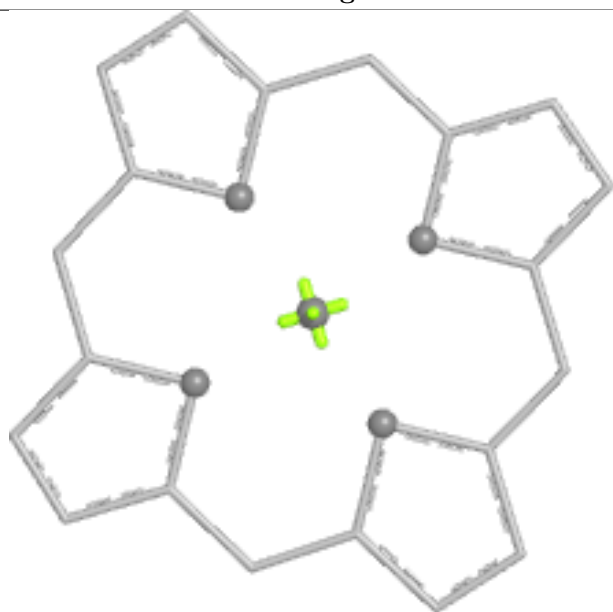
Ligand CLA P 5136



Bond lengths



Bond angles

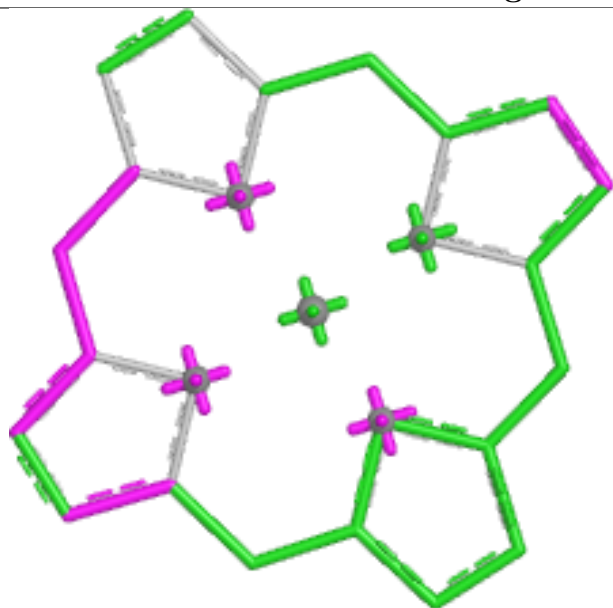


Torsions

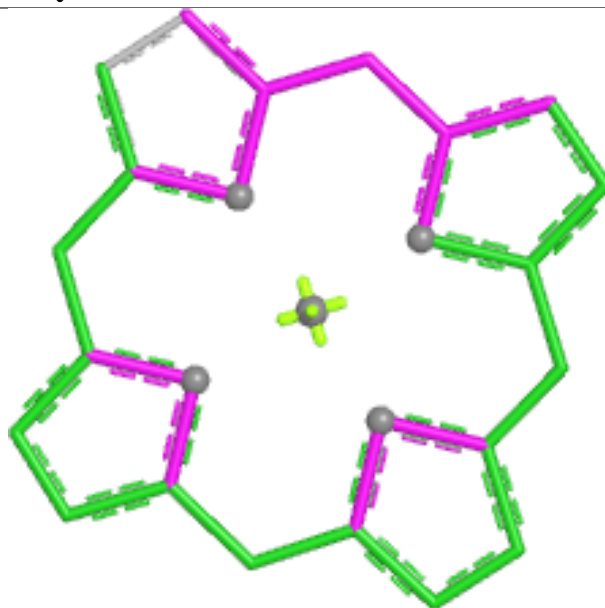


Rings

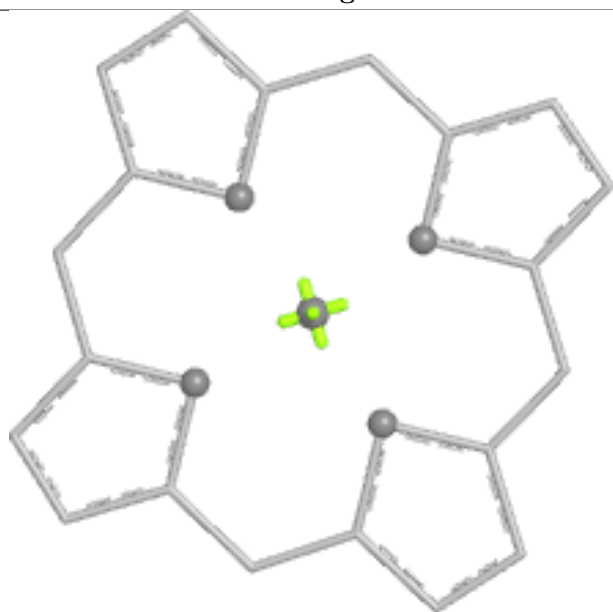
Ligand CLA Q 5021



Bond lengths



Bond angles

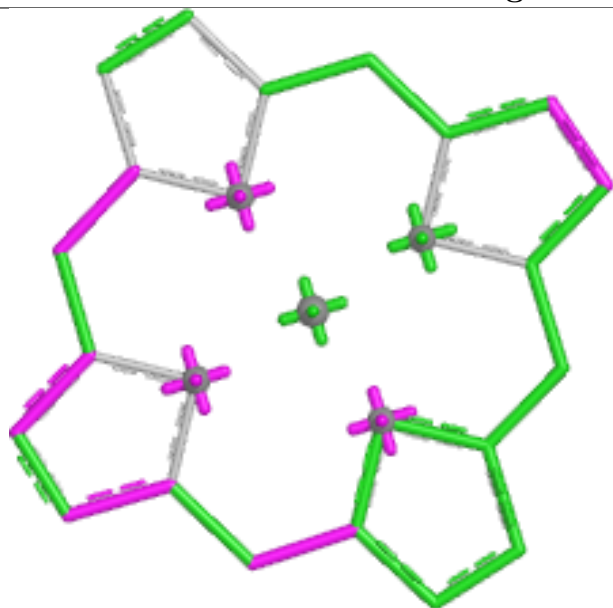


Torsions

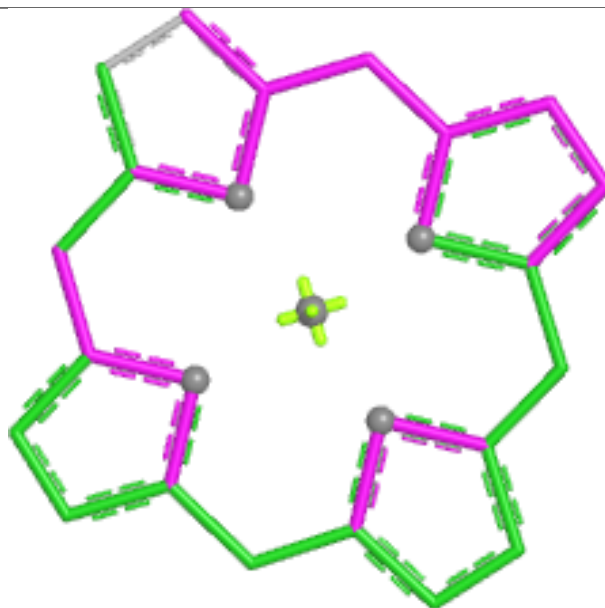


Rings

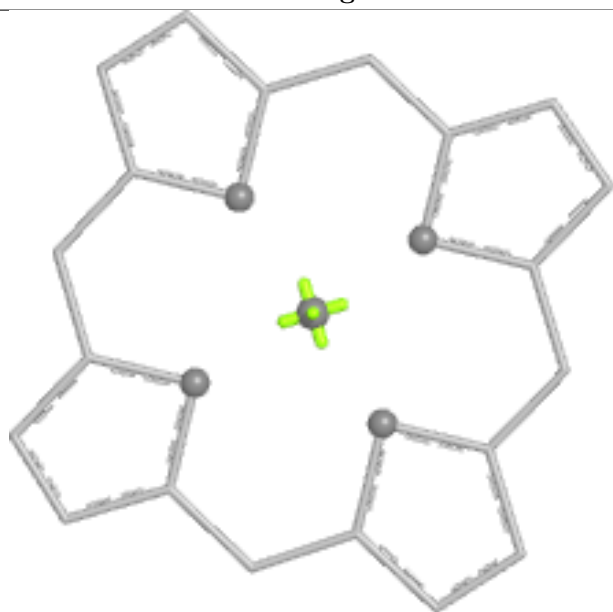
Ligand CLA P 5125



Bond lengths



Bond angles

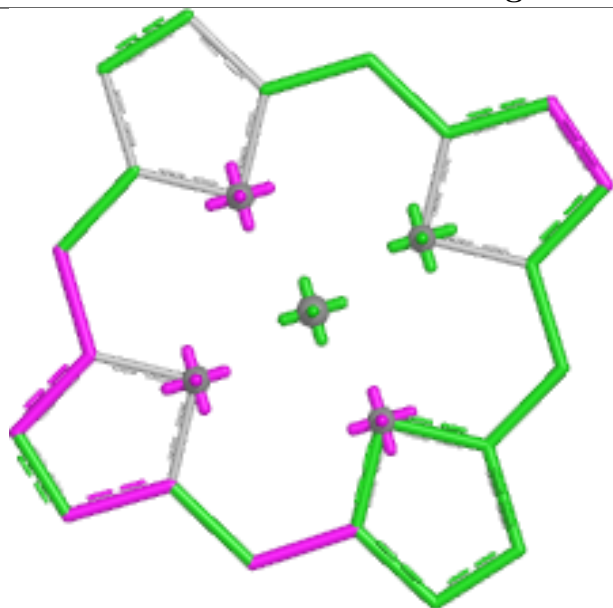


Torsions

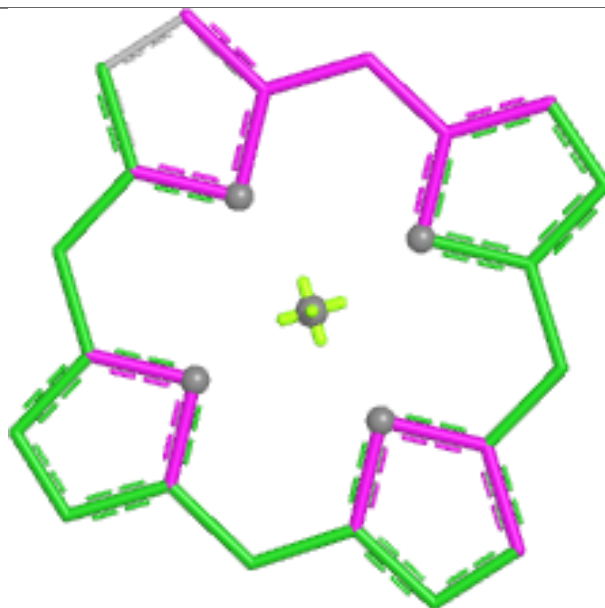


Rings

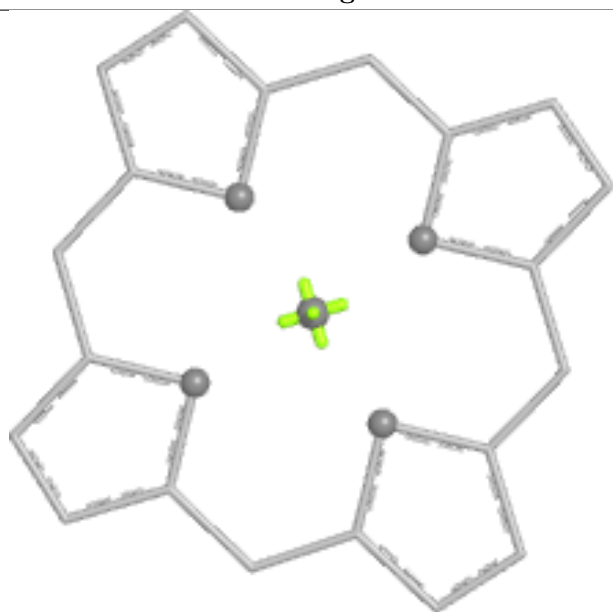
Ligand CLA B 1235



Bond lengths



Bond angles

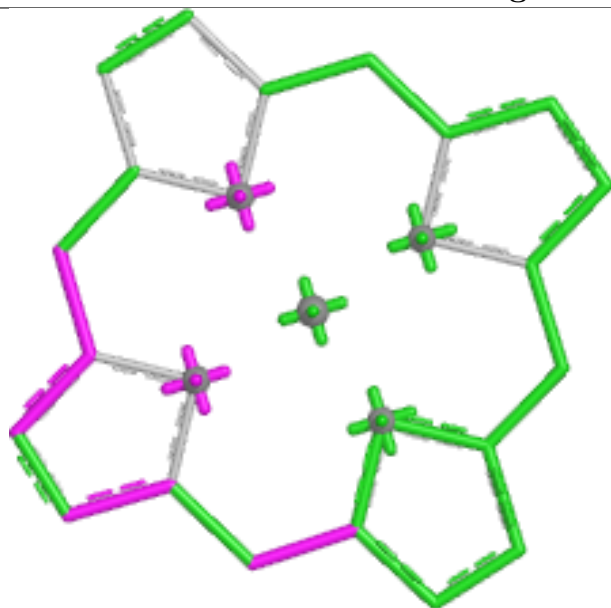


Torsions

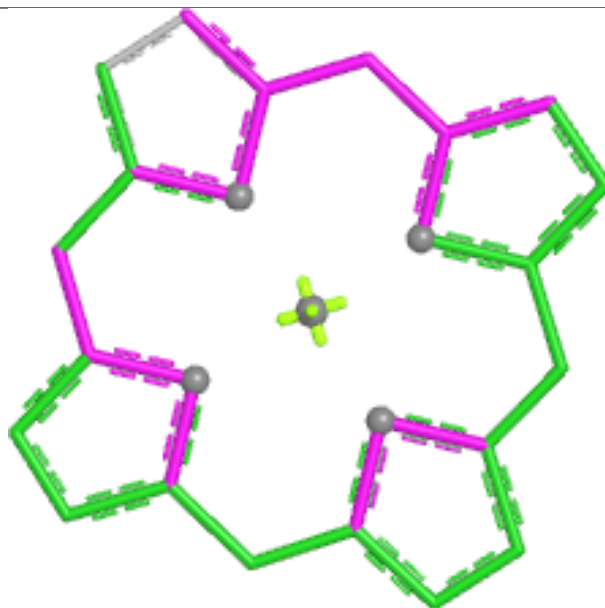


Rings

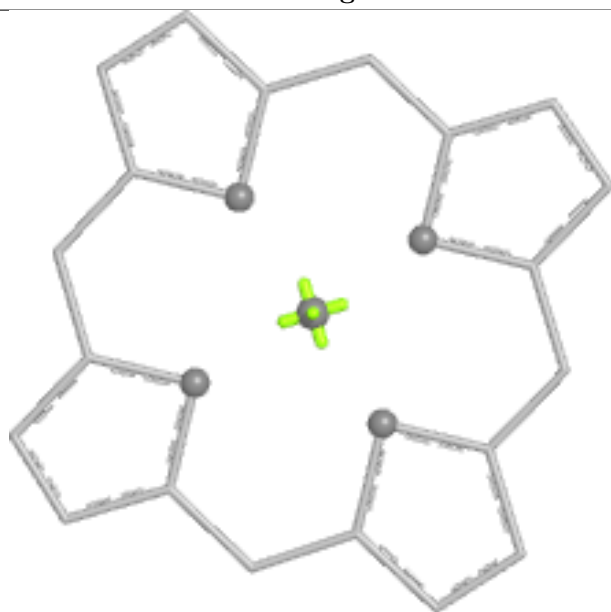
Ligand CLA 3 1011



Bond lengths



Bond angles

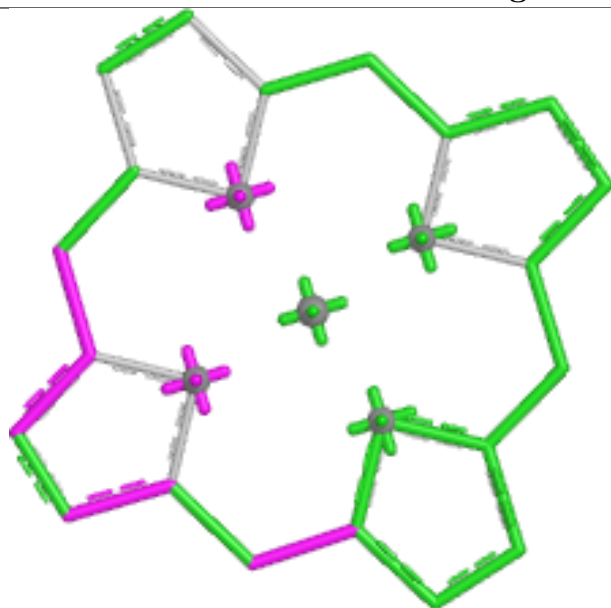


Torsions

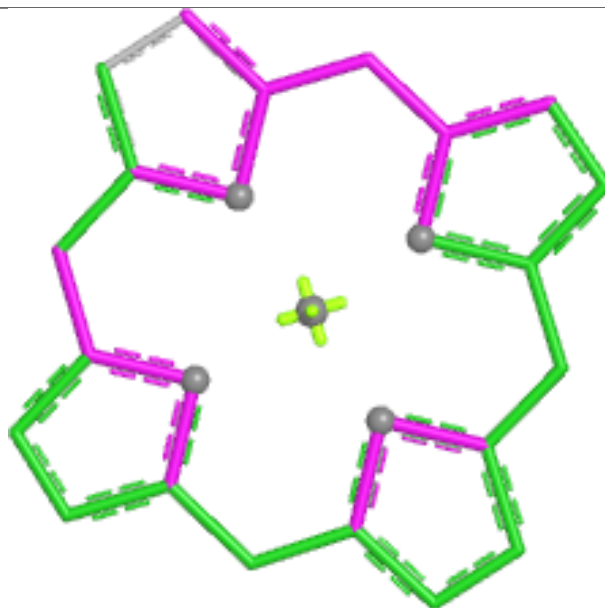


Rings

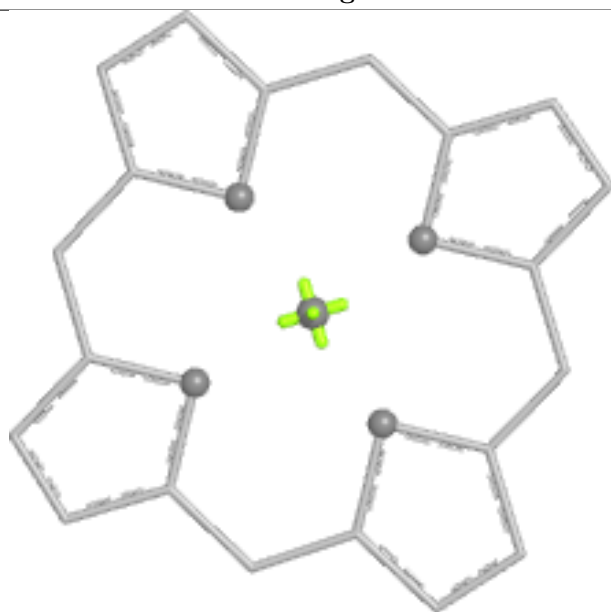
Ligand CLA 2 1017



Bond lengths



Bond angles

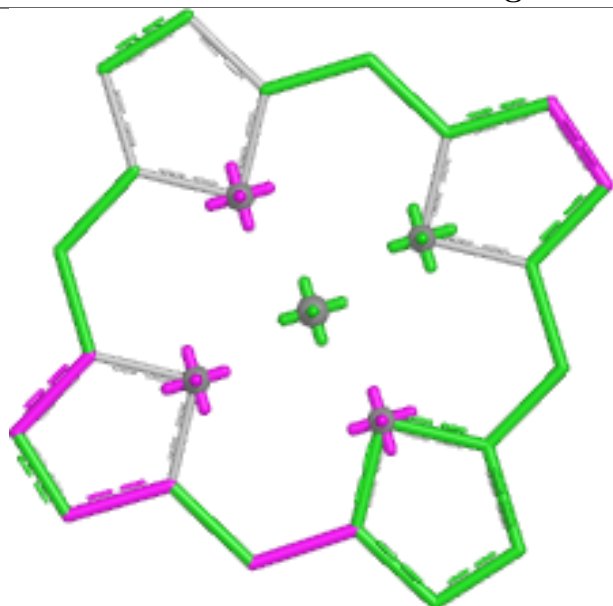


Torsions

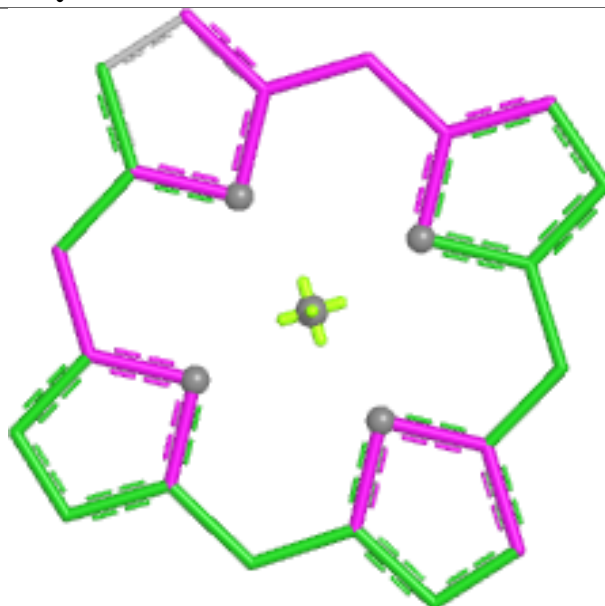


Rings

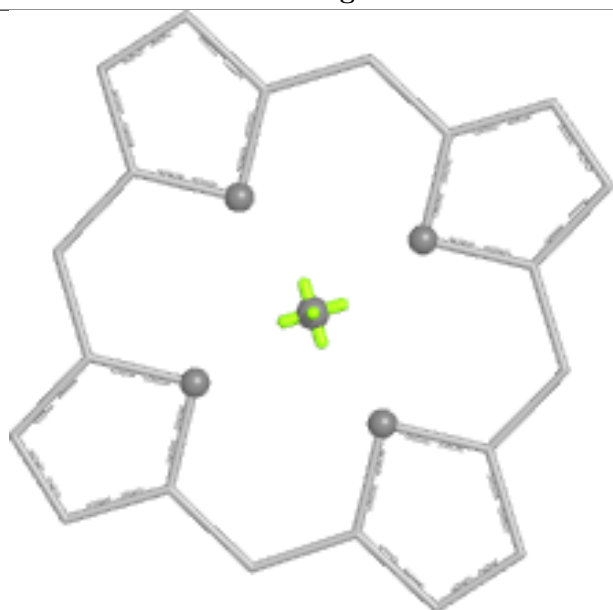
Ligand CLA Q 5213



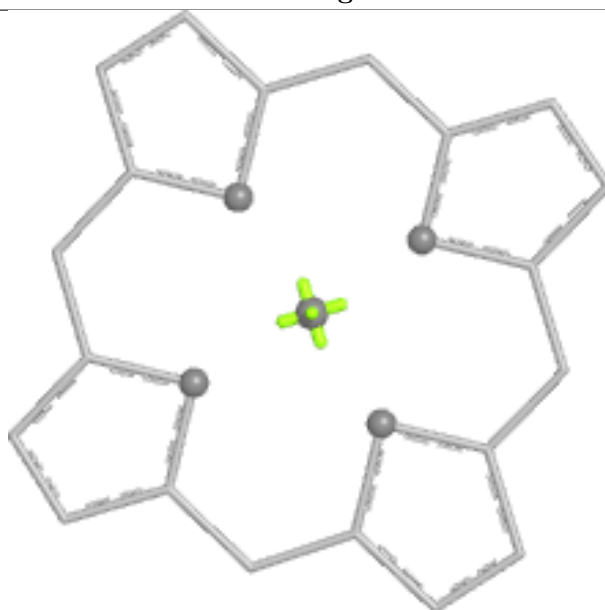
Bond lengths



Bond angles

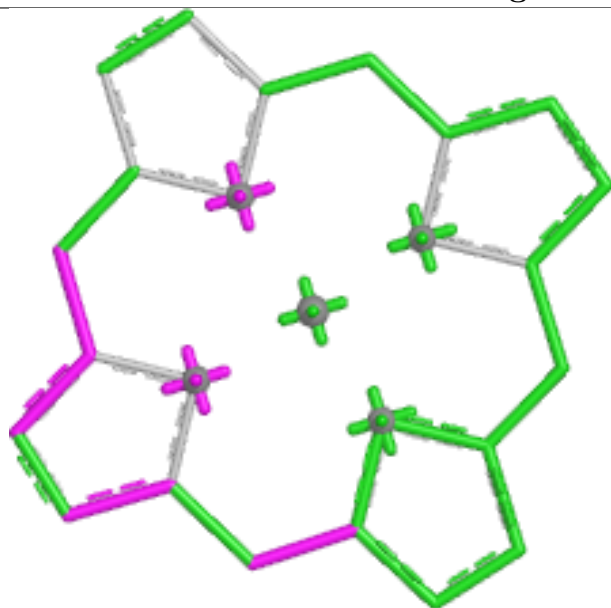


Torsions

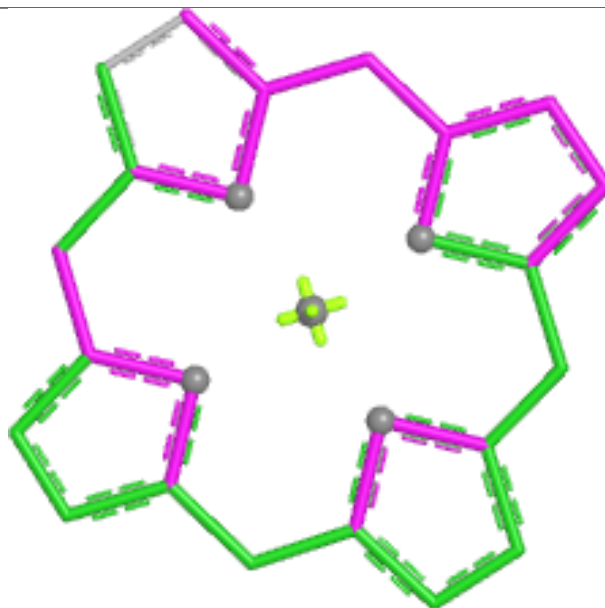


Rings

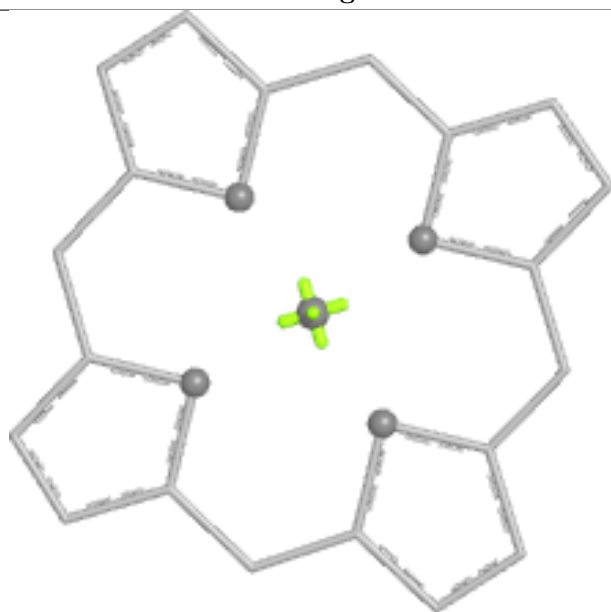
Ligand CLA 0 8002



Bond lengths



Bond angles

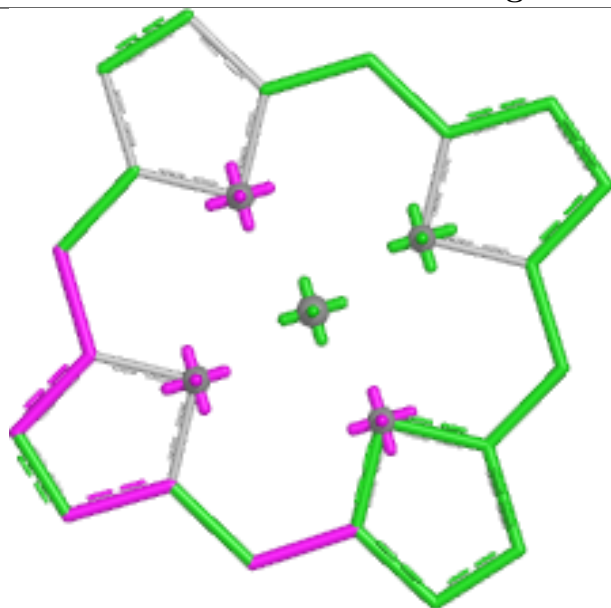


Torsions

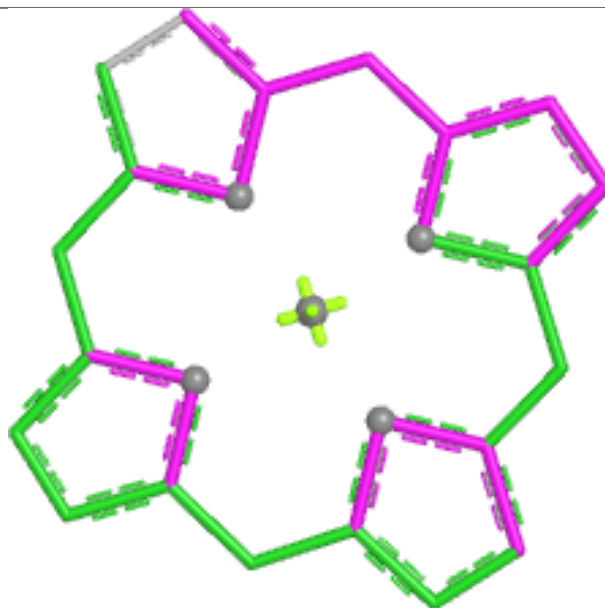


Rings

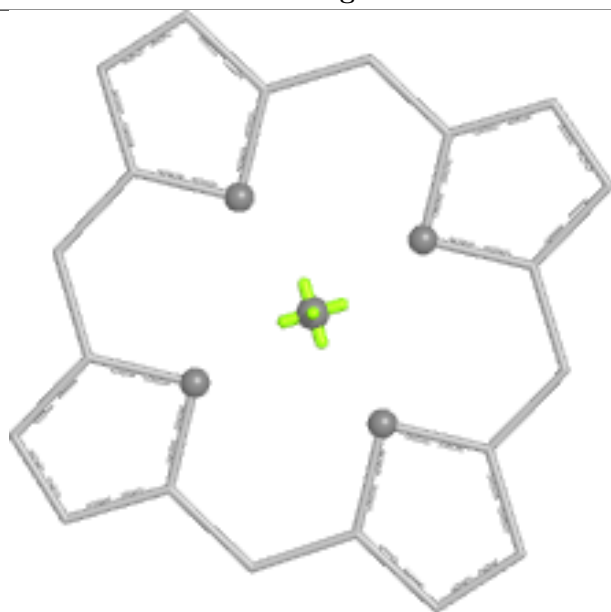
Ligand CLA P 5138



Bond lengths



Bond angles

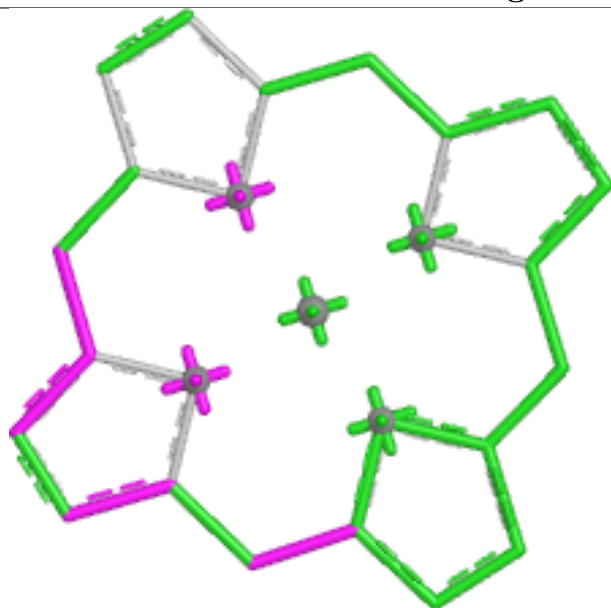


Torsions

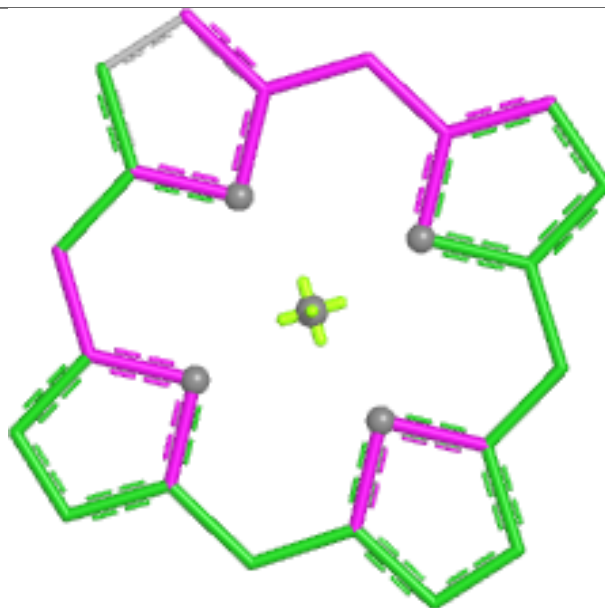


Rings

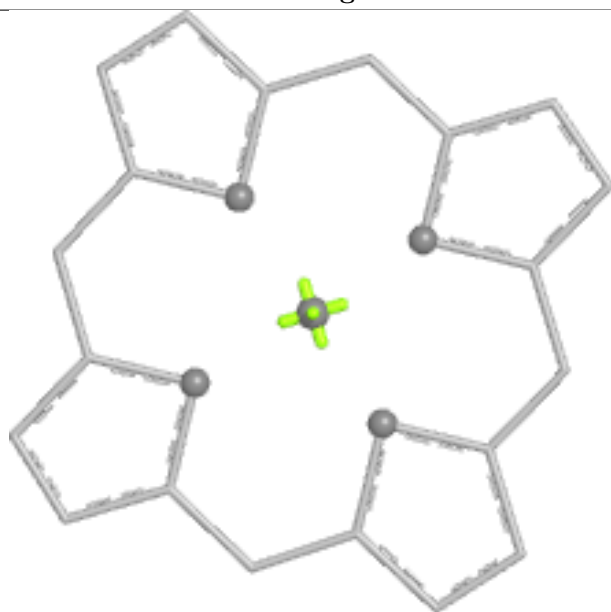
Ligand CLA Z 5101



Bond lengths



Bond angles

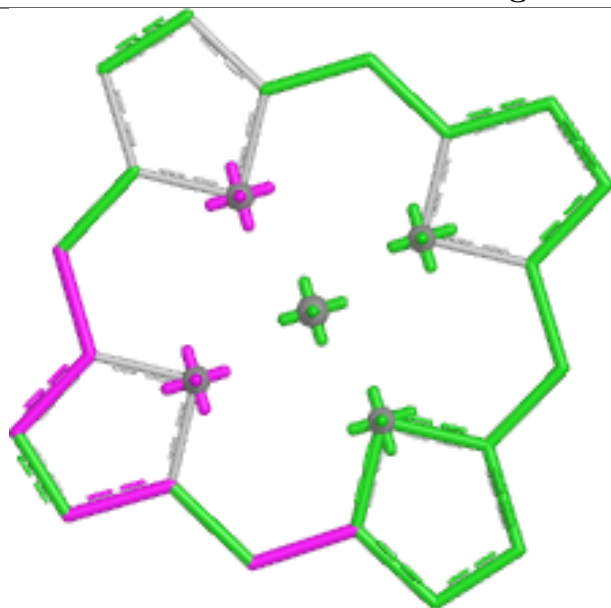


Torsions

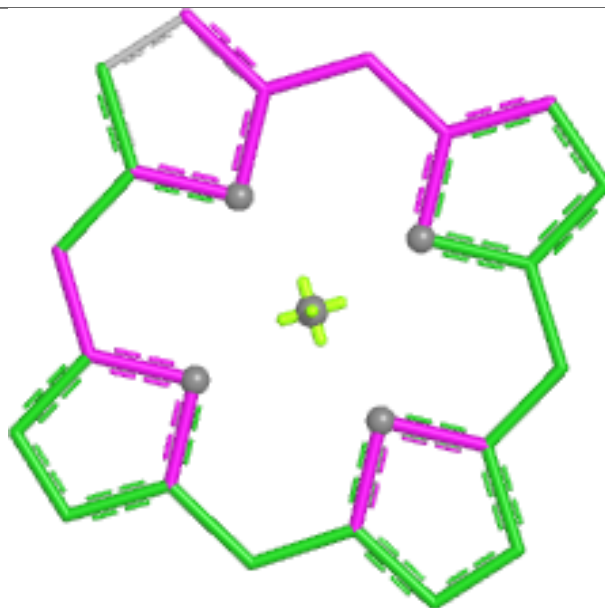


Rings

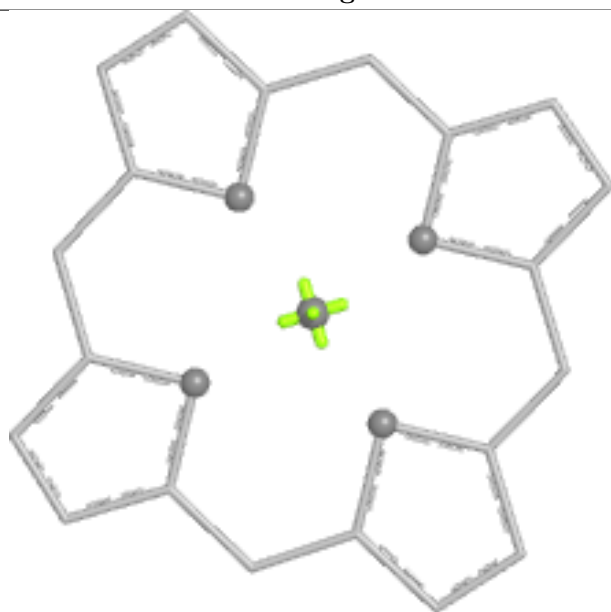
Ligand CLA 7 1031



Bond lengths



Bond angles

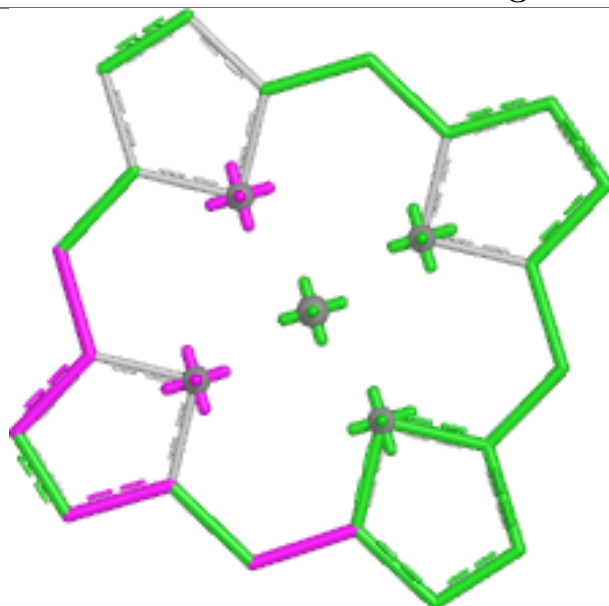


Torsions

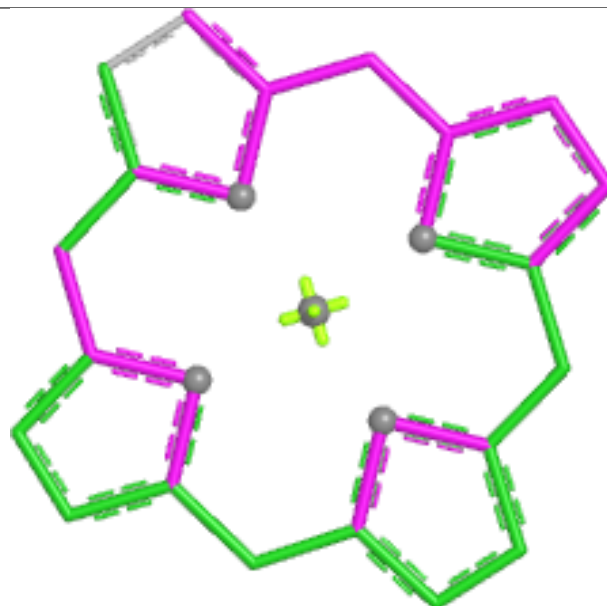


Rings

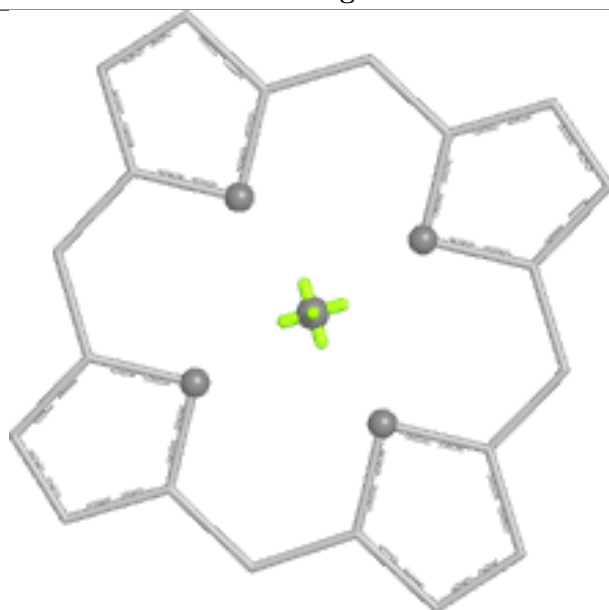
Ligand CLA 9 1021



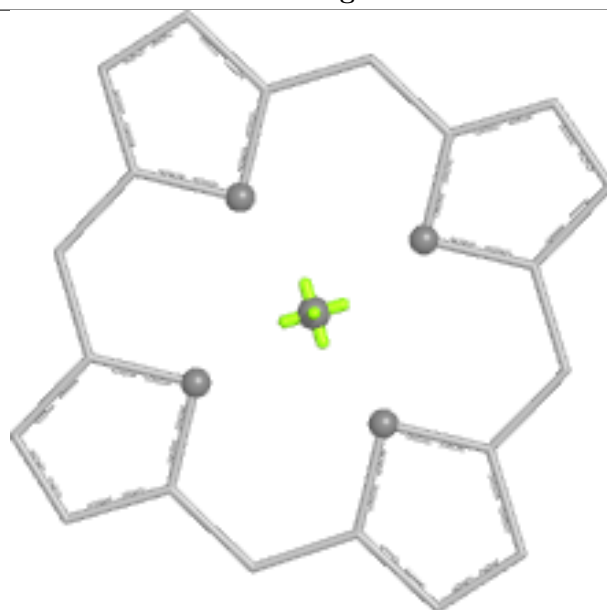
Bond lengths



Bond angles

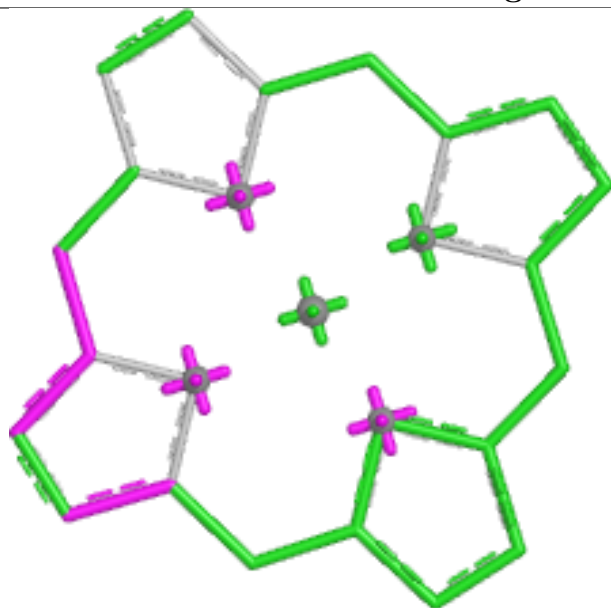


Torsions

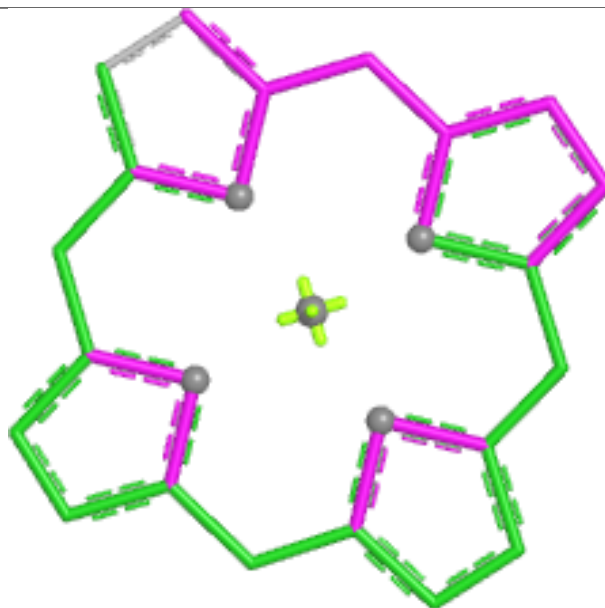


Rings

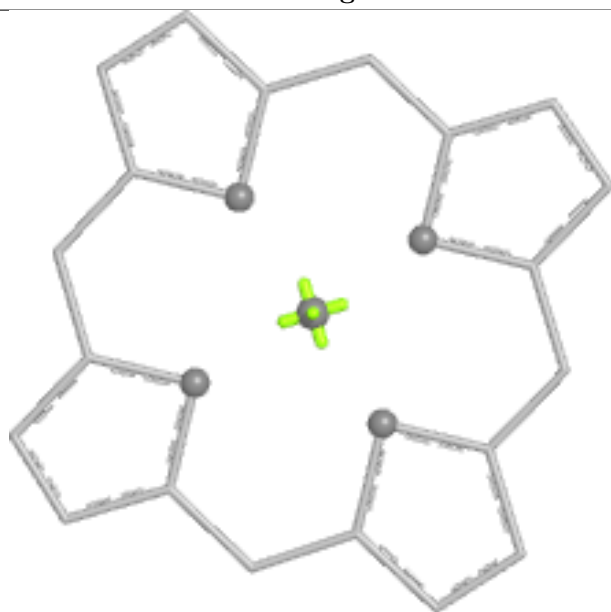
Ligand CLA A 1126



Bond lengths



Bond angles

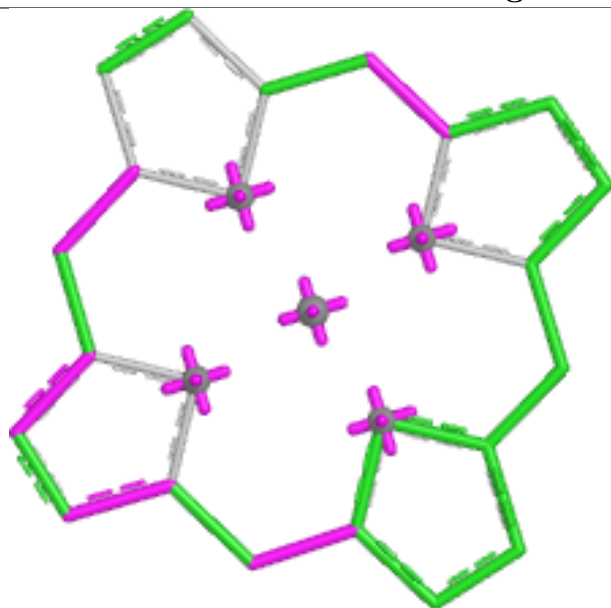


Torsions

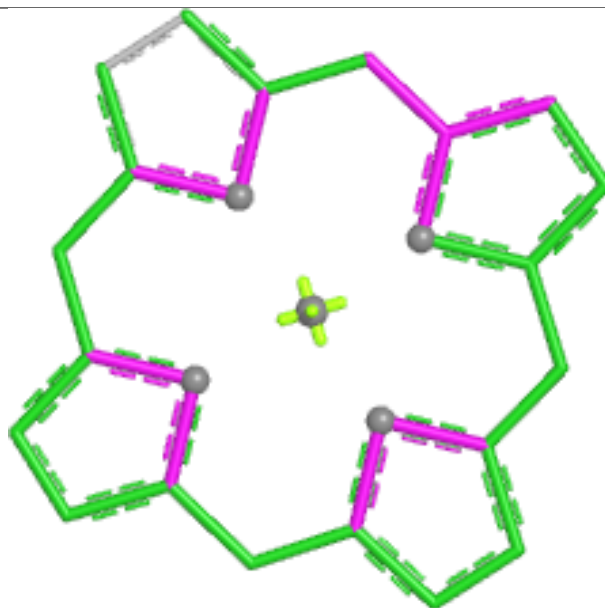


Rings

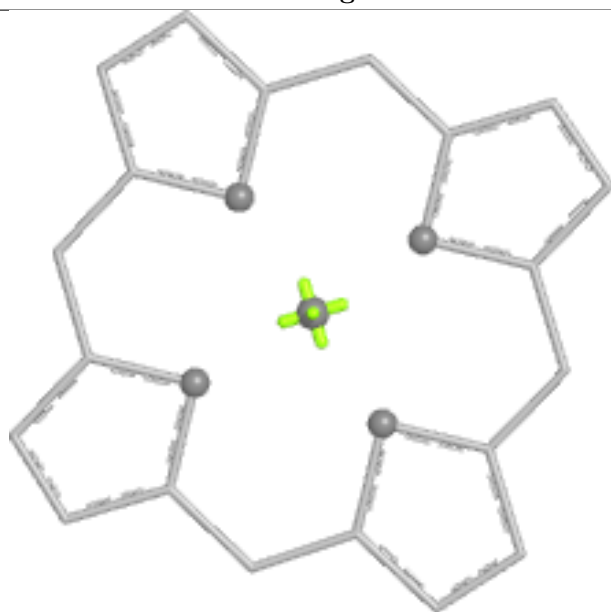
Ligand CLA P 5011



Bond lengths



Bond angles

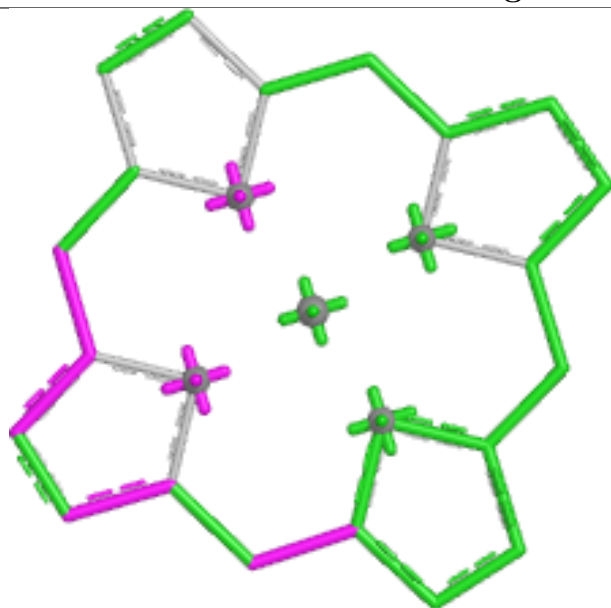


Torsions

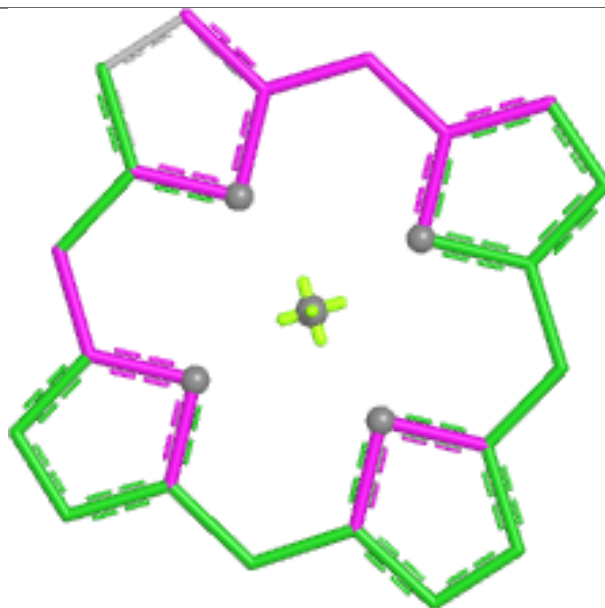


Rings

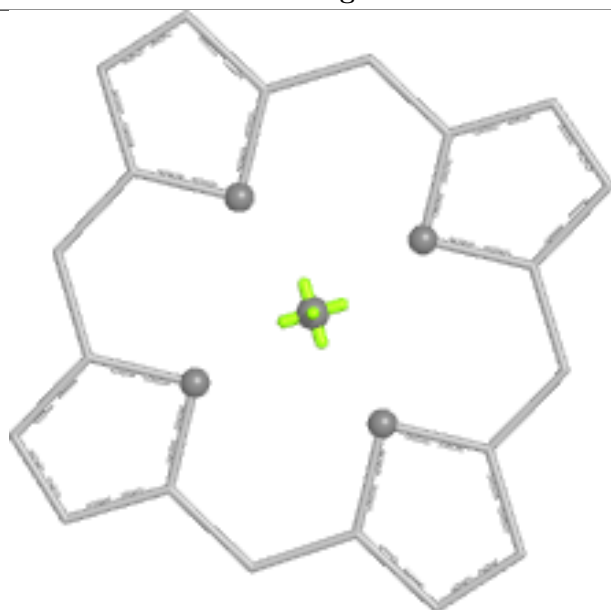
Ligand CLA U 8006



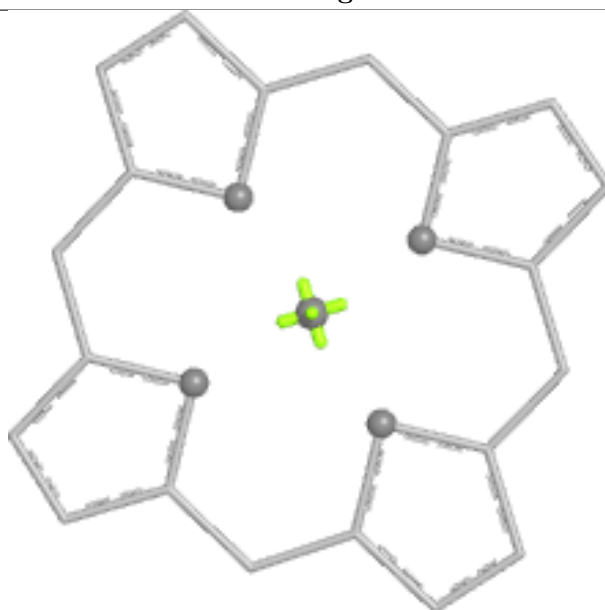
Bond lengths



Bond angles

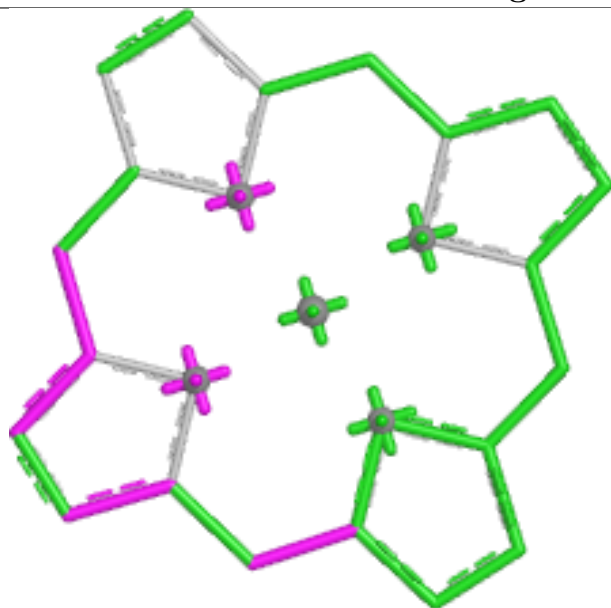


Torsions



Rings

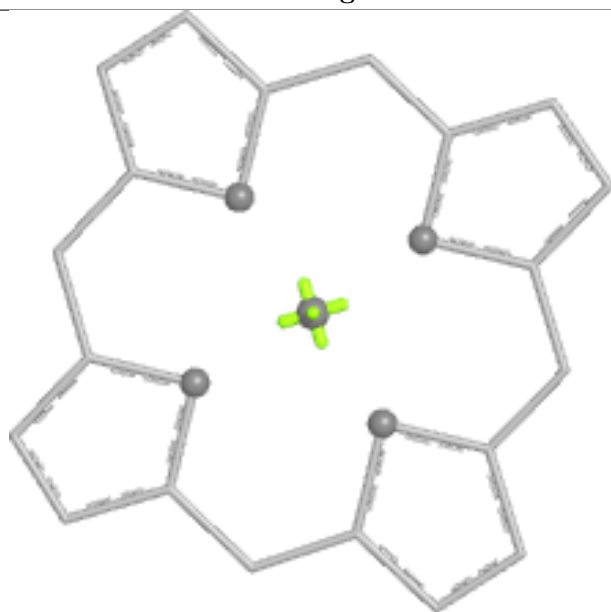
Ligand CLA 2 1016



Bond lengths



Bond angles

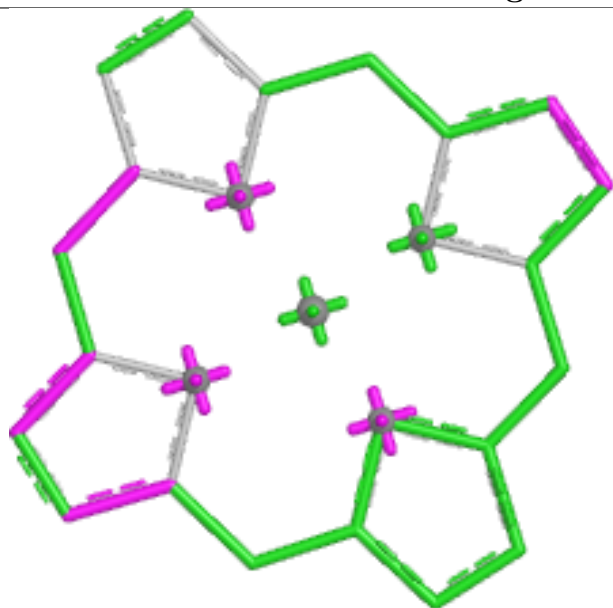


Torsions

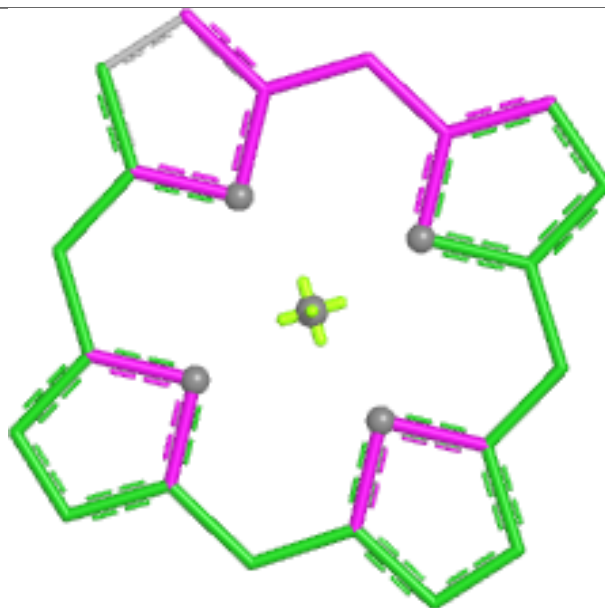


Rings

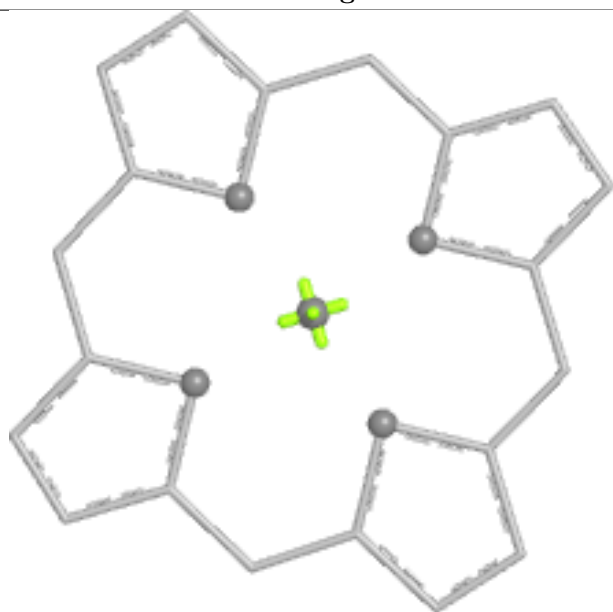
Ligand CLA P 5139



Bond lengths



Bond angles

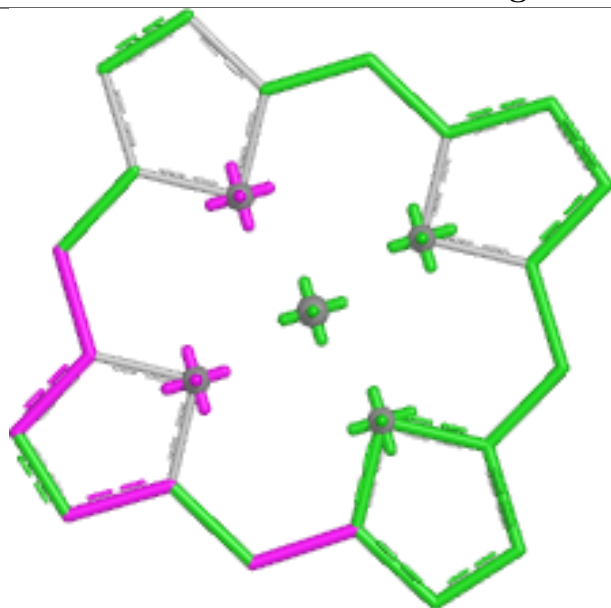


Torsions

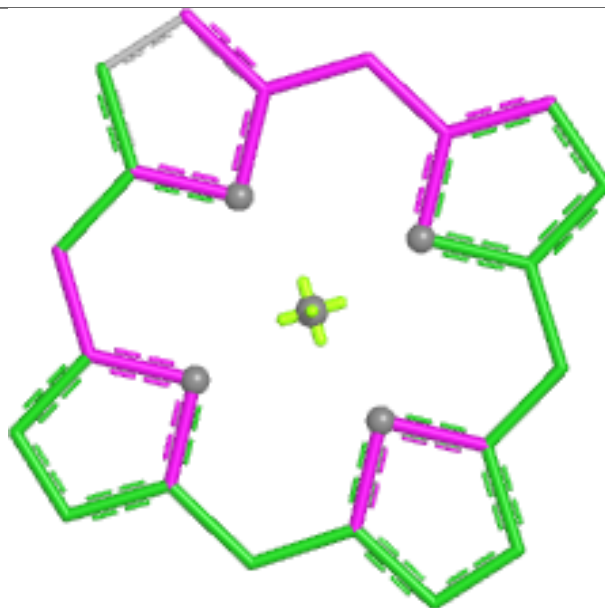


Rings

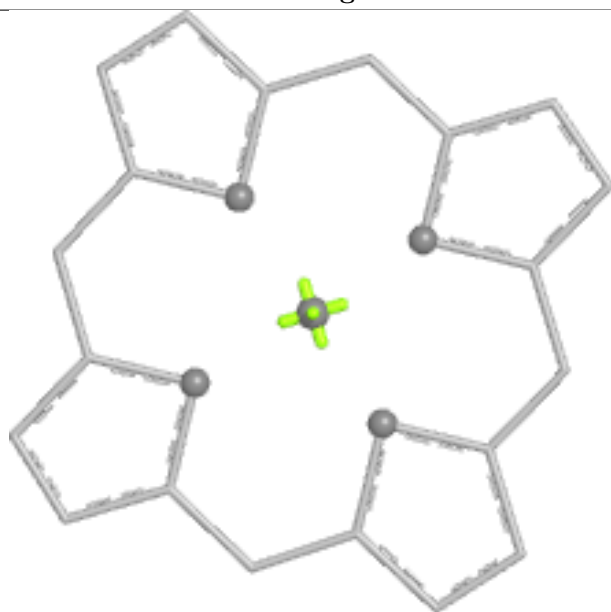
Ligand CLA 7 1017



Bond lengths



Bond angles

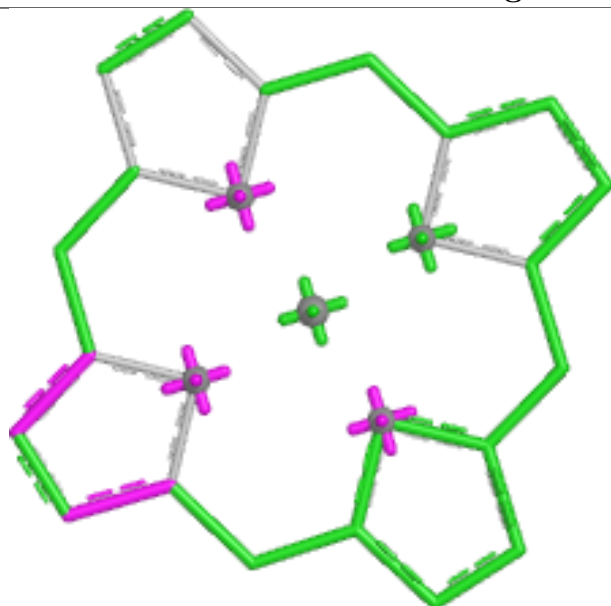


Torsions

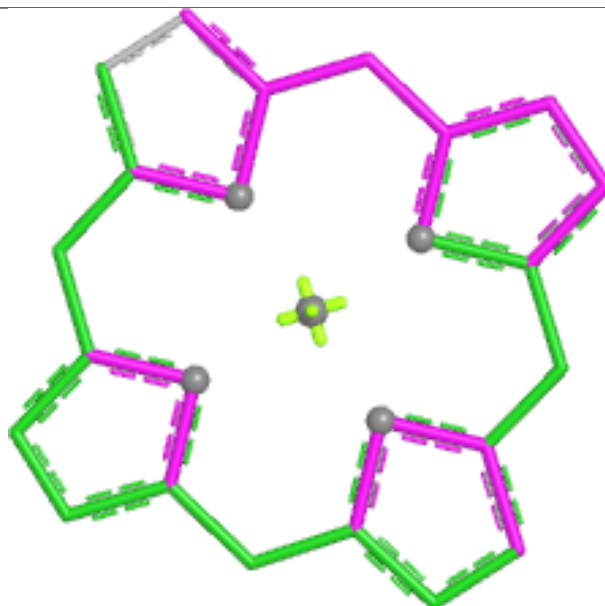


Rings

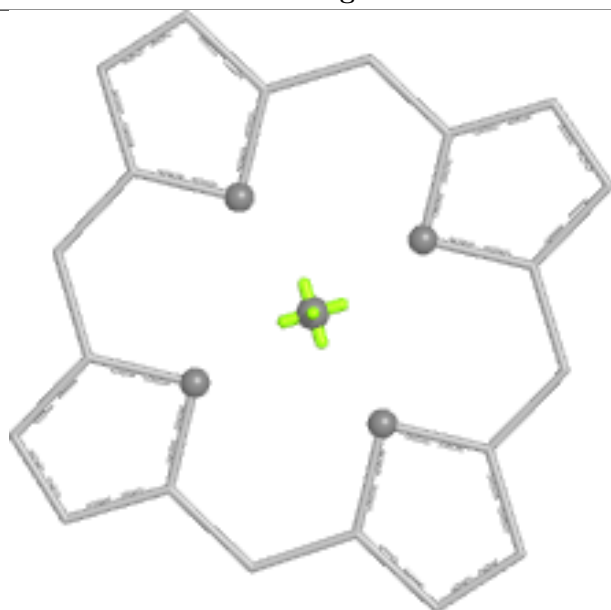
Ligand CLA A 1131



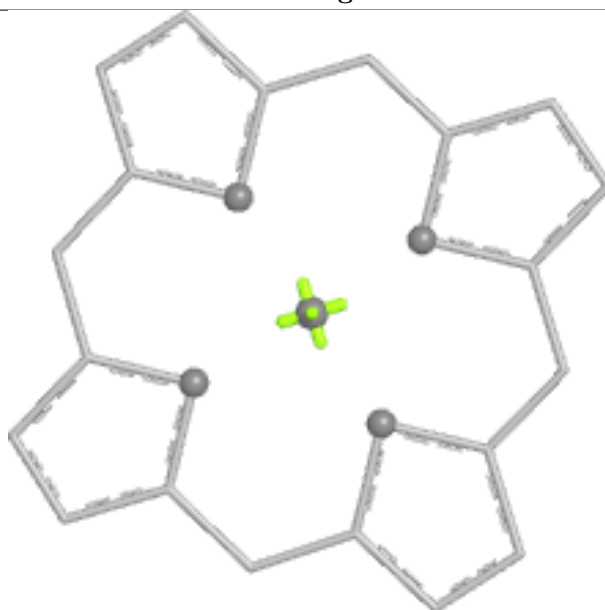
Bond lengths



Bond angles

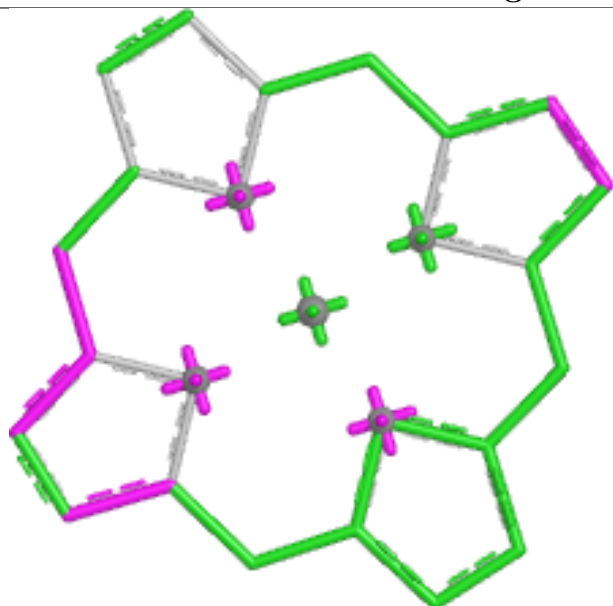


Torsions

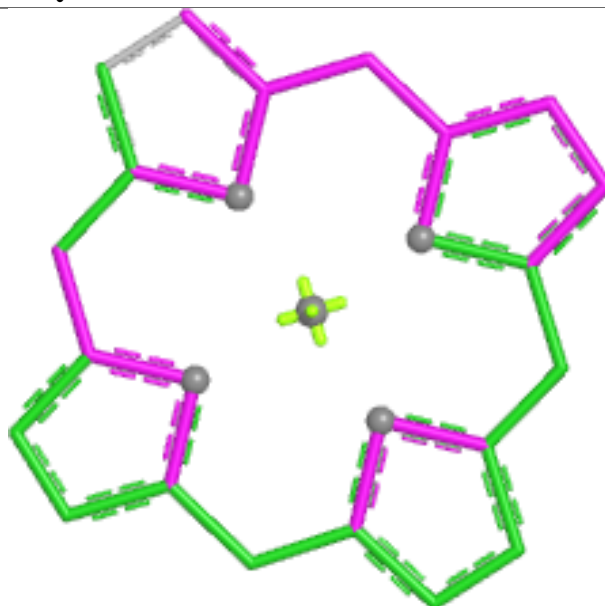


Rings

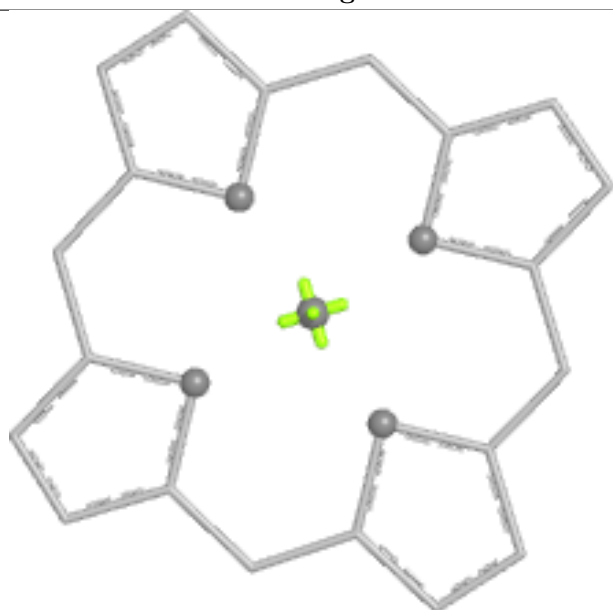
Ligand CLA Q 5225



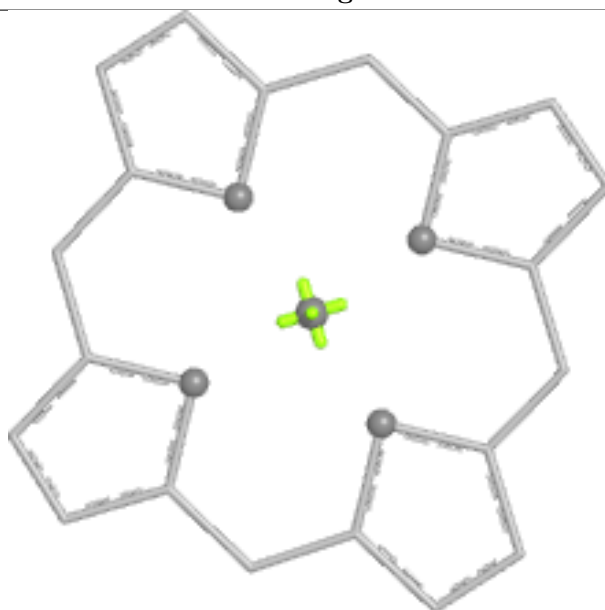
Bond lengths



Bond angles

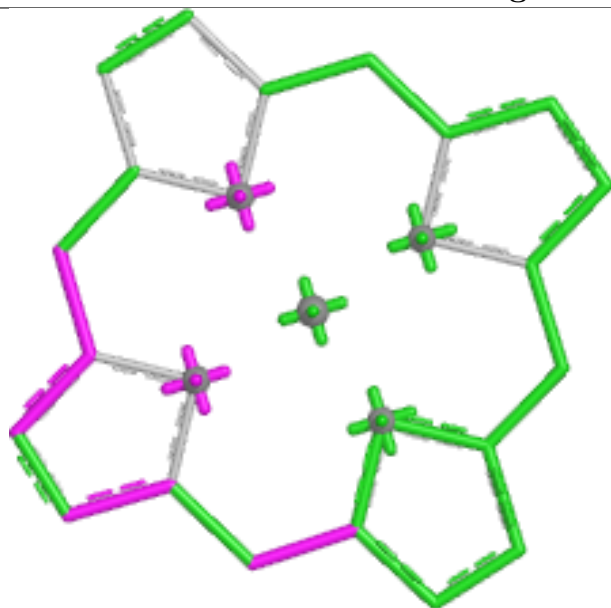


Torsions

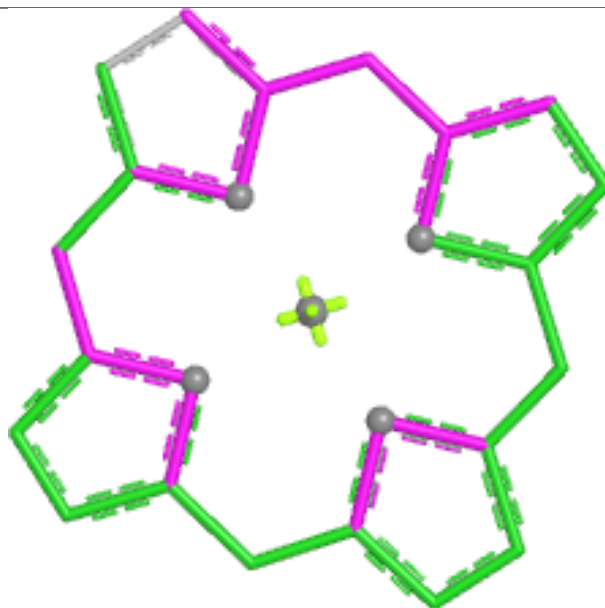


Rings

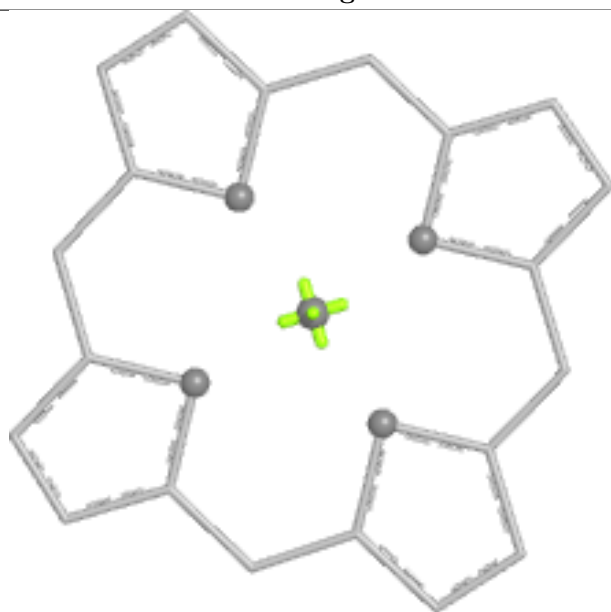
Ligand CLA 9 1017



Bond lengths



Bond angles

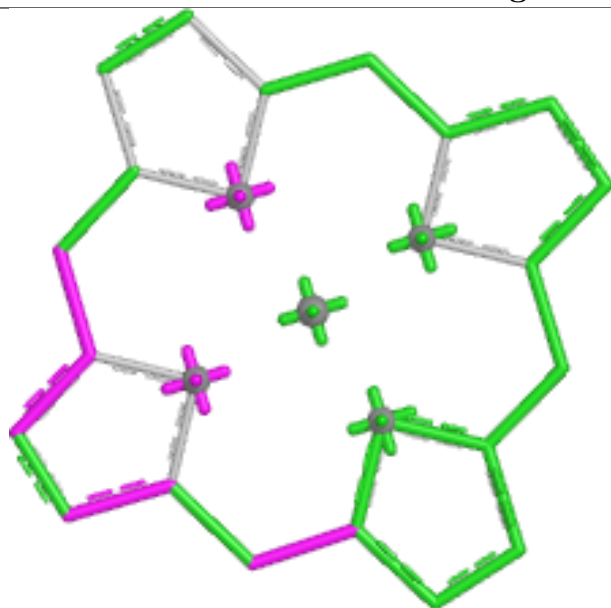


Torsions

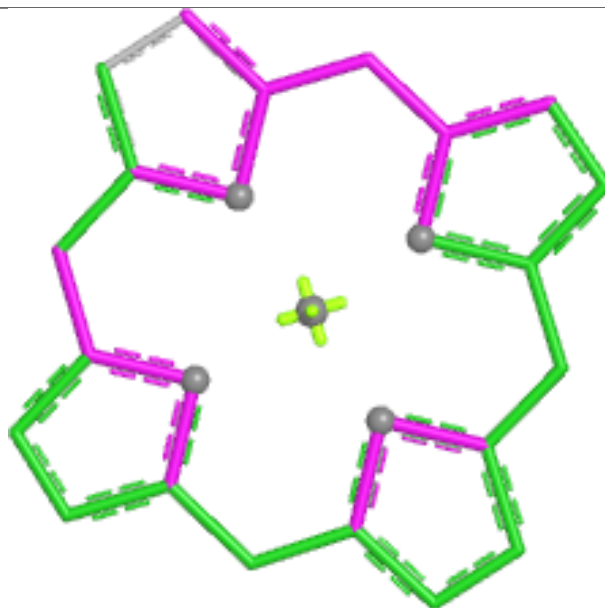


Rings

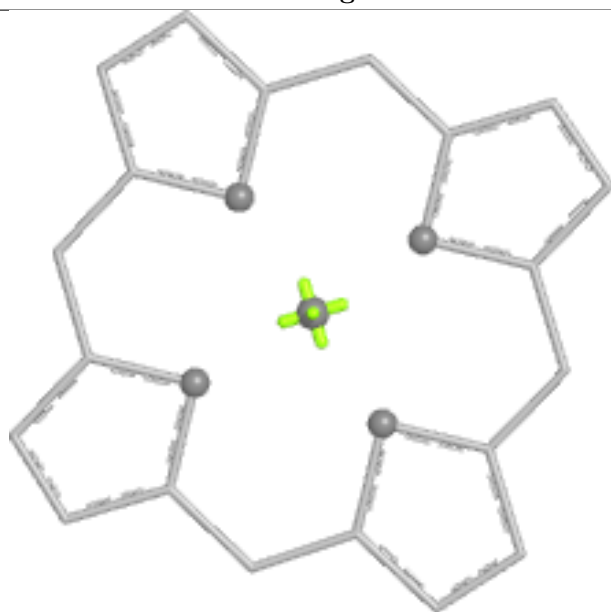
Ligand CLA 1 1016



Bond lengths



Bond angles

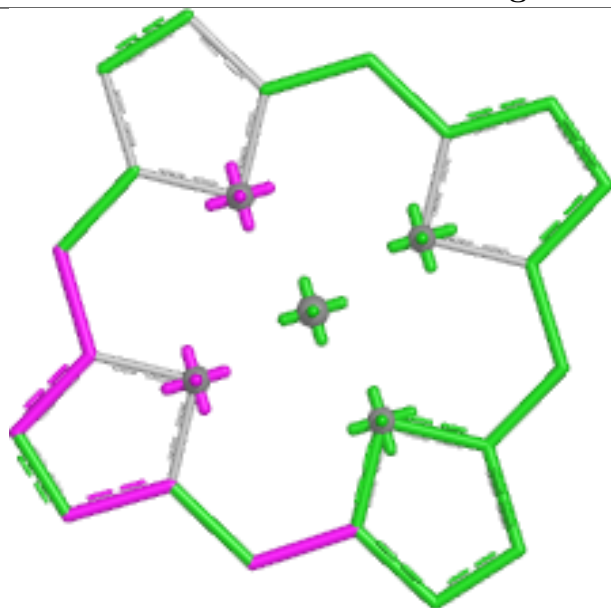


Torsions

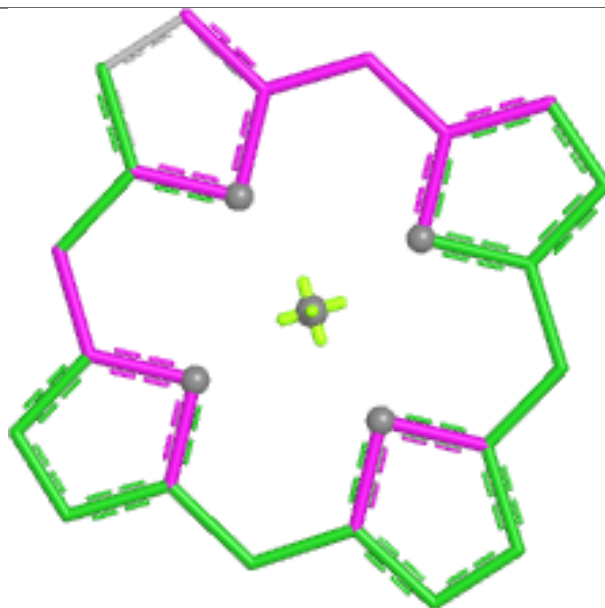


Rings

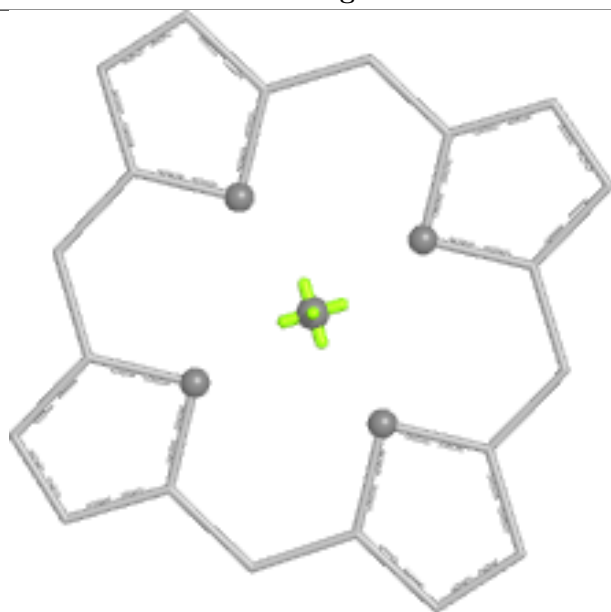
Ligand CLA 0 1021



Bond lengths



Bond angles

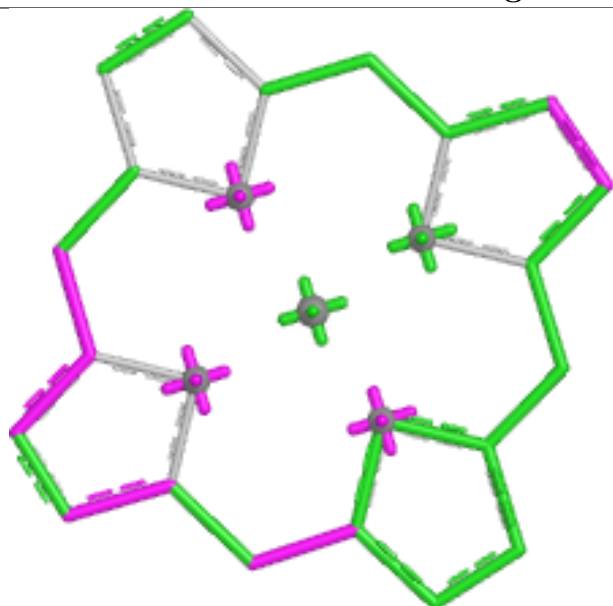


Torsions

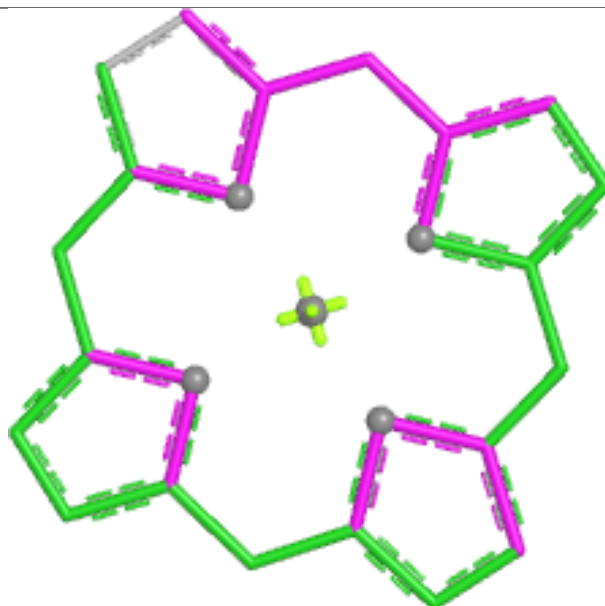


Rings

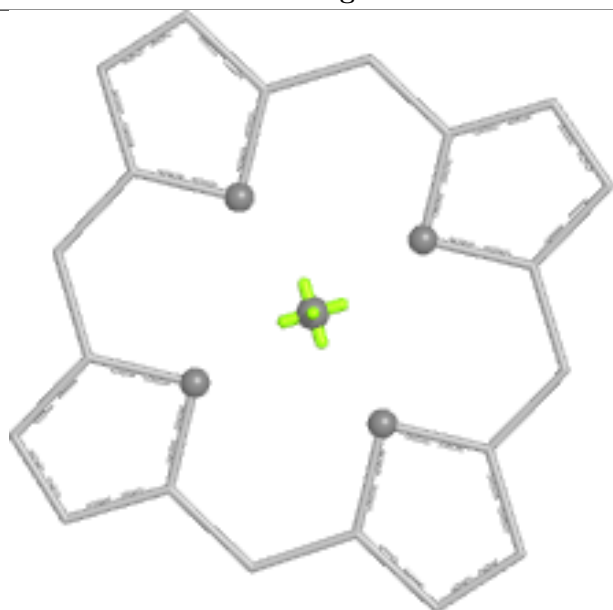
Ligand CLA A 1122



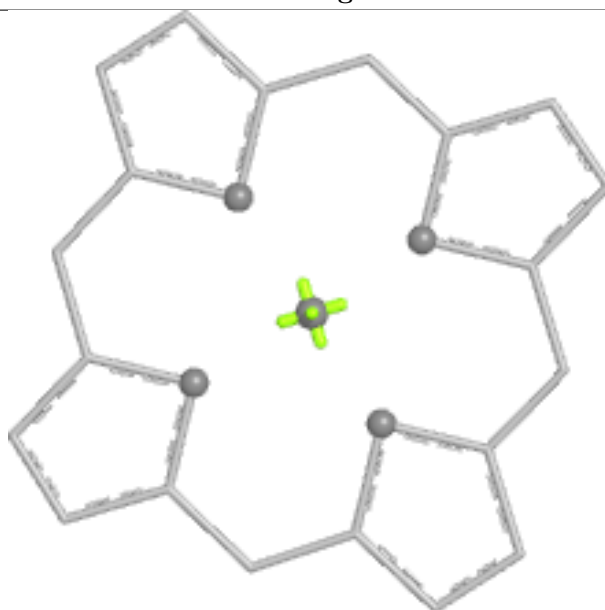
Bond lengths



Bond angles

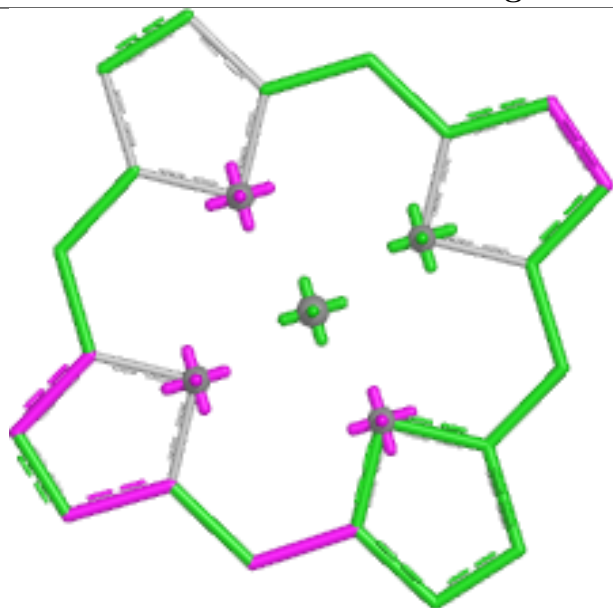


Torsions

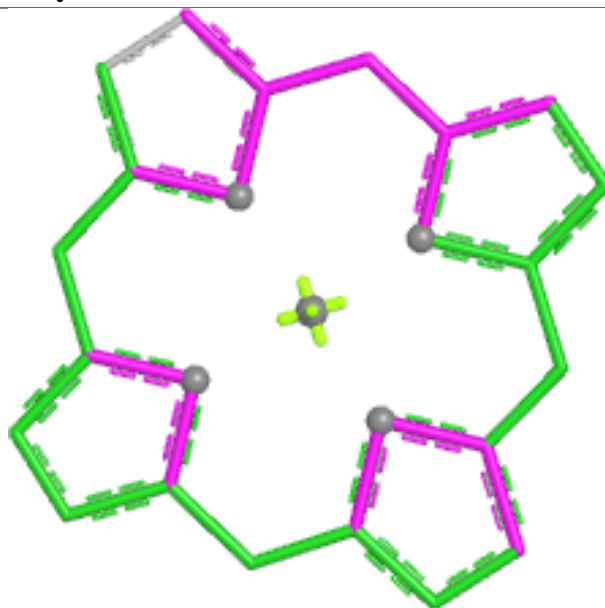


Rings

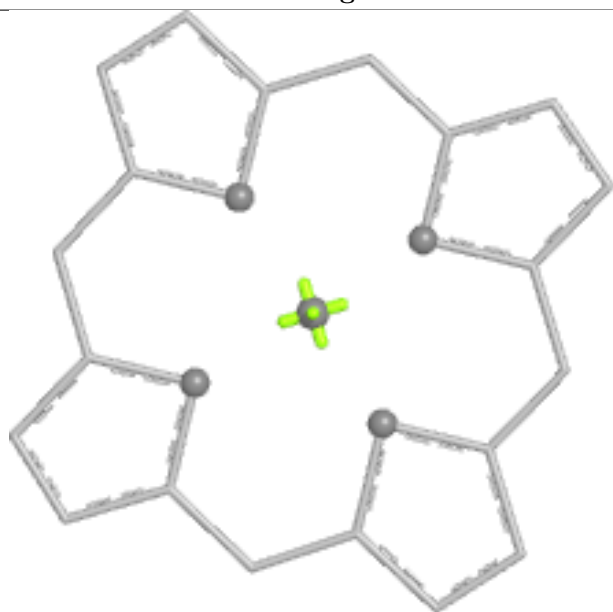
Ligand CLA Q 5220



Bond lengths



Bond angles

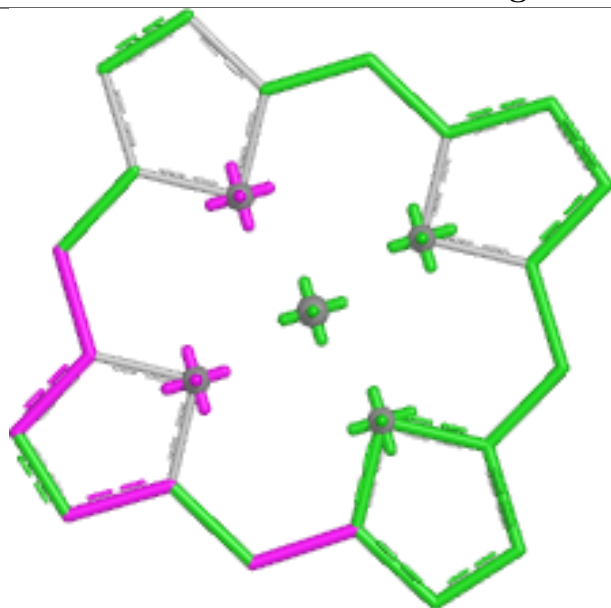


Torsions

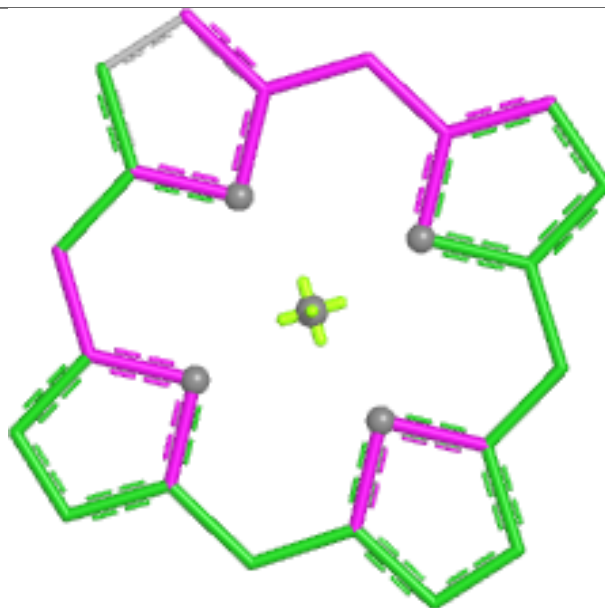


Rings

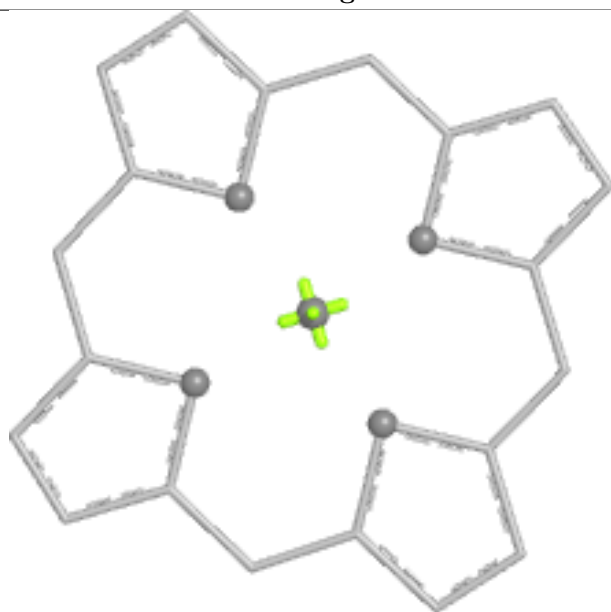
Ligand CLA 2 1026



Bond lengths



Bond angles

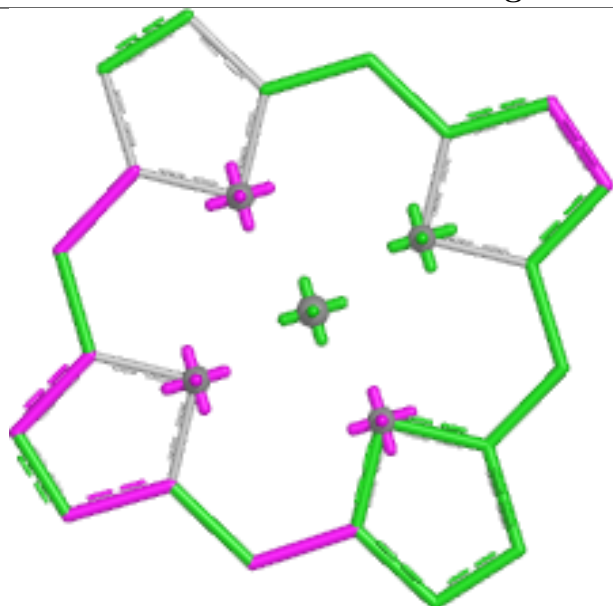


Torsions

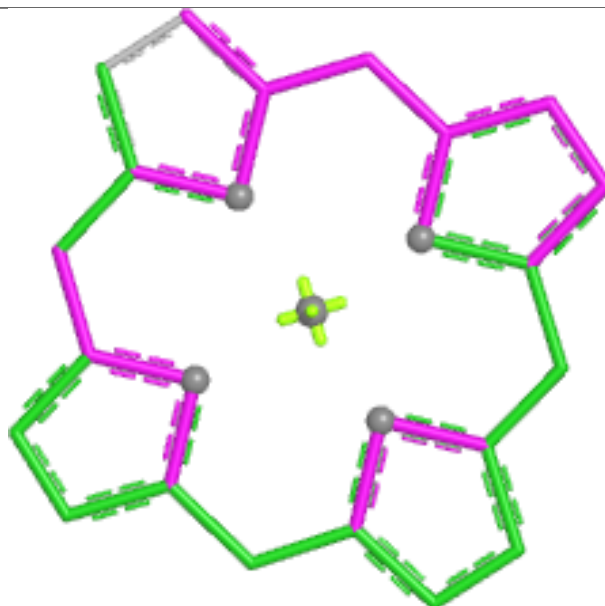


Rings

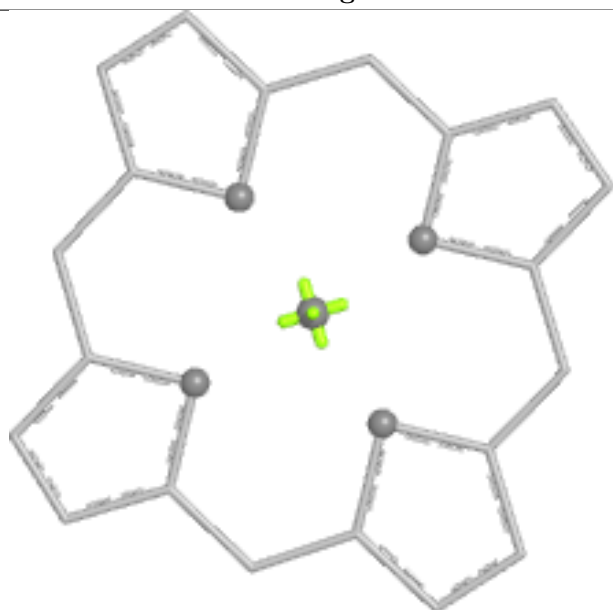
Ligand CLA A 1125



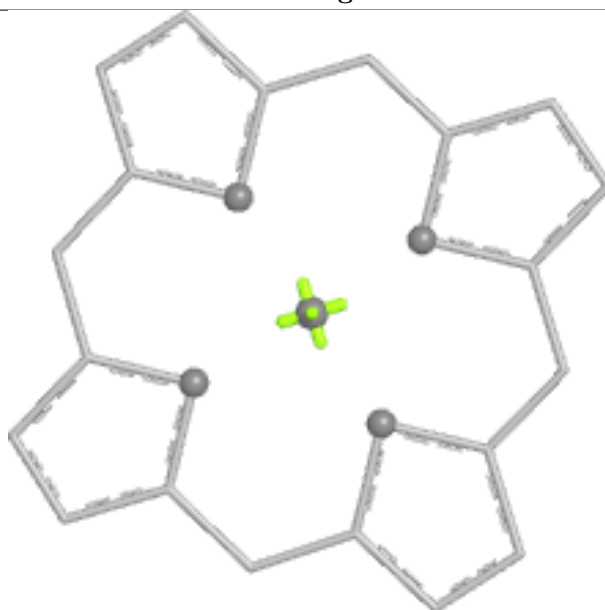
Bond lengths



Bond angles

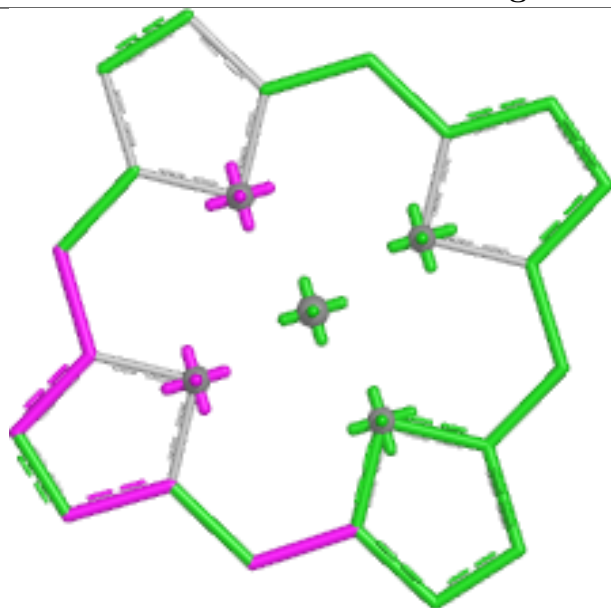


Torsions

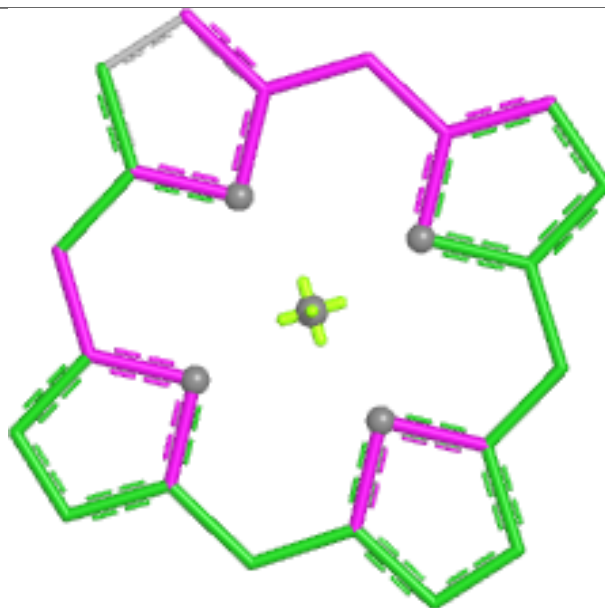


Rings

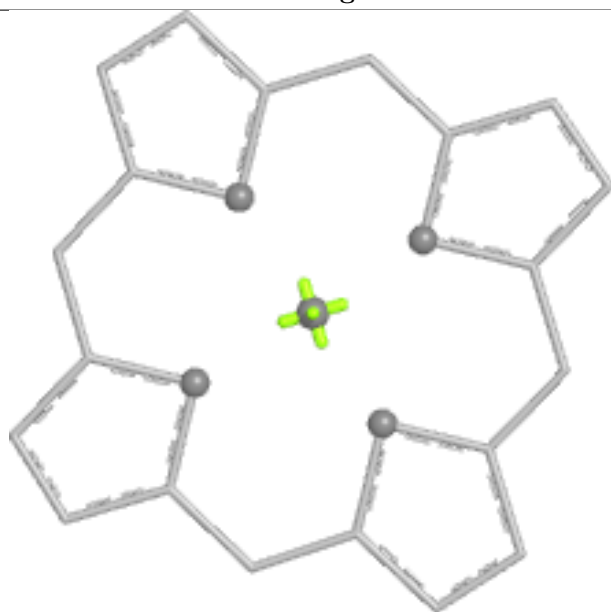
Ligand CLA 1 1011



Bond lengths



Bond angles

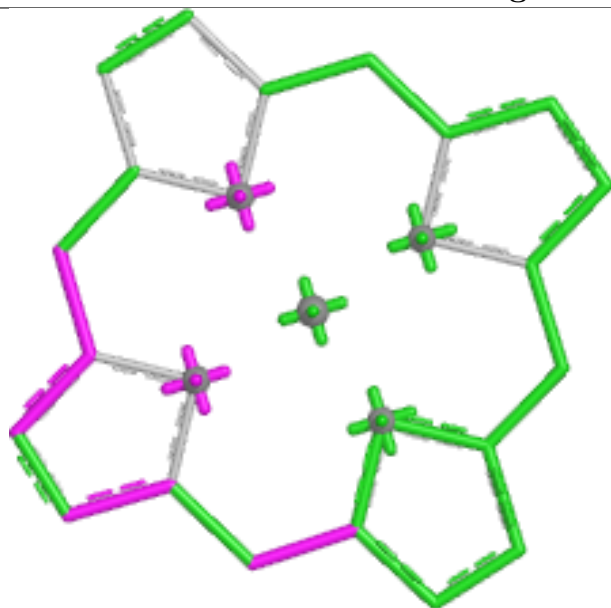


Torsions

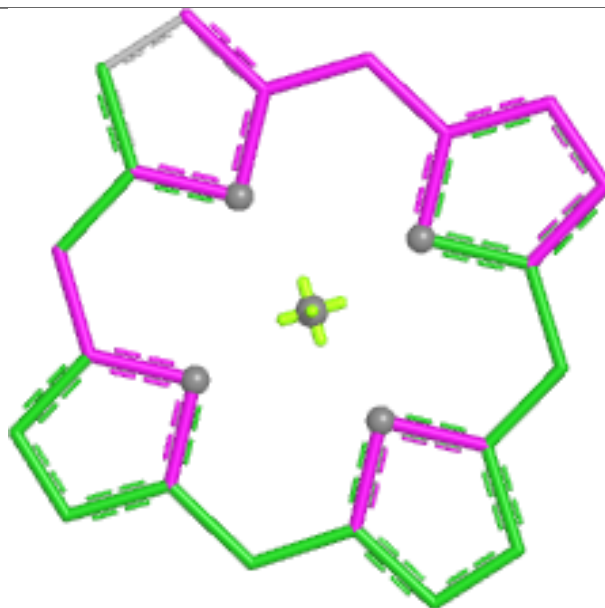


Rings

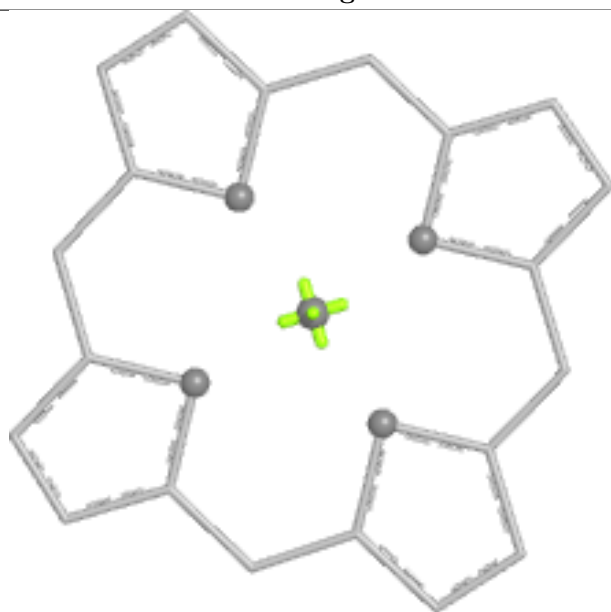
Ligand CLA 9 1016



Bond lengths



Bond angles

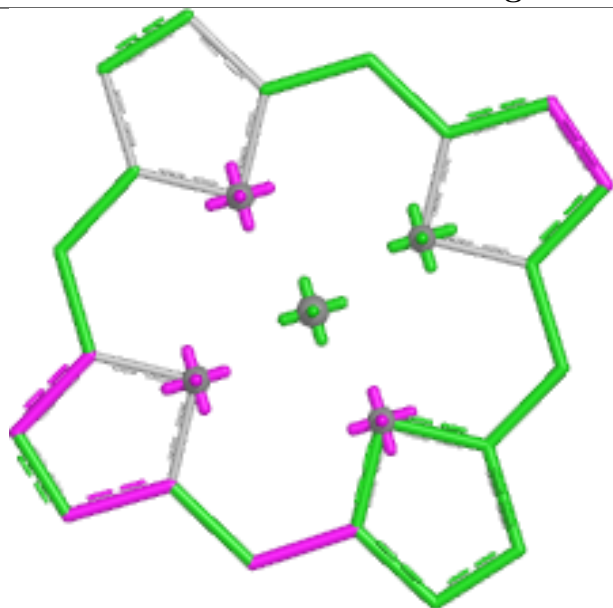


Torsions

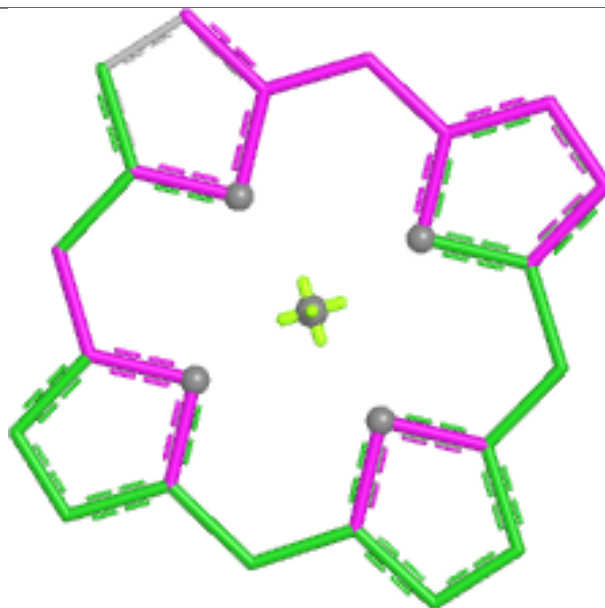


Rings

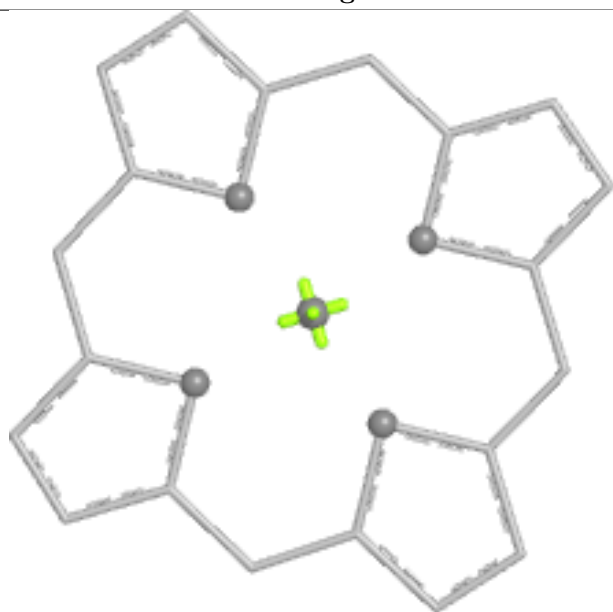
Ligand CLA A 1123



Bond lengths



Bond angles

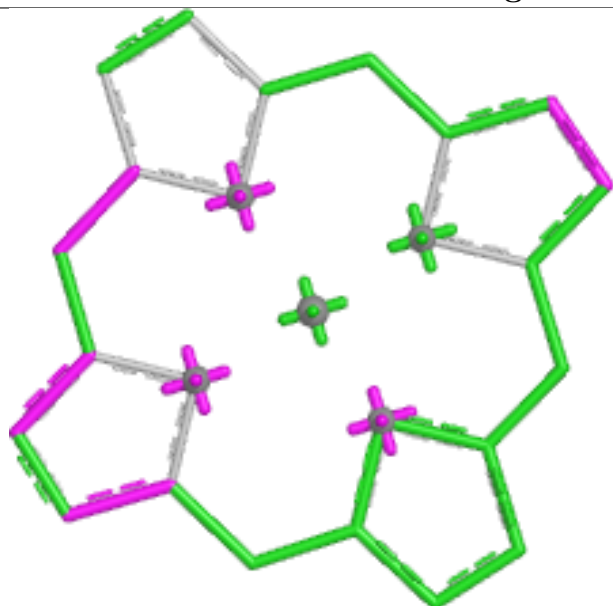


Torsions

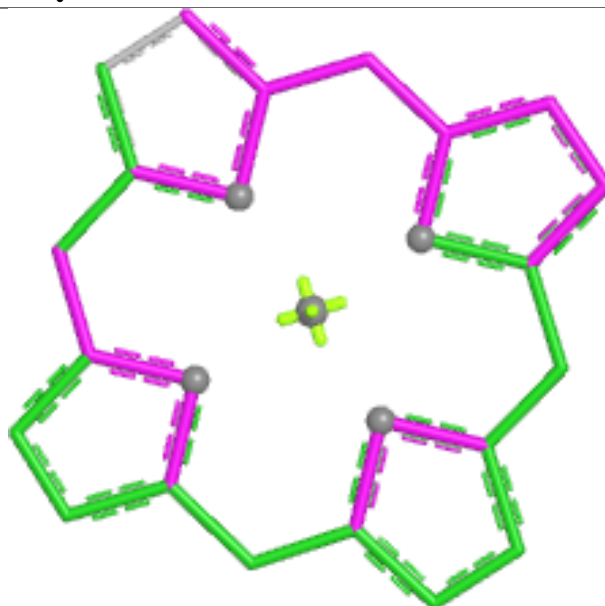


Rings

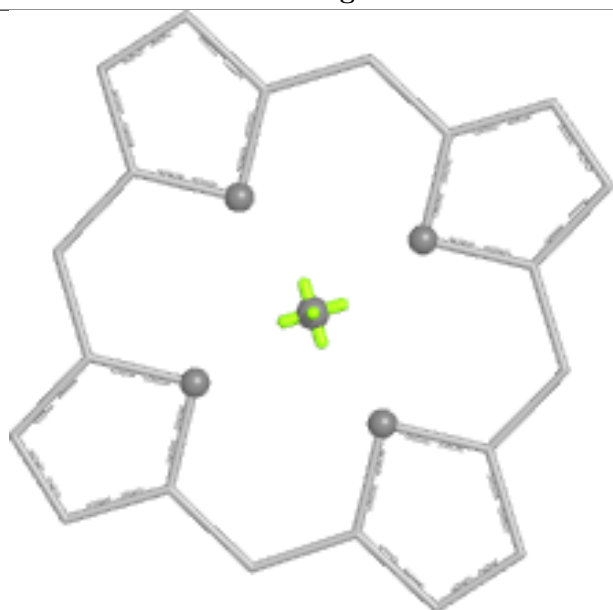
Ligand CLA Q 5226



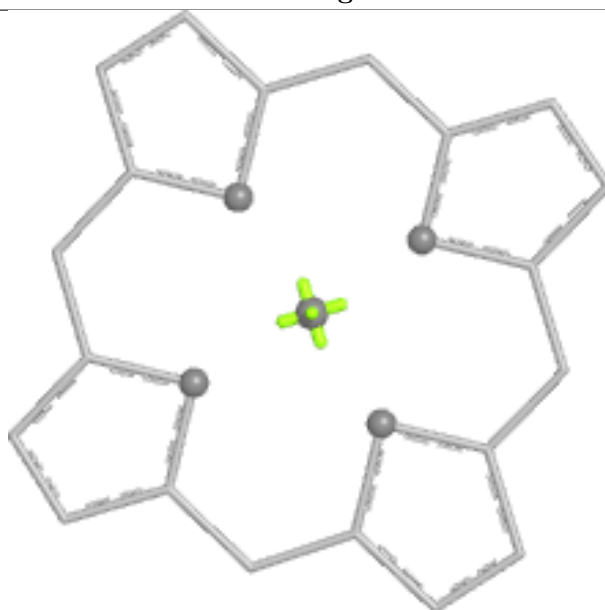
Bond lengths



Bond angles

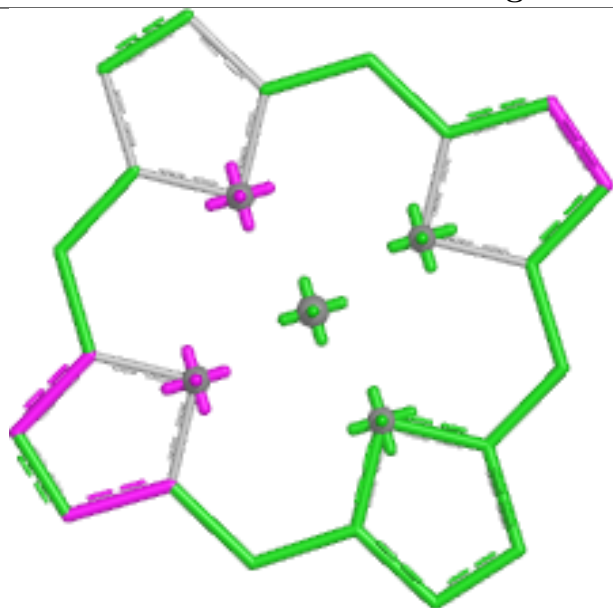


Torsions

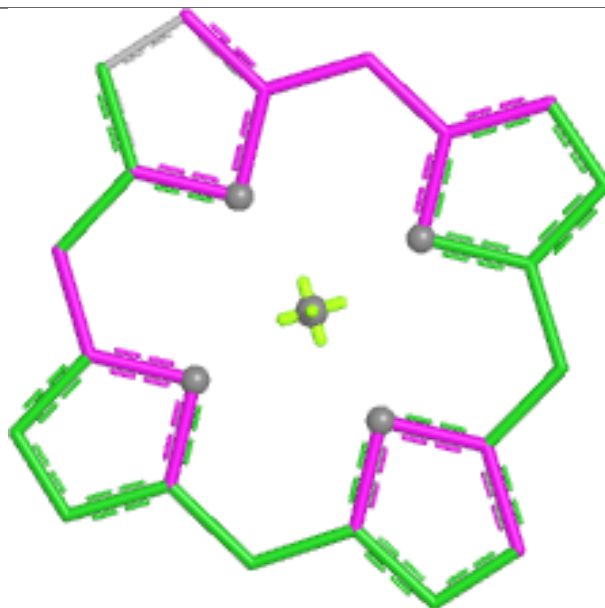


Rings

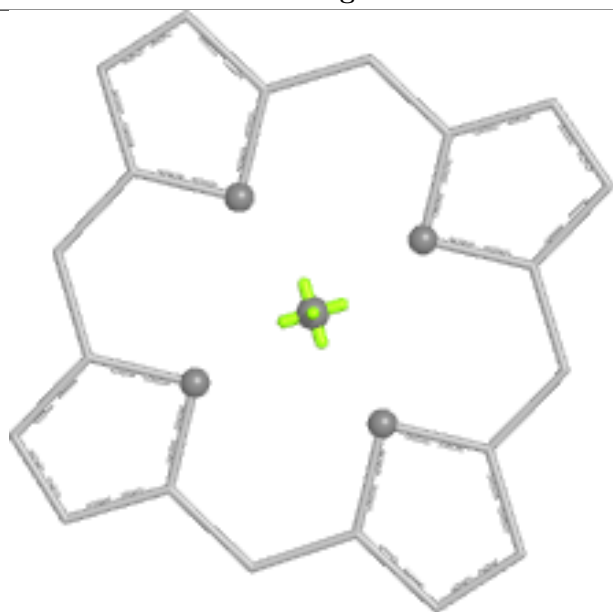
Ligand CLA P 5110



Bond lengths



Bond angles

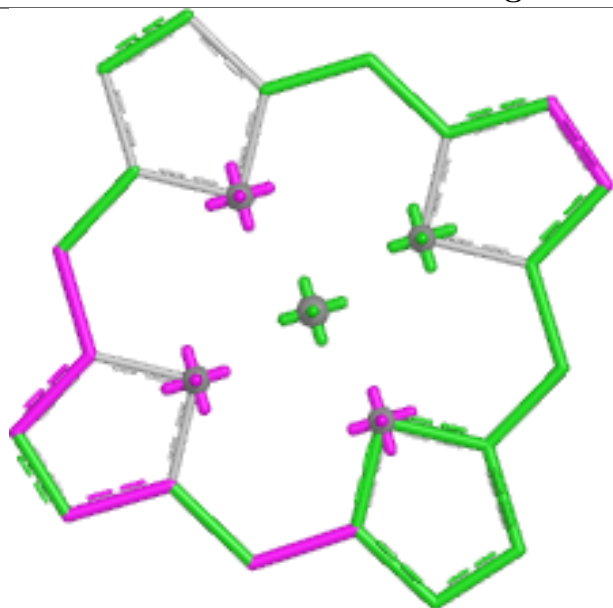


Torsions

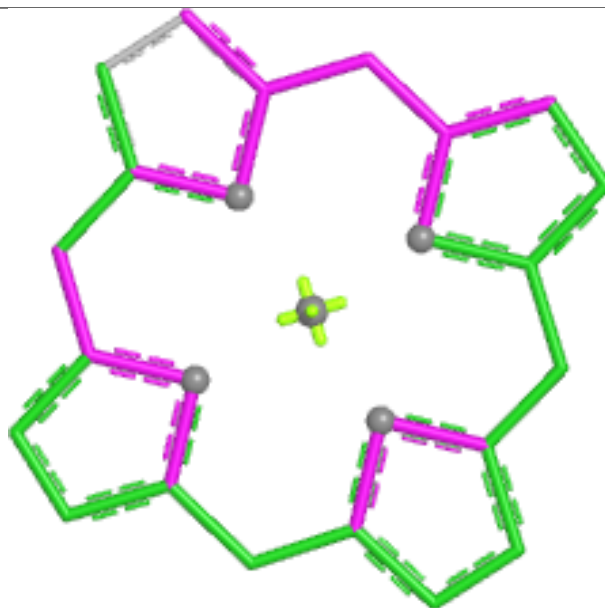


Rings

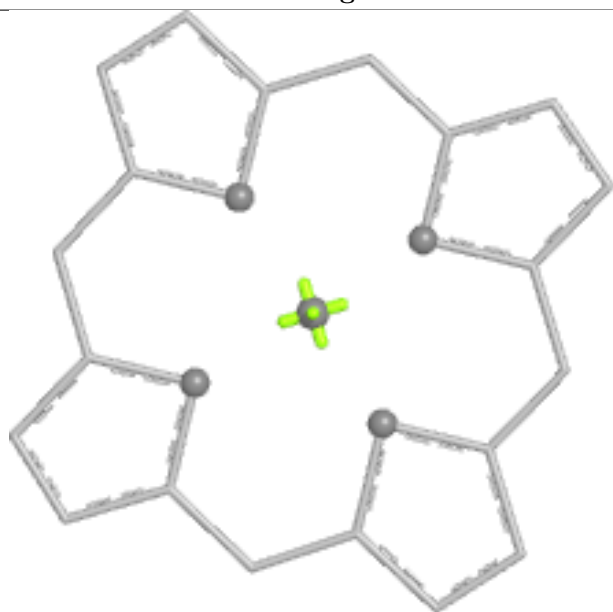
Ligand CLA A 1114



Bond lengths



Bond angles

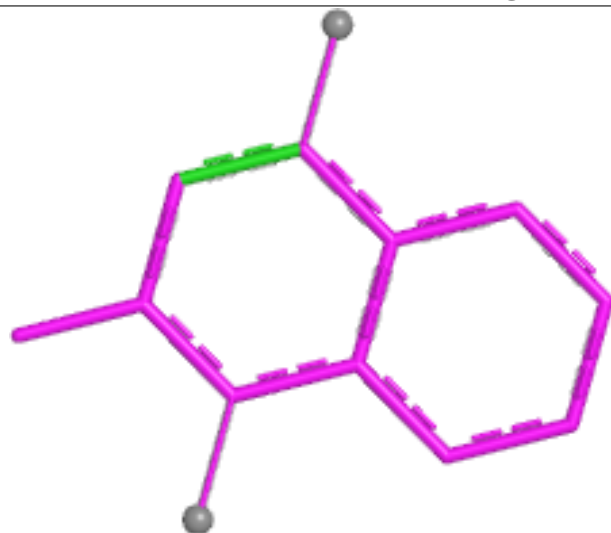


Torsions

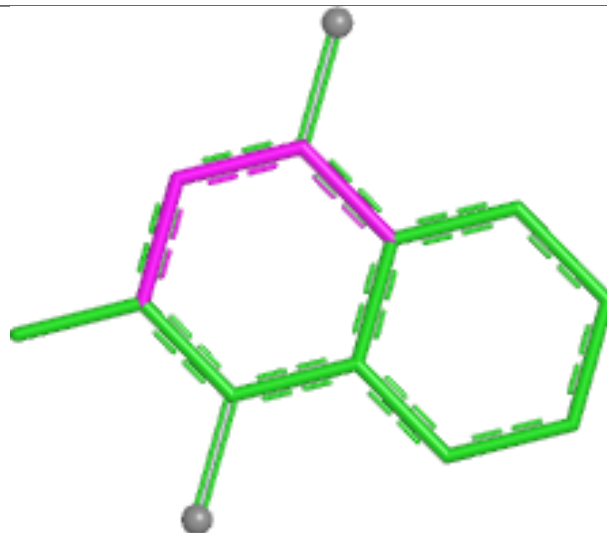


Rings

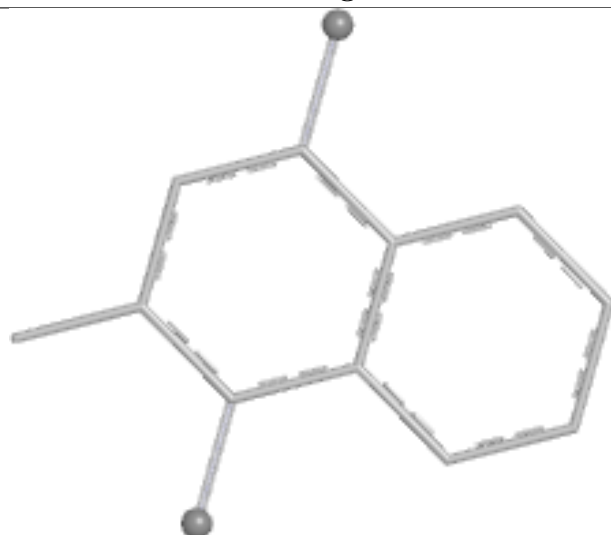
Ligand PQN B 2002



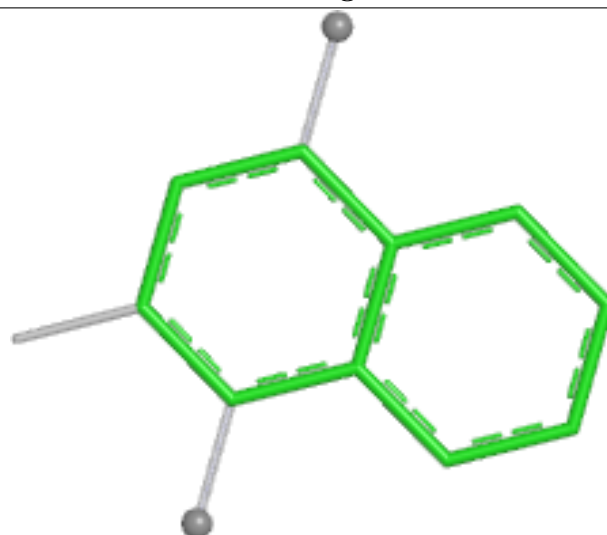
Bond lengths



Bond angles

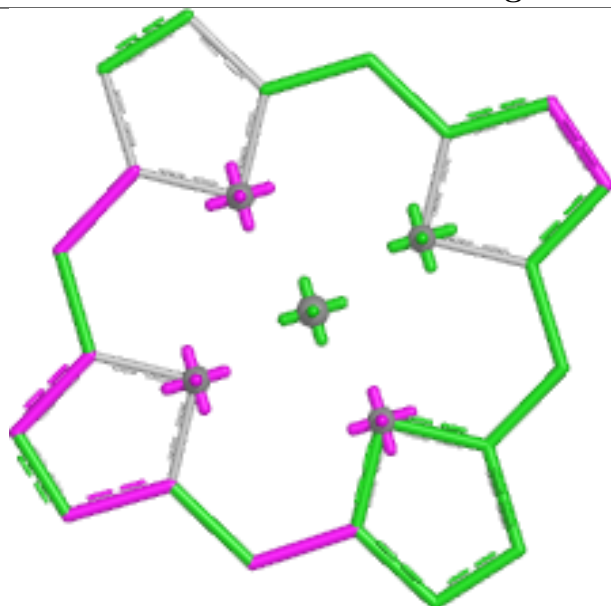


Torsions

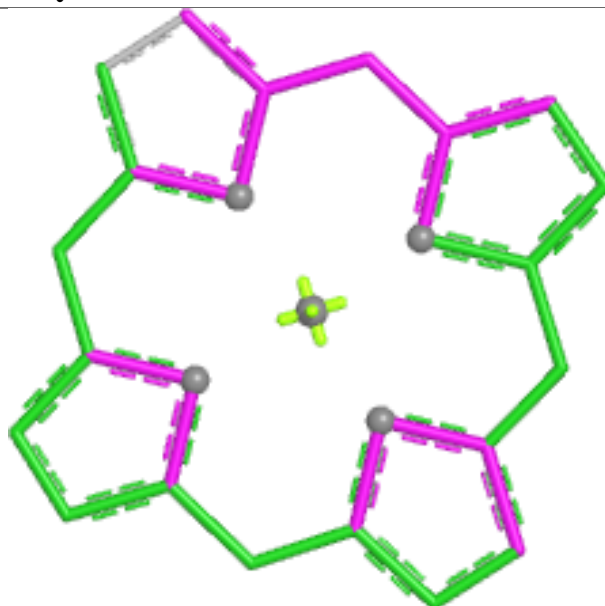


Rings

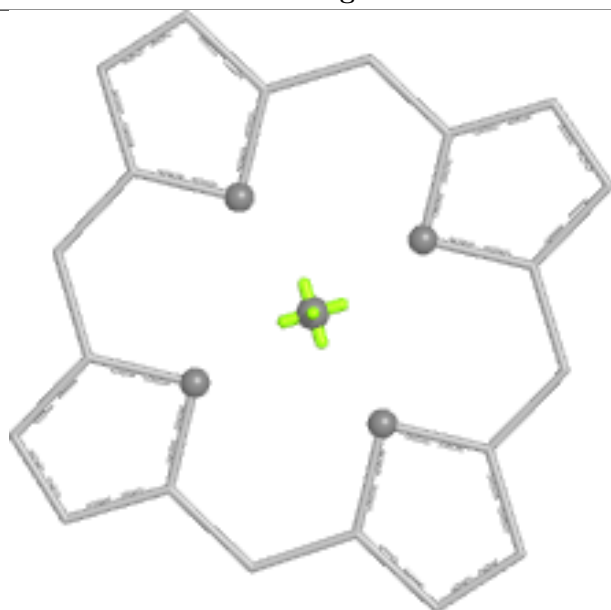
Ligand CLA Q 5217



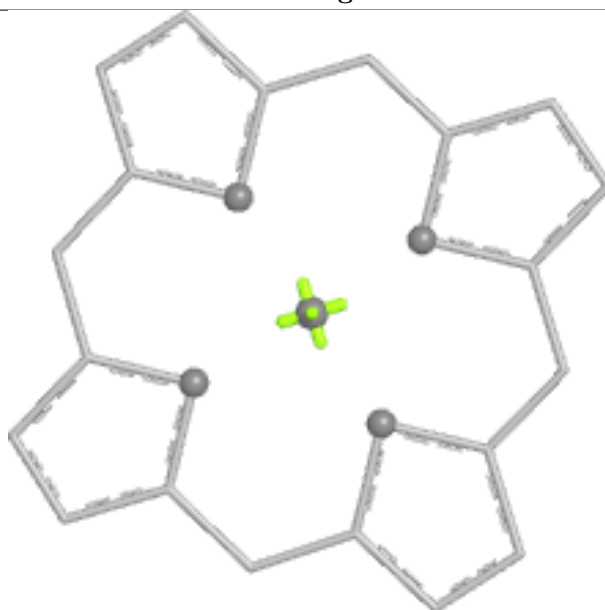
Bond lengths



Bond angles

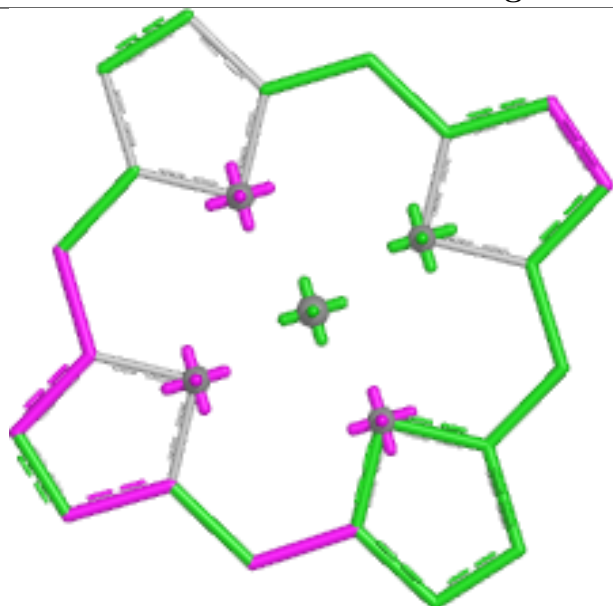


Torsions

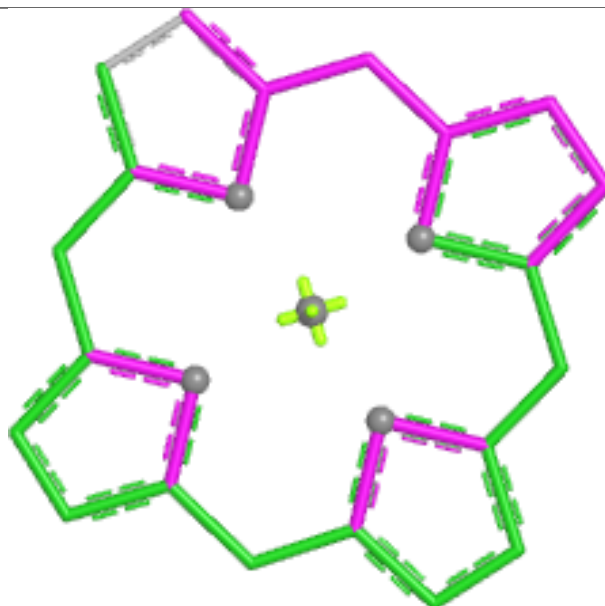


Rings

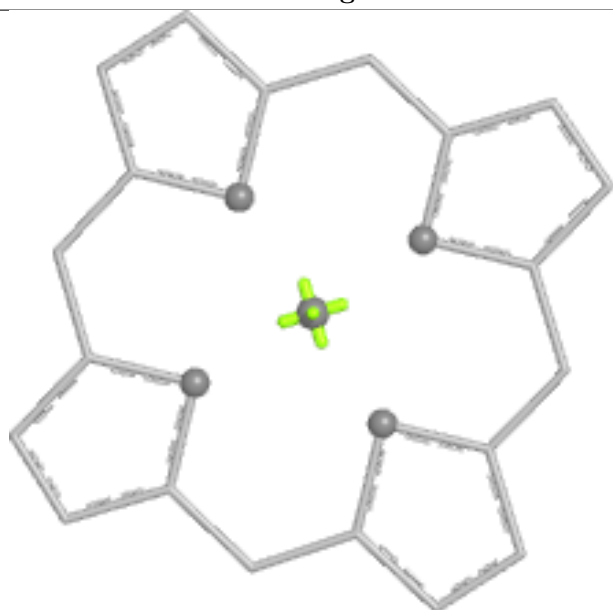
Ligand CLA A 1109



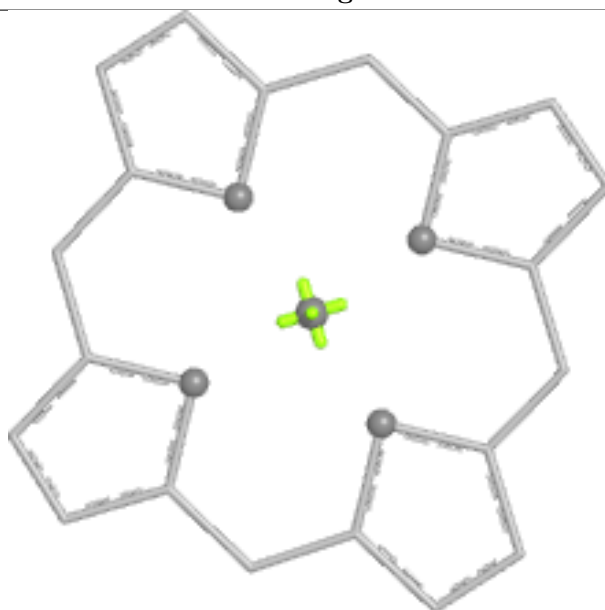
Bond lengths



Bond angles

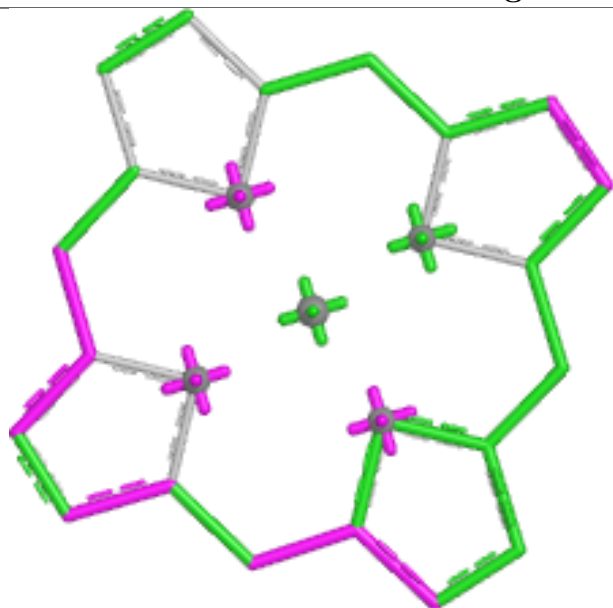


Torsions

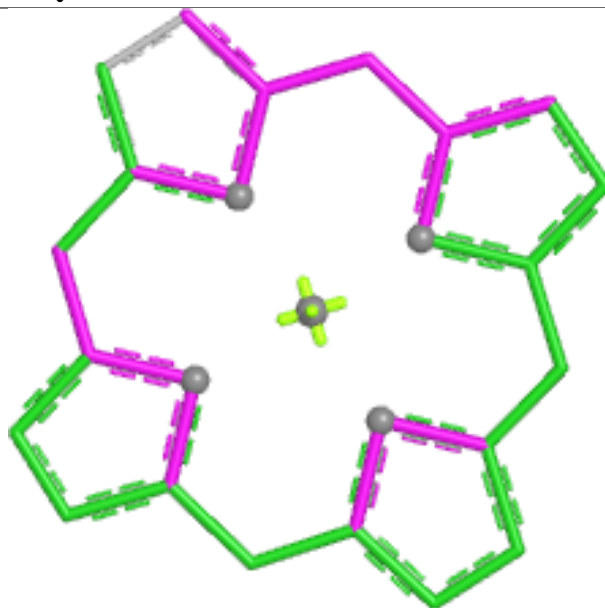


Rings

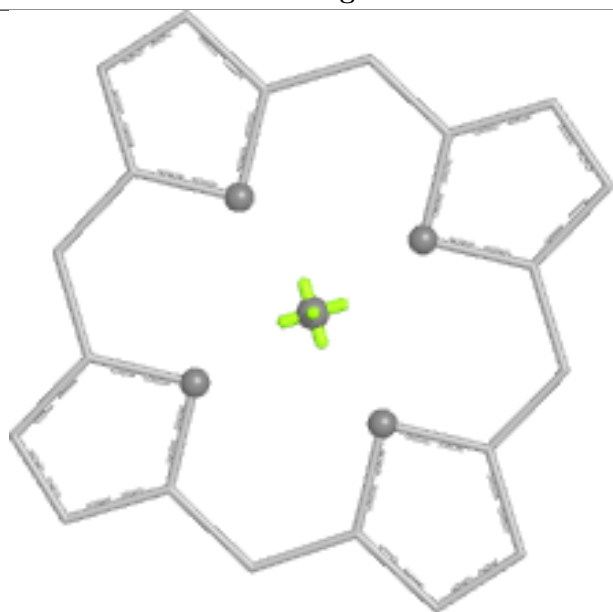
Ligand CLA Q 5221



Bond lengths



Bond angles

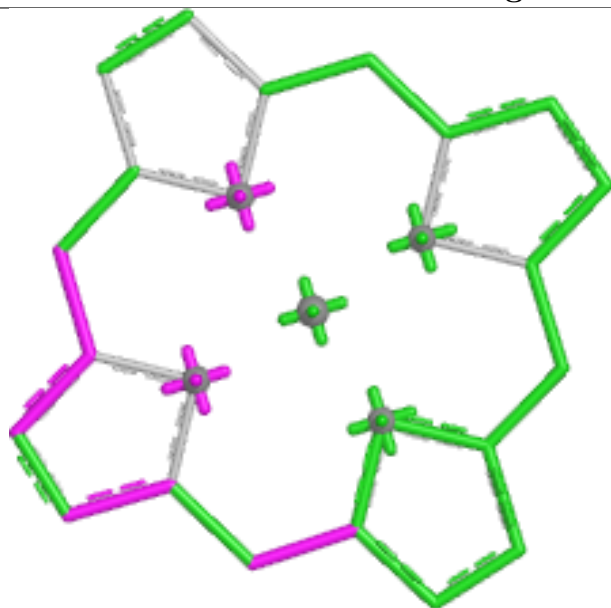


Torsions

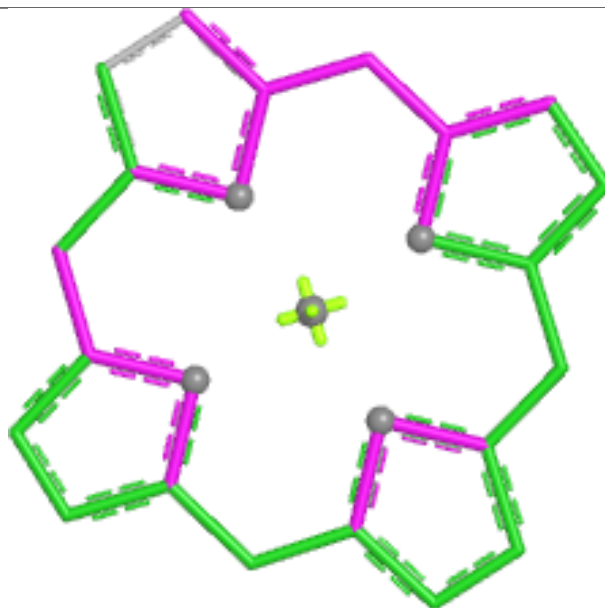


Rings

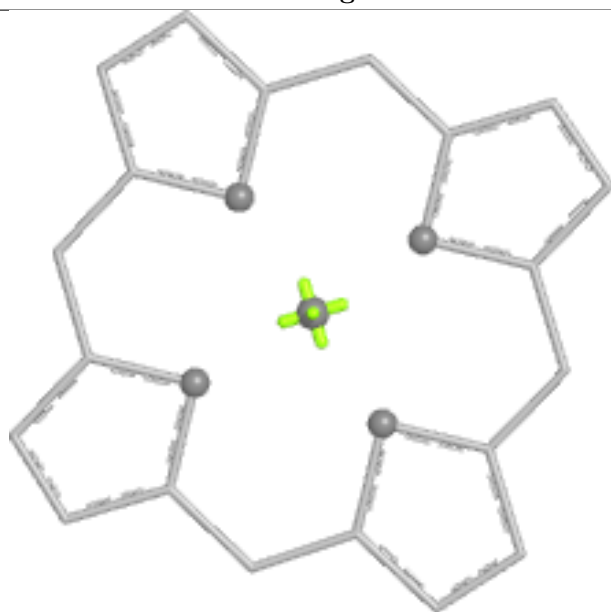
Ligand CLA B 1241



Bond lengths



Bond angles

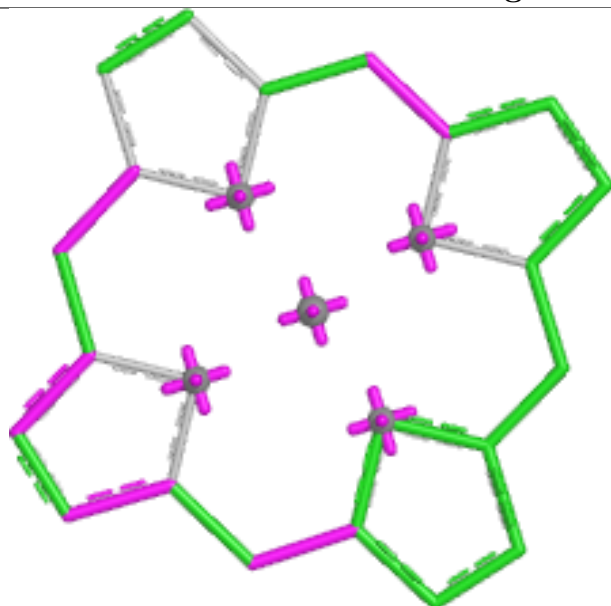


Torsions

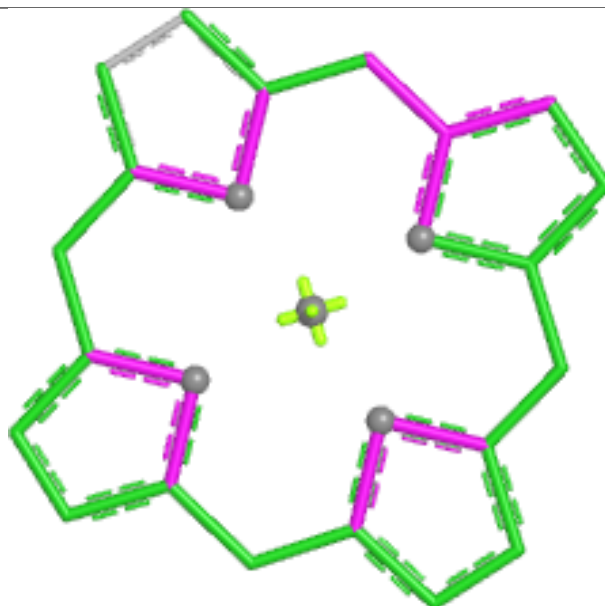


Rings

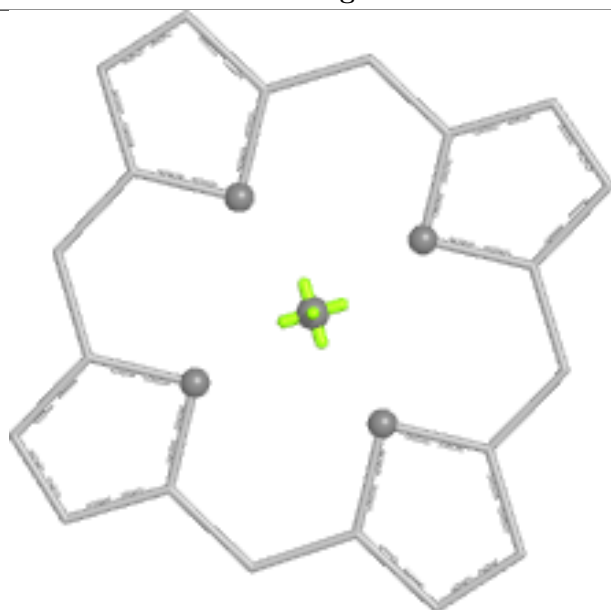
Ligand CLA A 1011



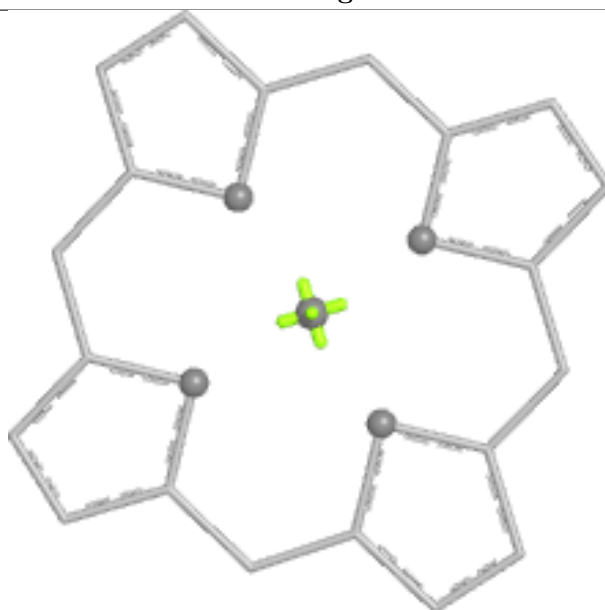
Bond lengths



Bond angles

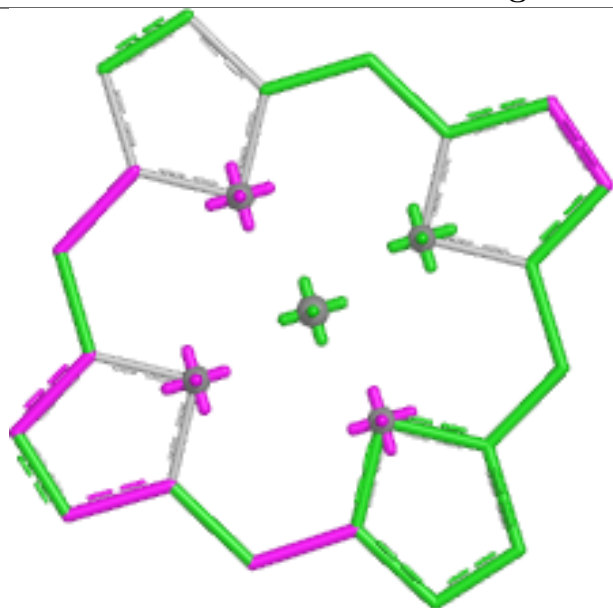


Torsions

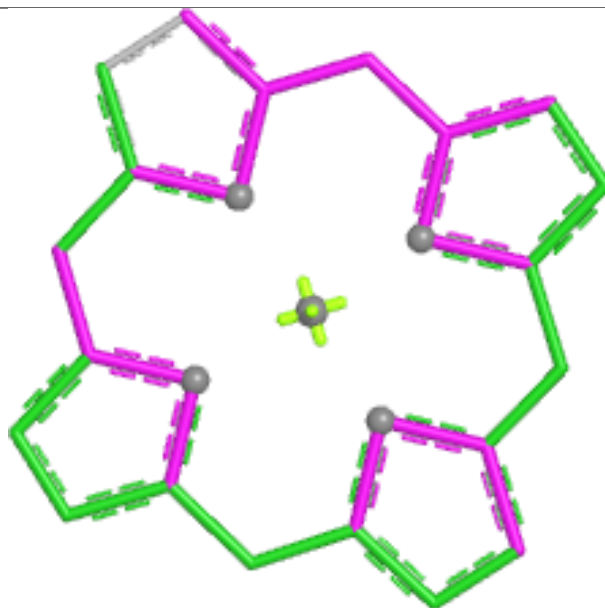


Rings

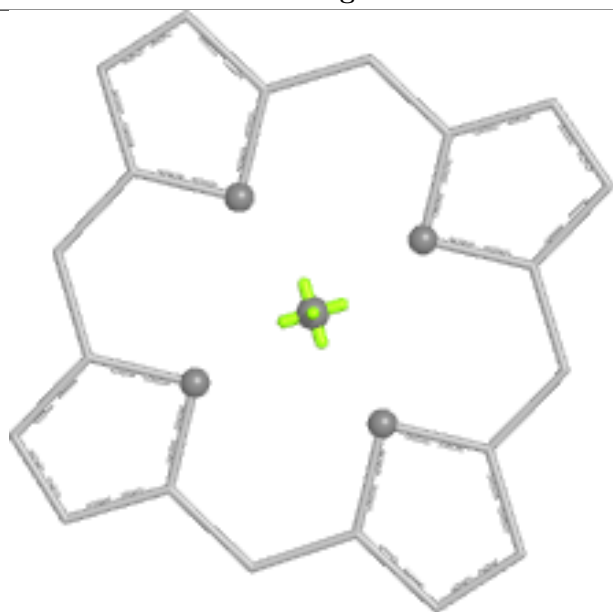
Ligand CLA J 1302



Bond lengths



Bond angles

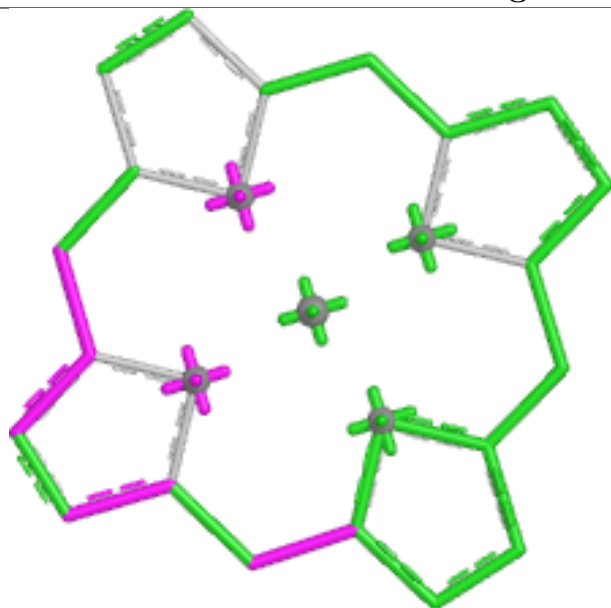


Torsions

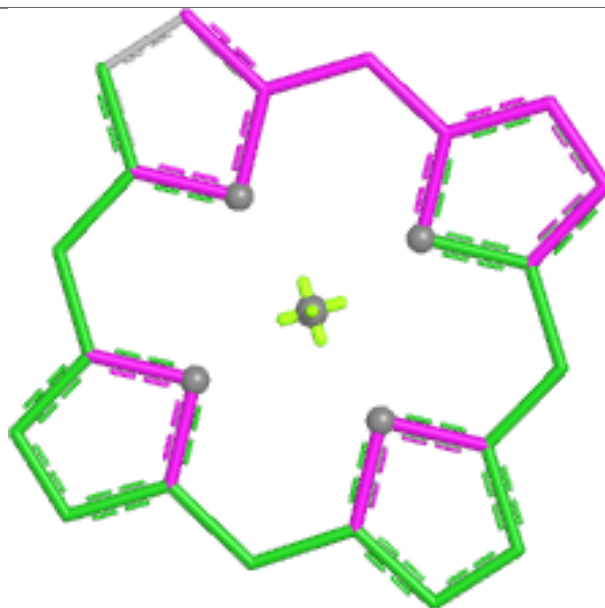


Rings

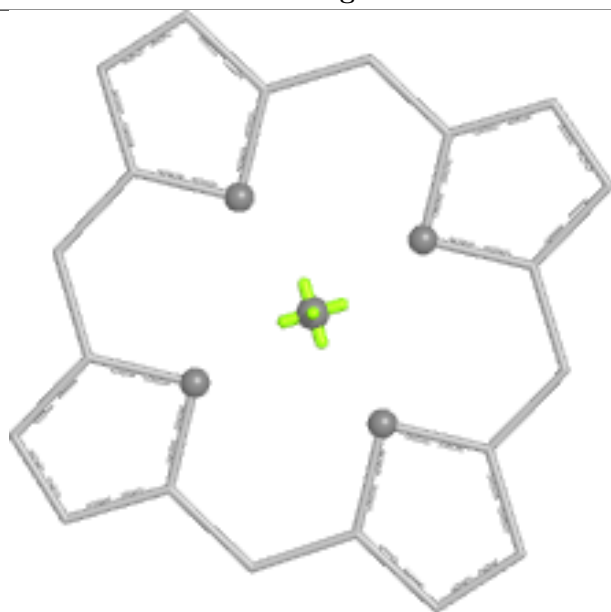
Ligand CLA 8 1014



Bond lengths



Bond angles

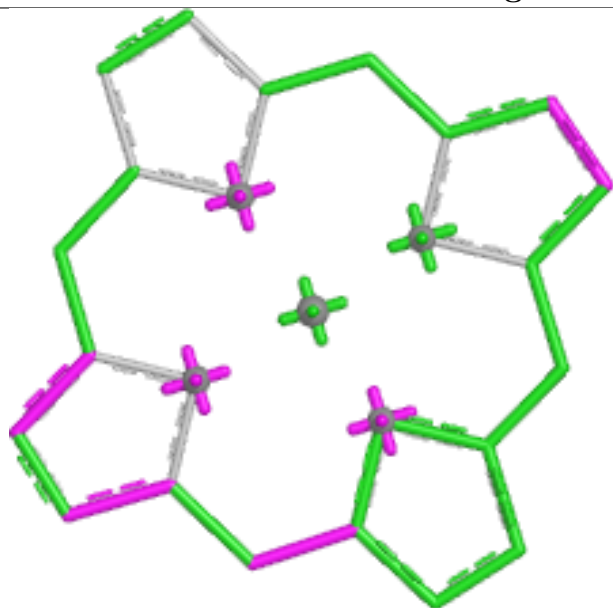


Torsions

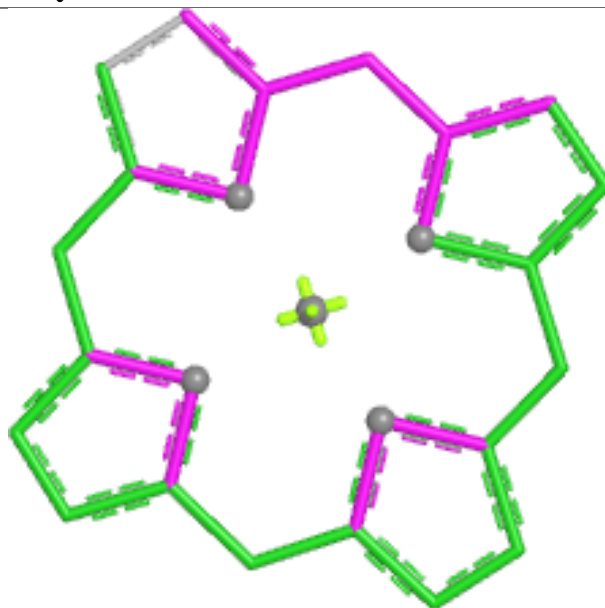


Rings

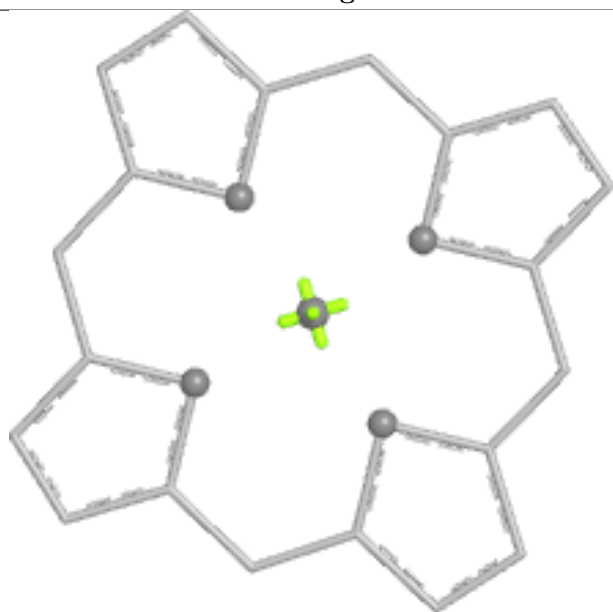
Ligand CLA Q 5222



Bond lengths



Bond angles

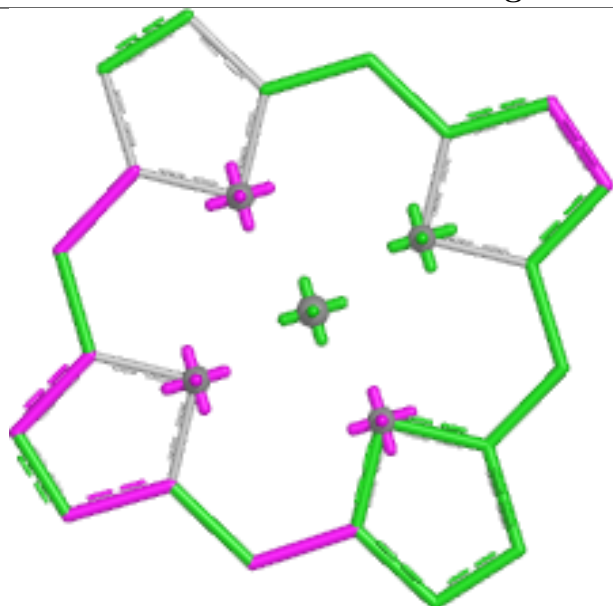


Torsions

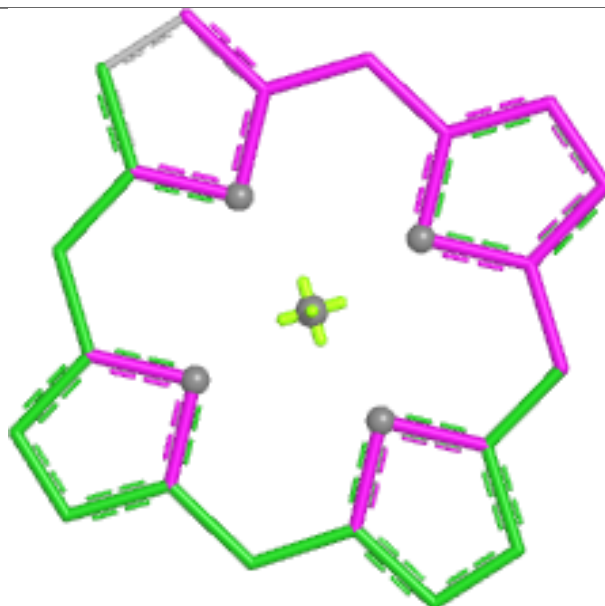


Rings

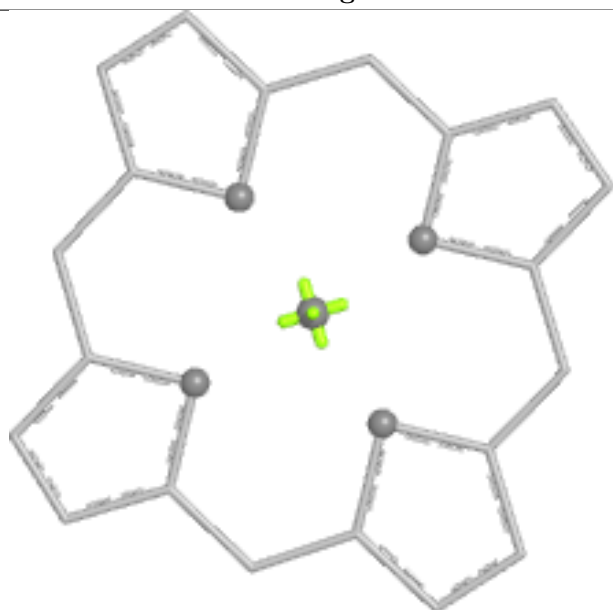
Ligand CLA A 1134



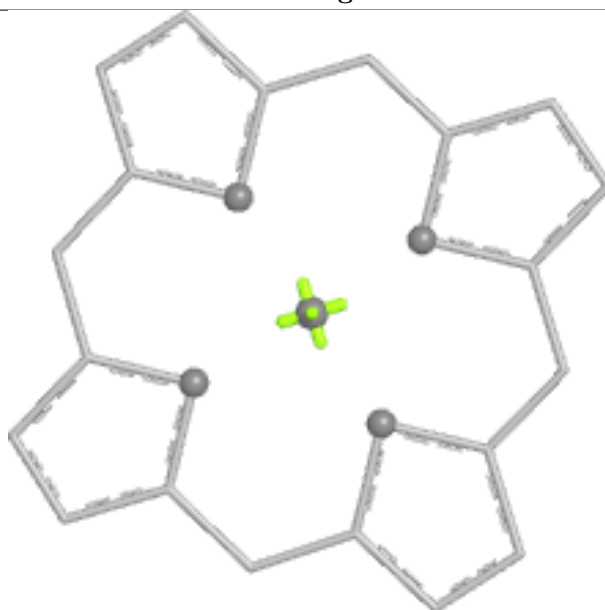
Bond lengths



Bond angles

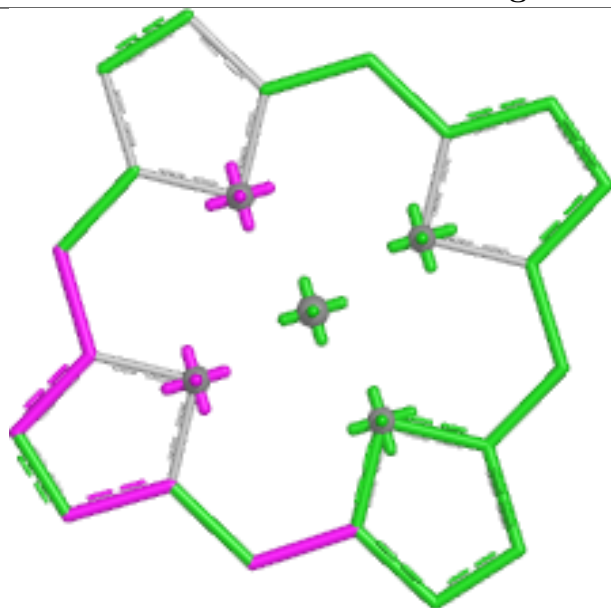


Torsions

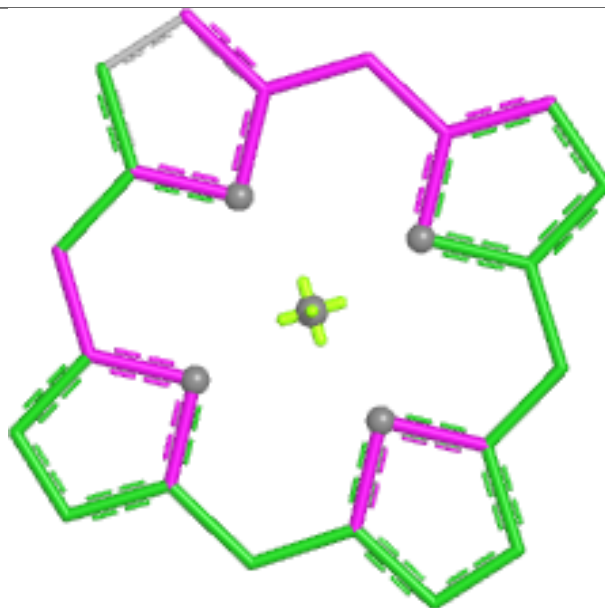


Rings

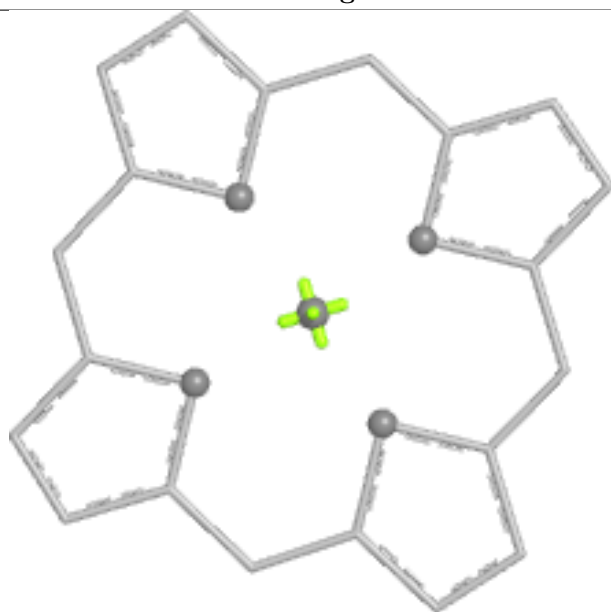
Ligand CLA 2 1015



Bond lengths



Bond angles

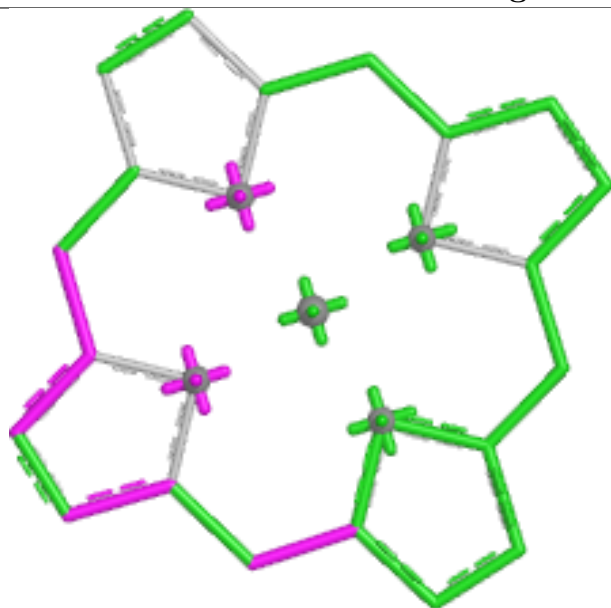


Torsions

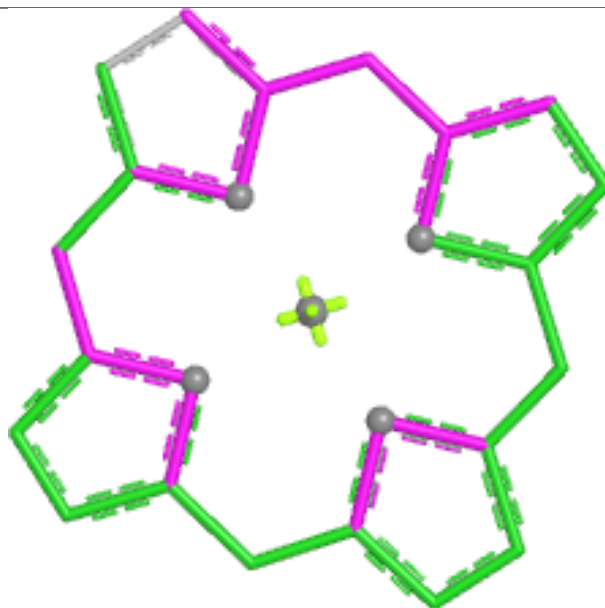


Rings

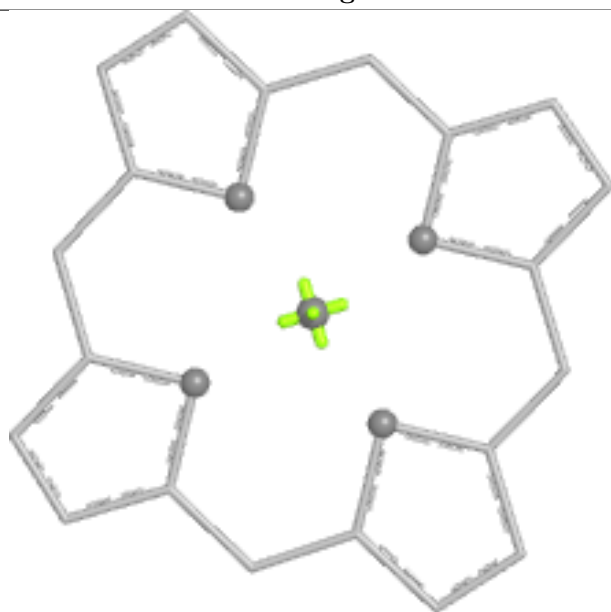
Ligand CLA 1 1012



Bond lengths



Bond angles

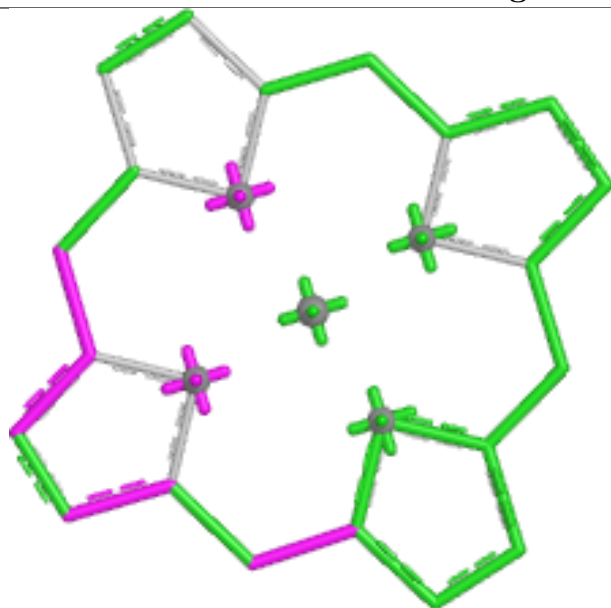


Torsions

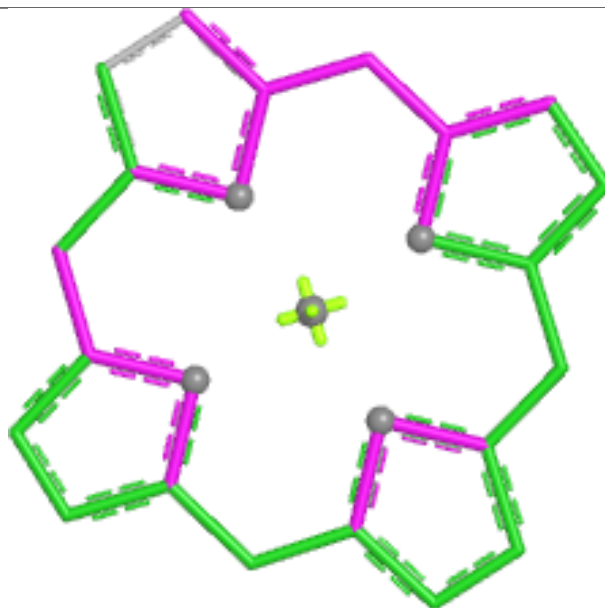


Rings

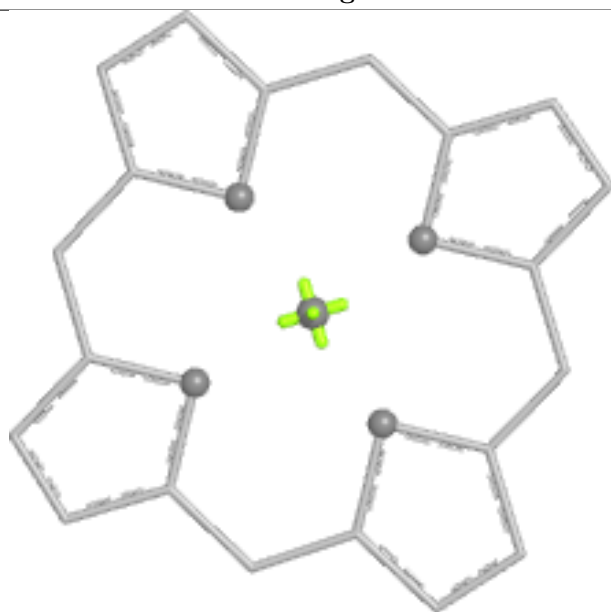
Ligand CLA 9 1033



Bond lengths



Bond angles

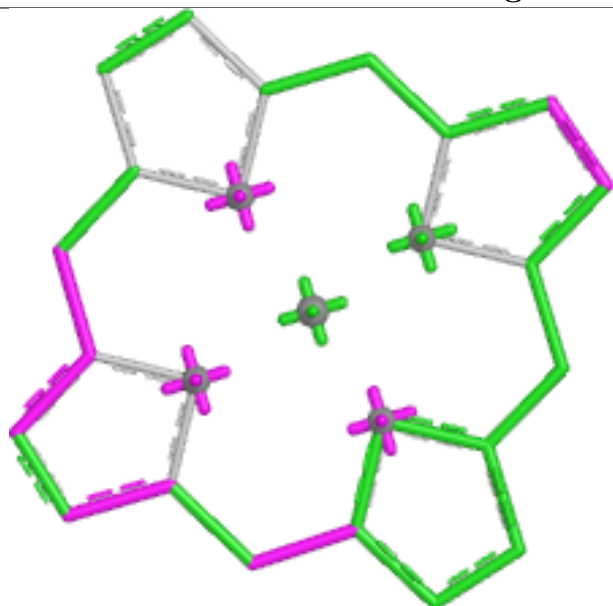


Torsions

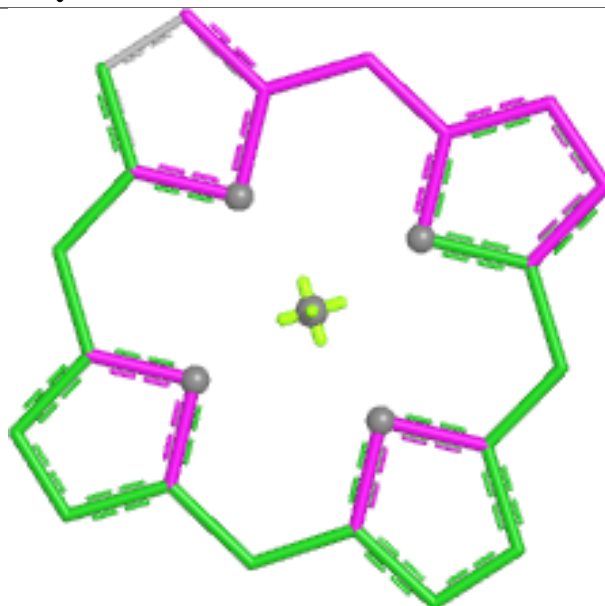


Rings

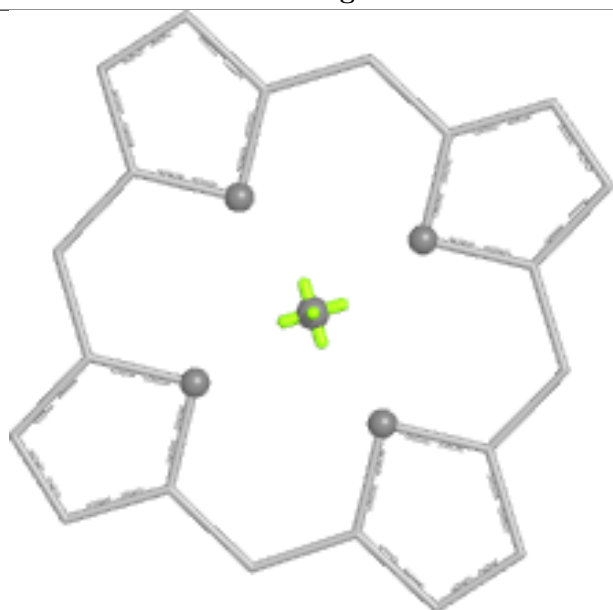
Ligand CLA Q 5208



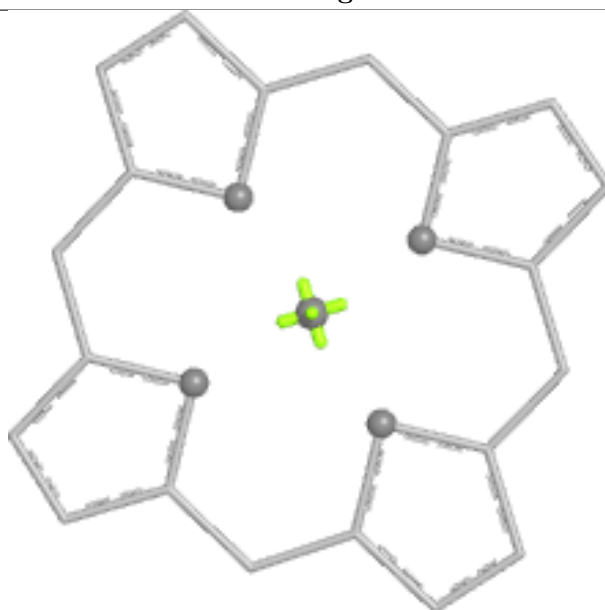
Bond lengths



Bond angles

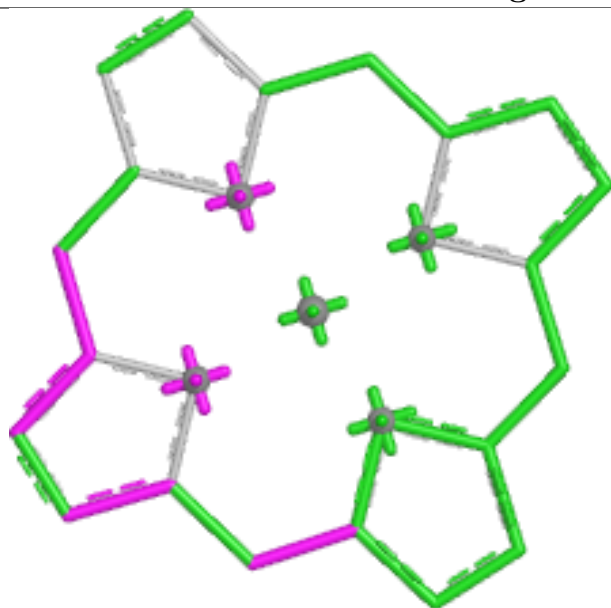


Torsions



Rings

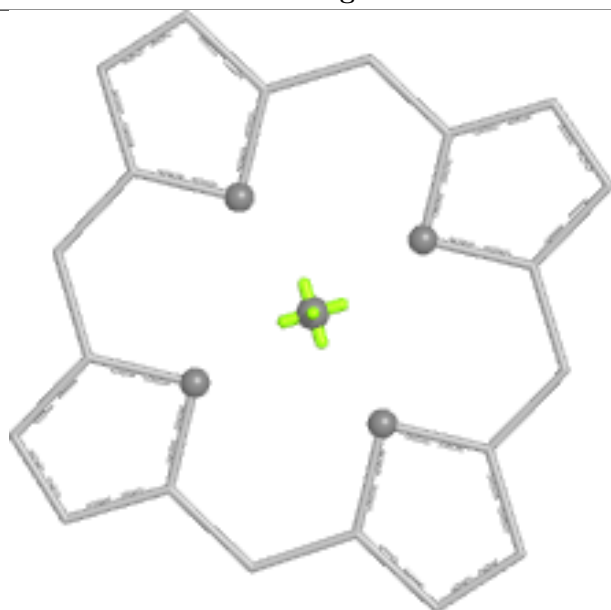
Ligand CLA 2 1023



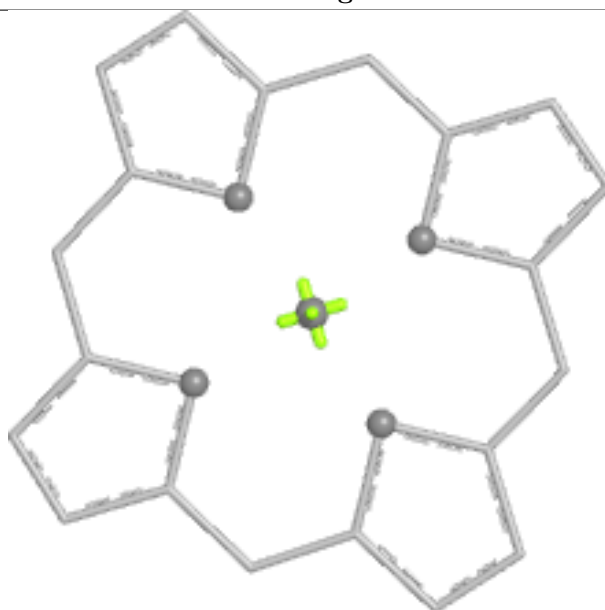
Bond lengths



Bond angles

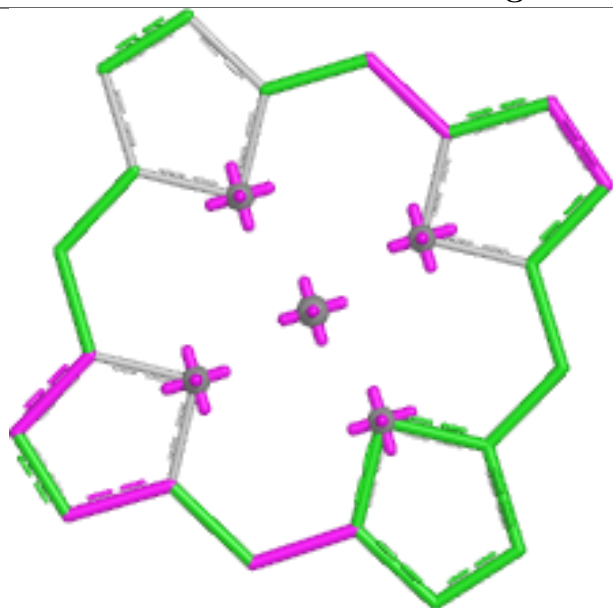


Torsions

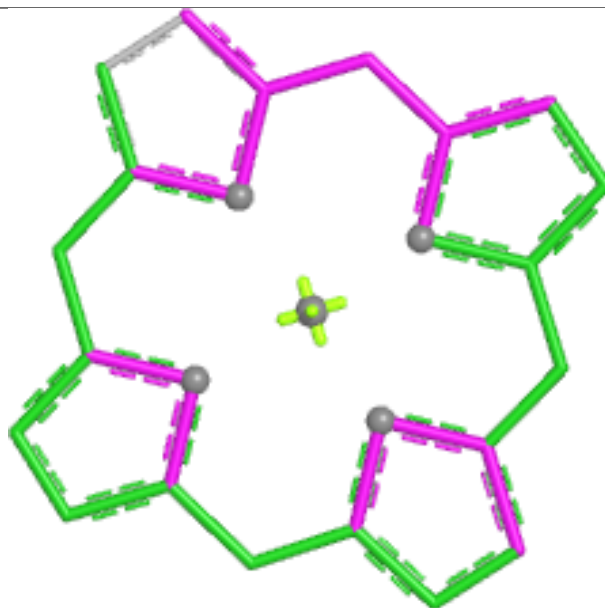


Rings

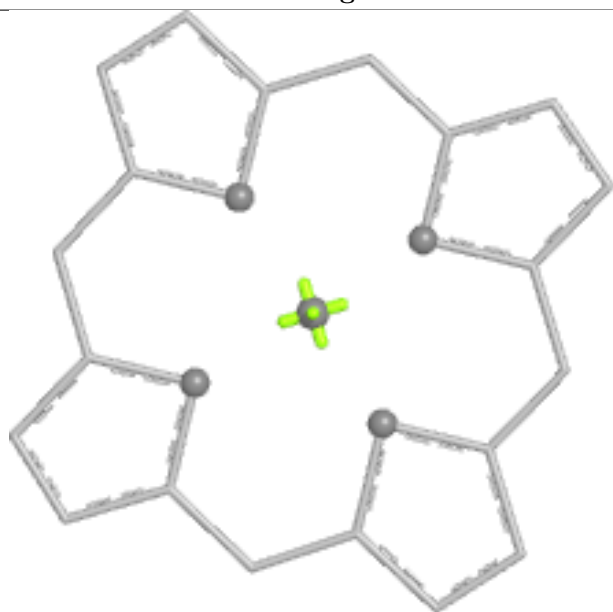
Ligand CLA P 5104



Bond lengths



Bond angles

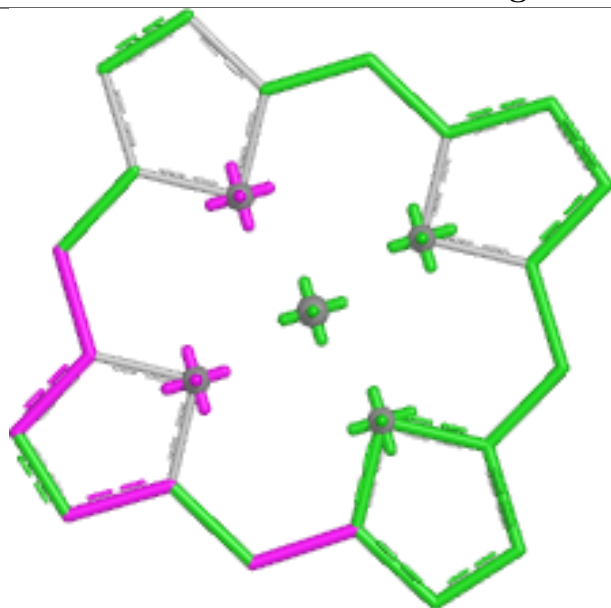


Torsions

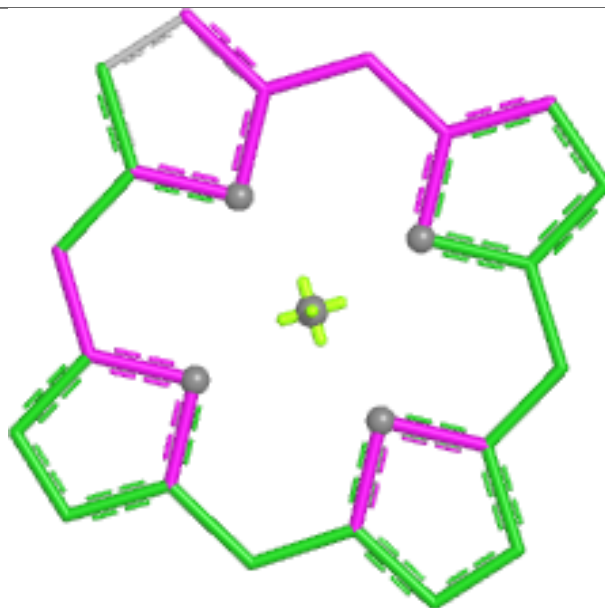


Rings

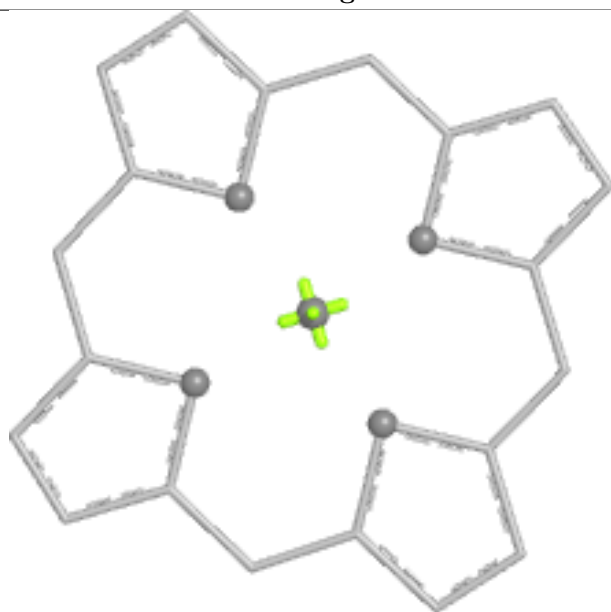
Ligand CLA 1 1015



Bond lengths



Bond angles

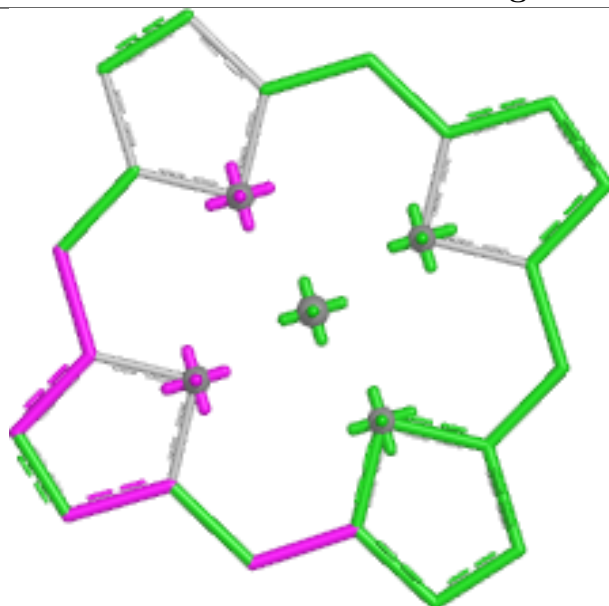


Torsions

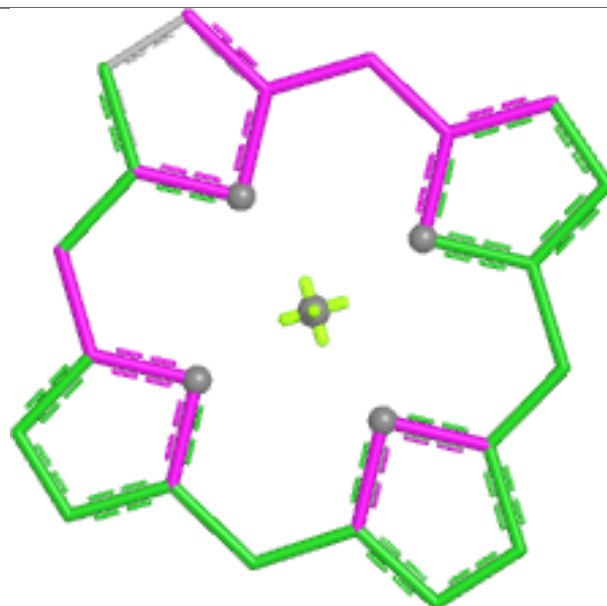


Rings

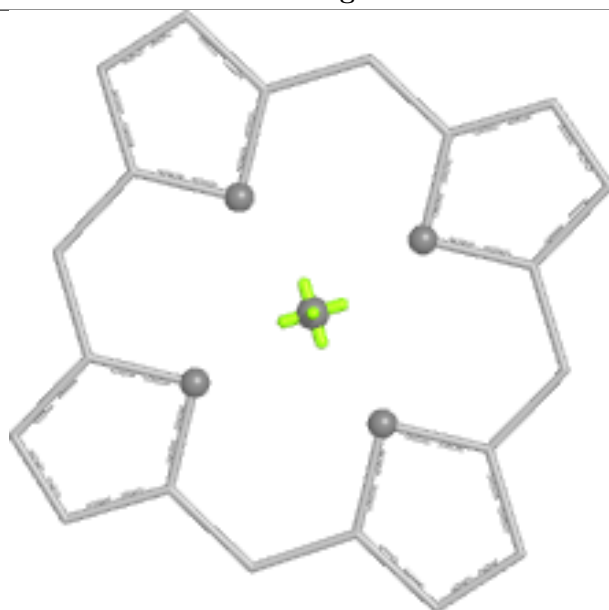
Ligand CLA 2 1012



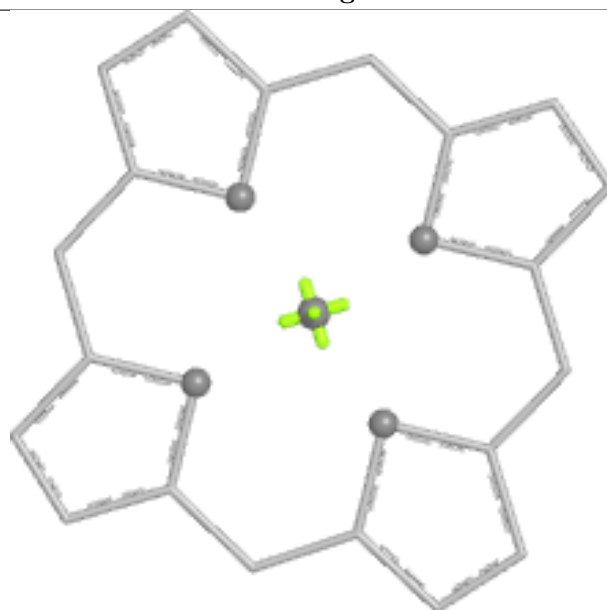
Bond lengths



Bond angles

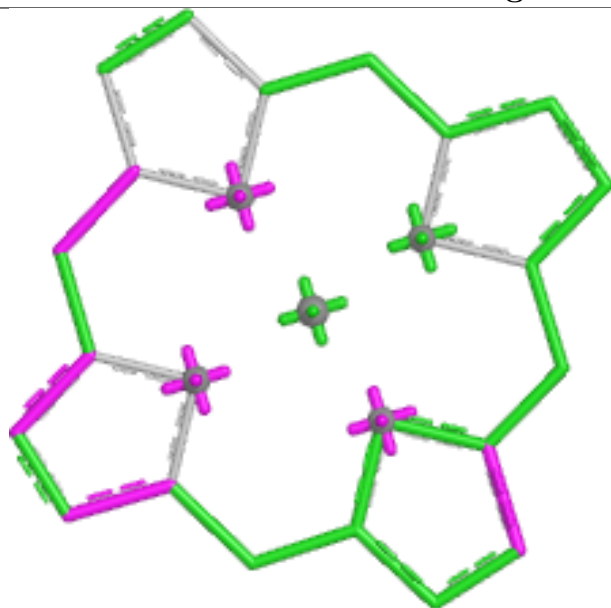


Torsions

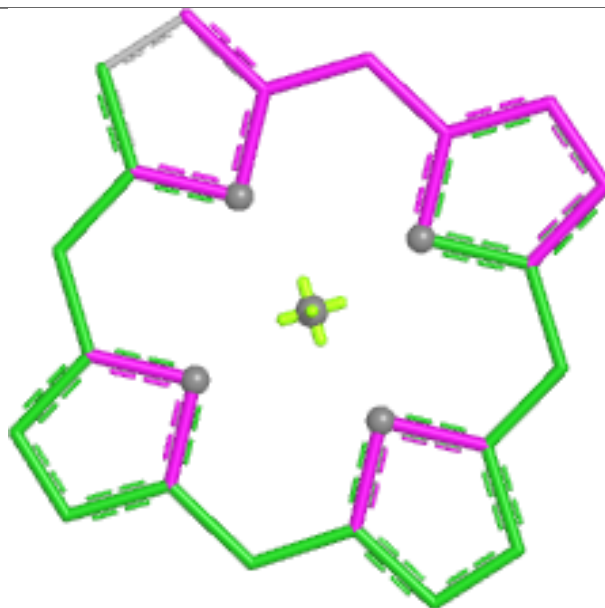


Rings

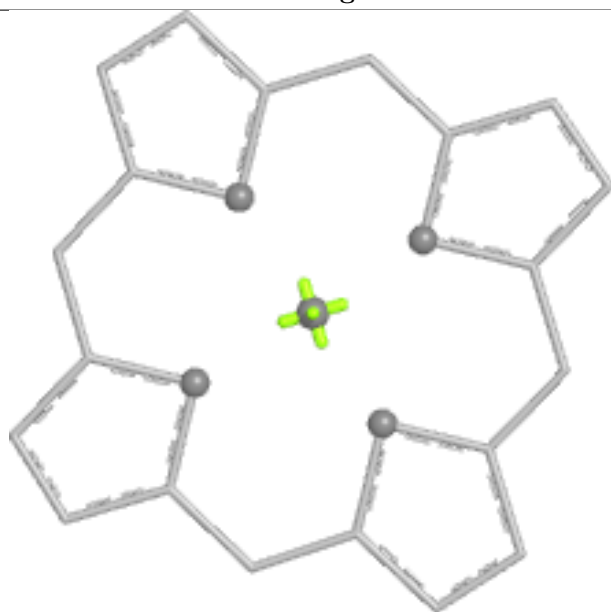
Ligand CLA P 5135



Bond lengths



Bond angles

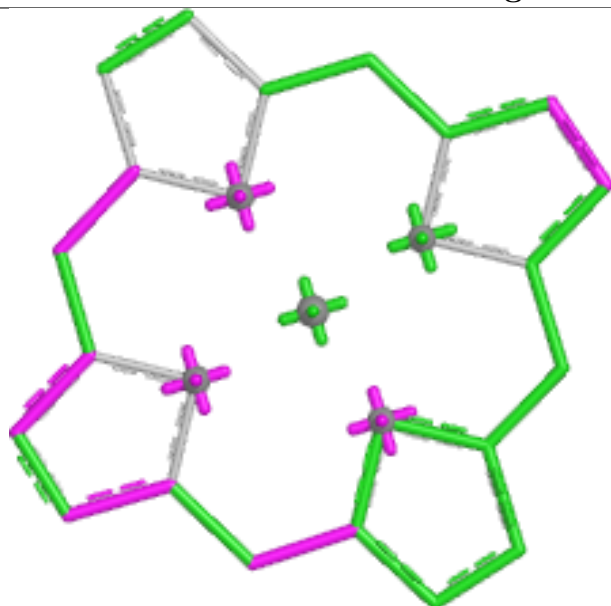


Torsions

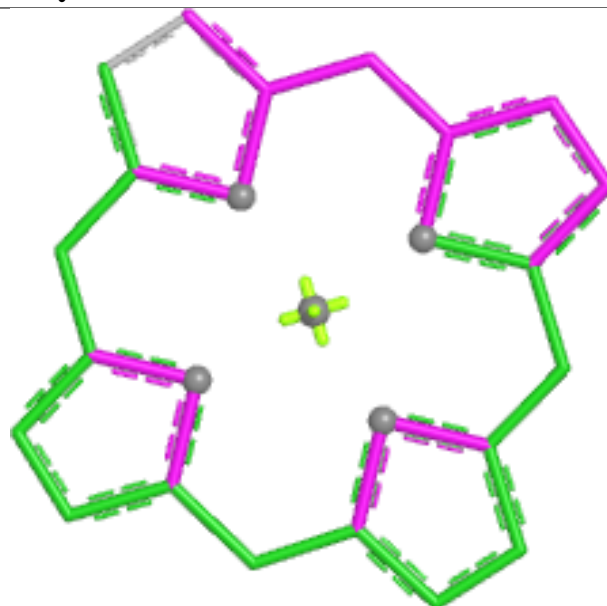


Rings

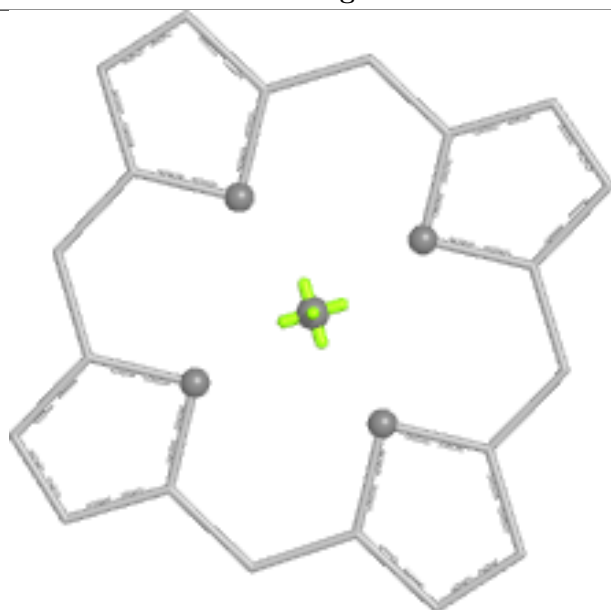
Ligand CLA Q 5230



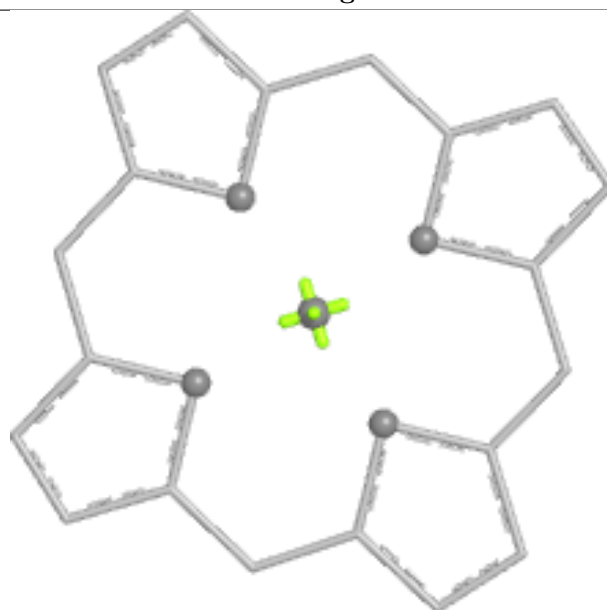
Bond lengths



Bond angles

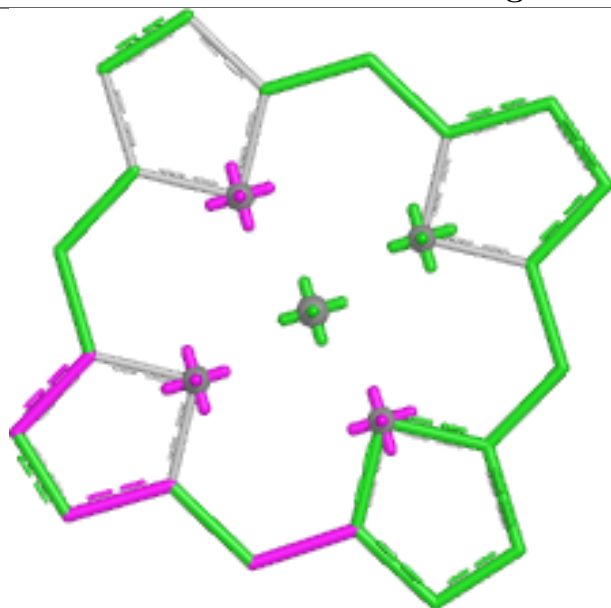


Torsions

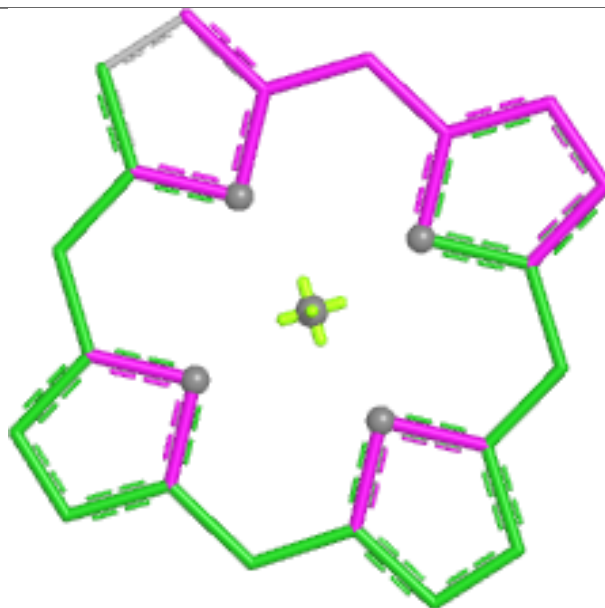


Rings

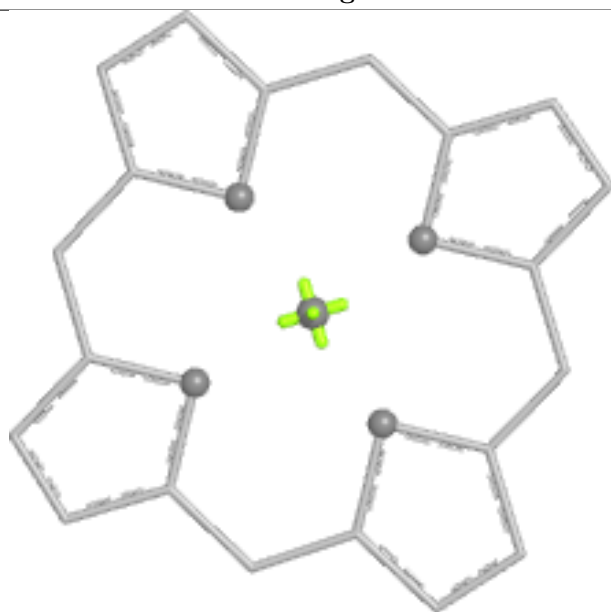
Ligand CLA P 5140



Bond lengths



Bond angles

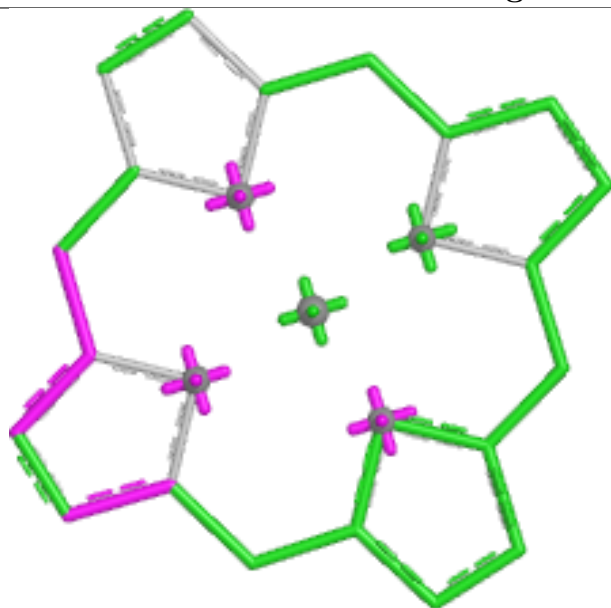


Torsions

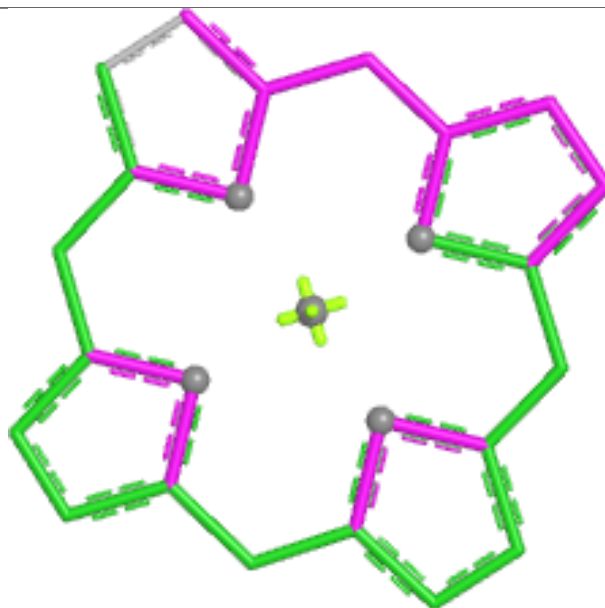


Rings

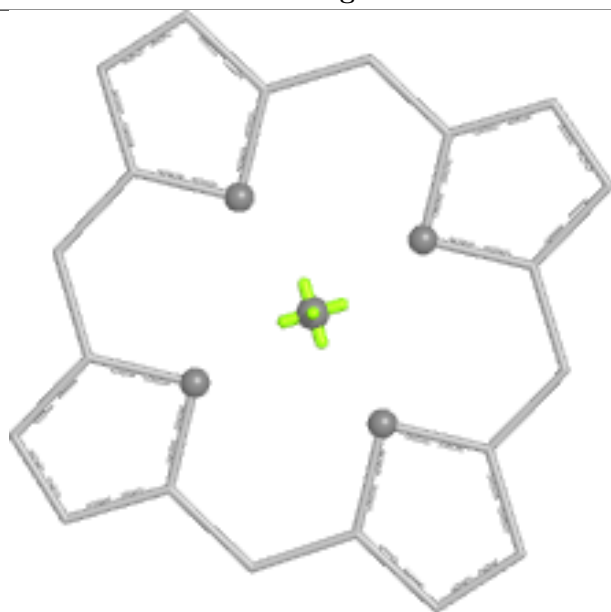
Ligand CLA P 5126



Bond lengths



Bond angles

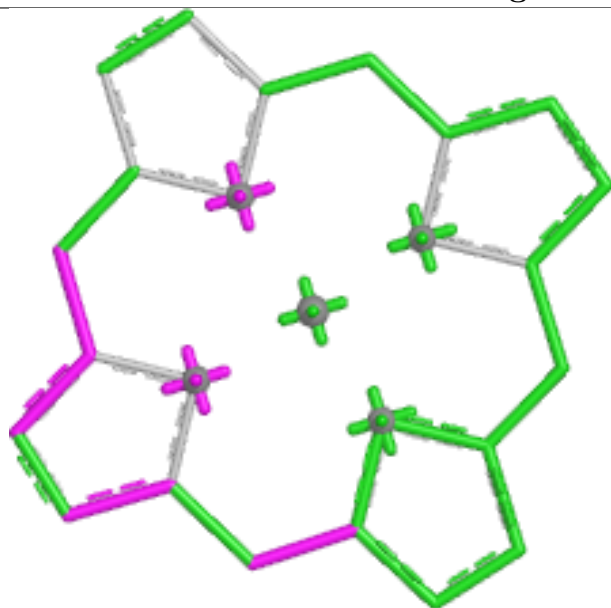


Torsions



Rings

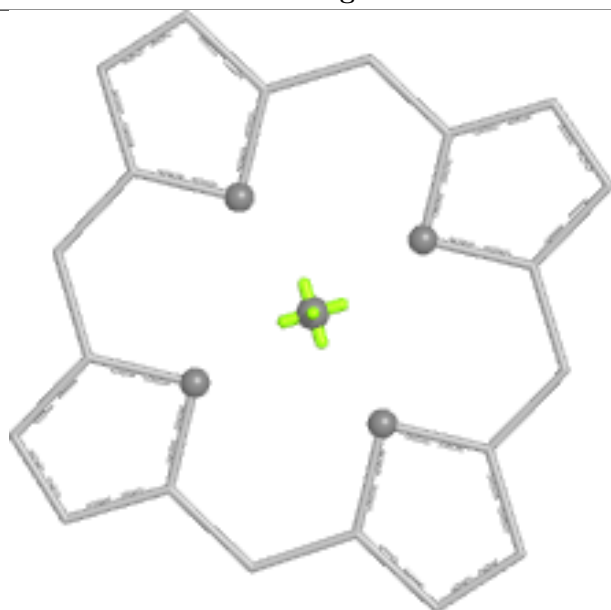
Ligand CLA 8 1026



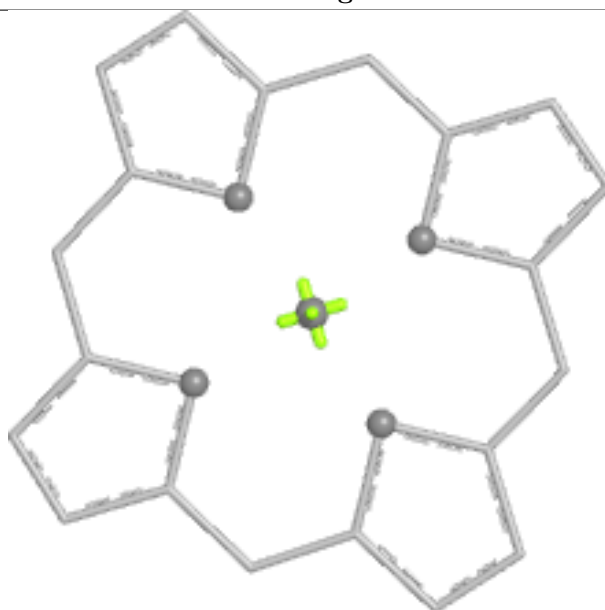
Bond lengths



Bond angles

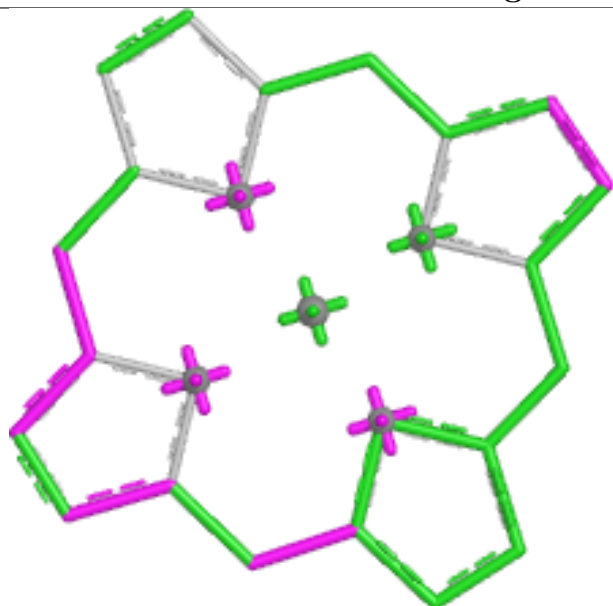


Torsions

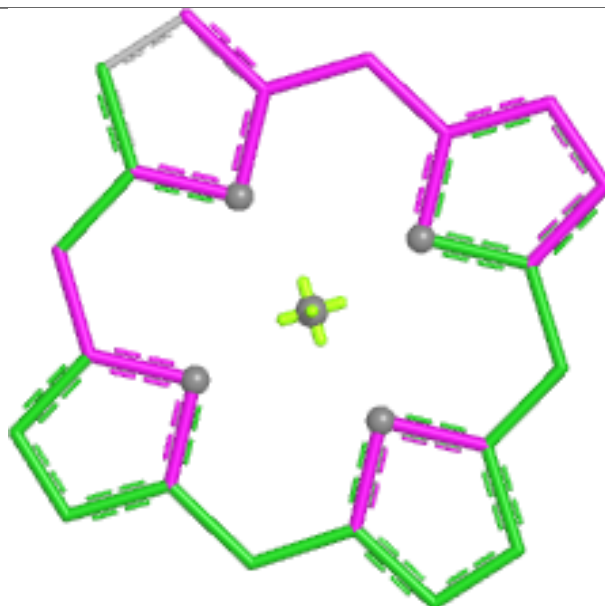


Rings

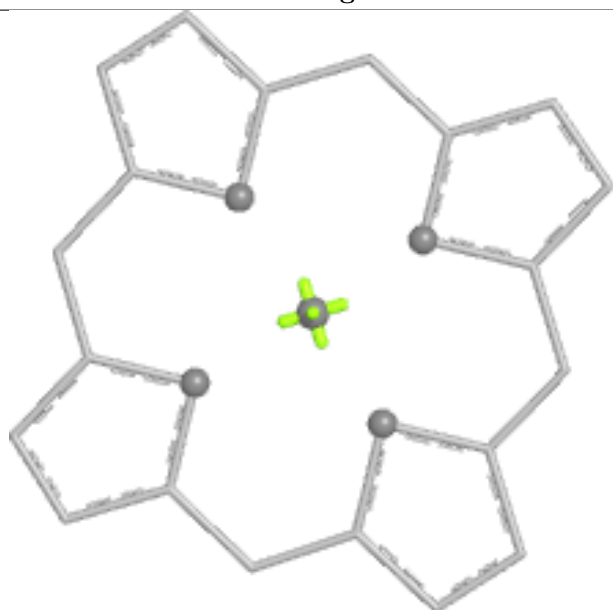
Ligand CLA K 1401



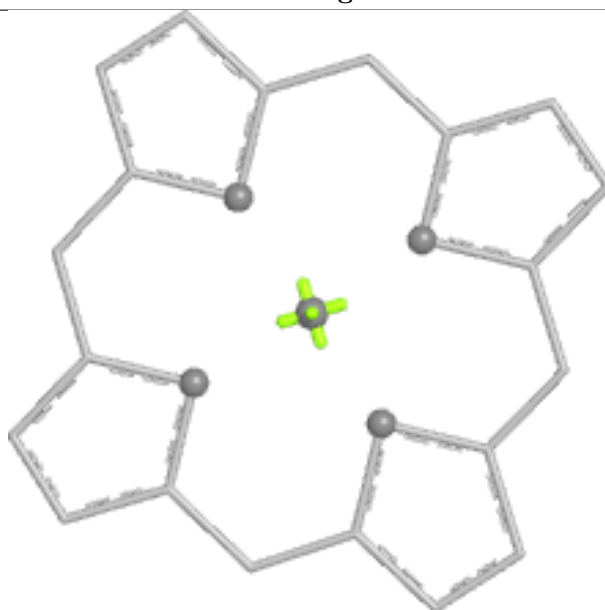
Bond lengths



Bond angles

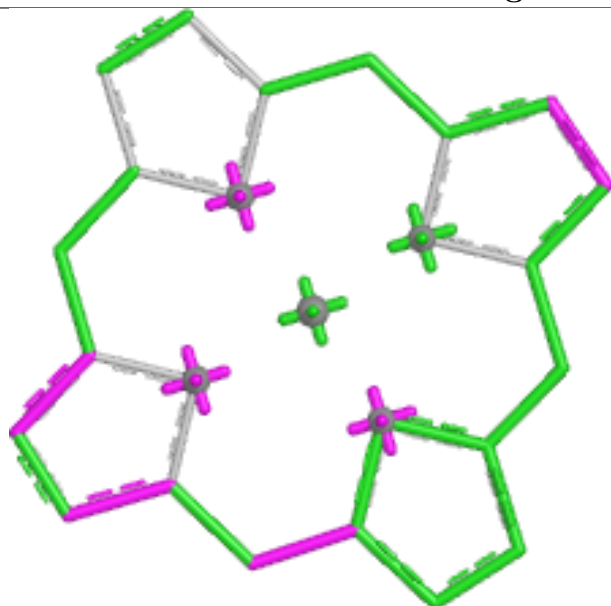


Torsions

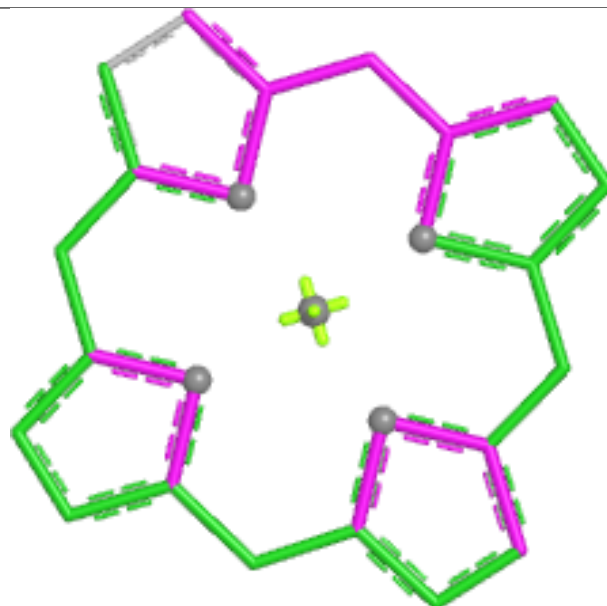


Rings

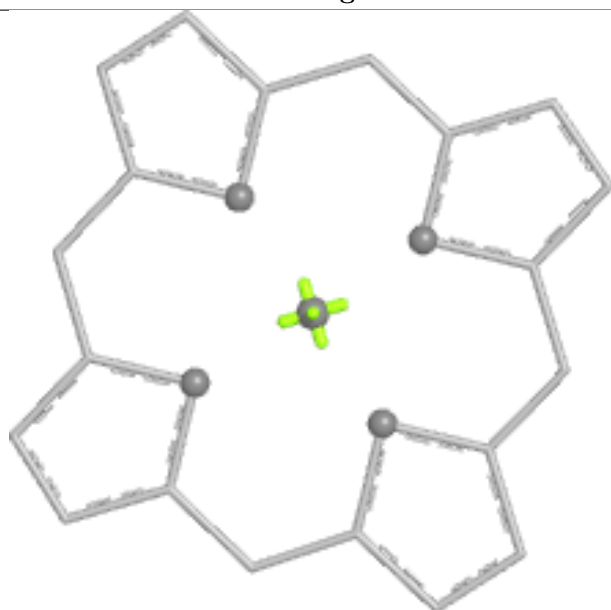
Ligand CLA B 1220



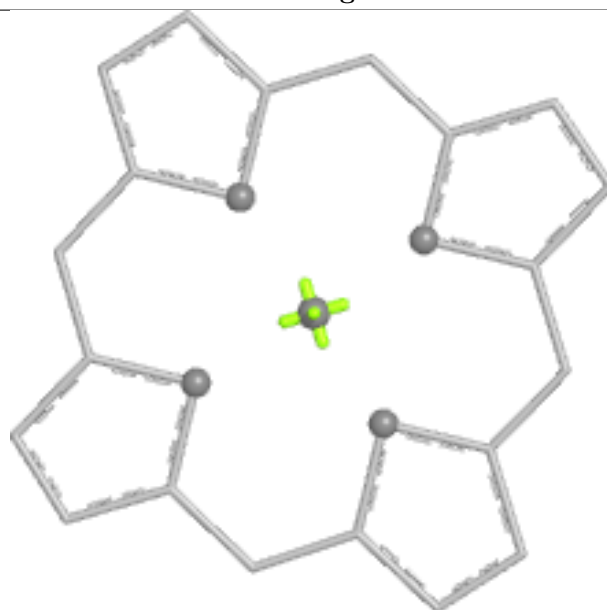
Bond lengths



Bond angles

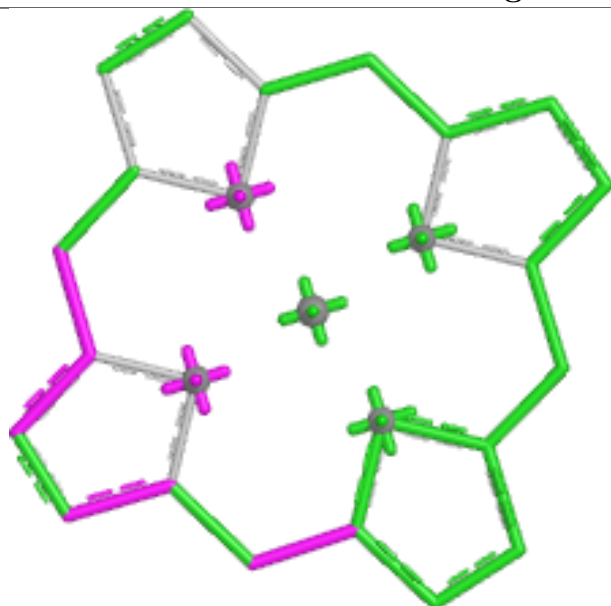


Torsions

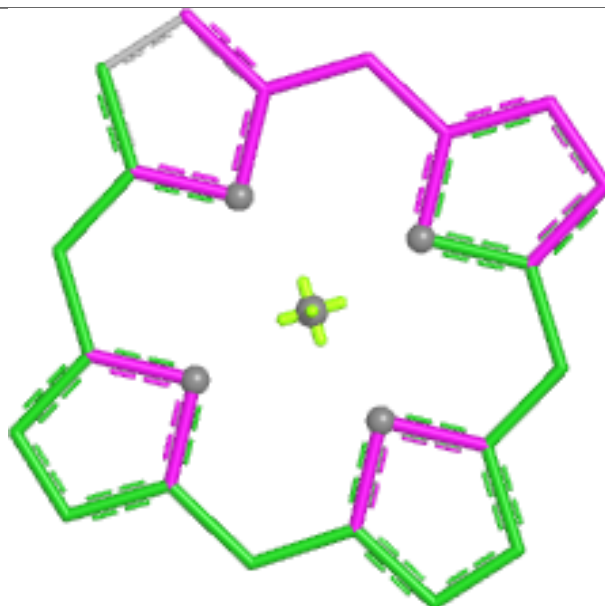


Rings

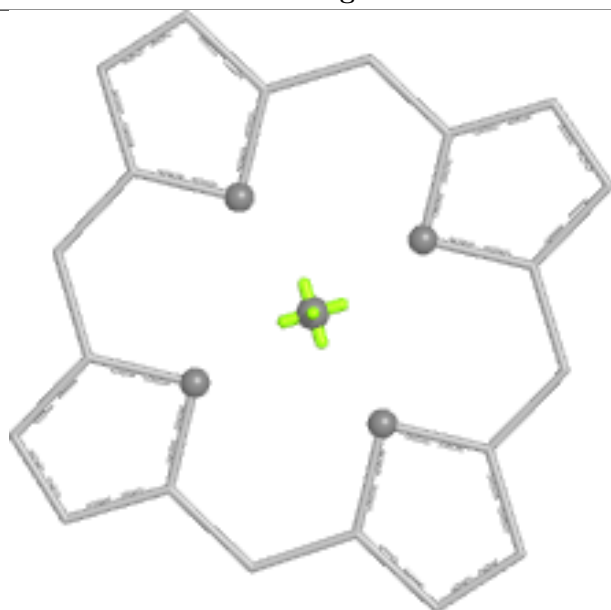
Ligand CLA A 1106



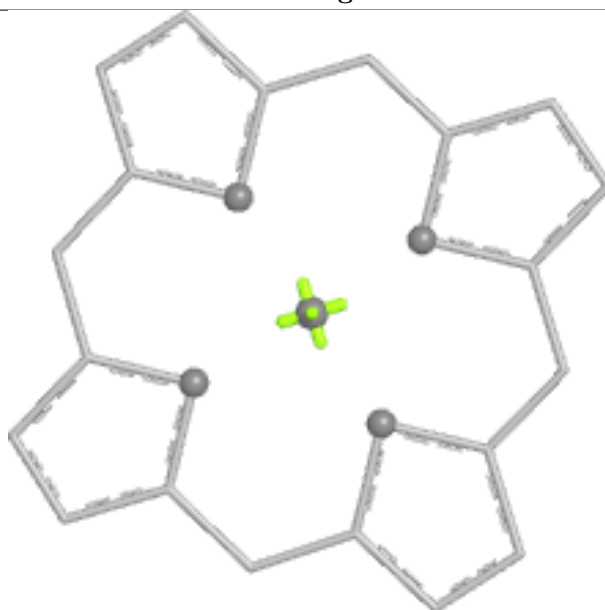
Bond lengths



Bond angles

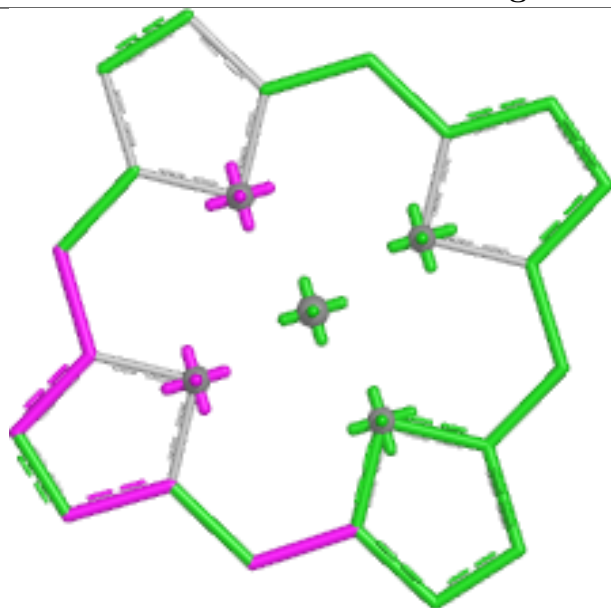


Torsions

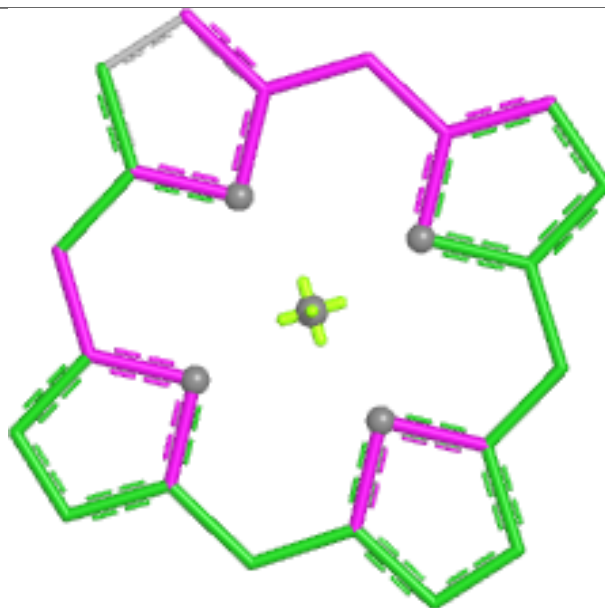


Rings

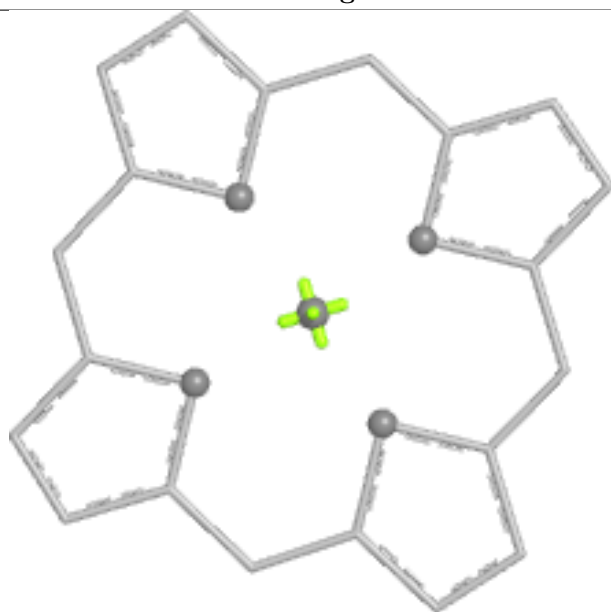
Ligand CLA 5 5404



Bond lengths



Bond angles

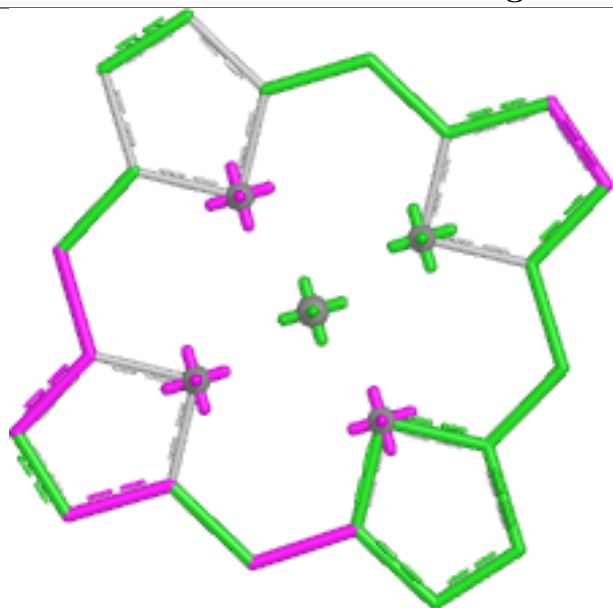


Torsions

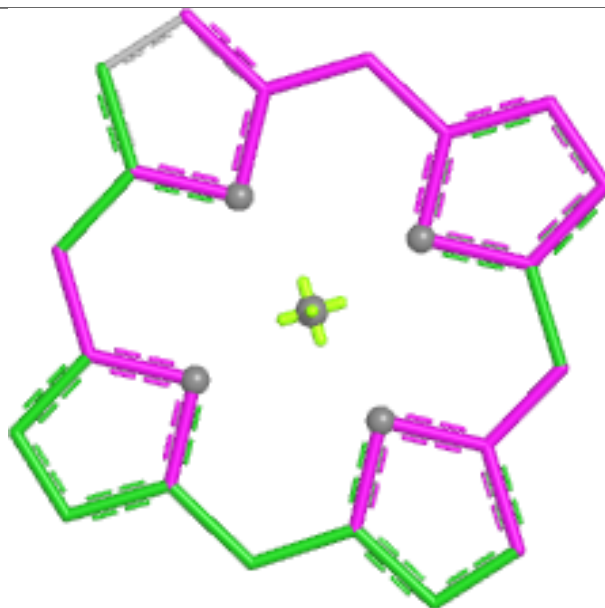


Rings

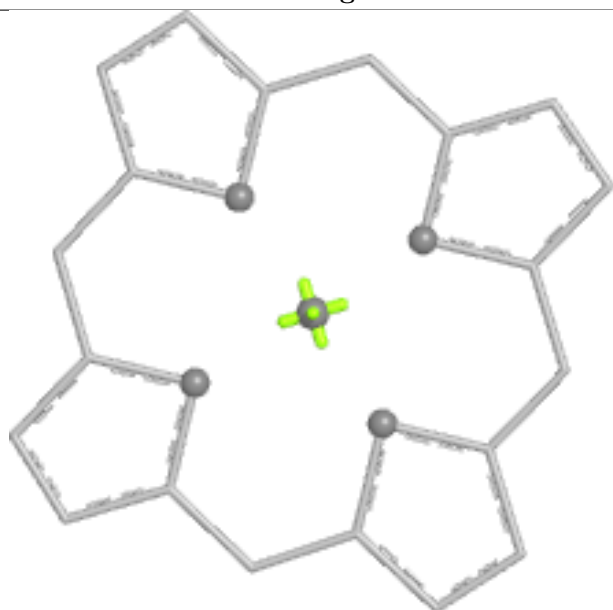
Ligand CLA P 5901



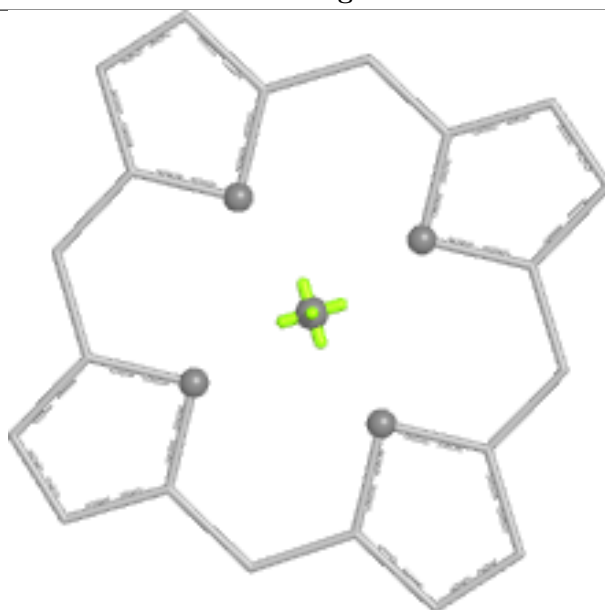
Bond lengths



Bond angles

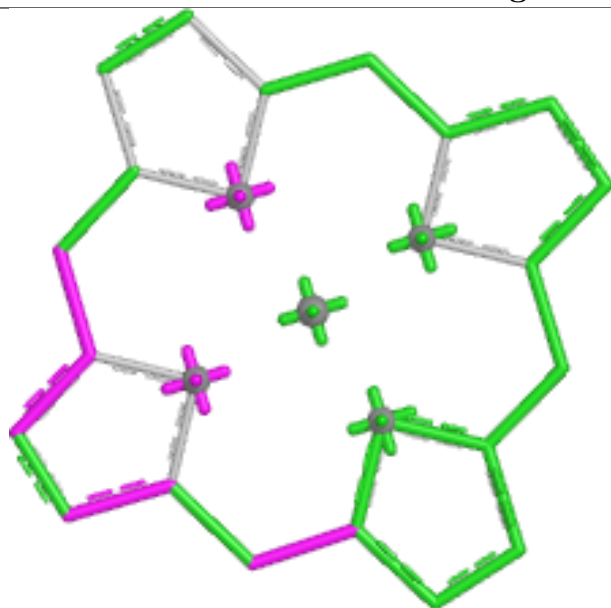


Torsions

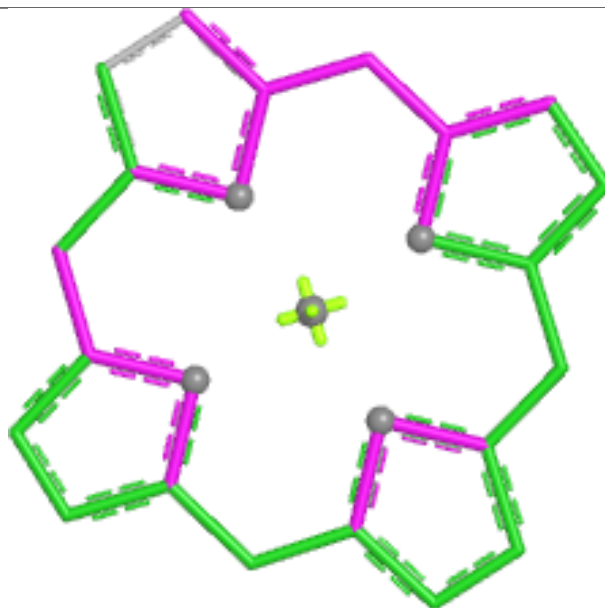


Rings

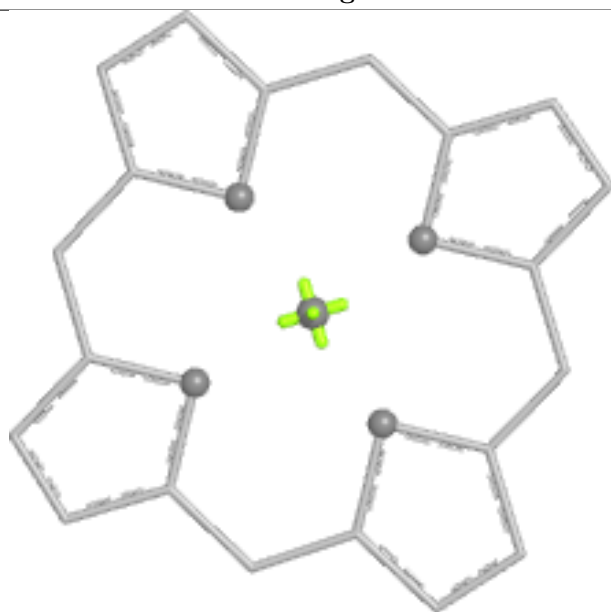
Ligand CLA 4 1017



Bond lengths



Bond angles

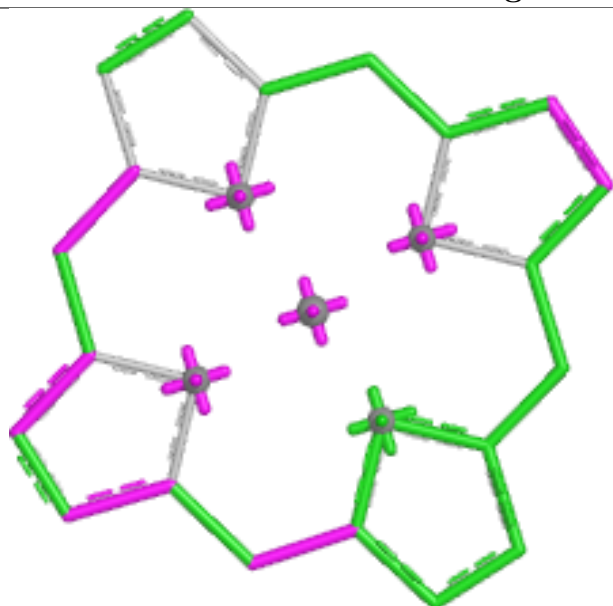


Torsions

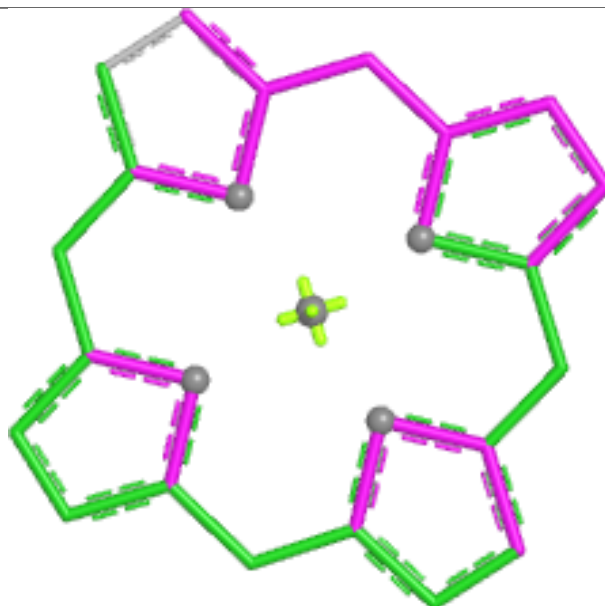


Rings

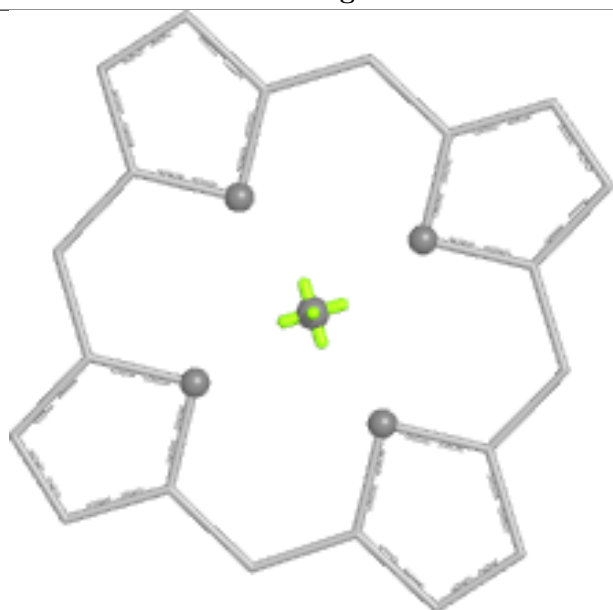
Ligand CLA A 1118



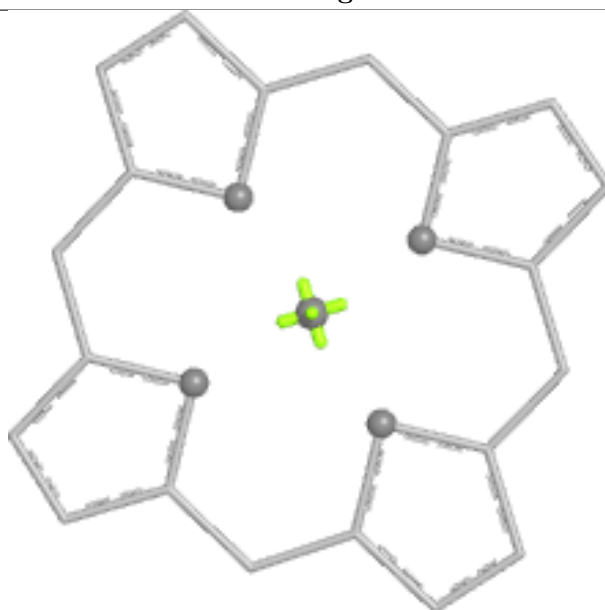
Bond lengths



Bond angles

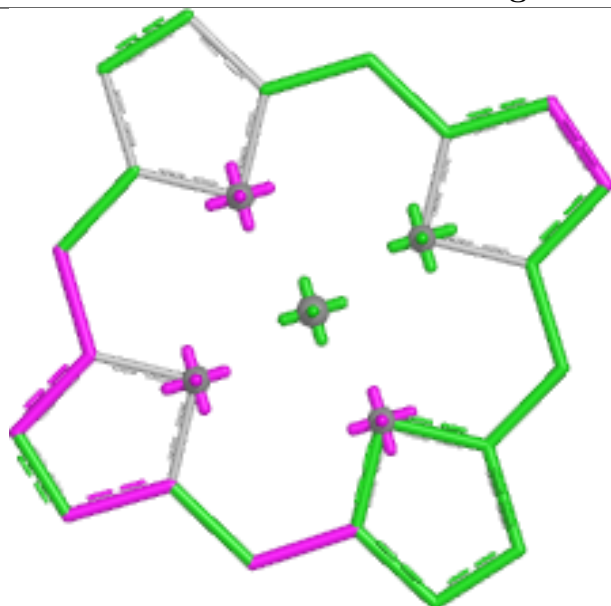


Torsions

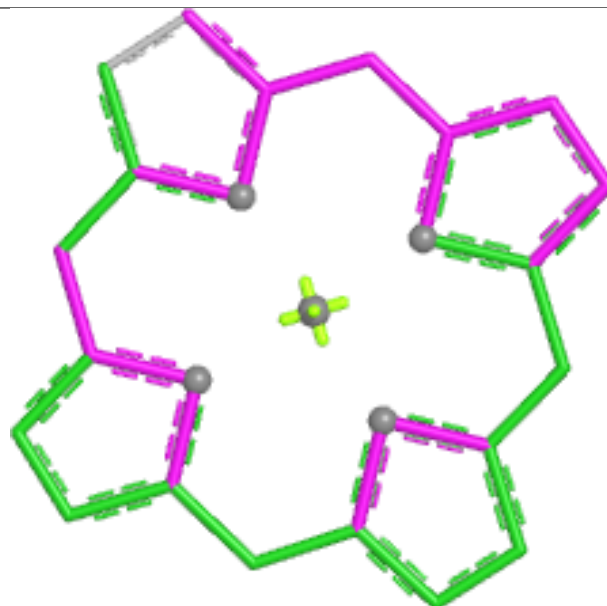


Rings

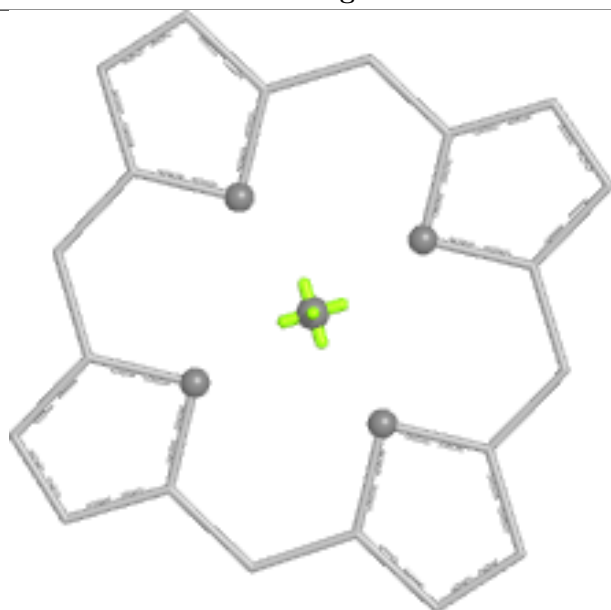
Ligand CLA 5 5401



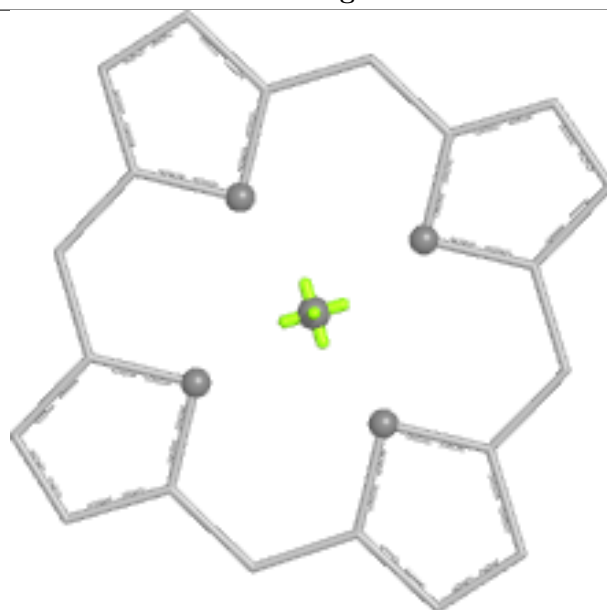
Bond lengths



Bond angles

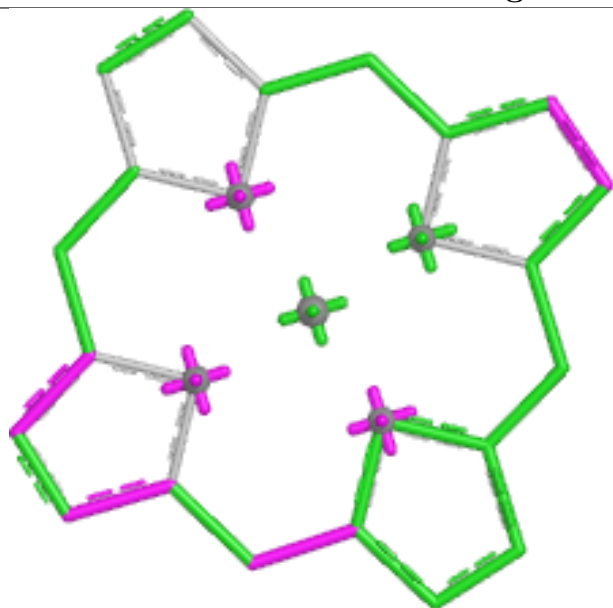


Torsions

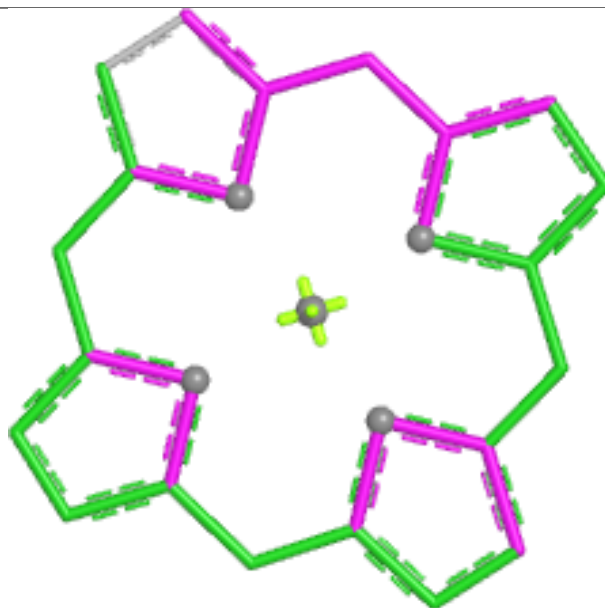


Rings

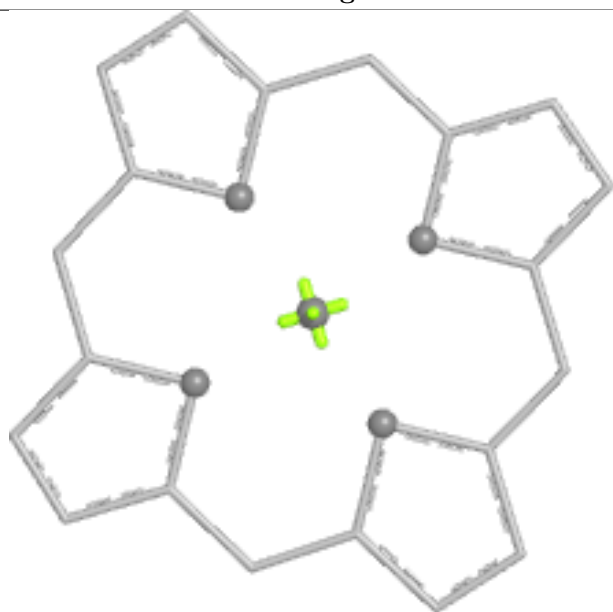
Ligand CLA P 5116



Bond lengths



Bond angles

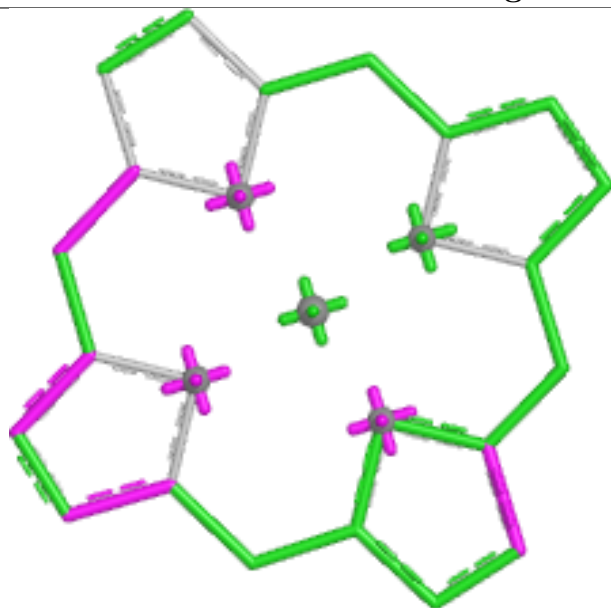


Torsions

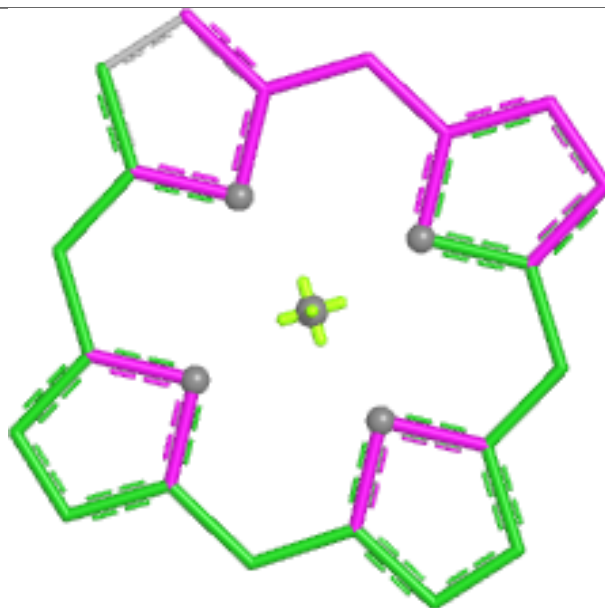


Rings

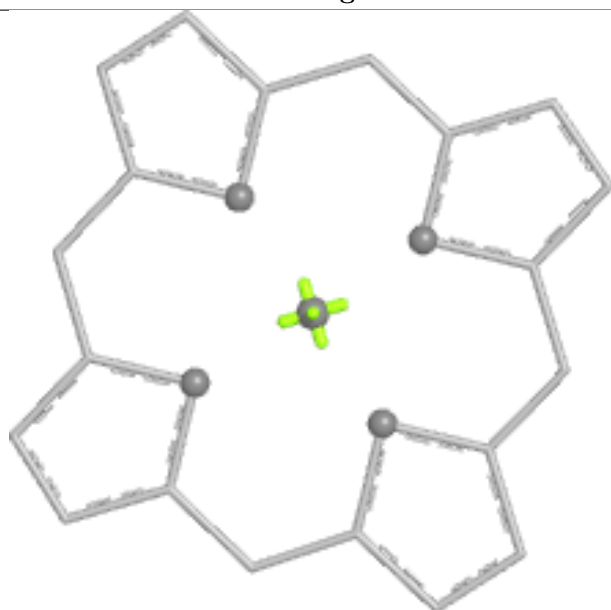
Ligand CLA A 1135



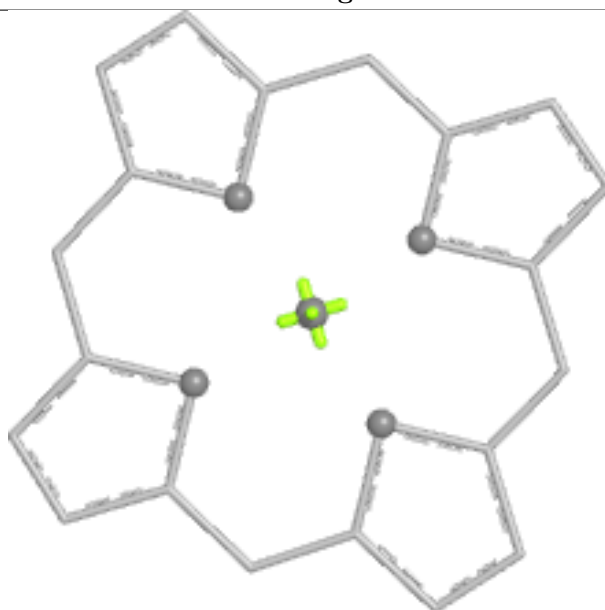
Bond lengths



Bond angles

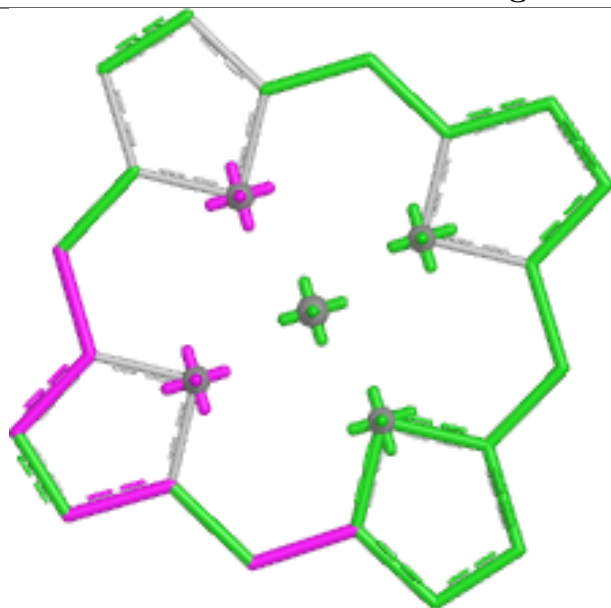


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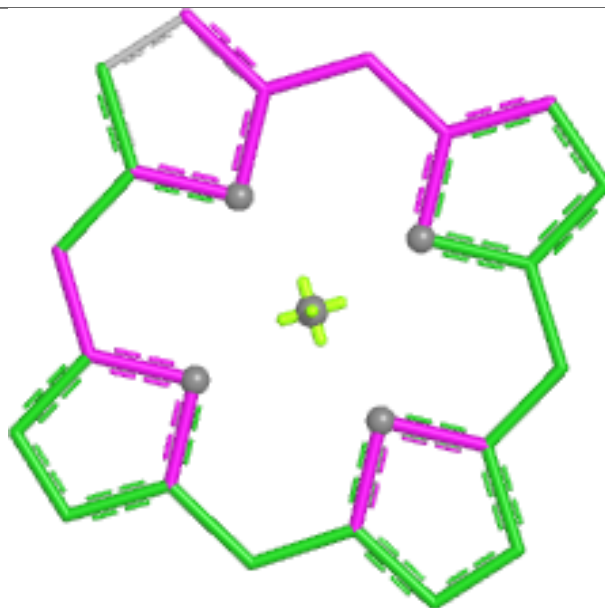


Rings

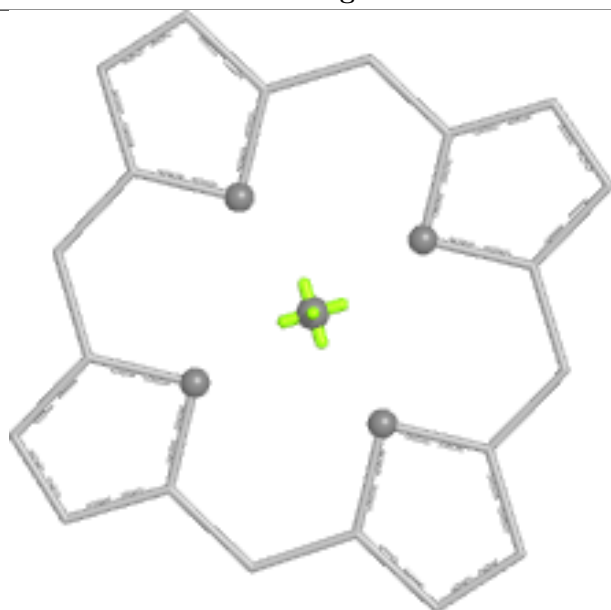
Ligand CLA 2 1033



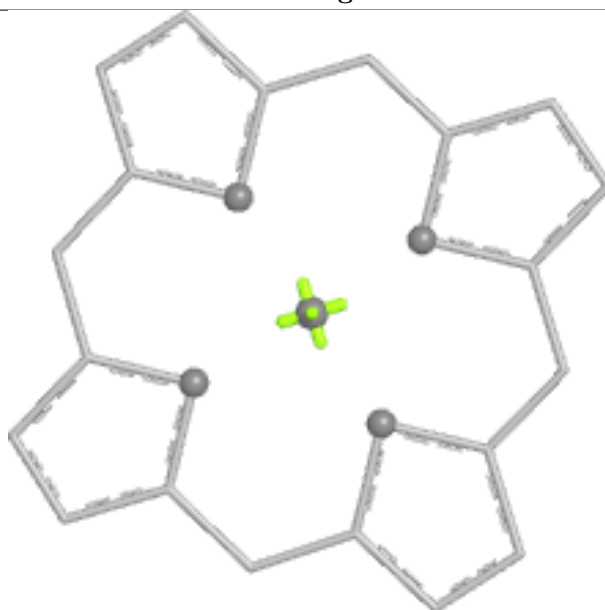
Bond lengths



Bond angles

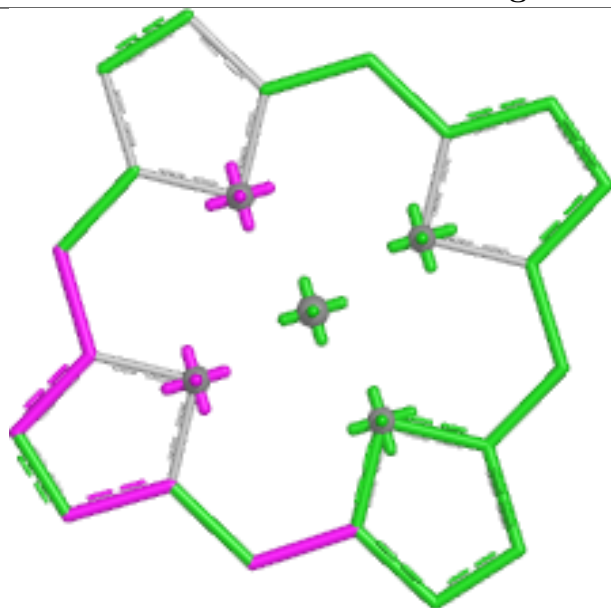


Torsions

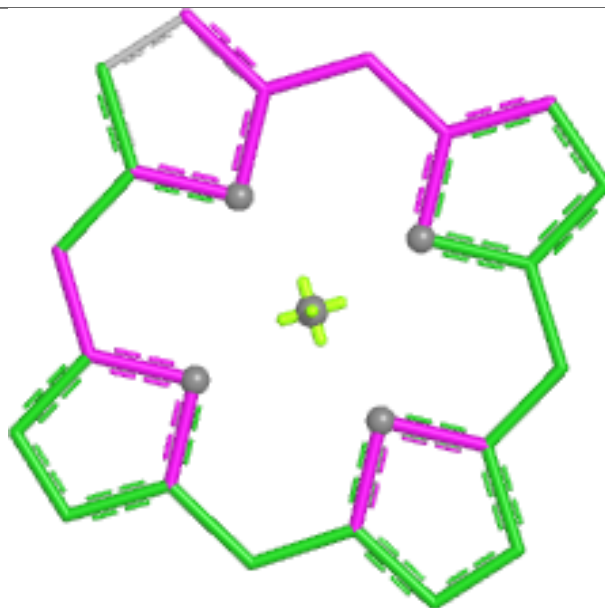


Rings

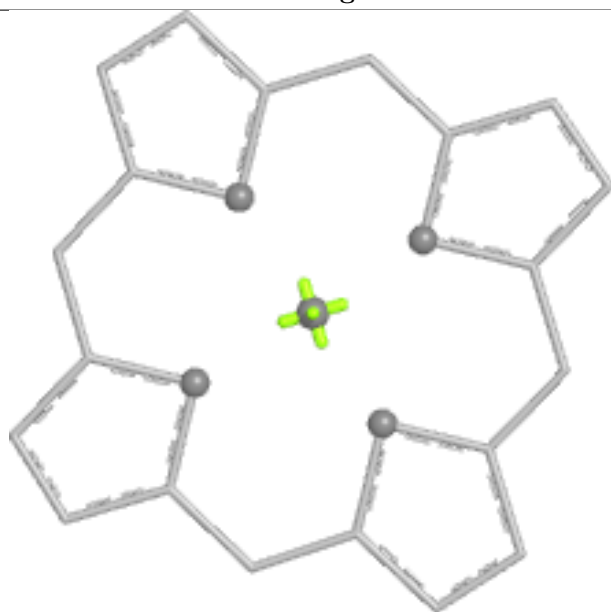
Ligand CLA 4 1015



Bond lengths



Bond angles

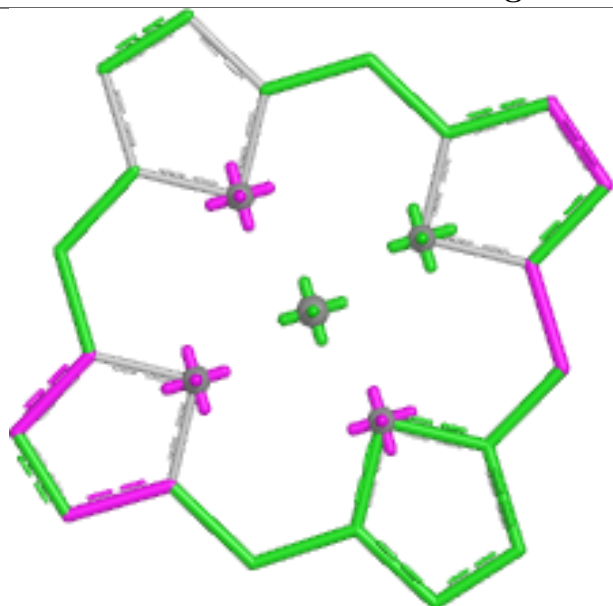


Torsions

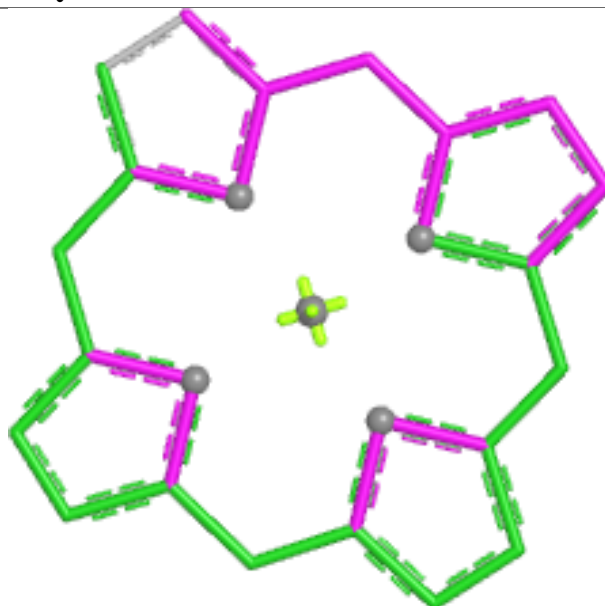


Rings

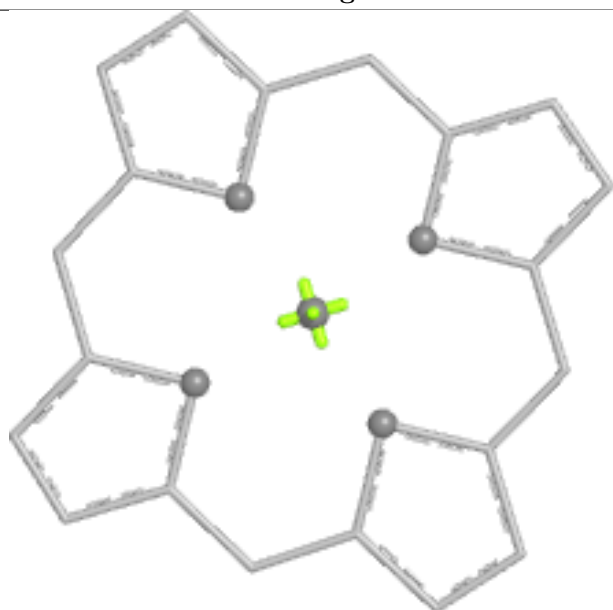
Ligand CLA Q 5203



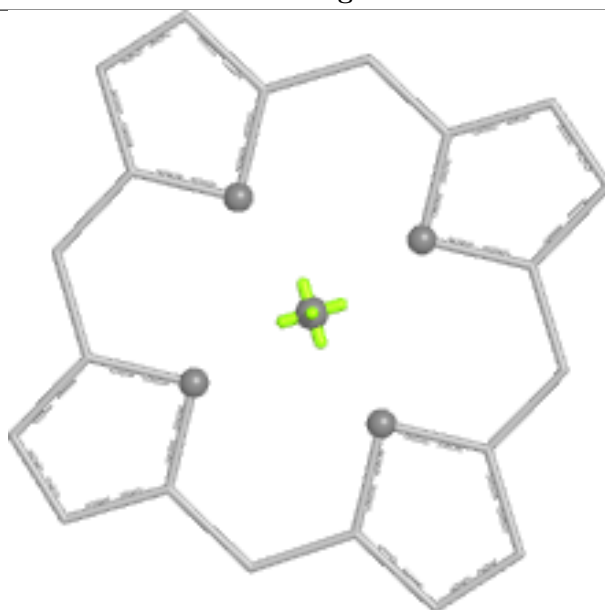
Bond lengths



Bond angles

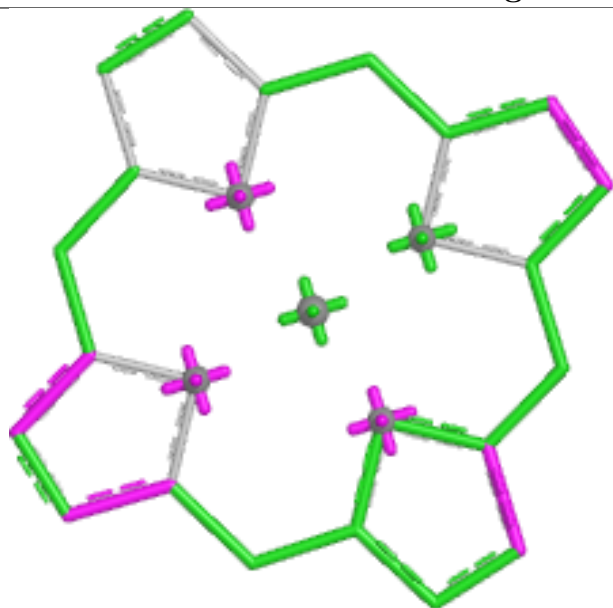


Torsions

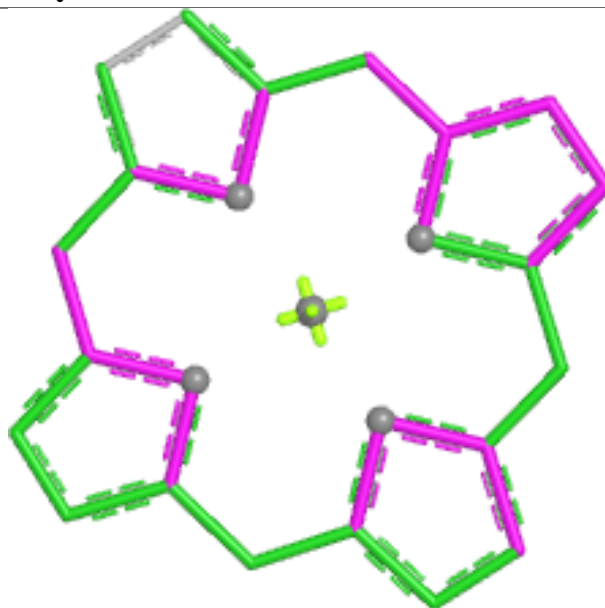


Rings

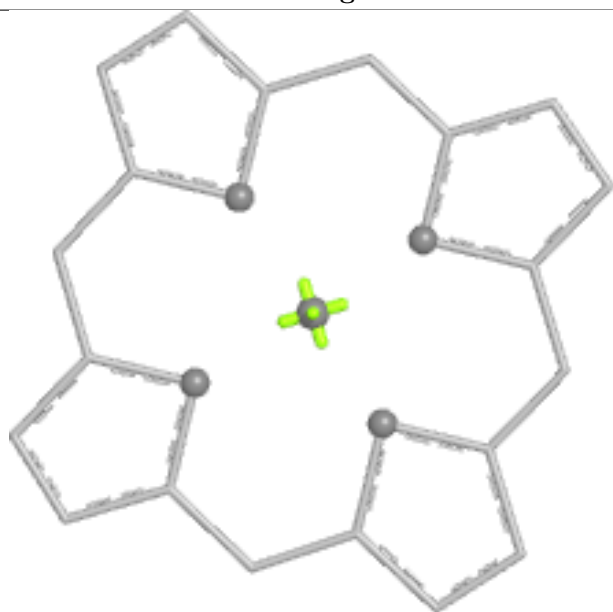
Ligand CLA Q 5238



Bond lengths



Bond angles

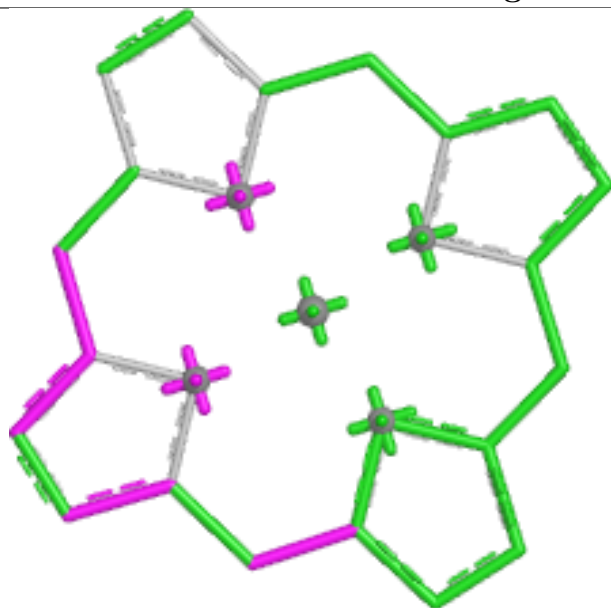


Torsions

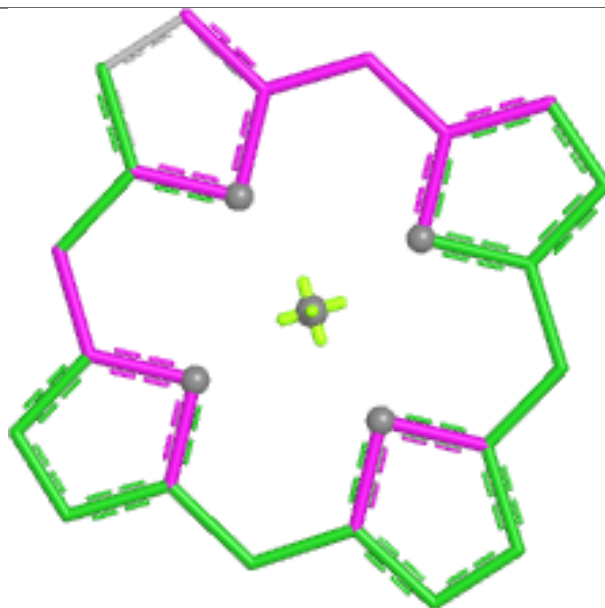


Rings

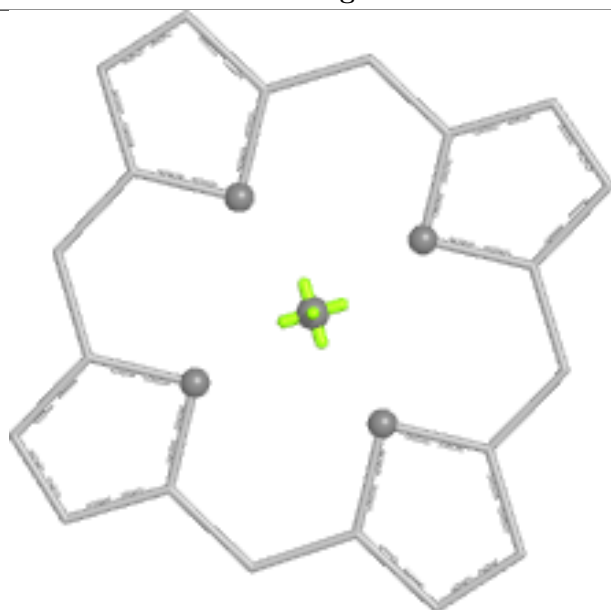
Ligand CLA G 1701



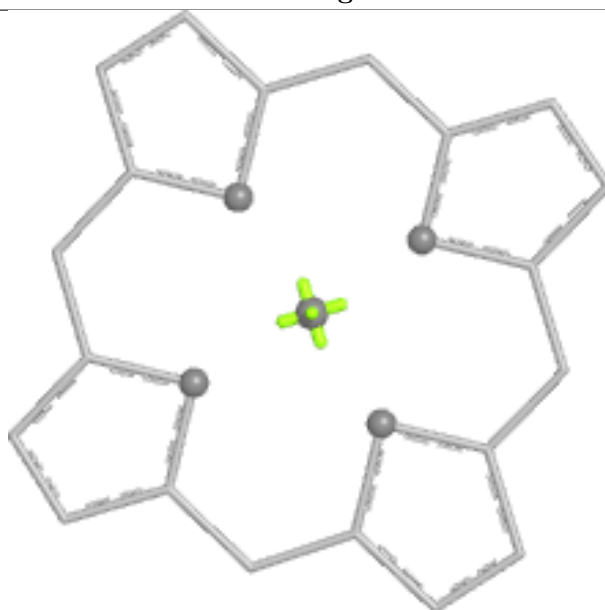
Bond lengths



Bond angles

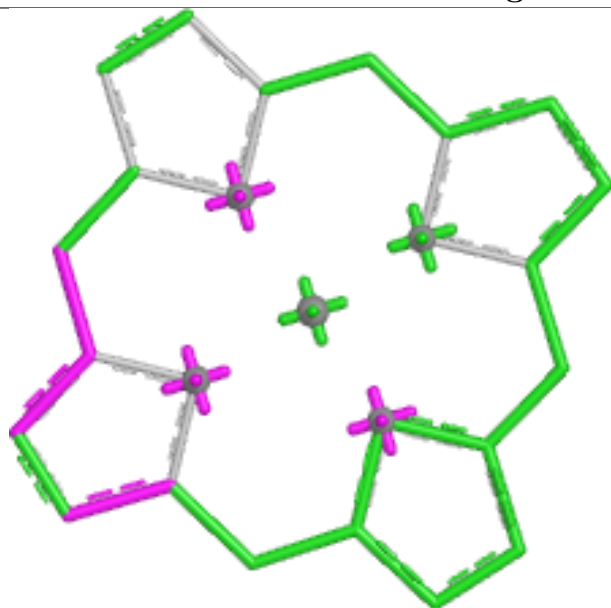


Torsions

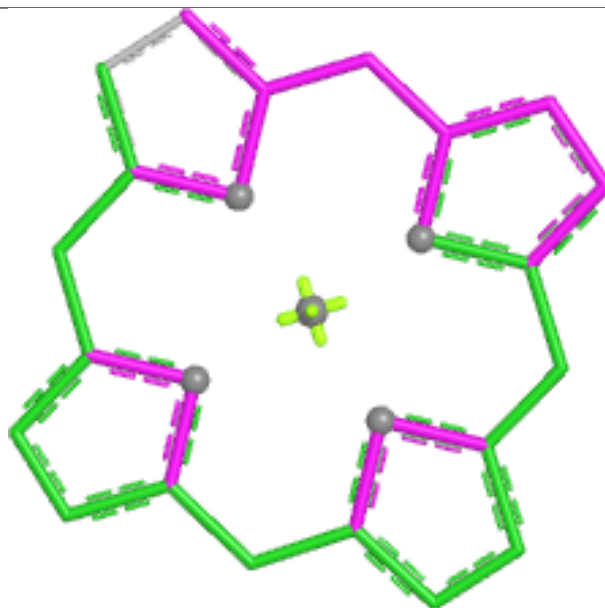


Rings

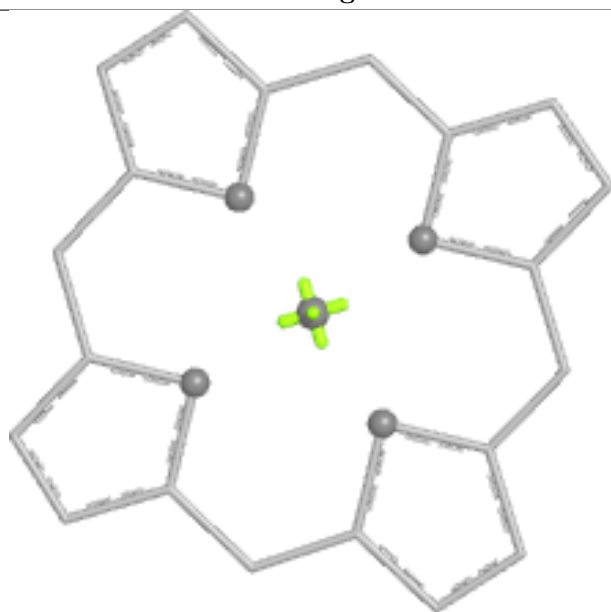
Ligand CLA P 5124



Bond lengths



Bond angles

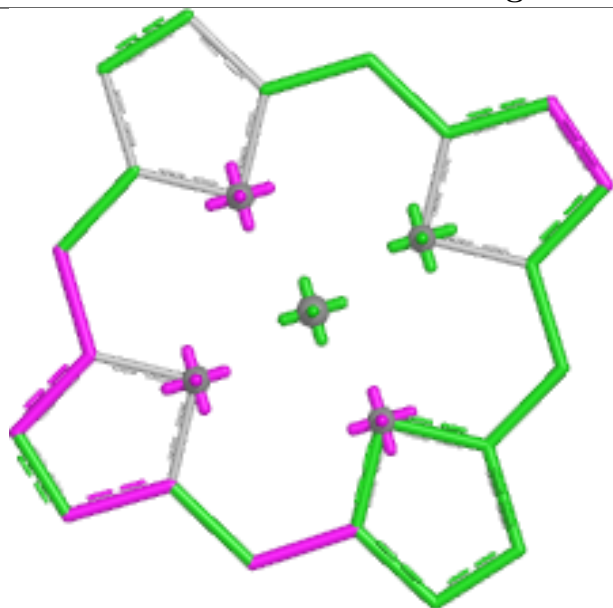


Torsions

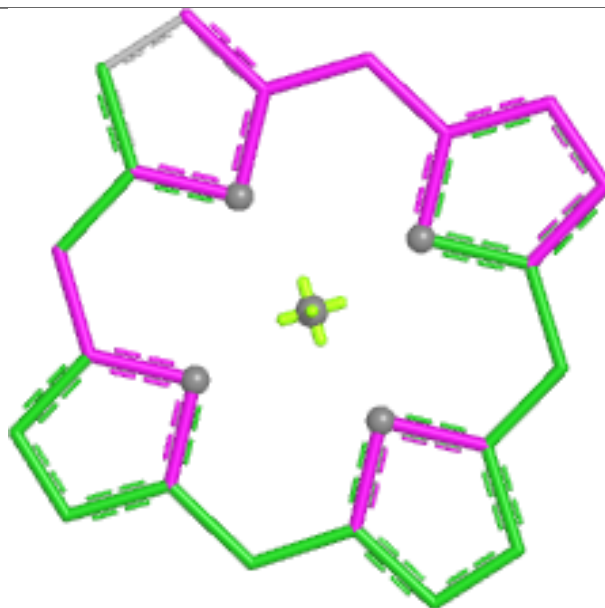


Rings

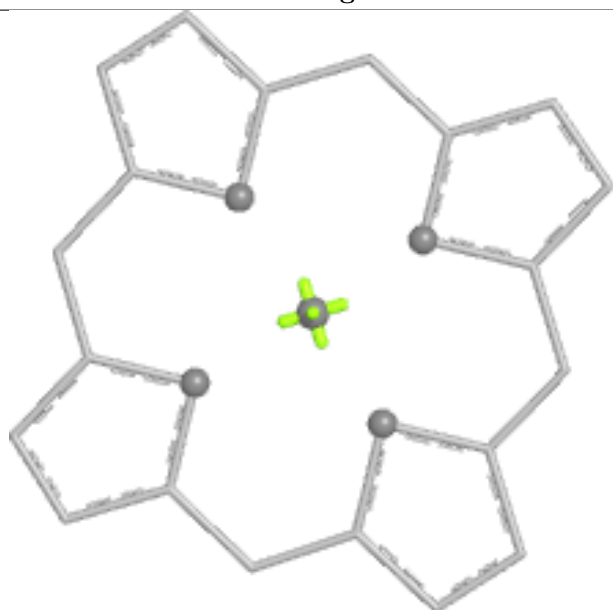
Ligand CLA P 5115



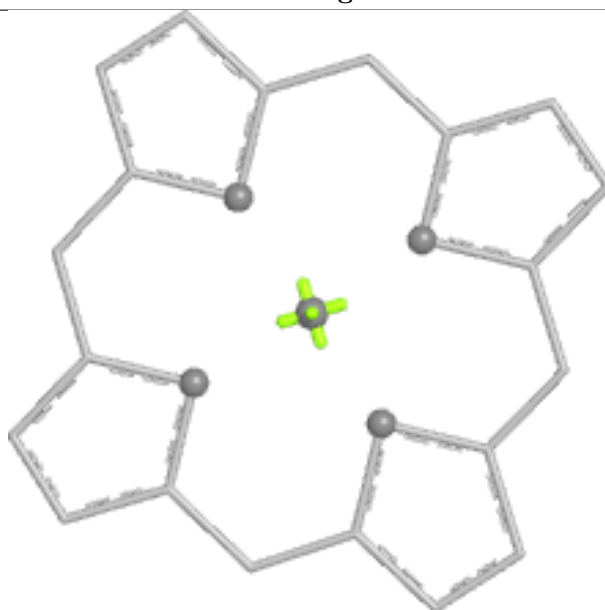
Bond lengths



Bond angles

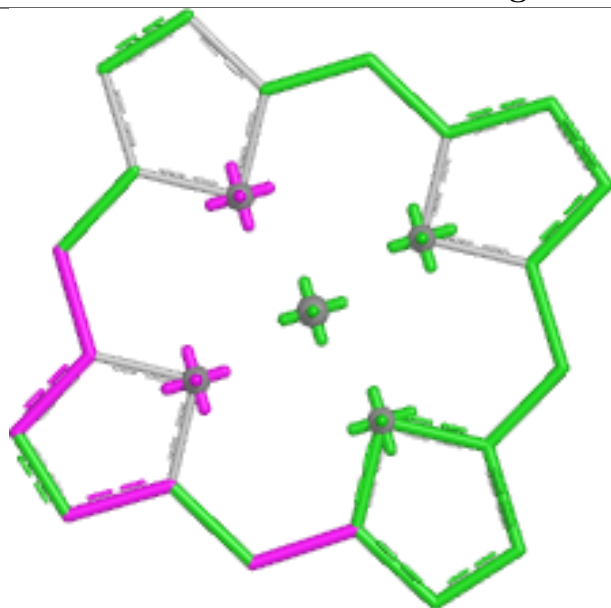


Torsions

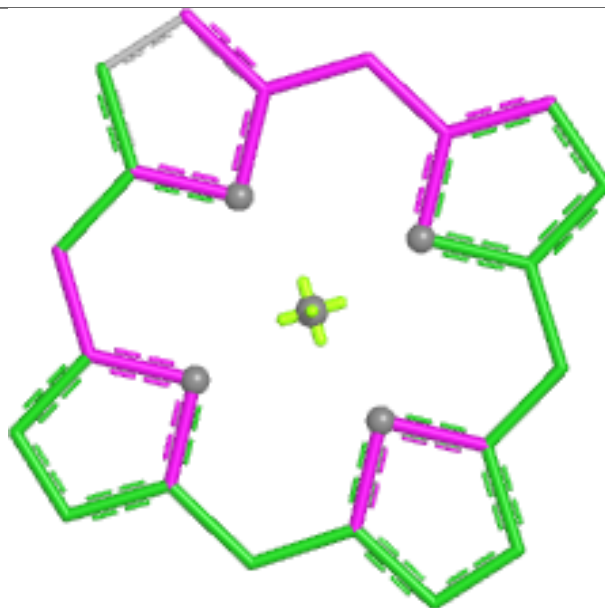


Rings

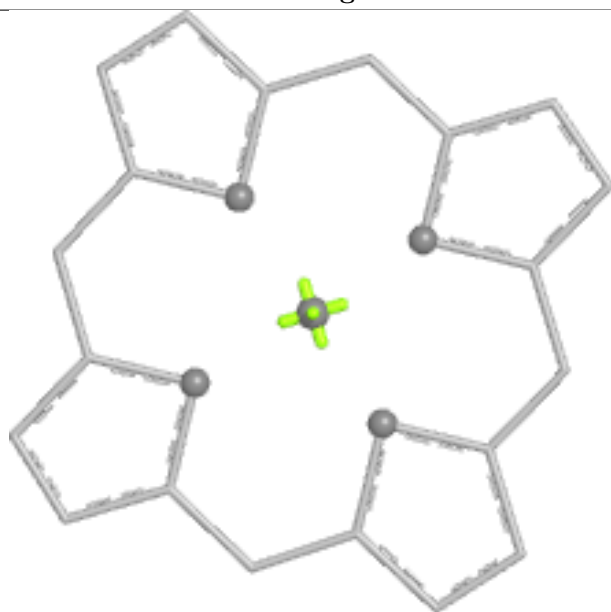
Ligand CLA 3 1015



Bond lengths



Bond angles

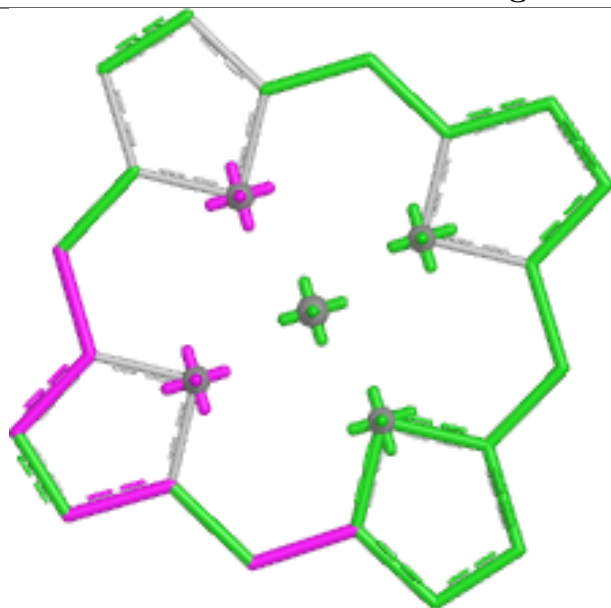


Torsions

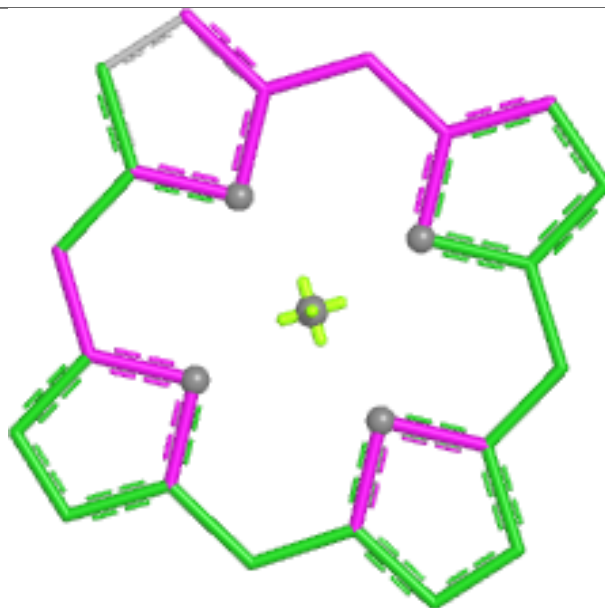


Rings

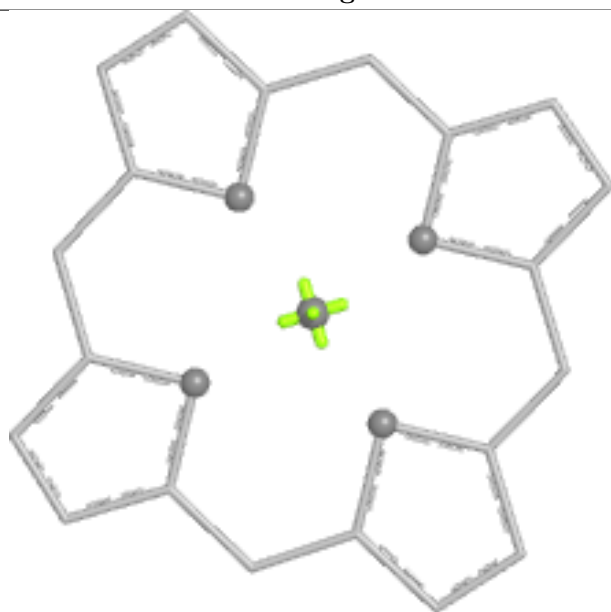
Ligand CLA 3 1021



Bond lengths



Bond angles

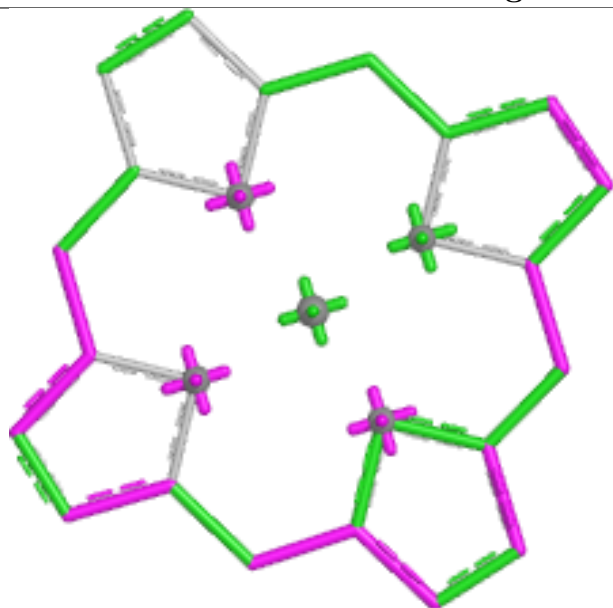


Torsions

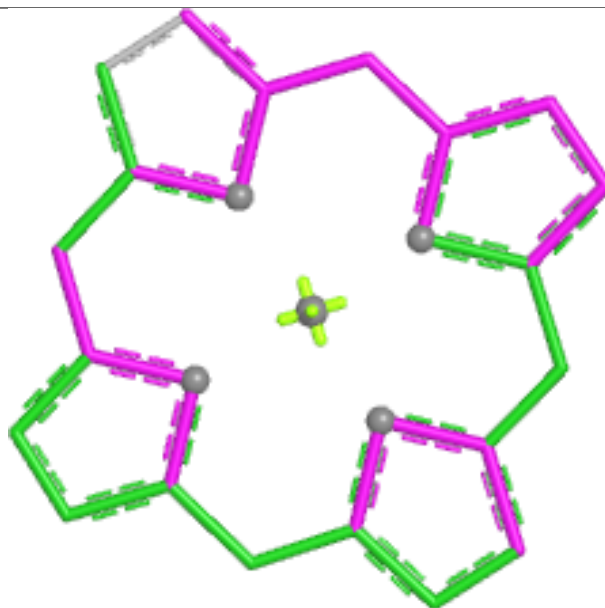


Rings

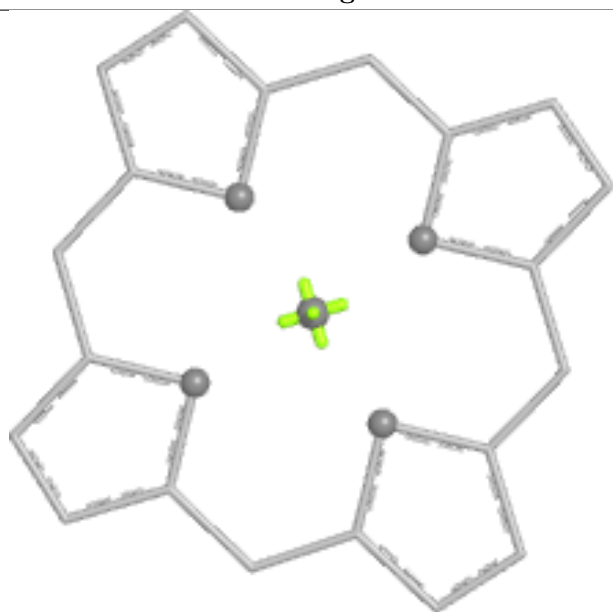
Ligand CLA B 1023



Bond lengths



Bond angles

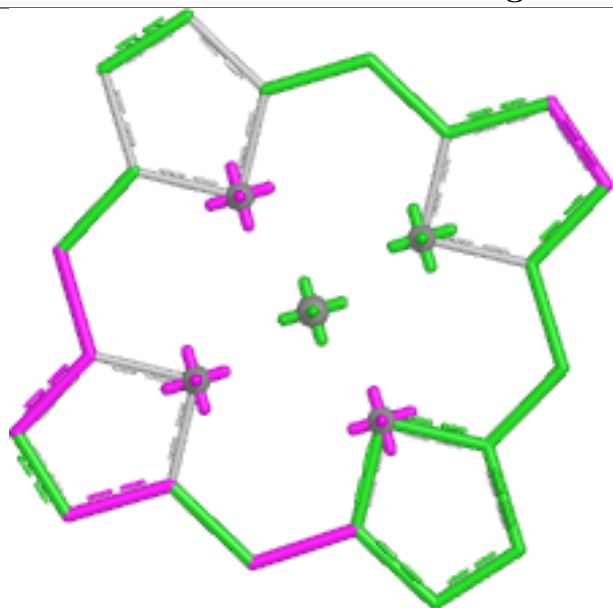


Torsions

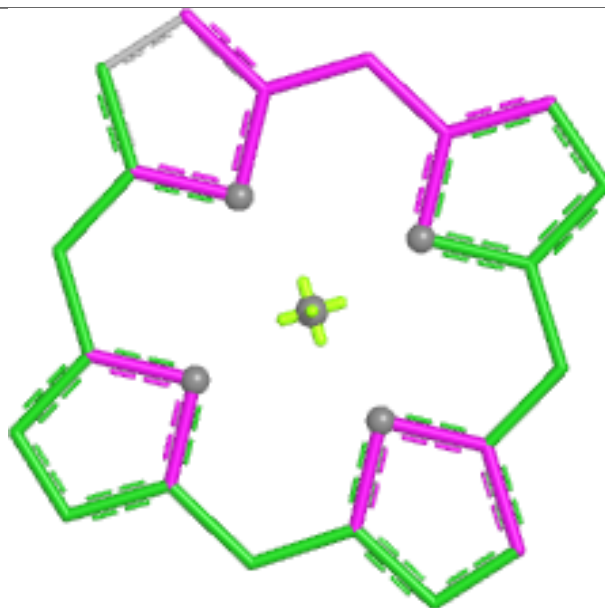


Rings

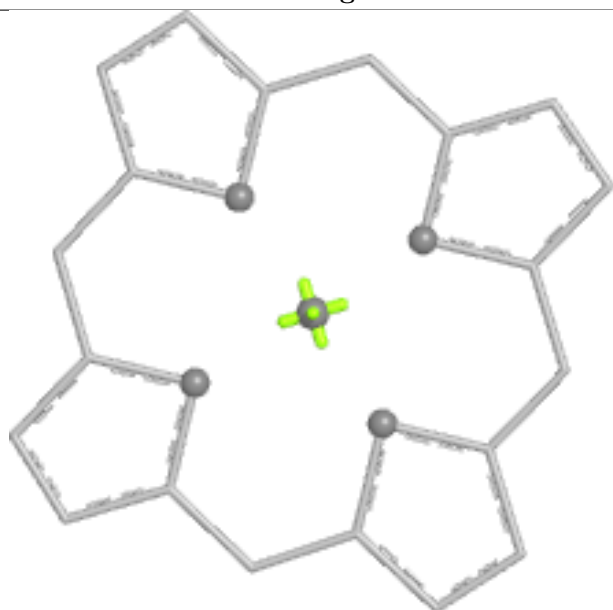
Ligand CLA P 5122



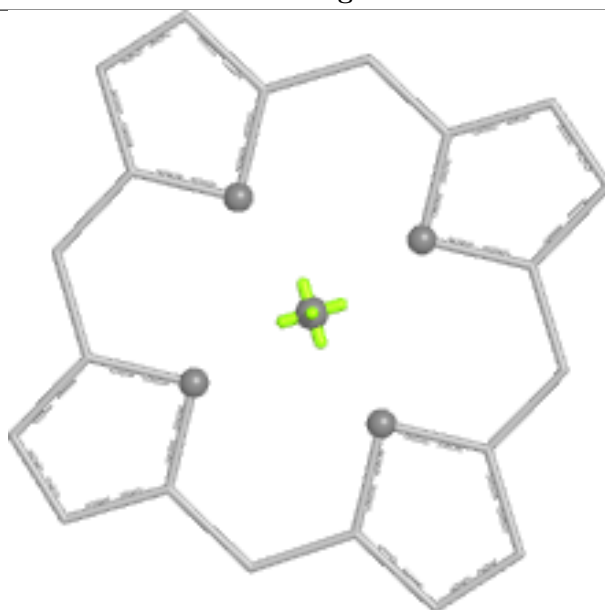
Bond lengths



Bond angles

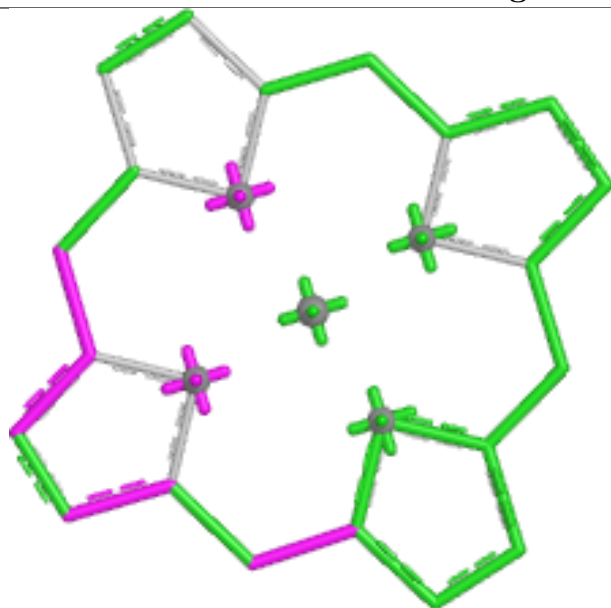


Torsions

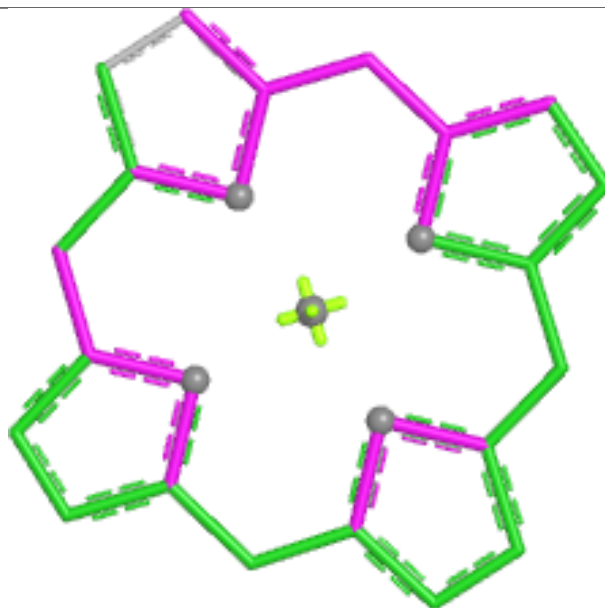


Rings

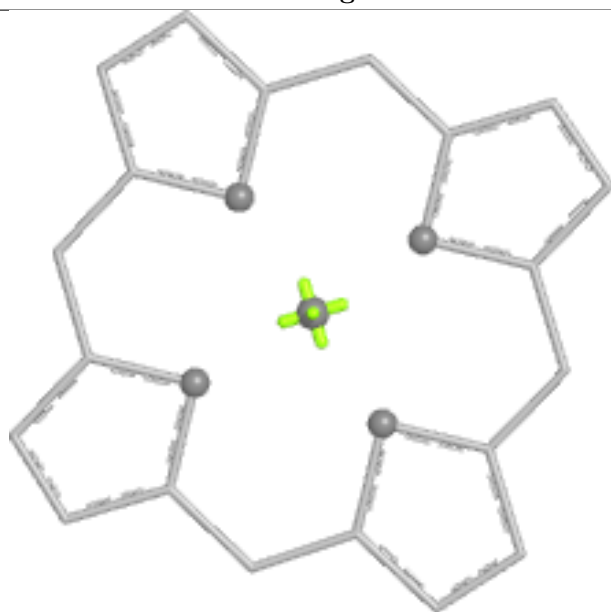
Ligand CLA 0 1015



Bond lengths



Bond angles

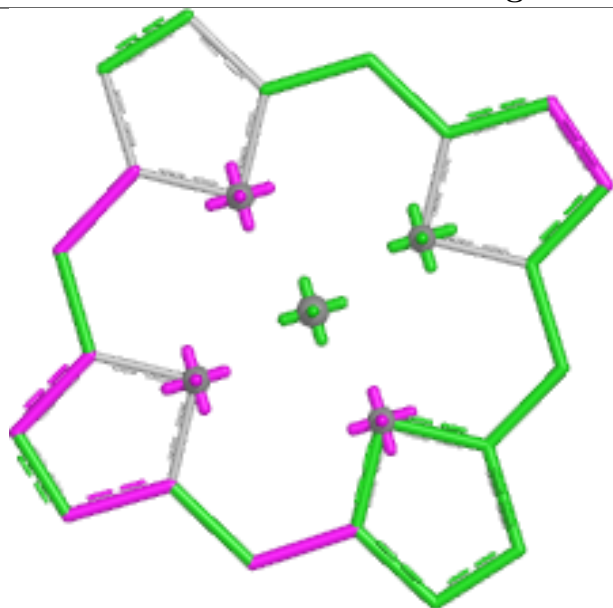


Torsions

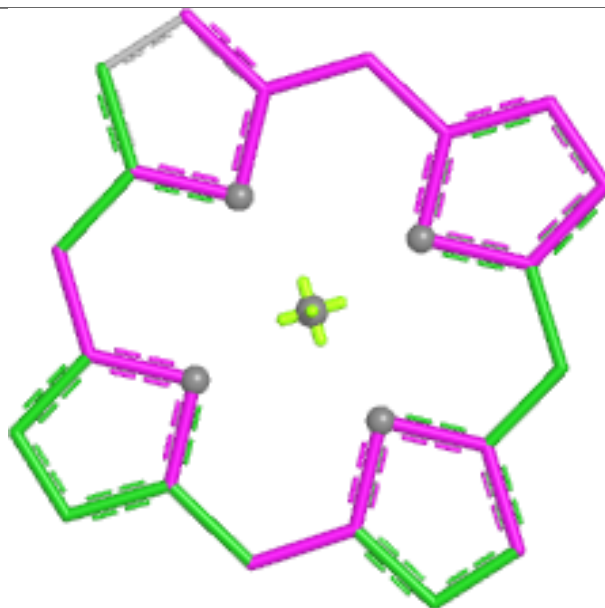


Rings

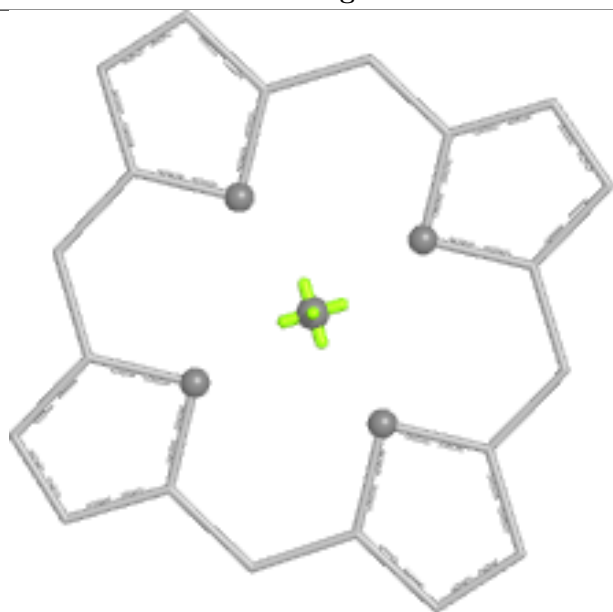
Ligand CLA P 5113



Bond lengths



Bond angles

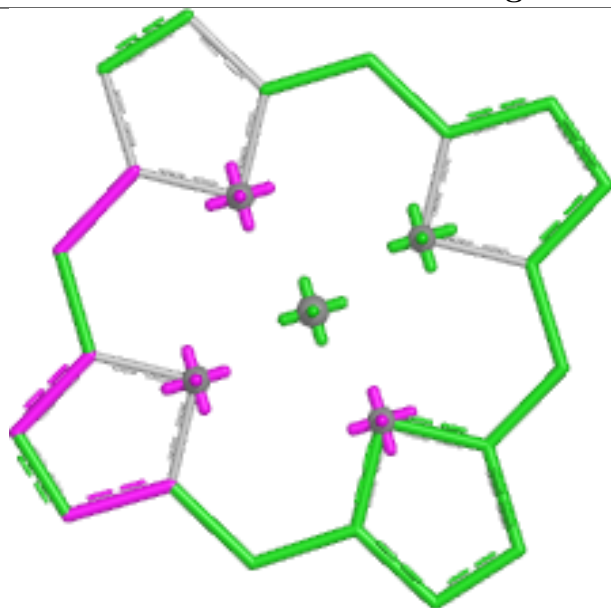


Torsions

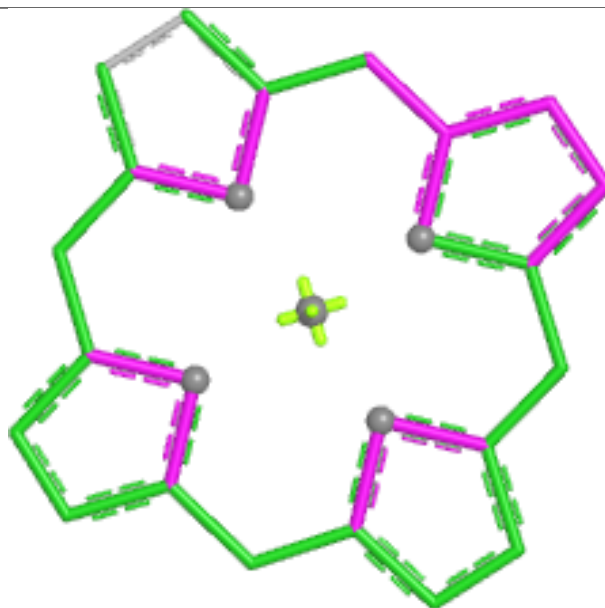


Rings

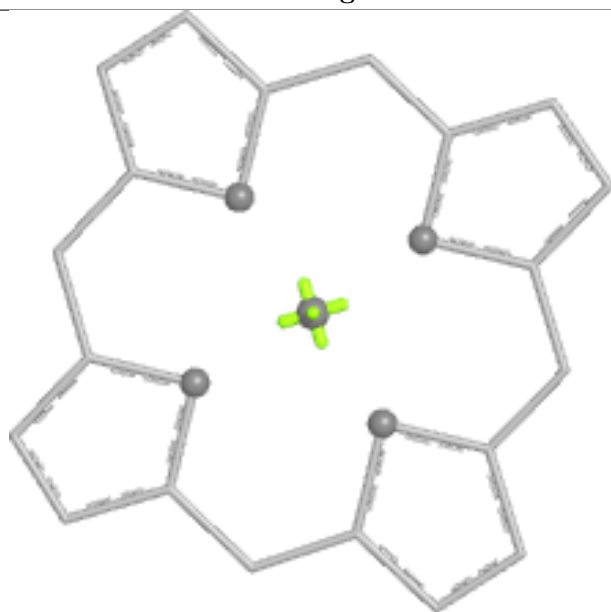
Ligand CLA B 1239



Bond lengths



Bond angles

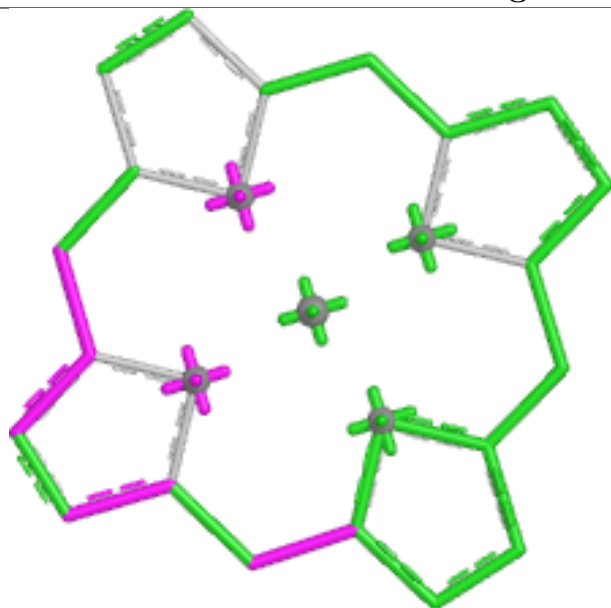


Torsions

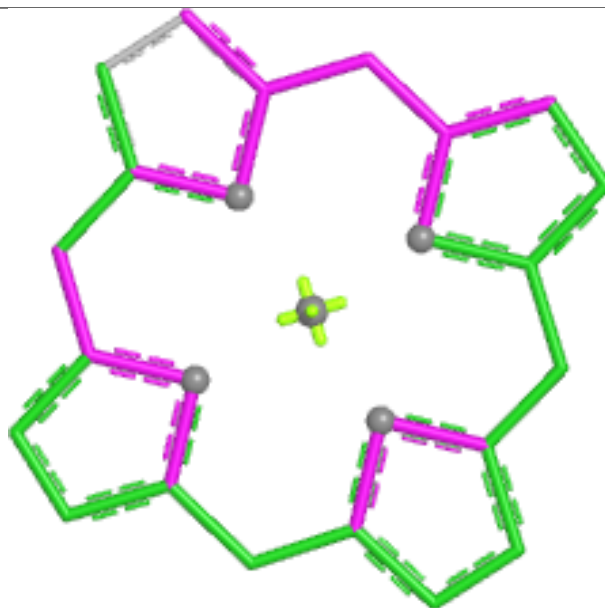


Rings

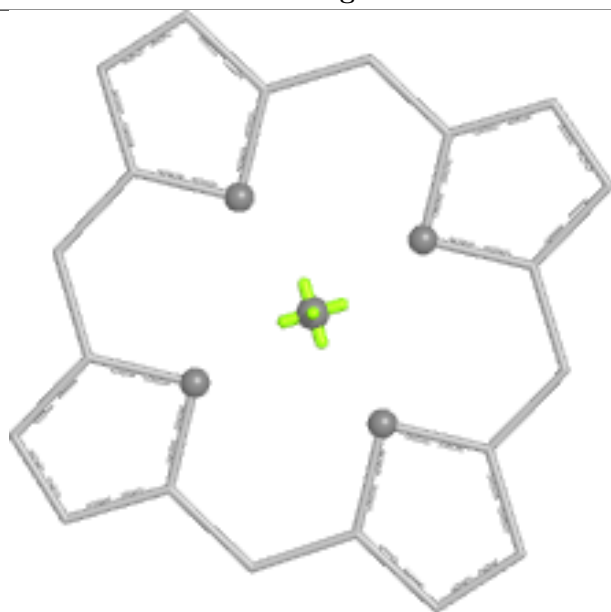
Ligand CLA 4 1016



Bond lengths



Bond angles

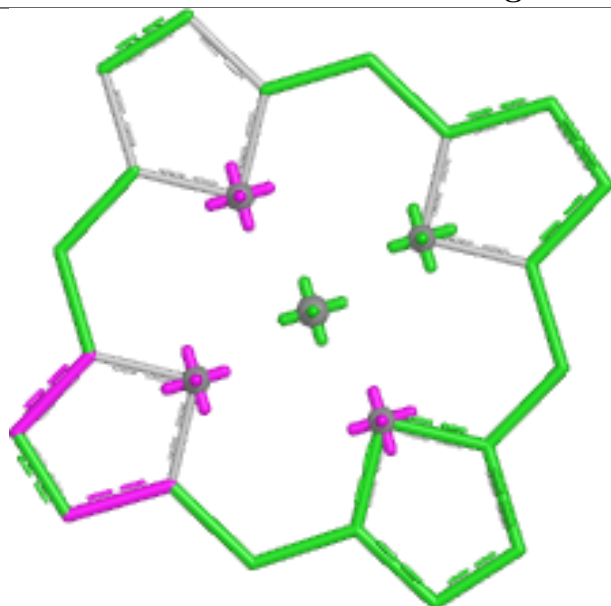


Torsions

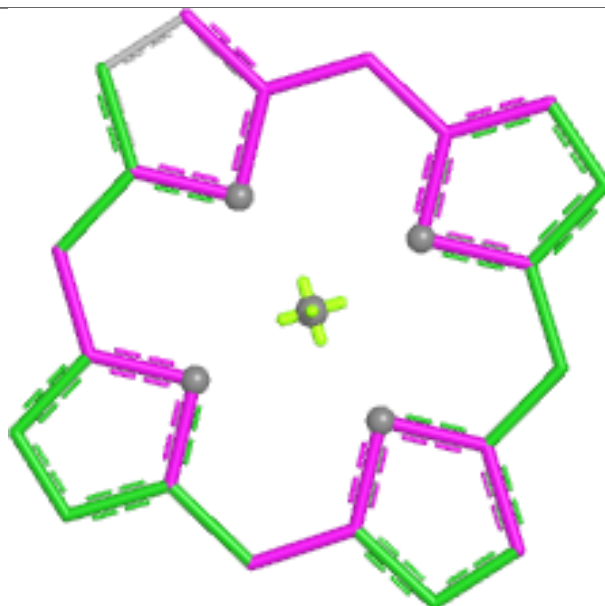


Rings

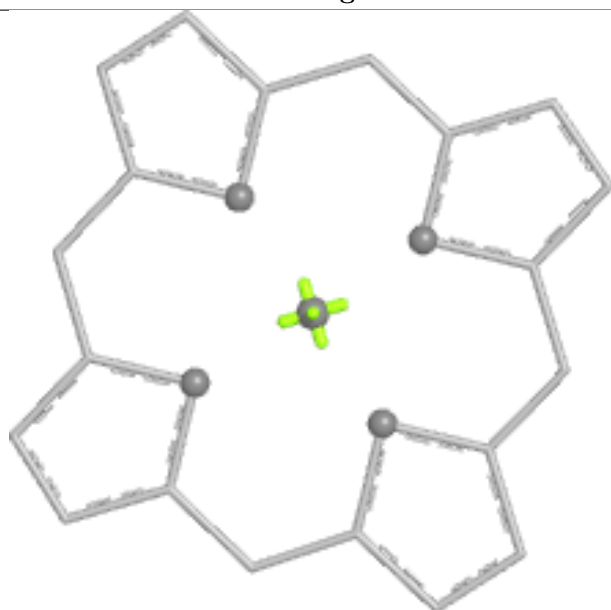
Ligand CLA A 1108



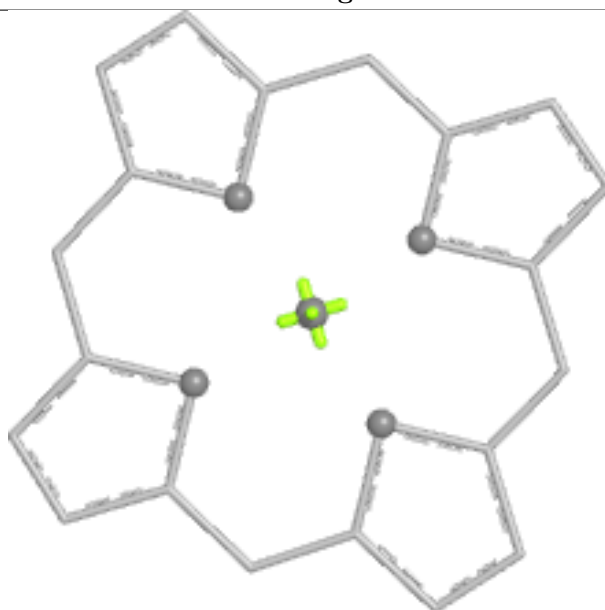
Bond lengths



Bond angles

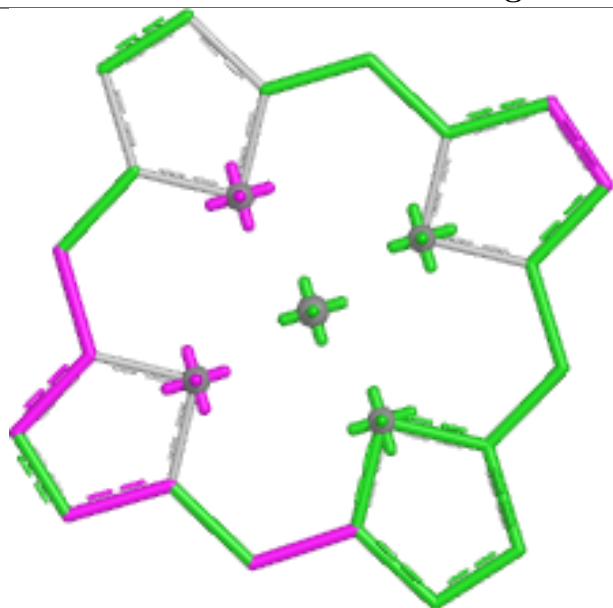


Torsions

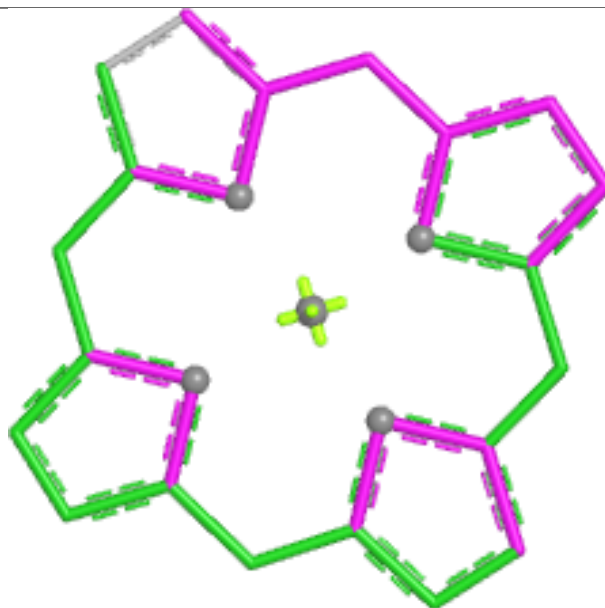


Rings

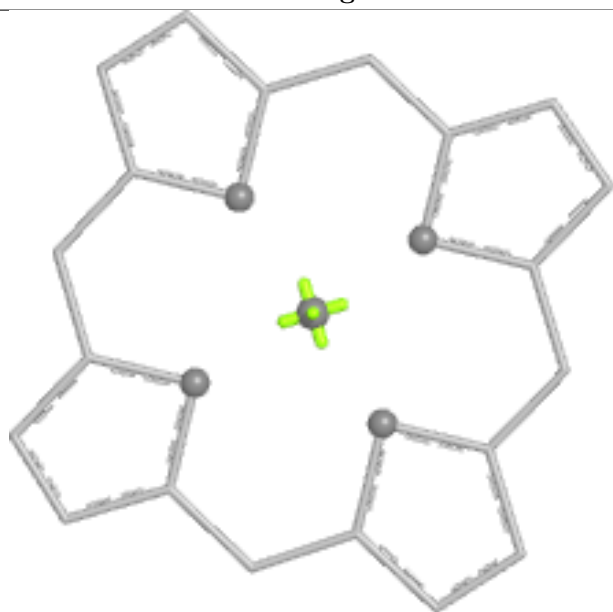
Ligand CLA A 1103



Bond lengths



Bond angles

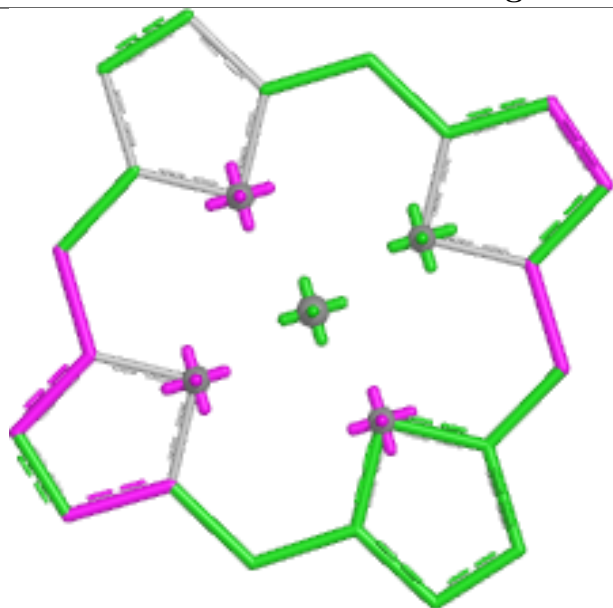


Torsions

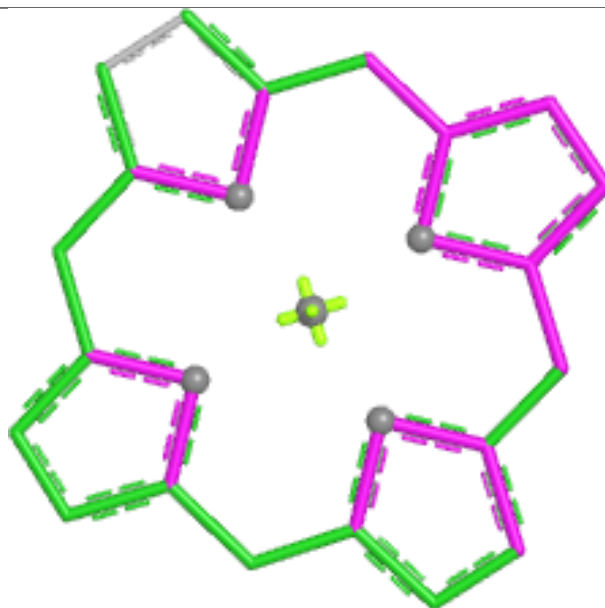


Rings

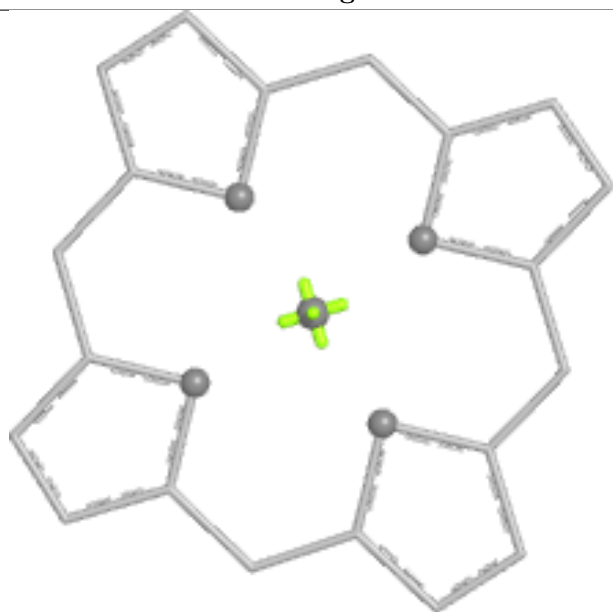
Ligand CLA B 1204



Bond lengths



Bond angles

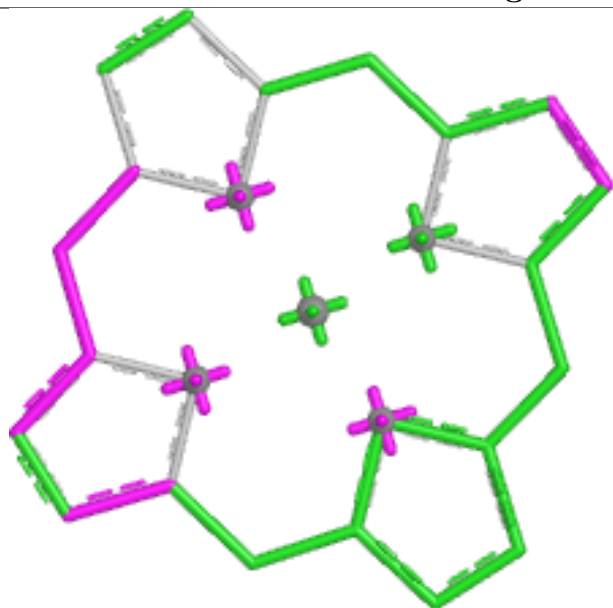


Torsions

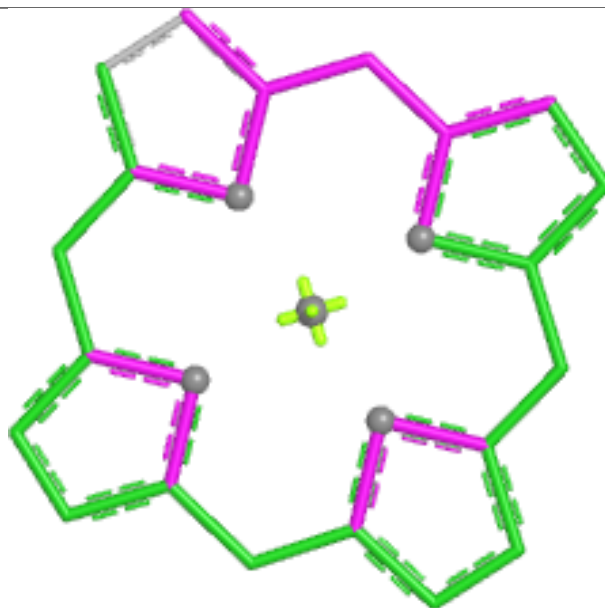


Rings

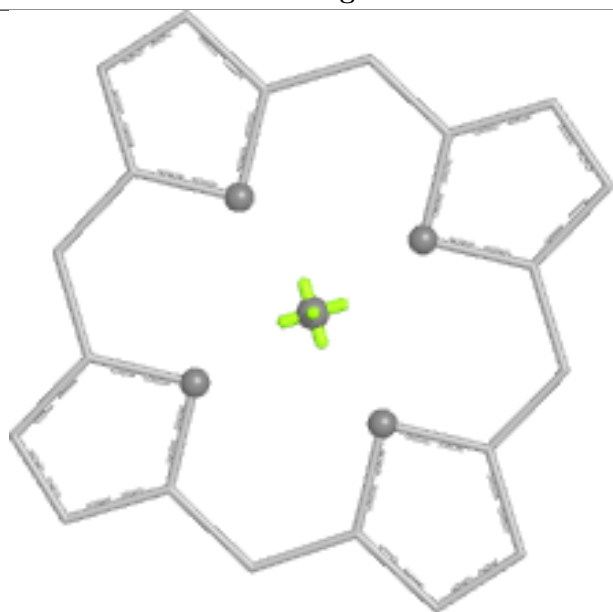
Ligand CLA B 1021



Bond lengths



Bond angles

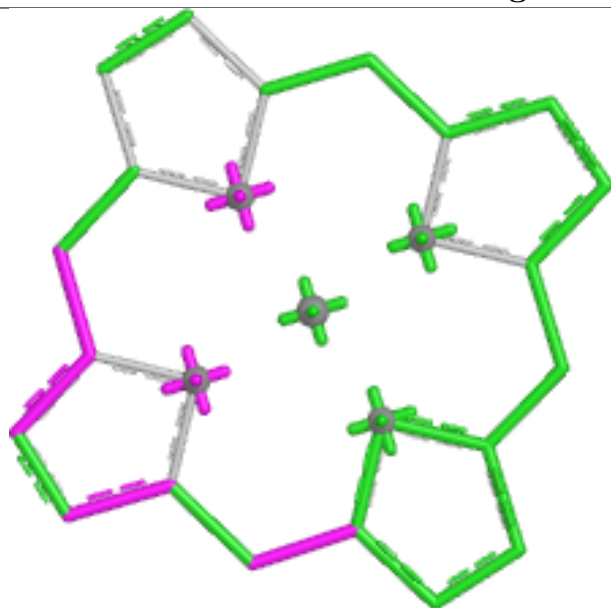


Torsions

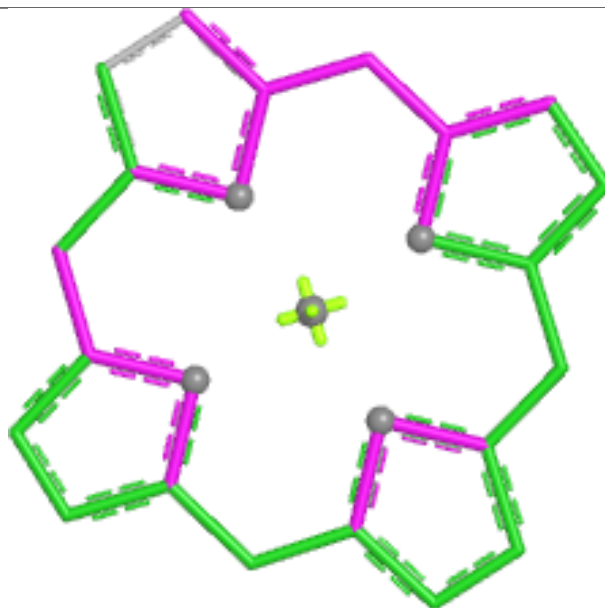


Rings

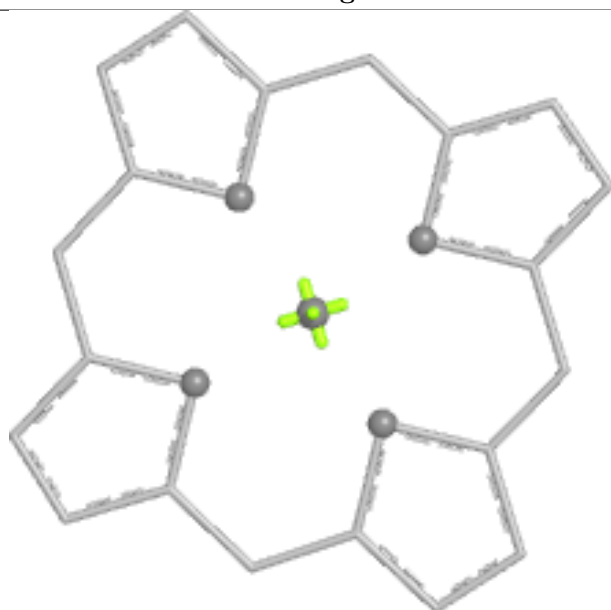
Ligand CLA J 4008



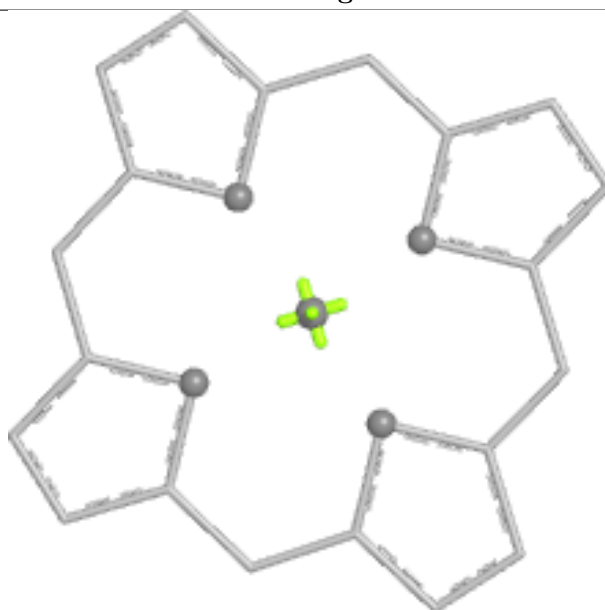
Bond lengths



Bond angles

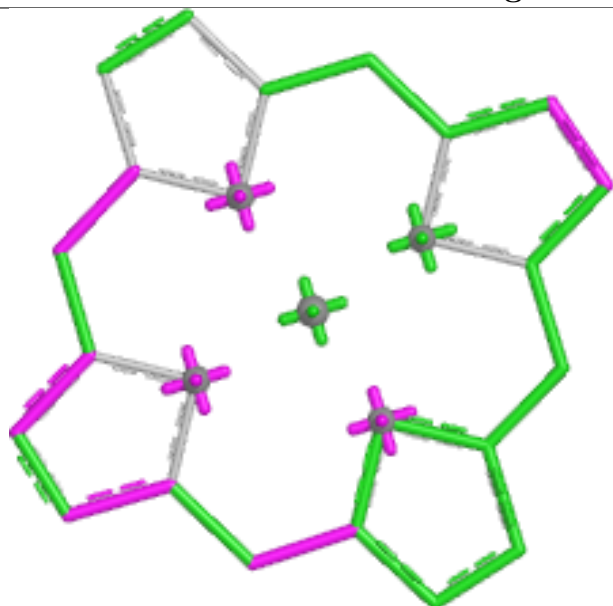


Torsions

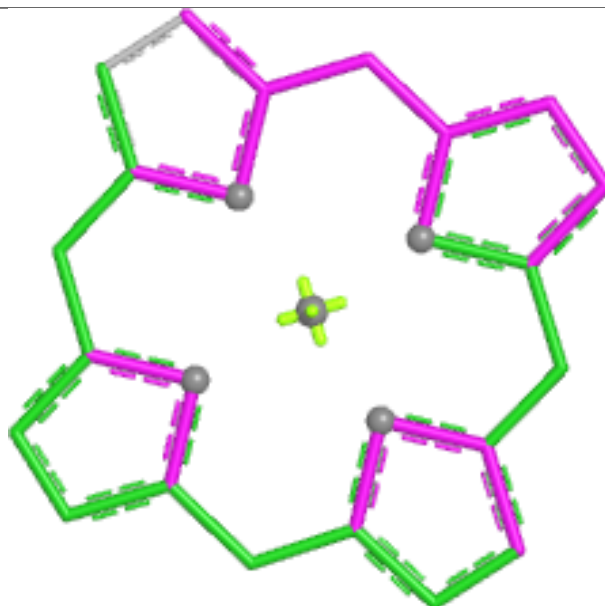


Rings

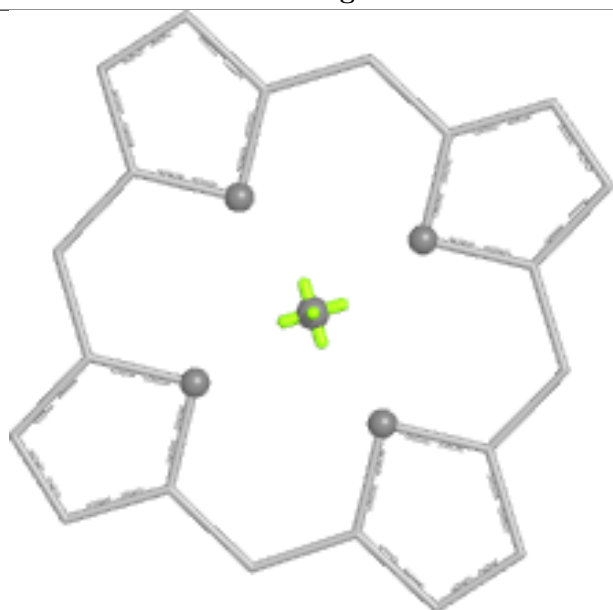
Ligand CLA A 1133



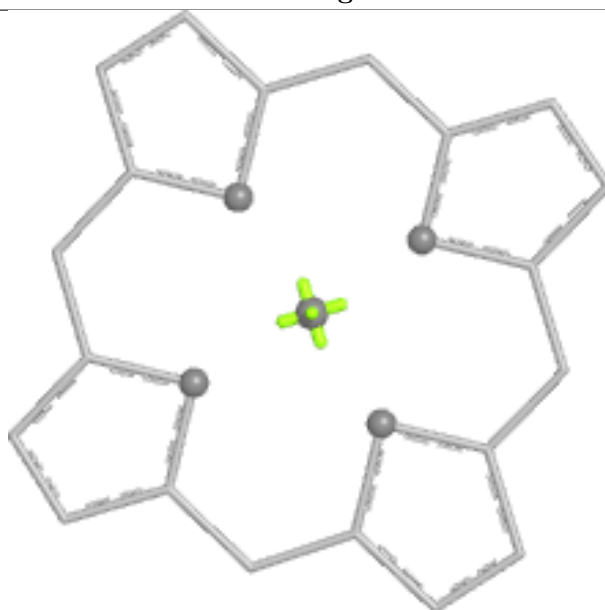
Bond lengths



Bond angles

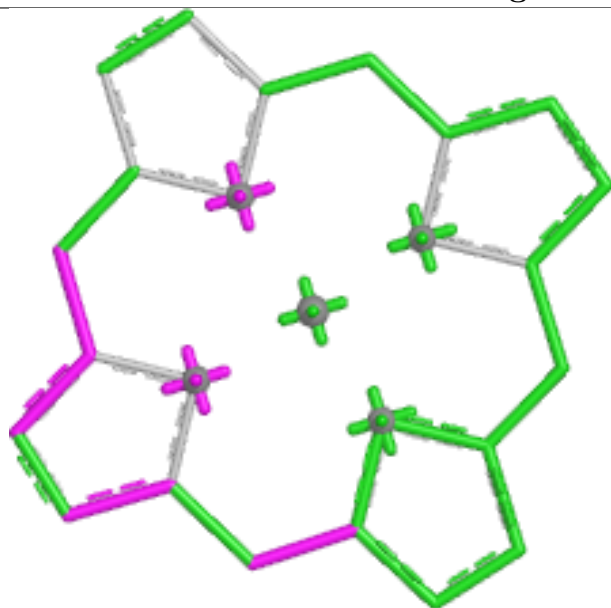


Torsions



Rings

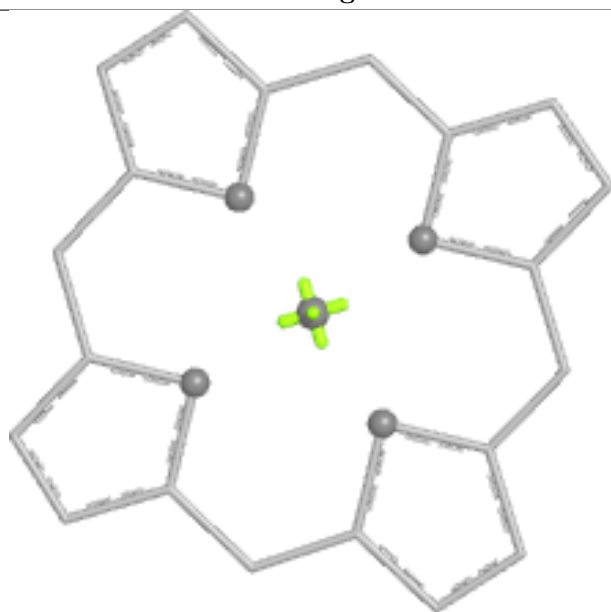
Ligand CLA 4 1032



Bond lengths



Bond angles

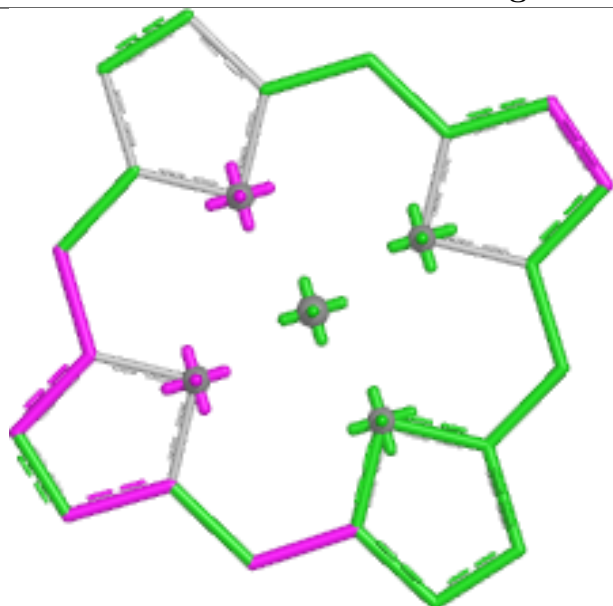


Torsions

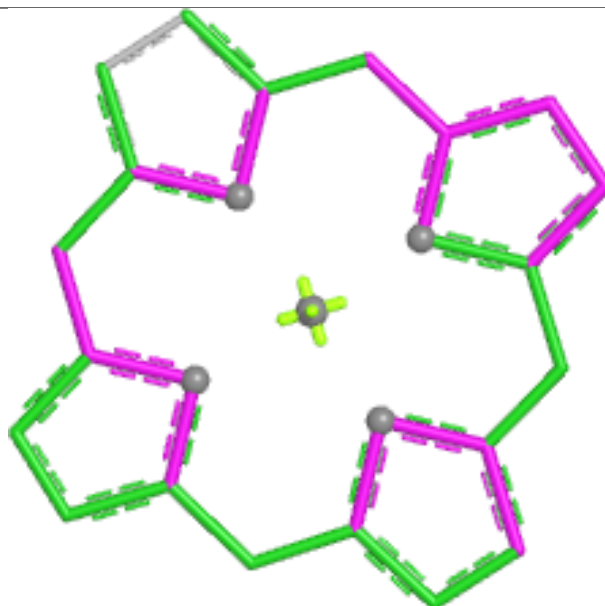


Rings

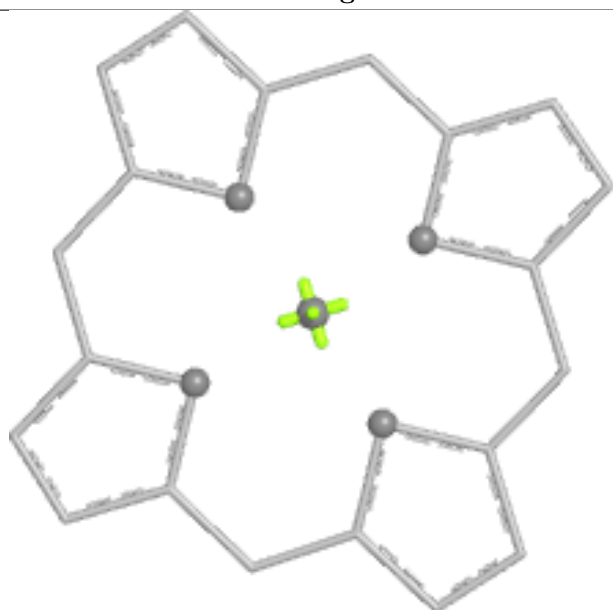
Ligand CLA 6 5502



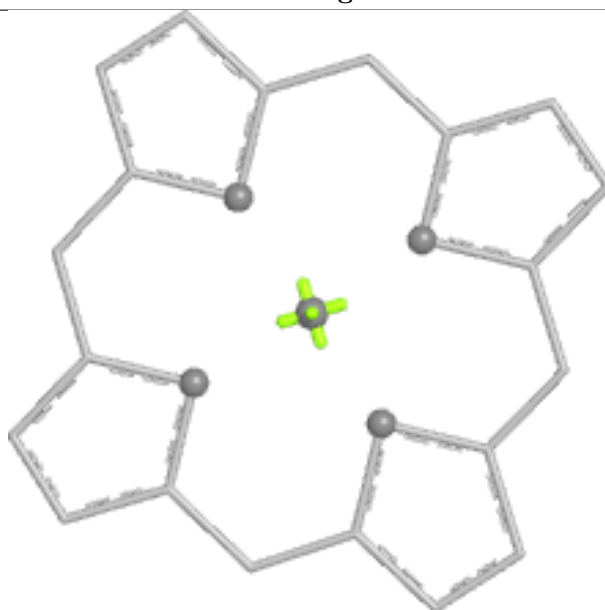
Bond lengths



Bond angles

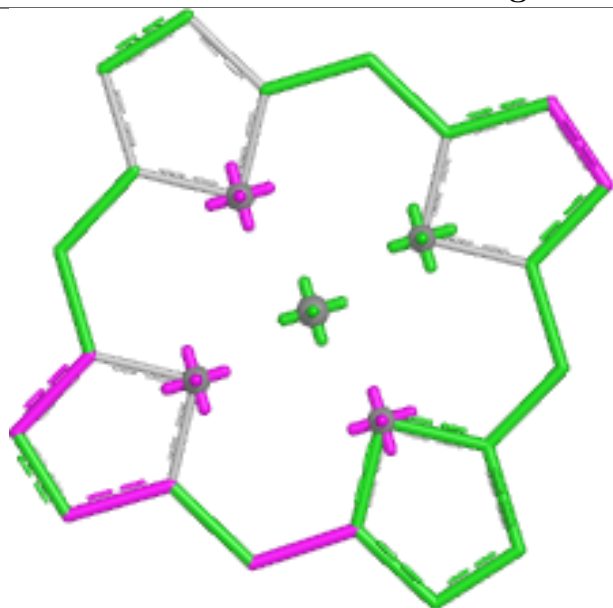


Torsions

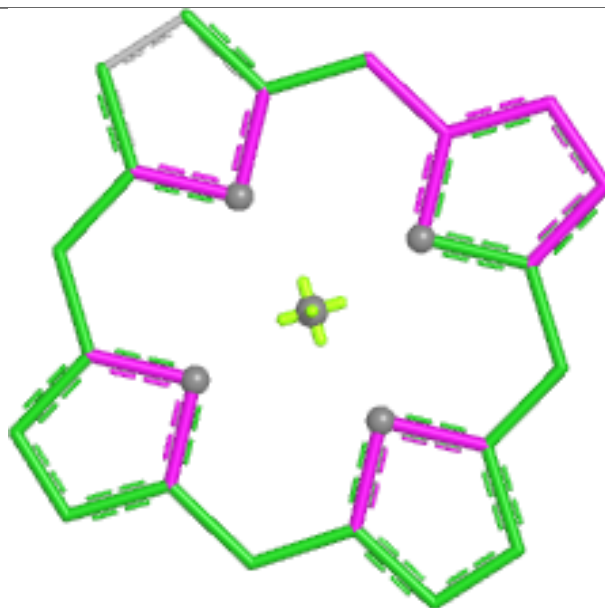


Rings

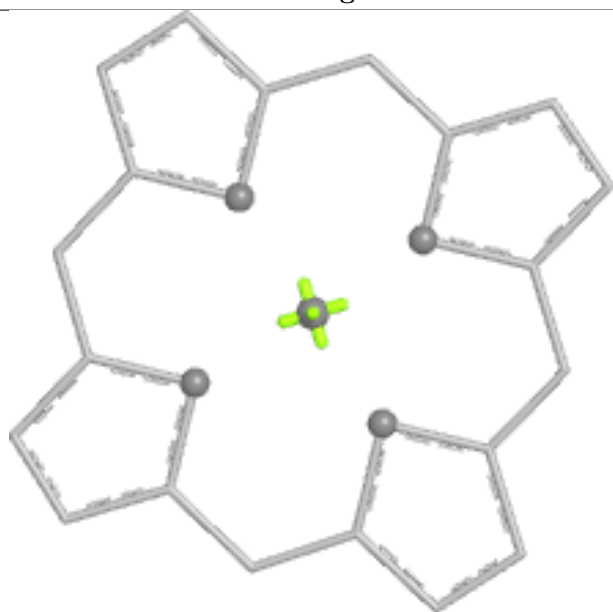
Ligand CLA 6 5503



Bond lengths



Bond angles

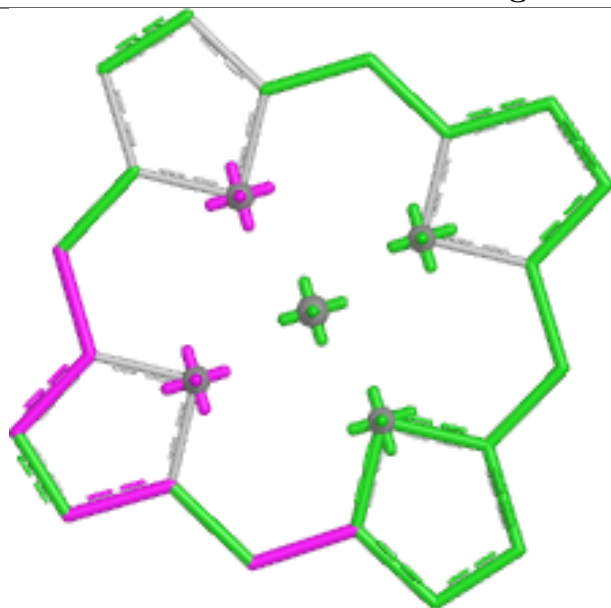


Torsions

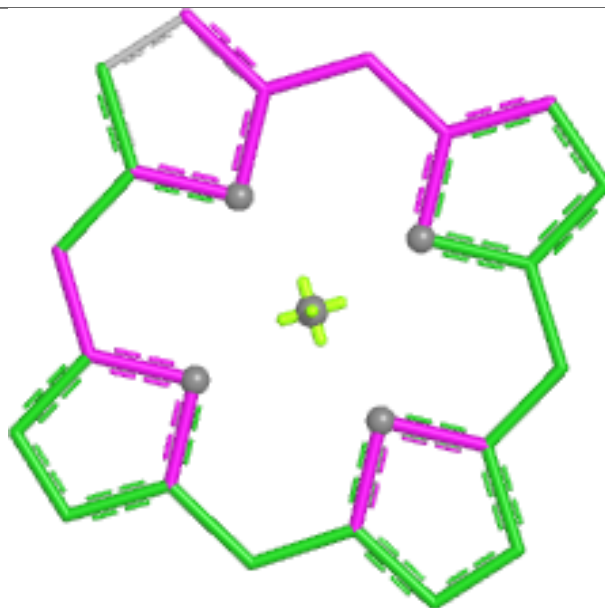


Rings

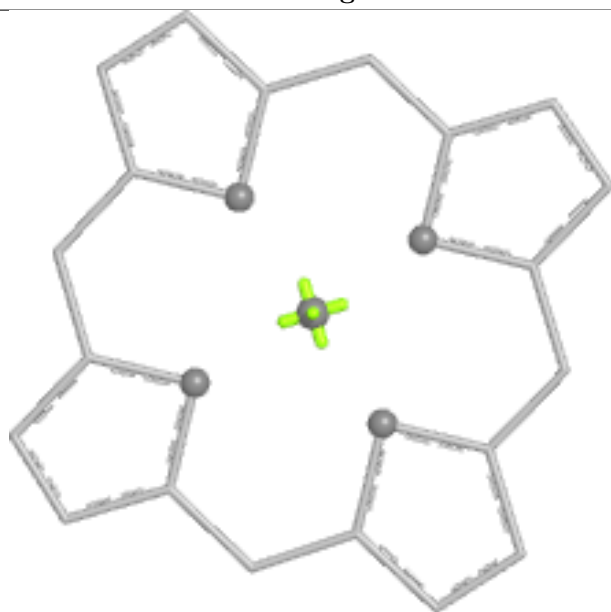
Ligand CLA 9 1041



Bond lengths



Bond angles

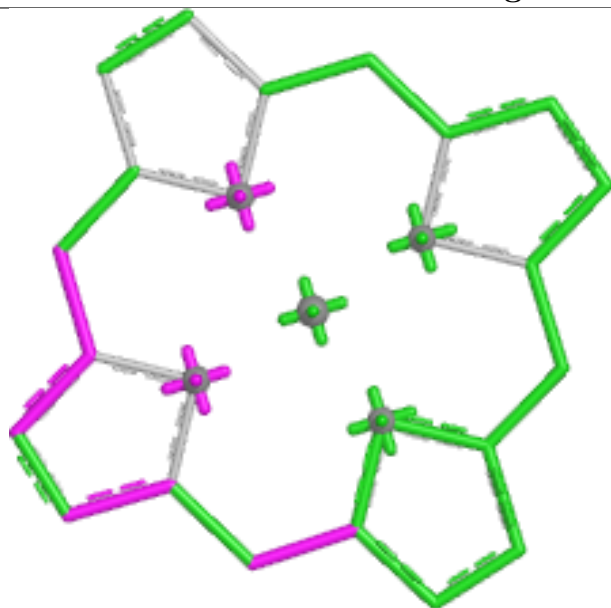


Torsions

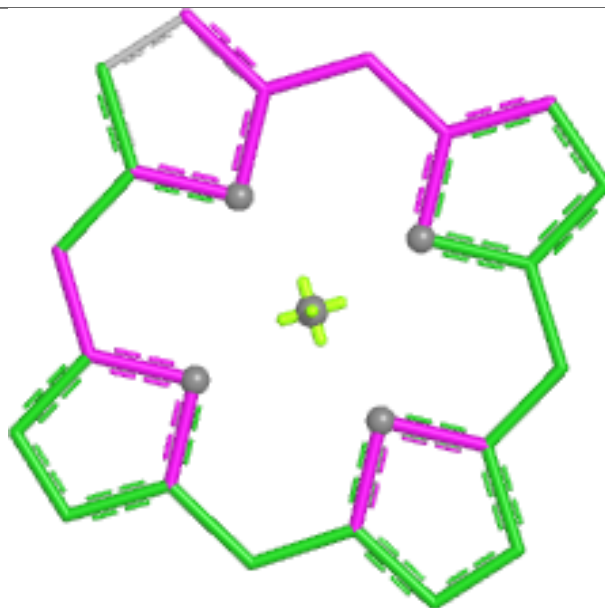


Rings

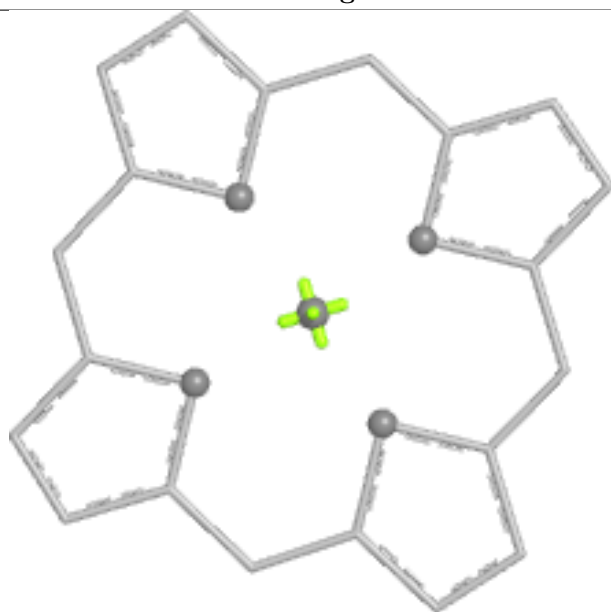
Ligand CLA U 8005



Bond lengths



Bond angles

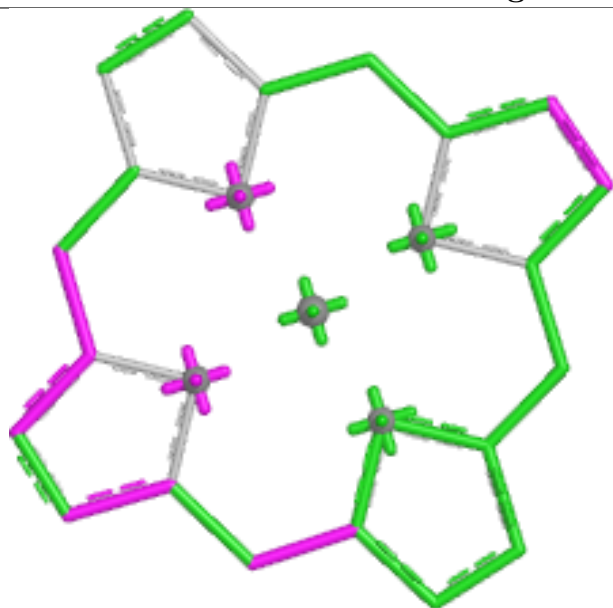


Torsions

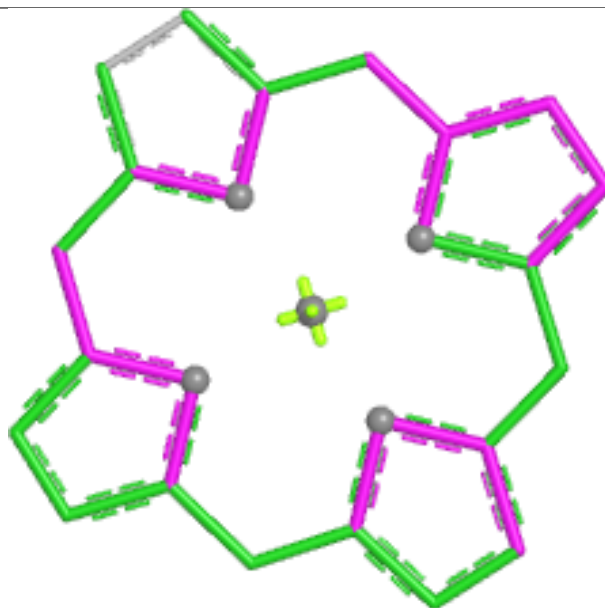


Rings

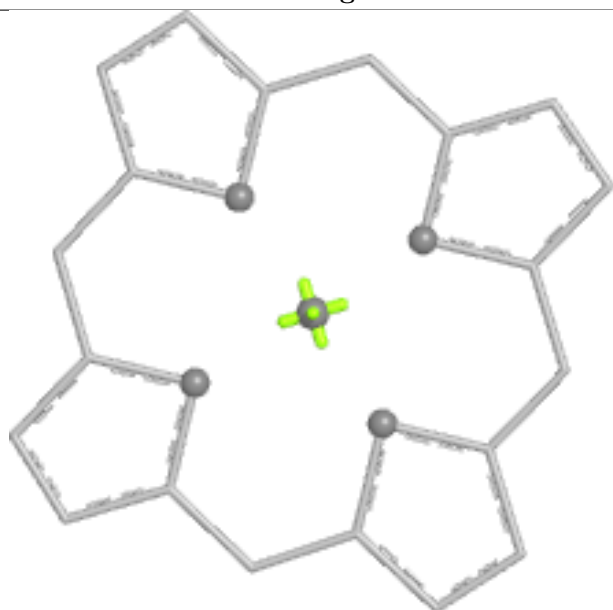
Ligand CLA L 1502



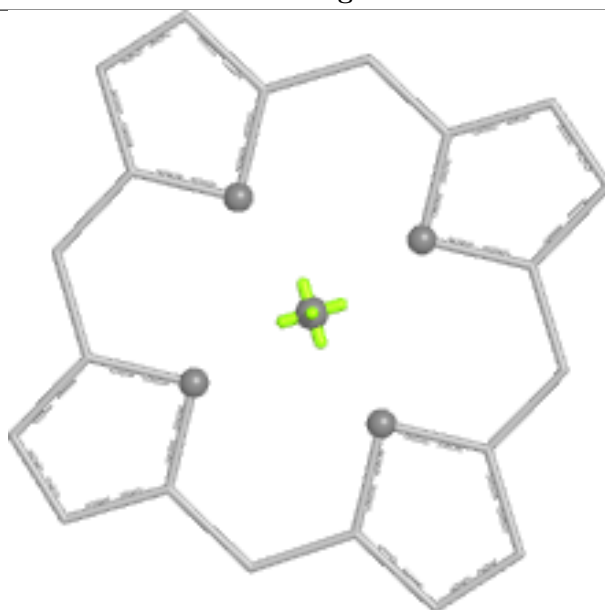
Bond lengths



Bond angles

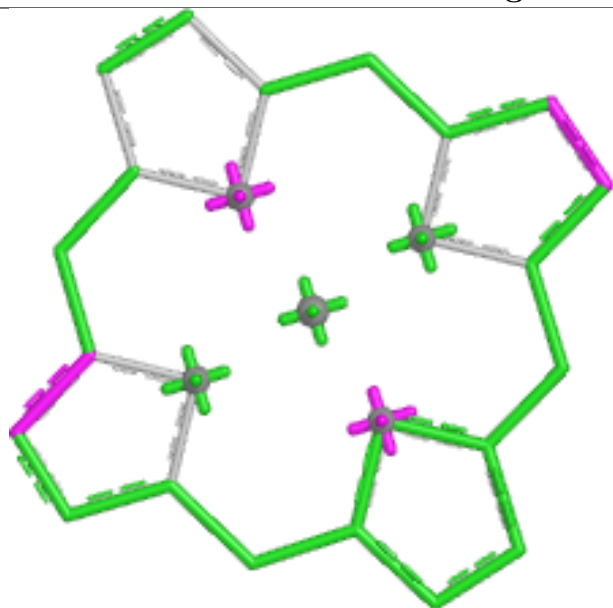


Torsions

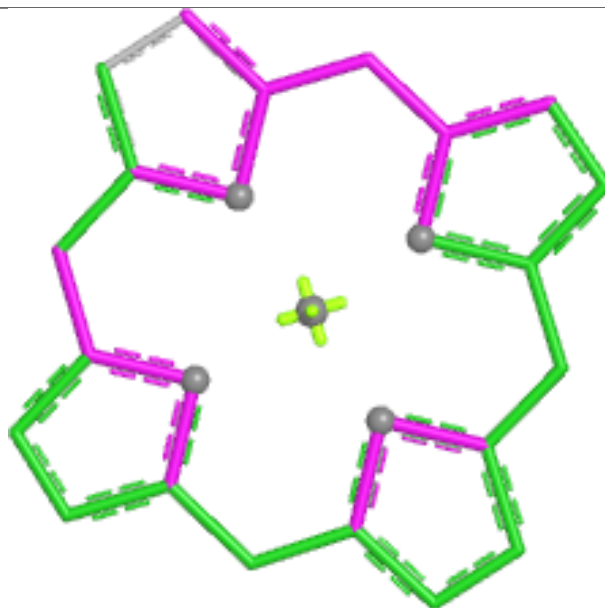


Rings

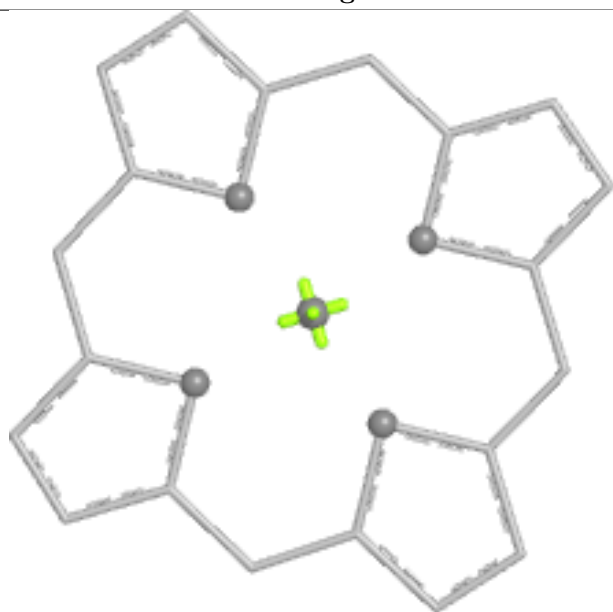
Ligand CLA B 1206



Bond lengths



Bond angles

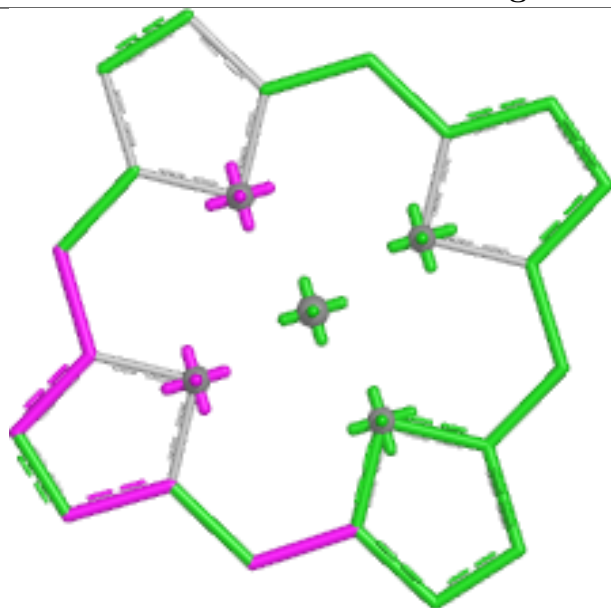


Torsions

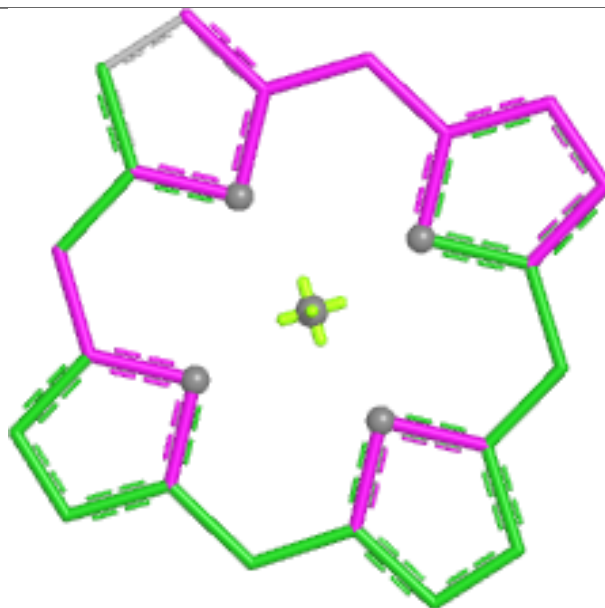


Rings

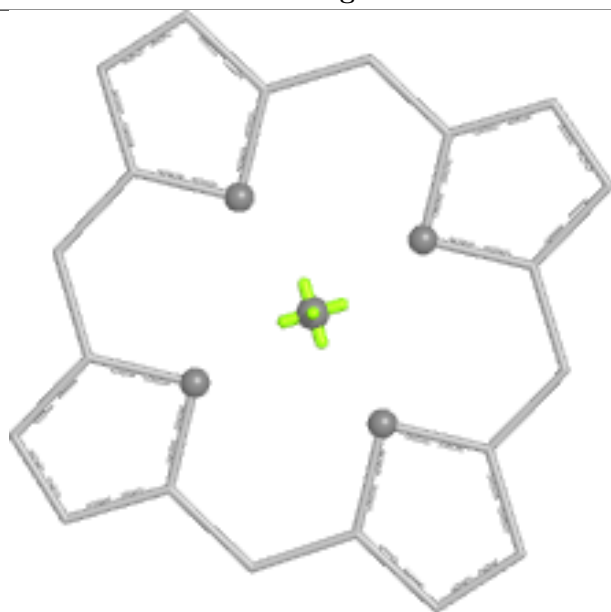
Ligand CLA 2 1014



Bond lengths



Bond angles

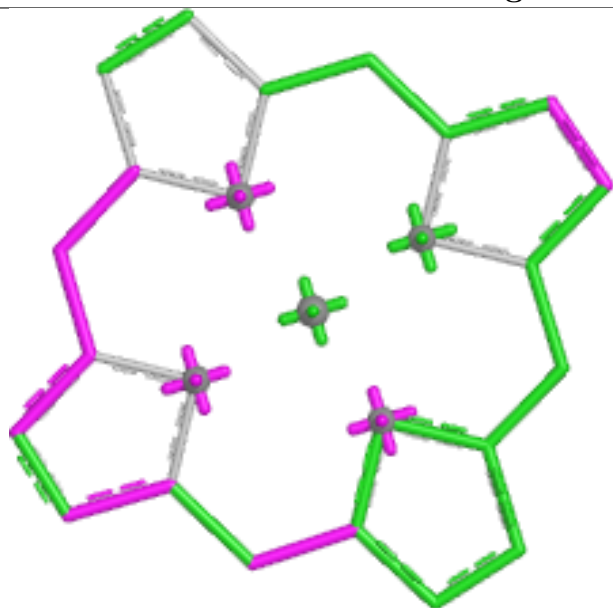


Torsions

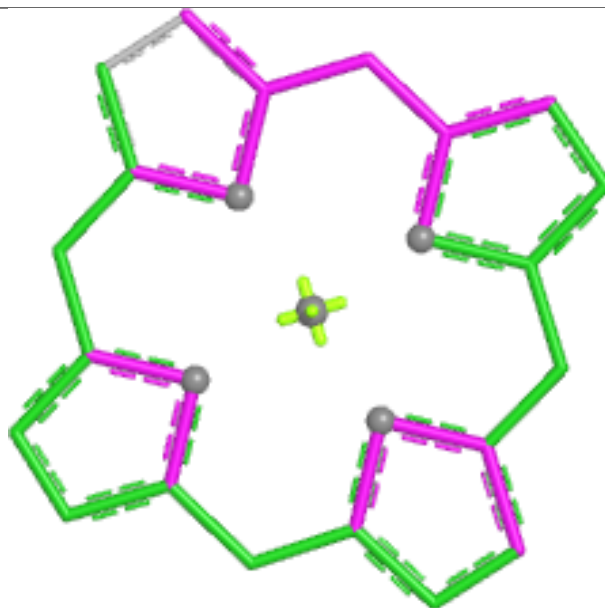


Rings

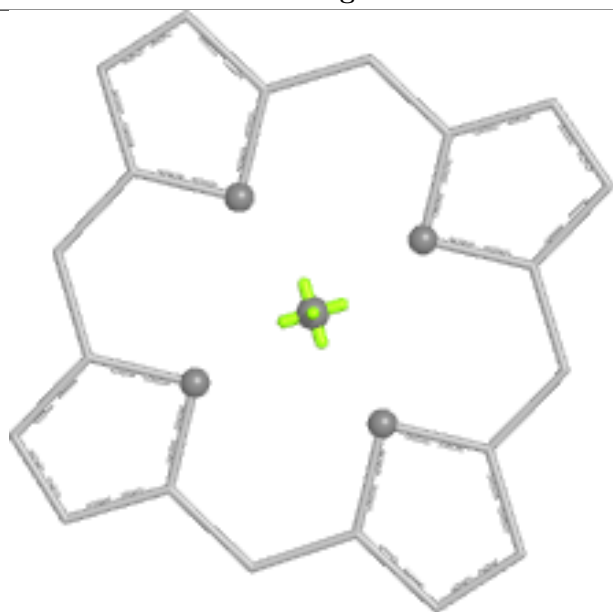
Ligand CLA B 1231



Bond lengths



Bond angles

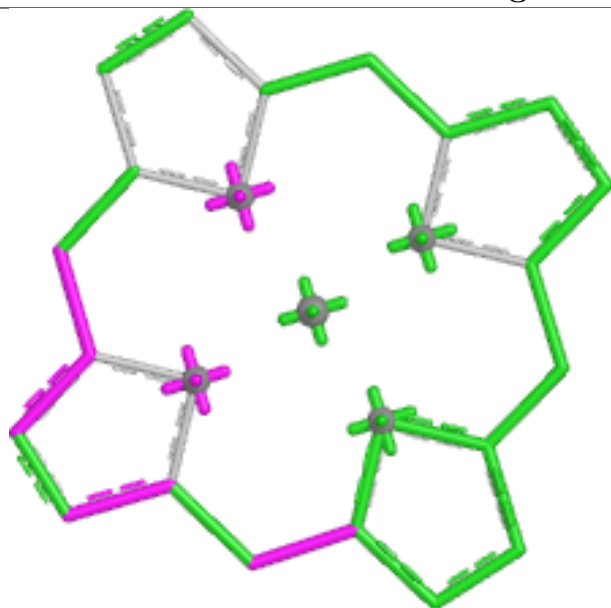


Torsions

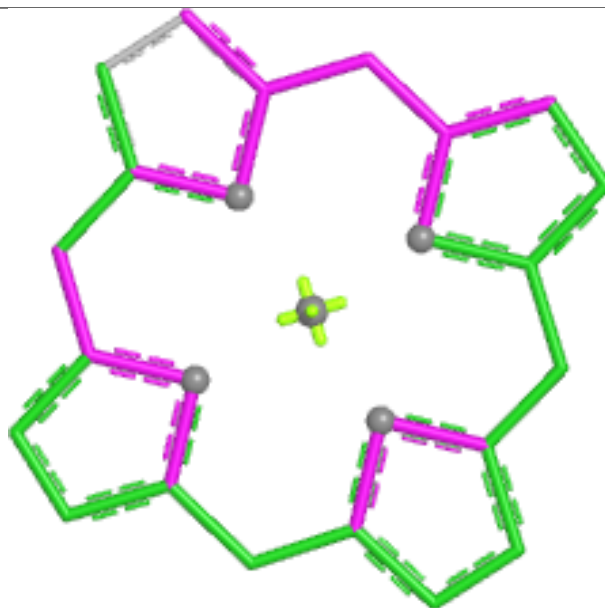


Rings

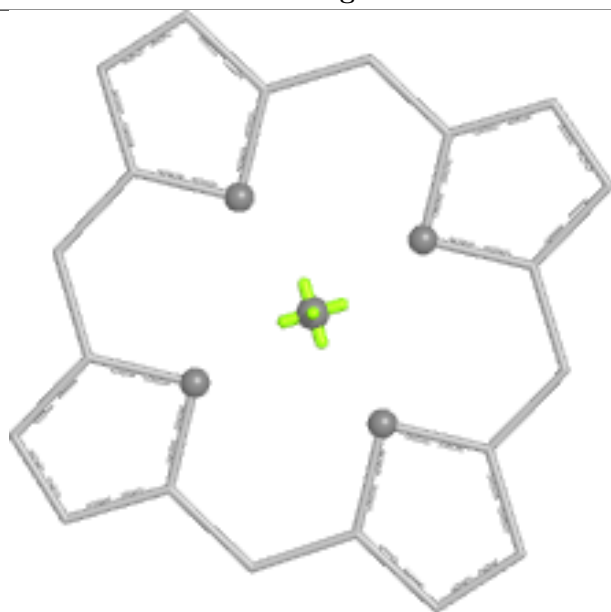
Ligand CLA 8 1011



Bond lengths



Bond angles

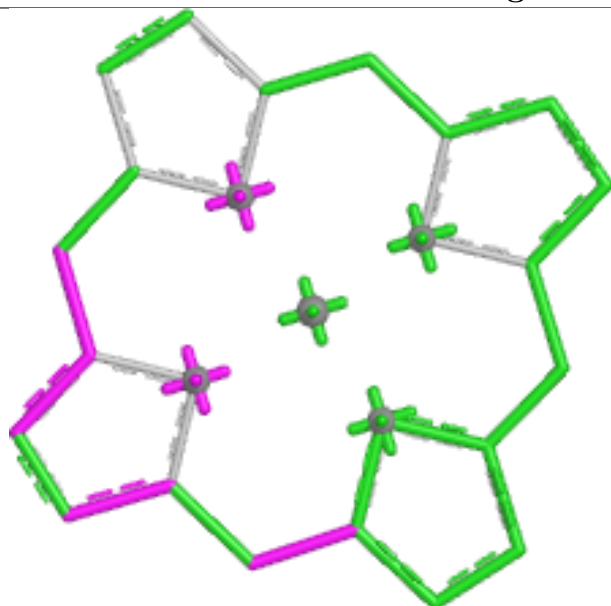


Torsions

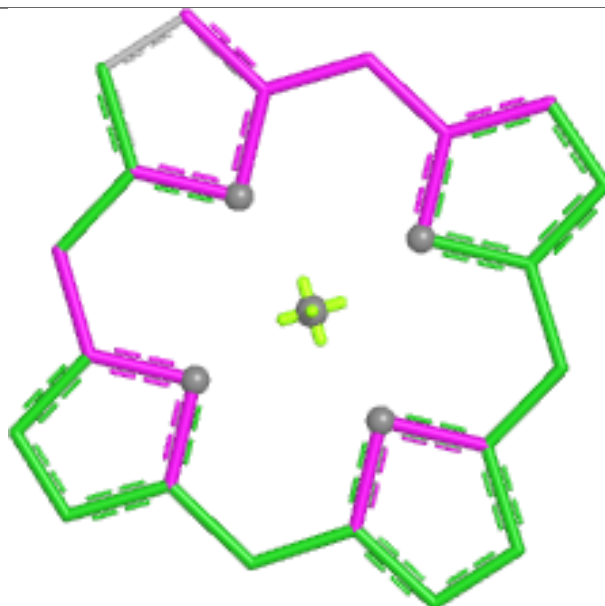


Rings

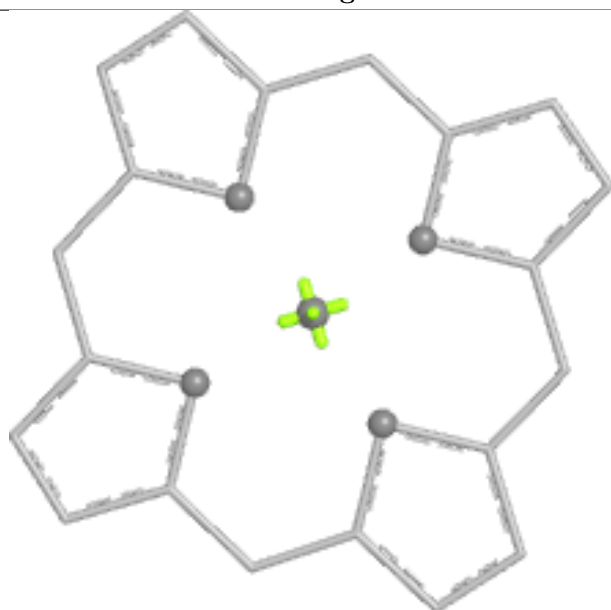
Ligand CLA F 4004



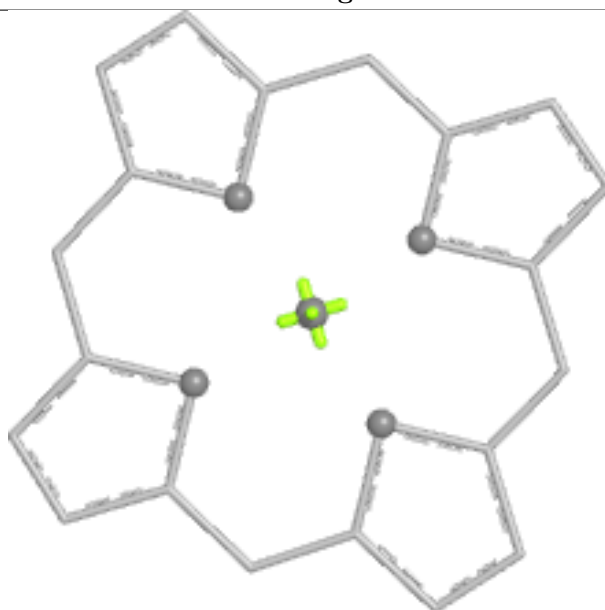
Bond lengths



Bond angles

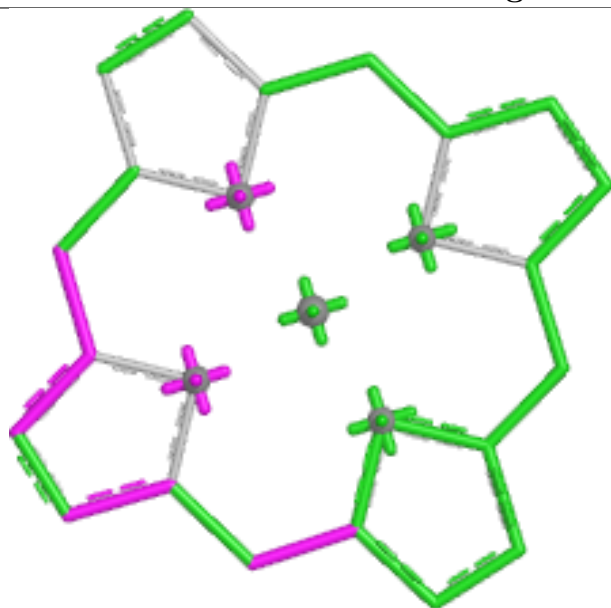


Torsions

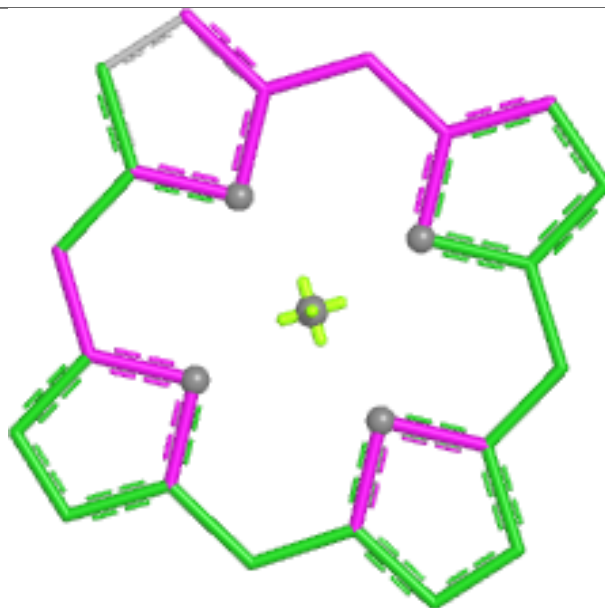


Rings

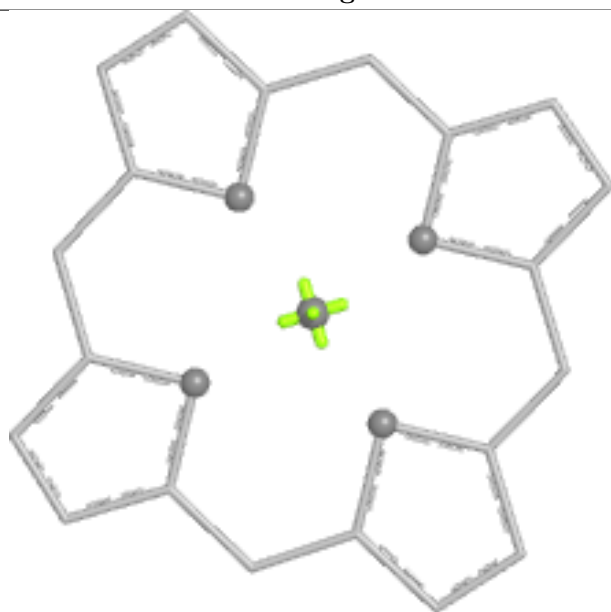
Ligand CLA P 8010



Bond lengths



Bond angles

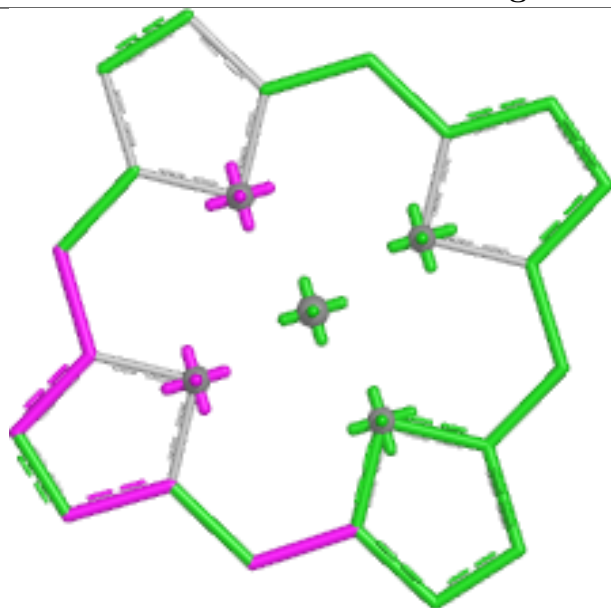


Torsions

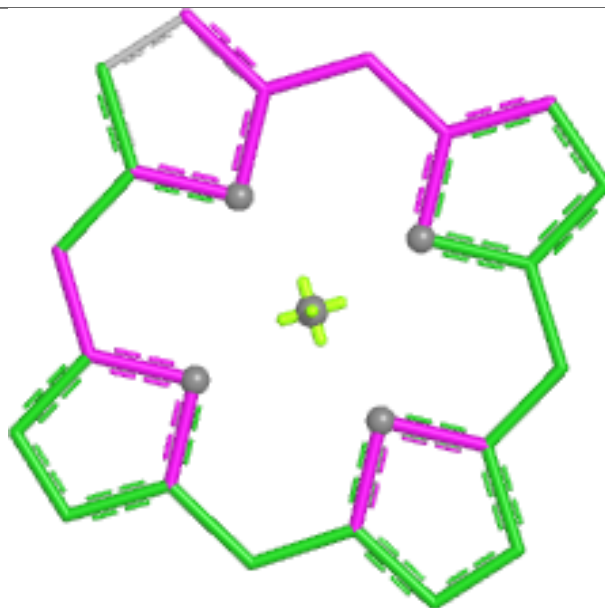


Rings

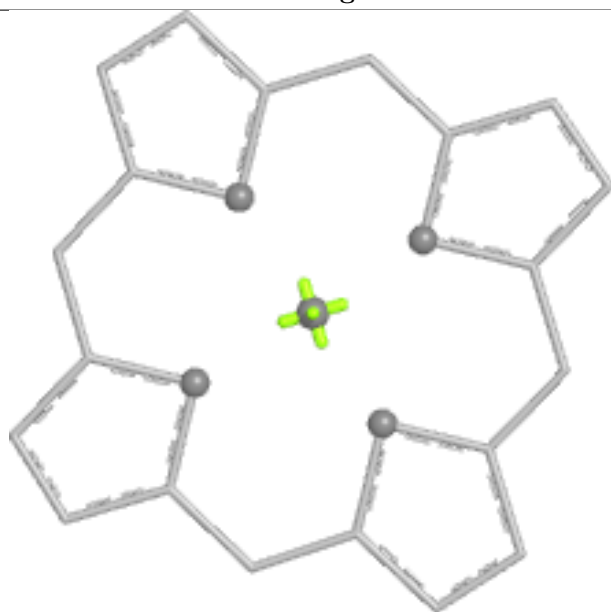
Ligand CLA 0 1033



Bond lengths



Bond angles

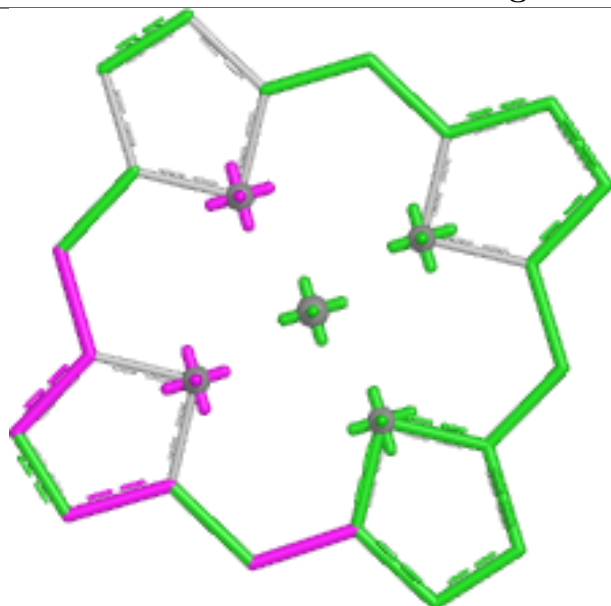


Torsions

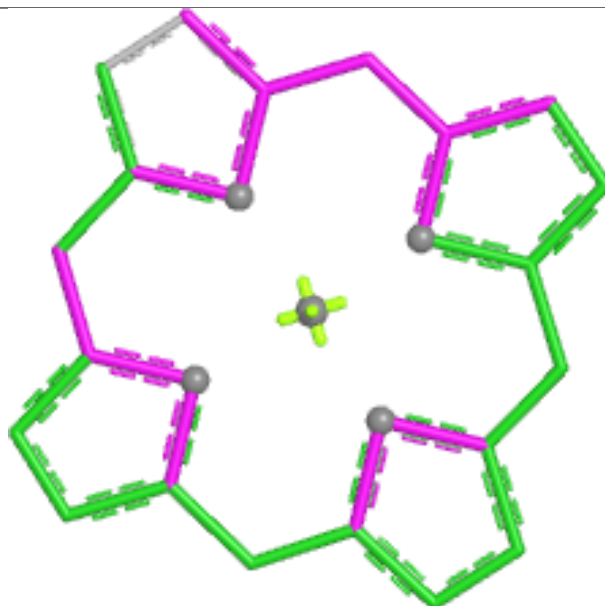


Rings

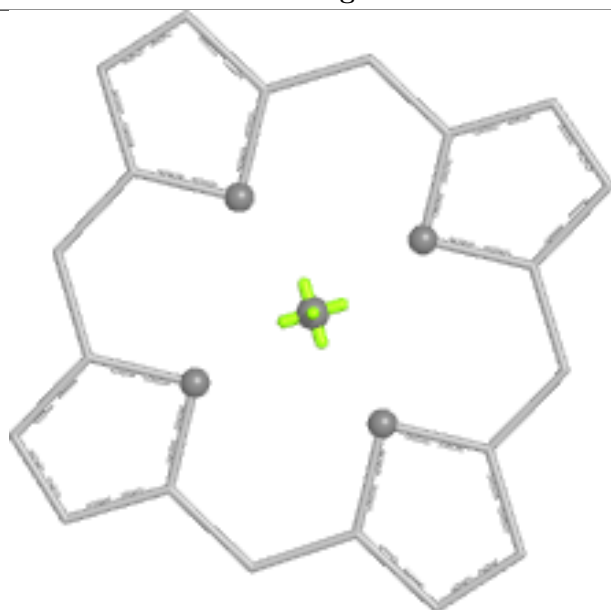
Ligand CLA 8 1023



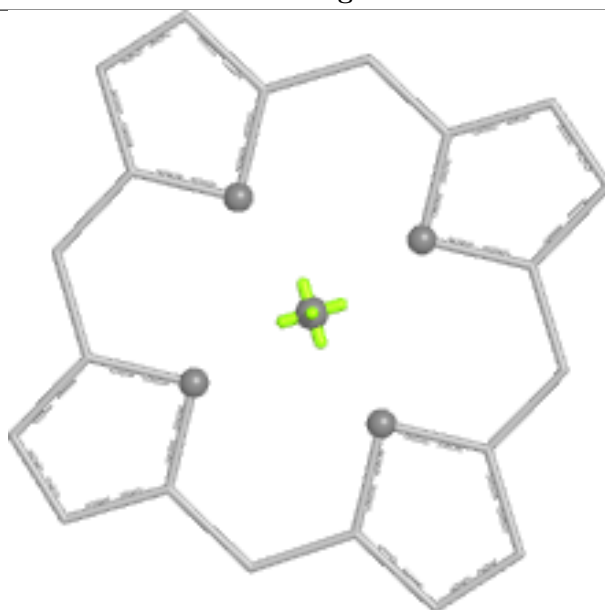
Bond lengths



Bond angles

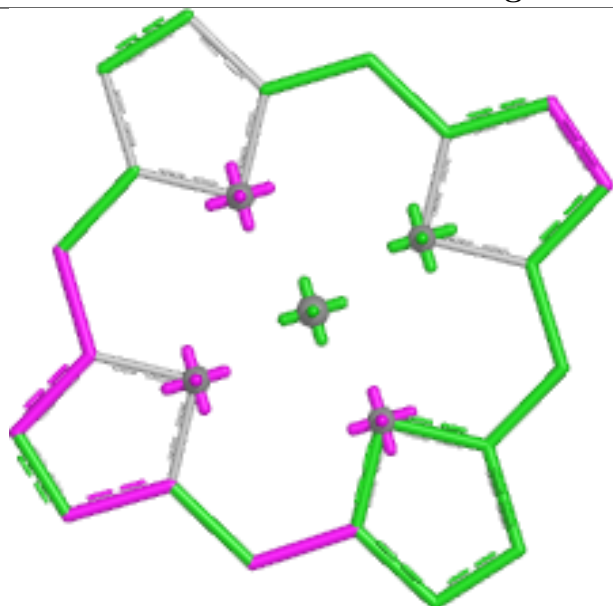


Torsions

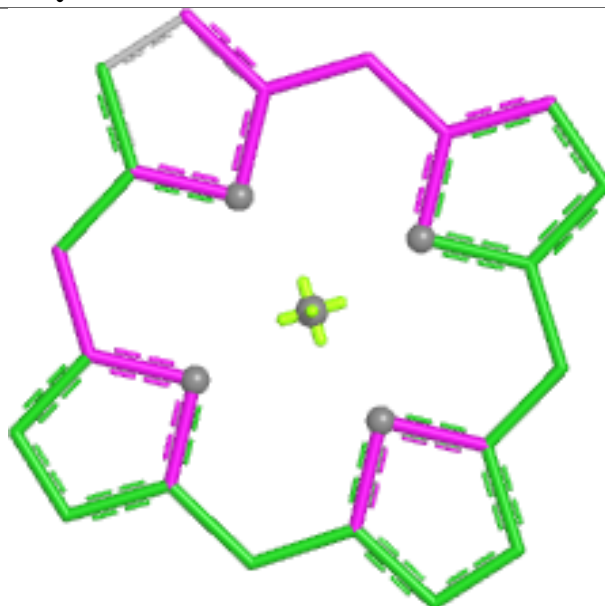


Rings

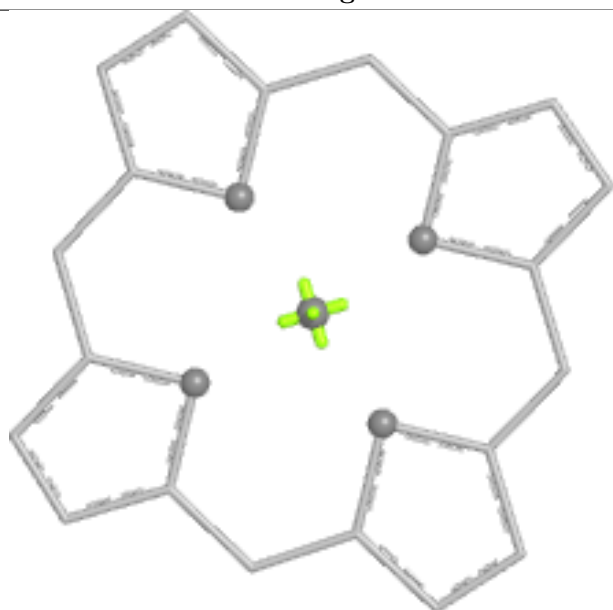
Ligand CLA Q 5232



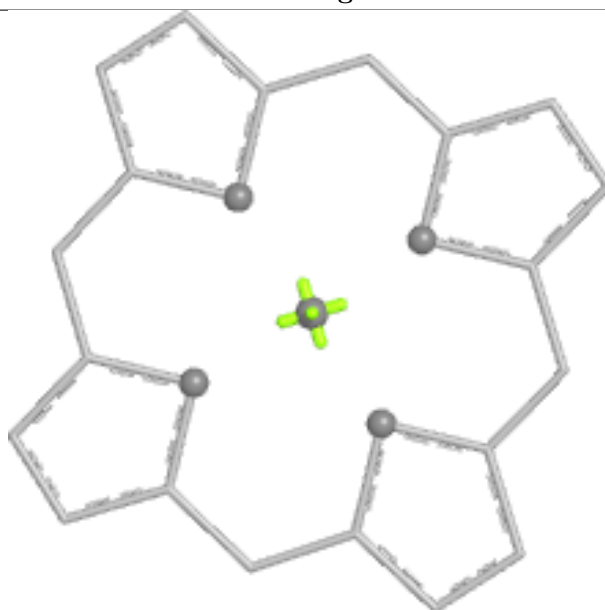
Bond lengths



Bond angles

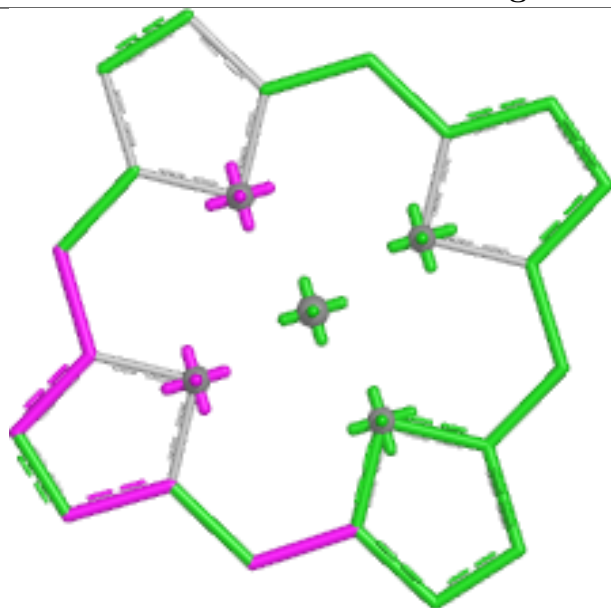


Torsions

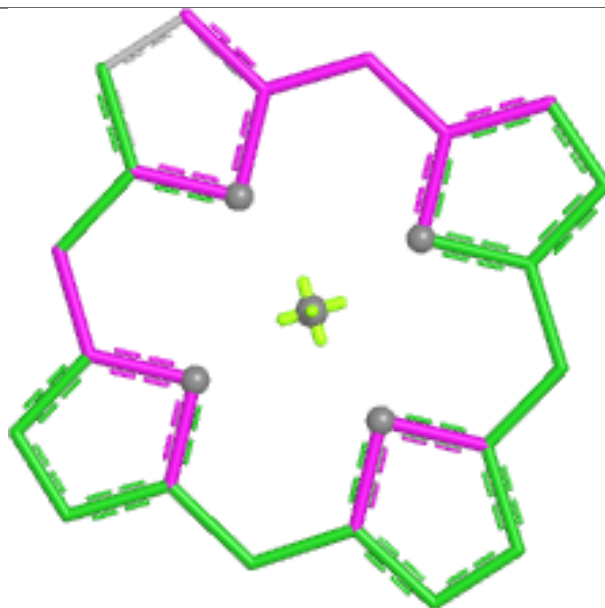


Rings

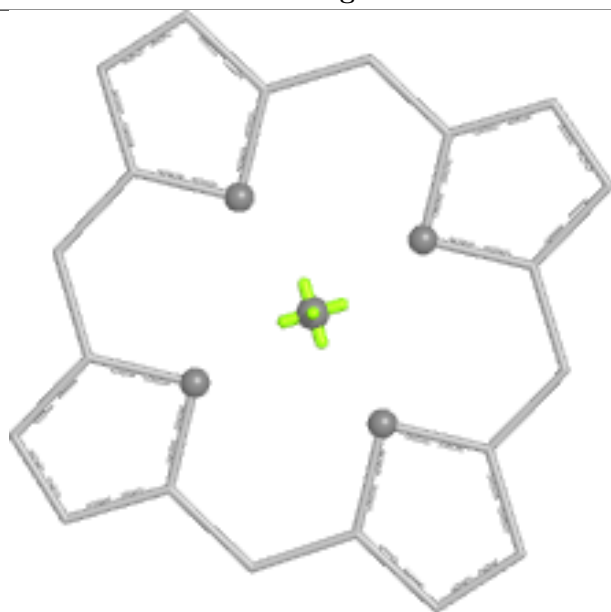
Ligand CLA 9 1032



Bond lengths



Bond angles

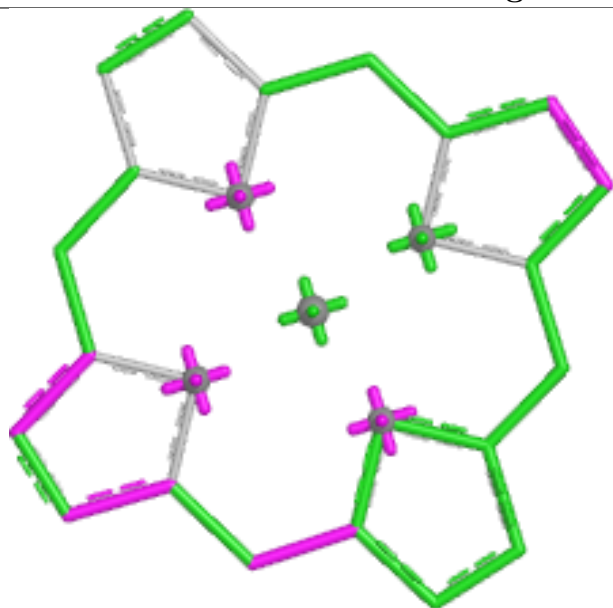


Torsions

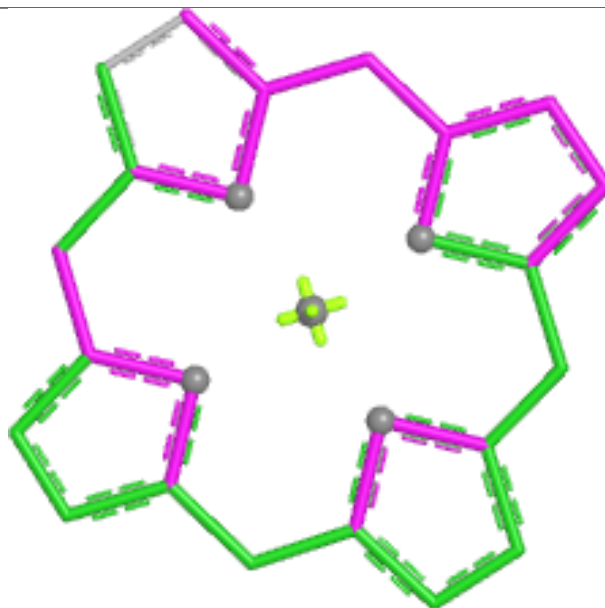


Rings

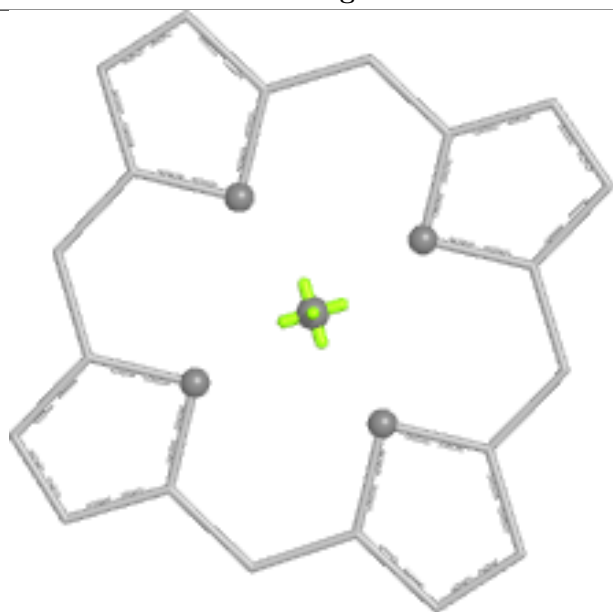
Ligand CLA P 5123



Bond lengths



Bond angles

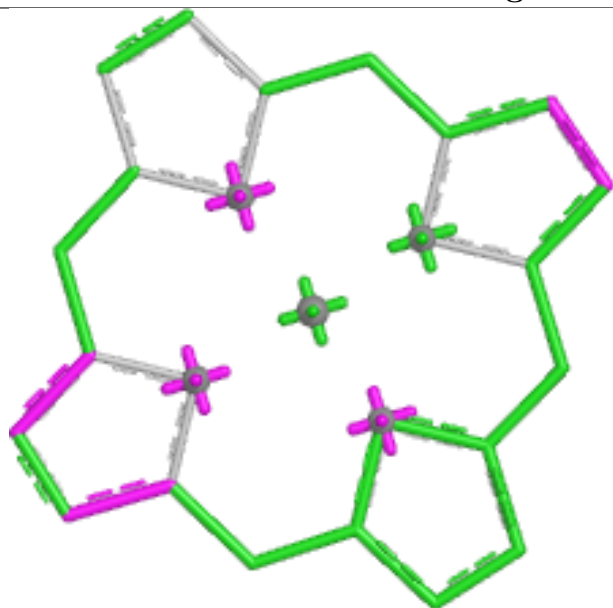


Torsions

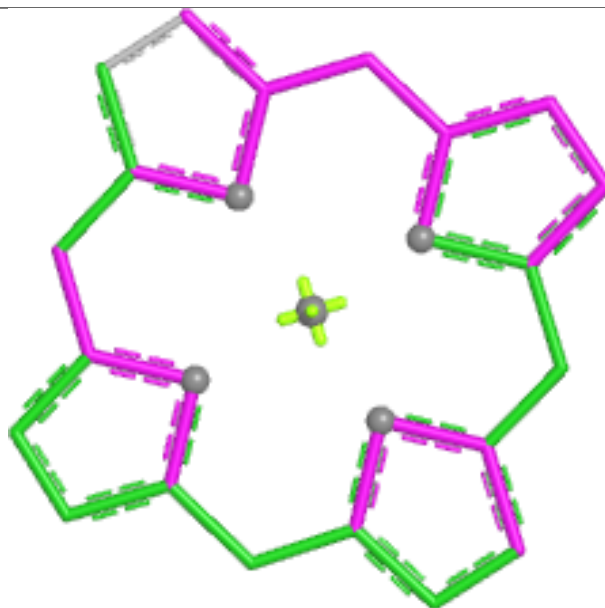


Rings

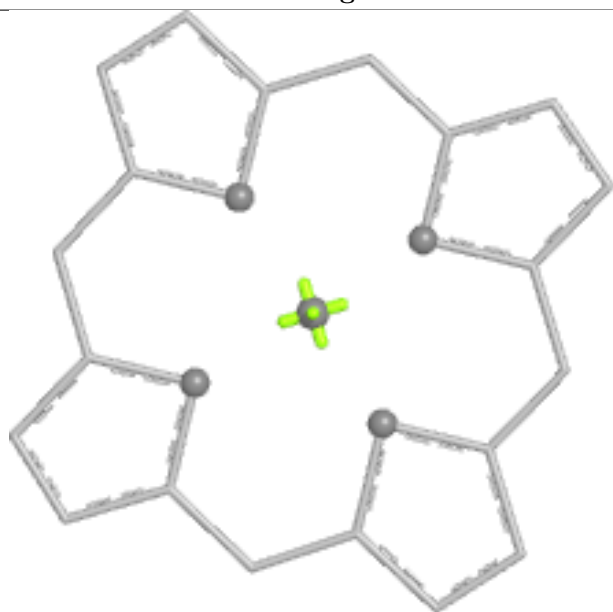
Ligand CLA P 5117



Bond lengths



Bond angles

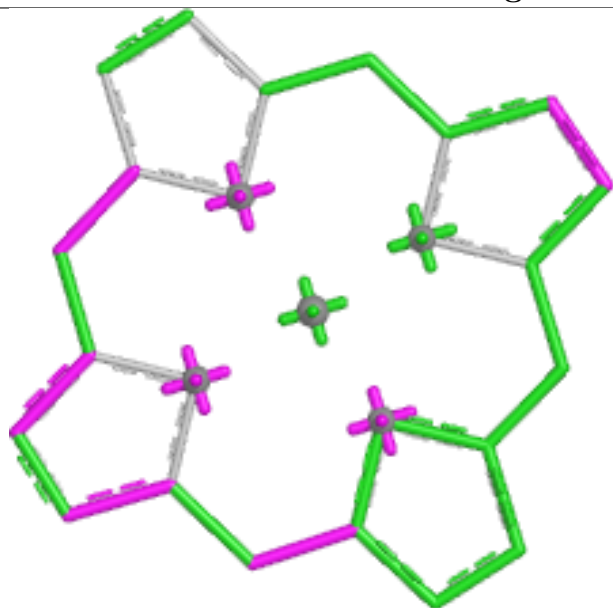


Torsions

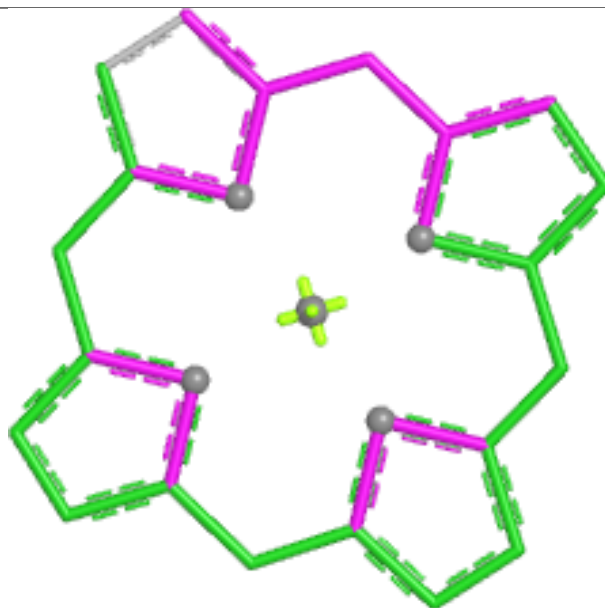


Rings

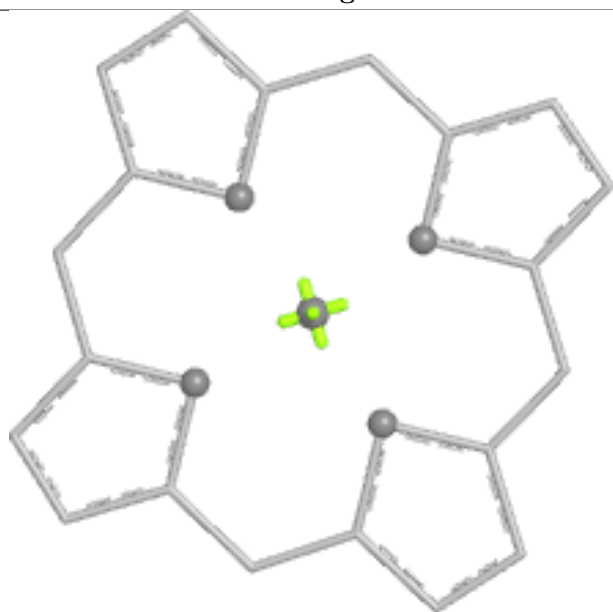
Ligand CLA V 5233



Bond lengths



Bond angles

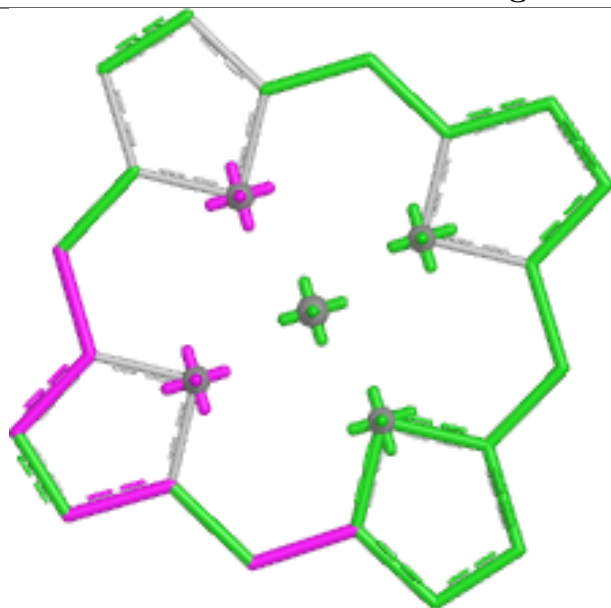


Torsions

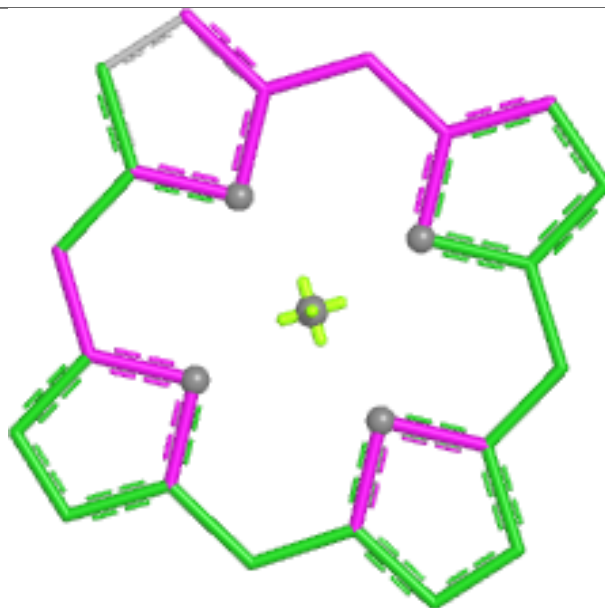


Rings

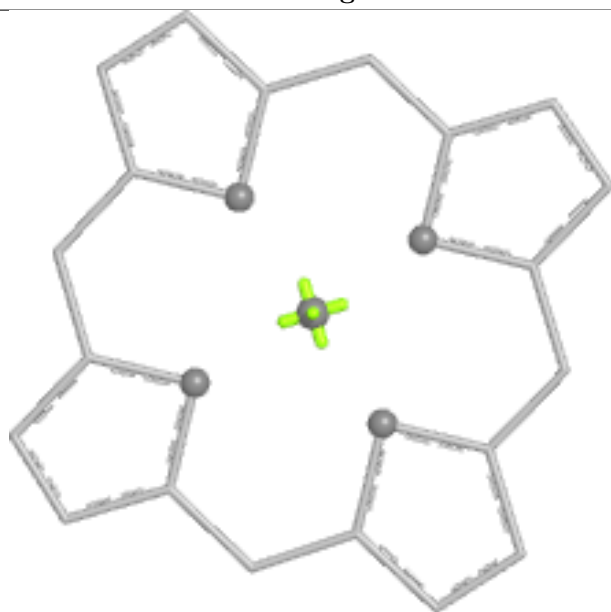
Ligand CLA 9 1015



Bond lengths



Bond angles

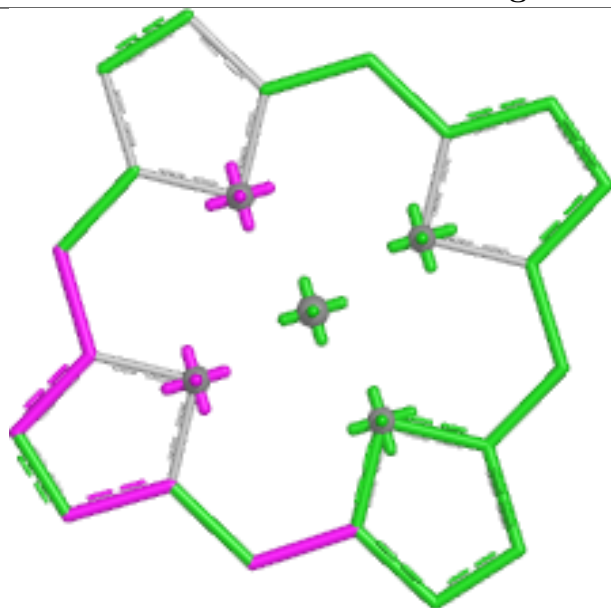


Torsions

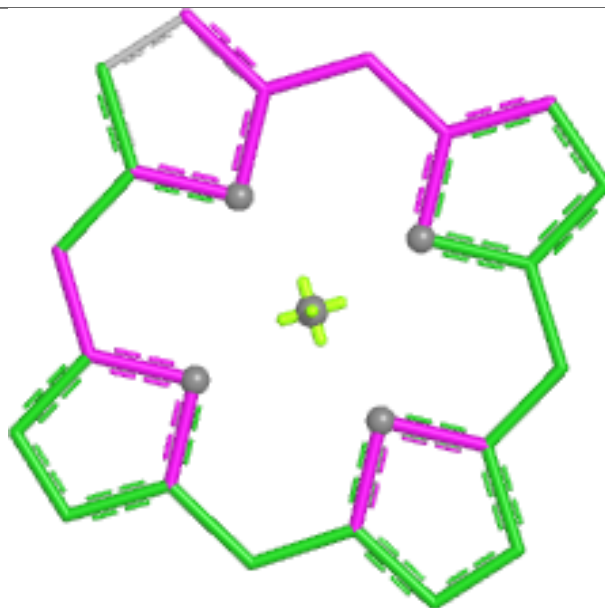


Rings

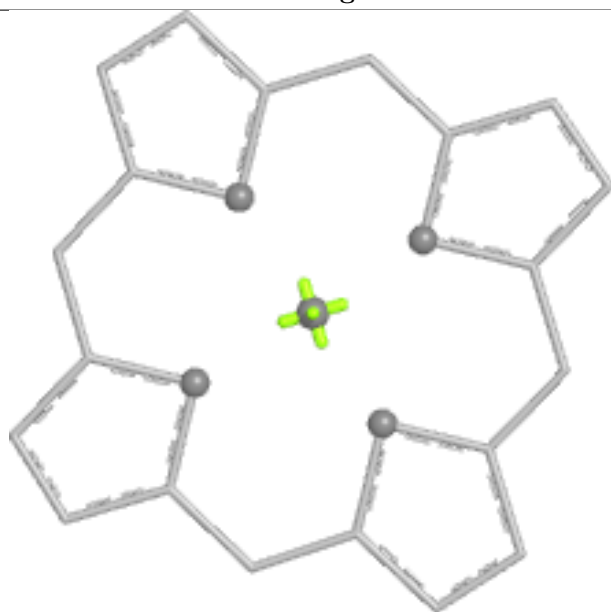
Ligand CLA 3 1031



Bond lengths



Bond angles

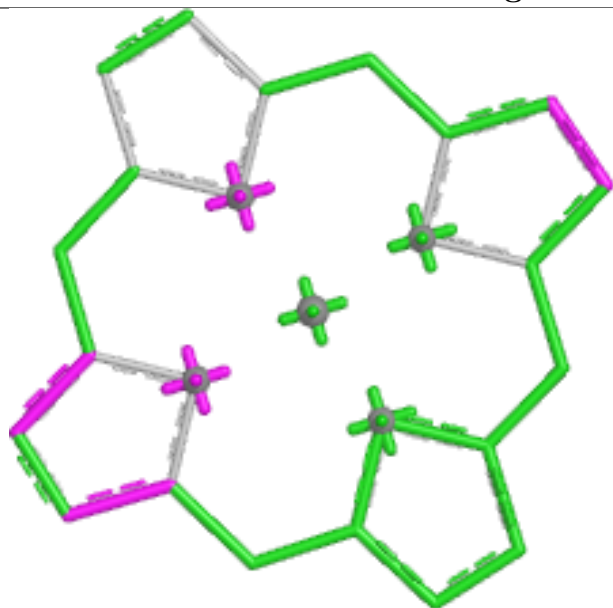


Torsions

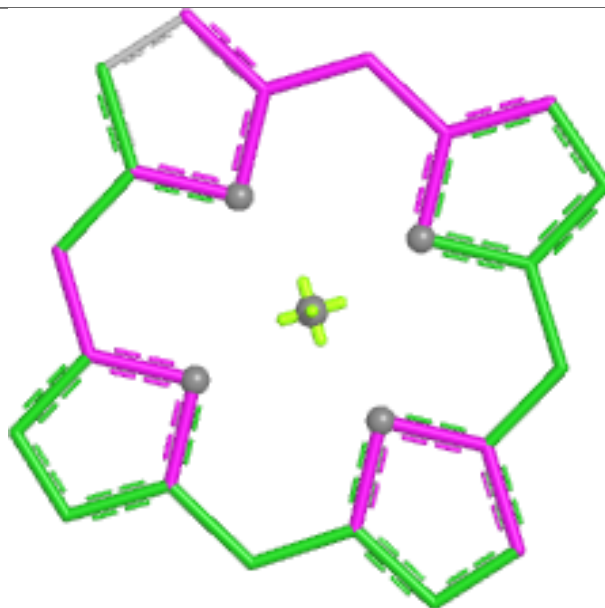


Rings

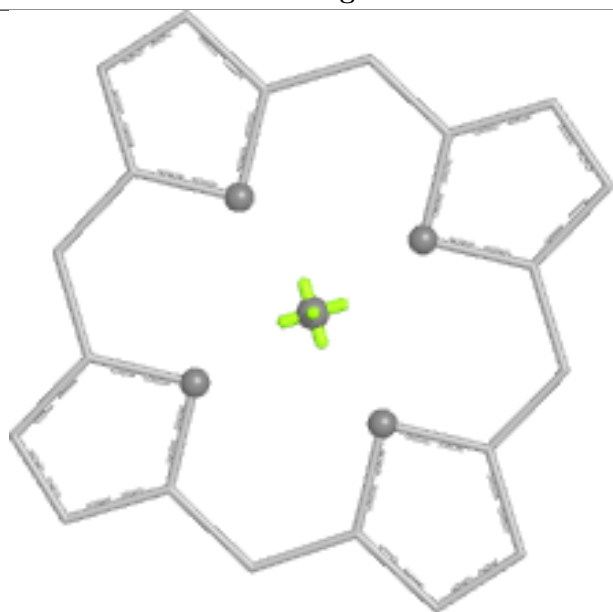
Ligand CLA A 1110



Bond lengths



Bond angles

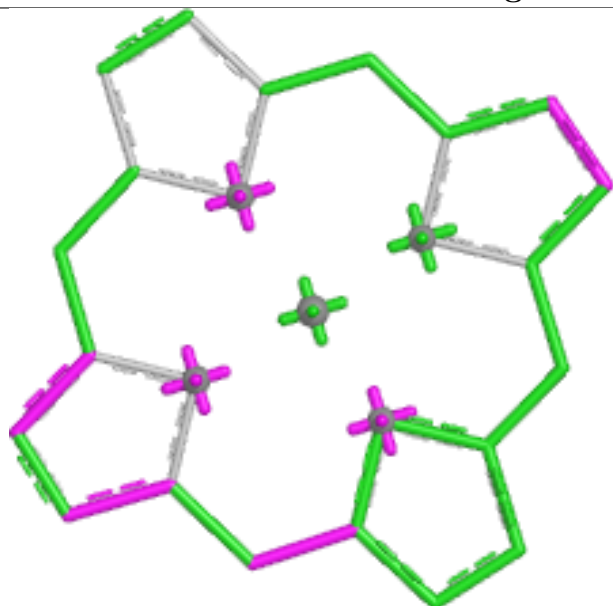


Torsions

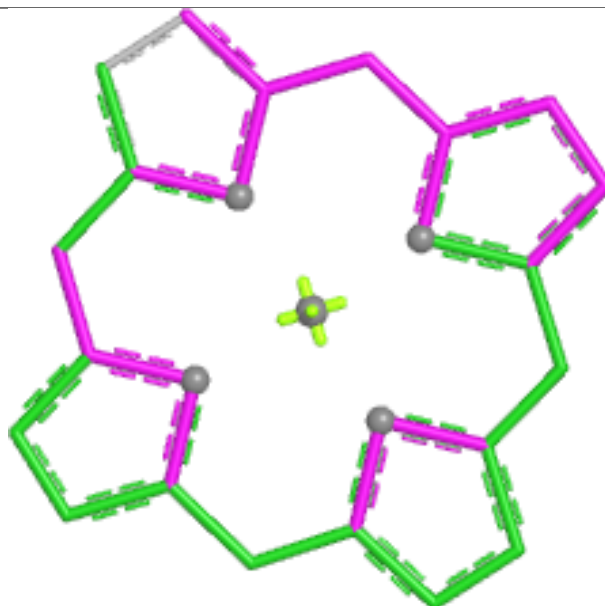


Rings

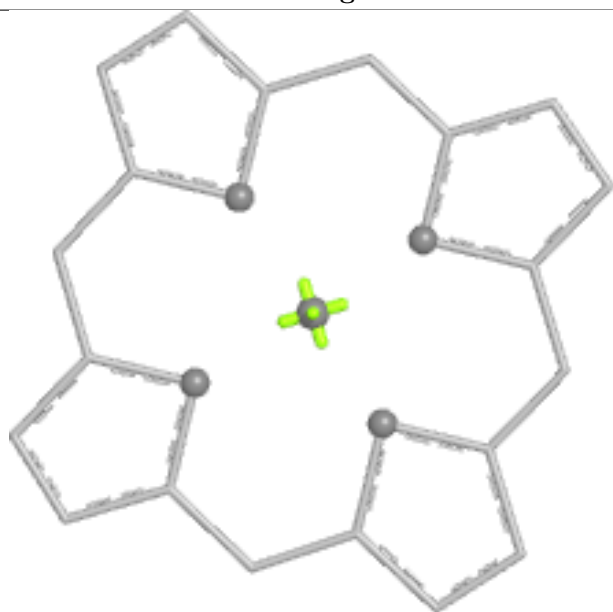
Ligand CLA A 1128



Bond lengths



Bond angles

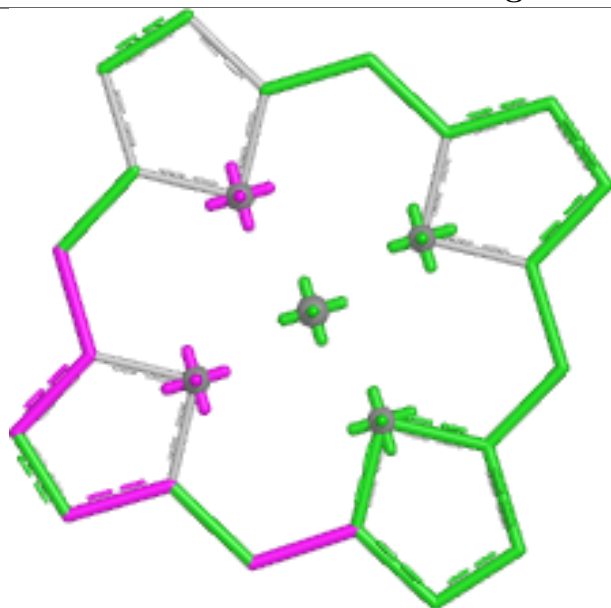


Torsions

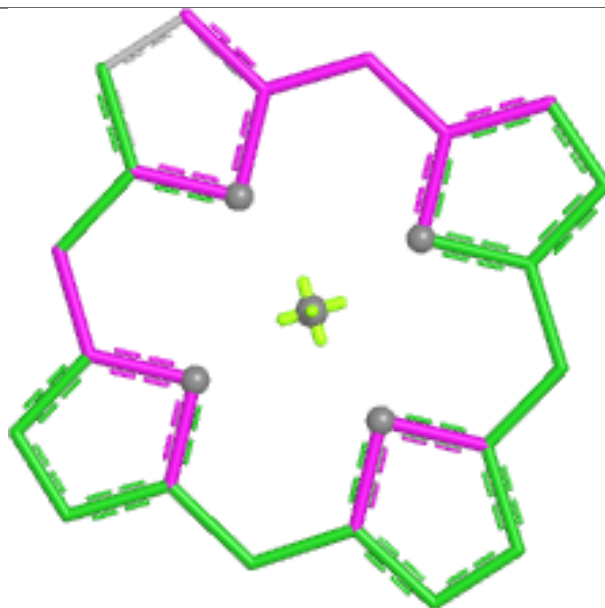


Rings

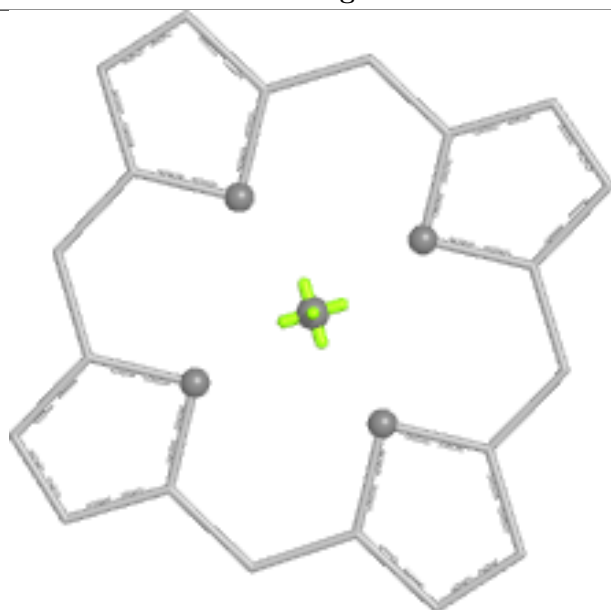
Ligand CLA B 1242



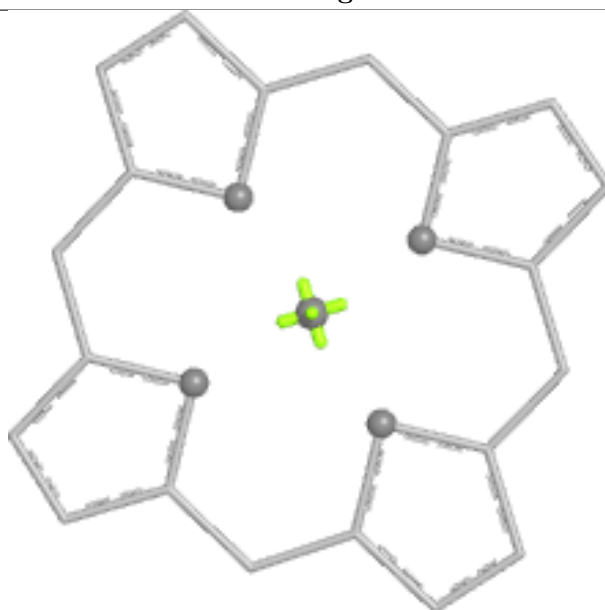
Bond lengths



Bond angles

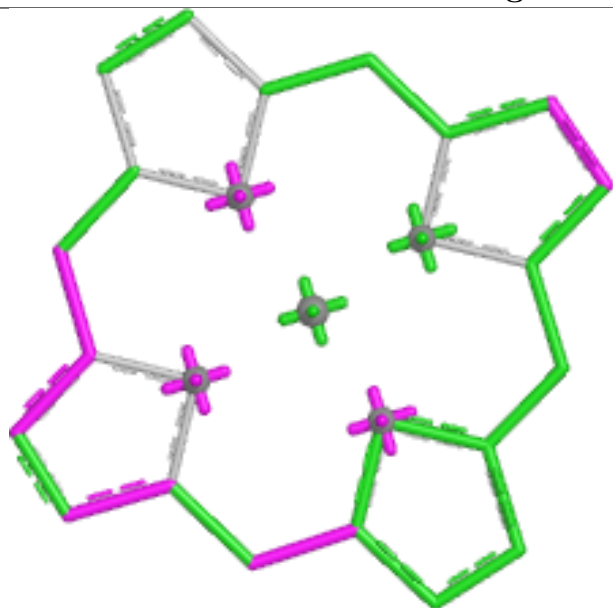


Torsions

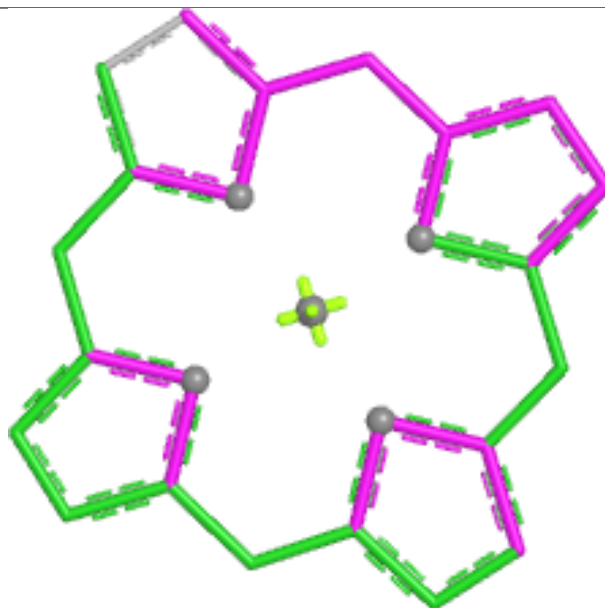


Rings

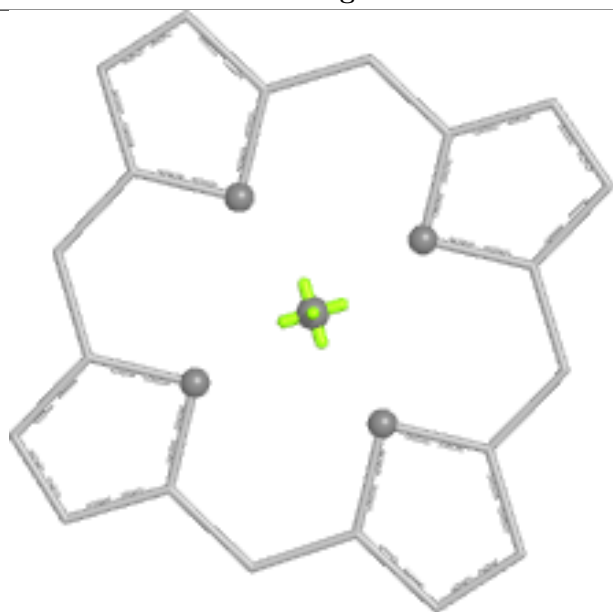
Ligand CLA P 5013



Bond lengths



Bond angles

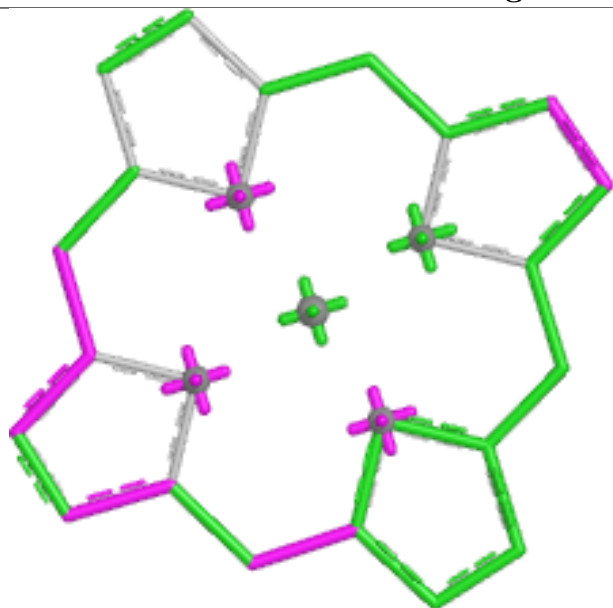


Torsions

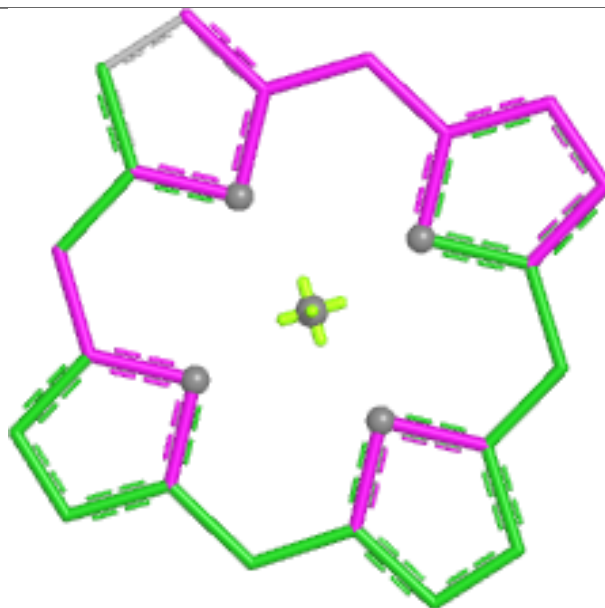


Rings

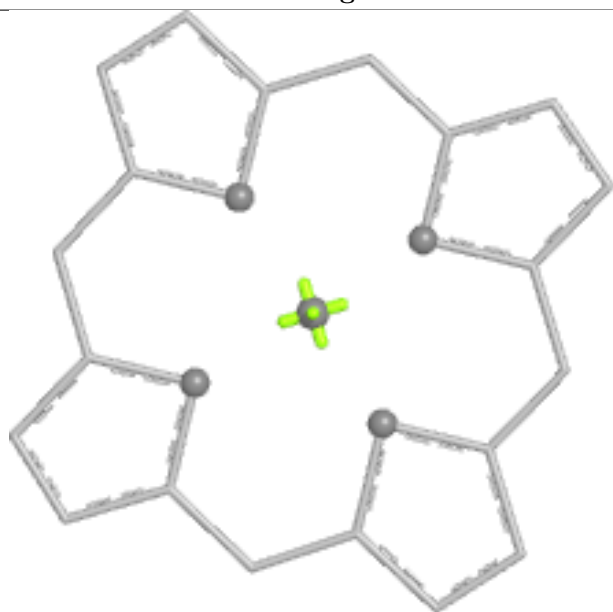
Ligand CLA B 1210



Bond lengths



Bond angles

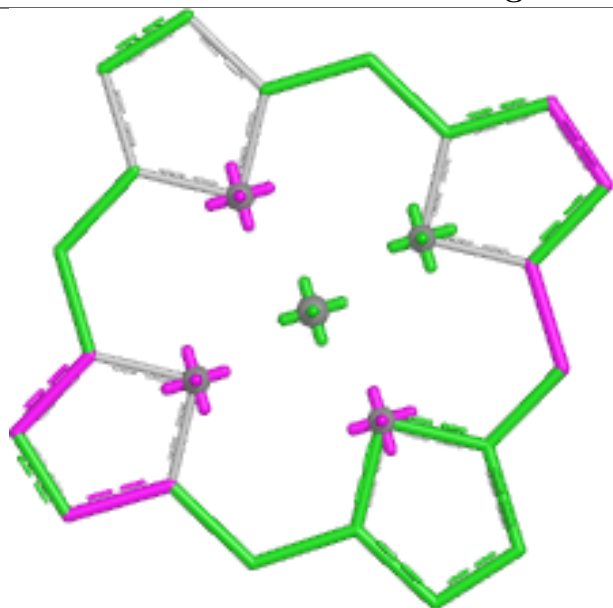


Torsions

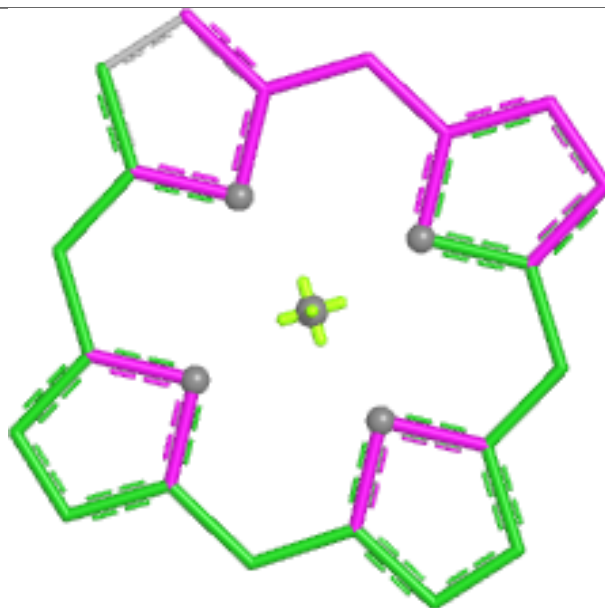


Rings

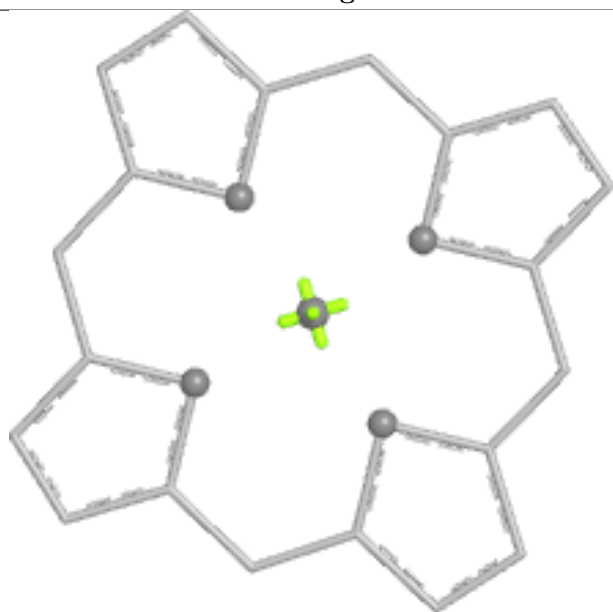
Ligand CLA B 1203



Bond lengths



Bond angles

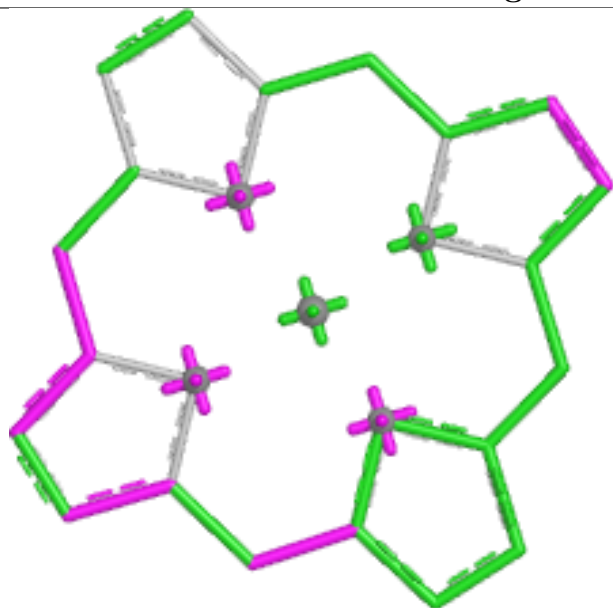


Torsions

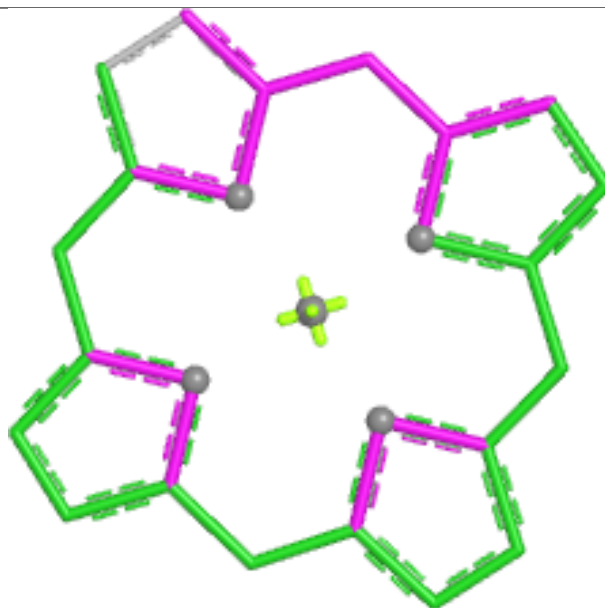


Rings

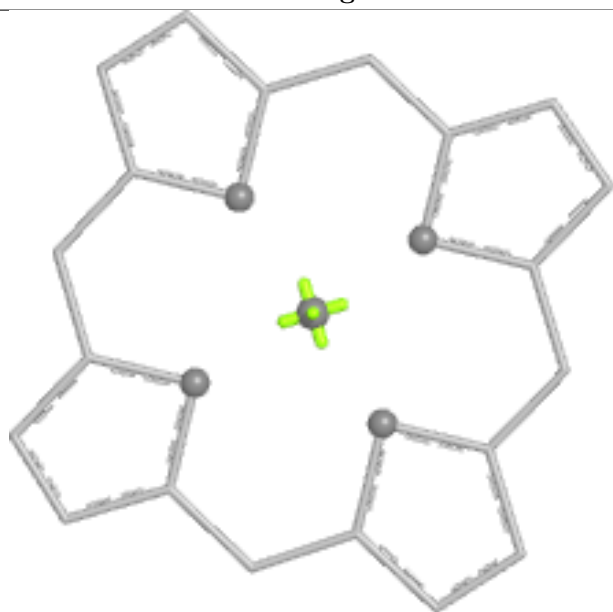
Ligand CLA A 1121



Bond lengths



Bond angles

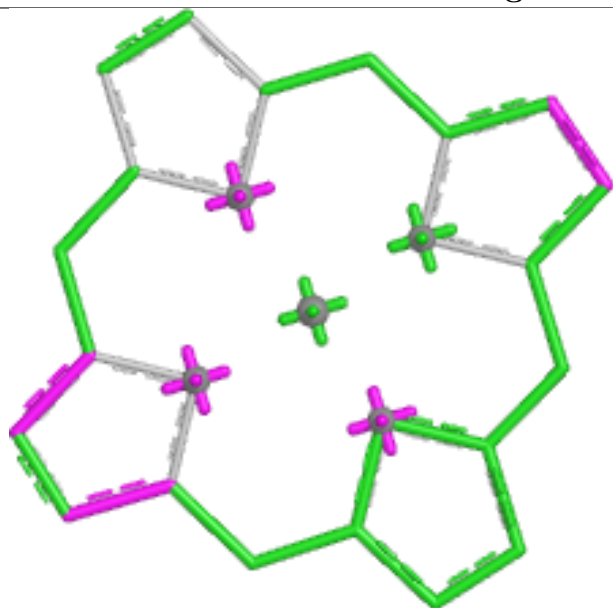


Torsions

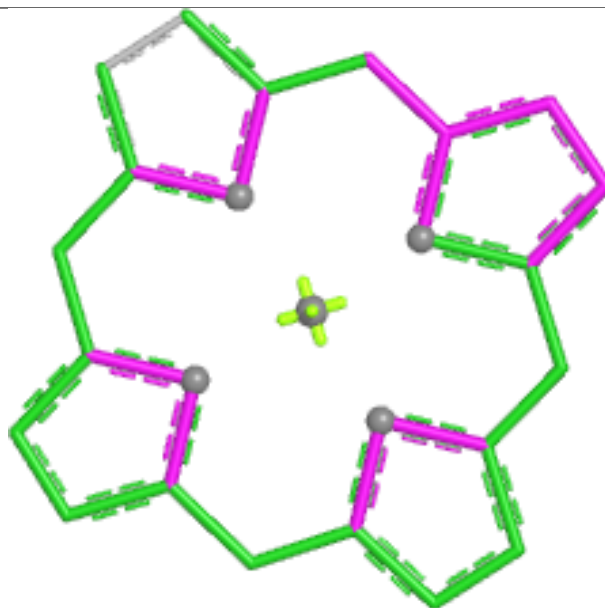


Rings

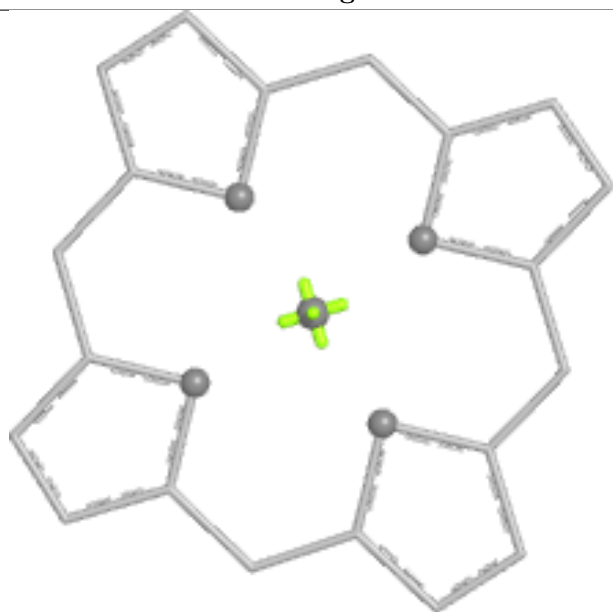
Ligand CLA B 1202



Bond lengths



Bond angles

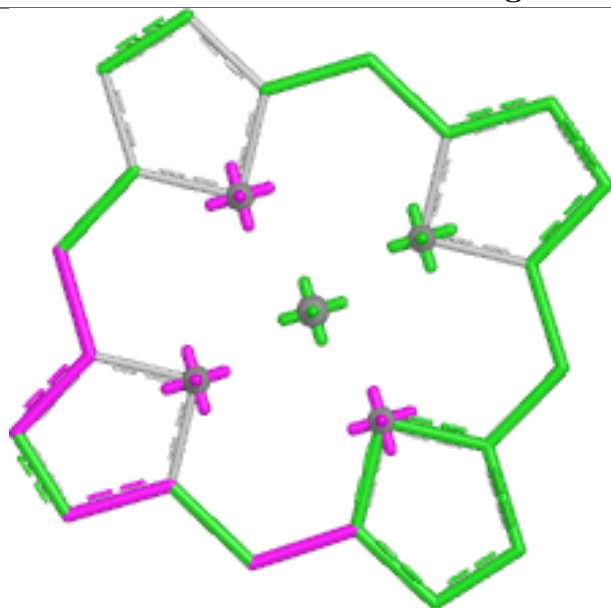


Torsions

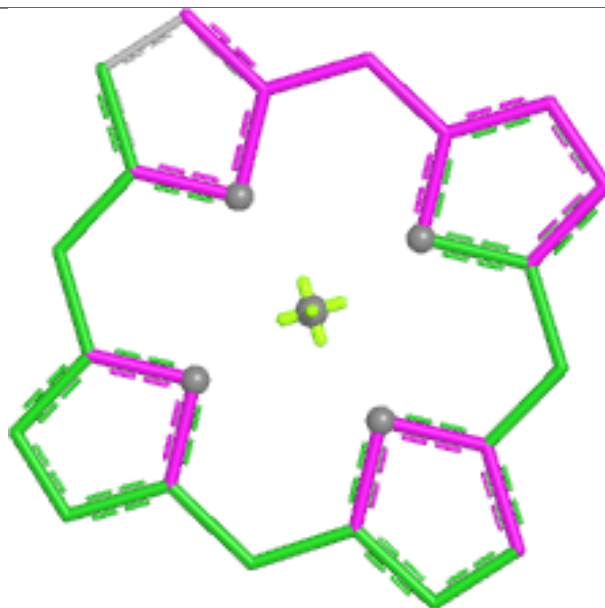


Rings

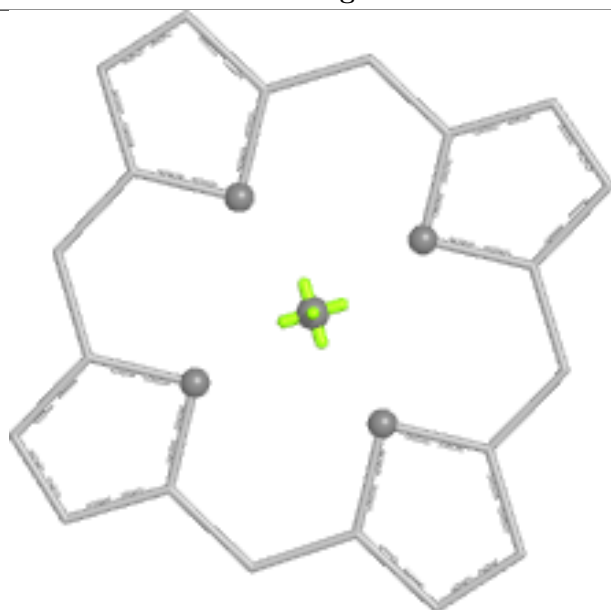
Ligand CLA A 1138



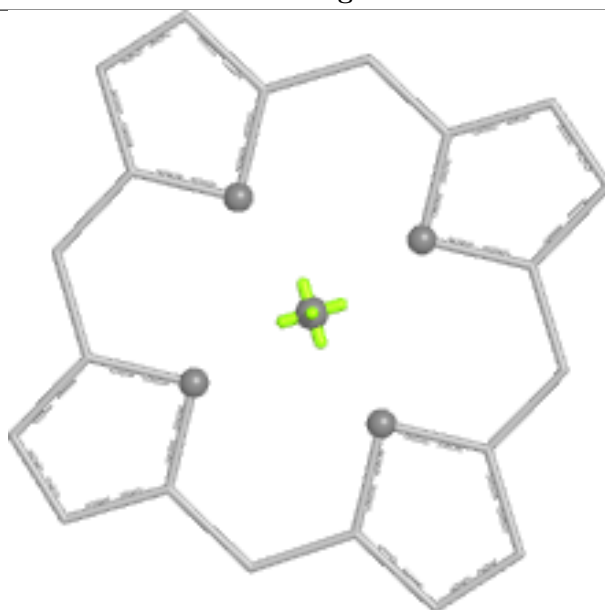
Bond lengths



Bond angles

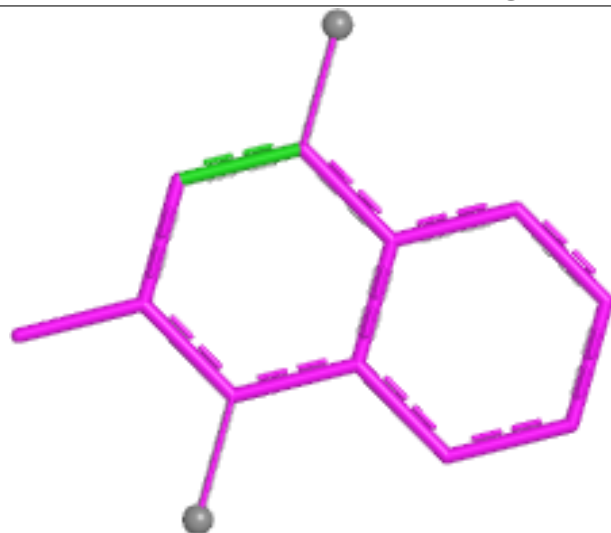


Torsions

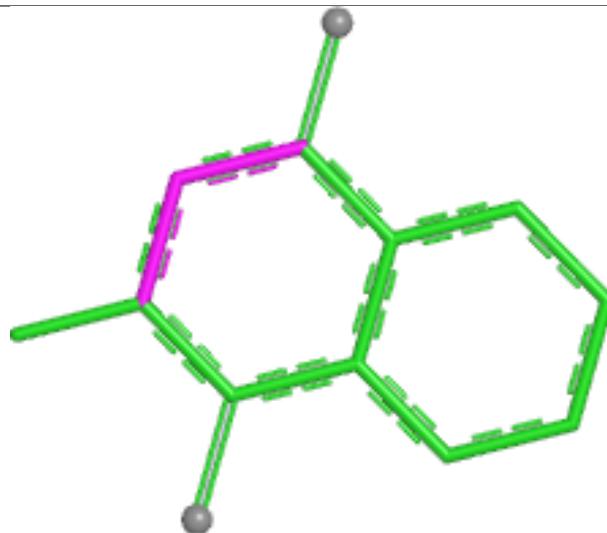


Rings

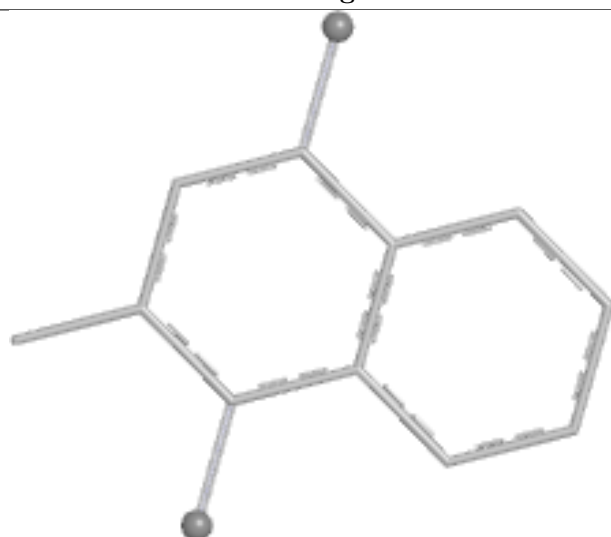
Ligand PQN A 2001



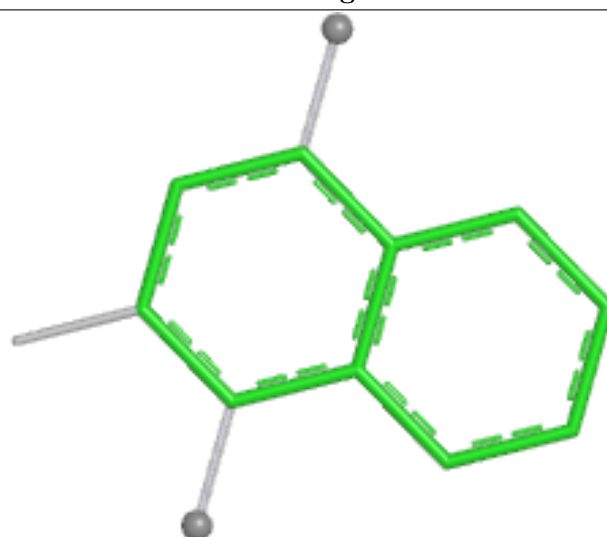
Bond lengths



Bond angles

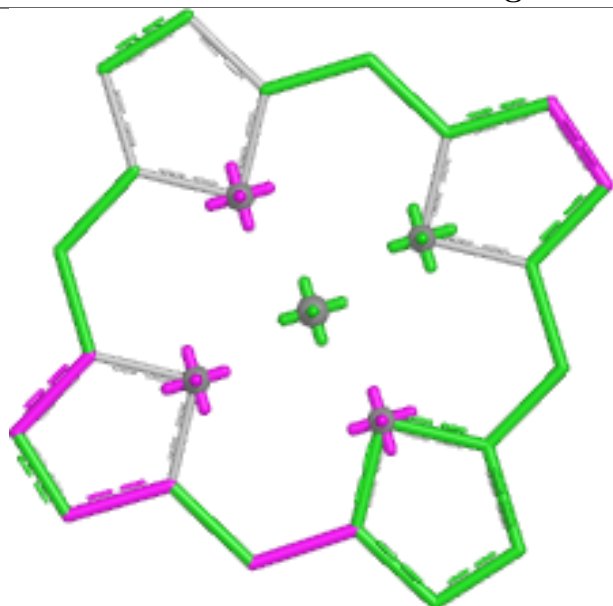


Torsions

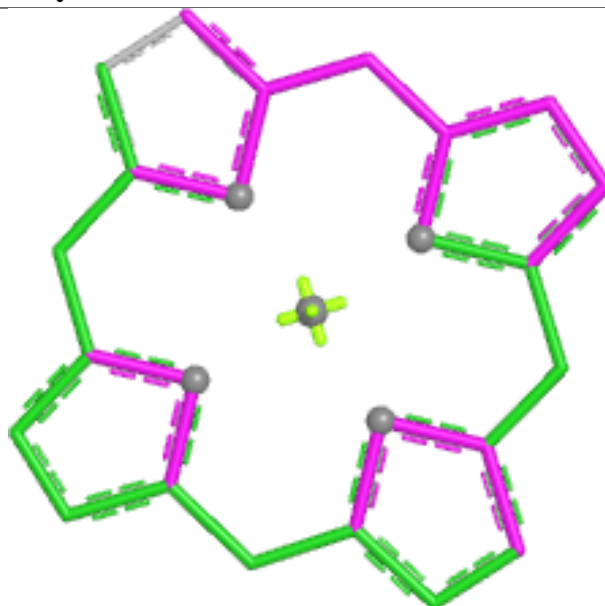


Rings

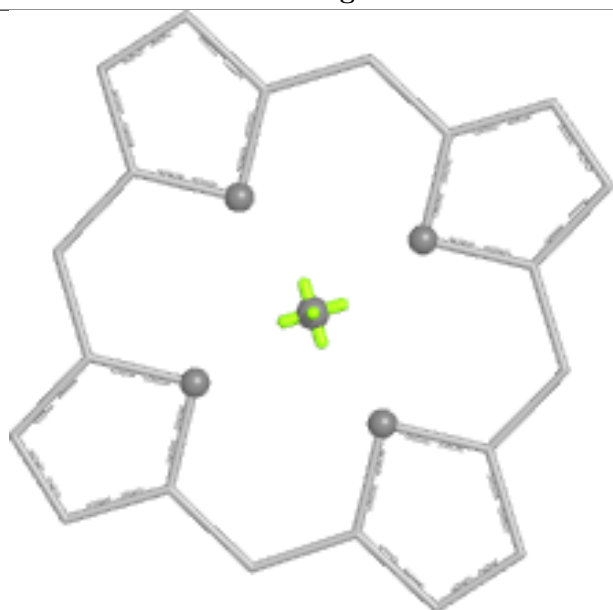
Ligand CLA Q 5201



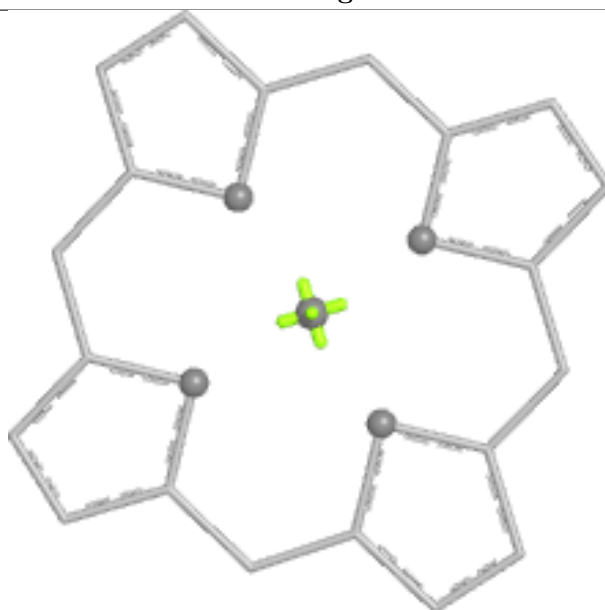
Bond lengths



Bond angles

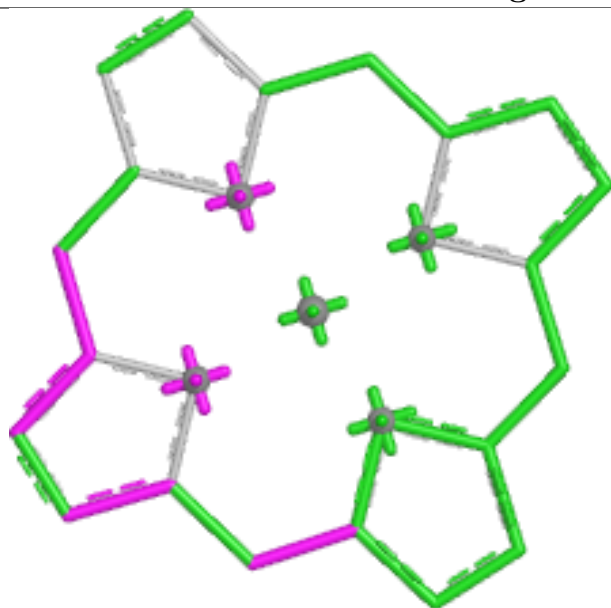


Torsions



Rings

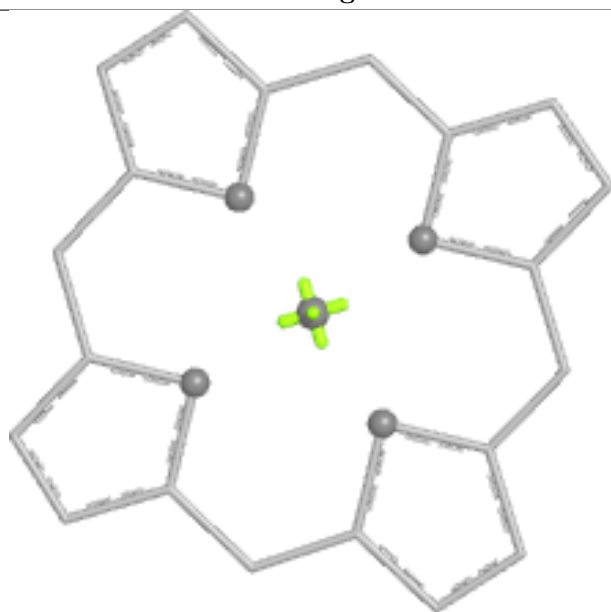
Ligand CLA 4 1033



Bond lengths



Bond angles

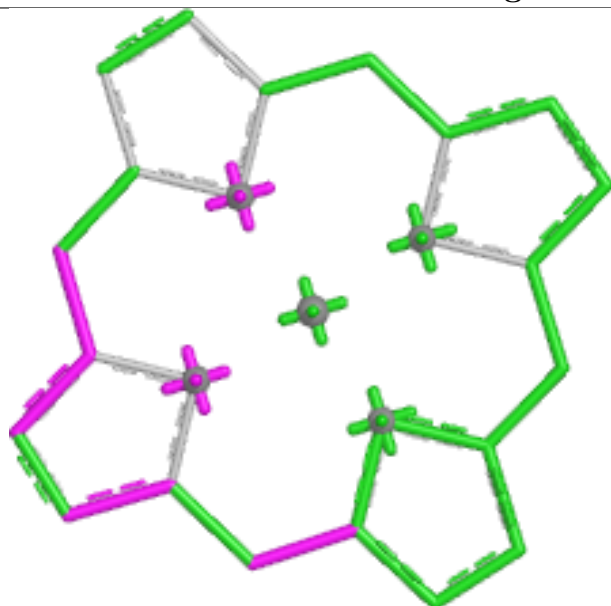


Torsions

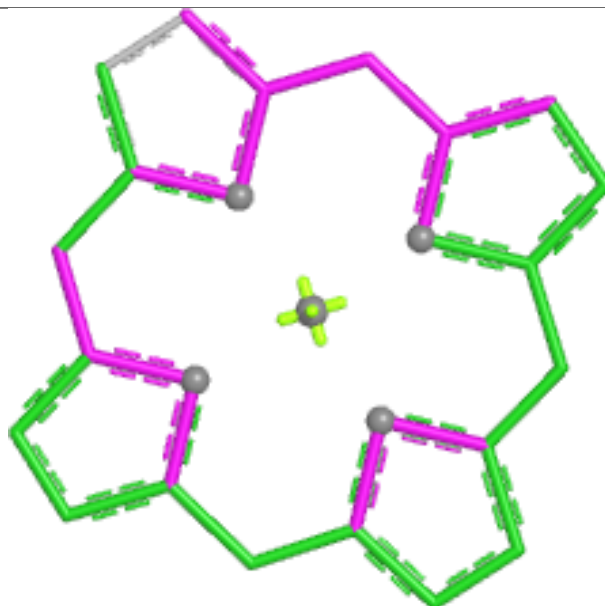


Rings

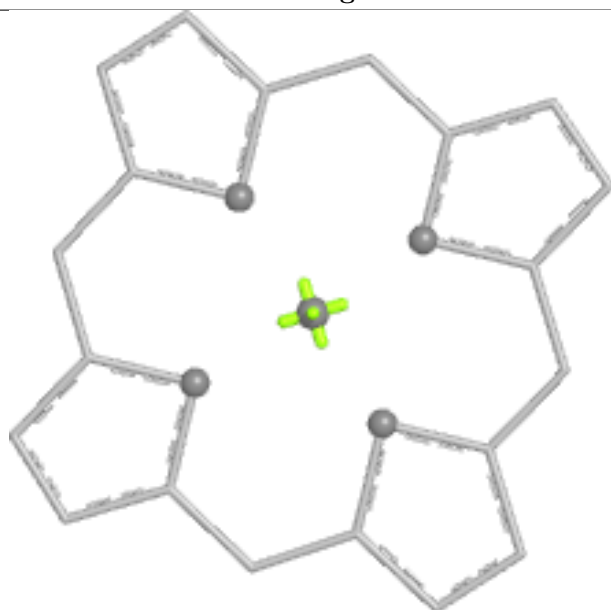
Ligand CLA U 8003



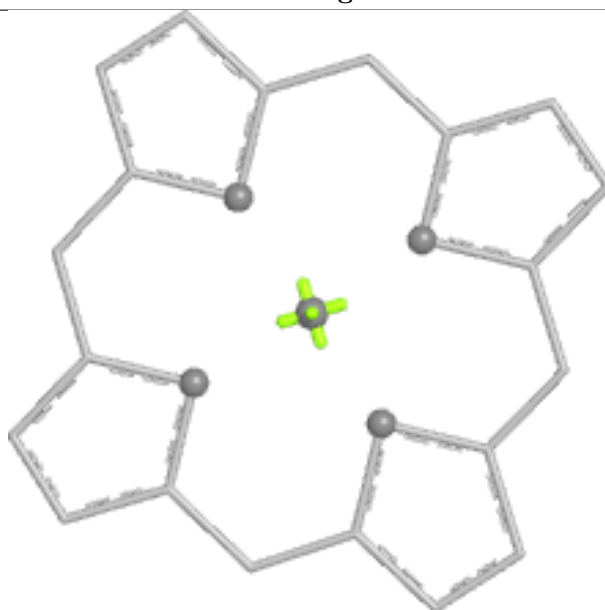
Bond lengths



Bond angles

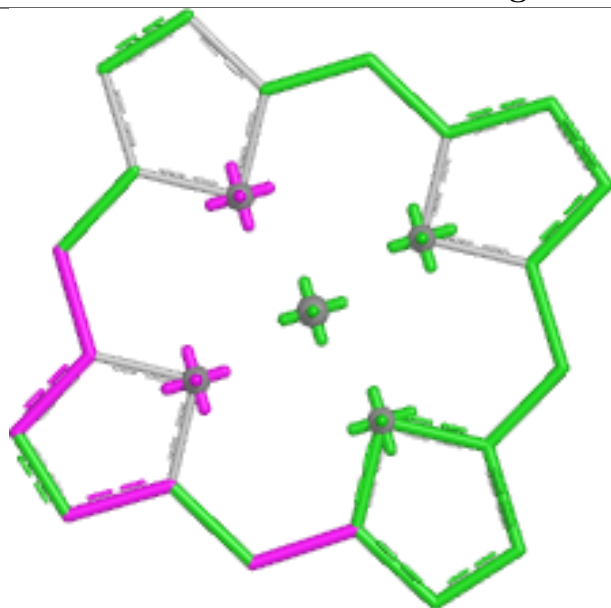


Torsions

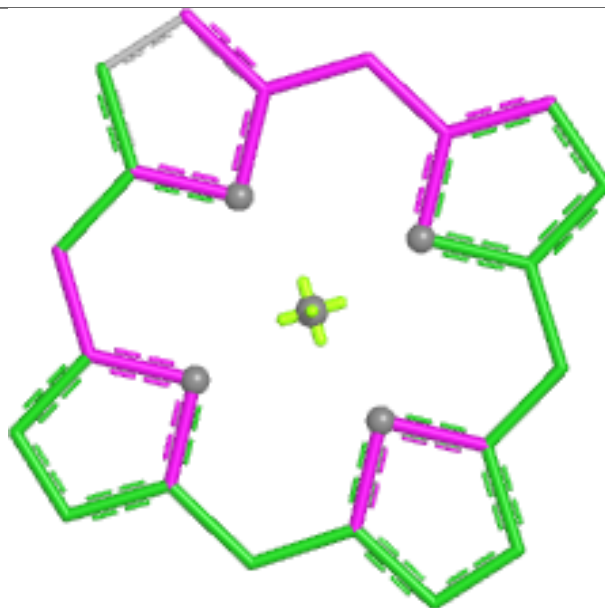


Rings

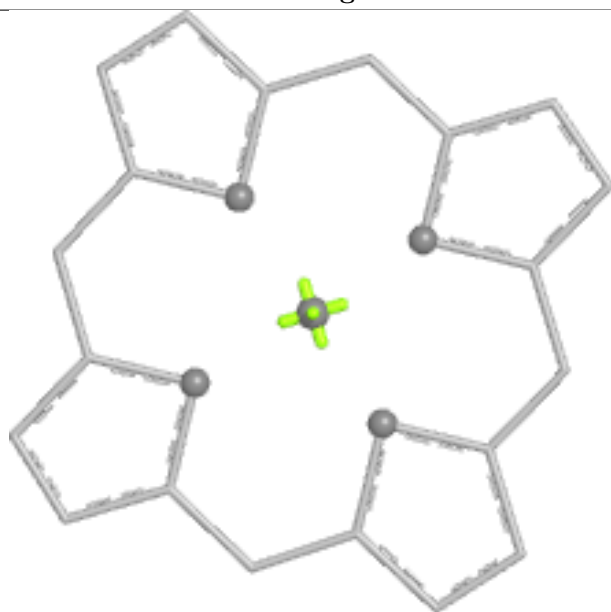
Ligand CLA 3 1022



Bond lengths



Bond angles

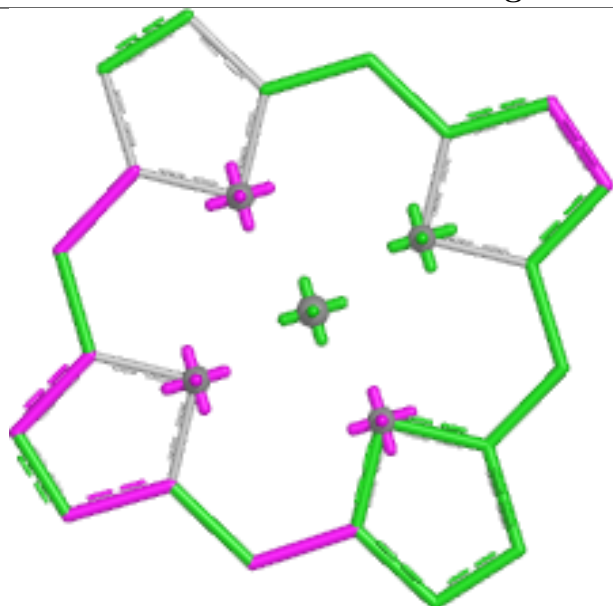


Torsions

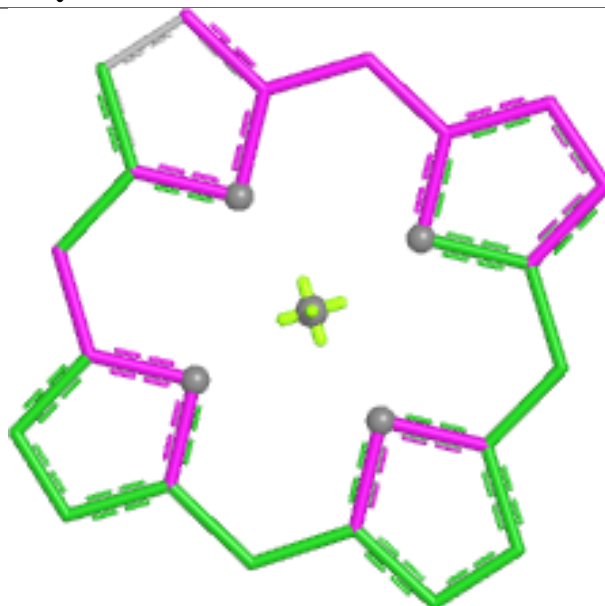


Rings

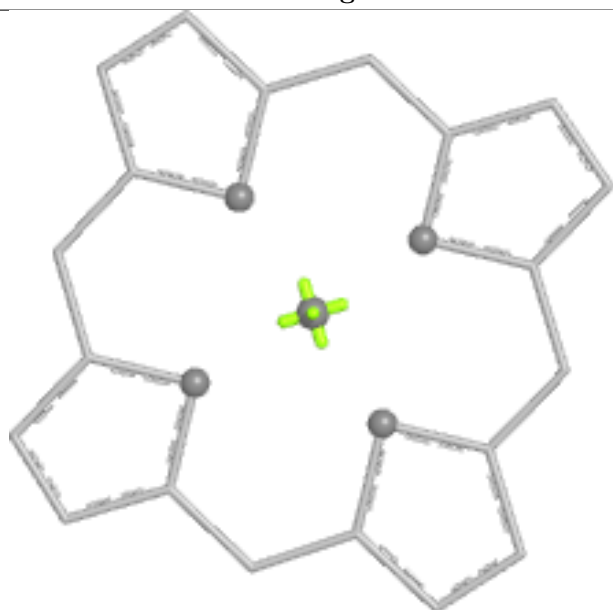
Ligand CLA Q 5223



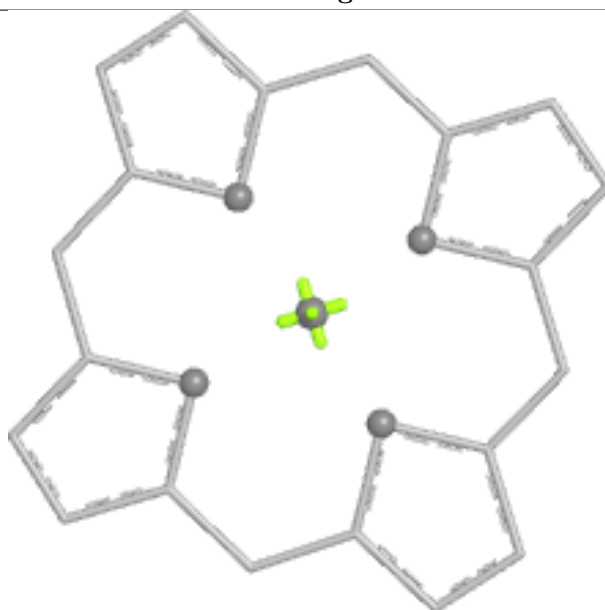
Bond lengths



Bond angles

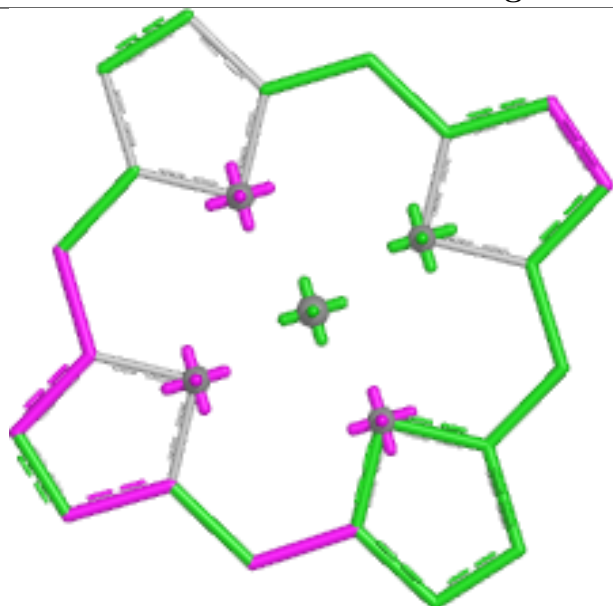


Torsions

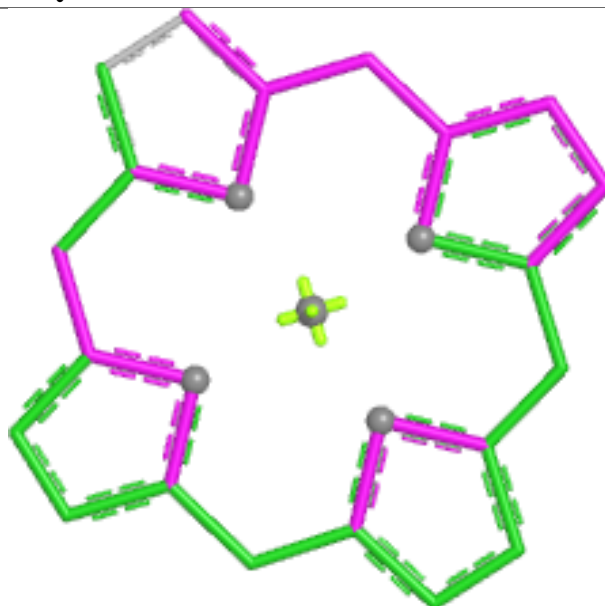


Rings

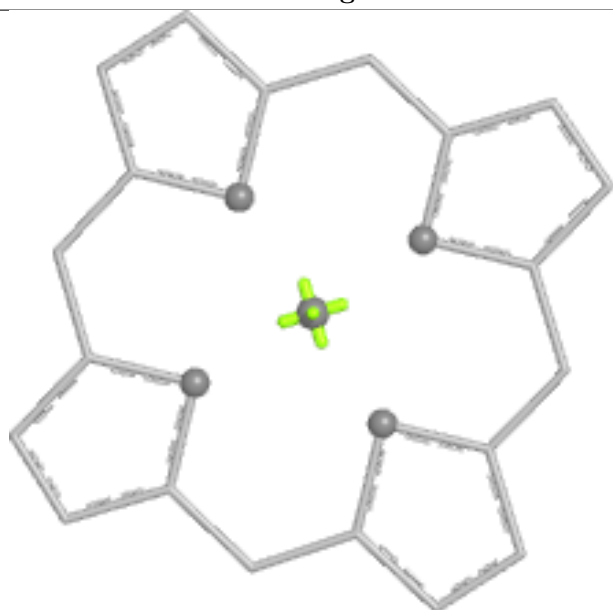
Ligand CLA Q 5210



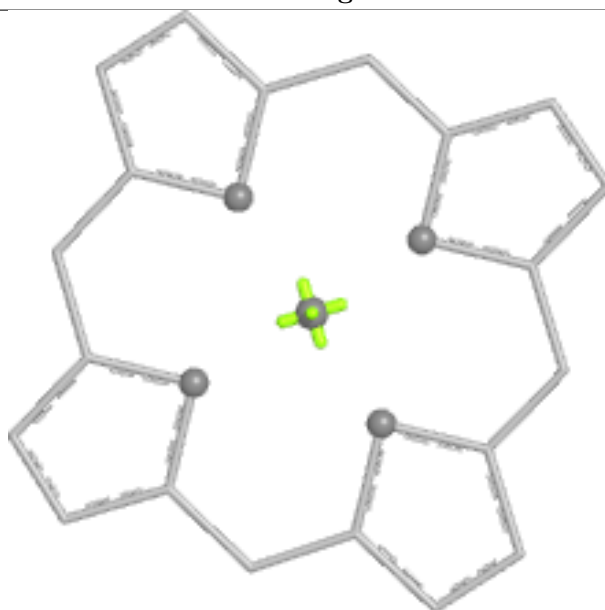
Bond lengths



Bond angles

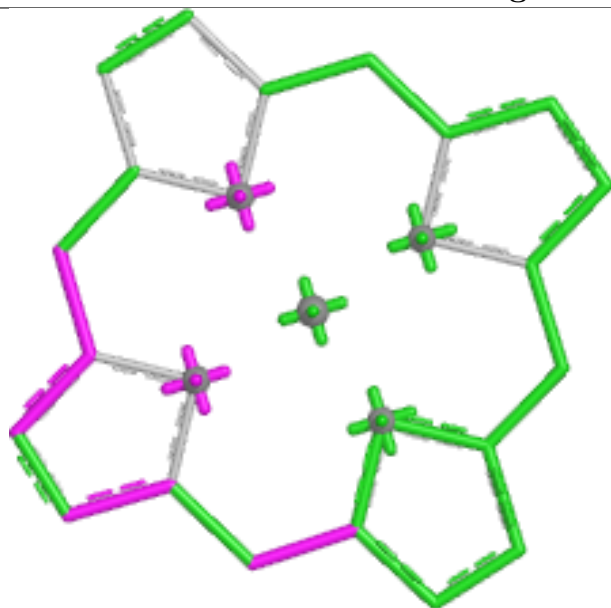


Torsions

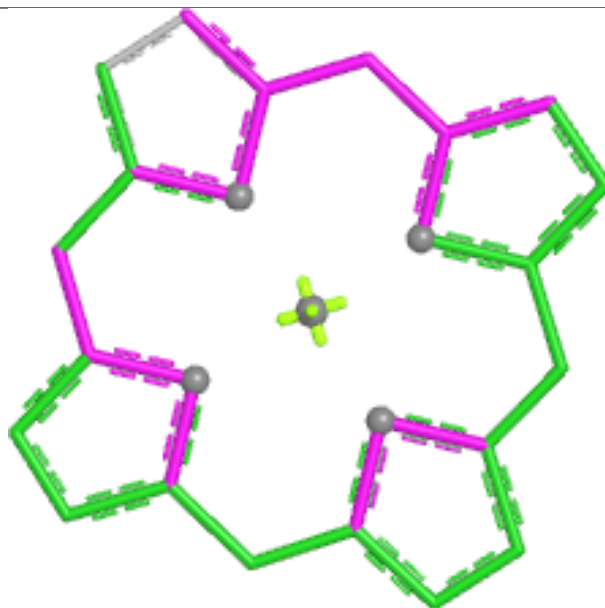


Rings

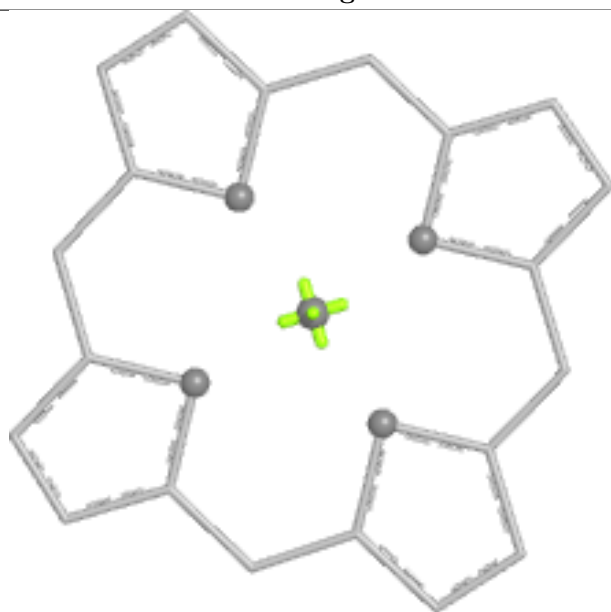
Ligand CLA 8 8007



Bond lengths



Bond angles

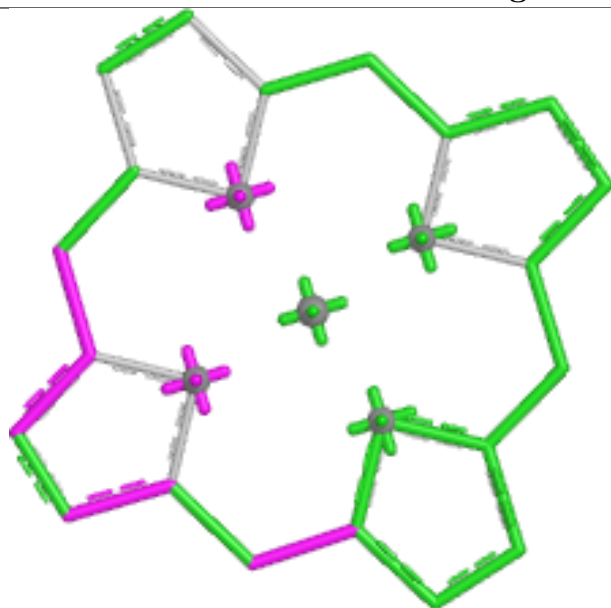


Torsions

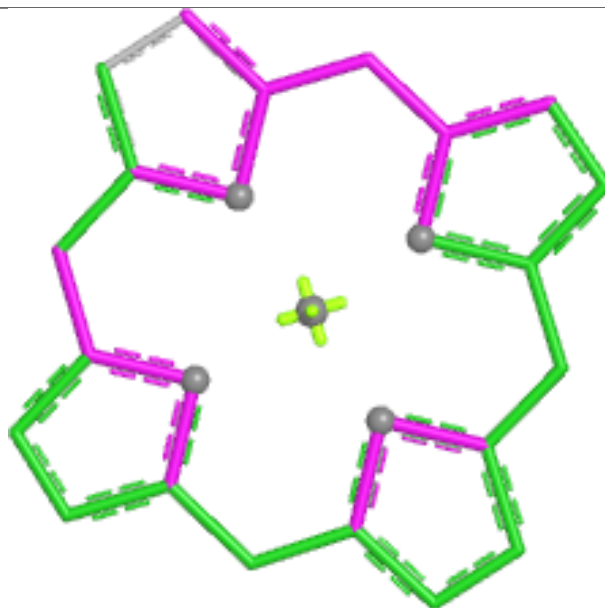


Rings

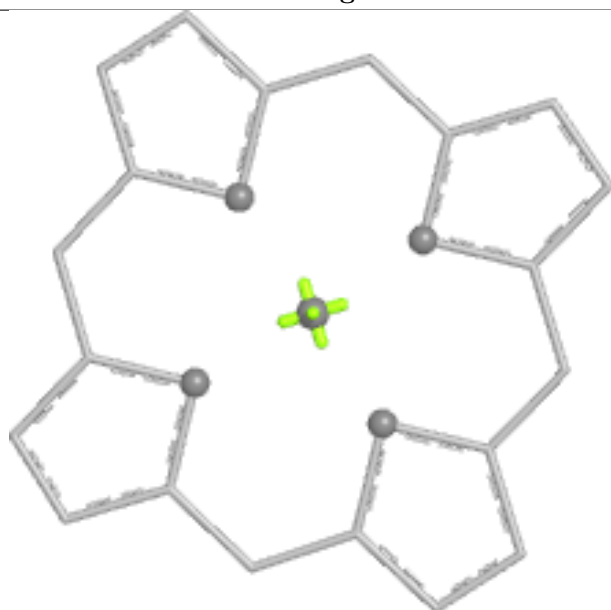
Ligand CLA 7 1016



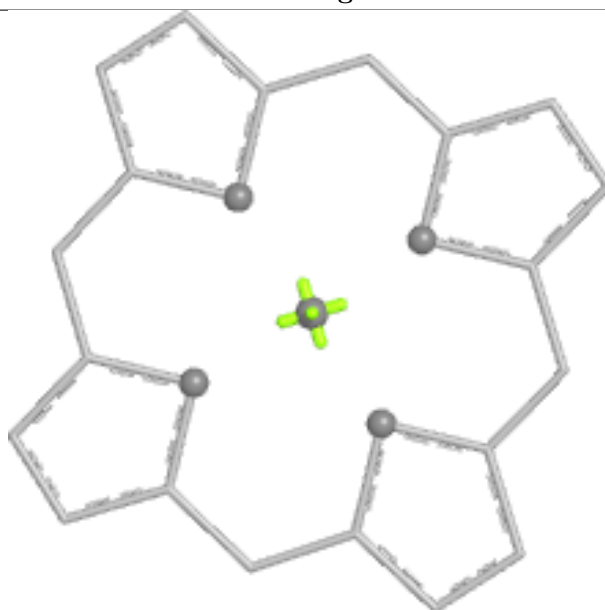
Bond lengths



Bond angles

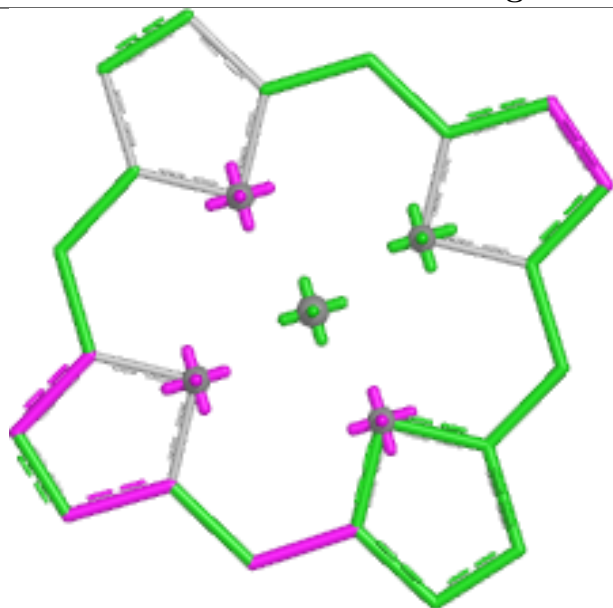


Torsions

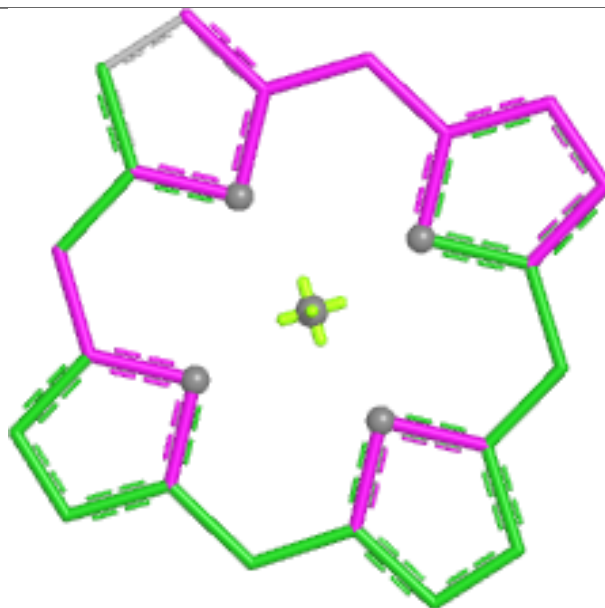


Rings

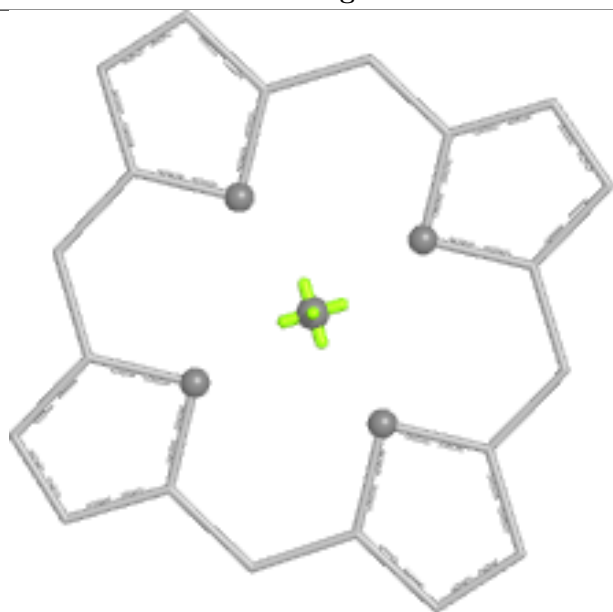
Ligand CLA P 5012



Bond lengths



Bond angles

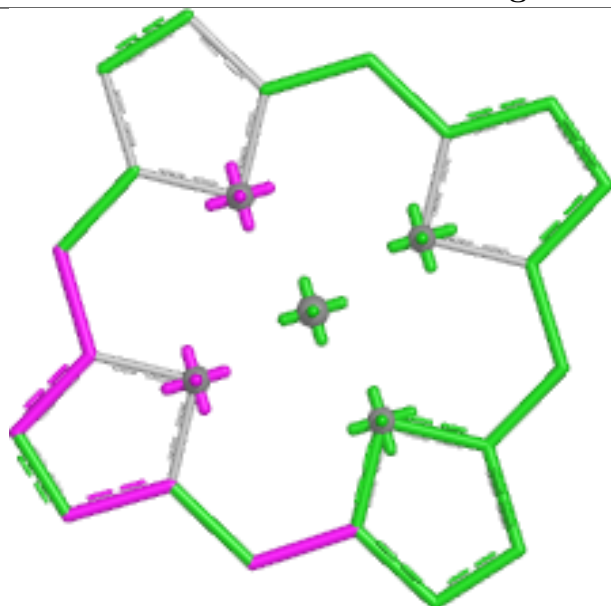


Torsions

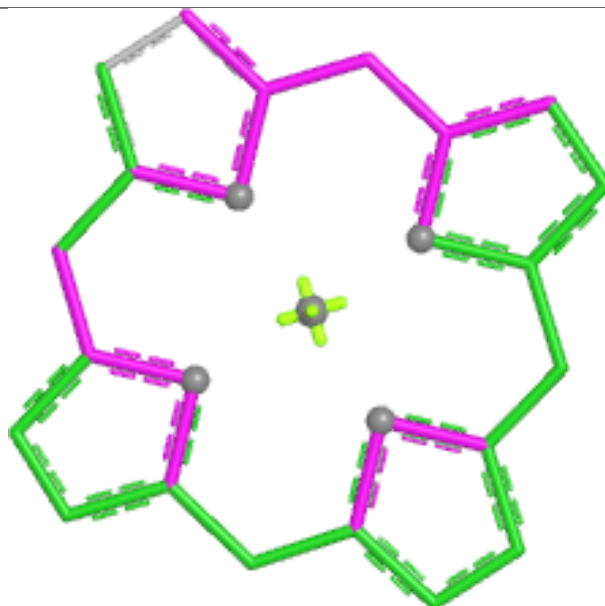


Rings

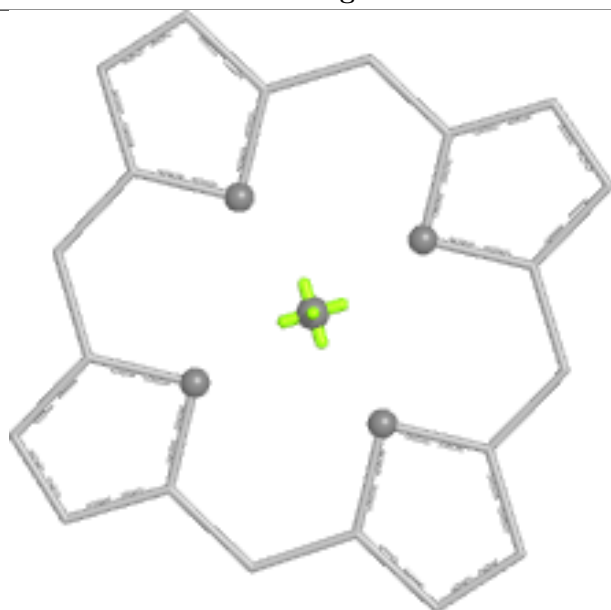
Ligand CLA 8 1021



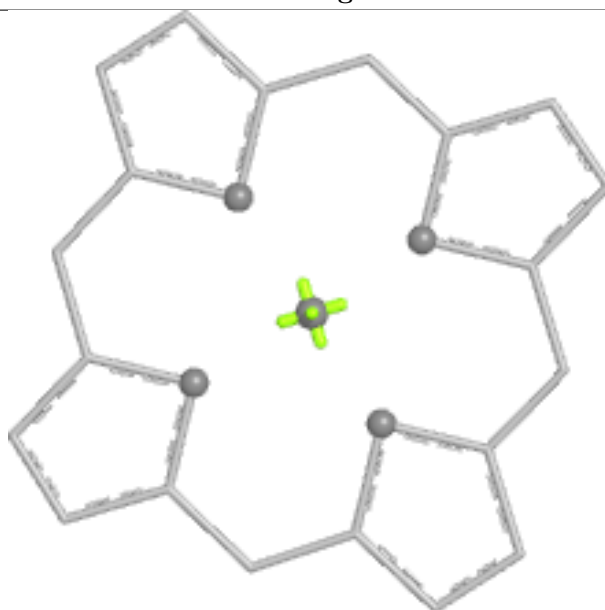
Bond lengths



Bond angles

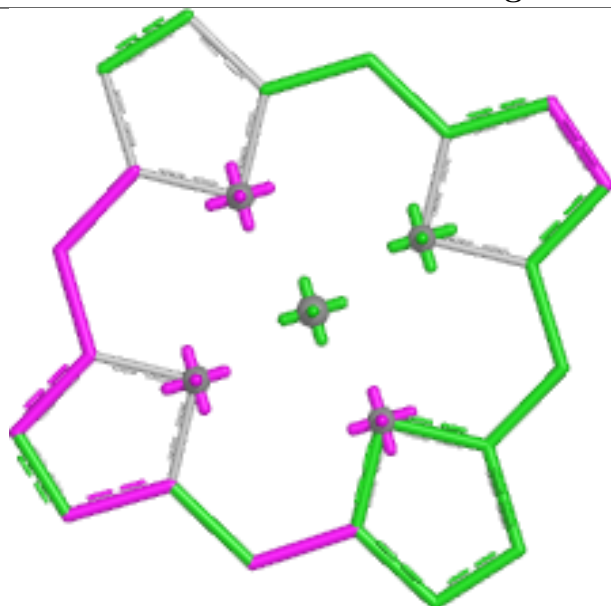


Torsions

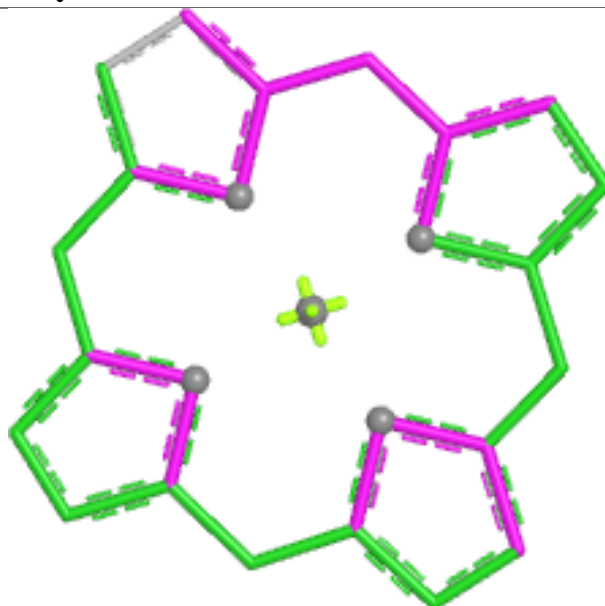


Rings

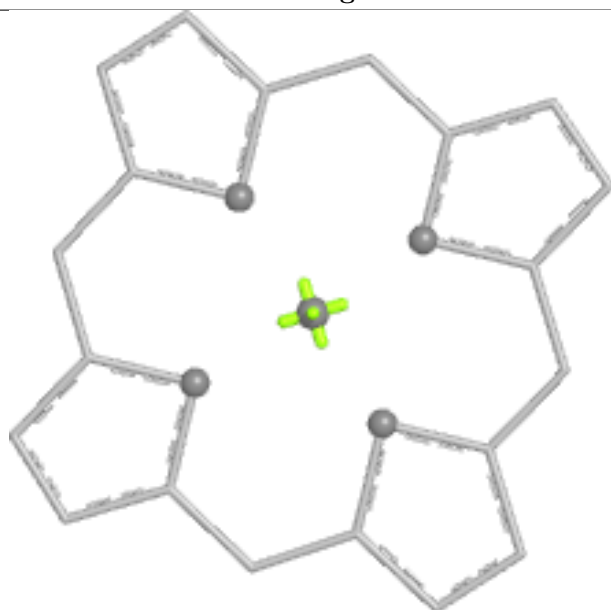
Ligand CLA Q 5231



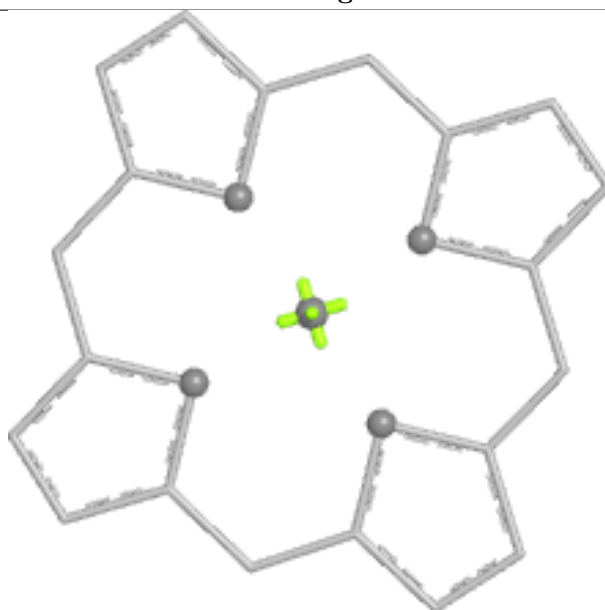
Bond lengths



Bond angles

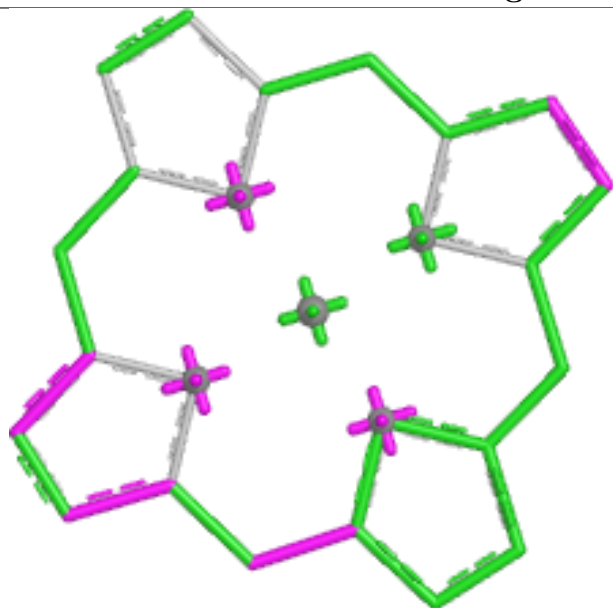


Torsions

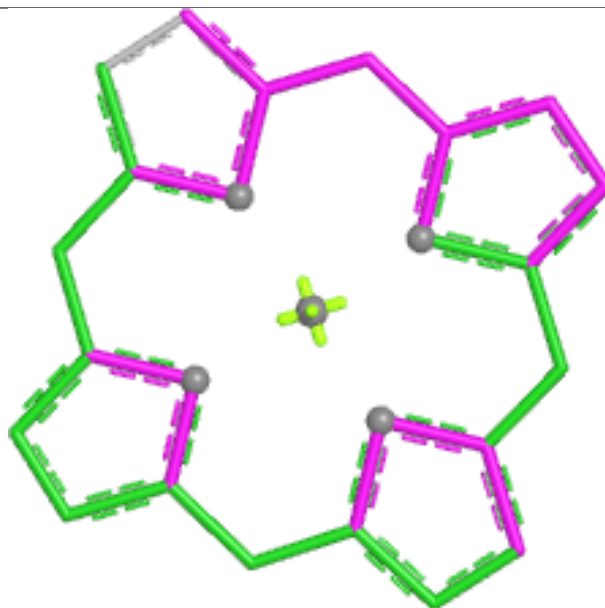


Rings

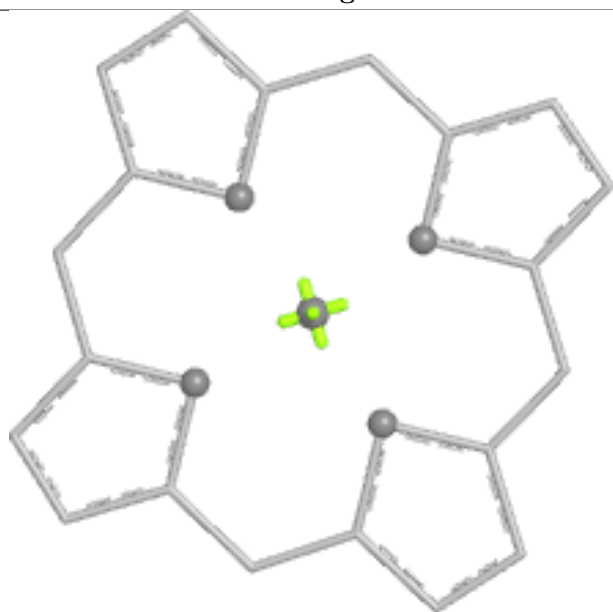
Ligand CLA B 1201



Bond lengths



Bond angles

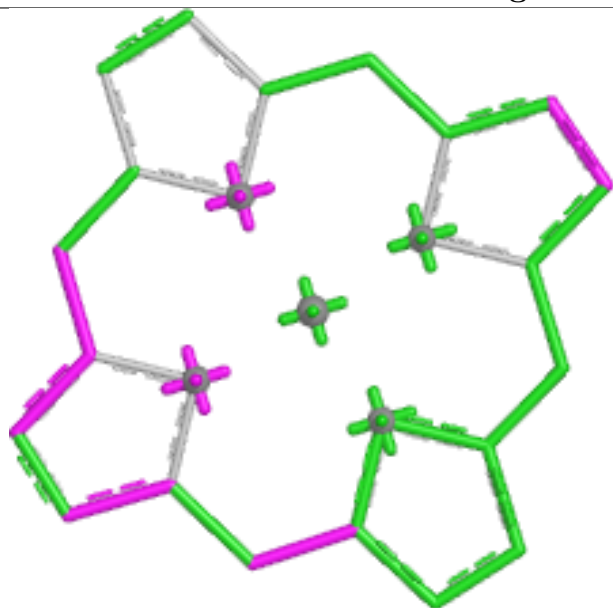


Torsions

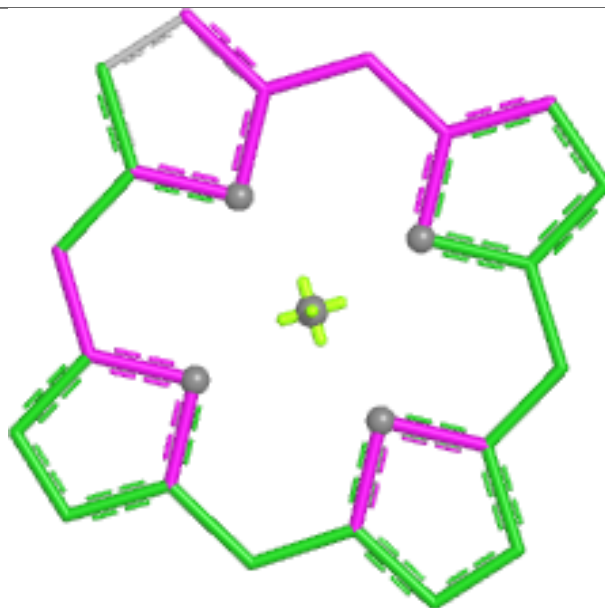


Rings

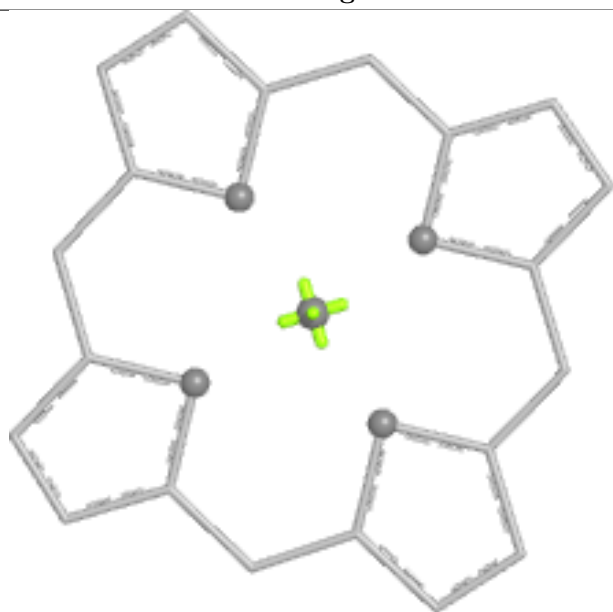
Ligand CLA 7 1015



Bond lengths



Bond angles

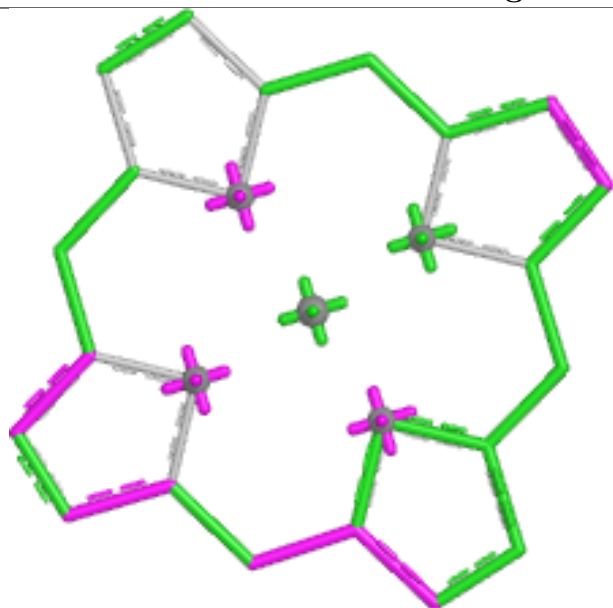


Torsions

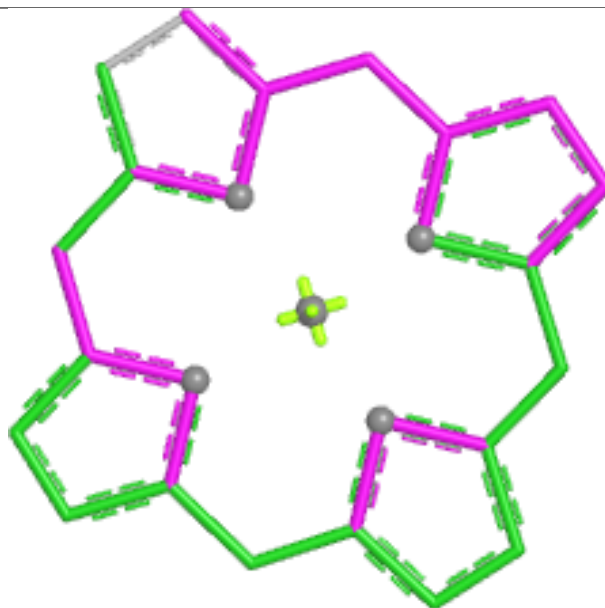


Rings

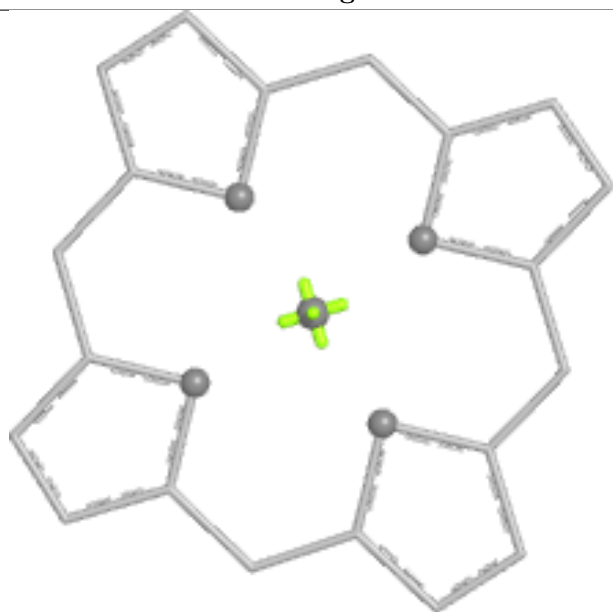
Ligand CLA B 1224



Bond lengths



Bond angles

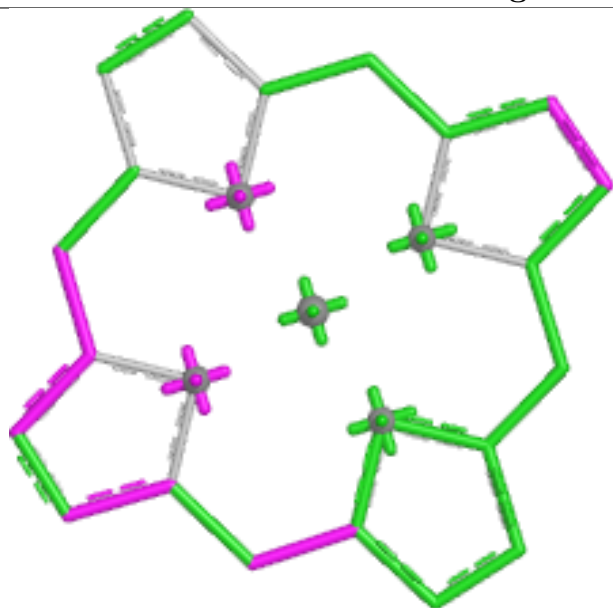


Torsions

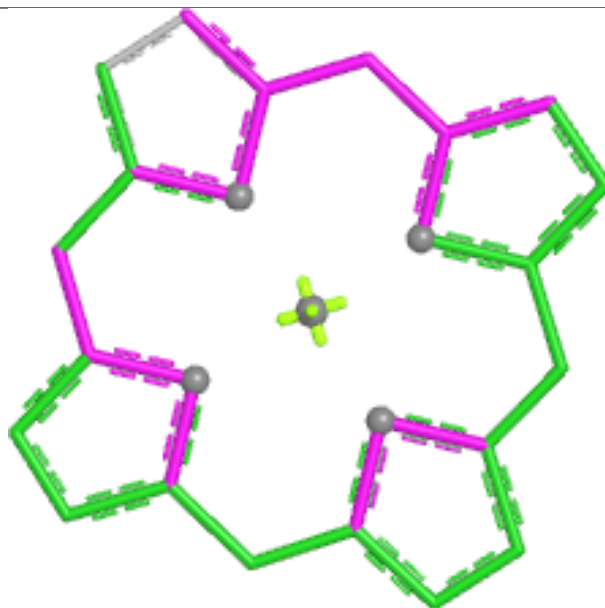


Rings

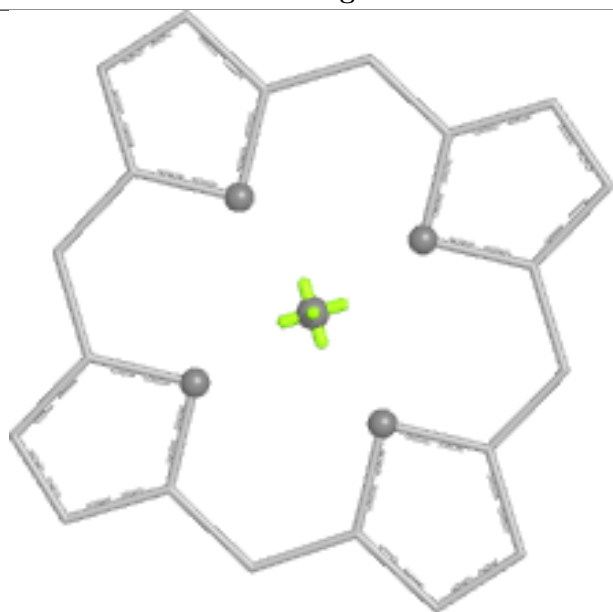
Ligand CLA 0 1031



Bond lengths



Bond angles

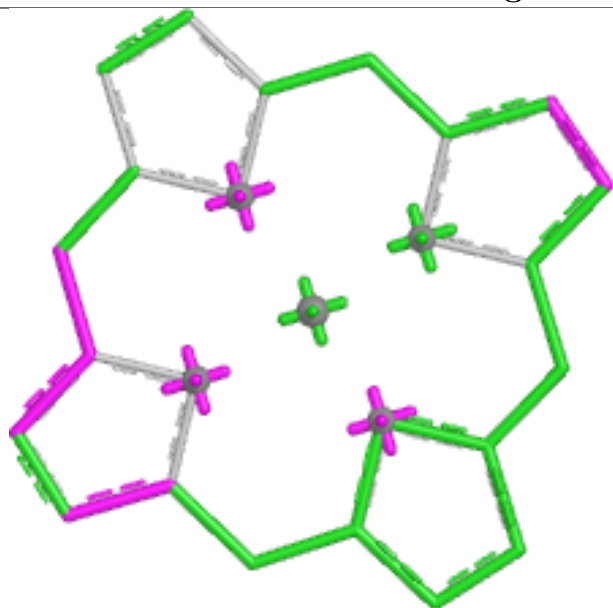


Torsions

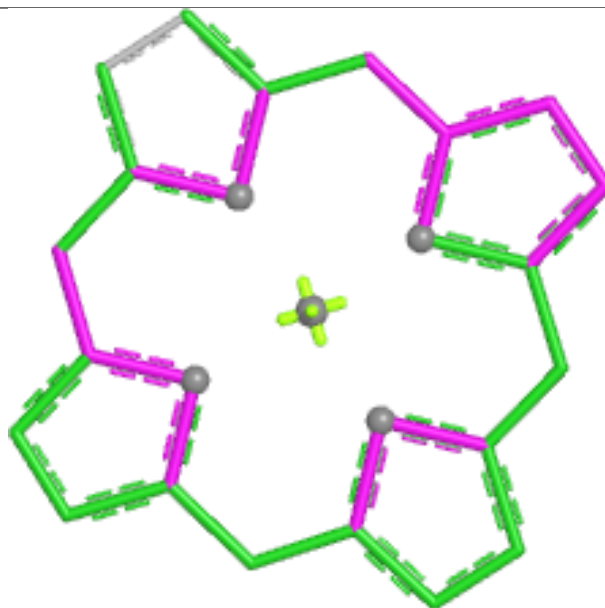


Rings

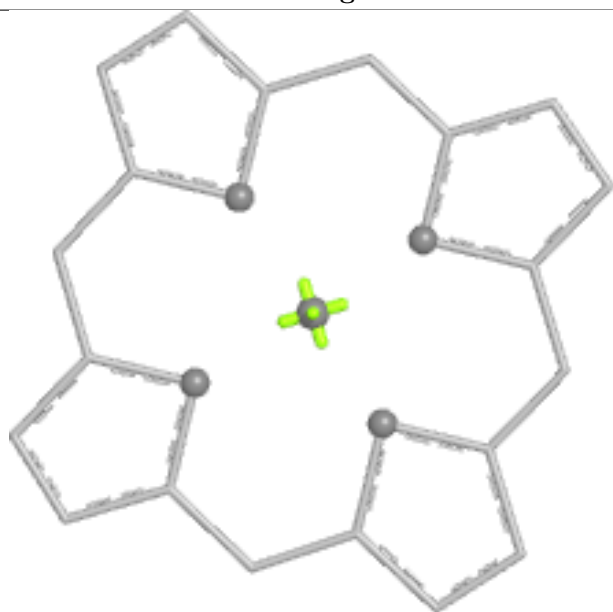
Ligand CLA A 1132



Bond lengths



Bond angles

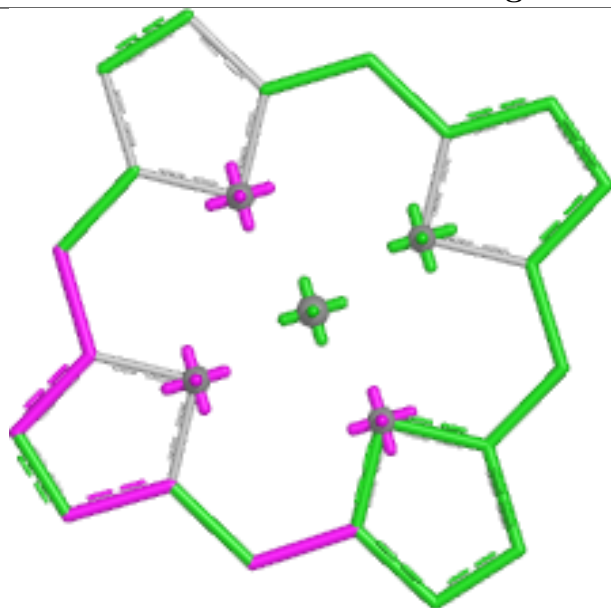


Torsions

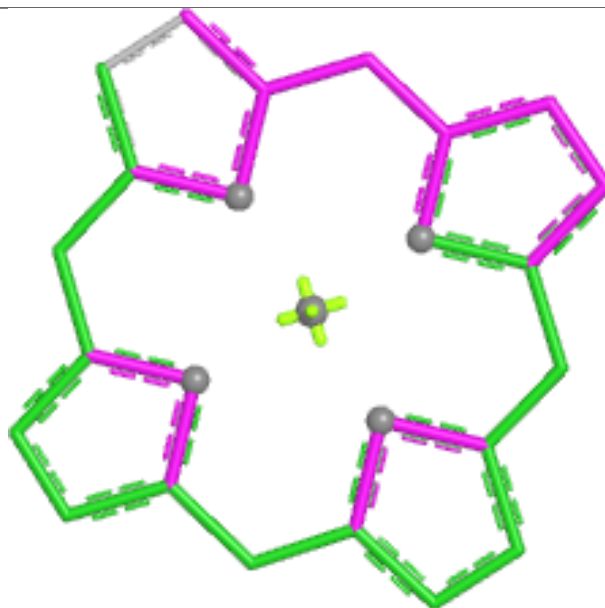


Rings

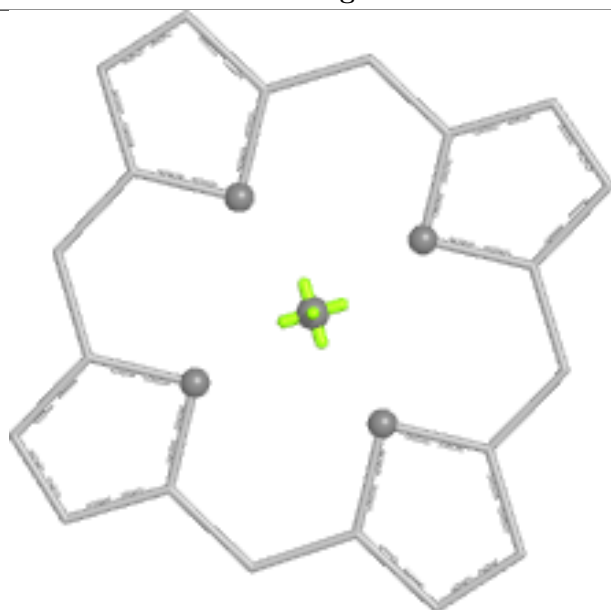
Ligand CLA B 1236



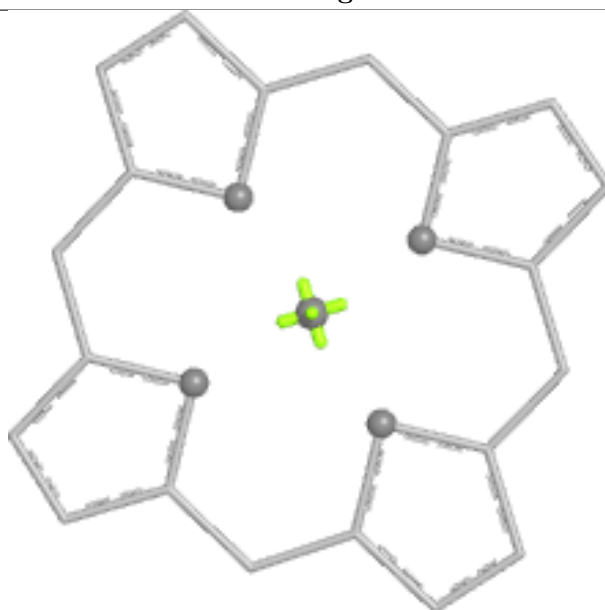
Bond lengths



Bond angles

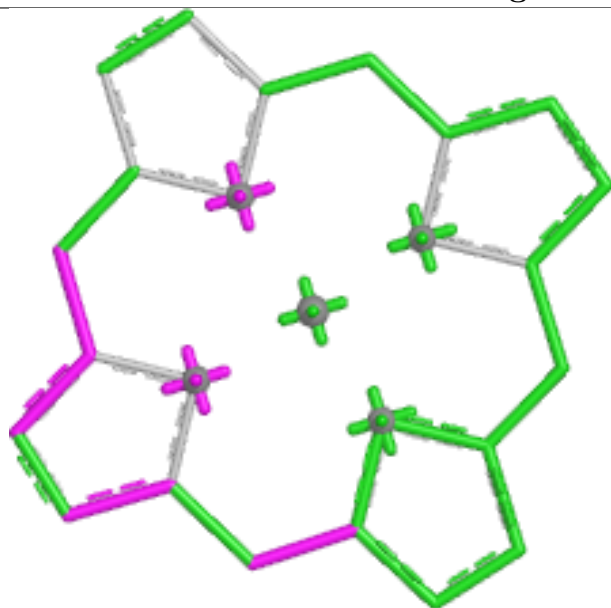


Torsions



Rings

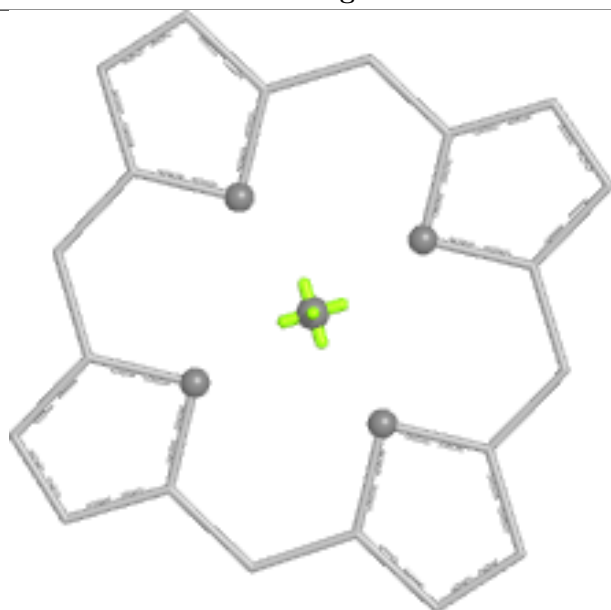
Ligand CLA 2 1031



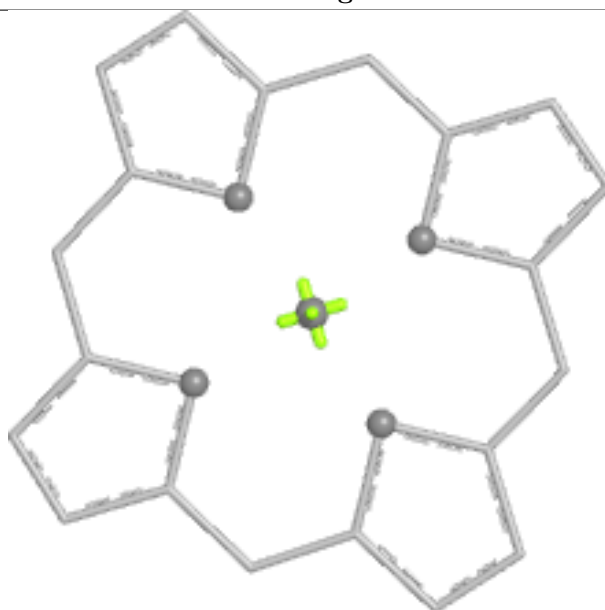
Bond lengths



Bond angles

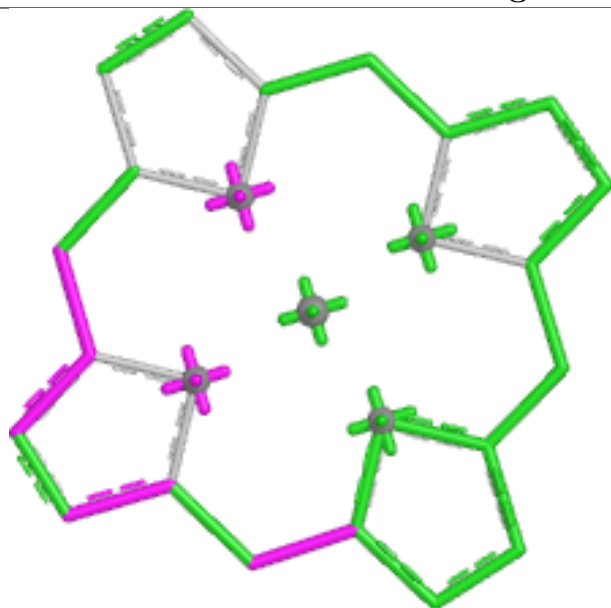


Torsions

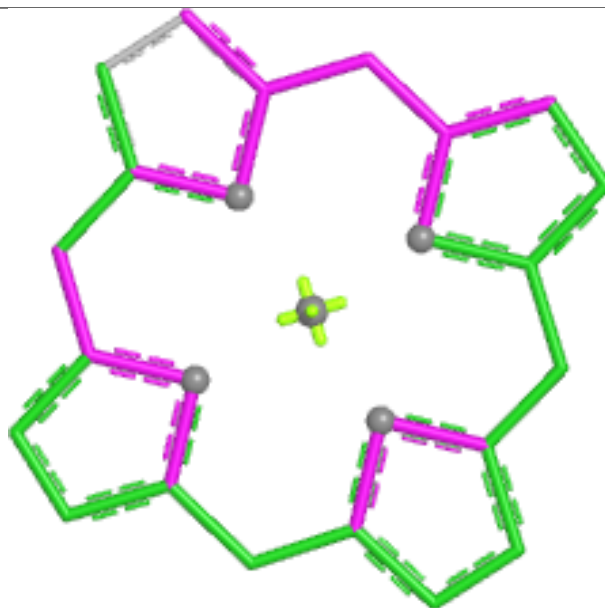


Rings

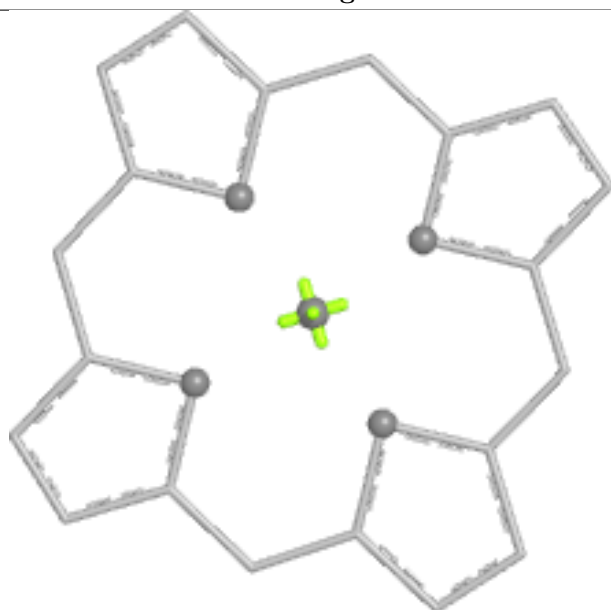
Ligand CLA 2 1021



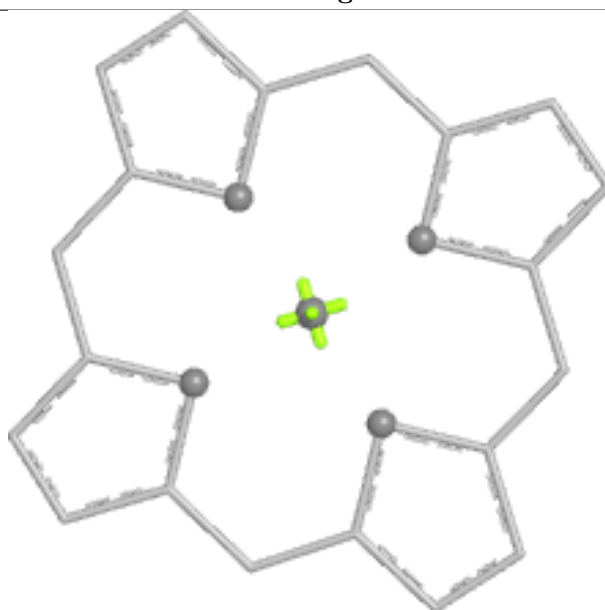
Bond lengths



Bond angles

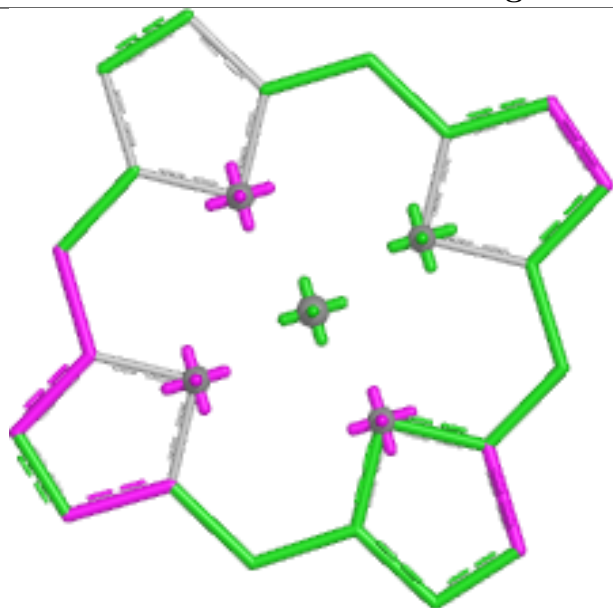


Torsions

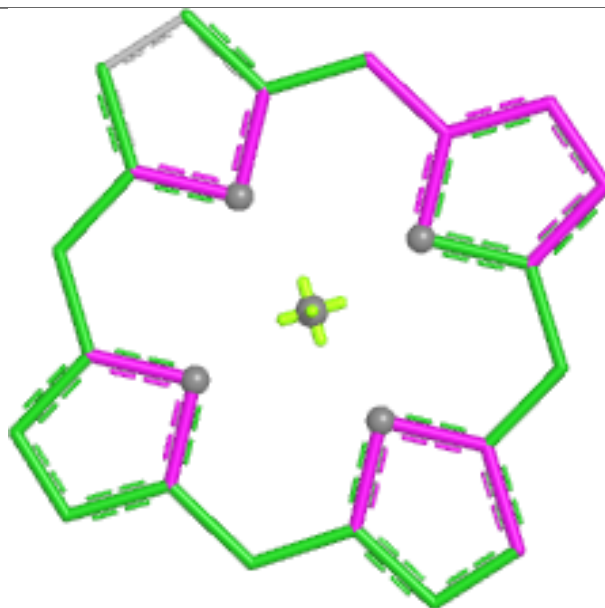


Rings

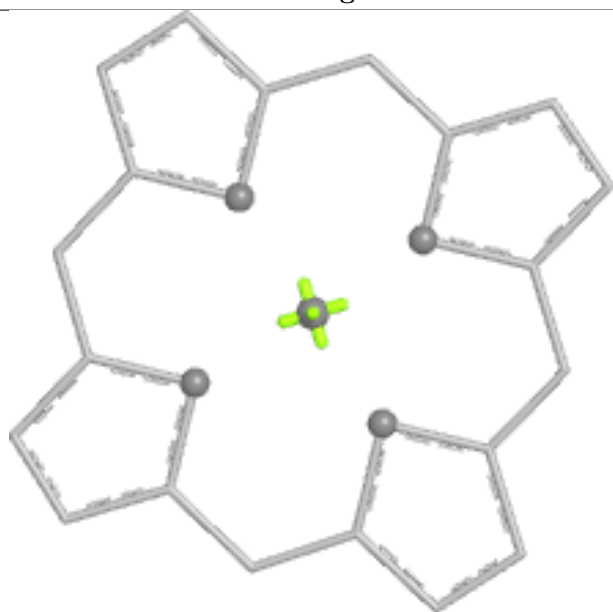
Ligand CLA B 1237



Bond lengths



Bond angles

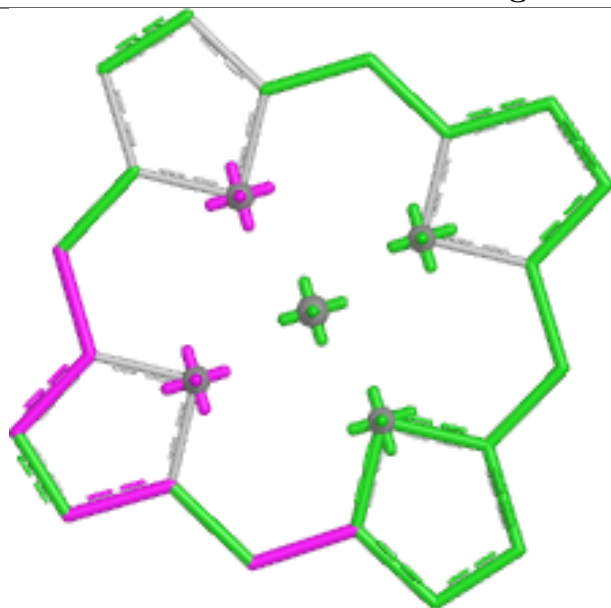


Torsions

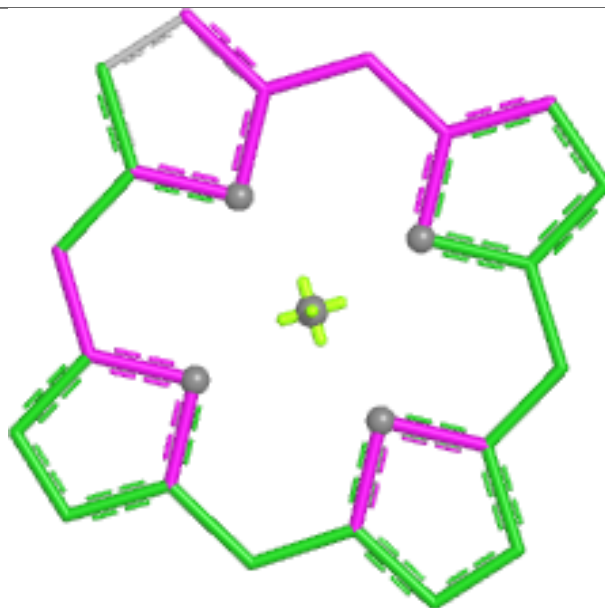


Rings

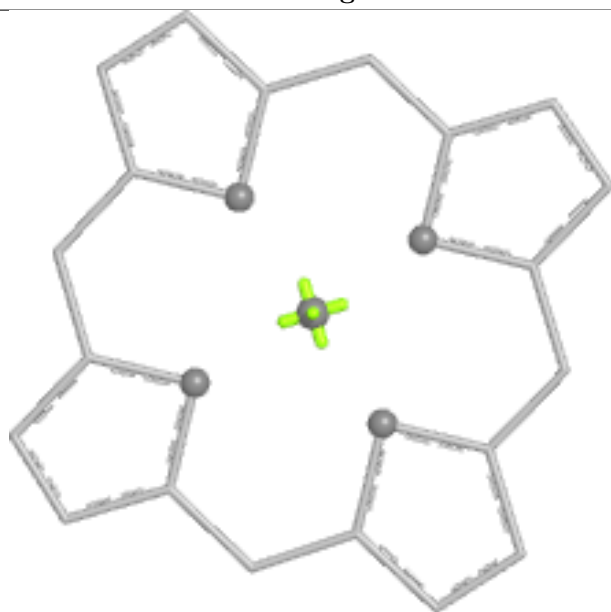
Ligand CLA 3 1025



Bond lengths



Bond angles

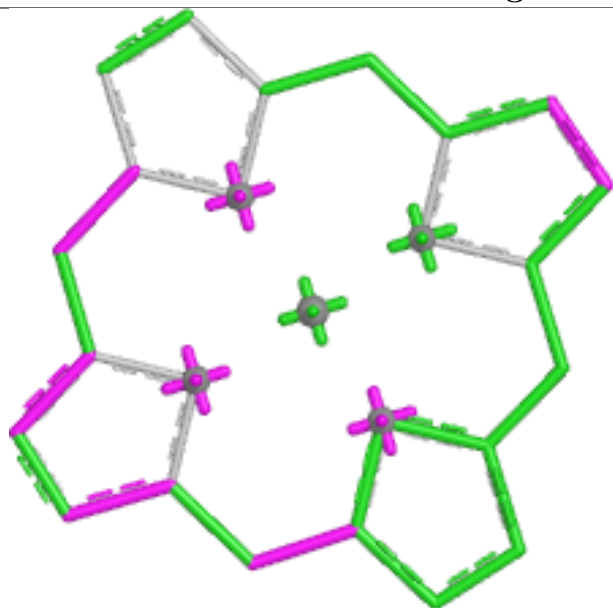


Torsions

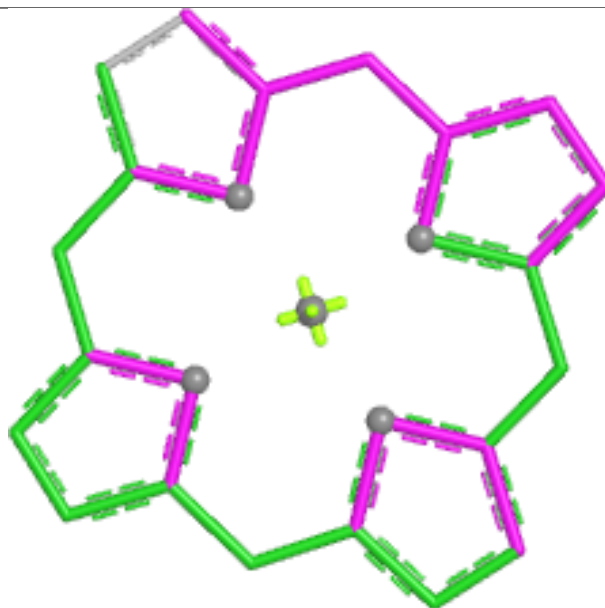


Rings

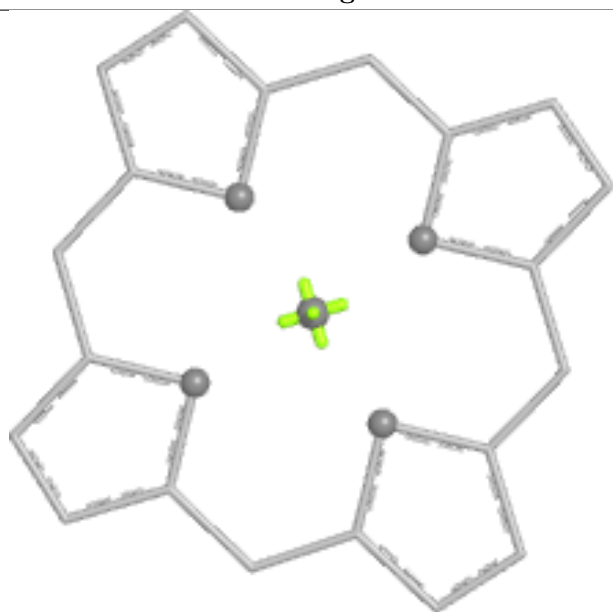
Ligand CLA P 5133



Bond lengths



Bond angles

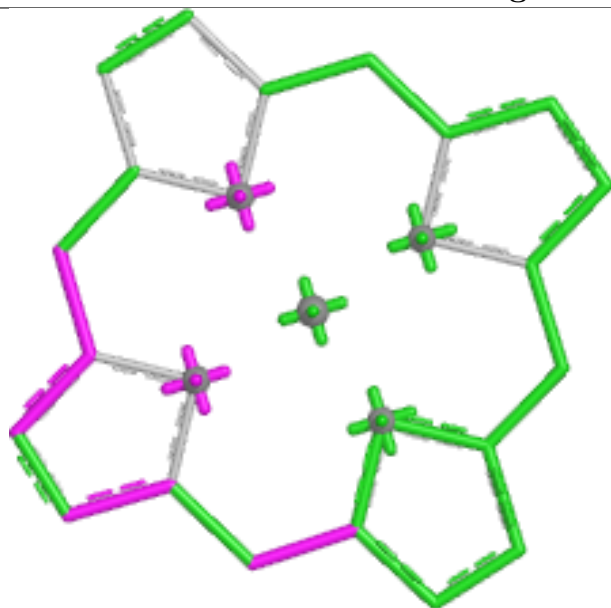


Torsions

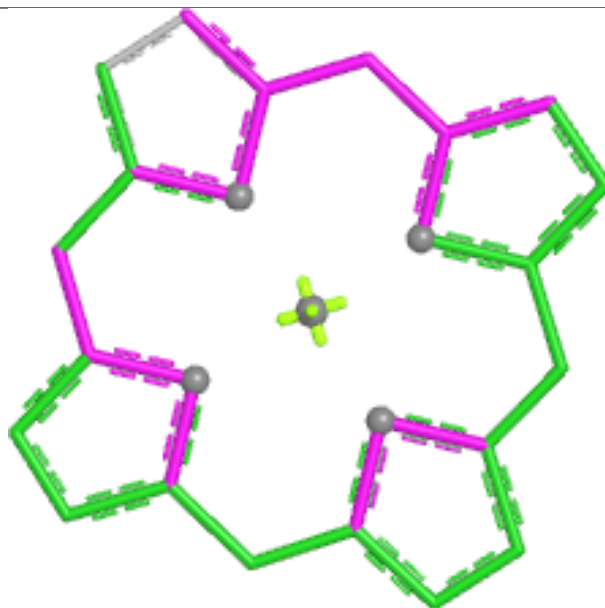


Rings

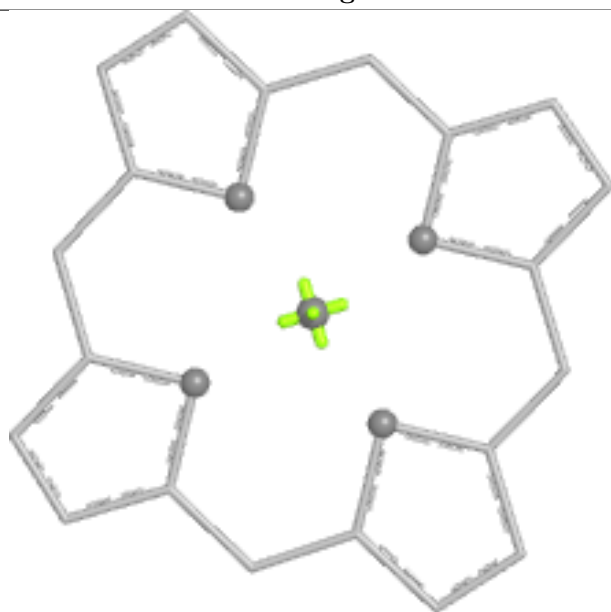
Ligand CLA 0 1011



Bond lengths



Bond angles

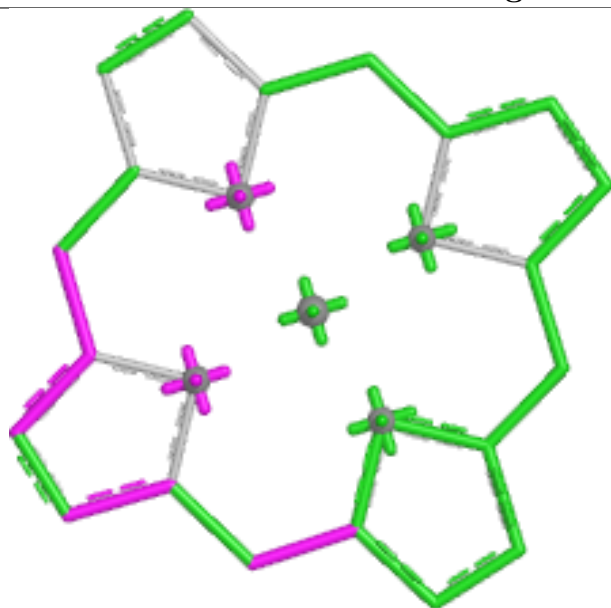


Torsions

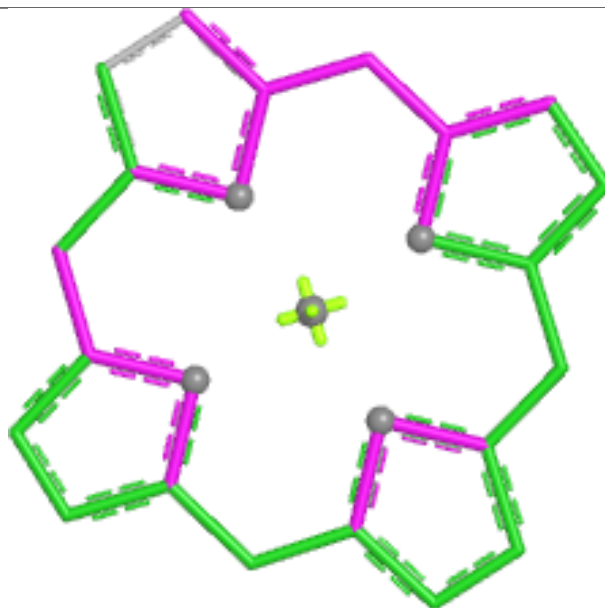


Rings

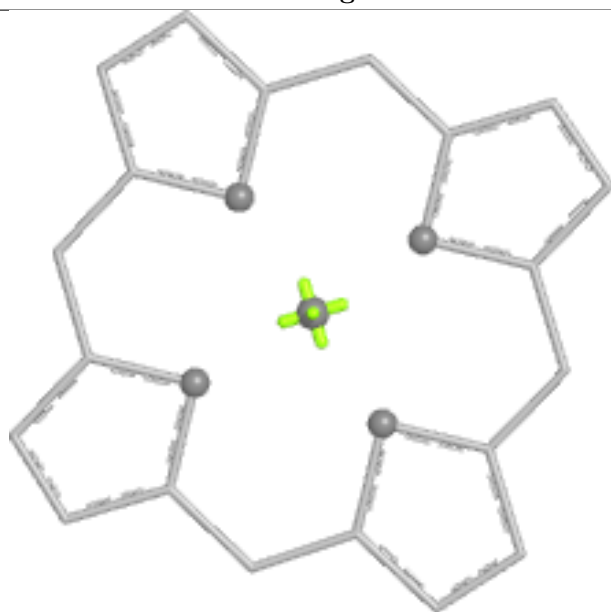
Ligand CLA B 1240



Bond lengths



Bond angles

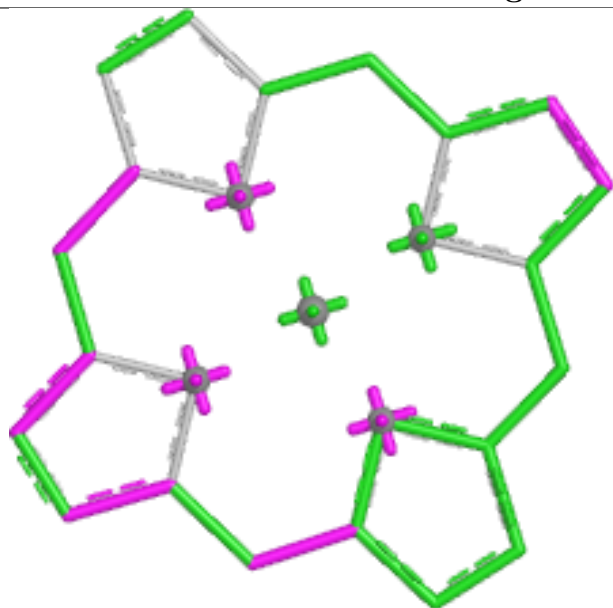


Torsions

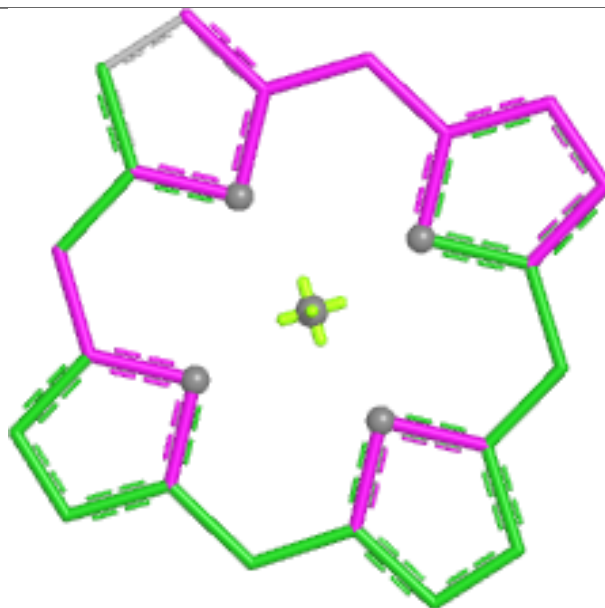


Rings

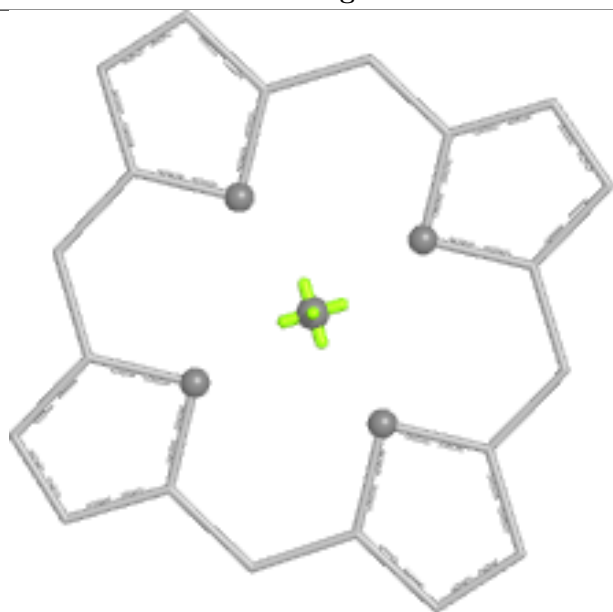
Ligand CLA B 1223



Bond lengths



Bond angles

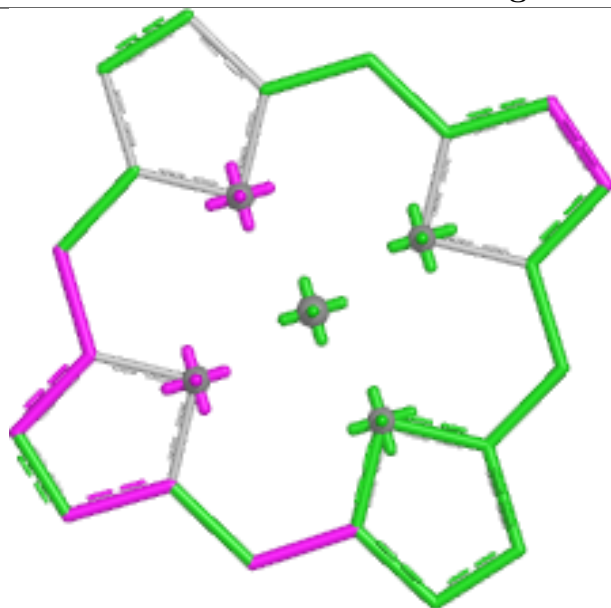


Torsions



Rings

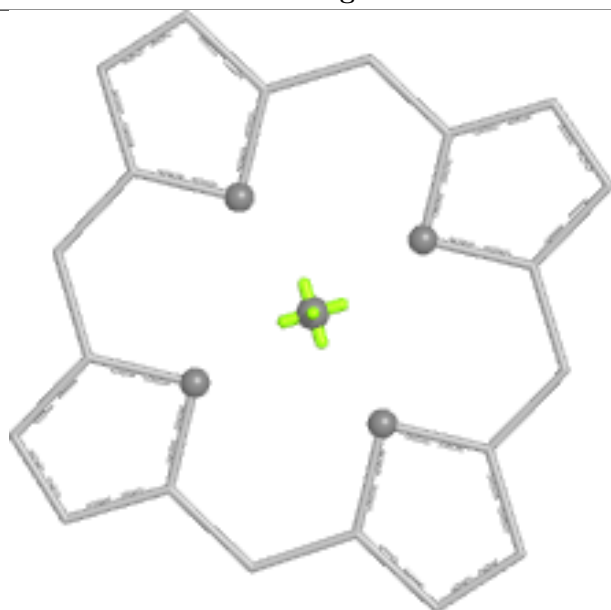
Ligand CLA 4 1031



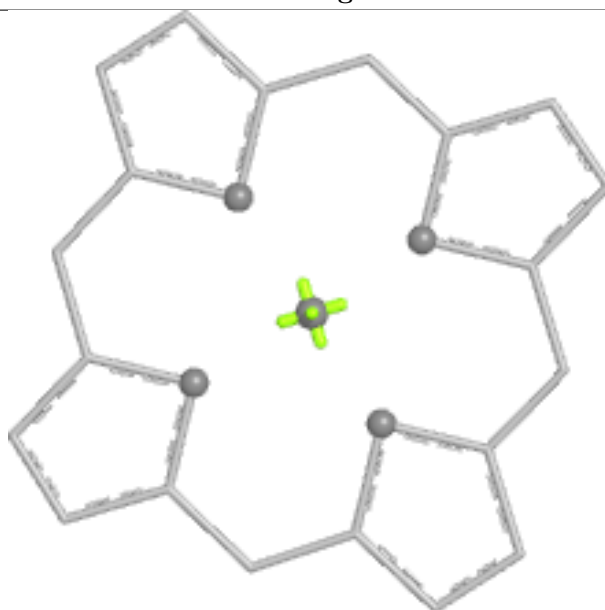
Bond lengths



Bond angles

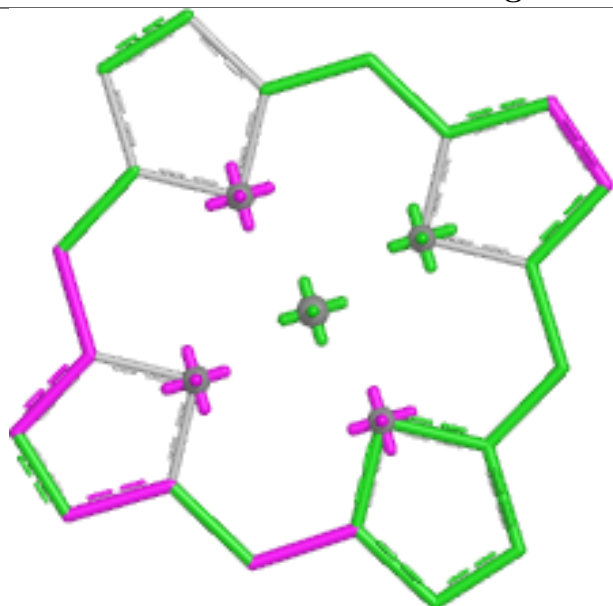


Torsions

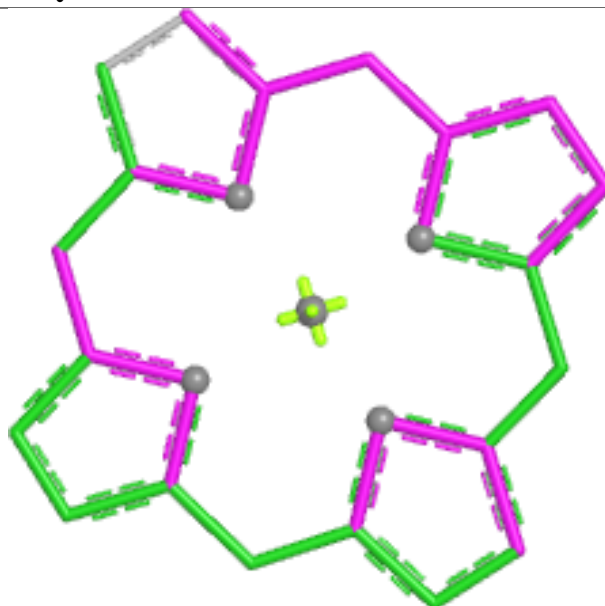


Rings

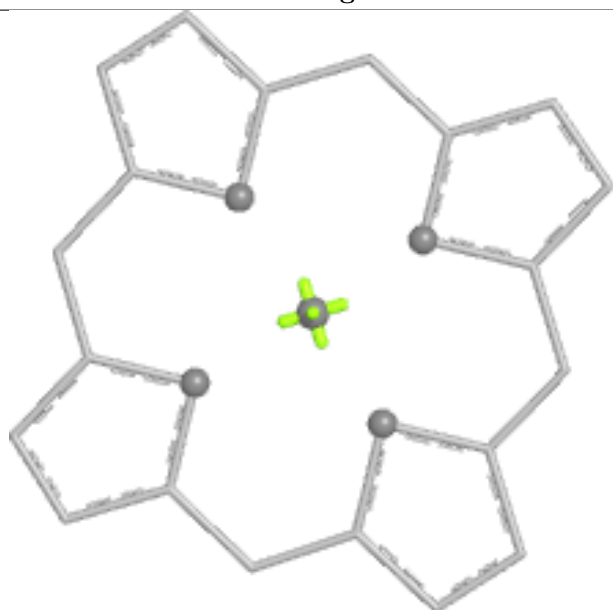
Ligand CLA Q 5228



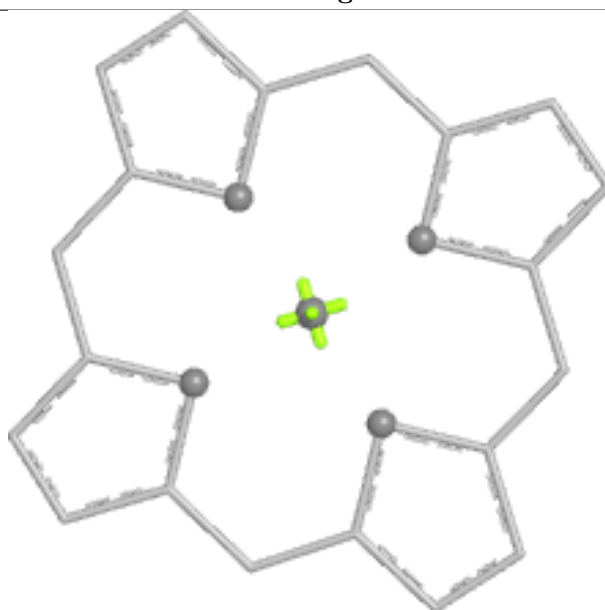
Bond lengths



Bond angles

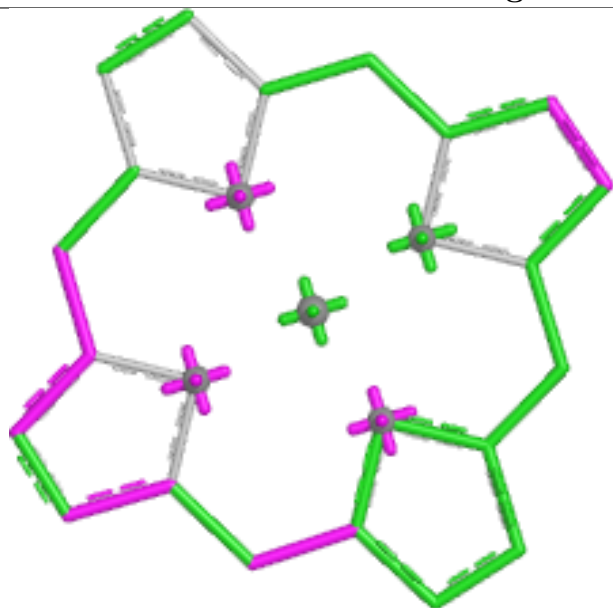


Torsions

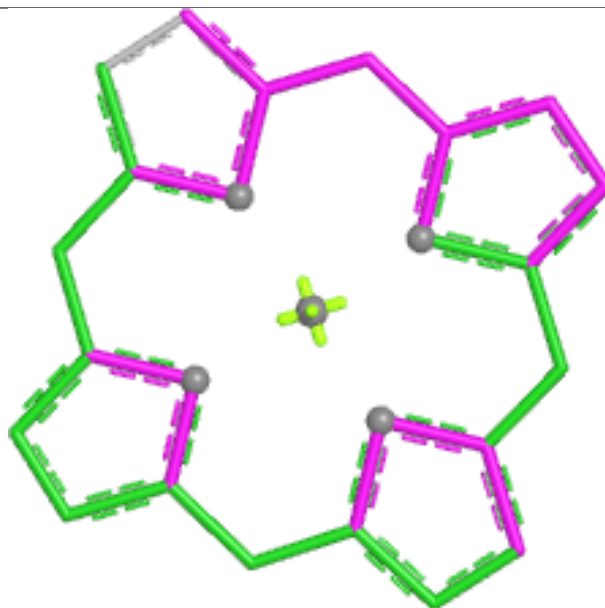


Rings

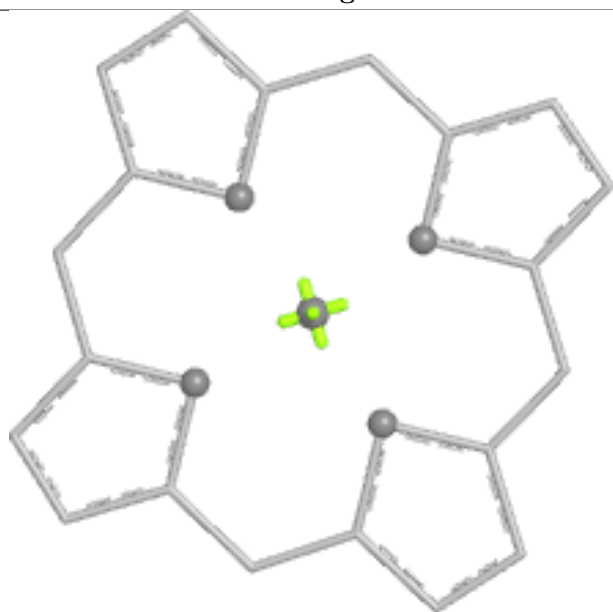
Ligand CLA P 5111



Bond lengths



Bond angles

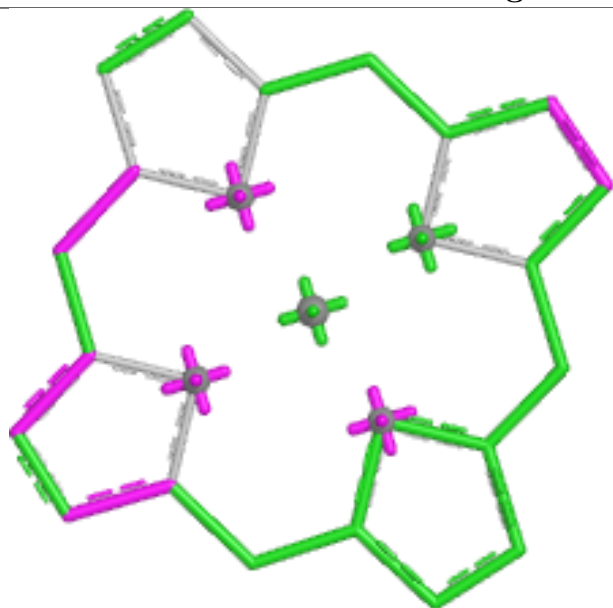


Torsions

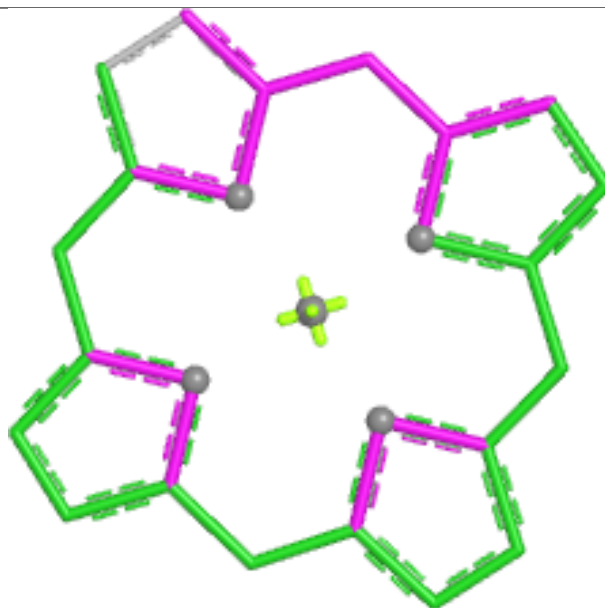


Rings

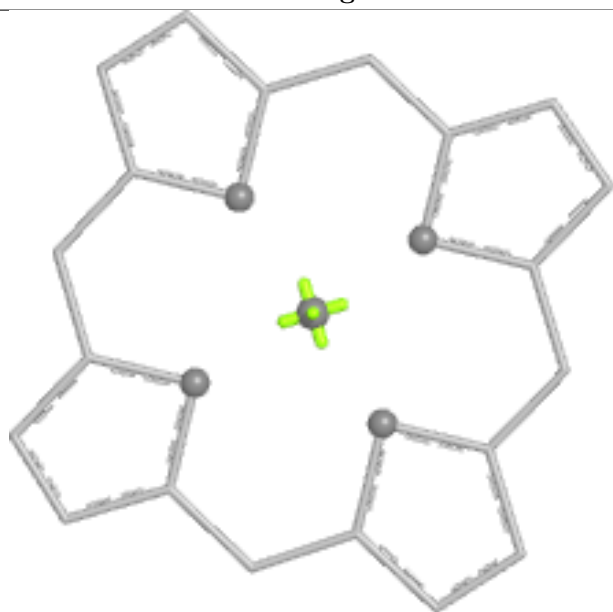
Ligand CLA P 5127



Bond lengths



Bond angles

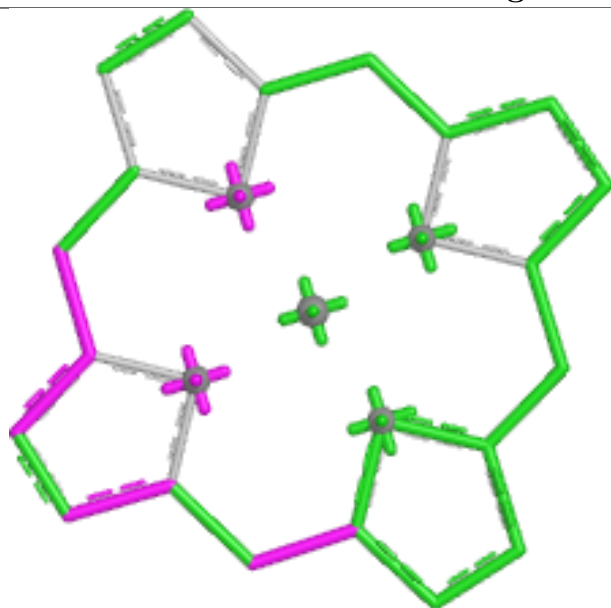


Torsions

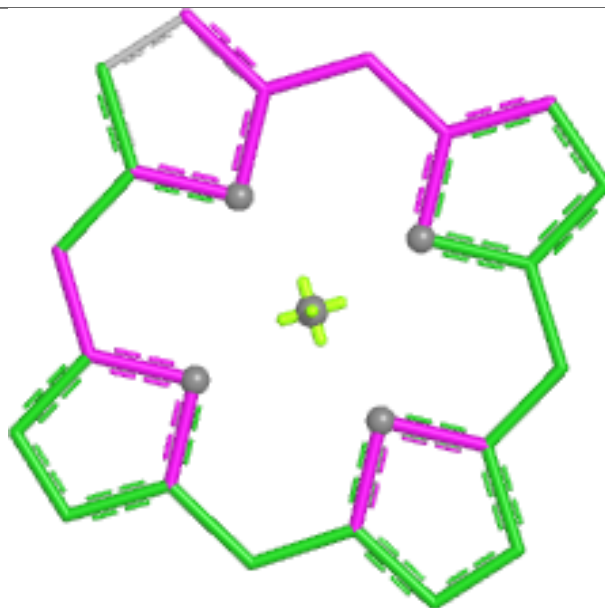


Rings

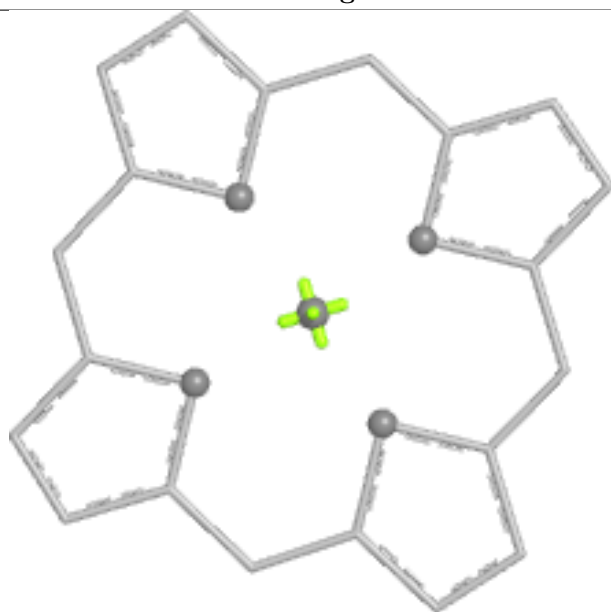
Ligand CLA F 4003



Bond lengths



Bond angles

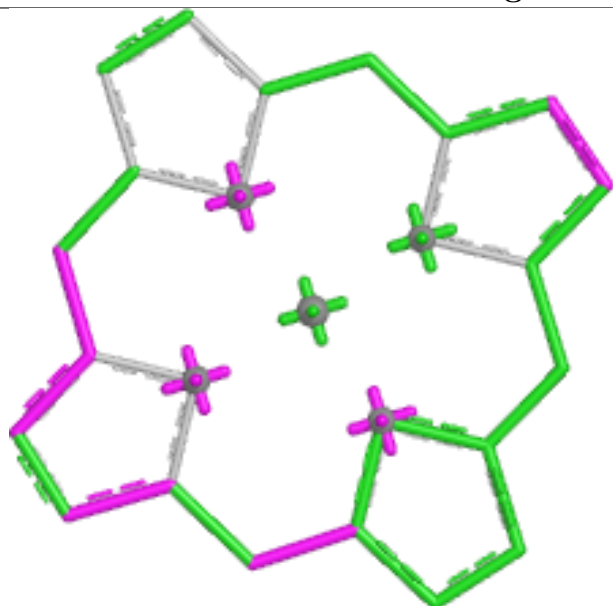


Torsions

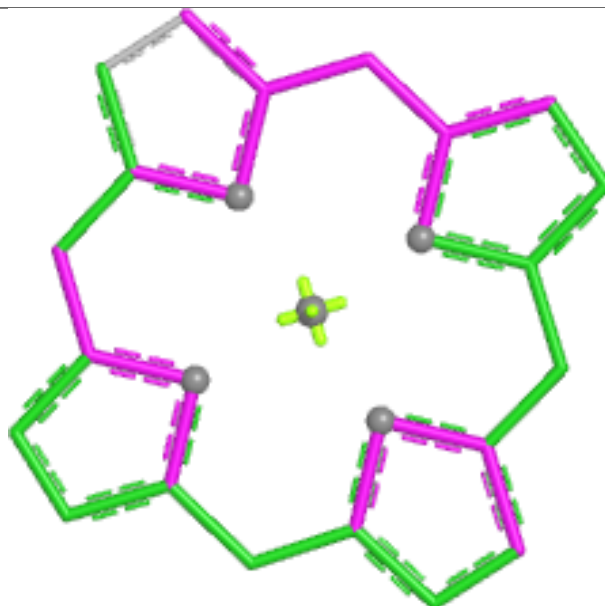


Rings

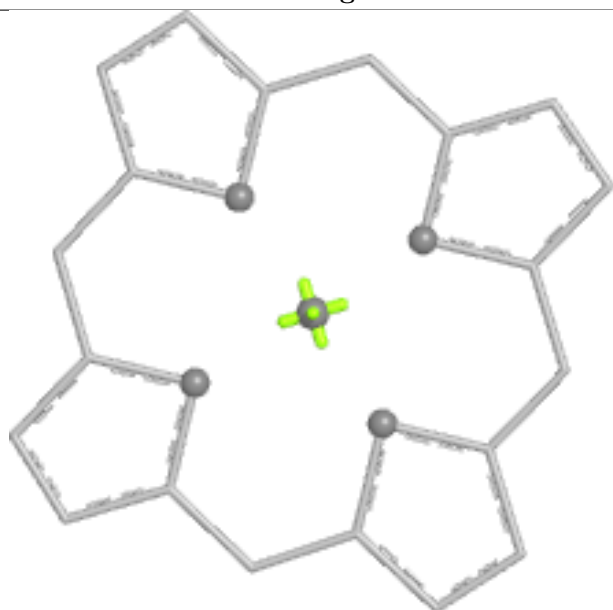
Ligand CLA A 1112



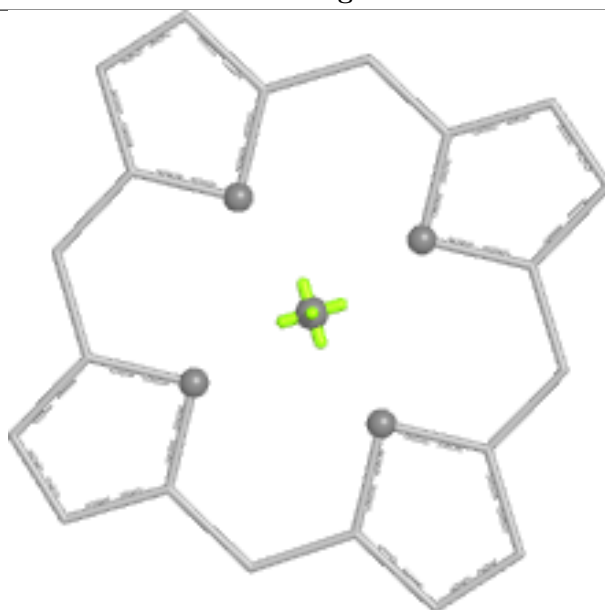
Bond lengths



Bond angles

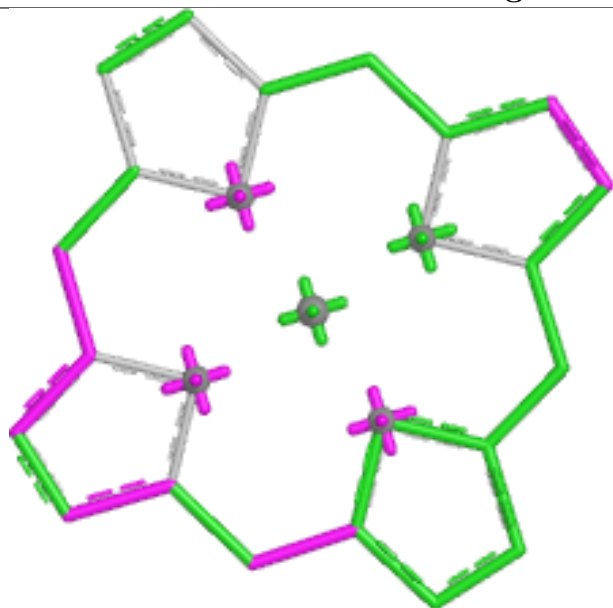


Torsions

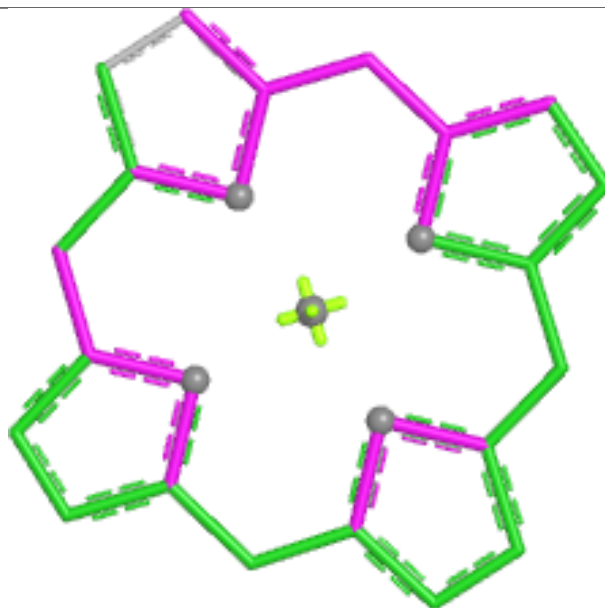


Rings

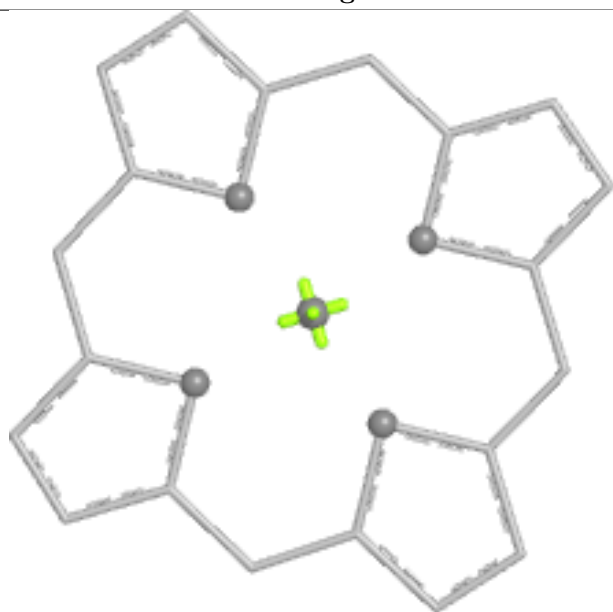
Ligand CLA B 1216



Bond lengths



Bond angles

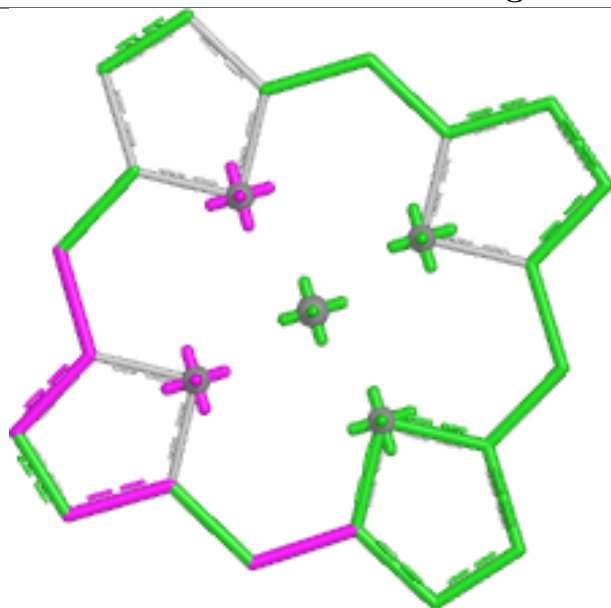


Torsions

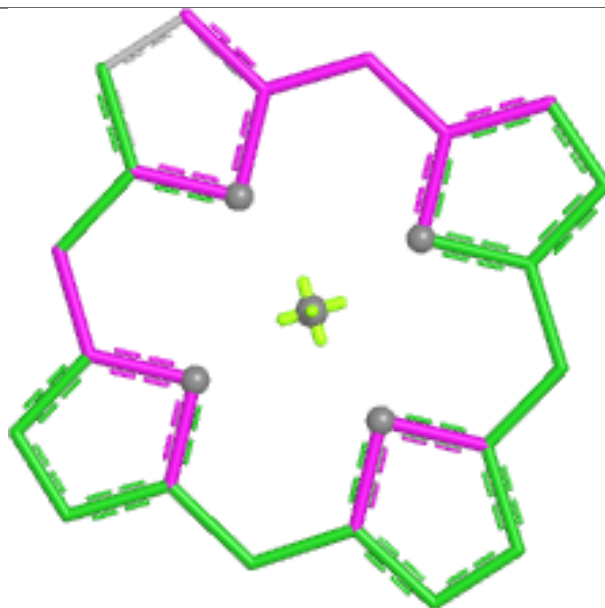


Rings

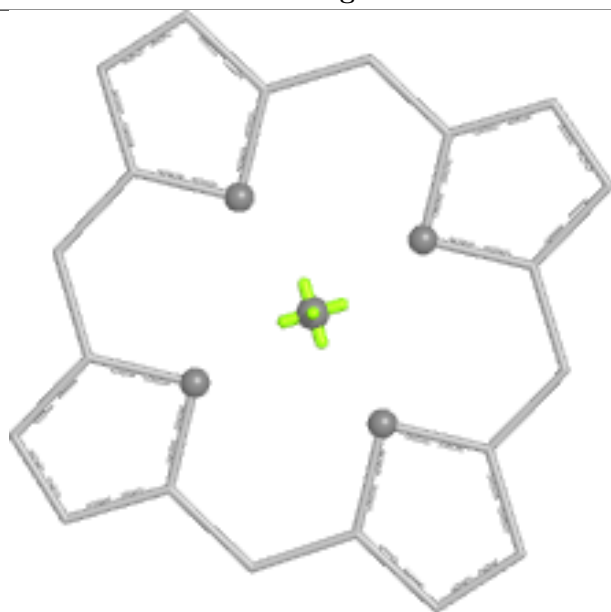
Ligand CLA P 8009



Bond lengths



Bond angles

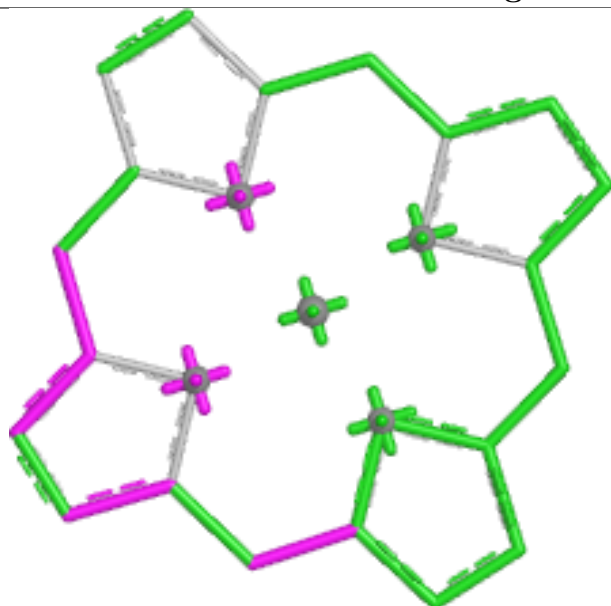


Torsions

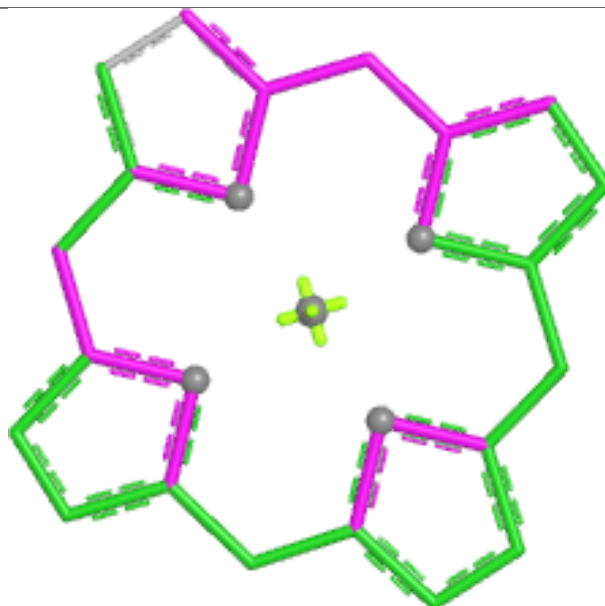


Rings

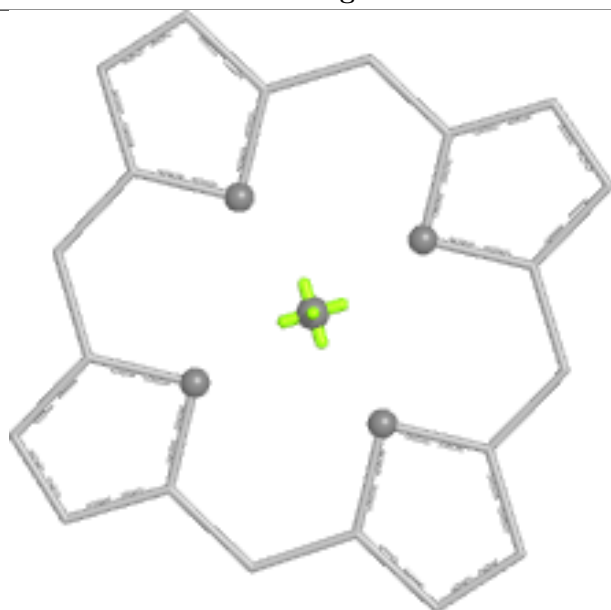
Ligand CLA V 5701



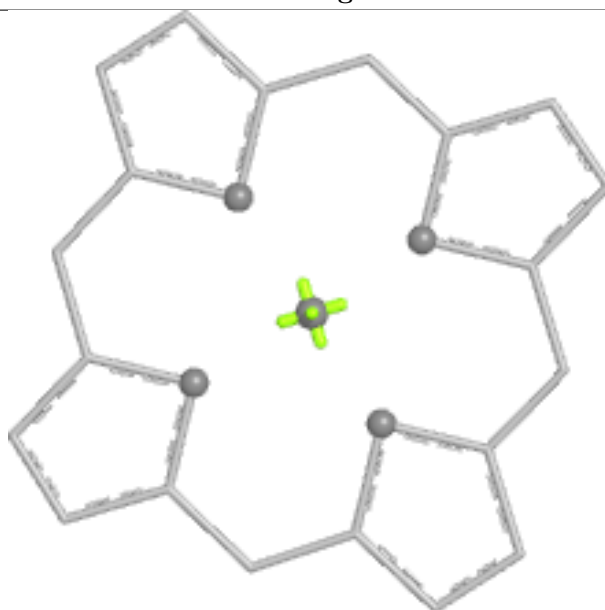
Bond lengths



Bond angles

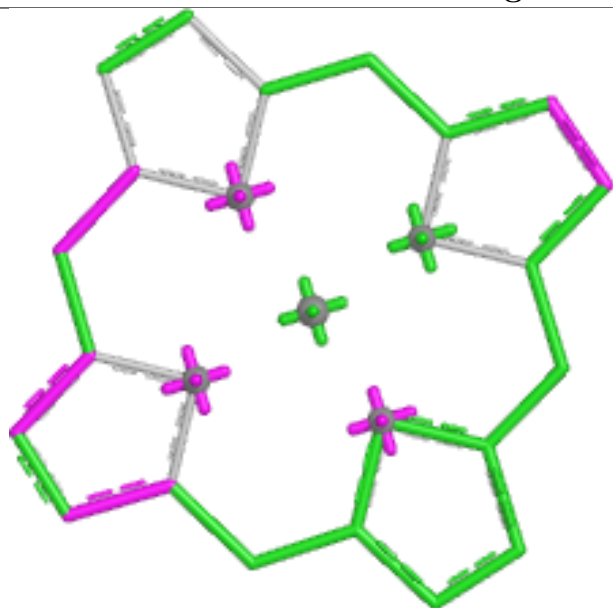


Torsions

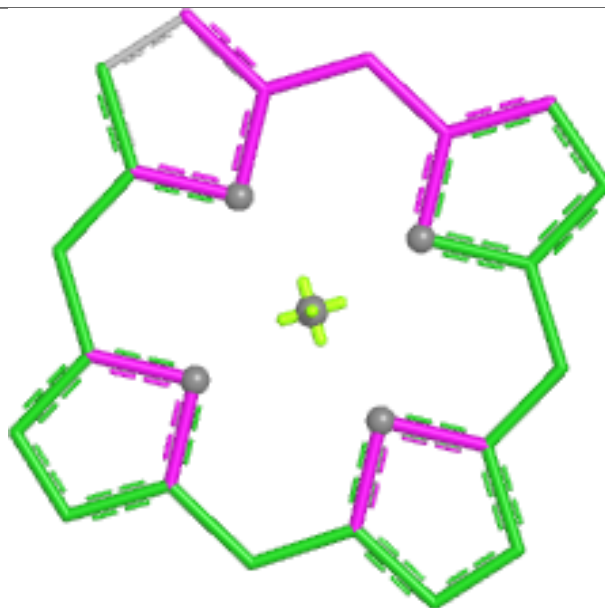


Rings

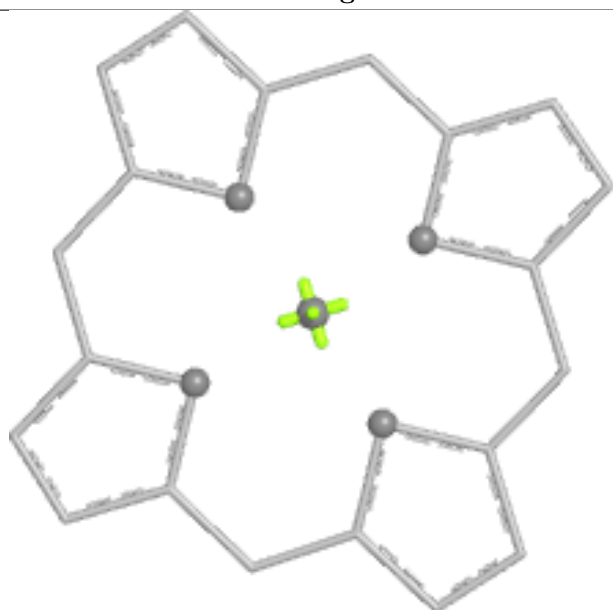
Ligand CLA A 1127



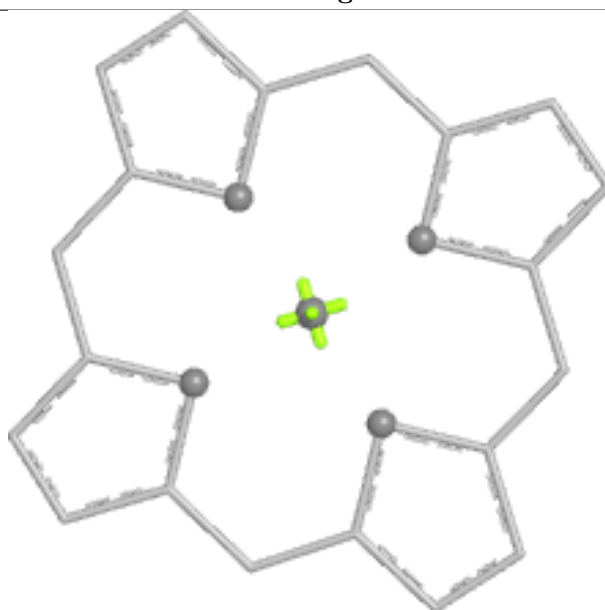
Bond lengths



Bond angles

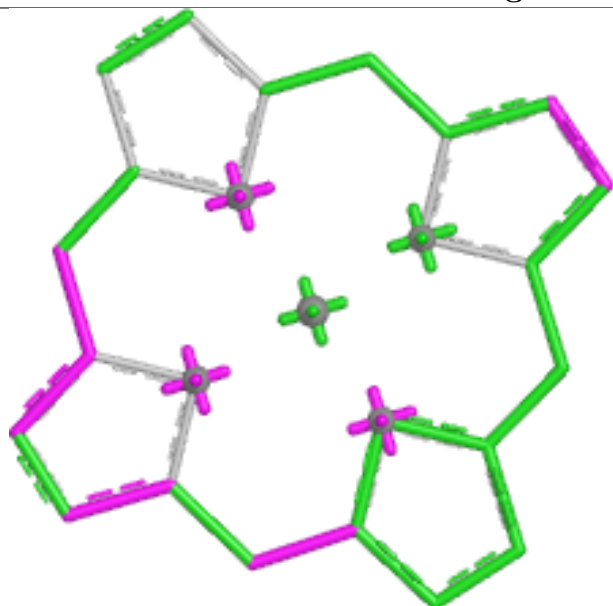


Torsions

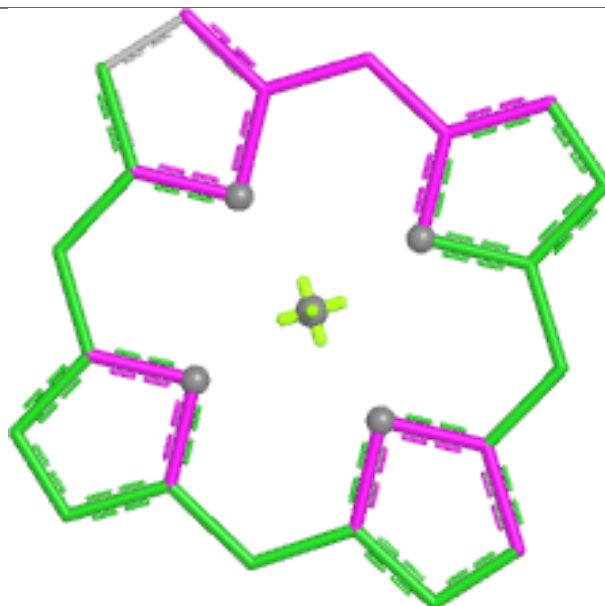


Rings

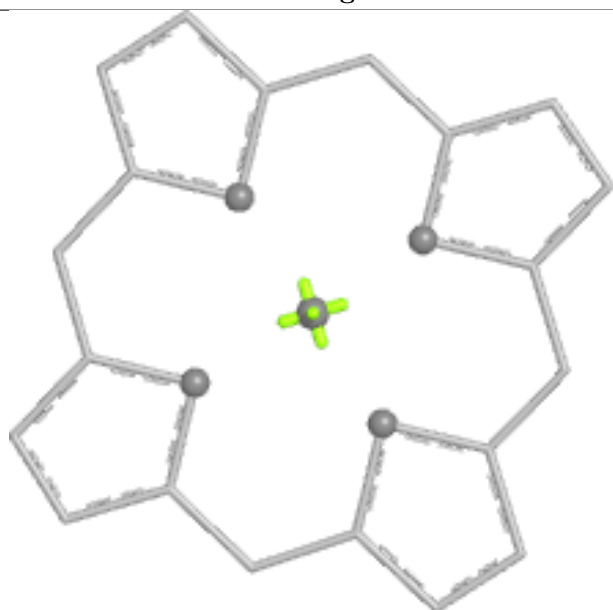
Ligand CLA B 1214



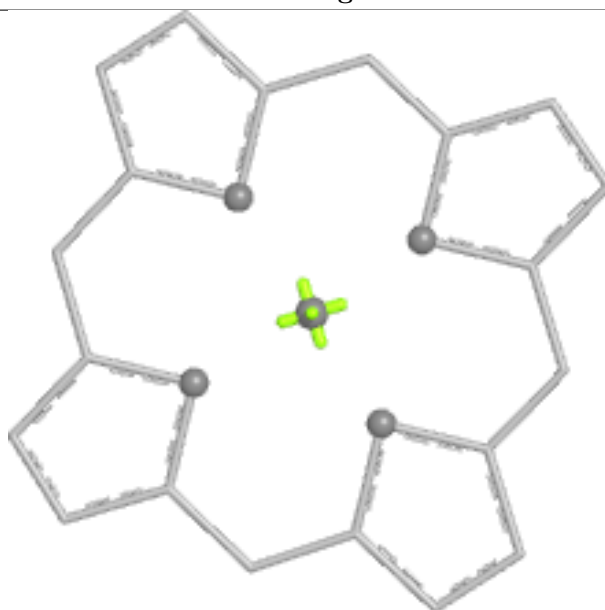
Bond lengths



Bond angles

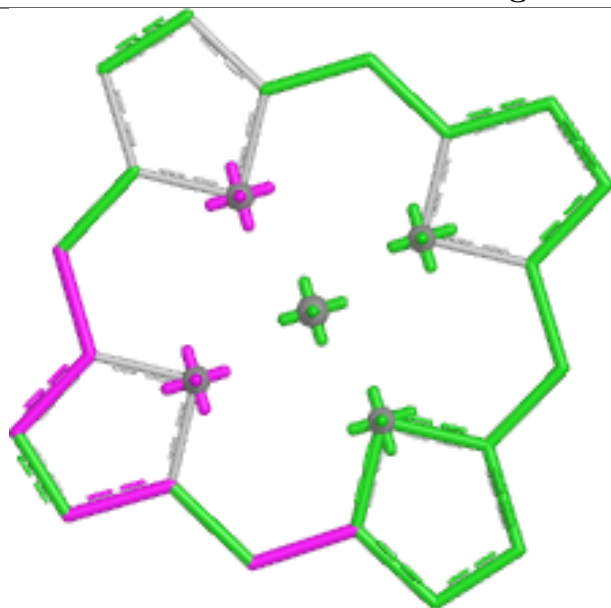


Torsions

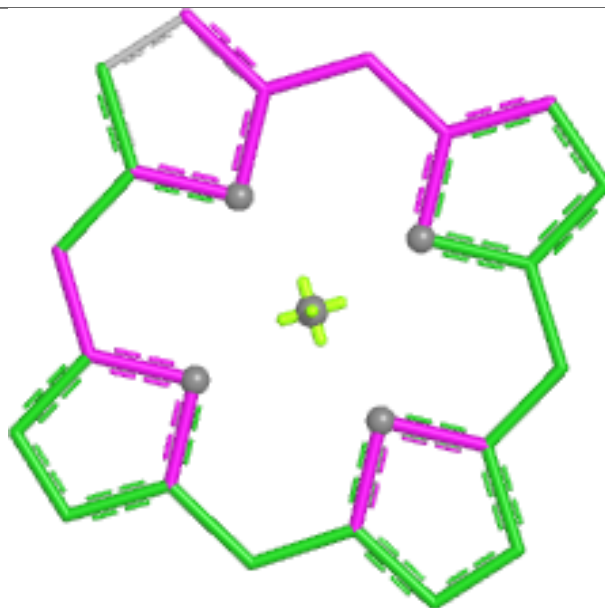


Rings

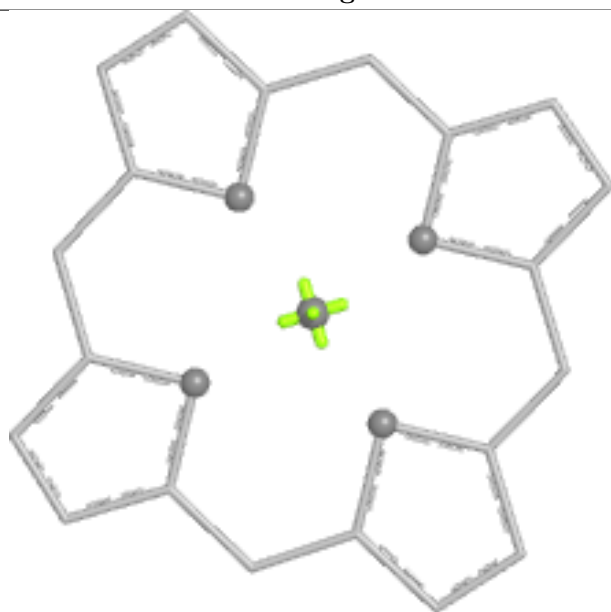
Ligand CLA 3 1017



Bond lengths



Bond angles

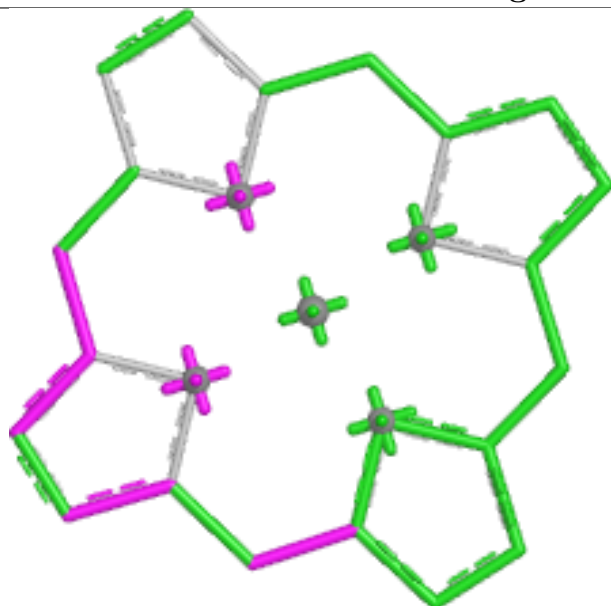


Torsions

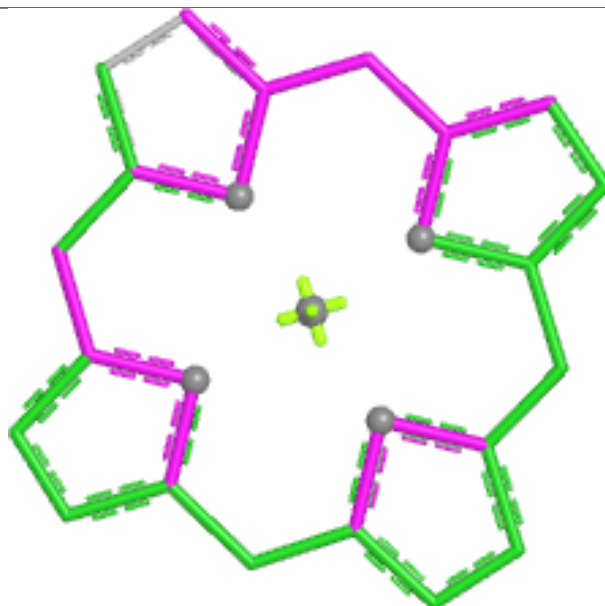


Rings

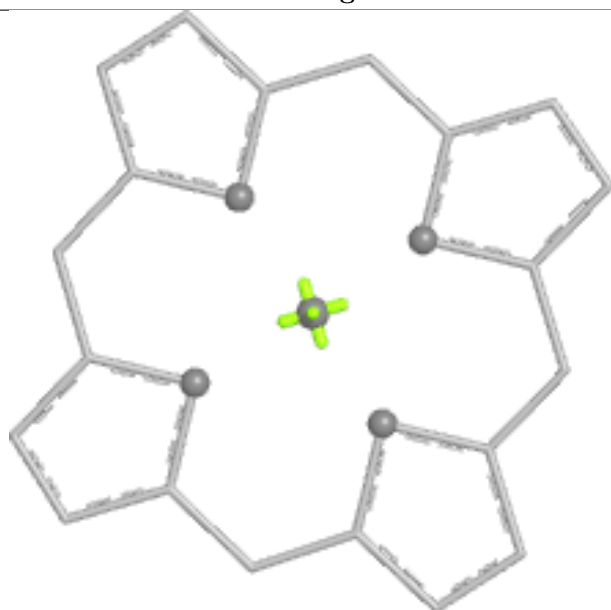
Ligand CLA 7 1011



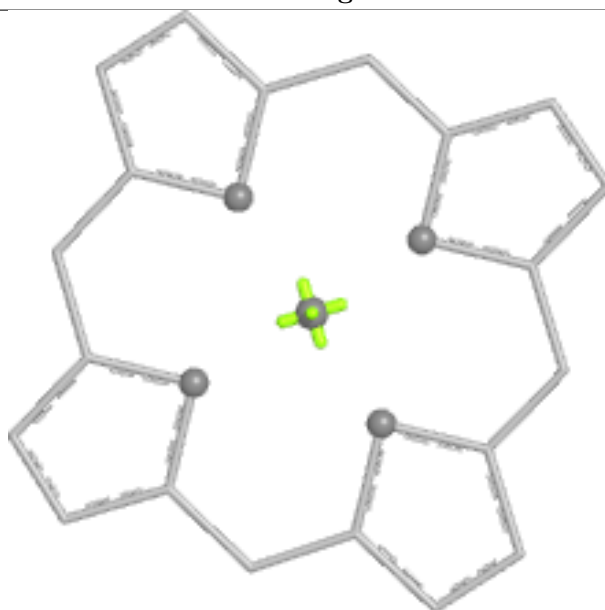
Bond lengths



Bond angles

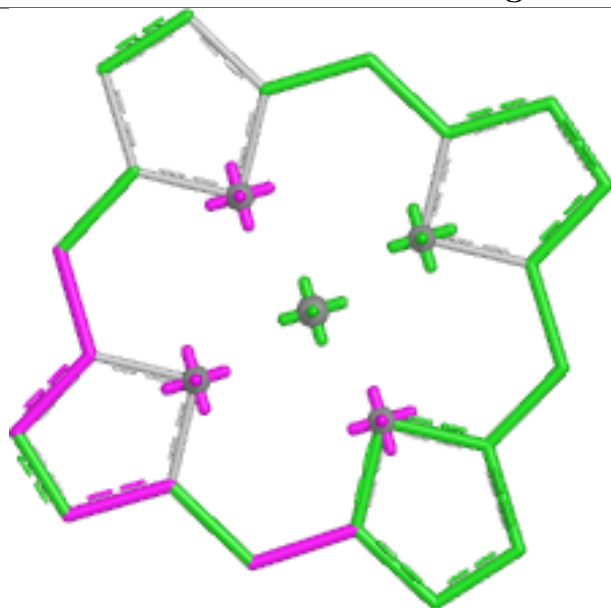


Torsions

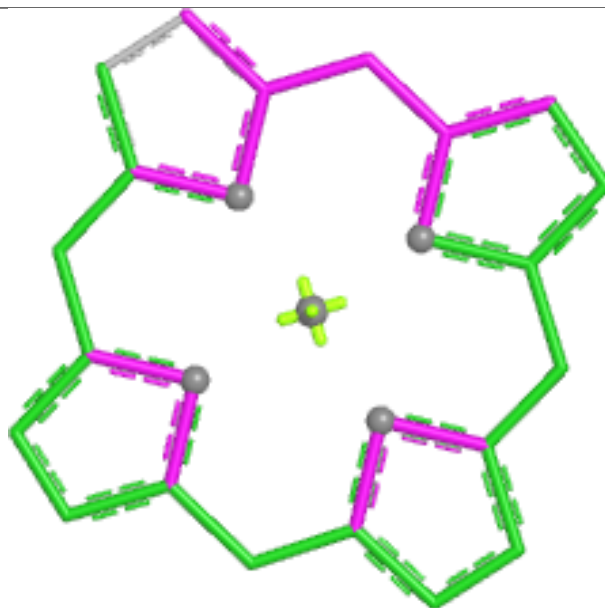


Rings

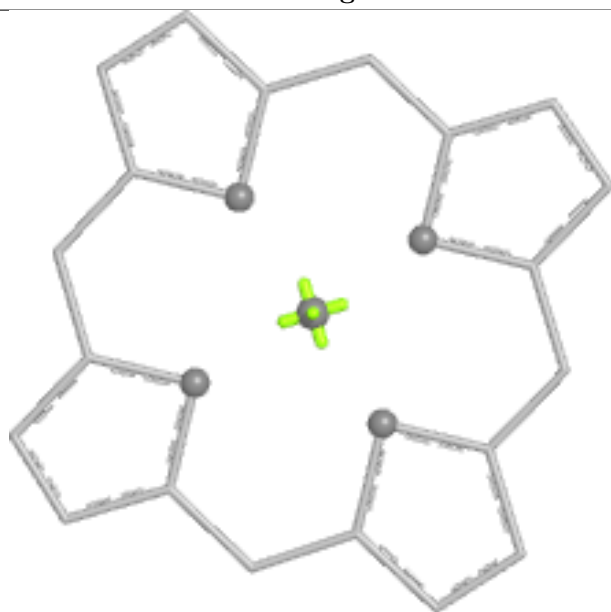
Ligand CLA B 1205



Bond lengths



Bond angles

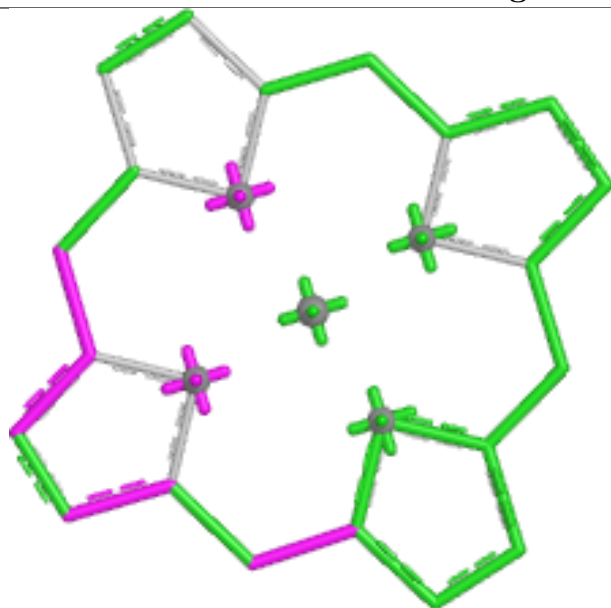


Torsions

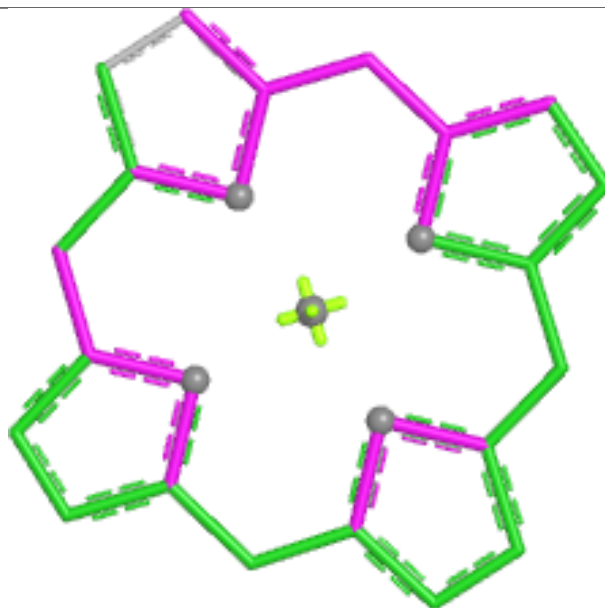


Rings

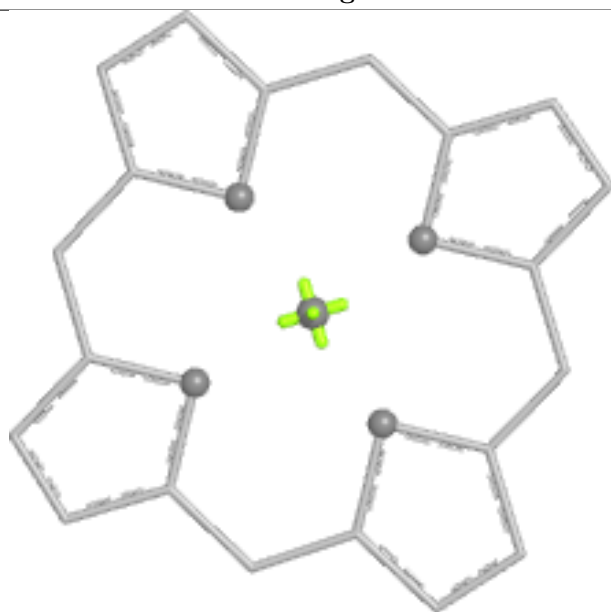
Ligand CLA 2 4007



Bond lengths



Bond angles

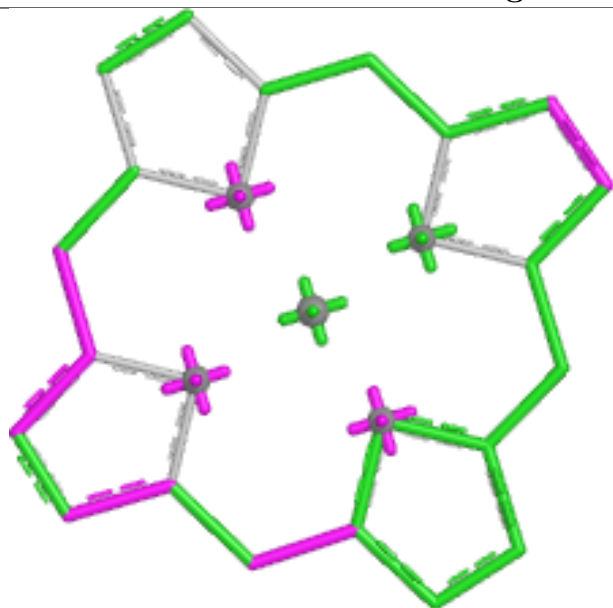


Torsions

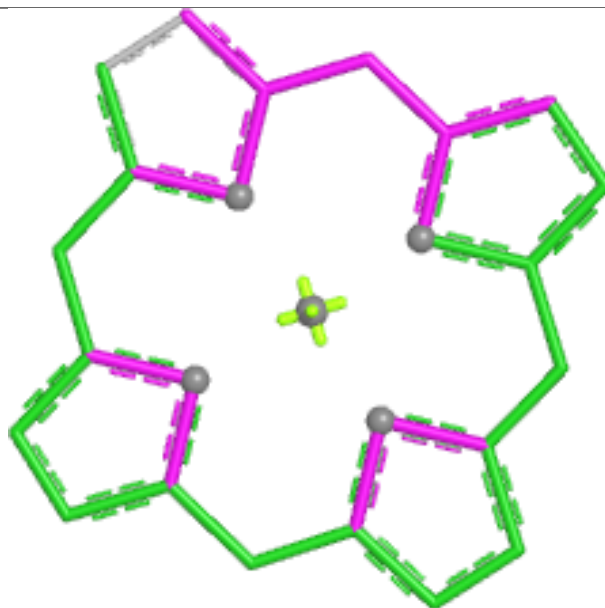


Rings

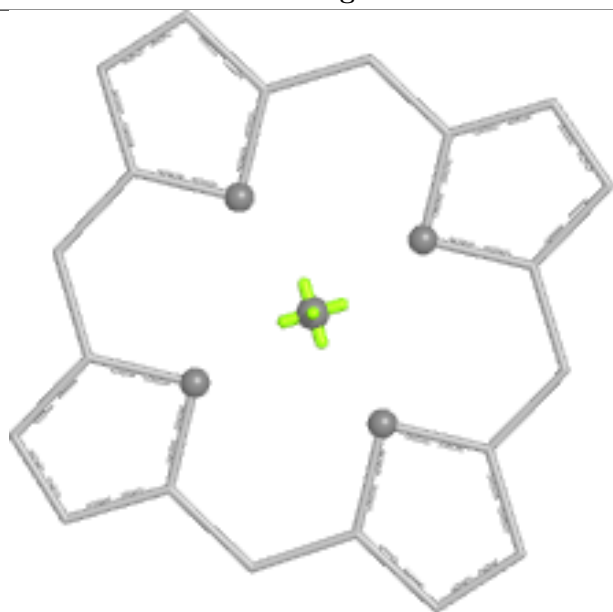
Ligand CLA P 5121



Bond lengths



Bond angles

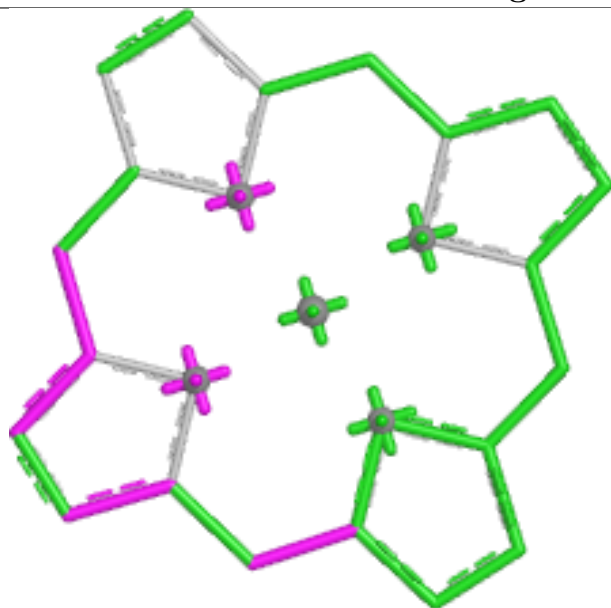


Torsions



Rings

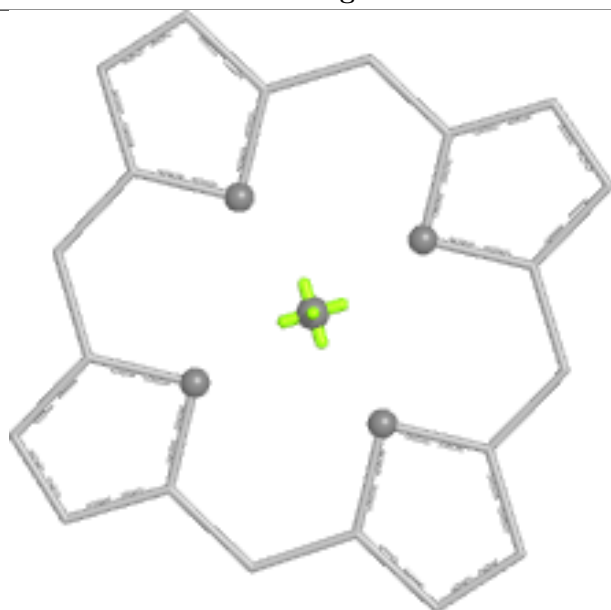
Ligand CLA 9 1031



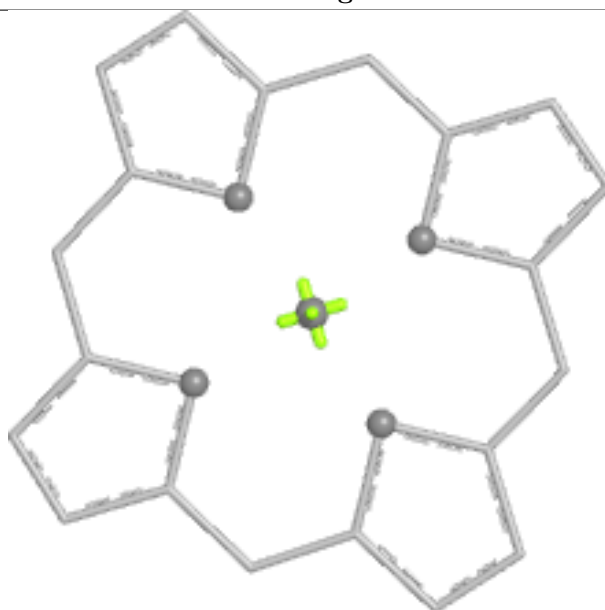
Bond lengths



Bond angles

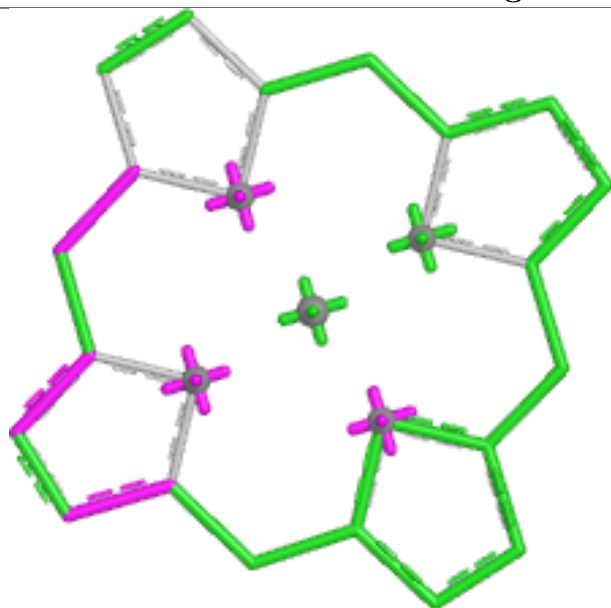


Torsions

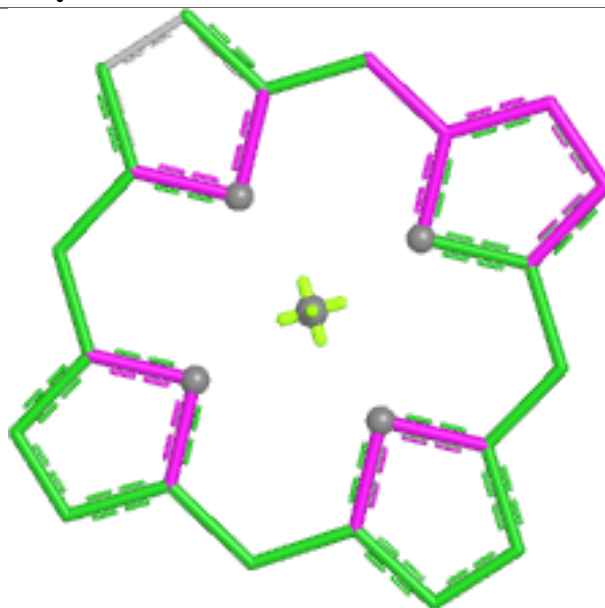


Rings

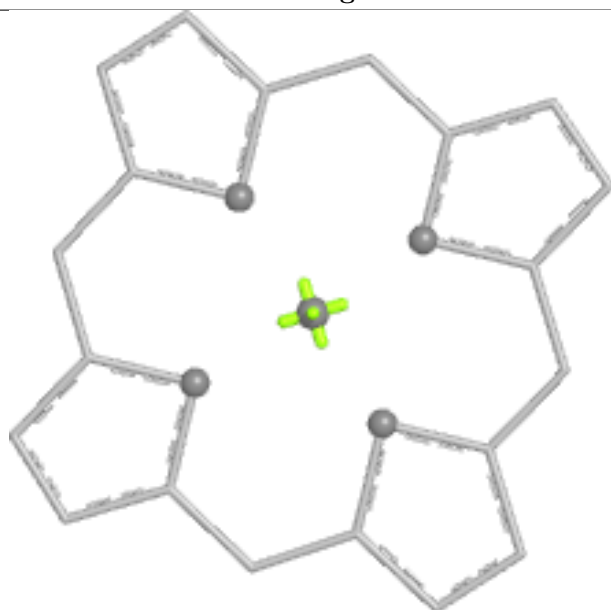
Ligand CLA Q 5239



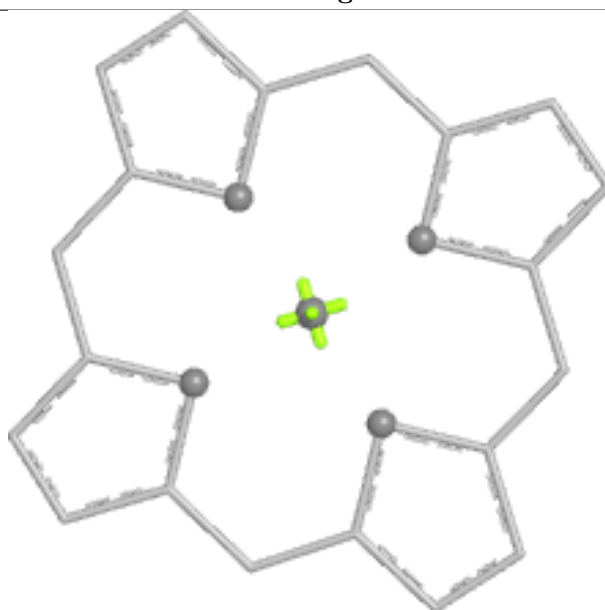
Bond lengths



Bond angles

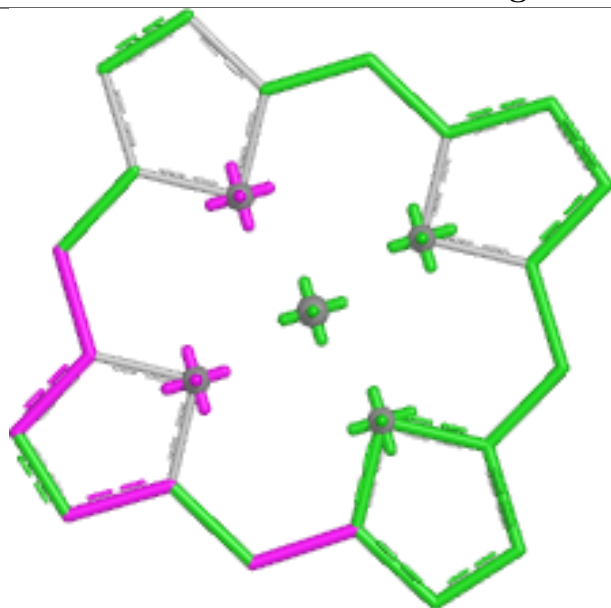


Torsions

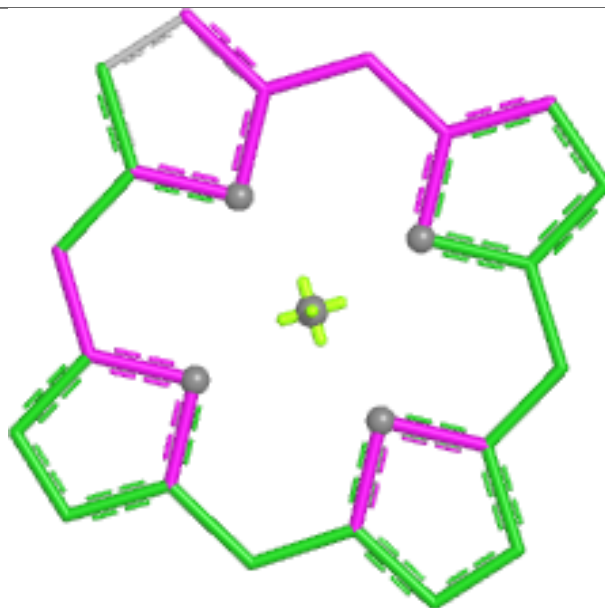


Rings

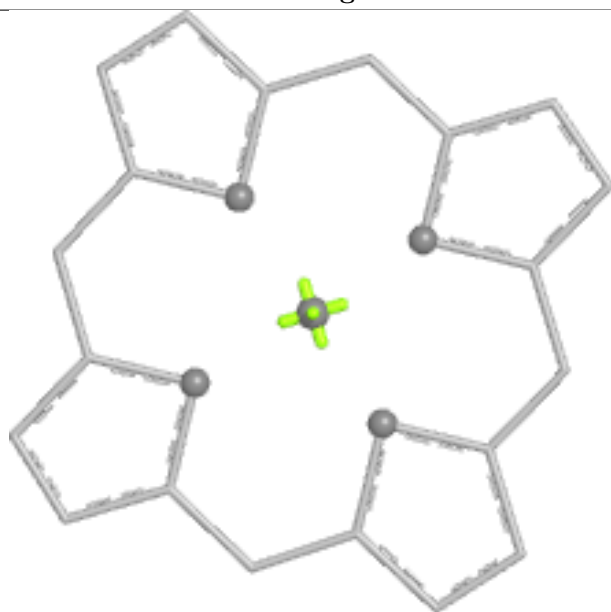
Ligand CLA 7 1022



Bond lengths



Bond angles

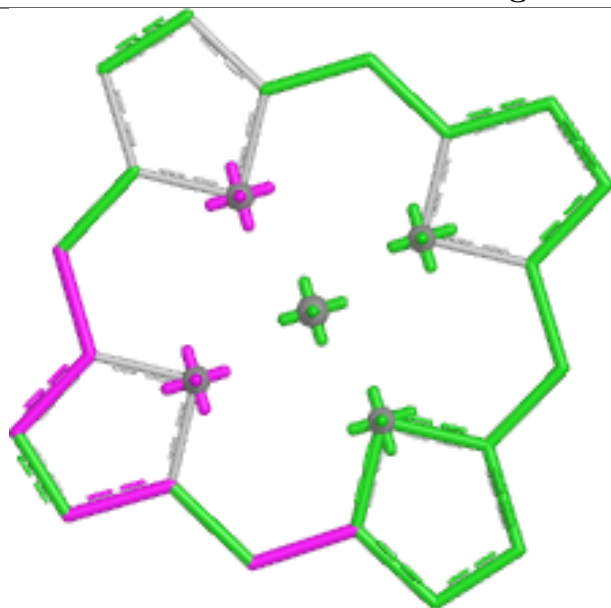


Torsions

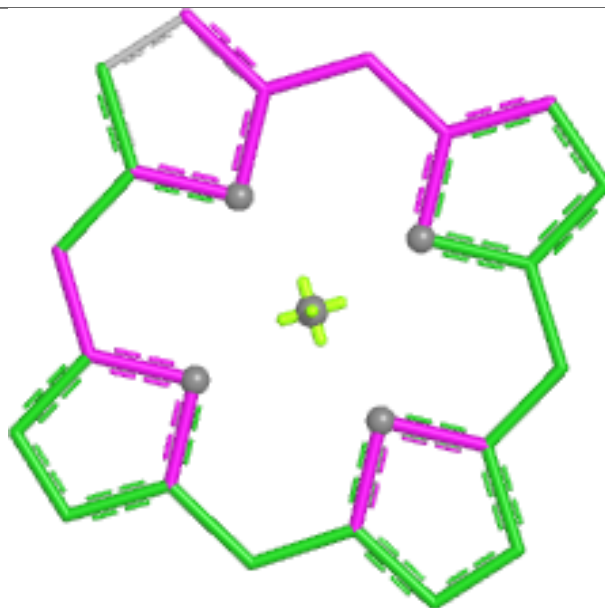


Rings

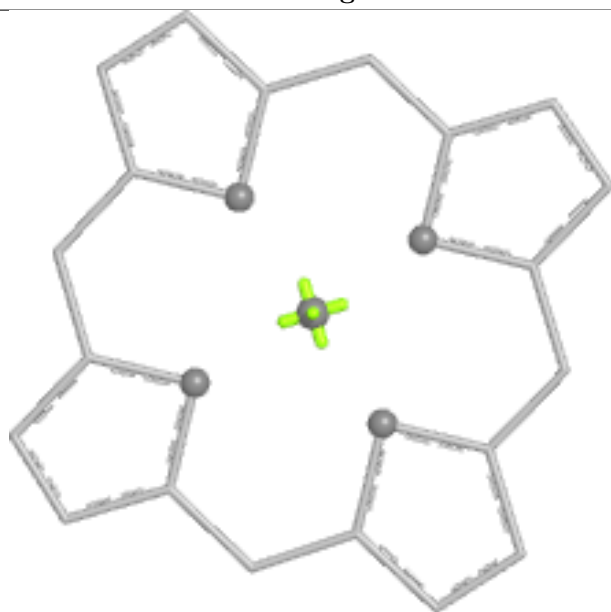
Ligand CLA 0 1026



Bond lengths



Bond angles

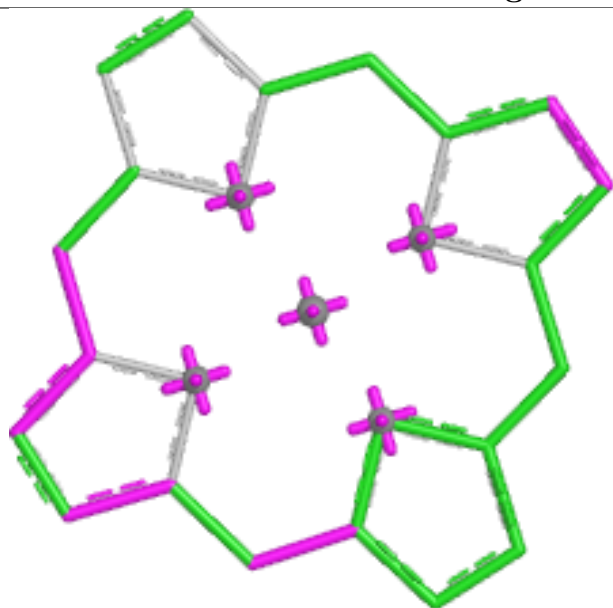


Torsions

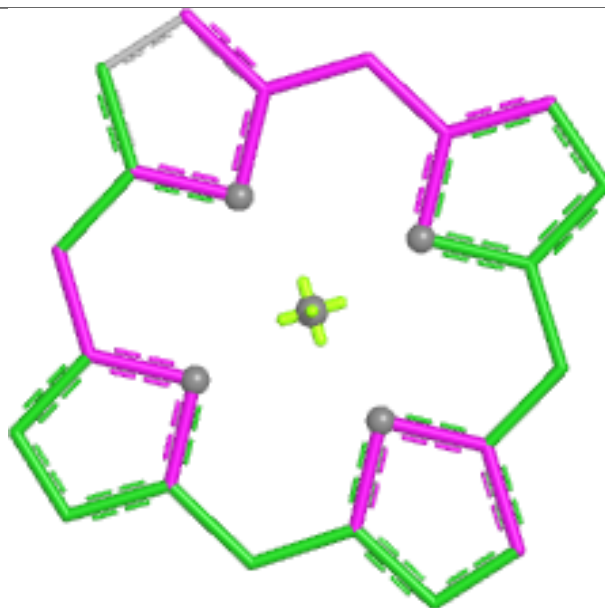


Rings

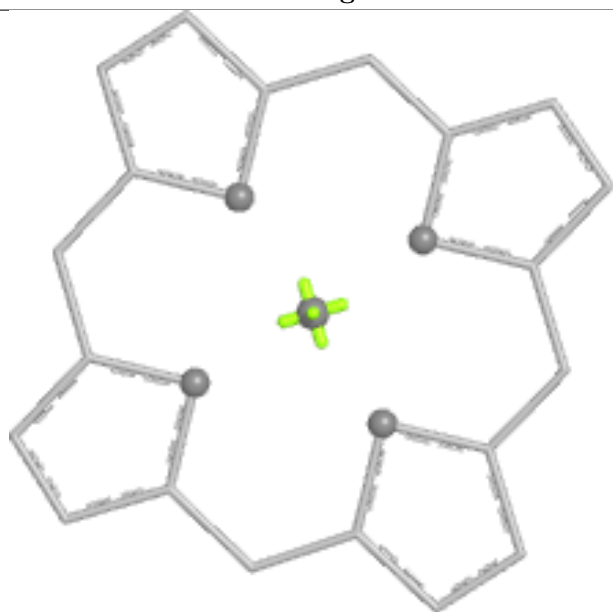
Ligand CLA B 1022



Bond lengths



Bond angles

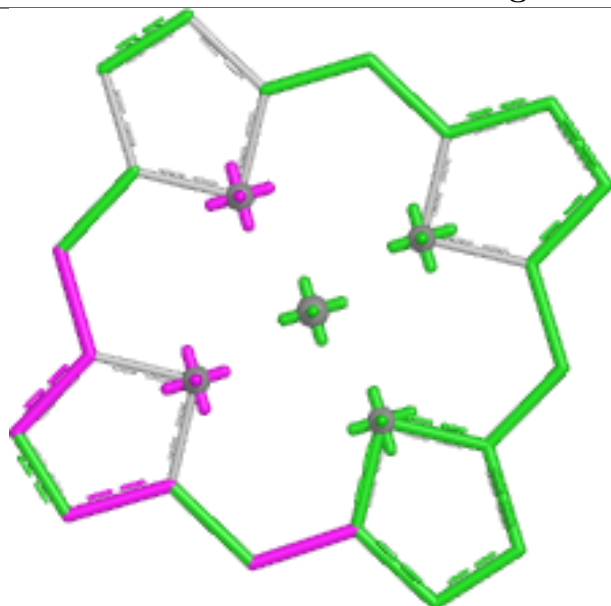


Torsions

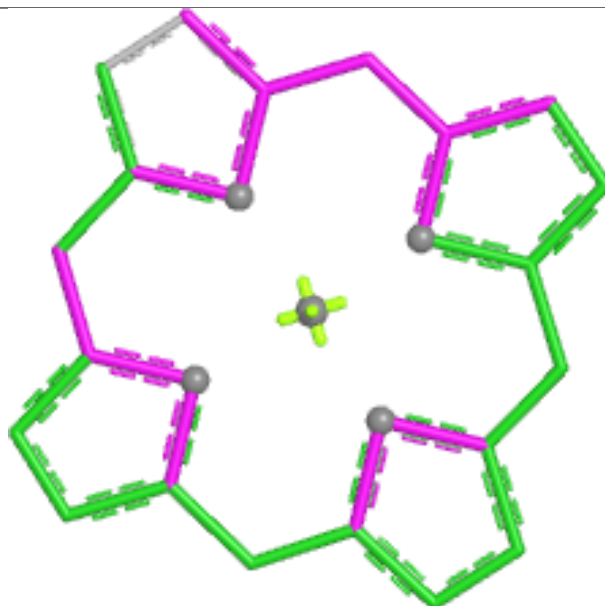


Rings

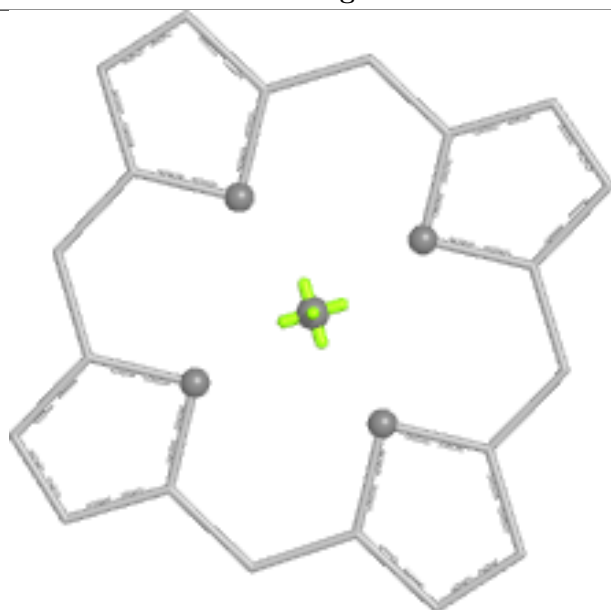
Ligand CLA 4 1022



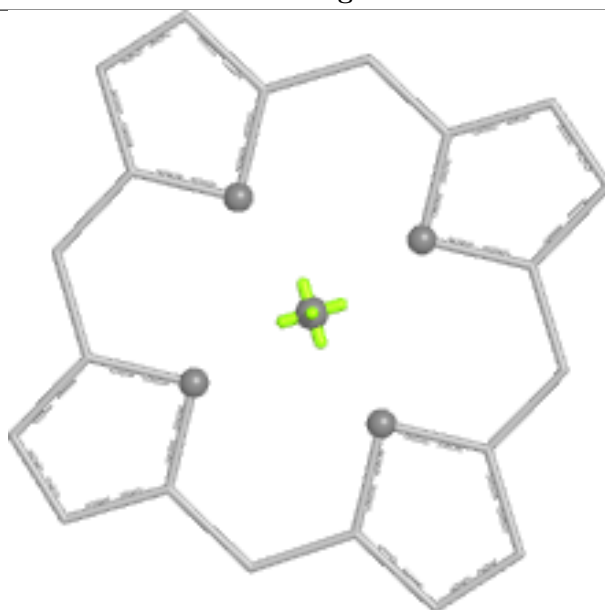
Bond lengths



Bond angles

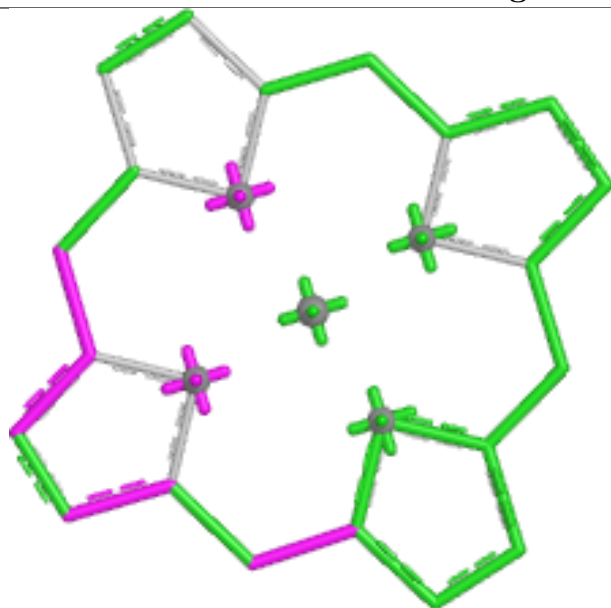


Torsions

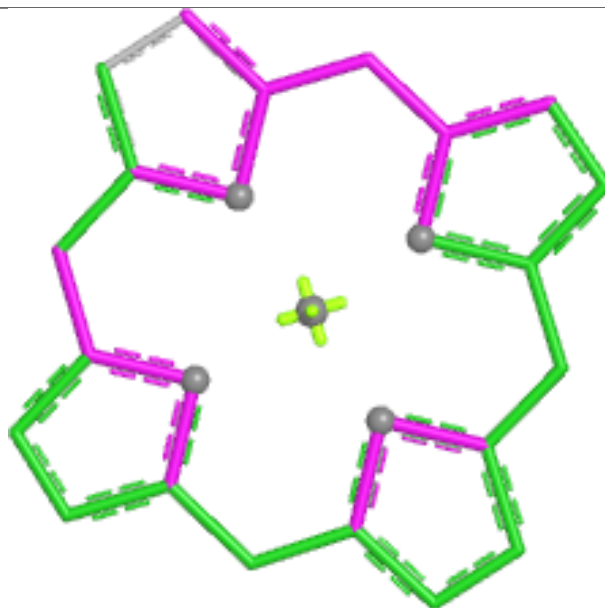


Rings

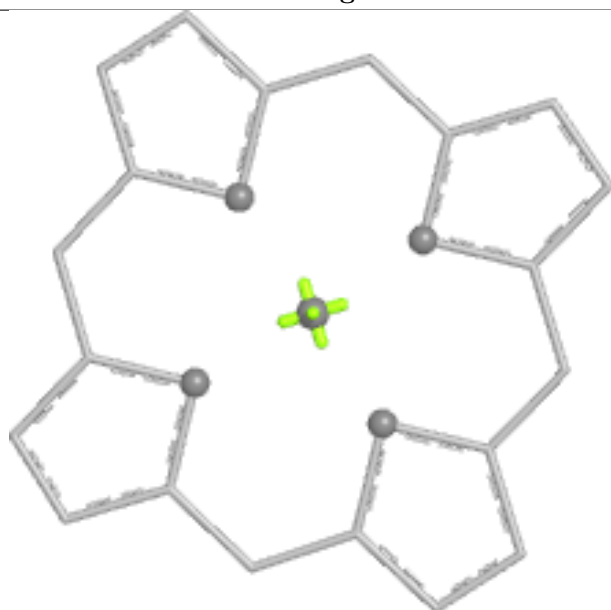
Ligand CLA 3 1032



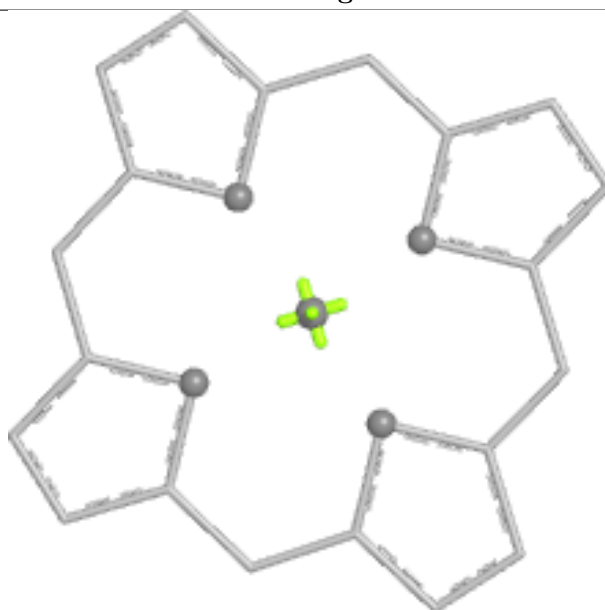
Bond lengths



Bond angles

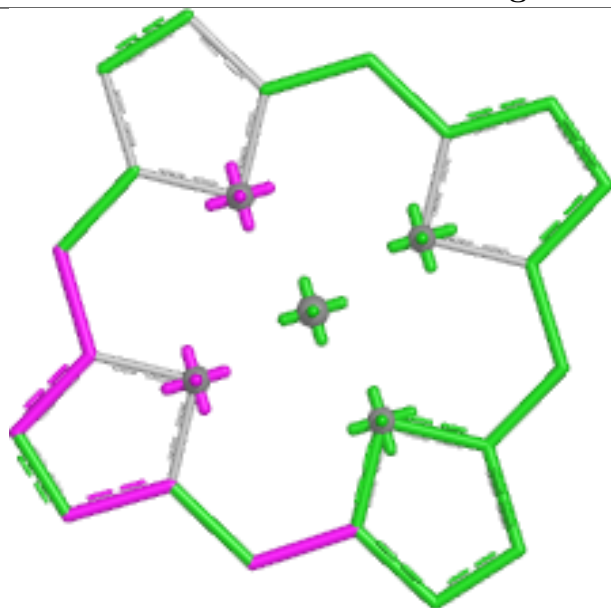


Torsions

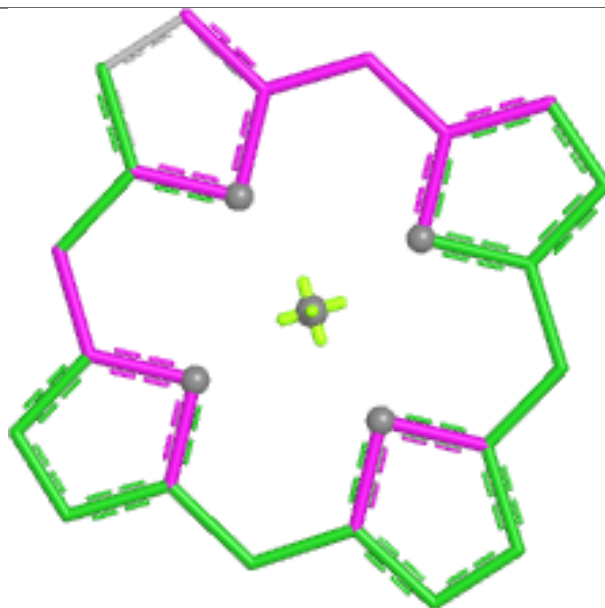


Rings

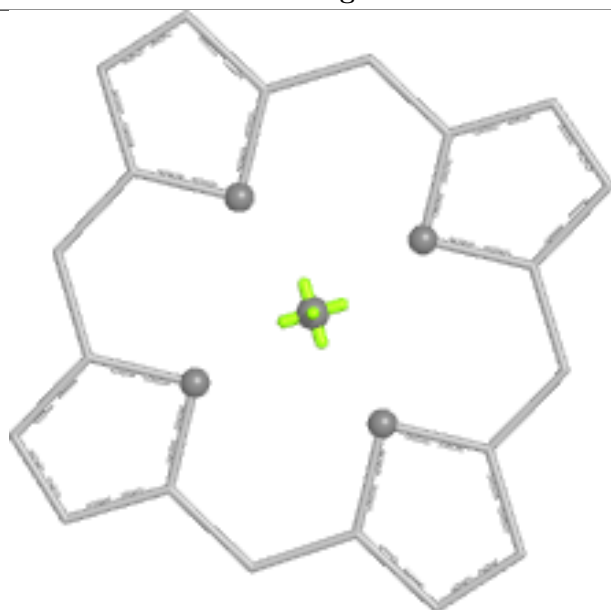
Ligand CLA 3 1012



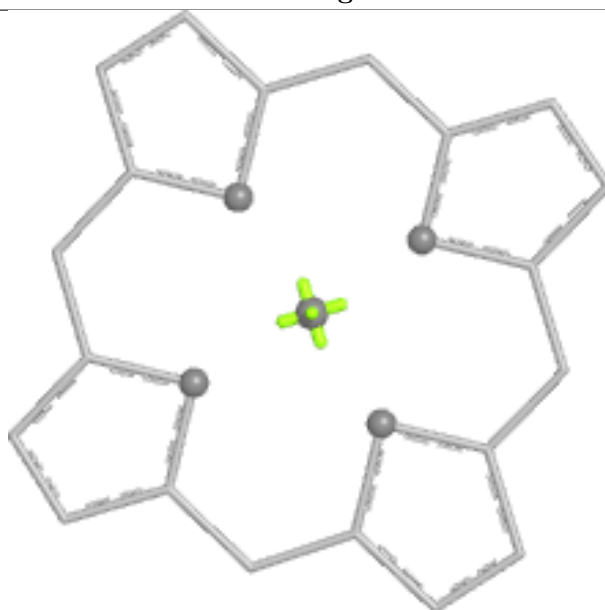
Bond lengths



Bond angles

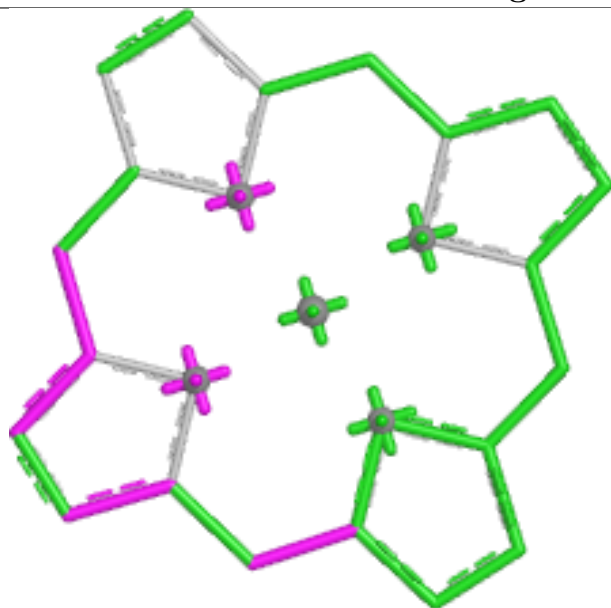


Torsions



Rings

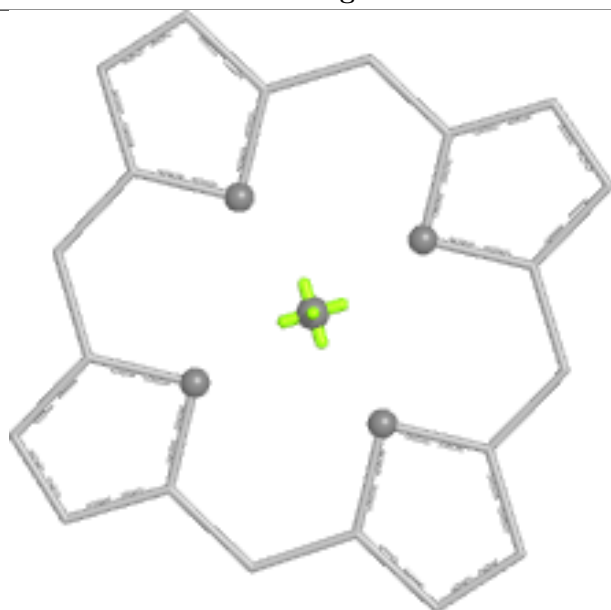
Ligand CLA 9 1011



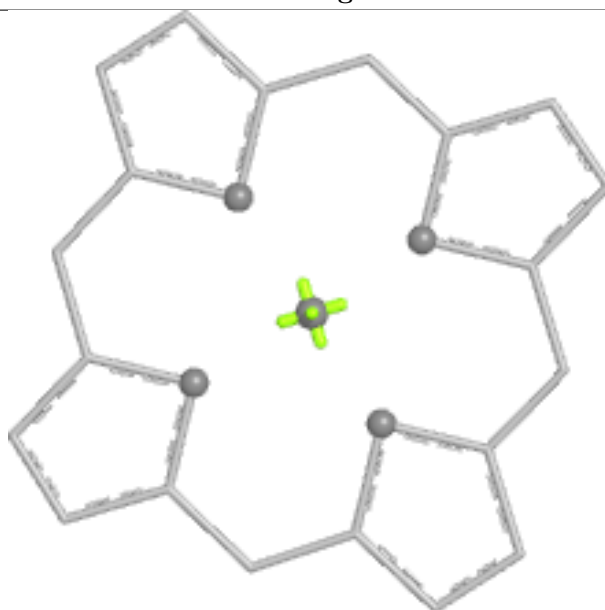
Bond lengths



Bond angles

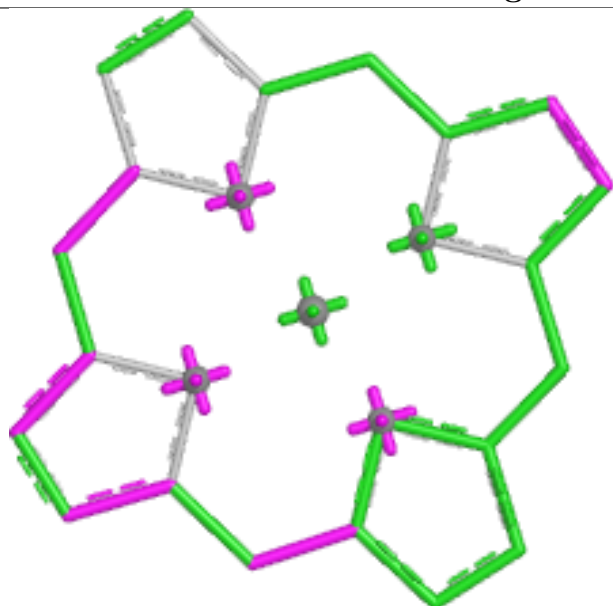


Torsions

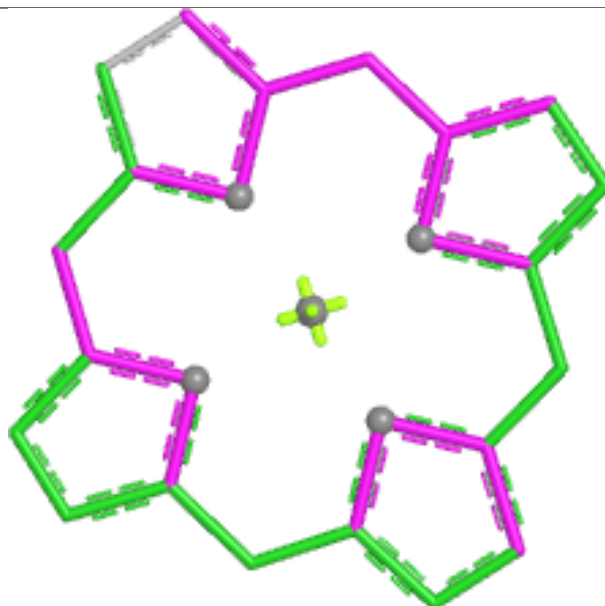


Rings

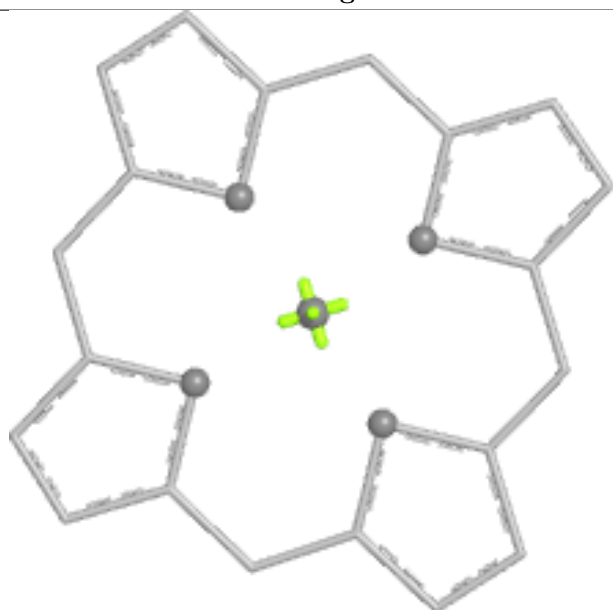
Ligand CLA A 1137



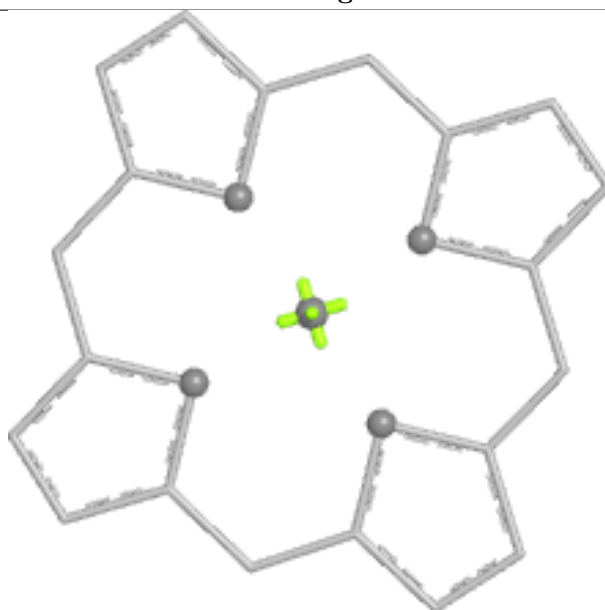
Bond lengths



Bond angles

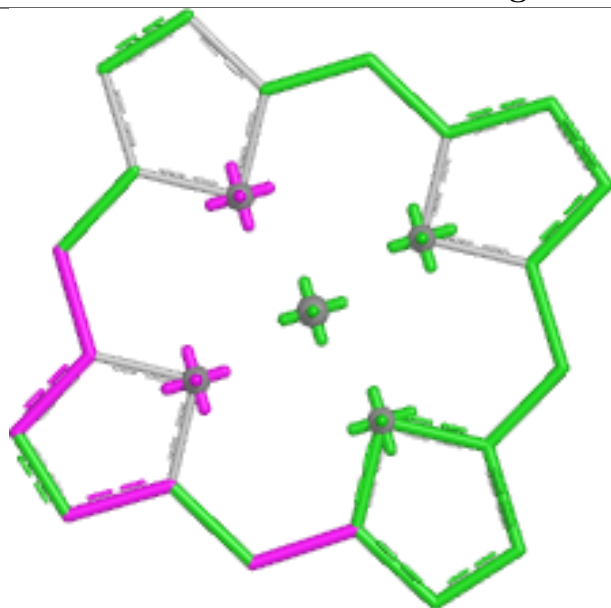


Torsions

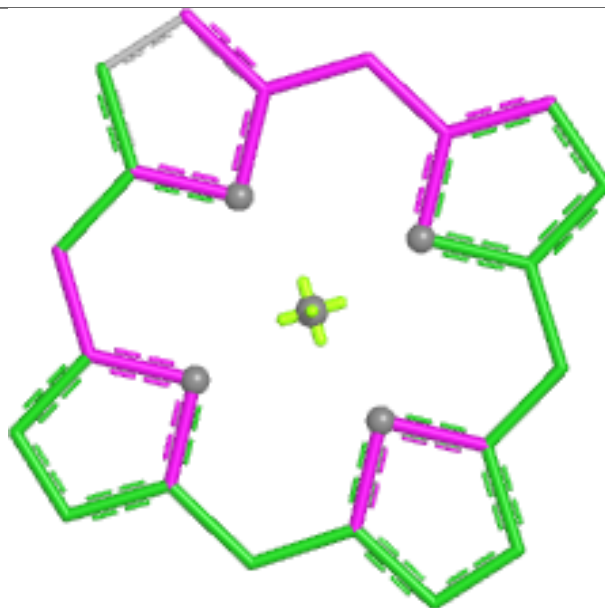


Rings

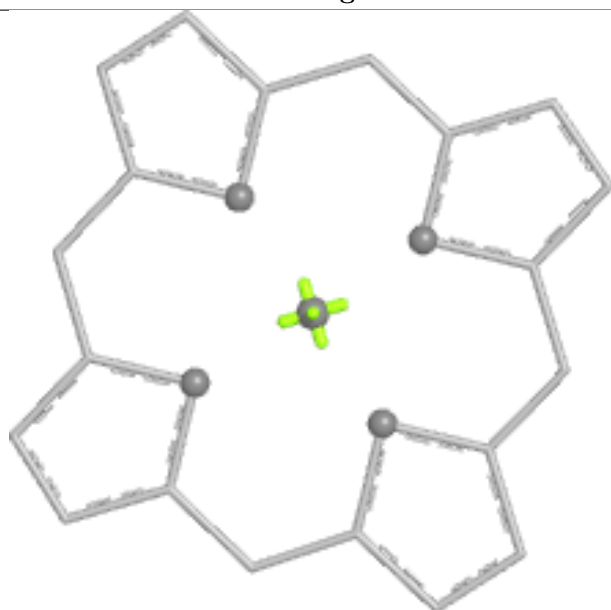
Ligand CLA 2 1011



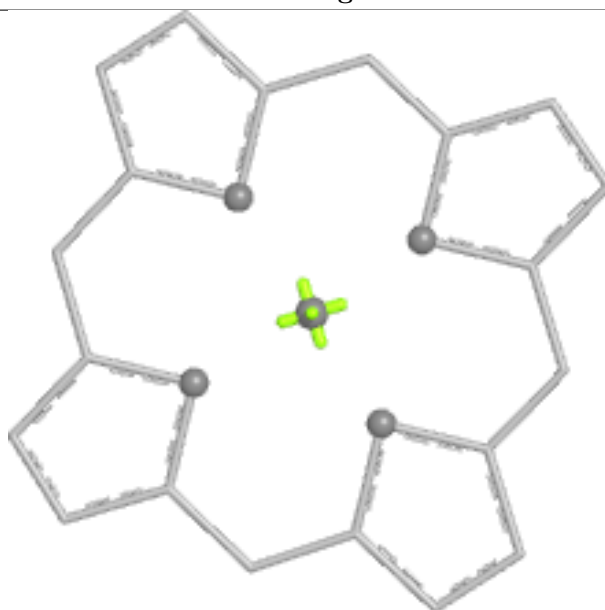
Bond lengths



Bond angles

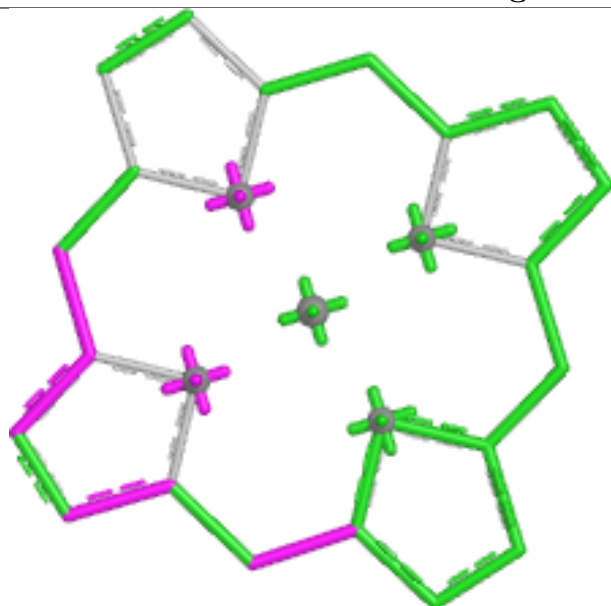


Torsions

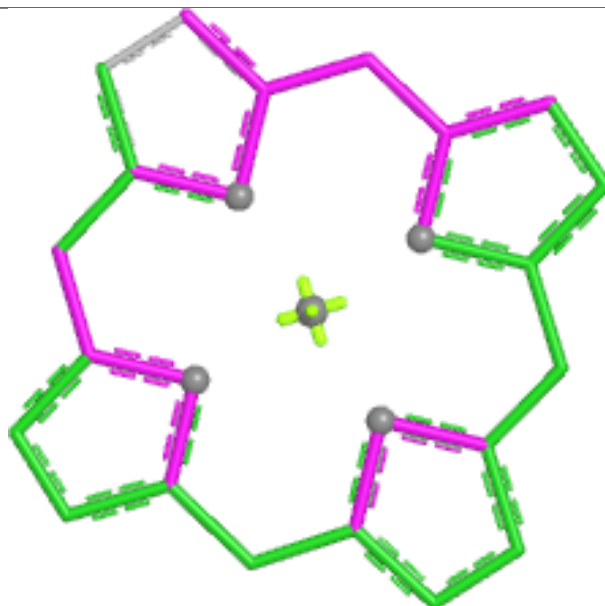


Rings

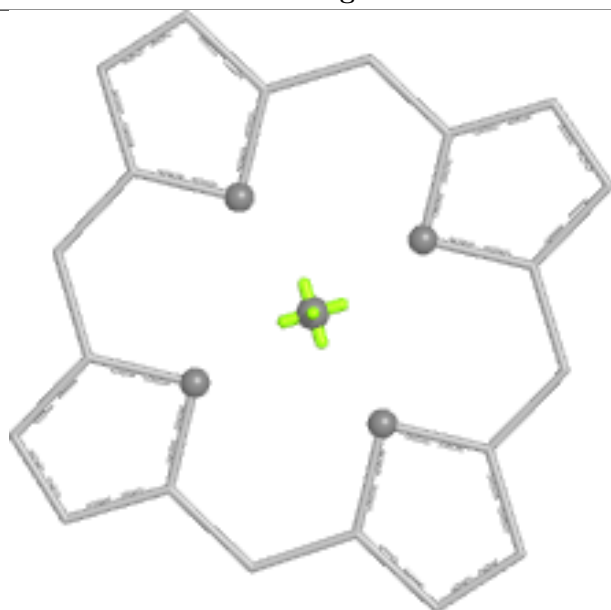
Ligand CLA 9 1025



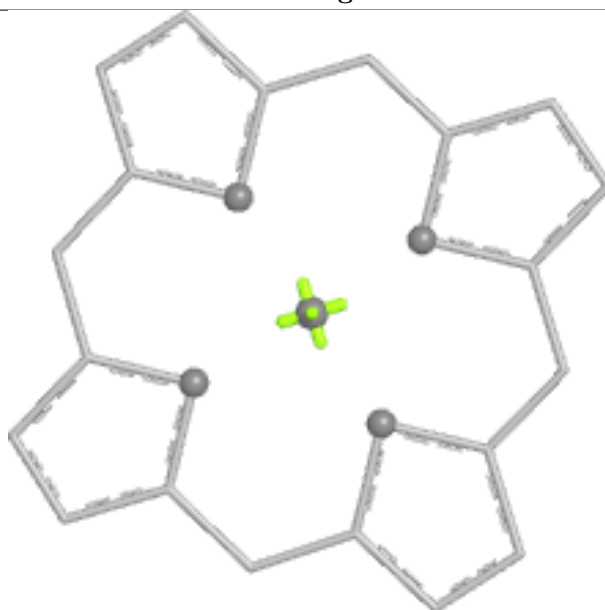
Bond lengths



Bond angles

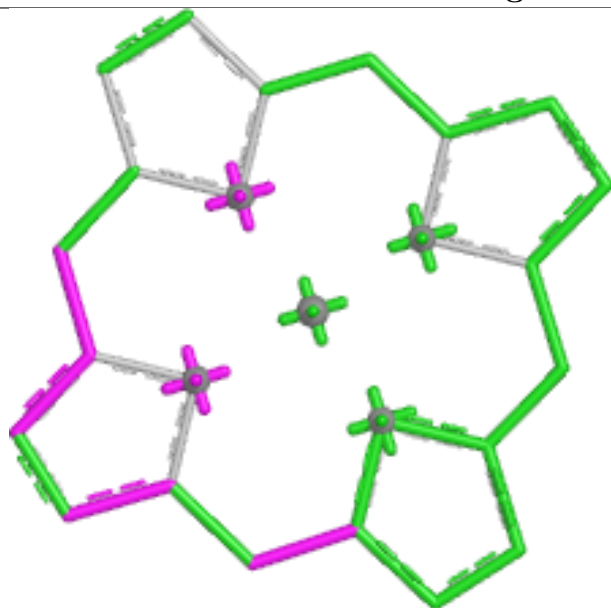


Torsions

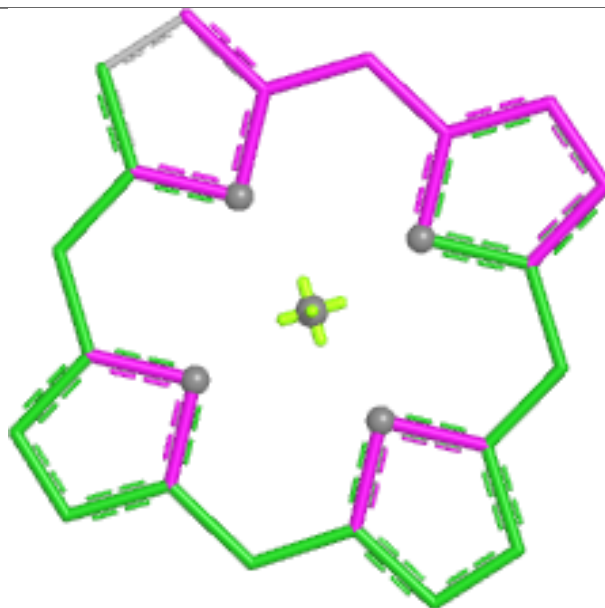


Rings

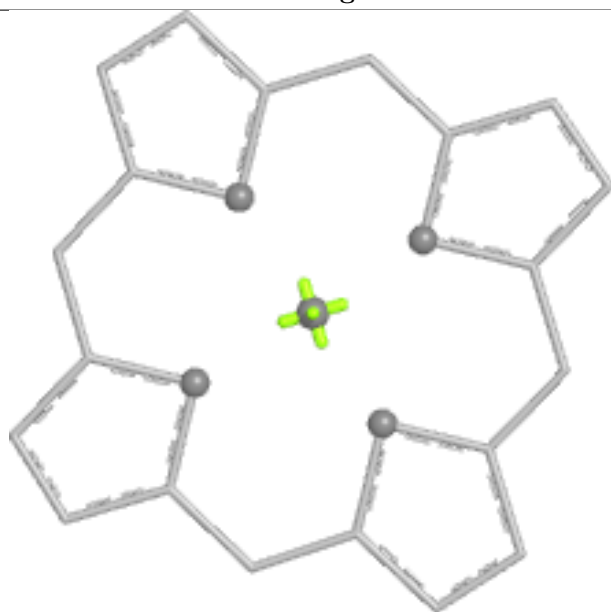
Ligand CLA P 5106



Bond lengths



Bond angles

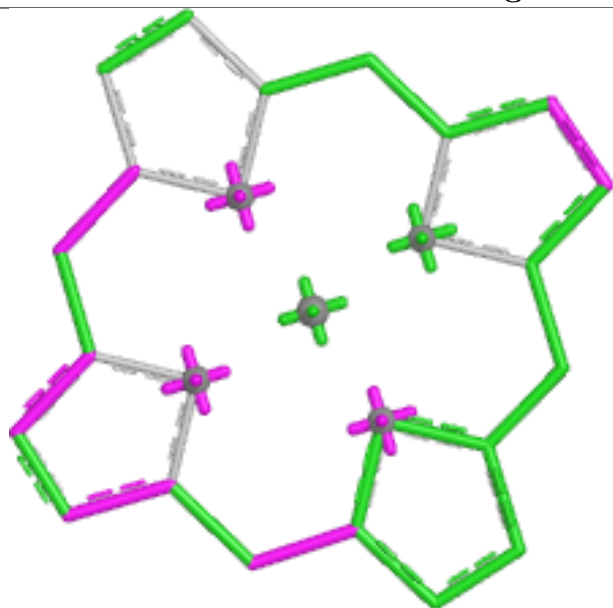


Torsions

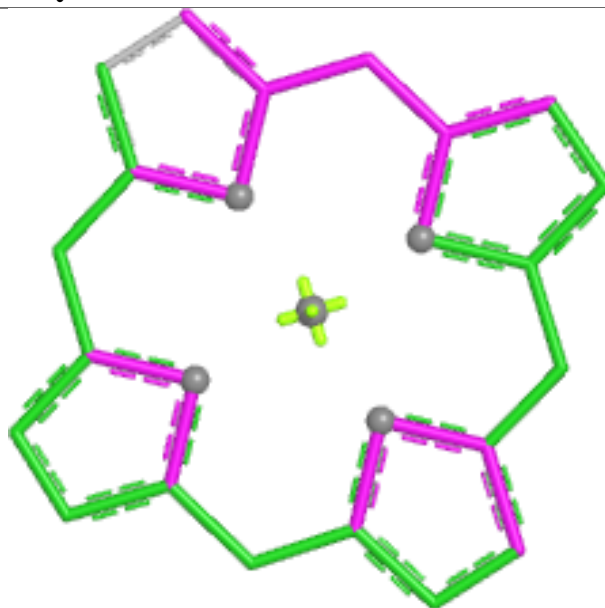


Rings

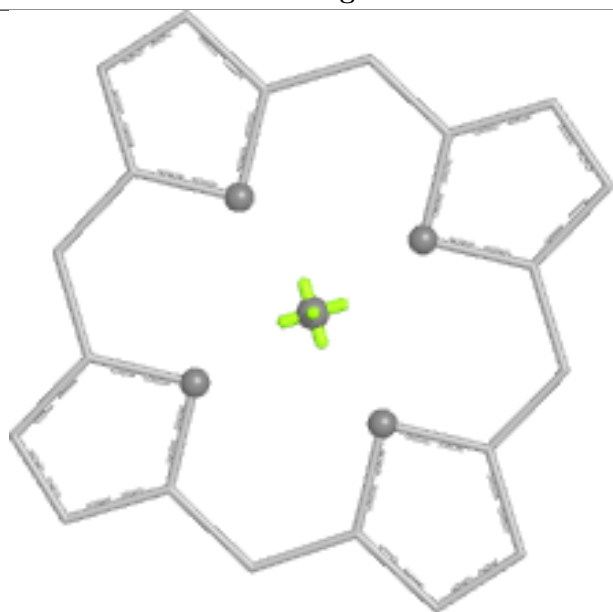
Ligand CLA Q 5209



Bond lengths



Bond angles

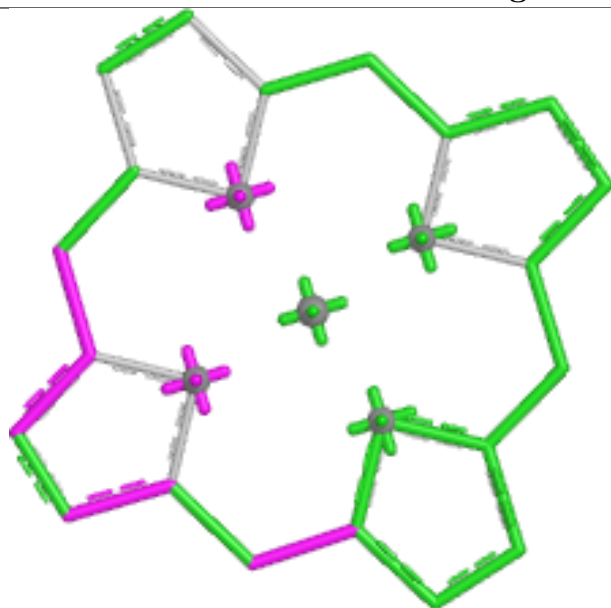


Torsions

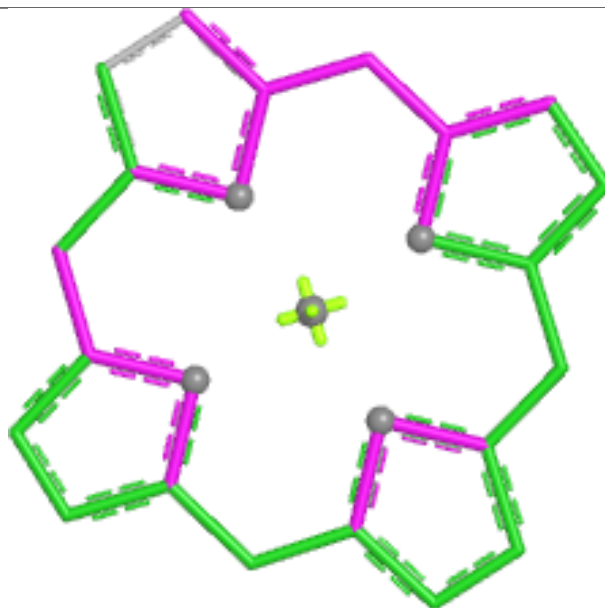


Rings

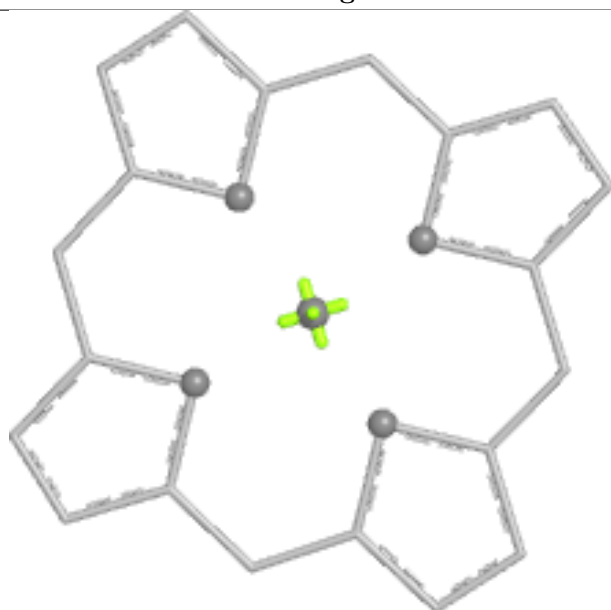
Ligand CLA 1 1013



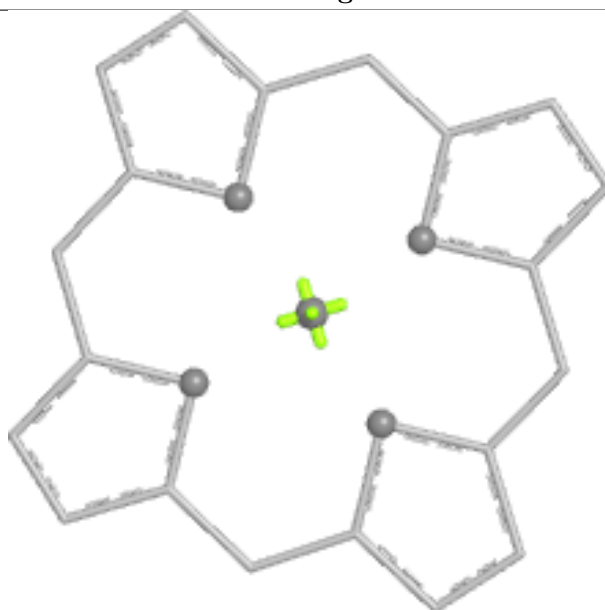
Bond lengths



Bond angles

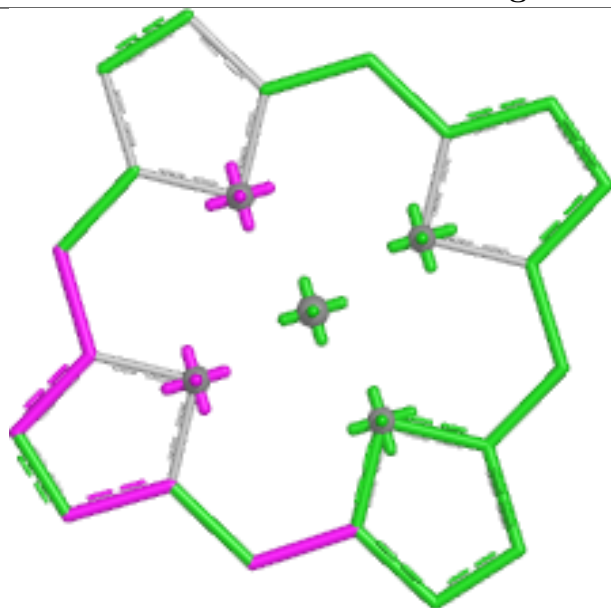


Torsions

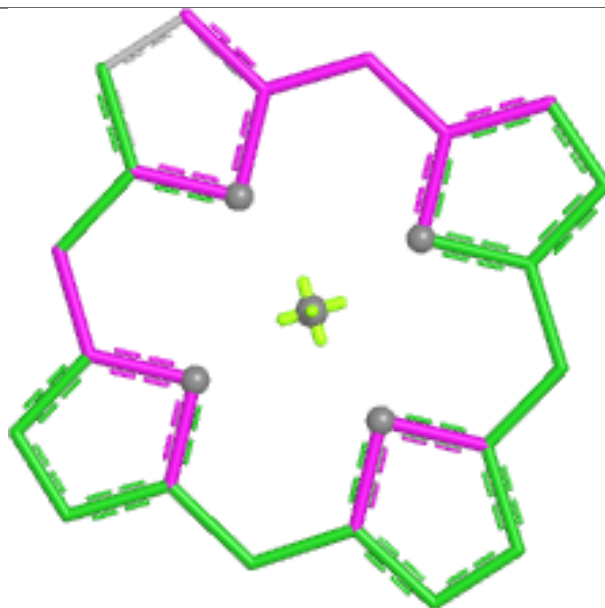


Rings

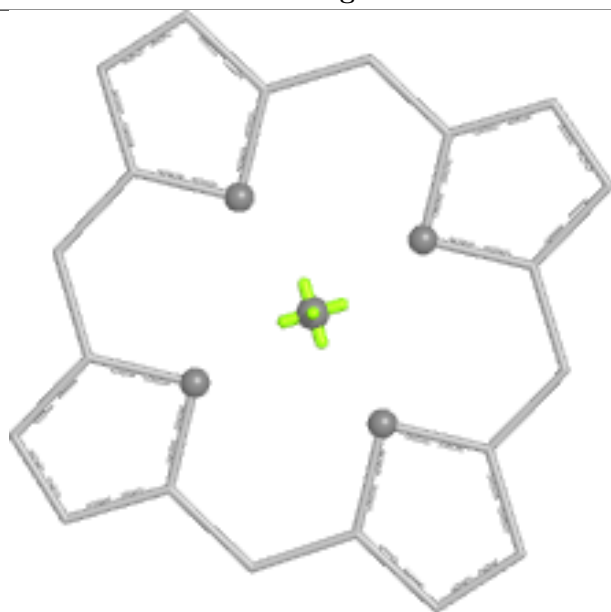
Ligand CLA 4 1013



Bond lengths



Bond angles

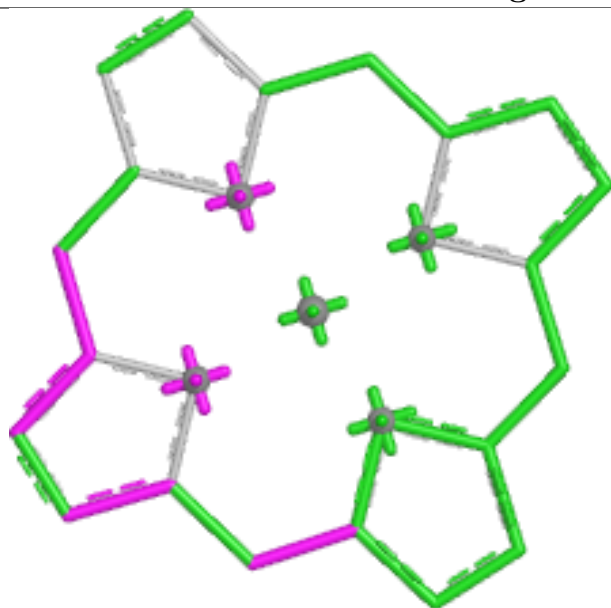


Torsions



Rings

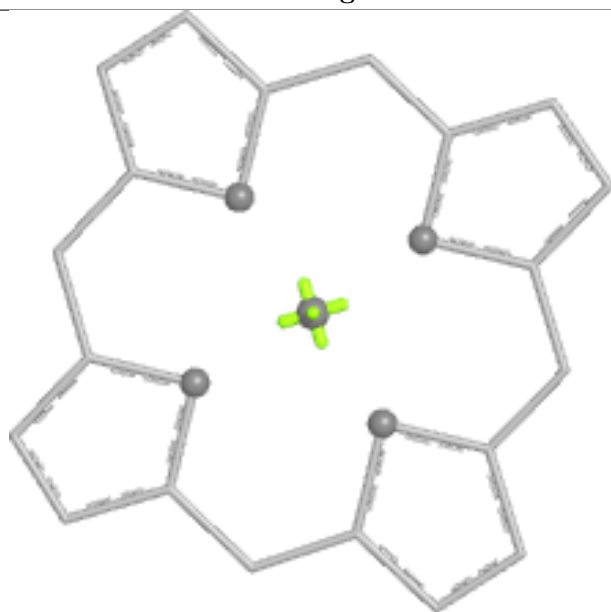
Ligand CLA 3 1014



Bond lengths



Bond angles

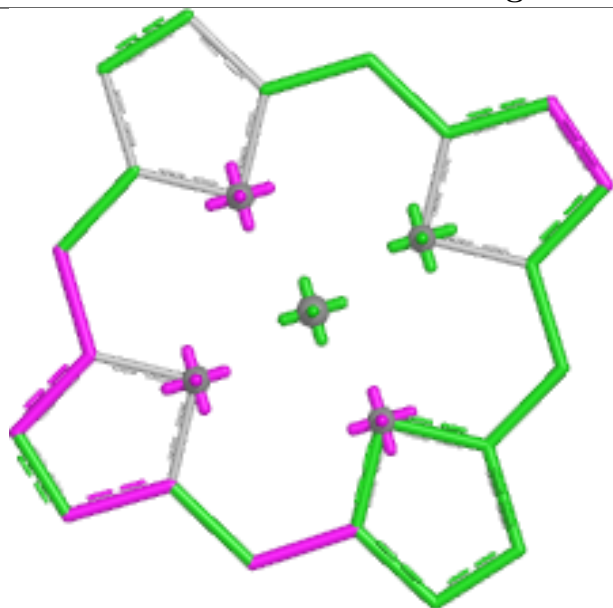


Torsions

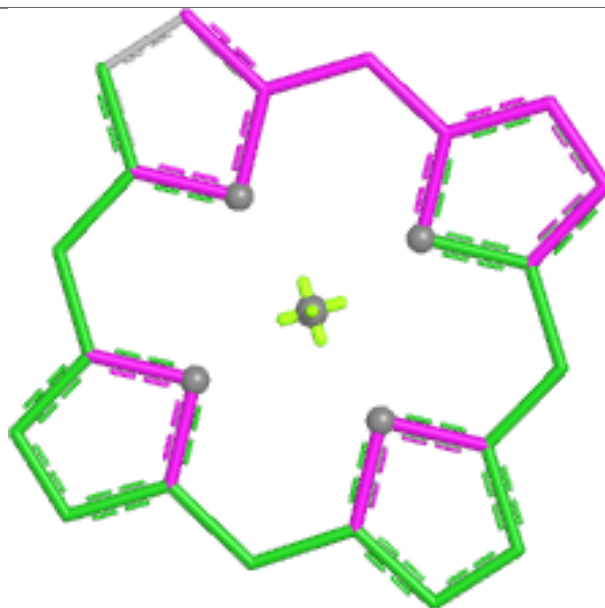


Rings

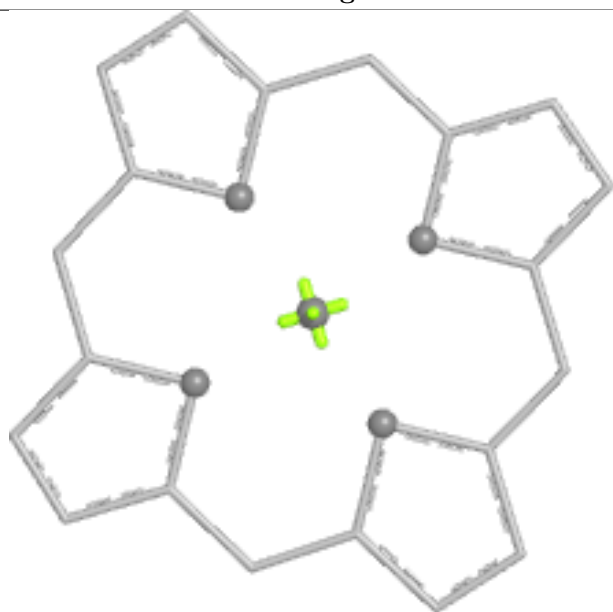
Ligand CLA P 5109



Bond lengths



Bond angles

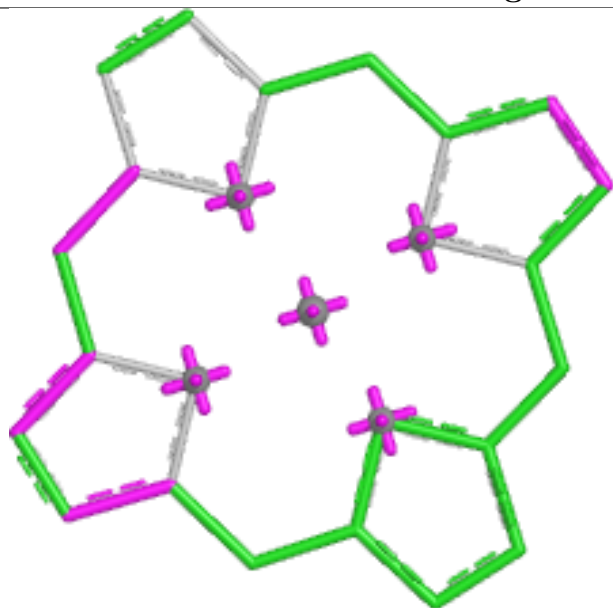


Torsions

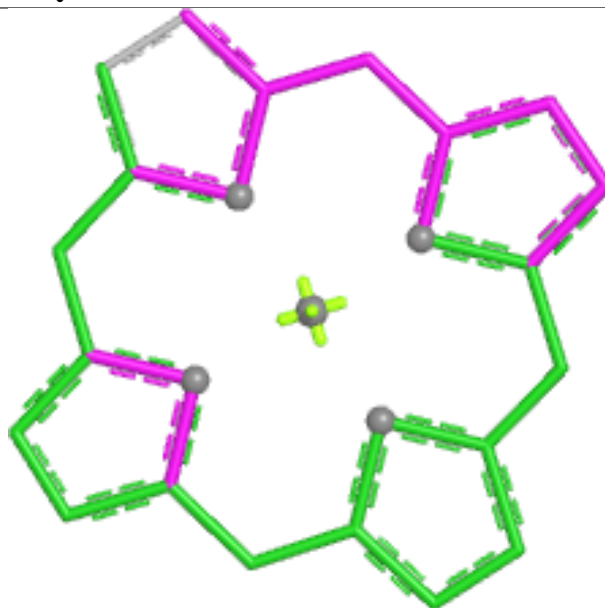


Rings

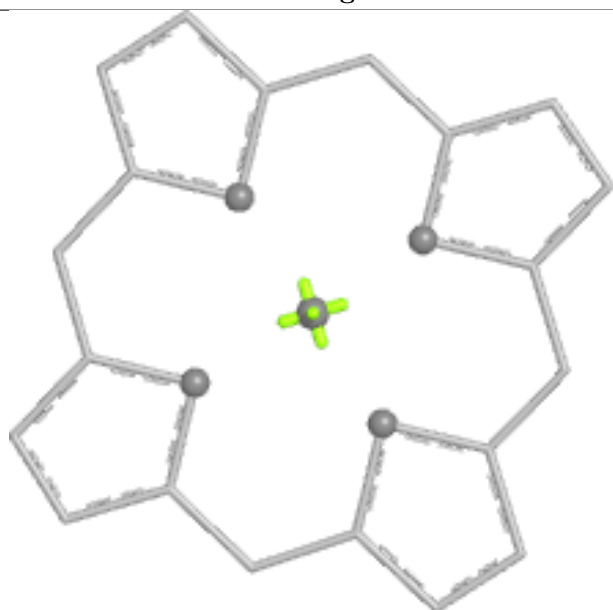
Ligand CLA Q 5207



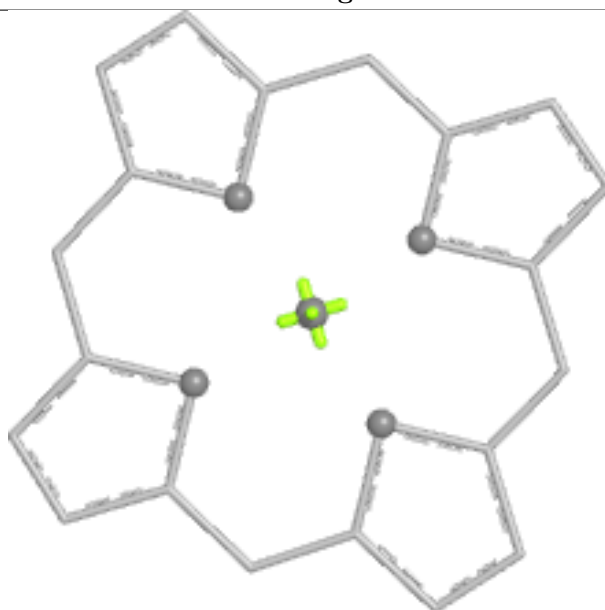
Bond lengths



Bond angles

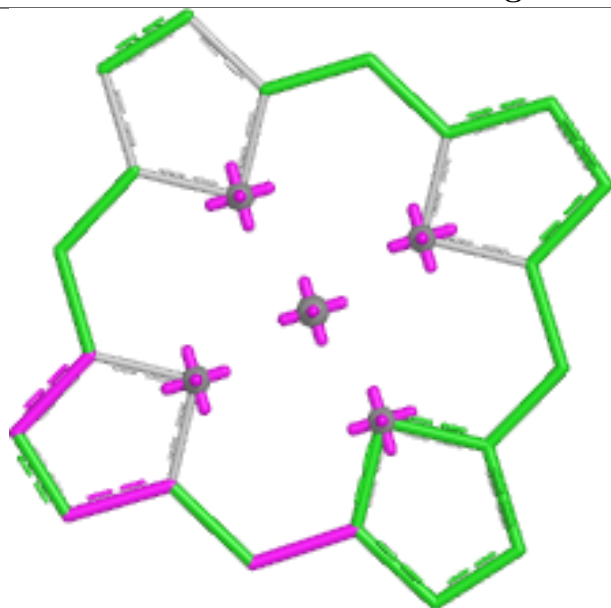


Torsions

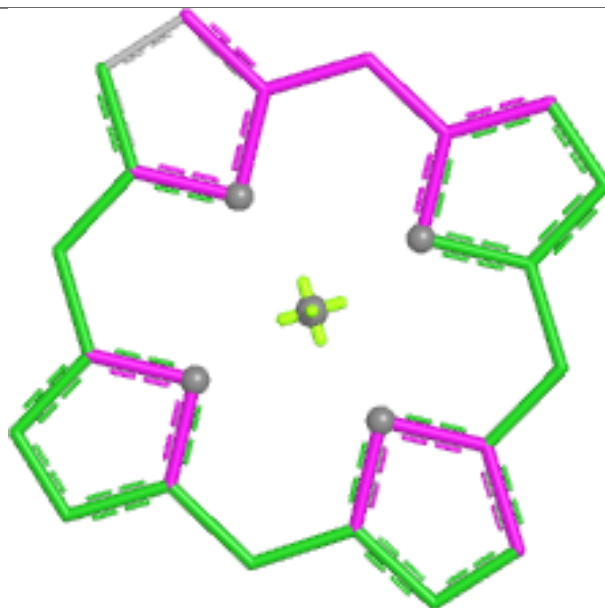


Rings

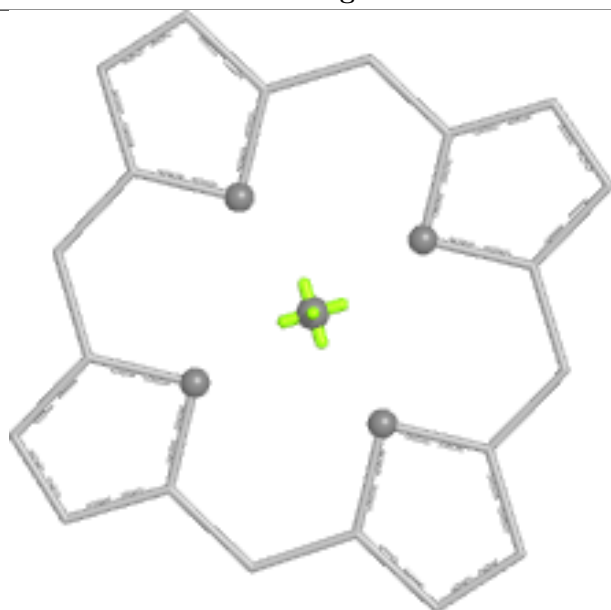
Ligand CLA A 1102



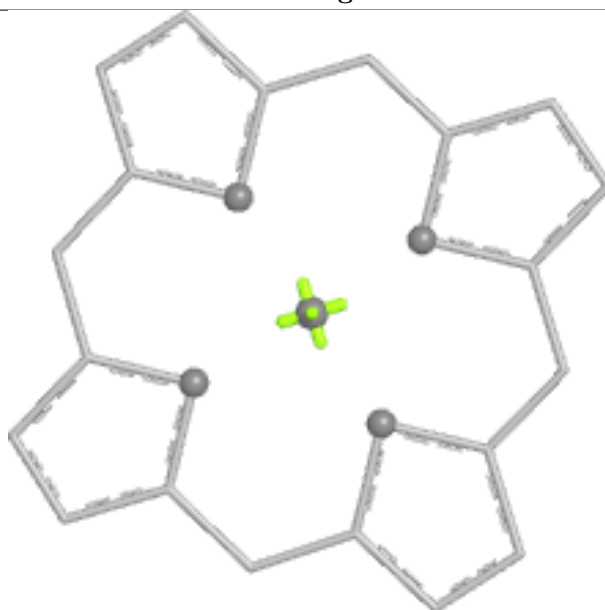
Bond lengths



Bond angles

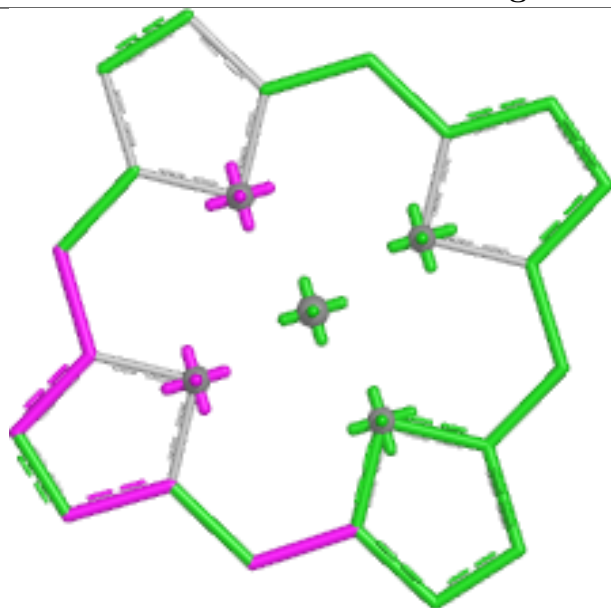


Torsions

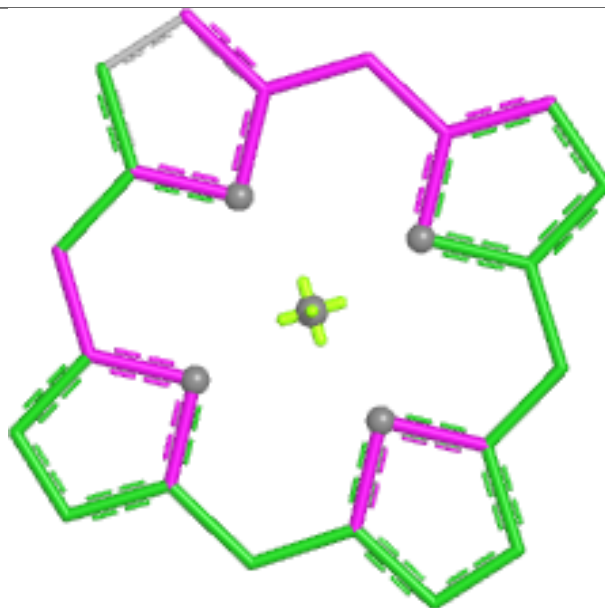


Rings

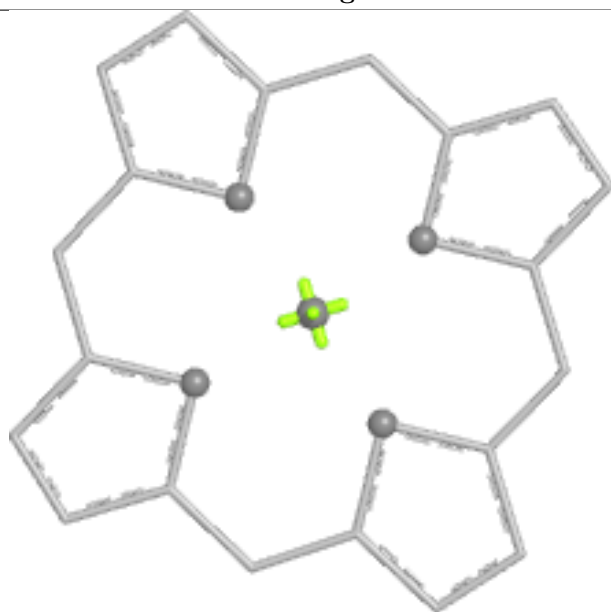
Ligand CLA 2 1022



Bond lengths



Bond angles

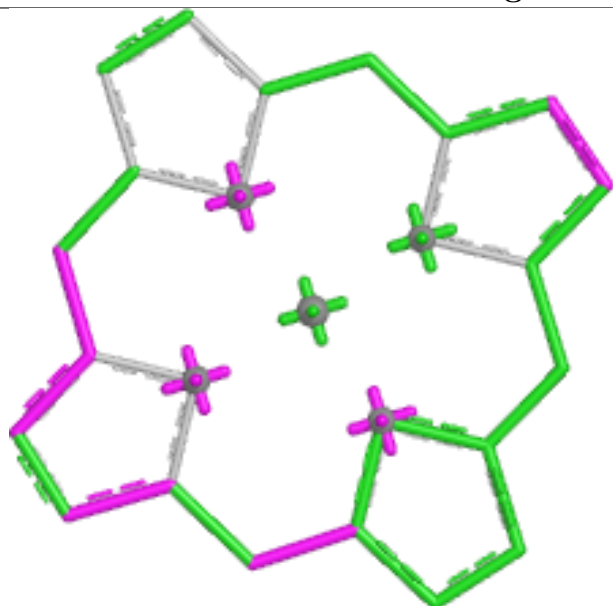


Torsions

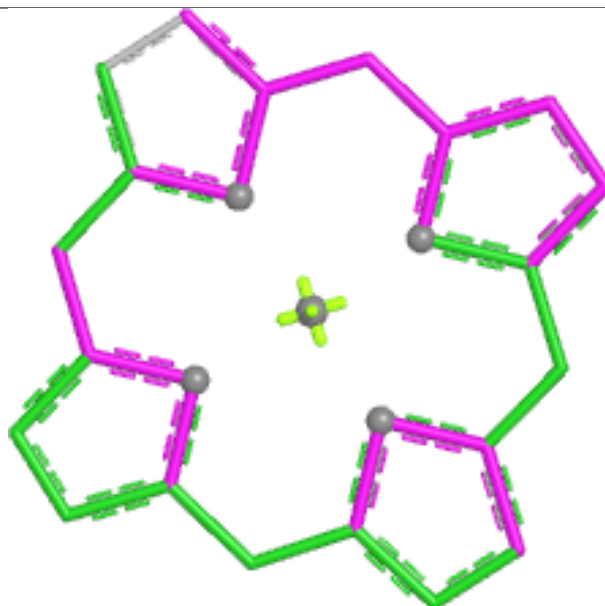


Rings

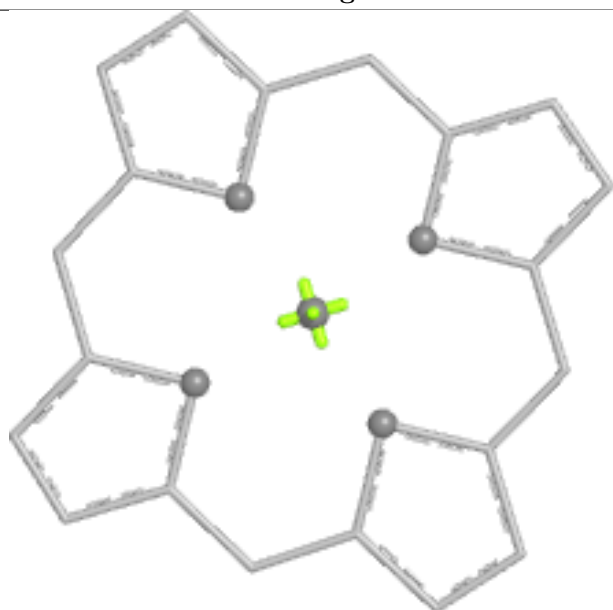
Ligand CLA A 1129



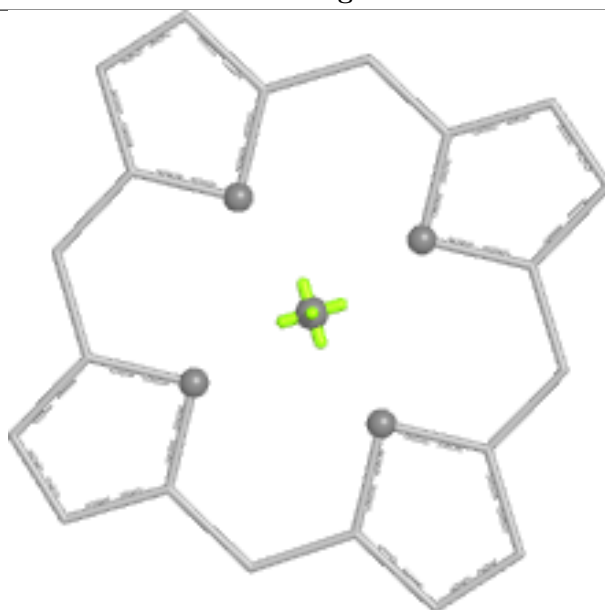
Bond lengths



Bond angles

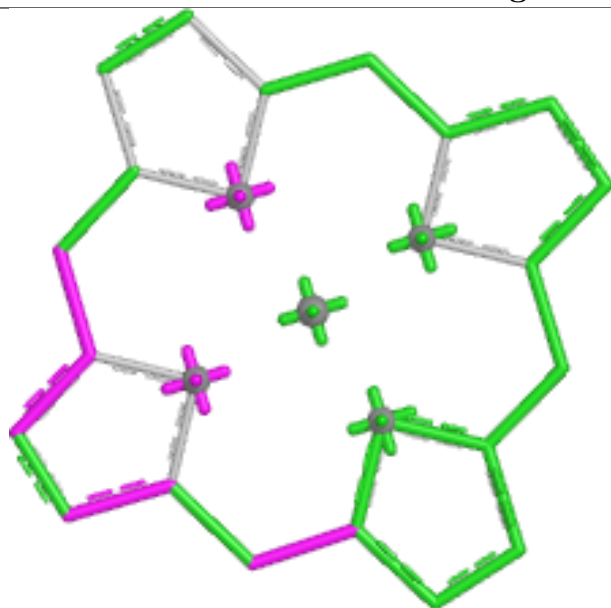


Torsions

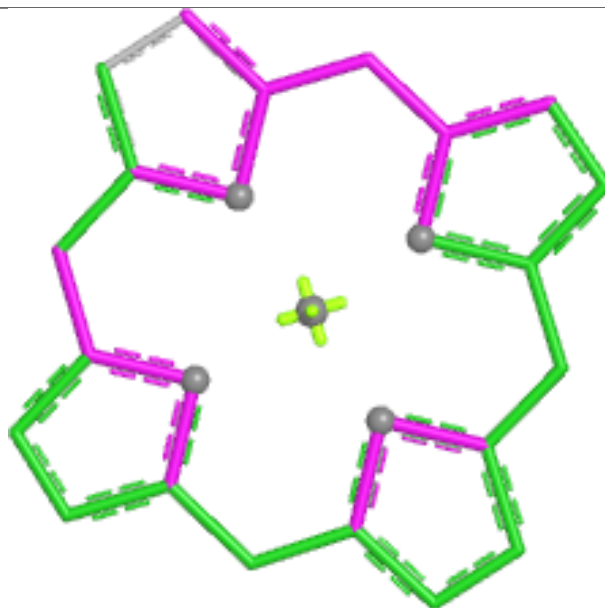


Rings

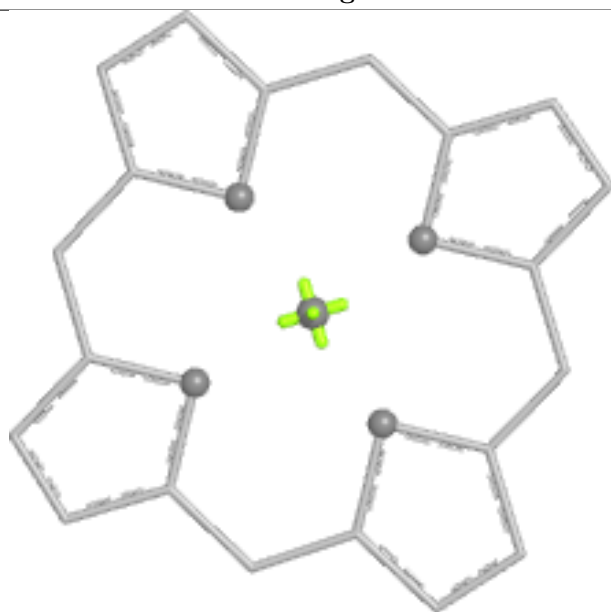
Ligand CLA 0 1025



Bond lengths



Bond angles

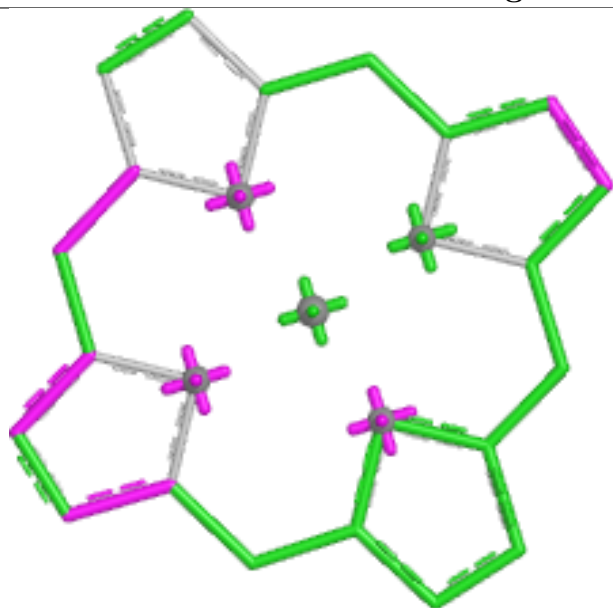


Torsions

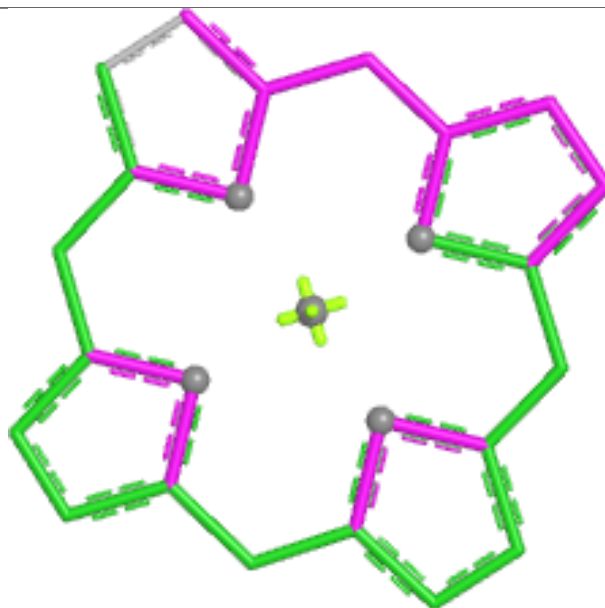


Rings

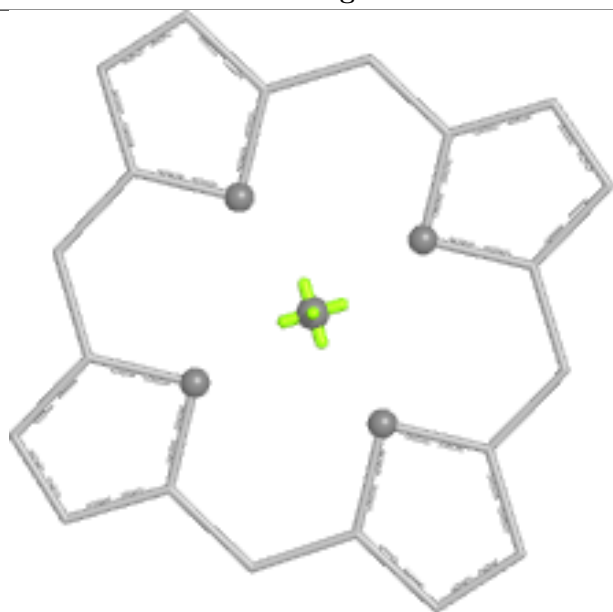
Ligand CLA B 1130



Bond lengths



Bond angles

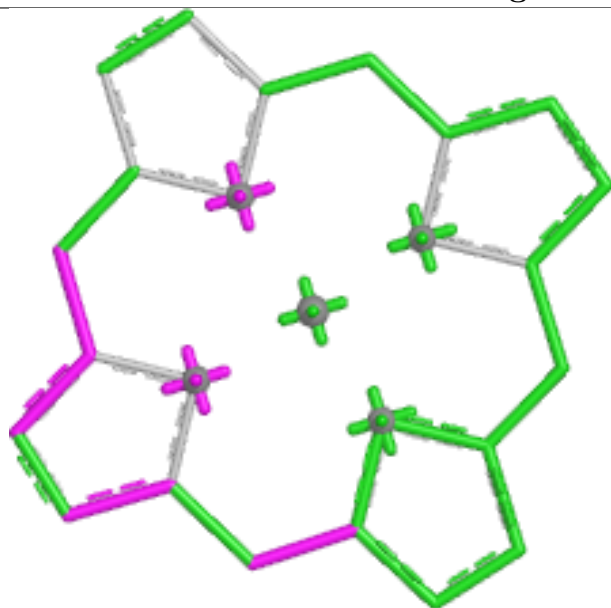


Torsions



Rings

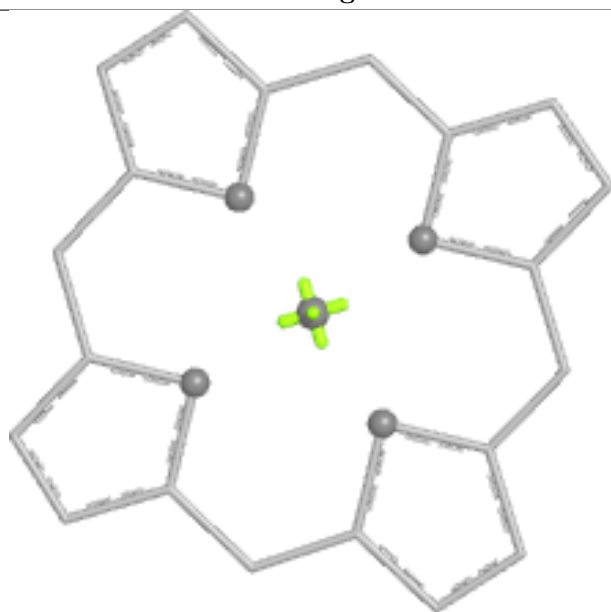
Ligand CLA 3 1033



Bond lengths



Bond angles

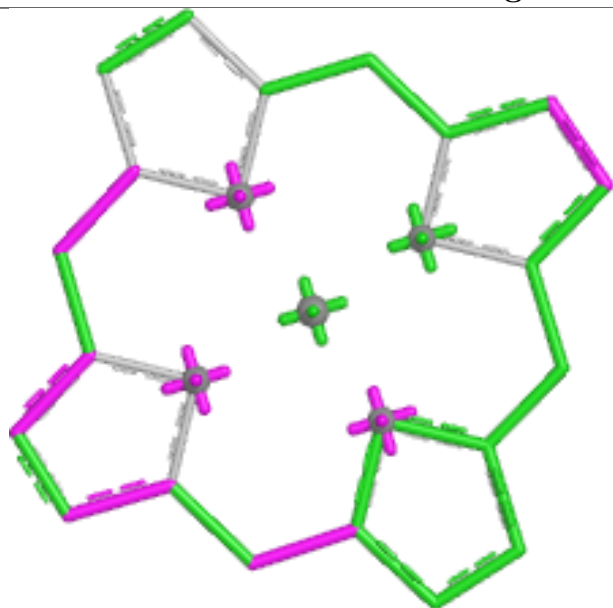


Torsions

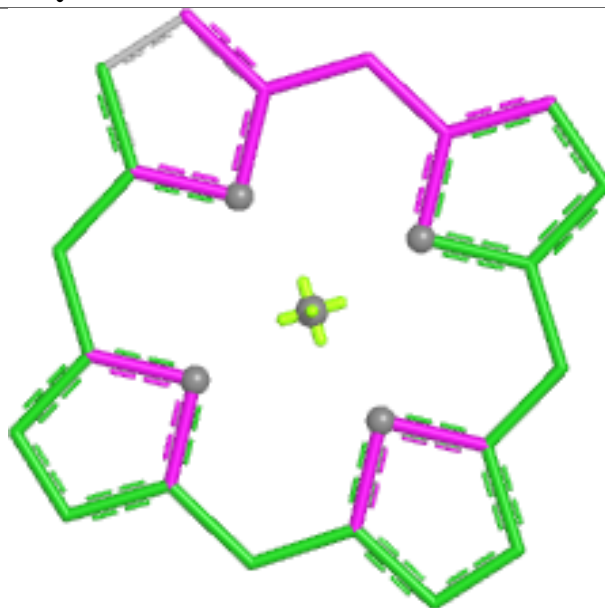


Rings

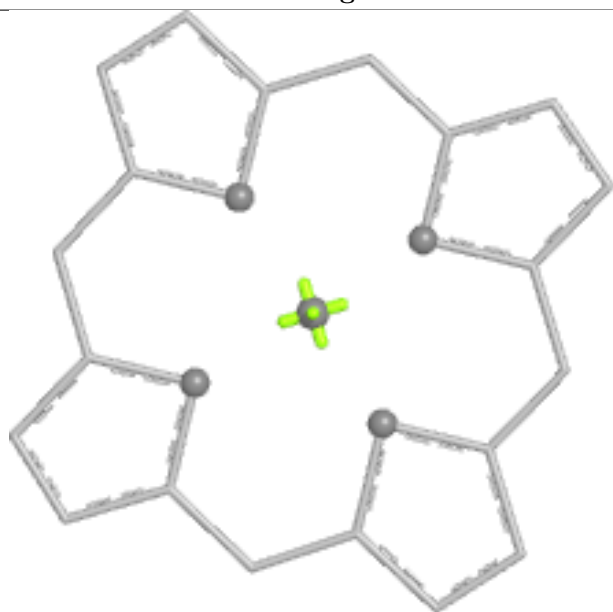
Ligand CLA Q 5234



Bond lengths



Bond angles

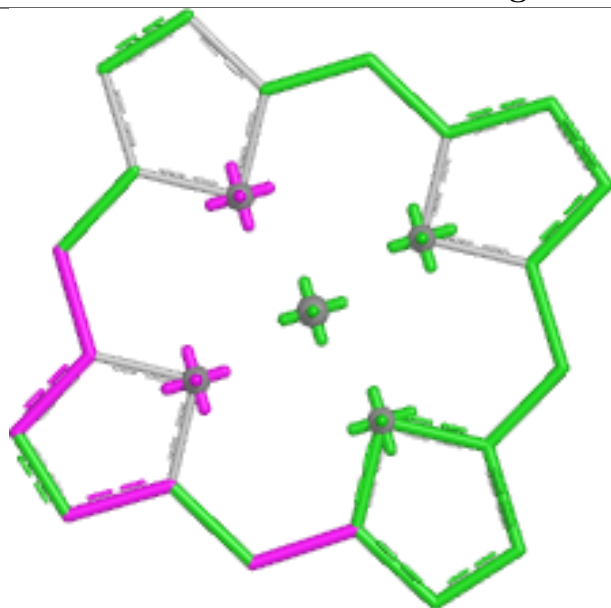


Torsions

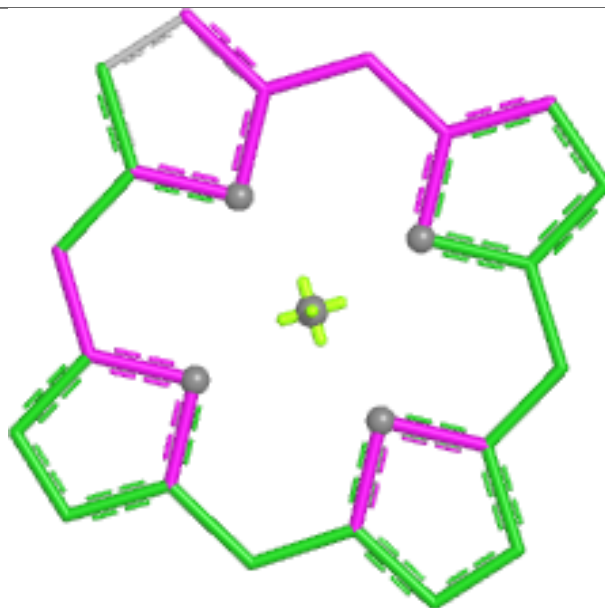


Rings

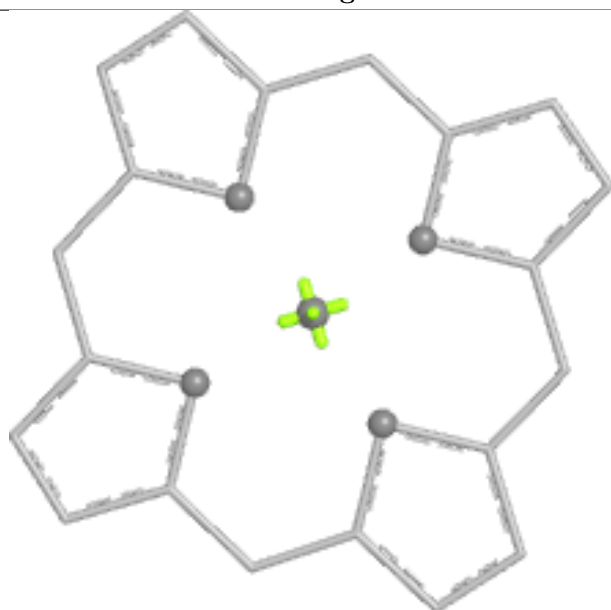
Ligand CLA 9 1012



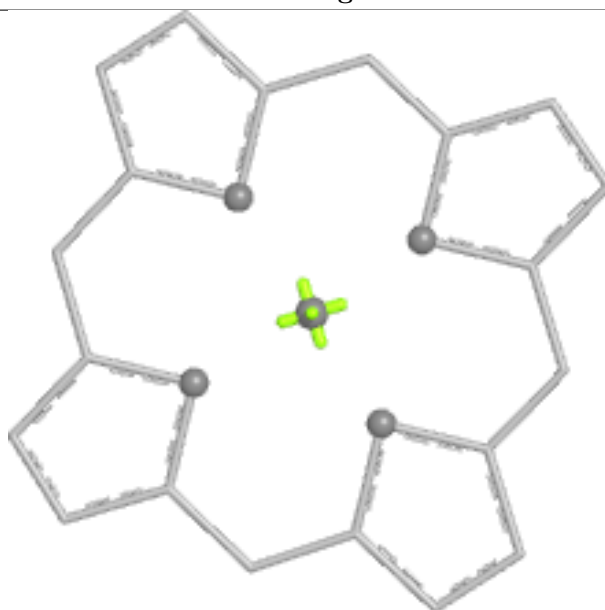
Bond lengths



Bond angles

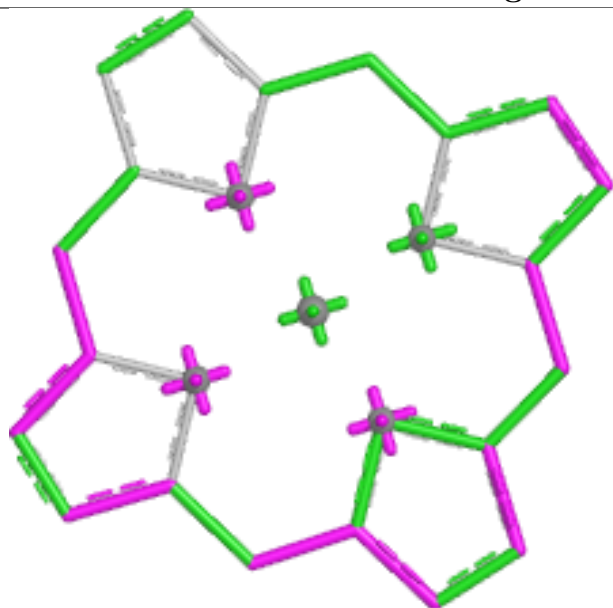


Torsions

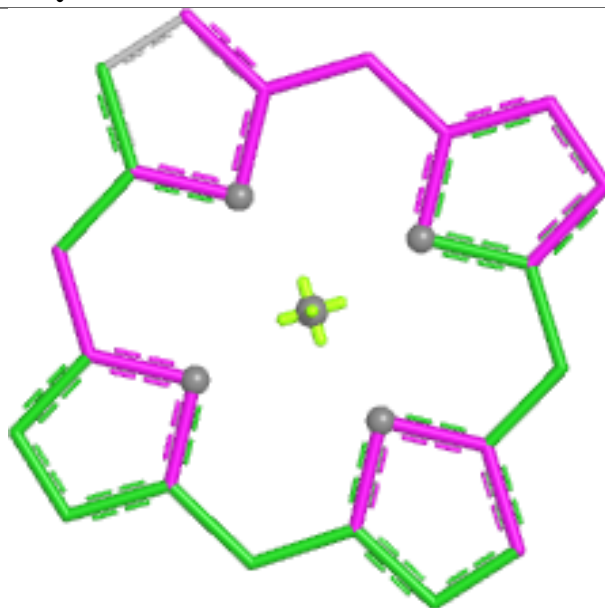


Rings

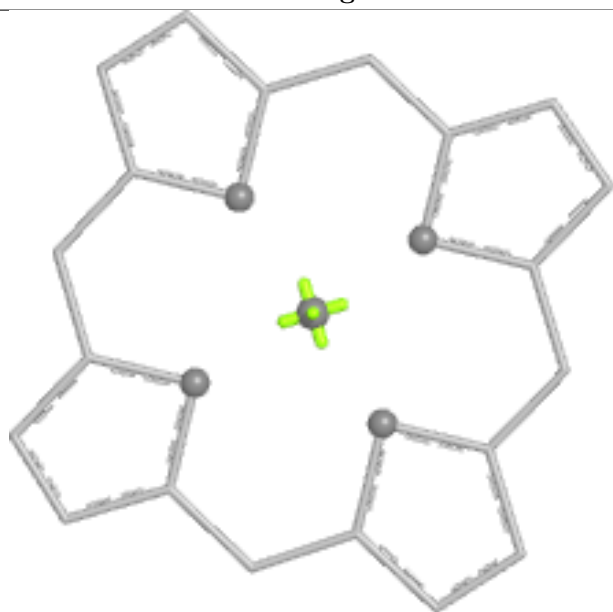
Ligand CLA Q 5023



Bond lengths



Bond angles

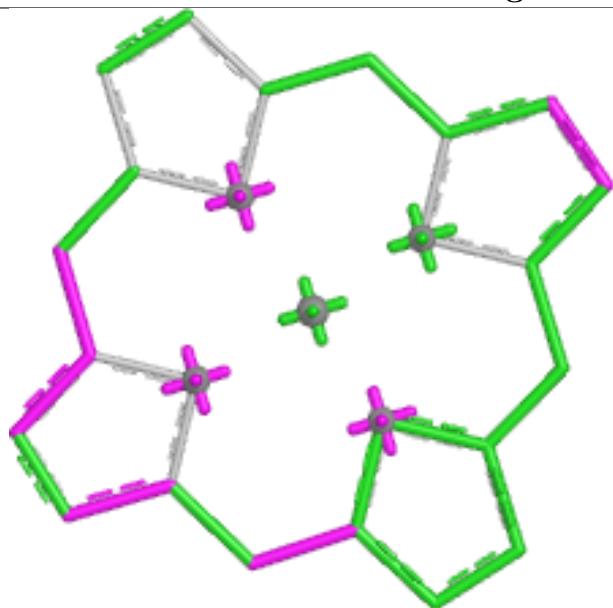


Torsions

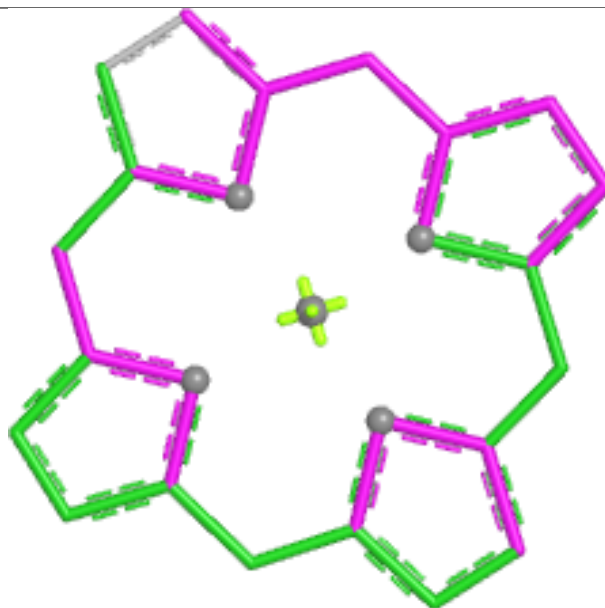


Rings

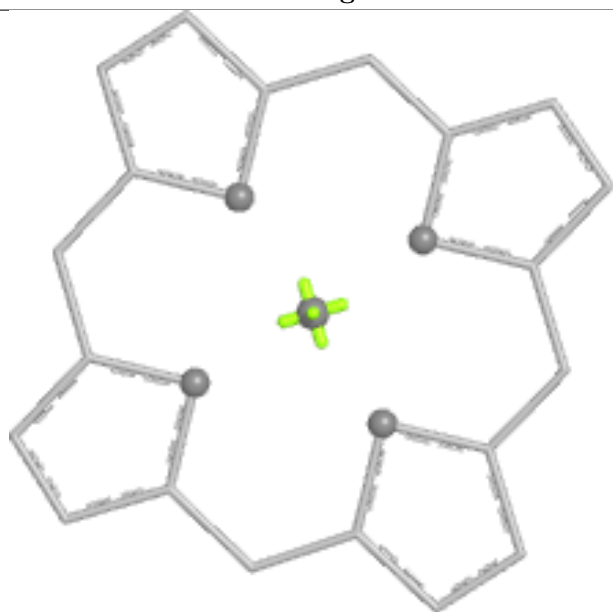
Ligand CLA P 5129



Bond lengths



Bond angles

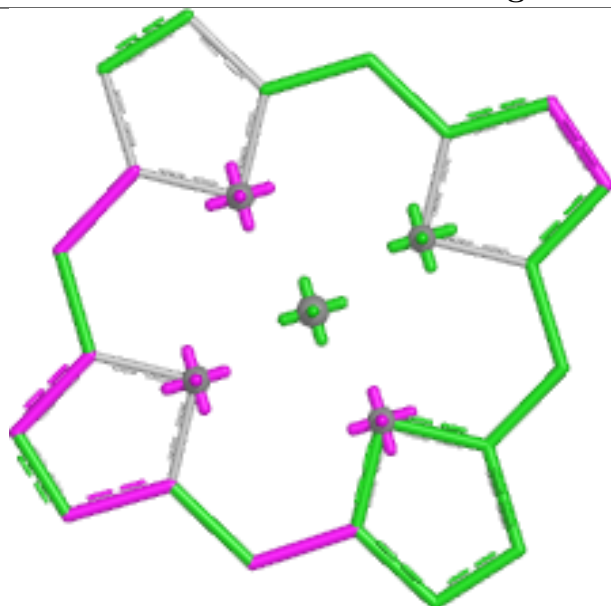


Torsions

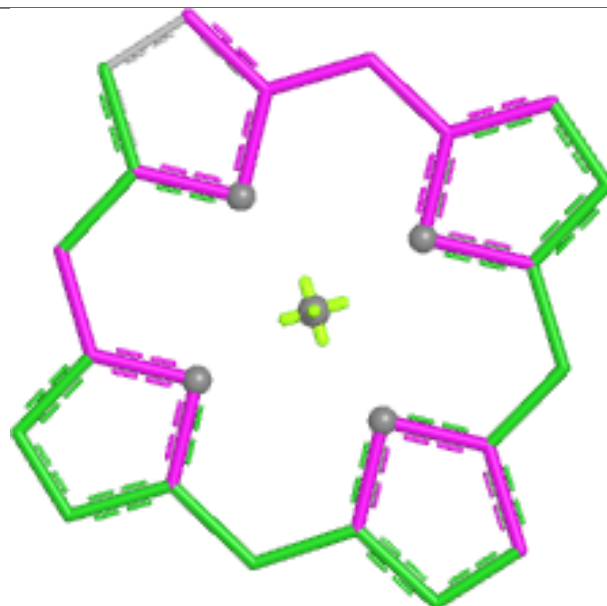


Rings

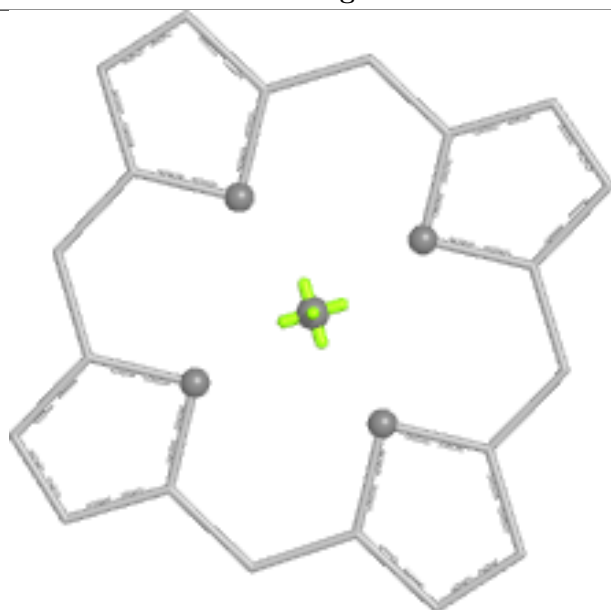
Ligand CLA Z 5302



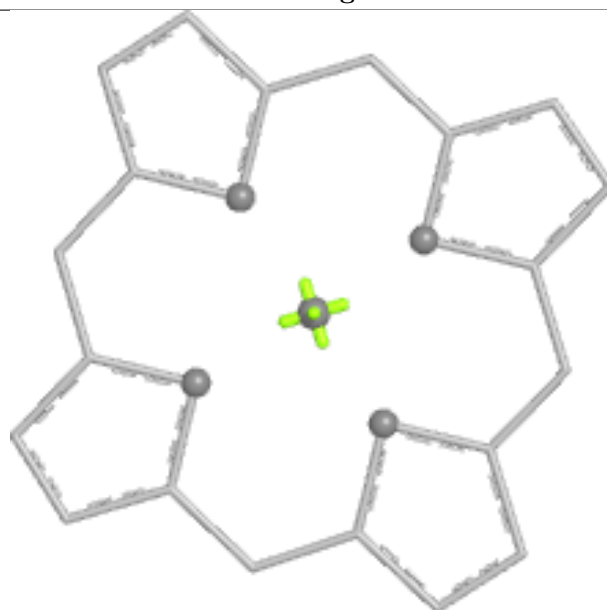
Bond lengths



Bond angles

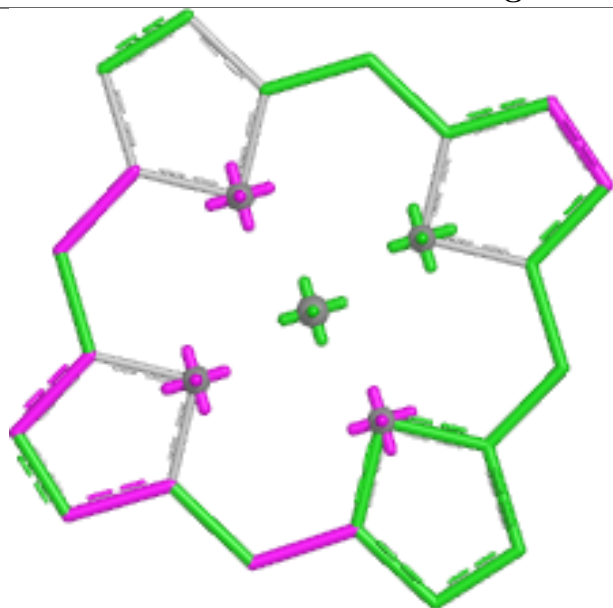


Torsions

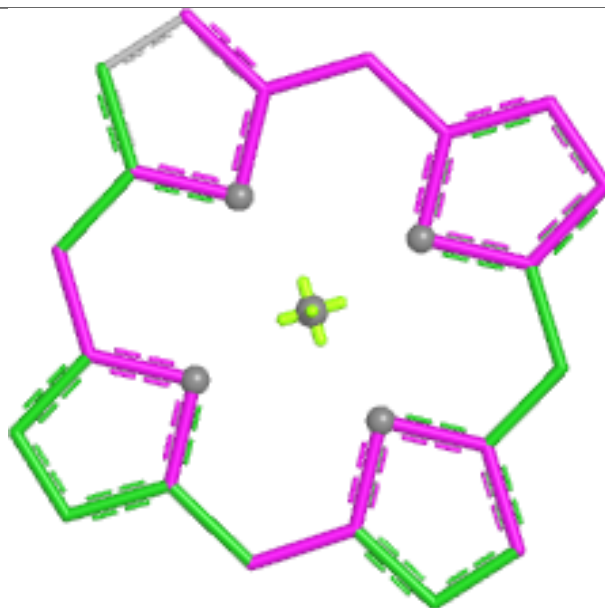


Rings

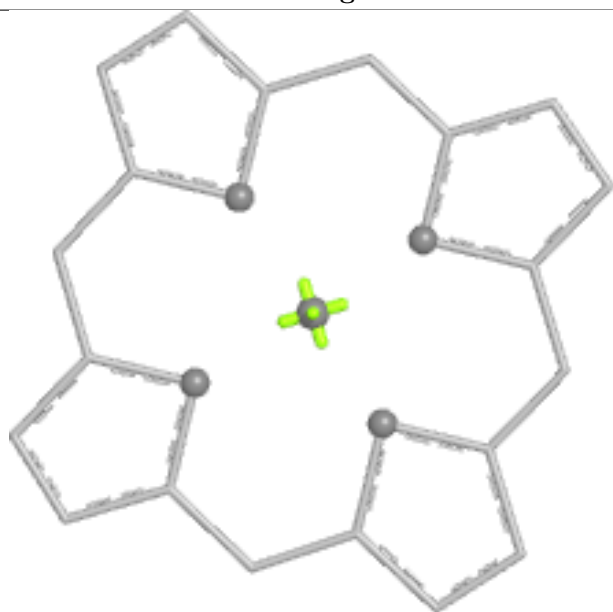
Ligand CLA A 1113



Bond lengths



Bond angles

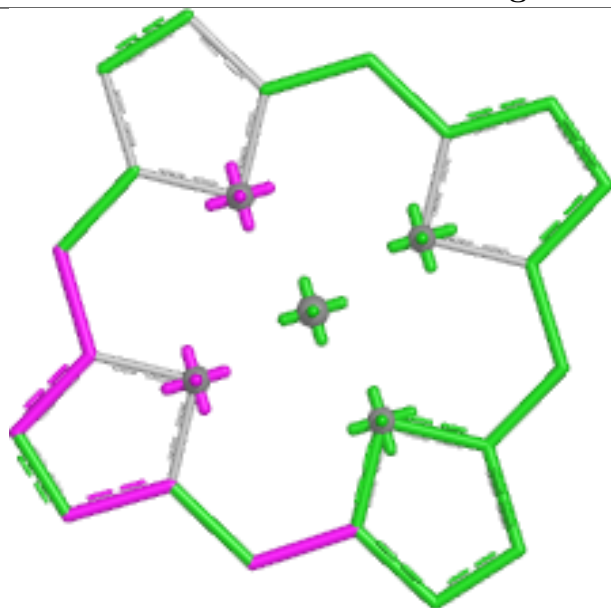


Torsions

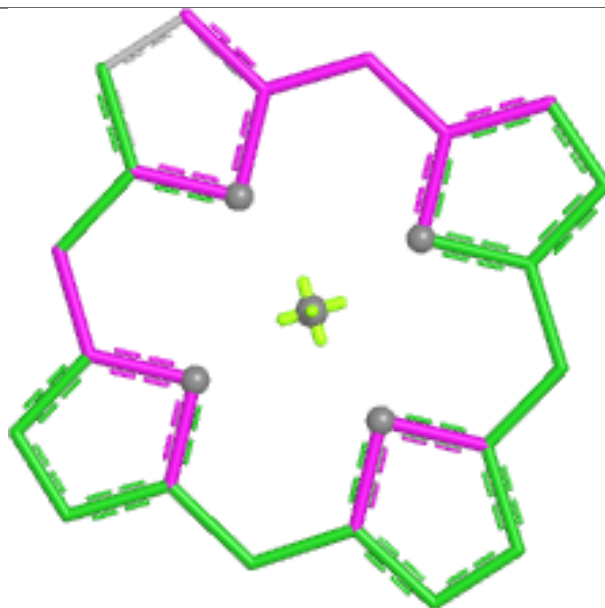


Rings

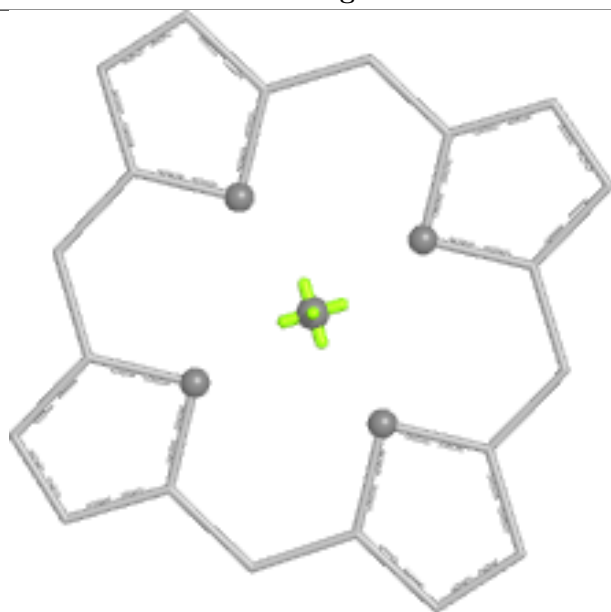
Ligand CLA 3 1026



Bond lengths



Bond angles

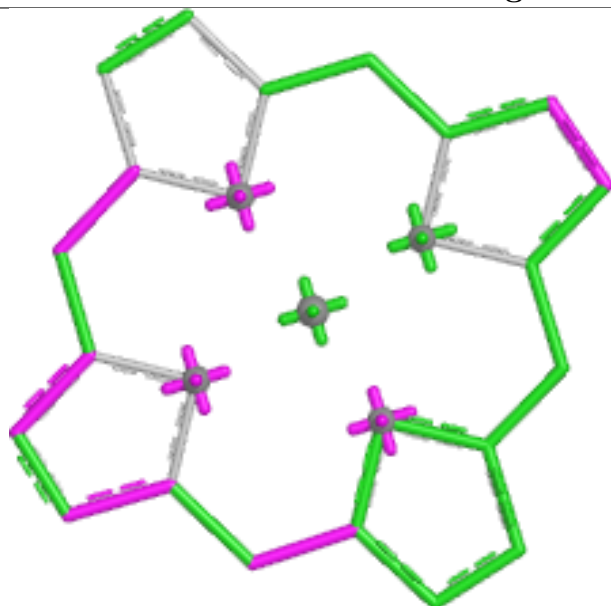


Torsions

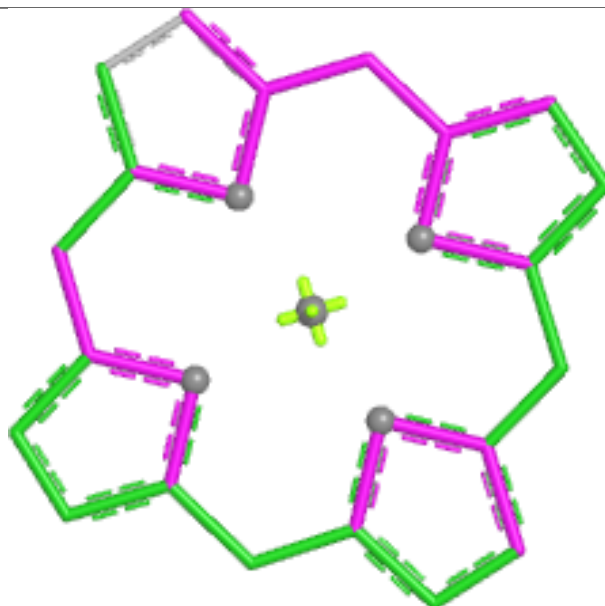


Rings

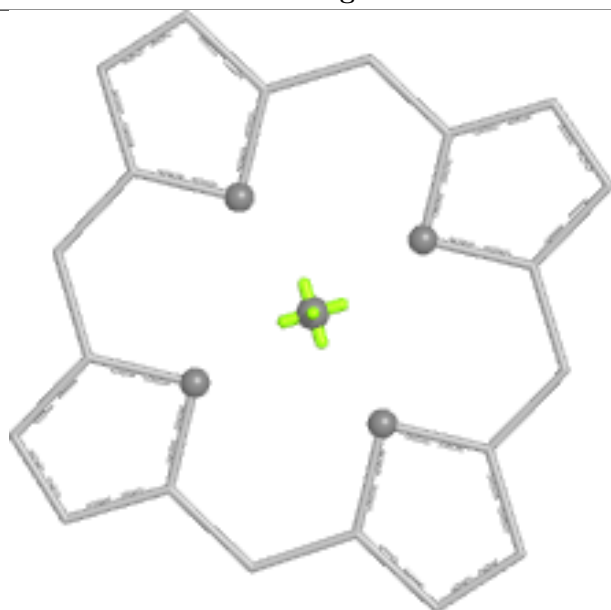
Ligand CLA B 1219



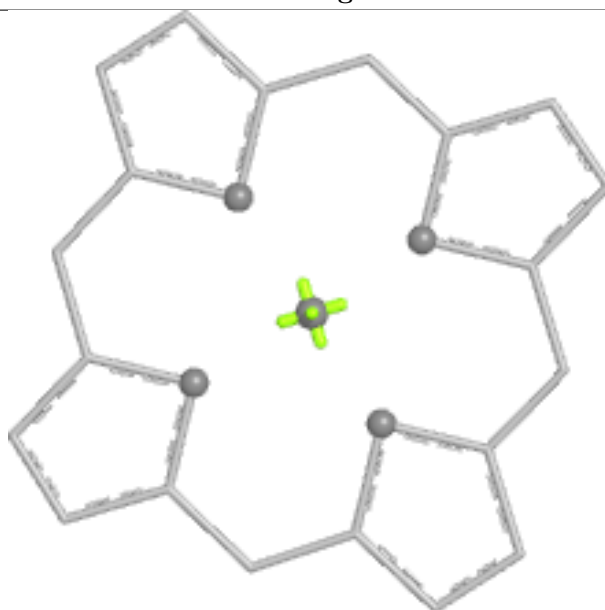
Bond lengths



Bond angles

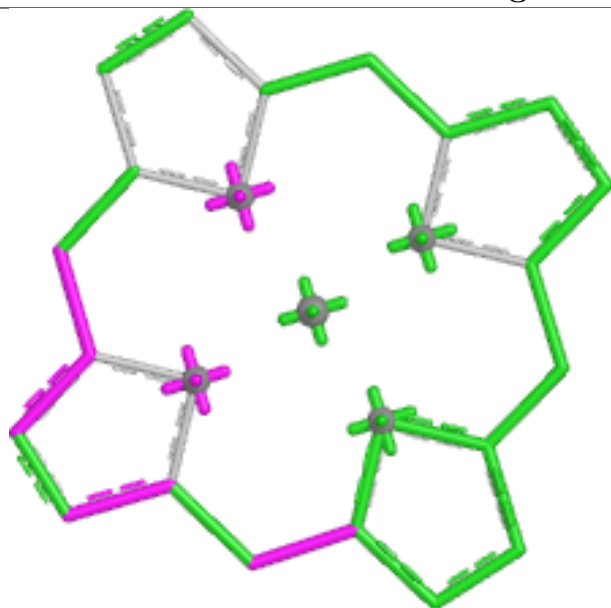


Torsions

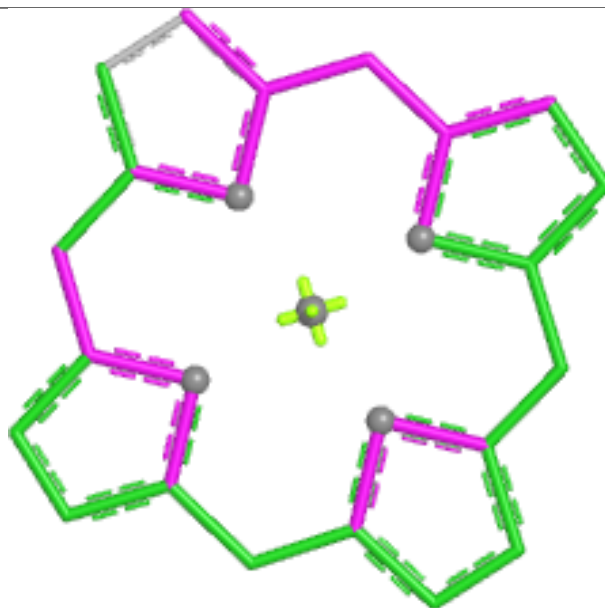


Rings

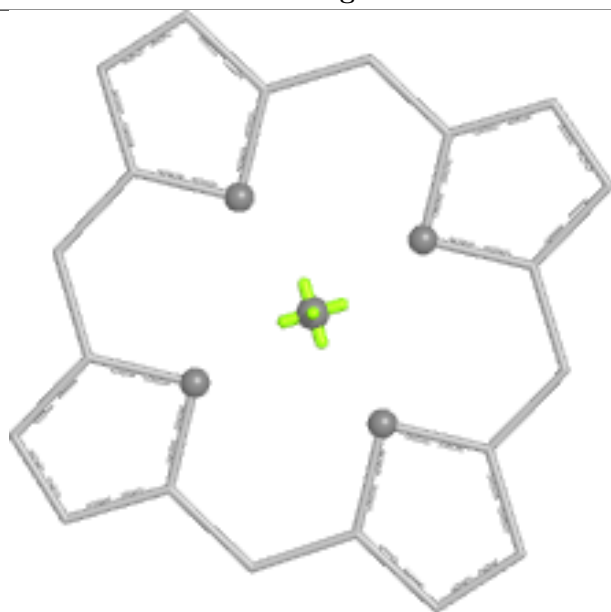
Ligand CLA 0 1012



Bond lengths



Bond angles

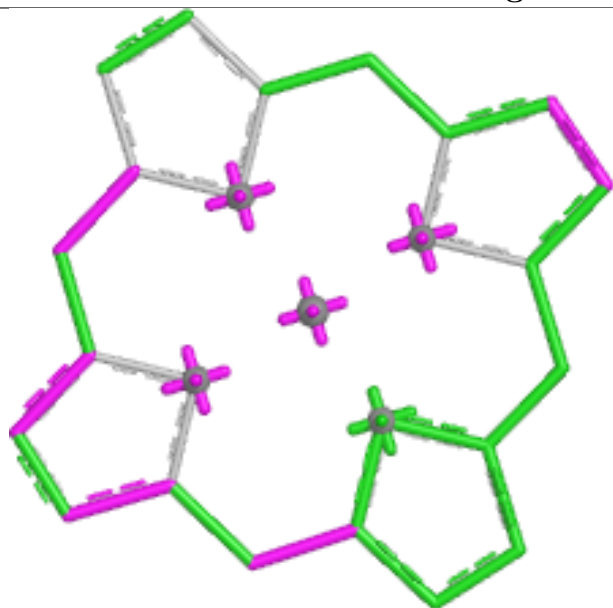


Torsions

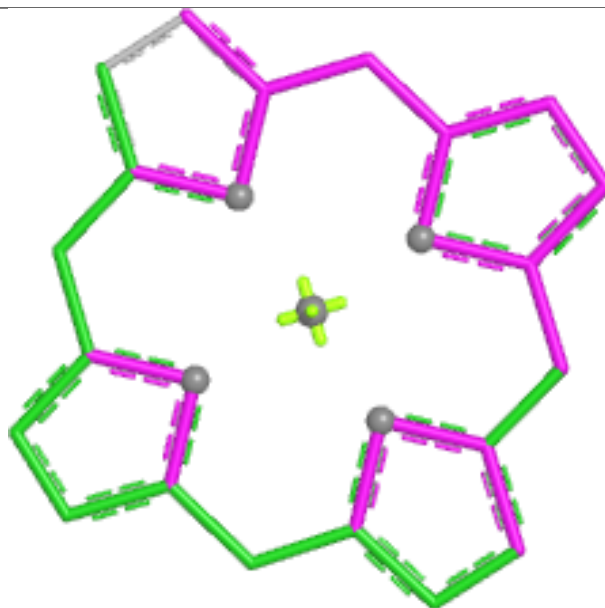


Rings

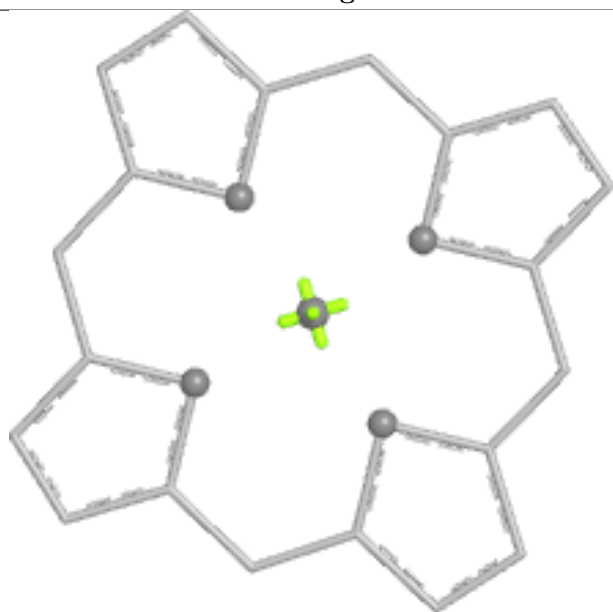
Ligand CLA P 5118



Bond lengths



Bond angles

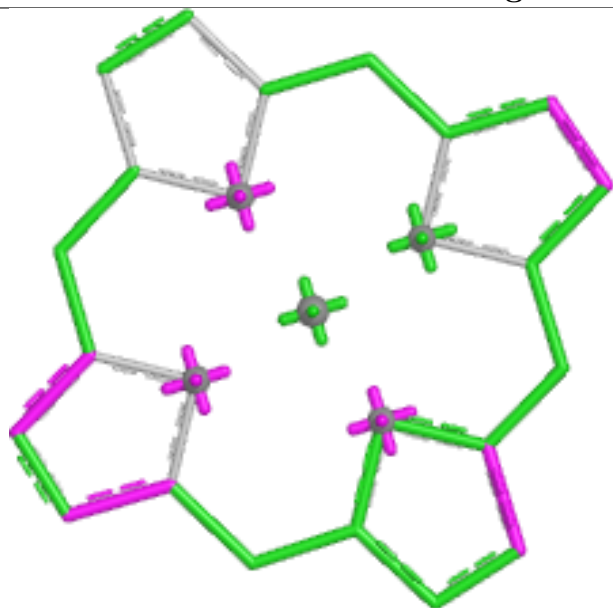


Torsions

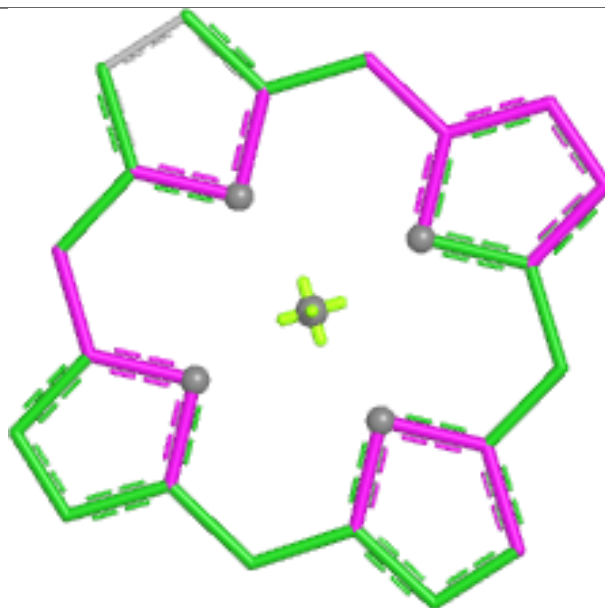


Rings

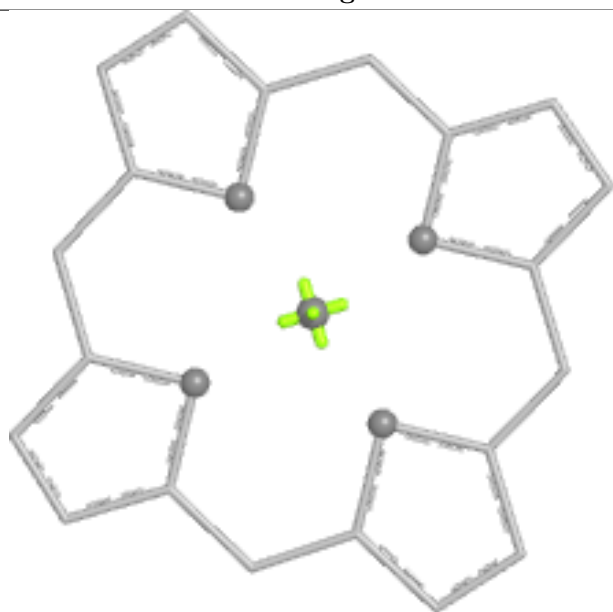
Ligand CLA B 1238



Bond lengths



Bond angles

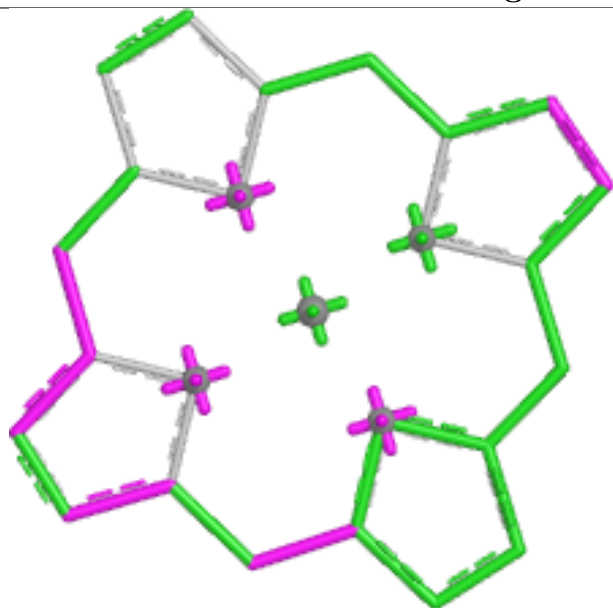


Torsions

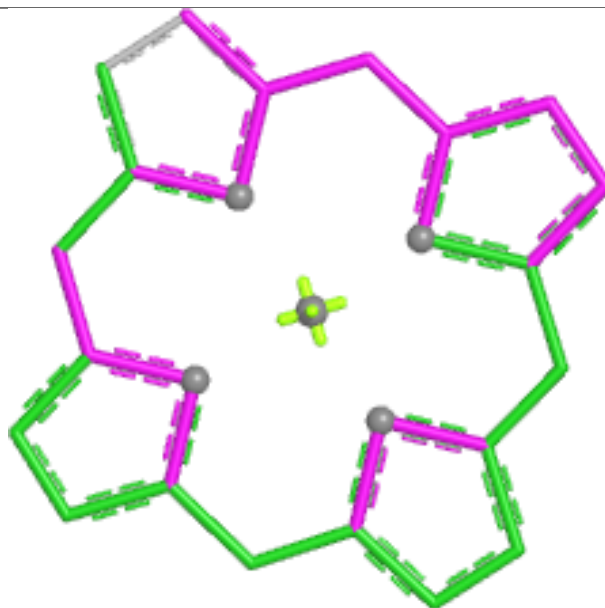


Rings

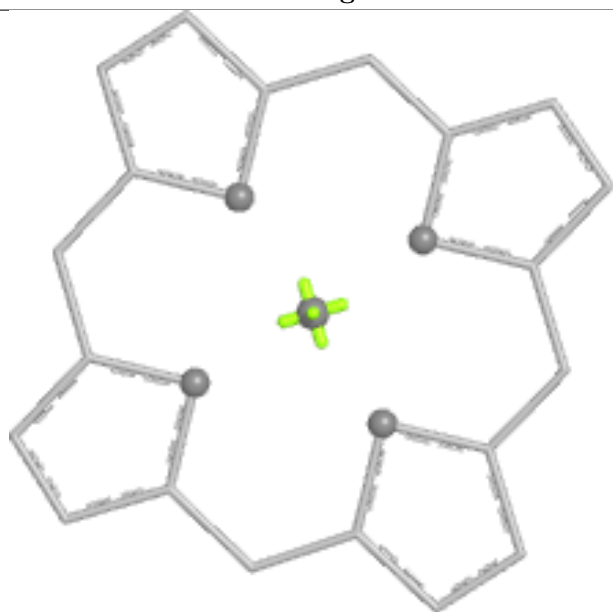
Ligand CLA A 1115



Bond lengths



Bond angles

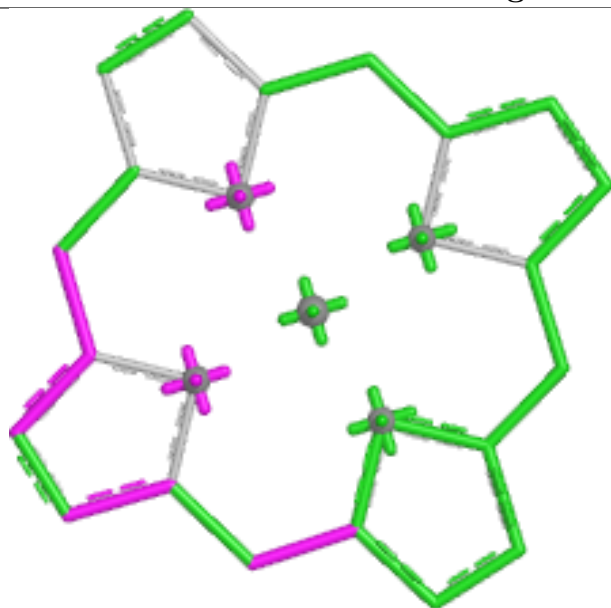


Torsions

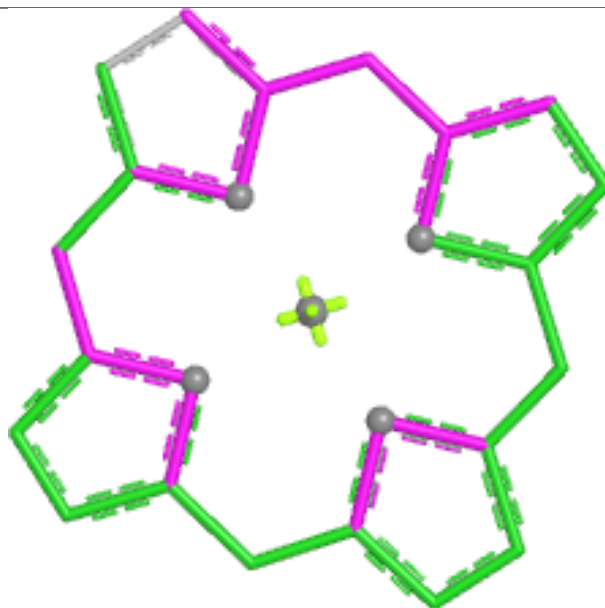


Rings

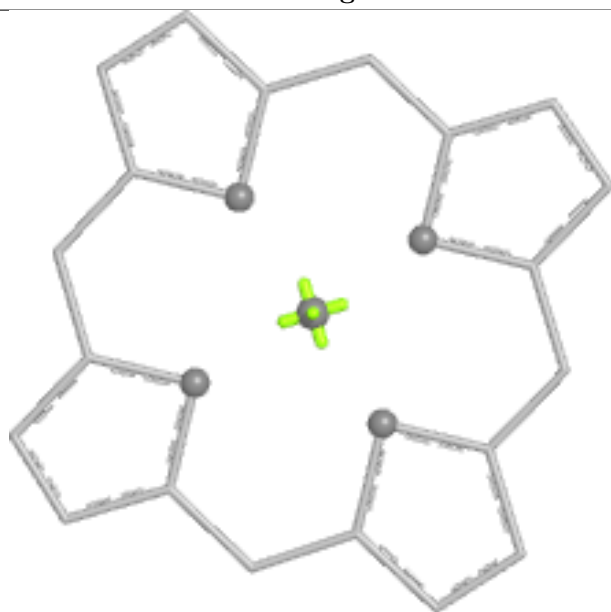
Ligand CLA F 4006



Bond lengths



Bond angles

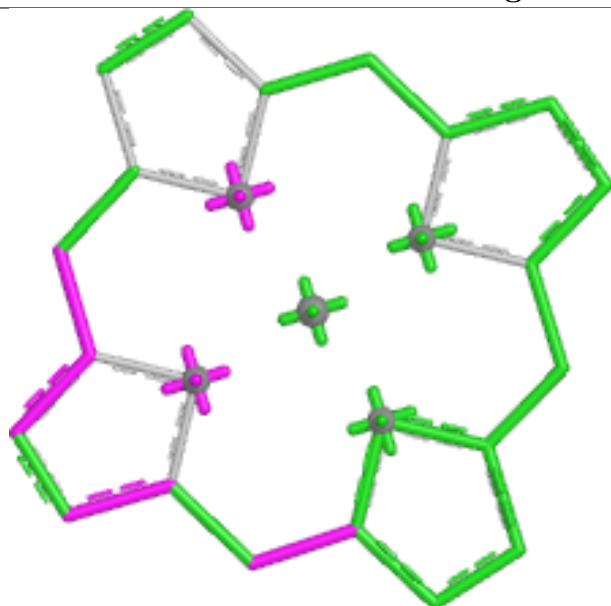


Torsions

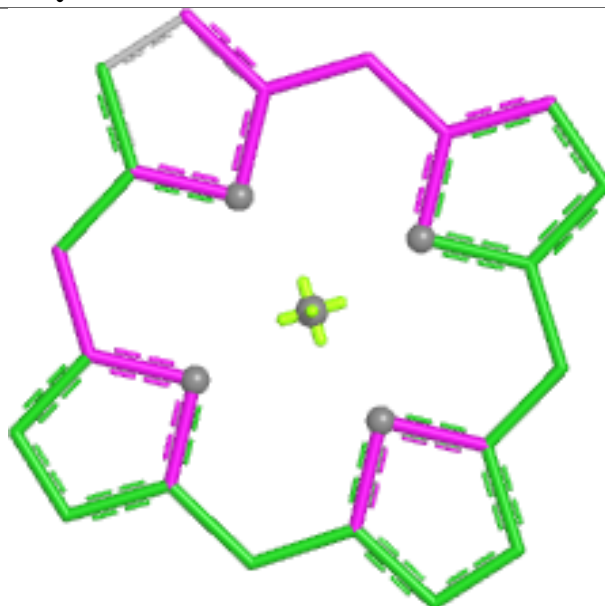


Rings

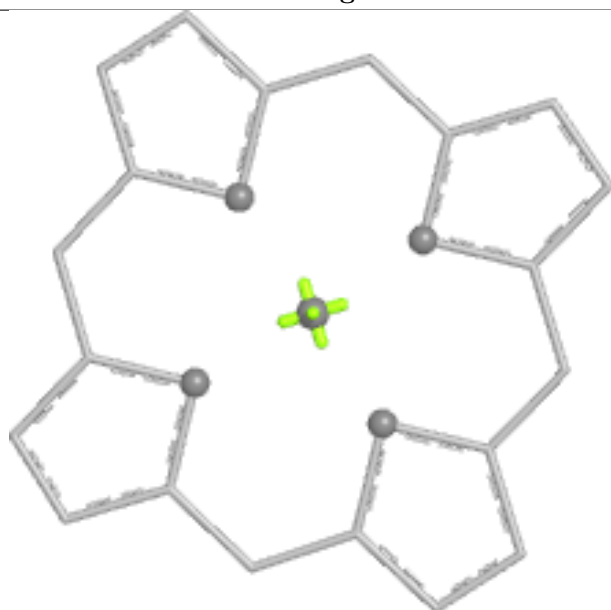
Ligand CLA Q 5241



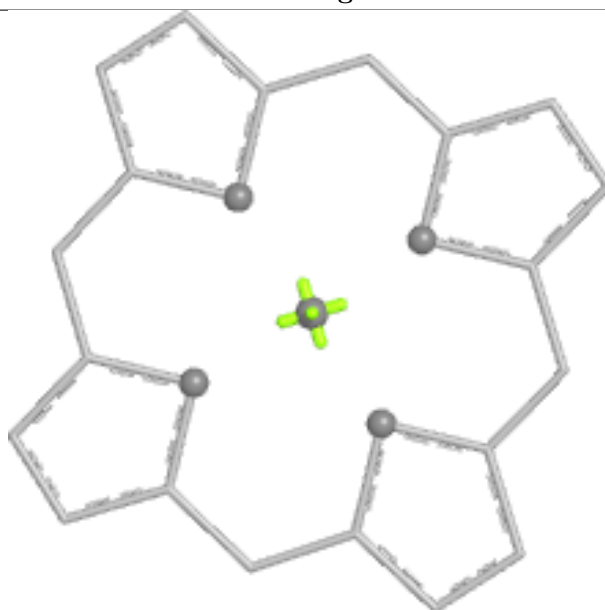
Bond lengths



Bond angles

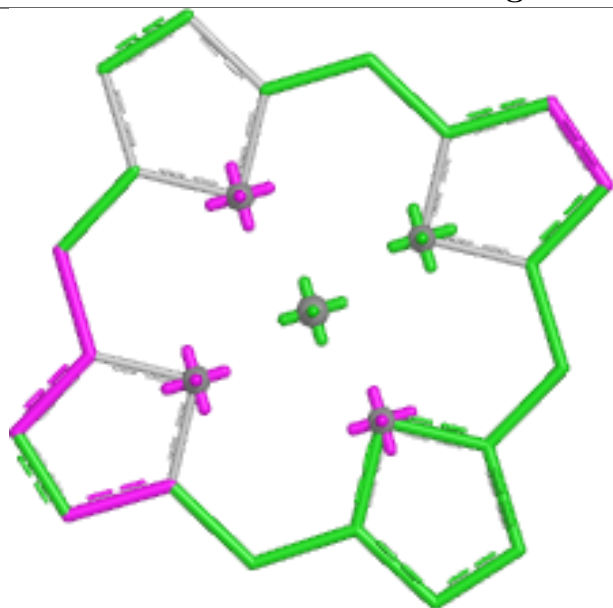


Torsions

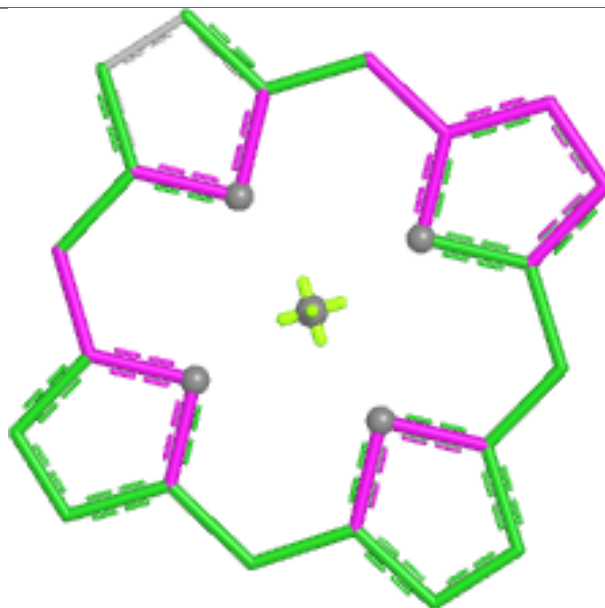


Rings

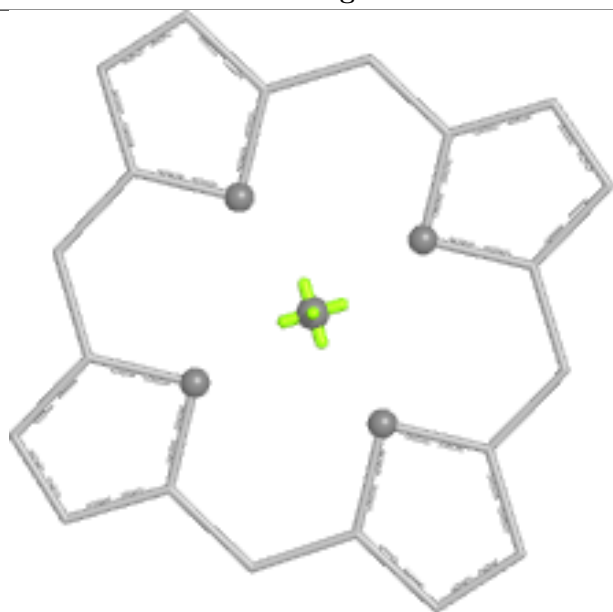
Ligand CLA P 5132



Bond lengths



Bond angles

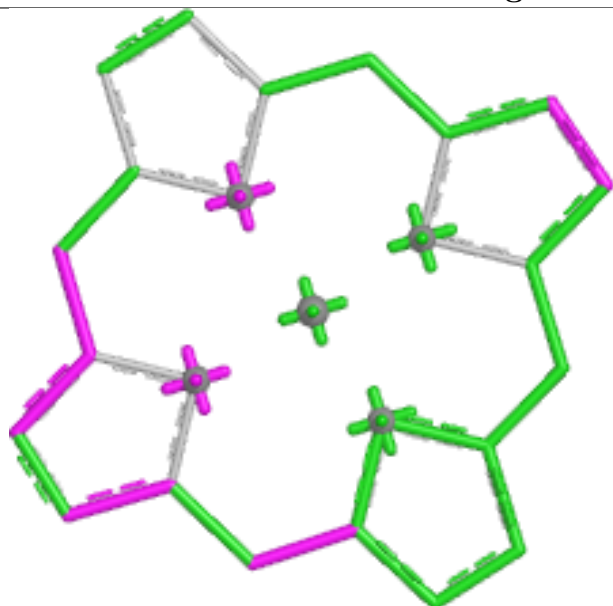


Torsions

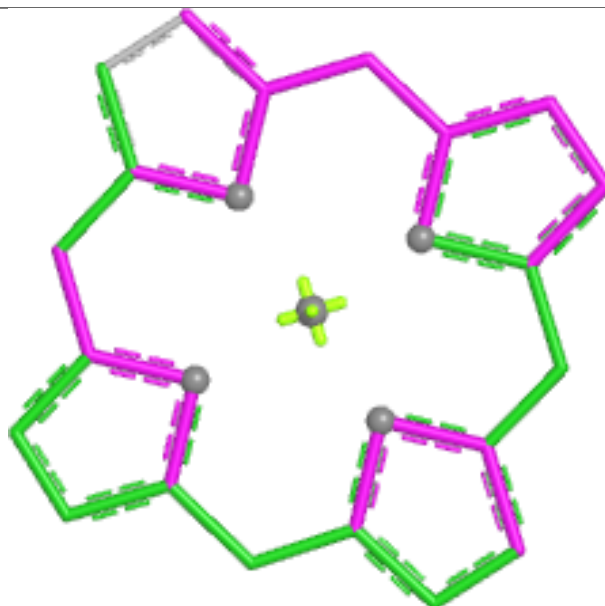


Rings

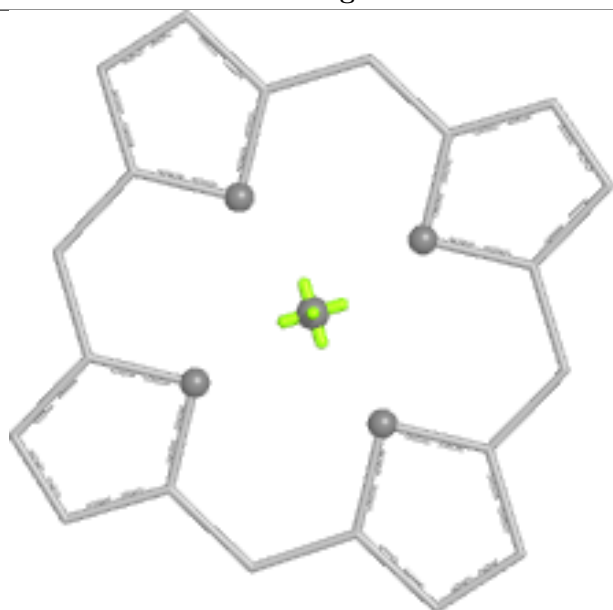
Ligand CLA B 1227



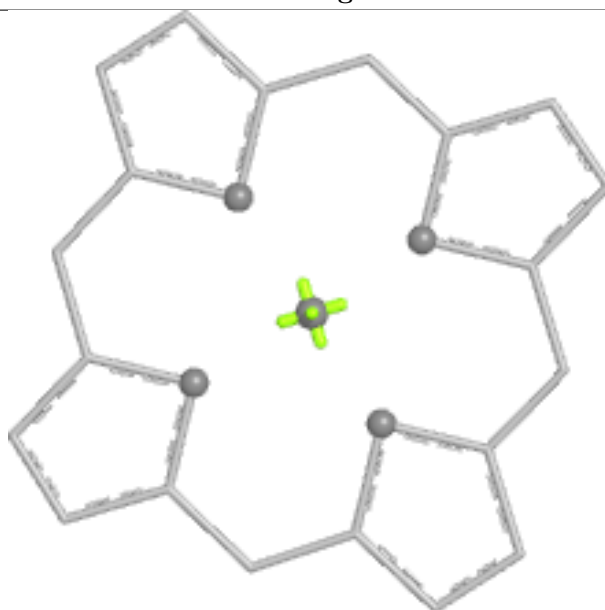
Bond lengths



Bond angles

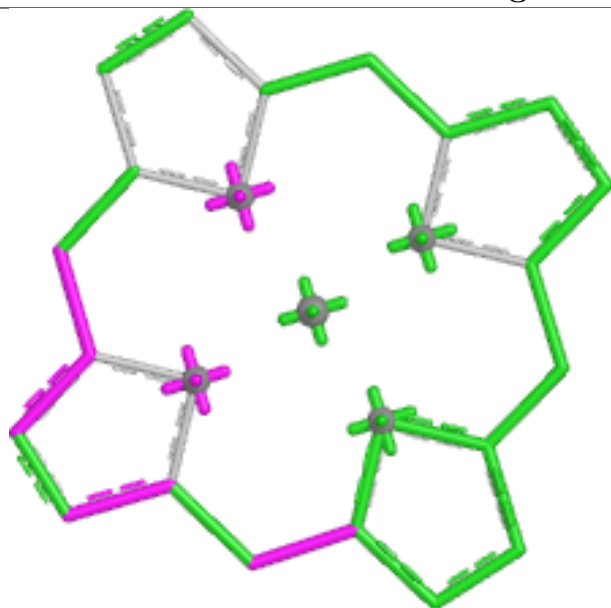


Torsions

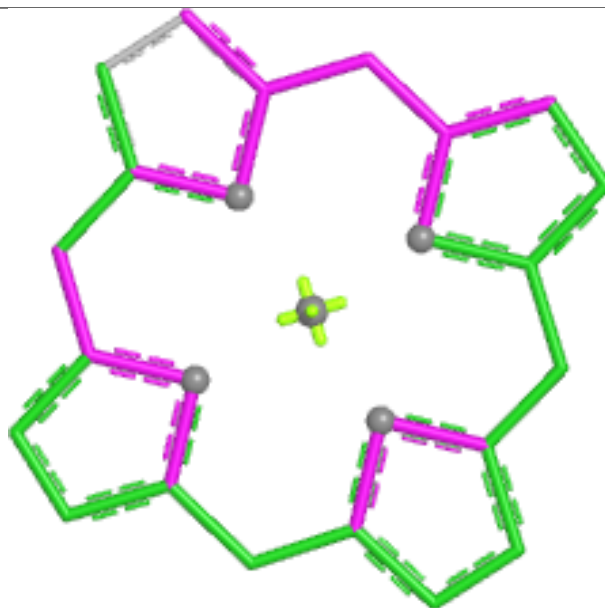


Rings

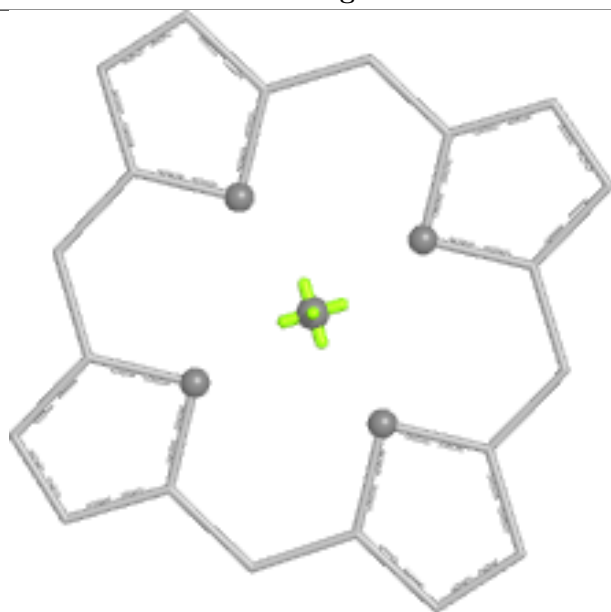
Ligand CLA 8 1025



Bond lengths



Bond angles

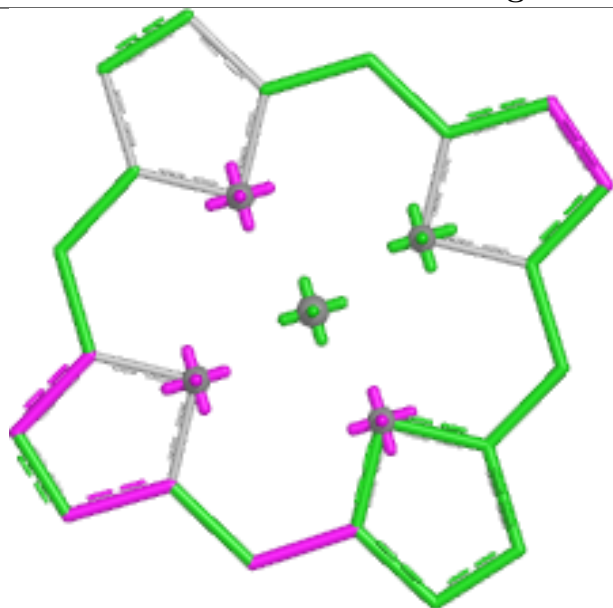


Torsions

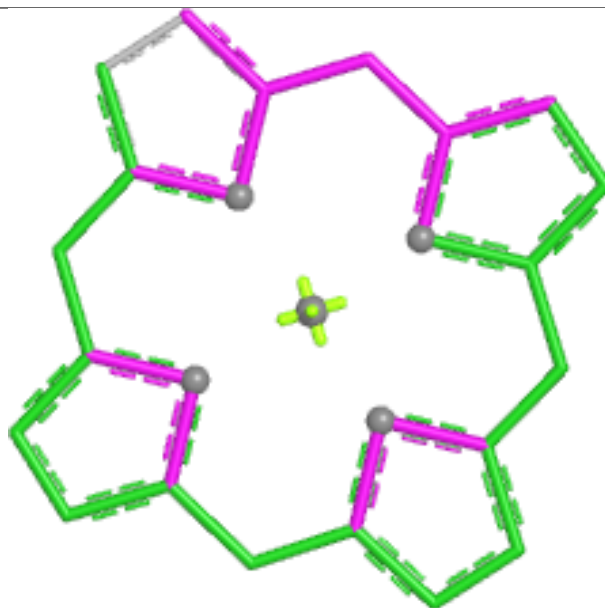


Rings

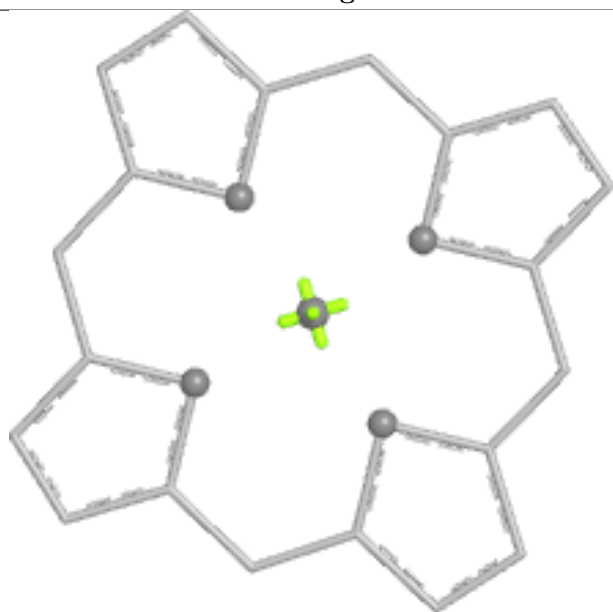
Ligand CLA F 1301



Bond lengths



Bond angles

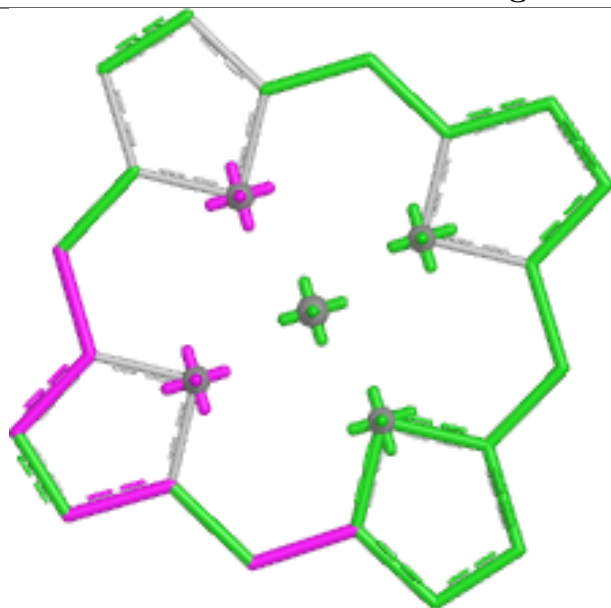


Torsions

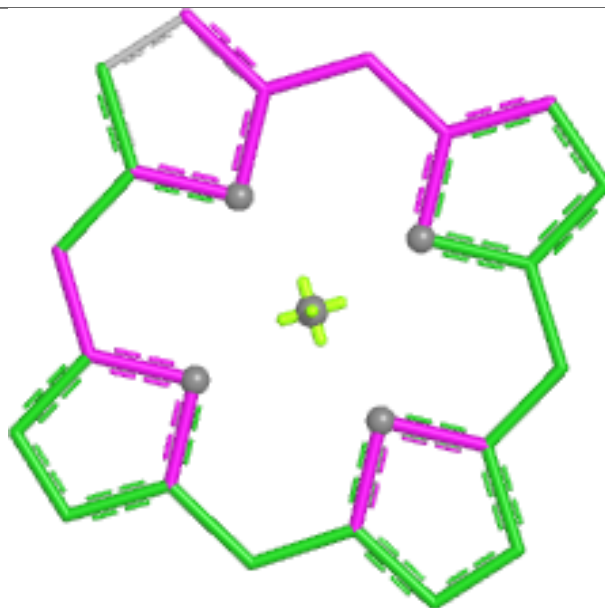


Rings

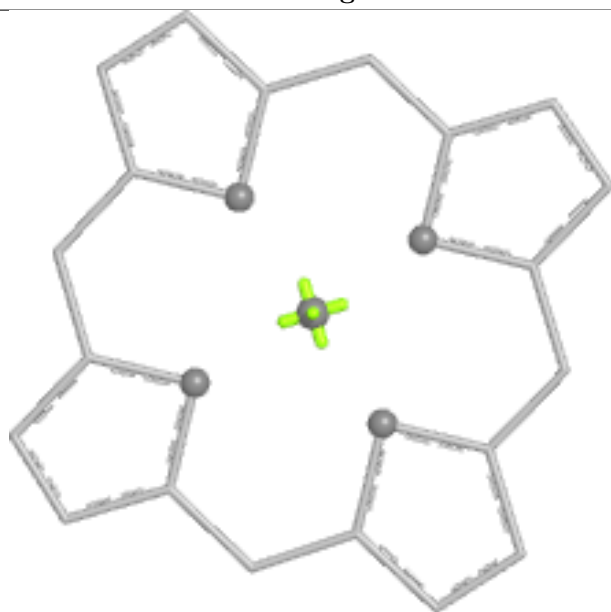
Ligand CLA 0 1014



Bond lengths



Bond angles

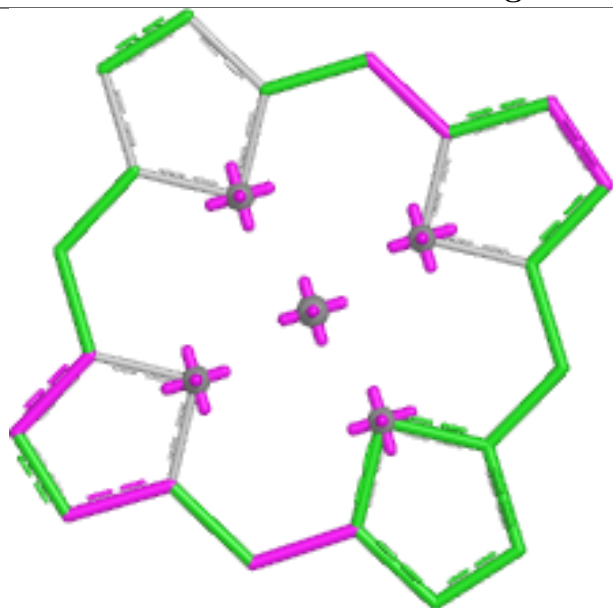


Torsions

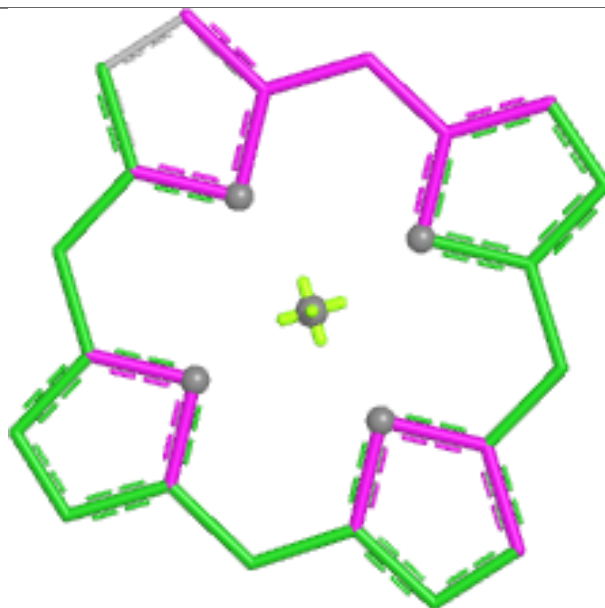


Rings

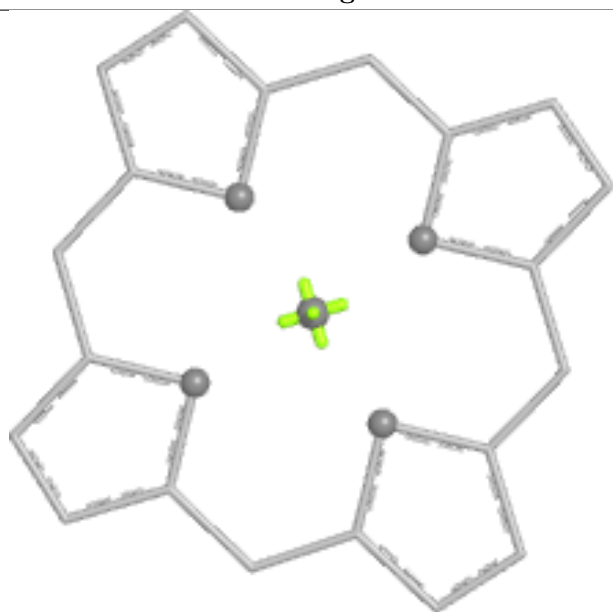
Ligand CLA A 1104



Bond lengths



Bond angles

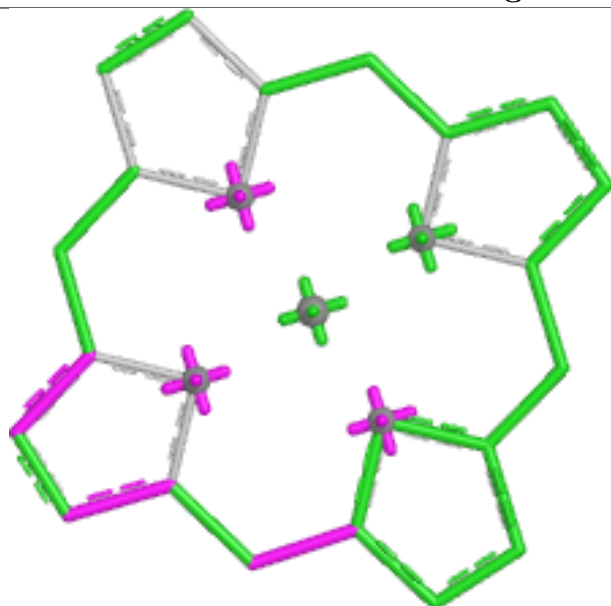


Torsions

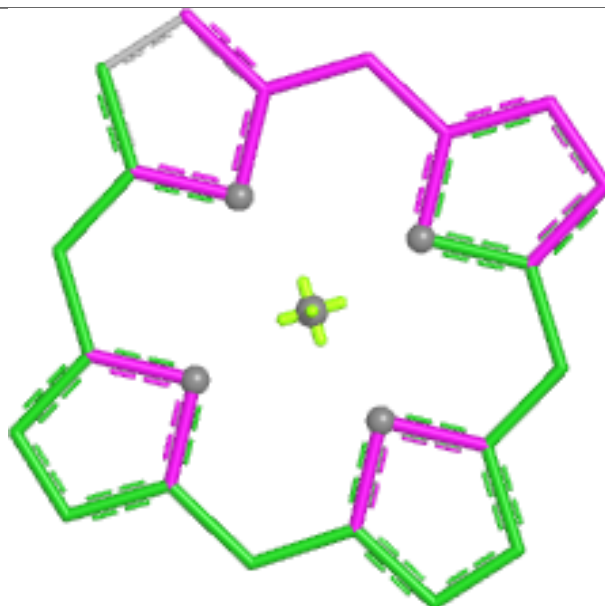


Rings

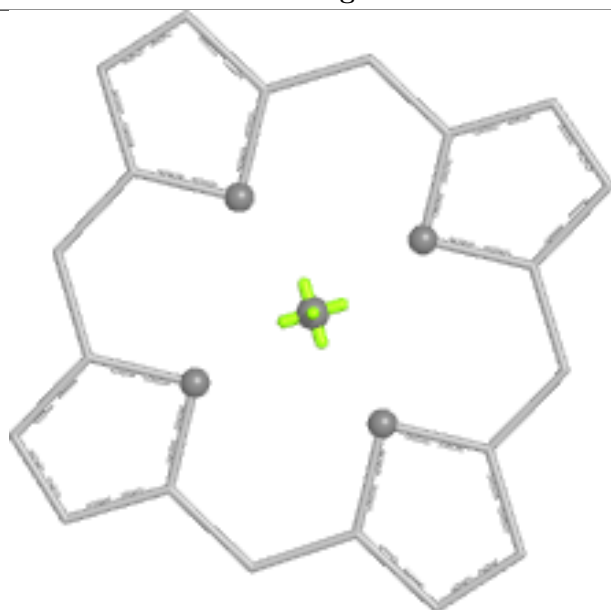
Ligand CLA A 1140



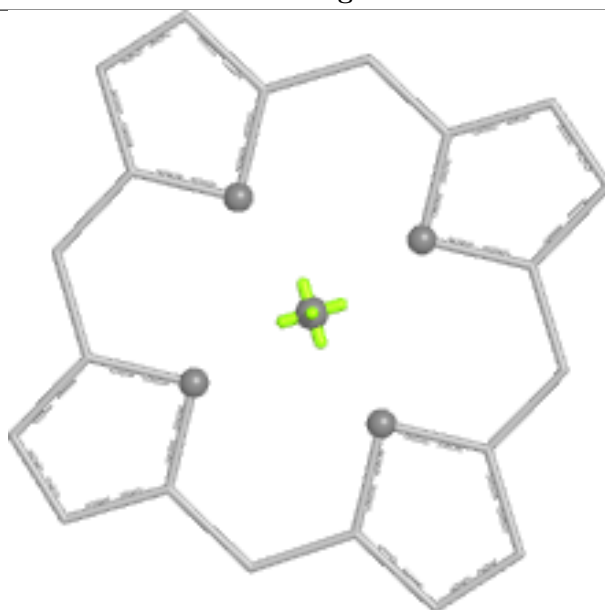
Bond lengths



Bond angles

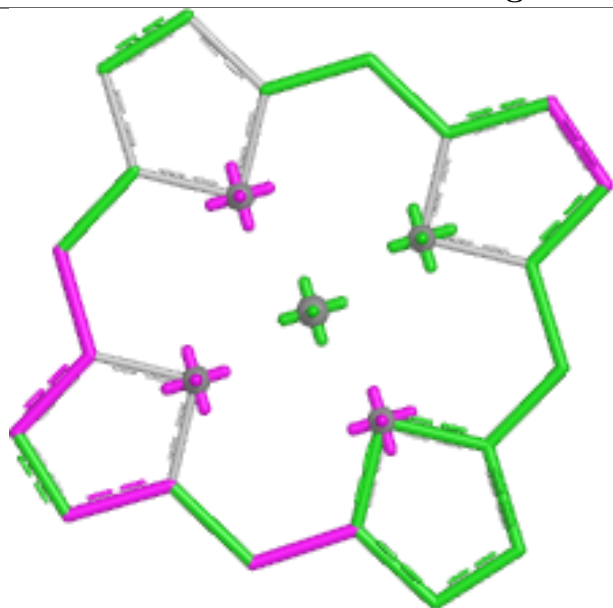


Torsions

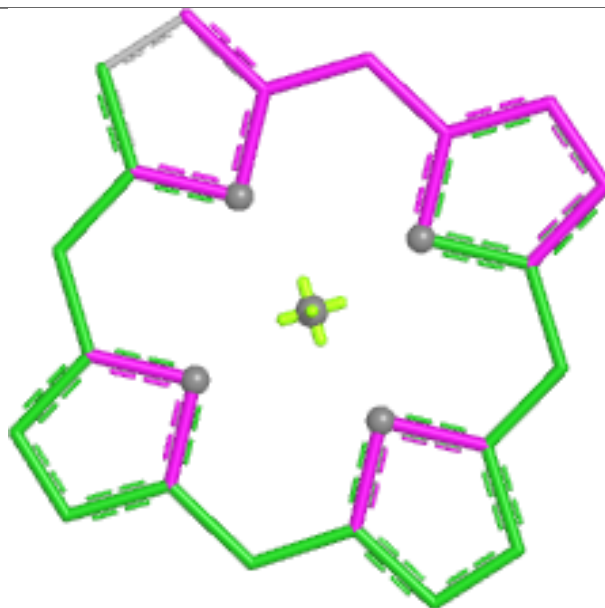


Rings

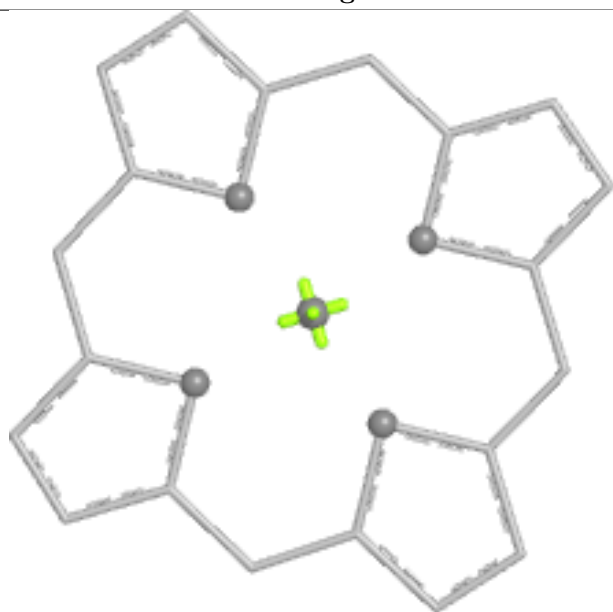
Ligand CLA P 5120



Bond lengths



Bond angles

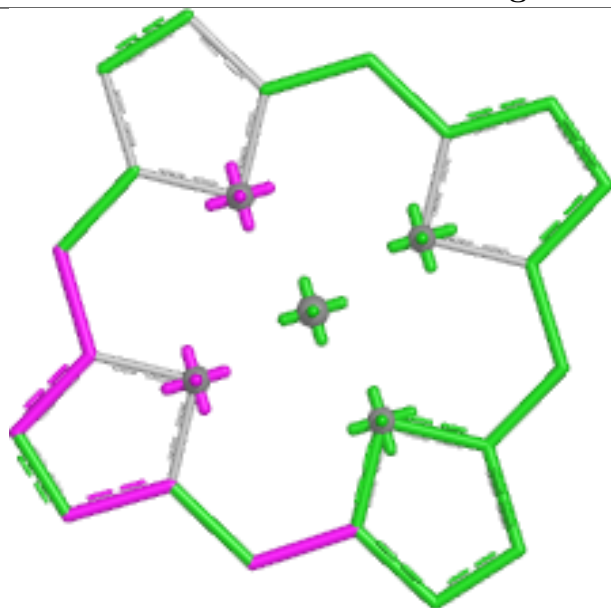


Torsions

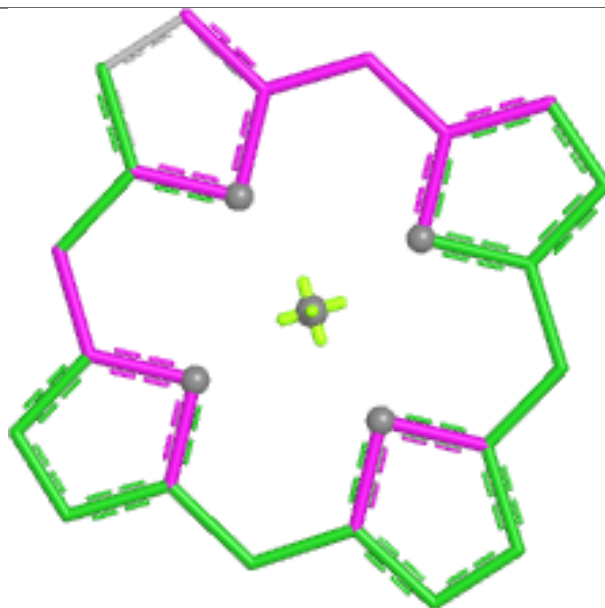


Rings

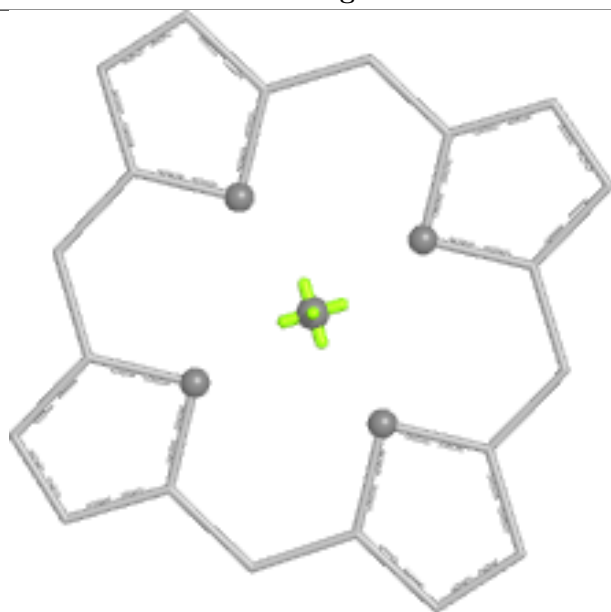
Ligand CLA 9 1026



Bond lengths



Bond angles

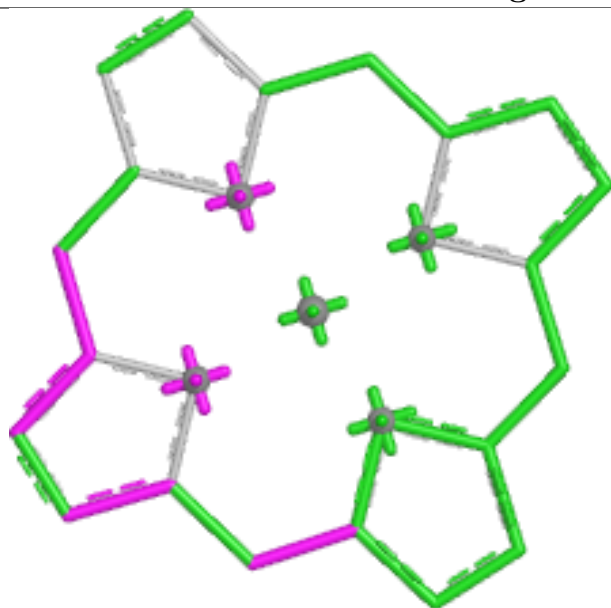


Torsions



Rings

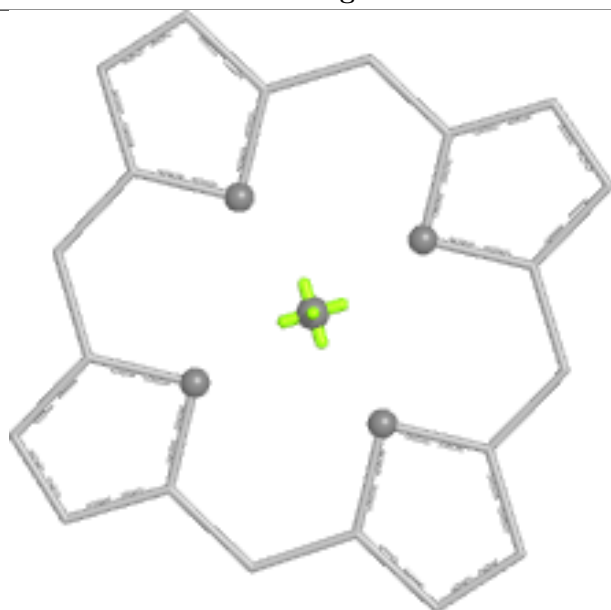
Ligand CLA 7 1014



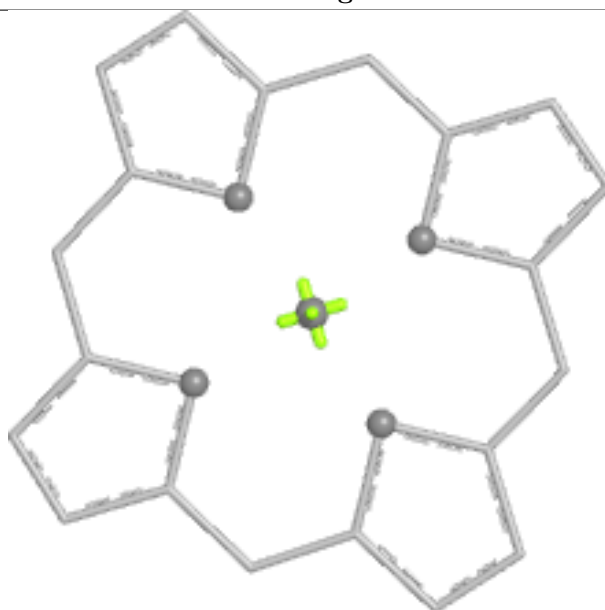
Bond lengths



Bond angles

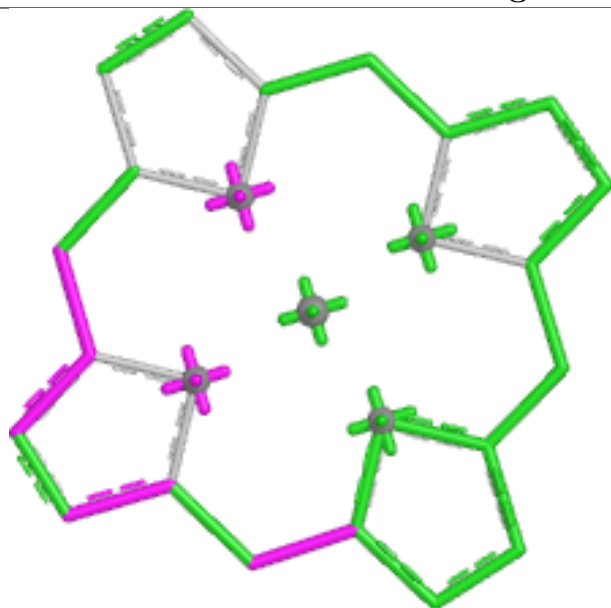


Torsions

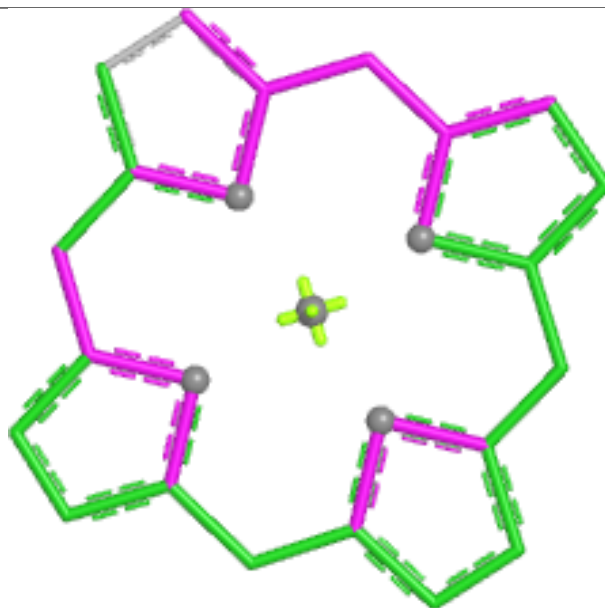


Rings

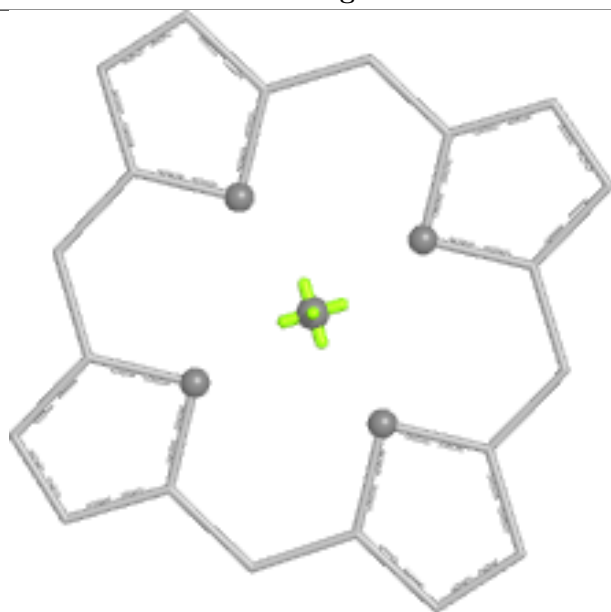
Ligand CLA 5 5403



Bond lengths



Bond angles

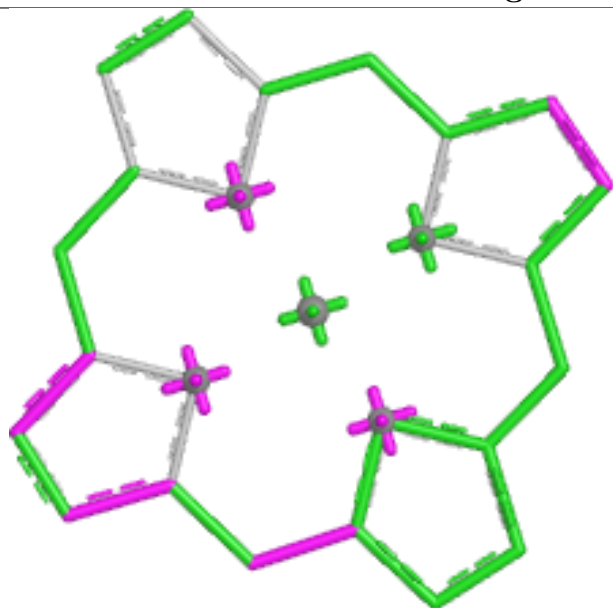


Torsions

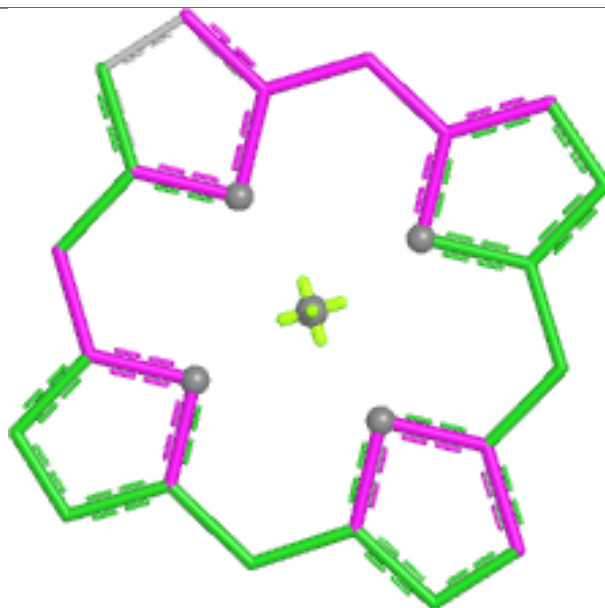


Rings

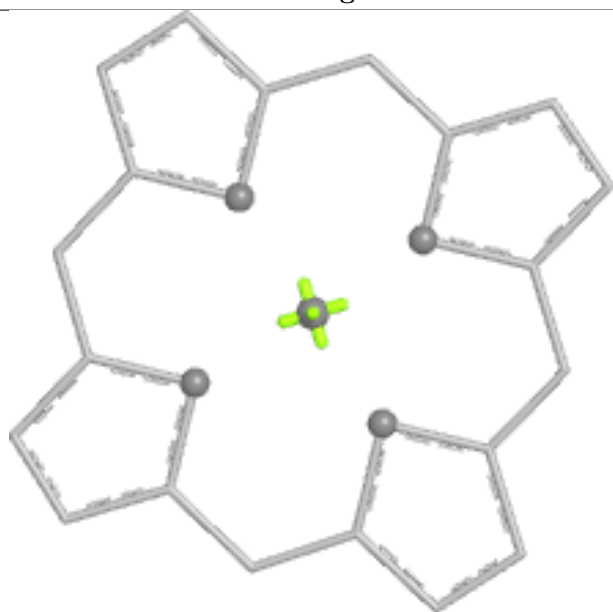
Ligand CLA B 1213



Bond lengths



Bond angles

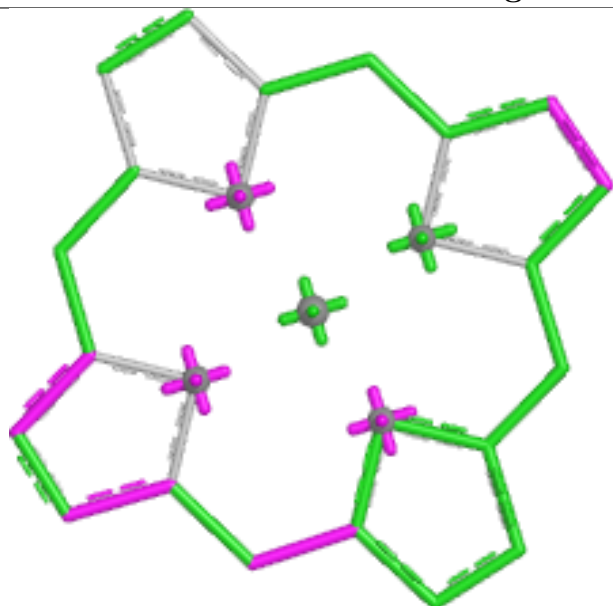


Torsions

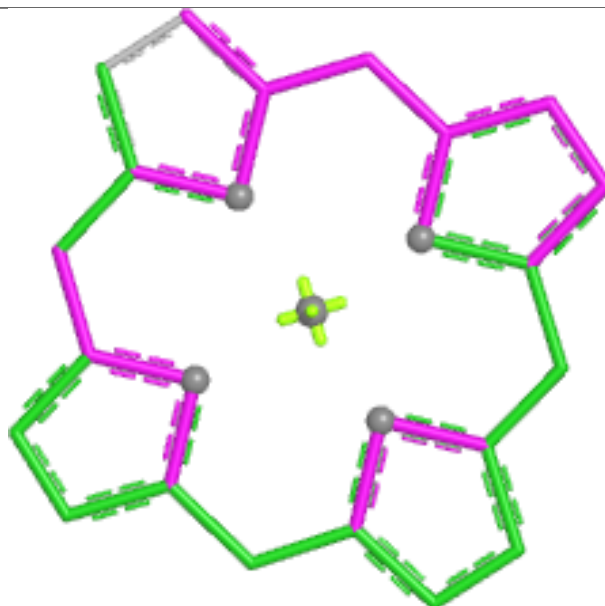


Rings

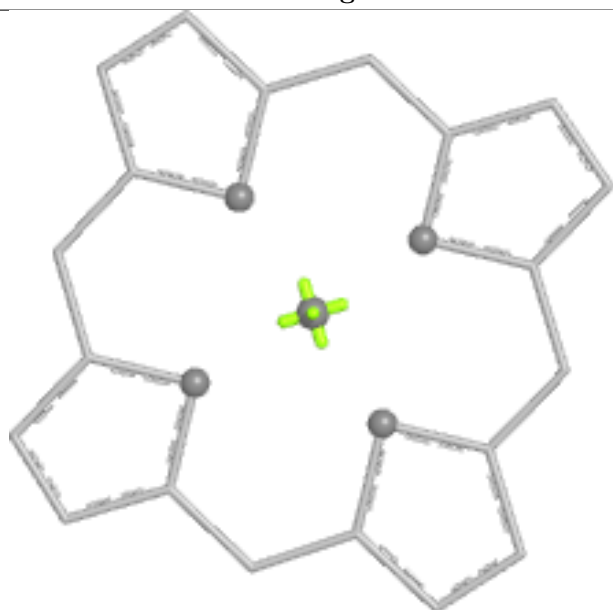
Ligand CLA A 1012



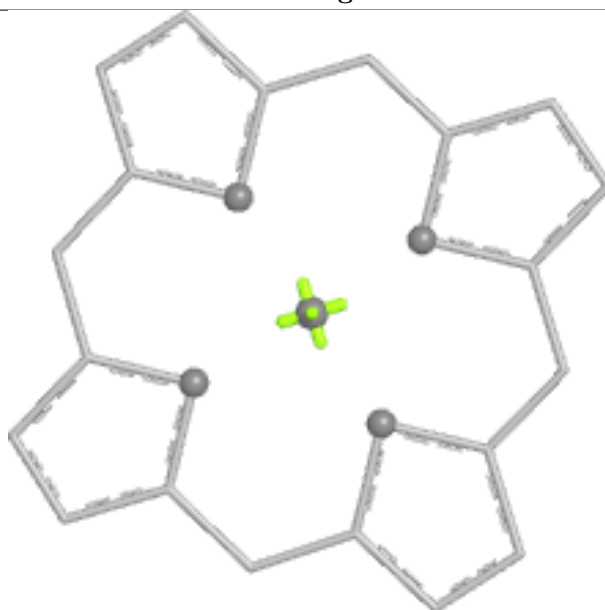
Bond lengths



Bond angles

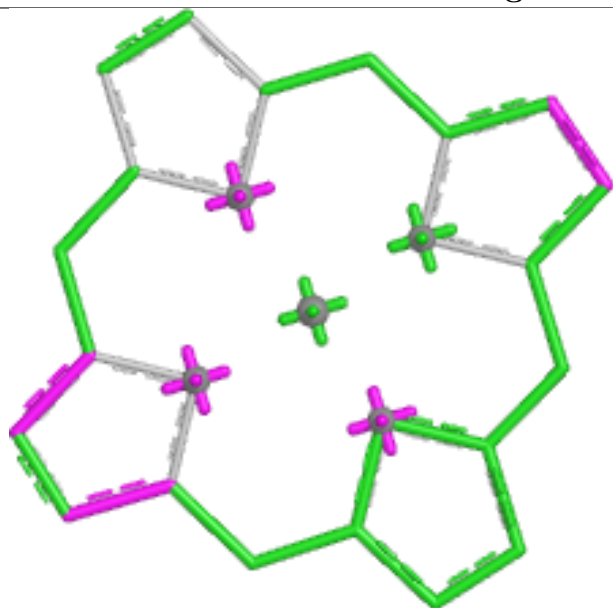


Torsions

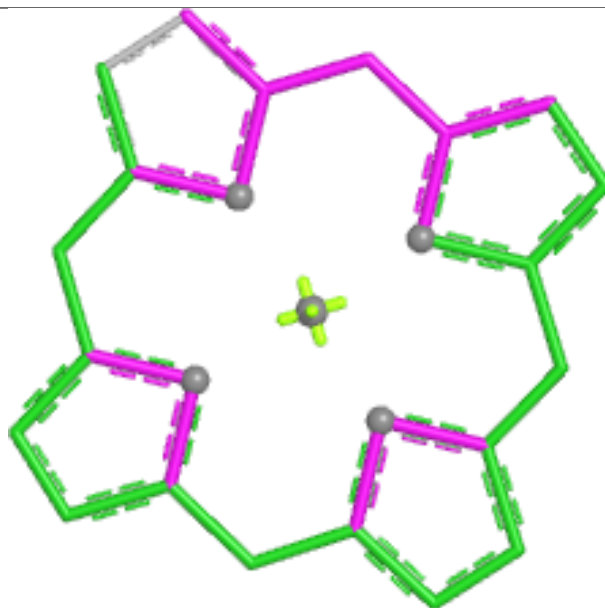


Rings

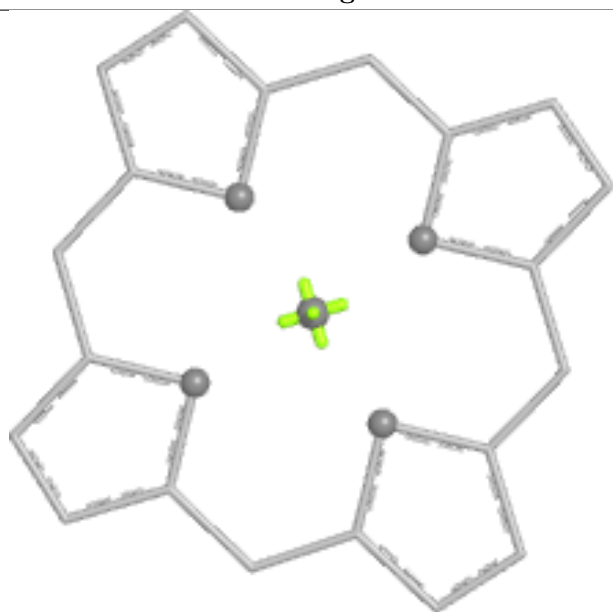
Ligand CLA B 1222



Bond lengths



Bond angles

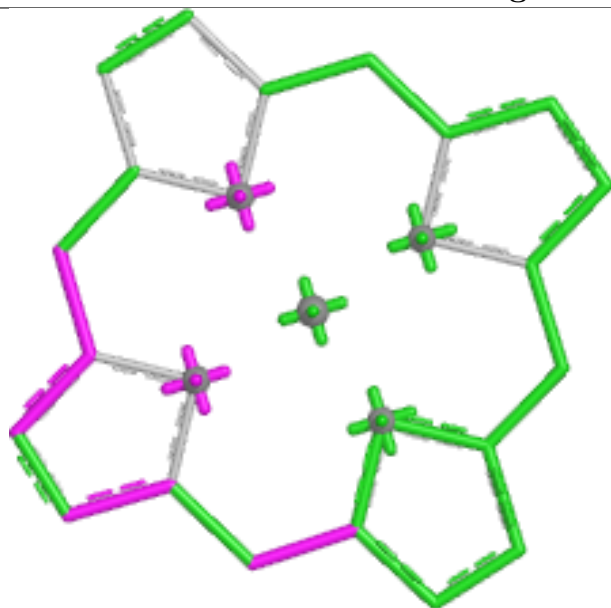


Torsions

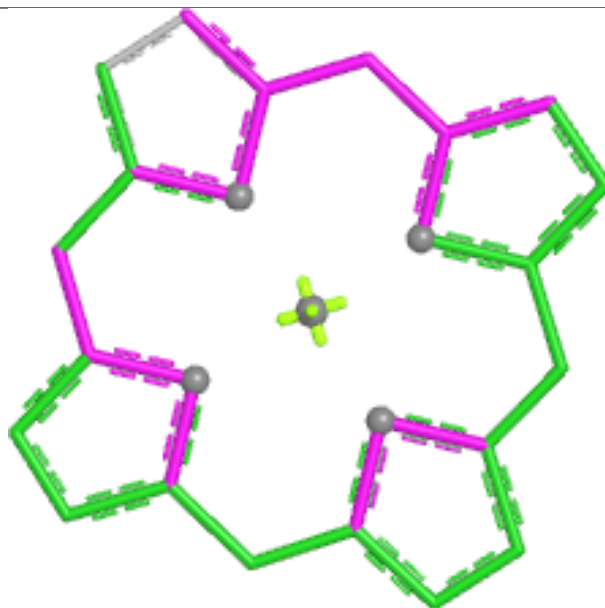


Rings

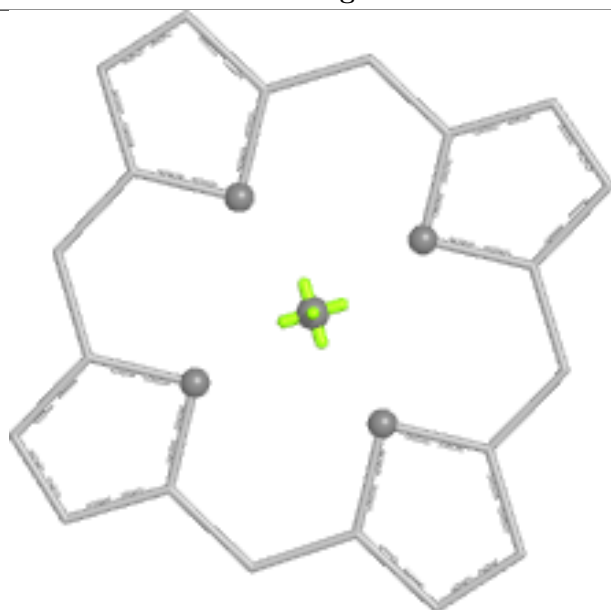
Ligand CLA 1 1031



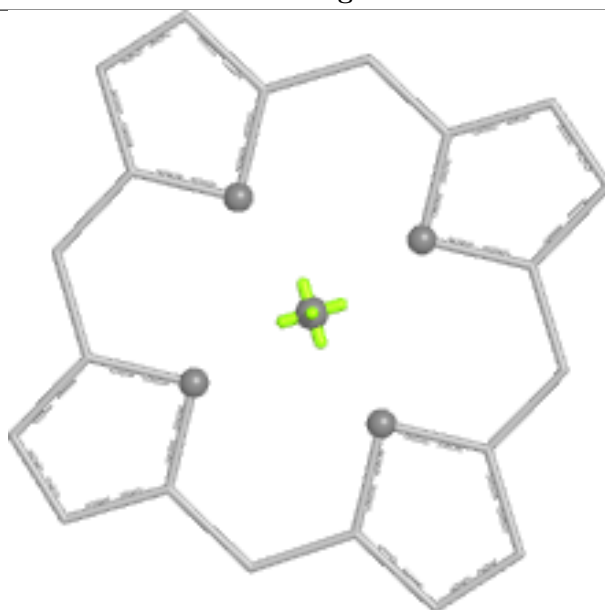
Bond lengths



Bond angles

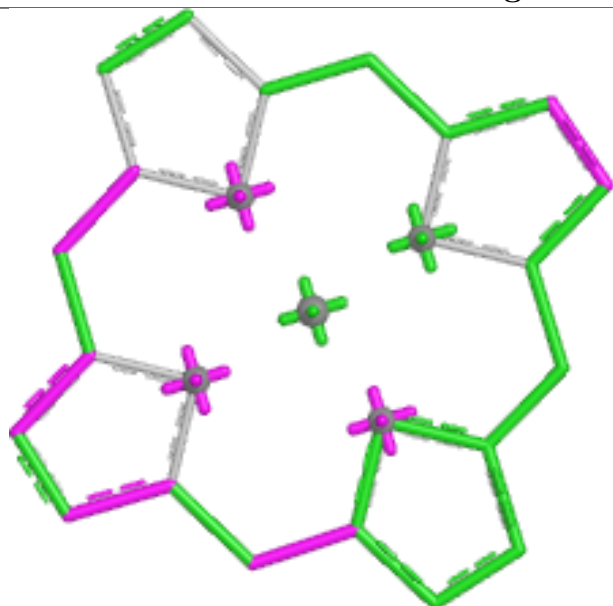


Torsions

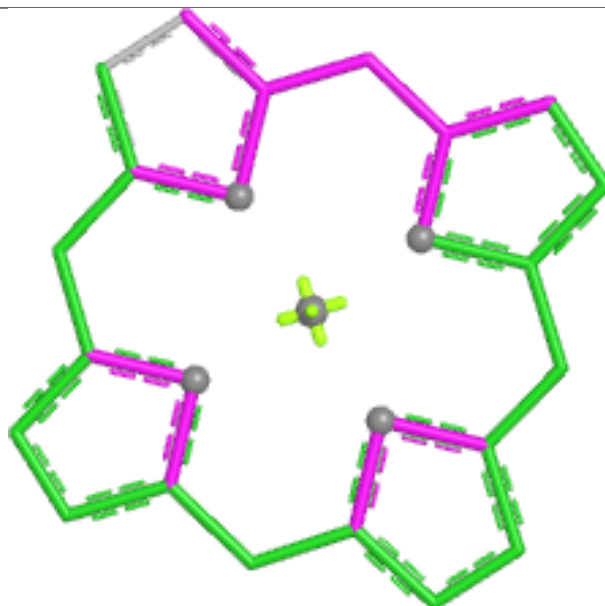


Rings

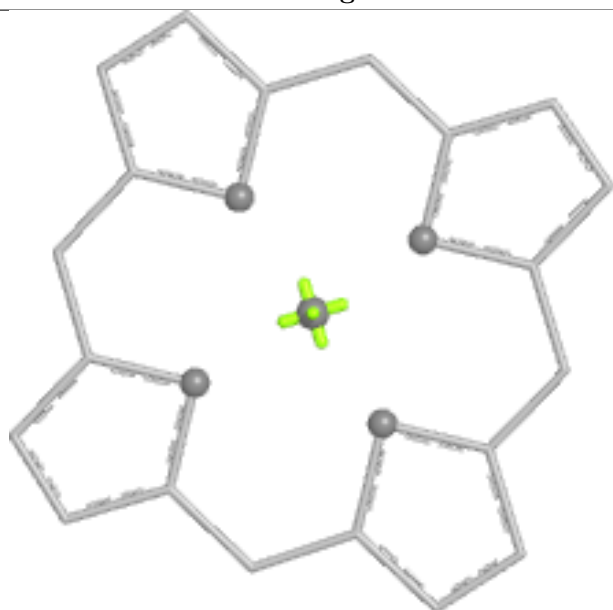
Ligand CLA G 1233



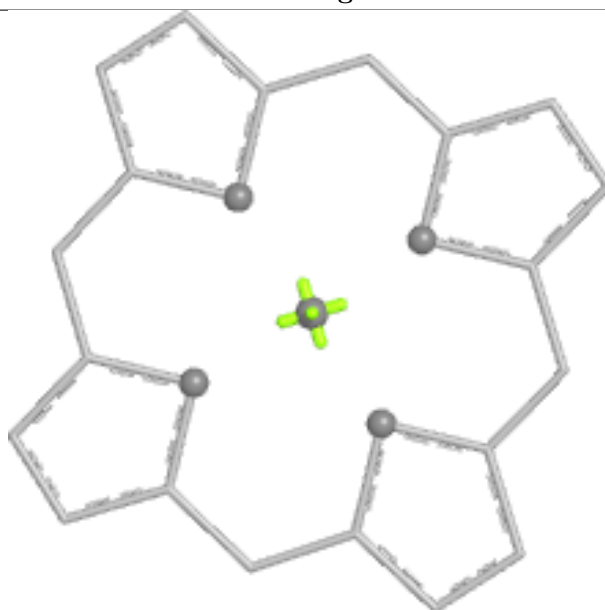
Bond lengths



Bond angles

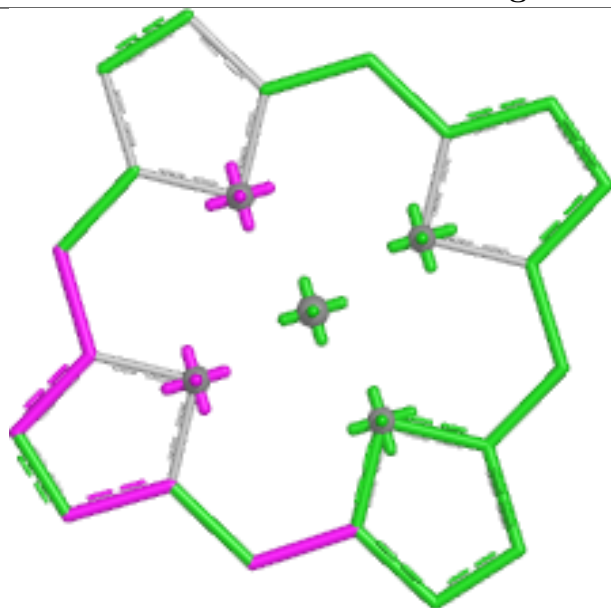


Torsions

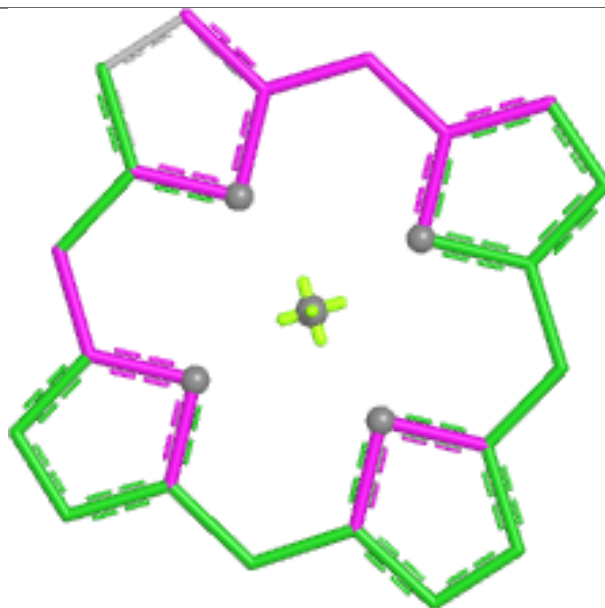


Rings

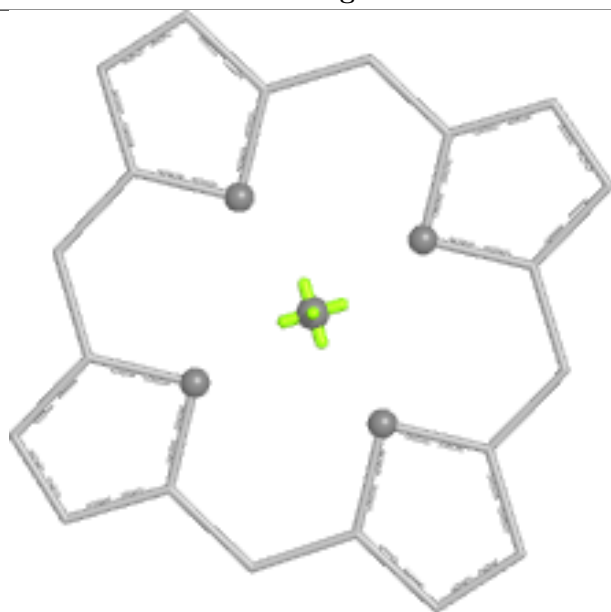
Ligand CLA 8 1012



Bond lengths



Bond angles

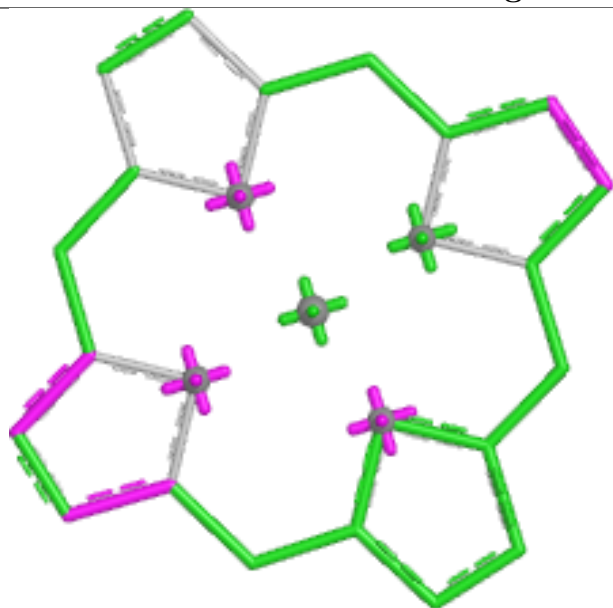


Torsions

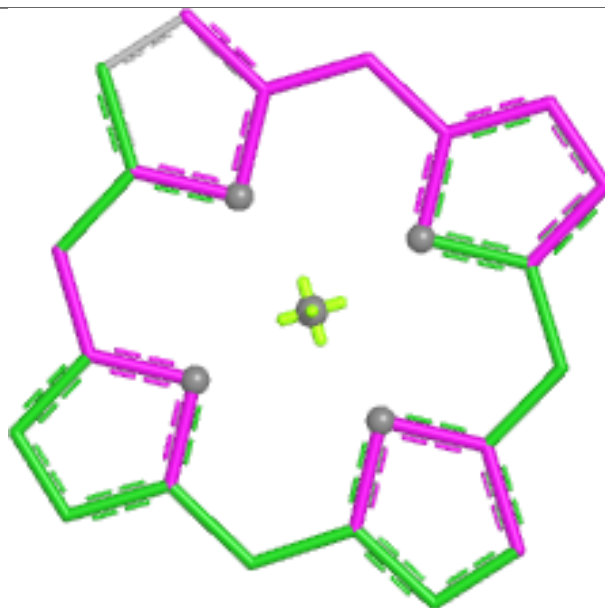


Rings

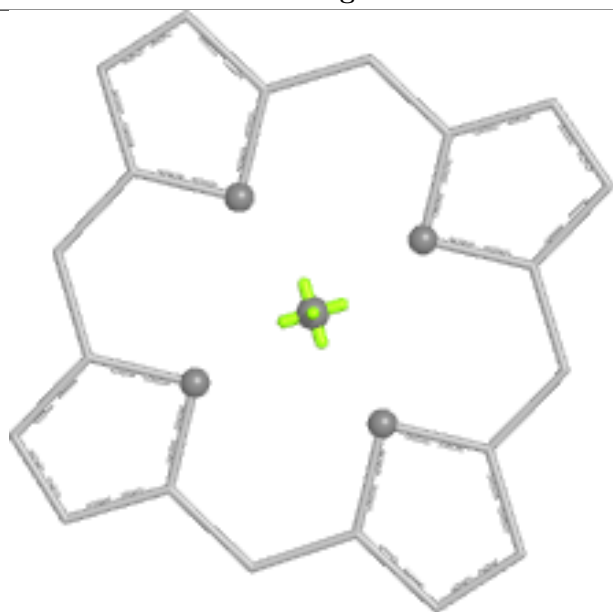
Ligand CLA A 1117



Bond lengths



Bond angles

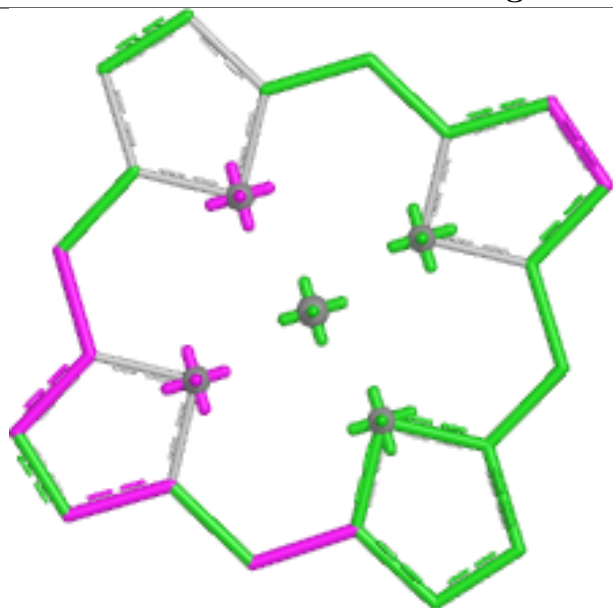


Torsions

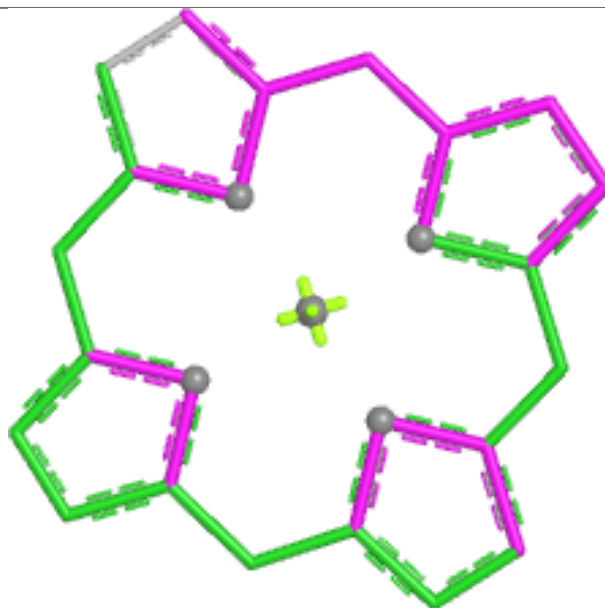


Rings

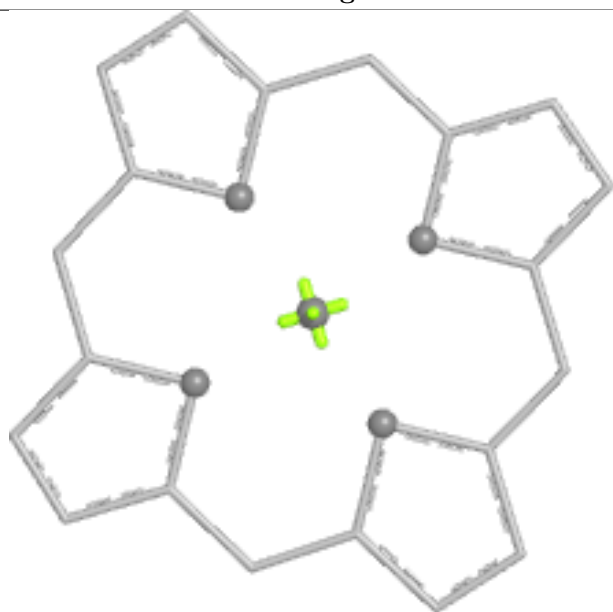
Ligand CLA P 5103



Bond lengths



Bond angles

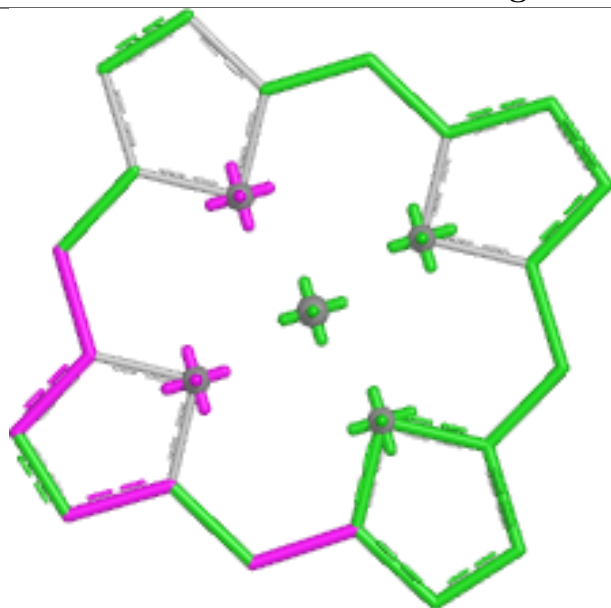


Torsions

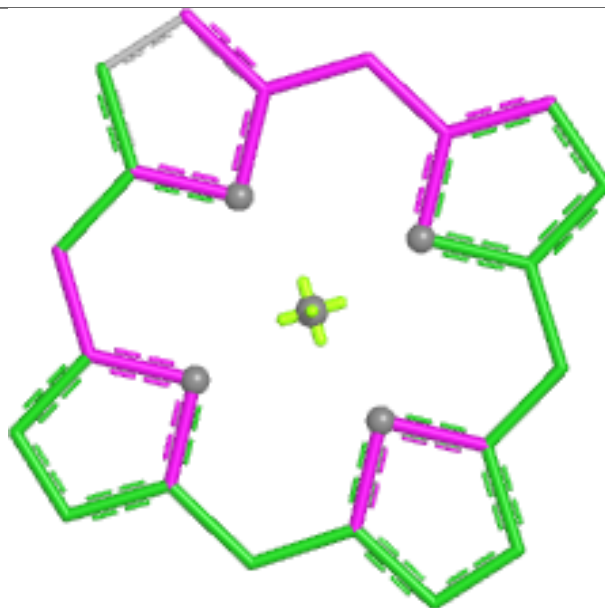


Rings

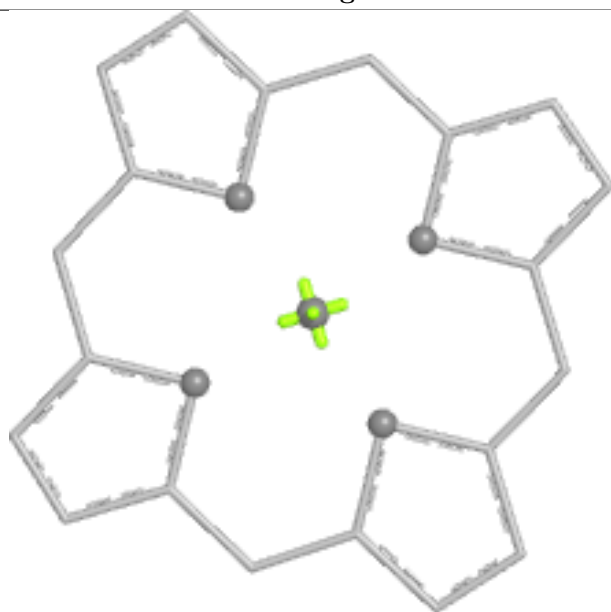
Ligand CLA 7 1013



Bond lengths



Bond angles

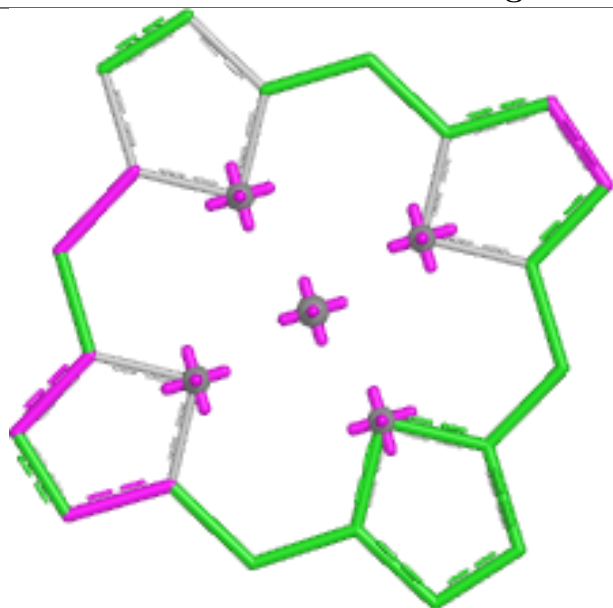


Torsions

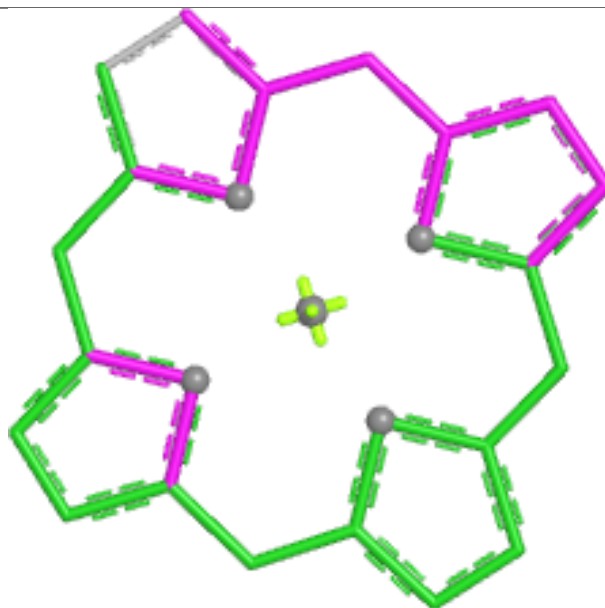


Rings

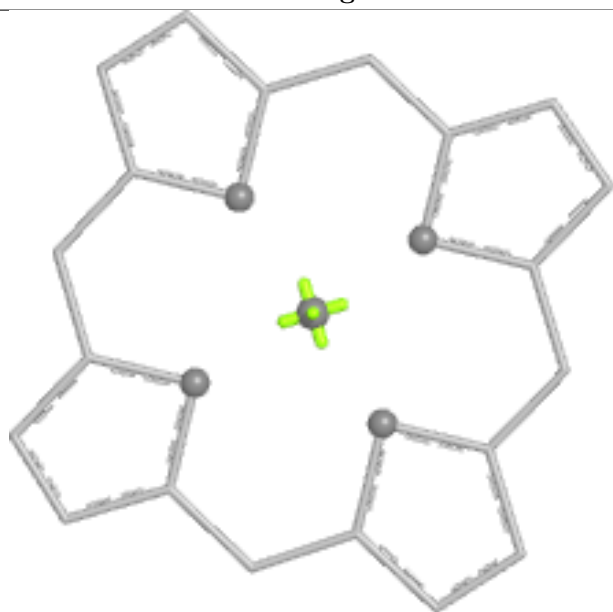
Ligand CLA B 1207



Bond lengths



Bond angles

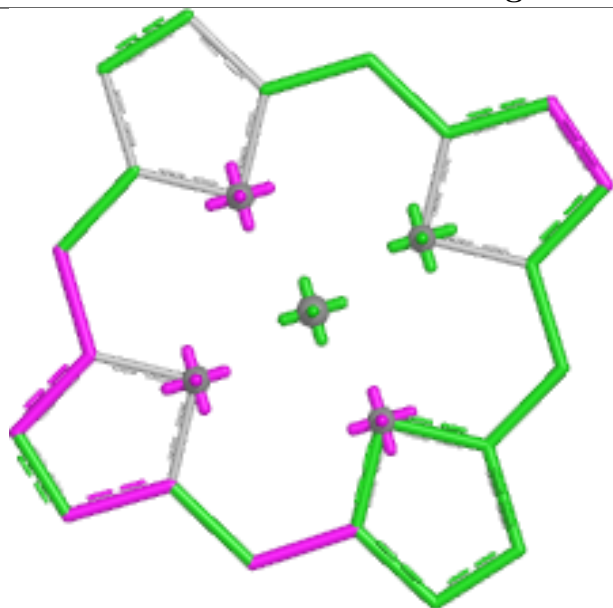


Torsions

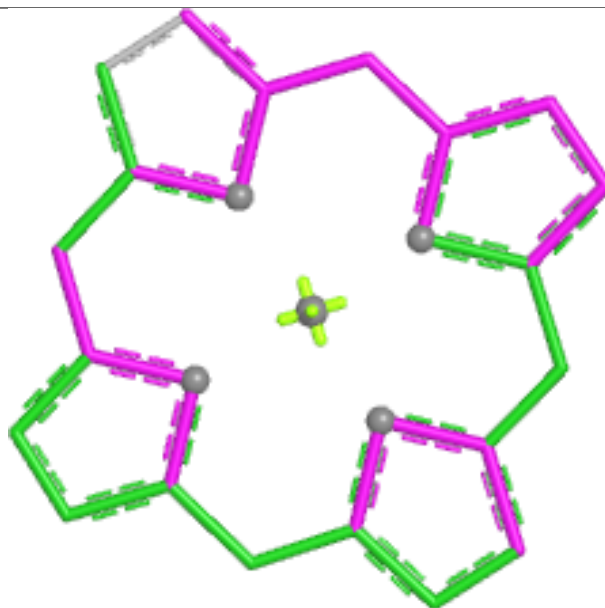


Rings

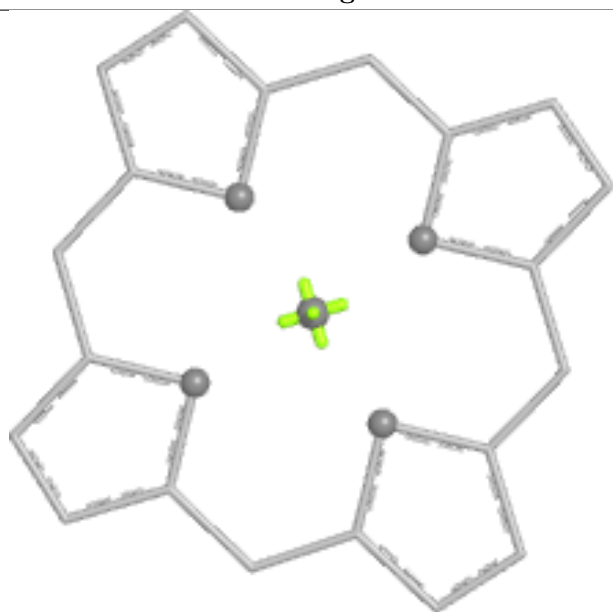
Ligand CLA B 1228



Bond lengths



Bond angles

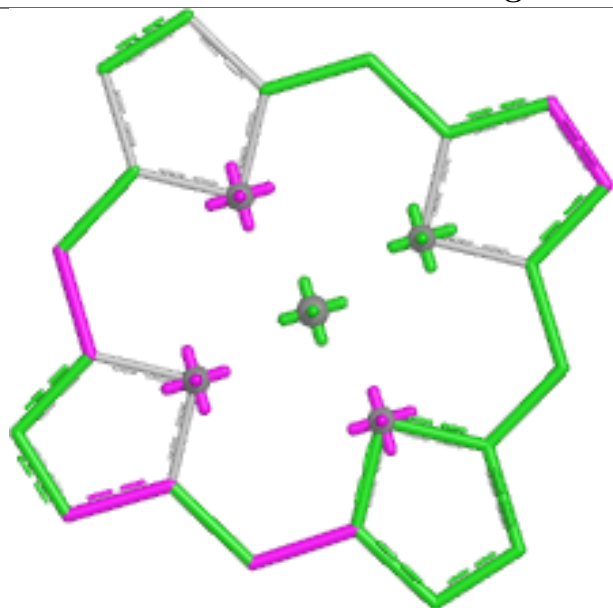


Torsions

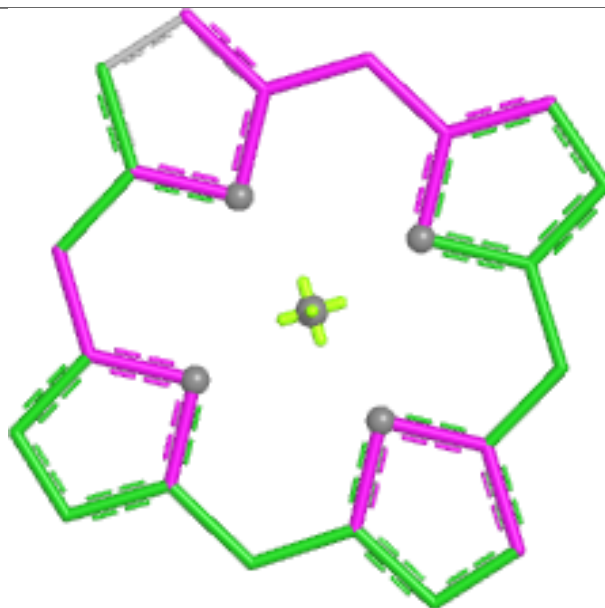


Rings

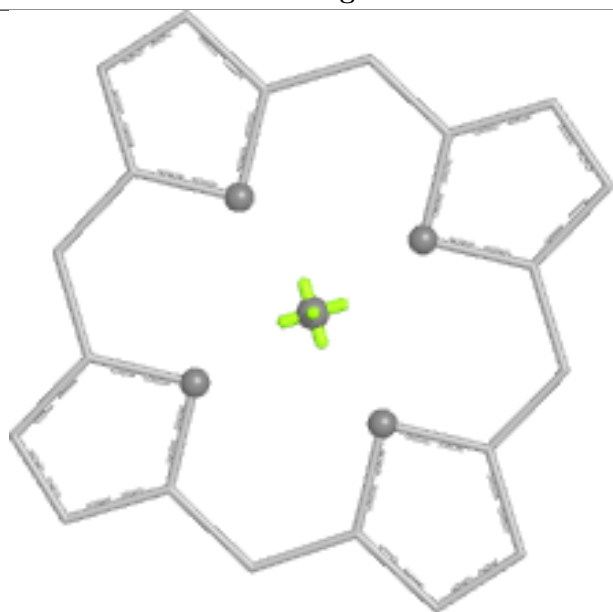
Ligand CLA A 1119



Bond lengths



Bond angles

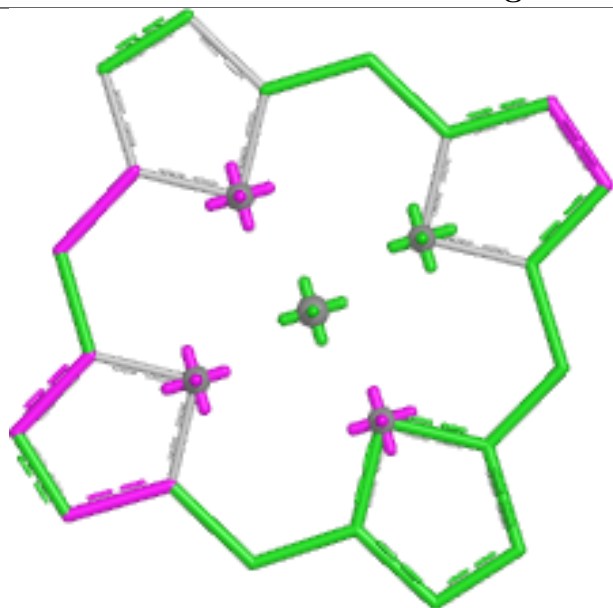


Torsions

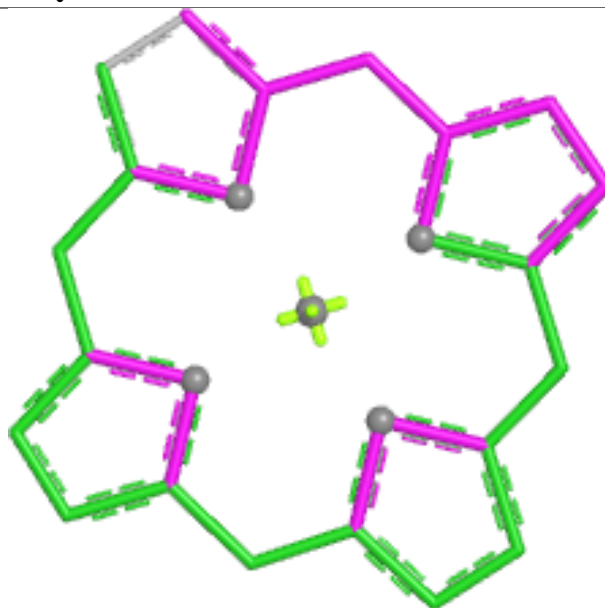


Rings

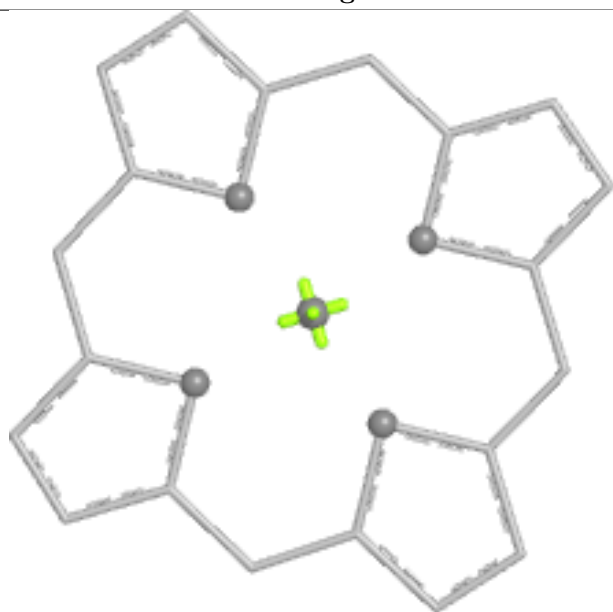
Ligand CLA Q 5130



Bond lengths



Bond angles

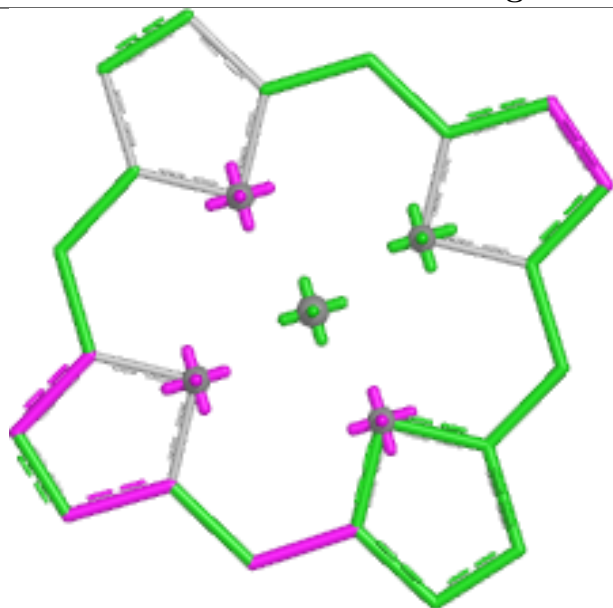


Torsions

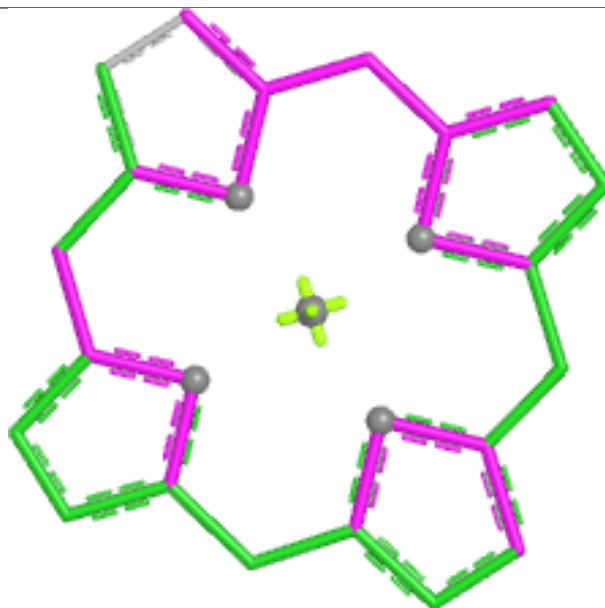


Rings

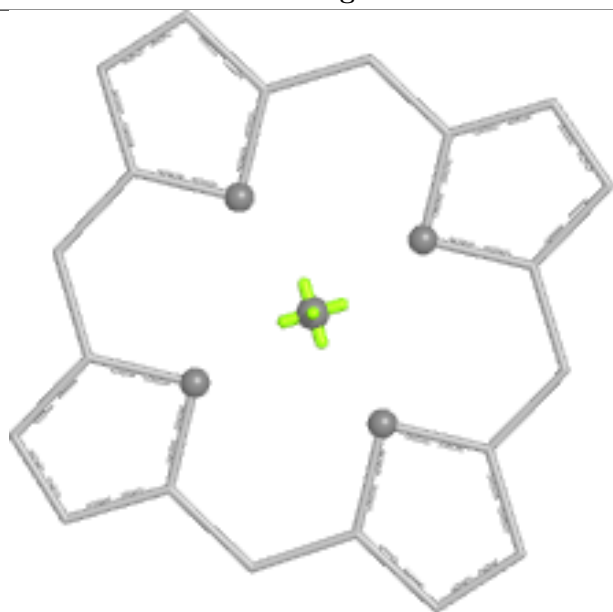
Ligand CLA P 5137



Bond lengths



Bond angles

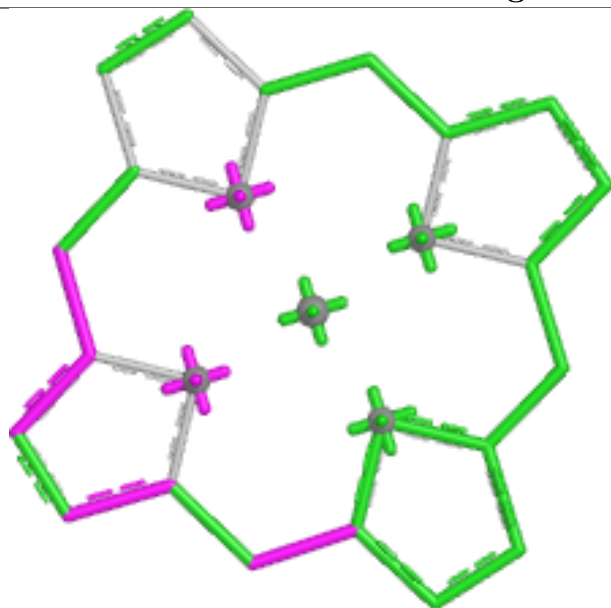


Torsions



Rings

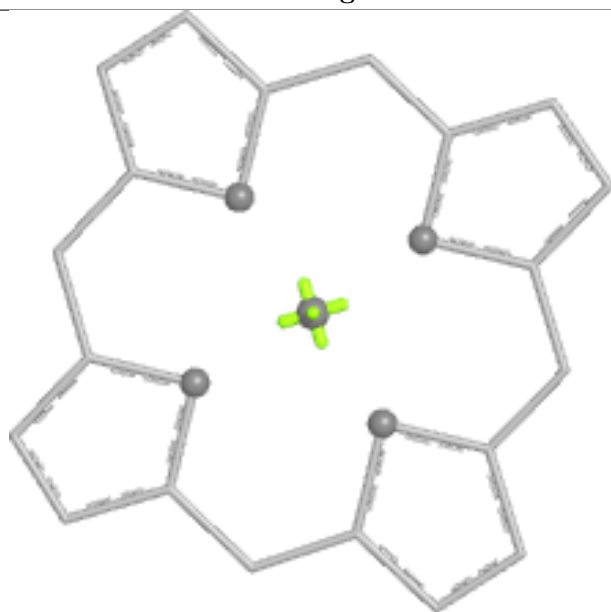
Ligand CLA Z 8008



Bond lengths



Bond angles

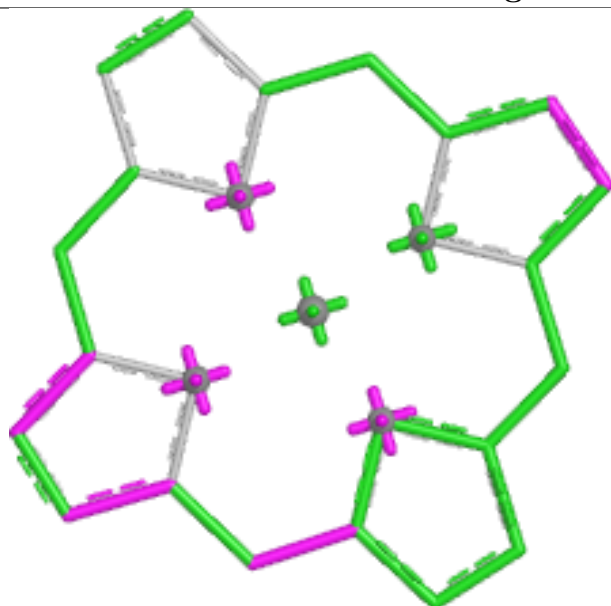


Torsions

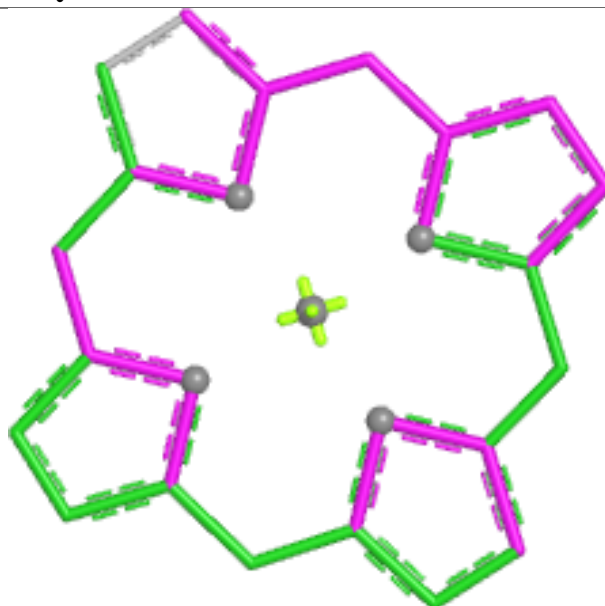


Rings

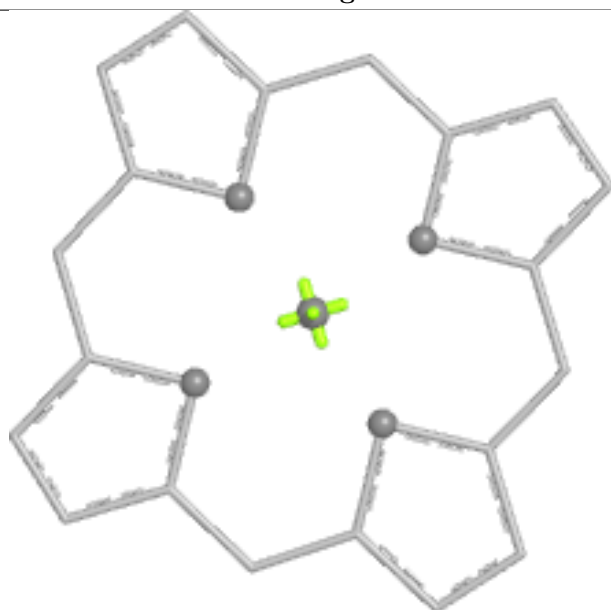
Ligand CLA Q 5218



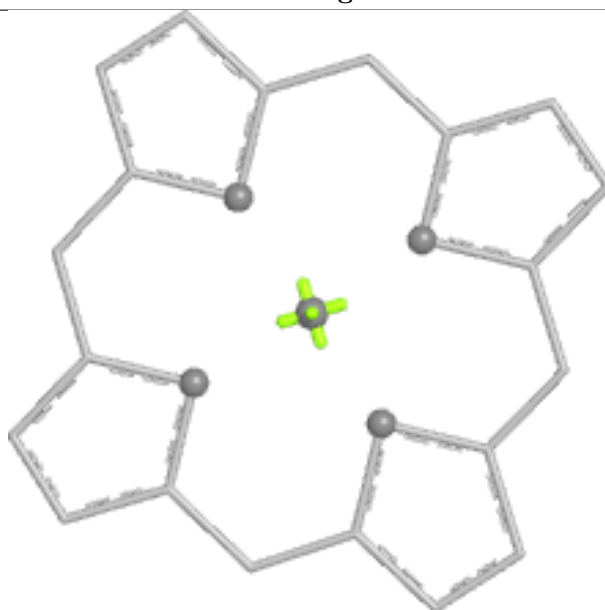
Bond lengths



Bond angles

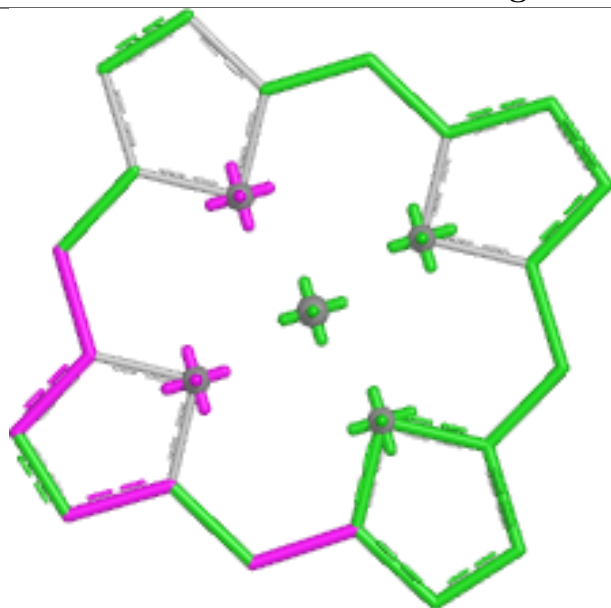


Torsions

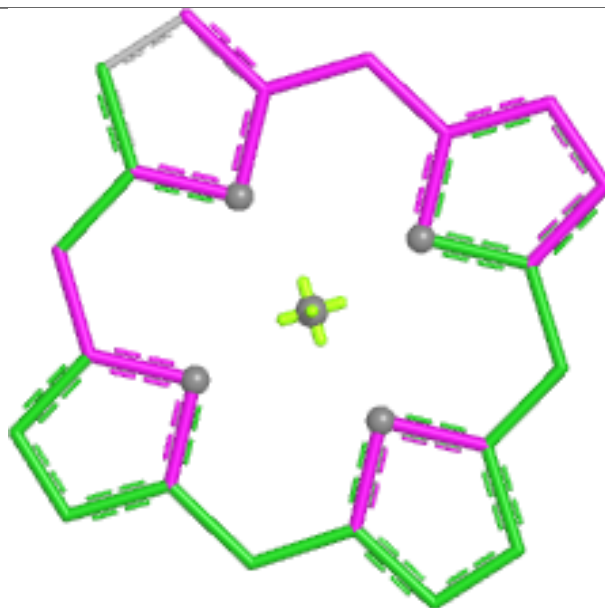


Rings

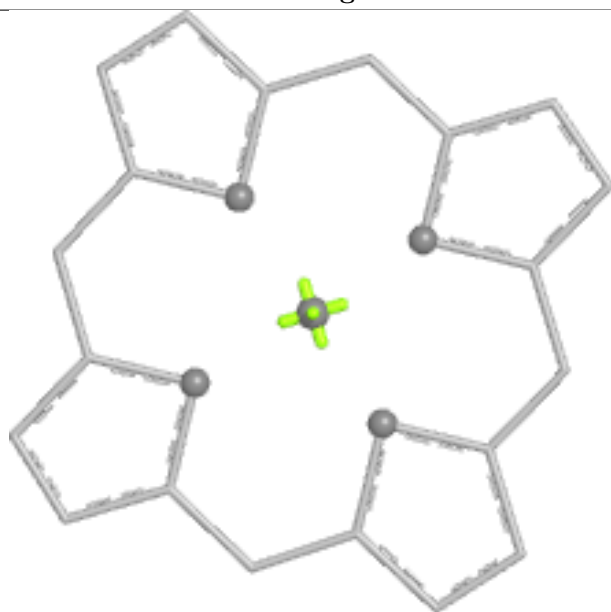
Ligand CLA 8 1015



Bond lengths



Bond angles

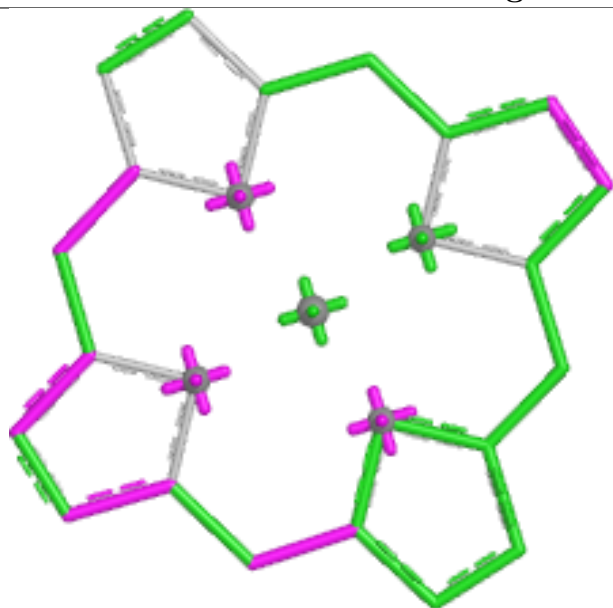


Torsions

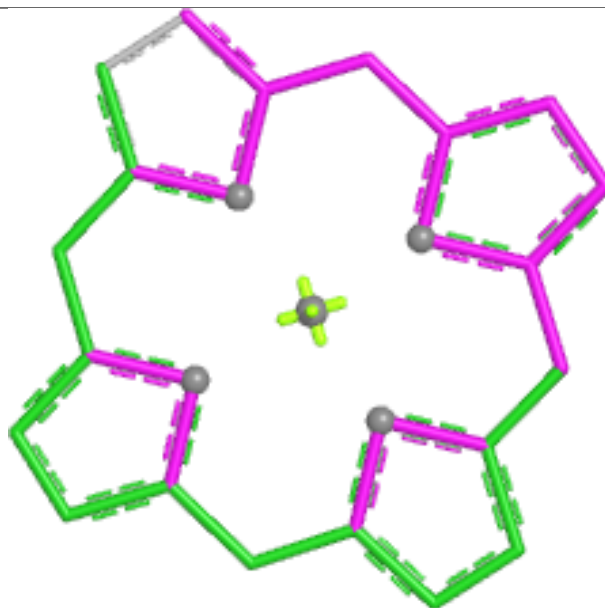


Rings

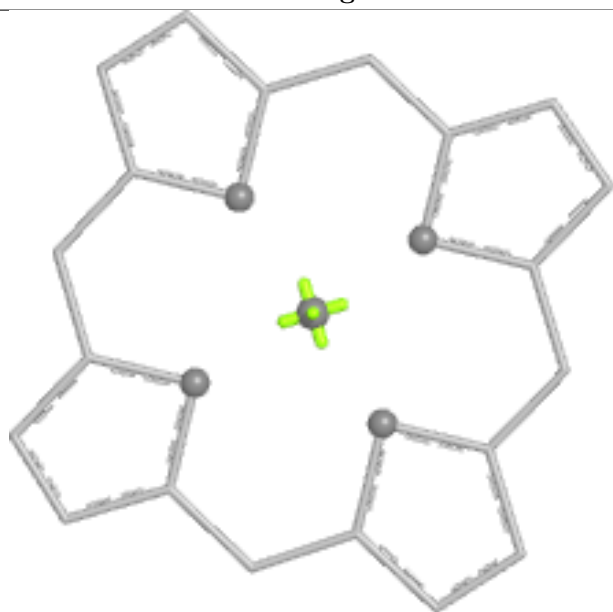
Ligand CLA P 5134



Bond lengths



Bond angles

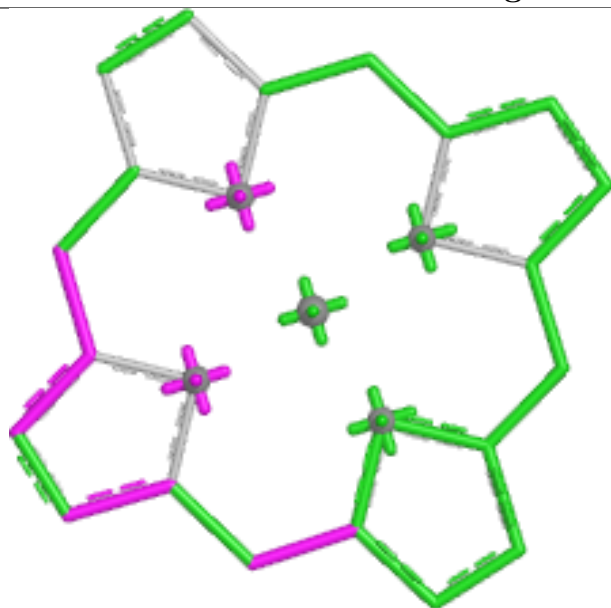


Torsions

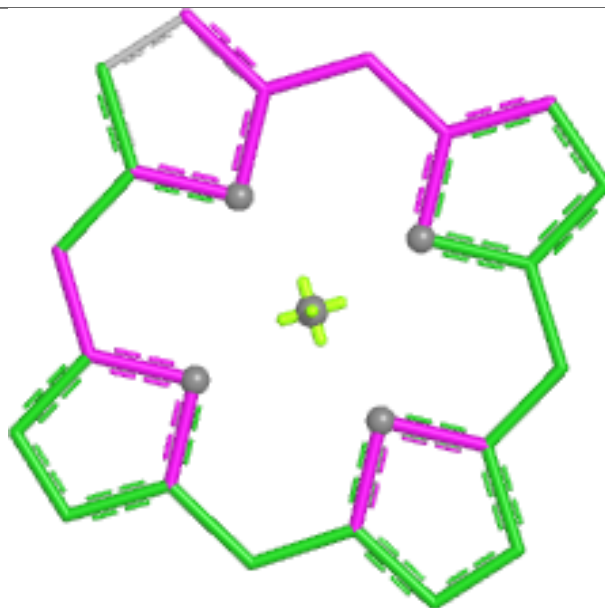


Rings

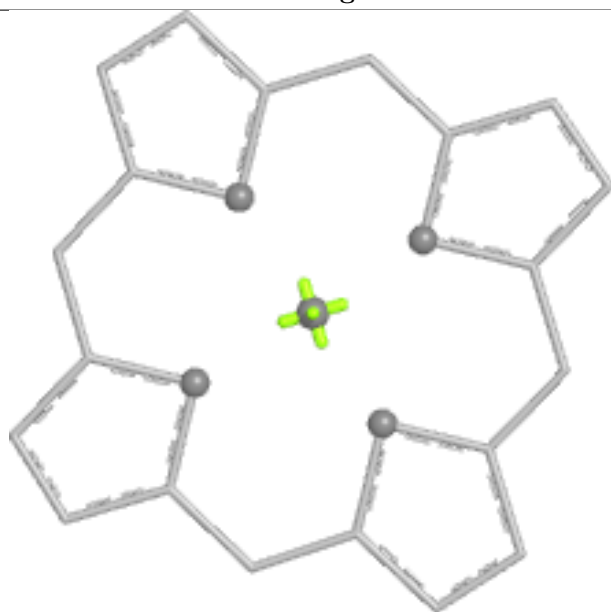
Ligand CLA K 1404



Bond lengths



Bond angles

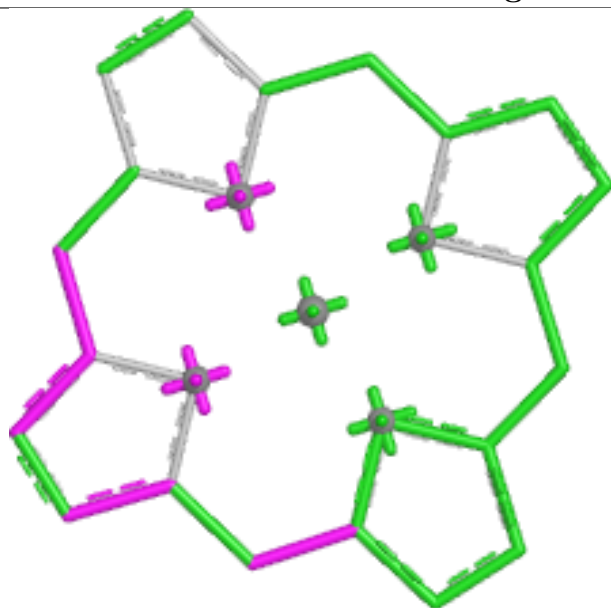


Torsions

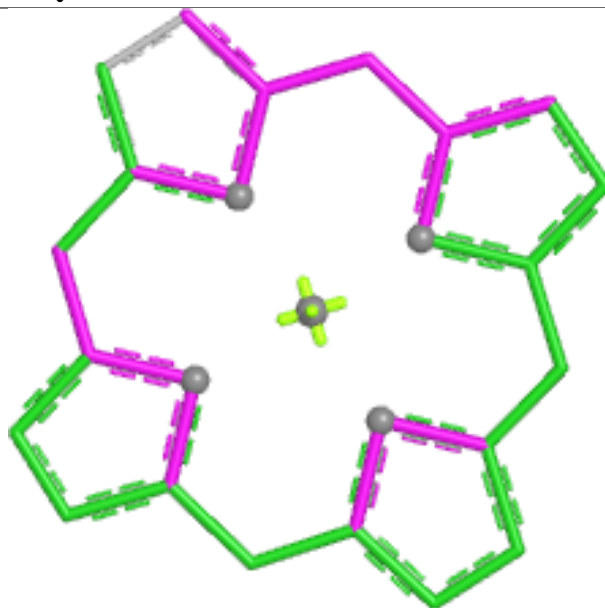


Rings

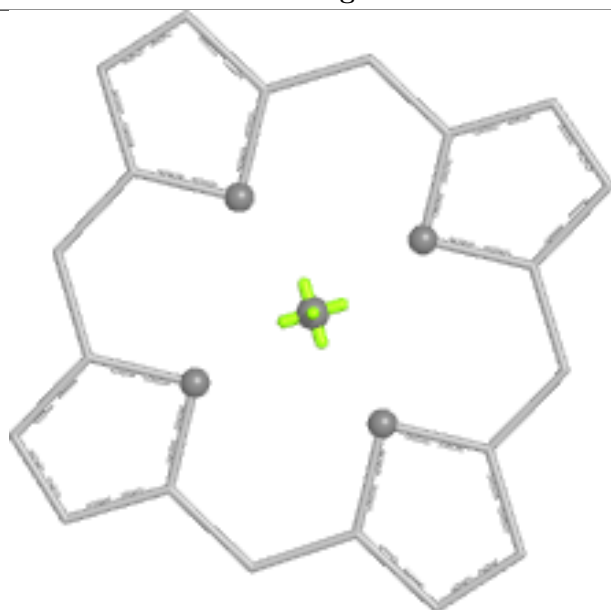
Ligand CLA Q 8001



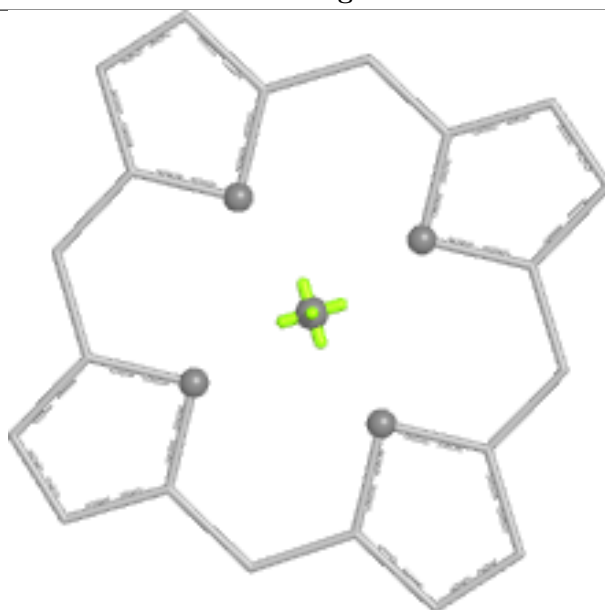
Bond lengths



Bond angles

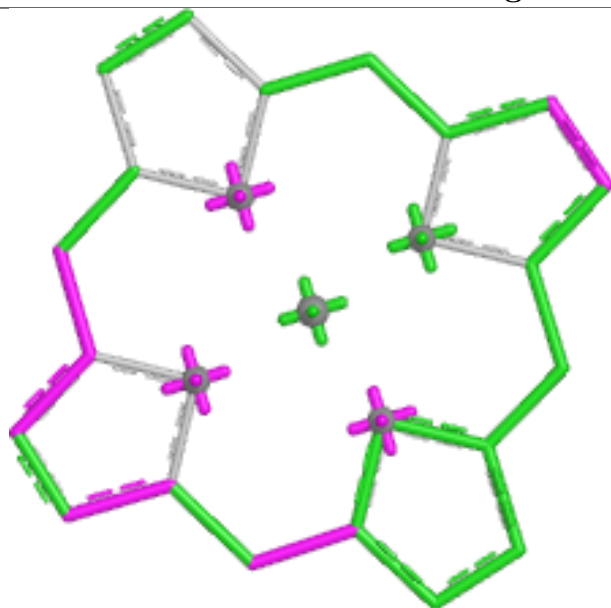


Torsions

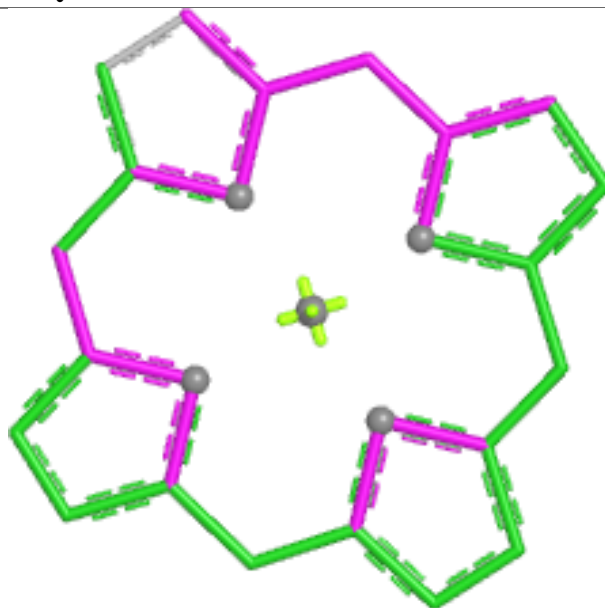


Rings

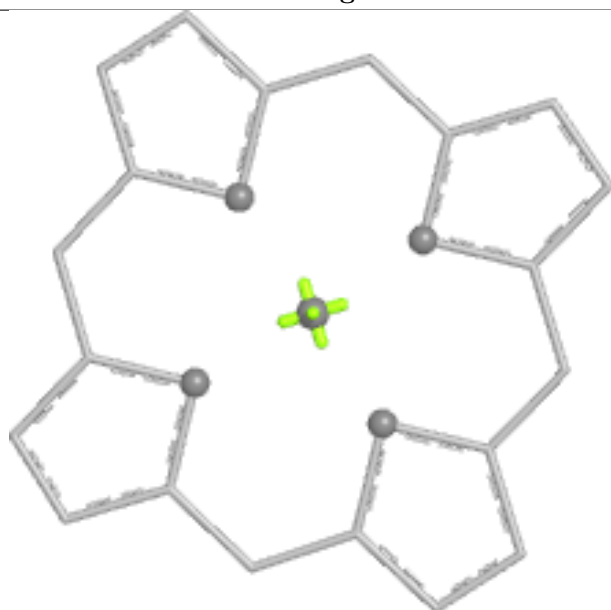
Ligand CLA Q 5216



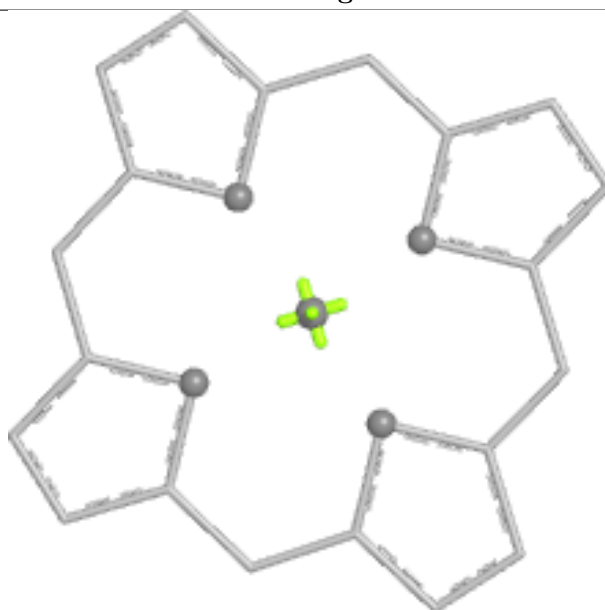
Bond lengths



Bond angles

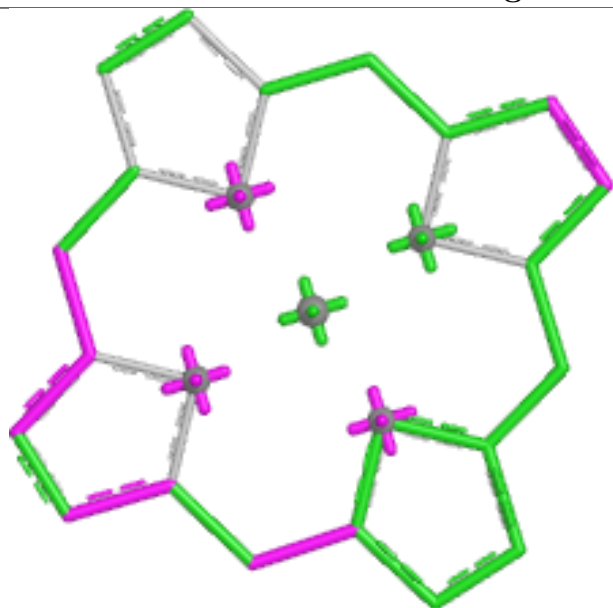


Torsions

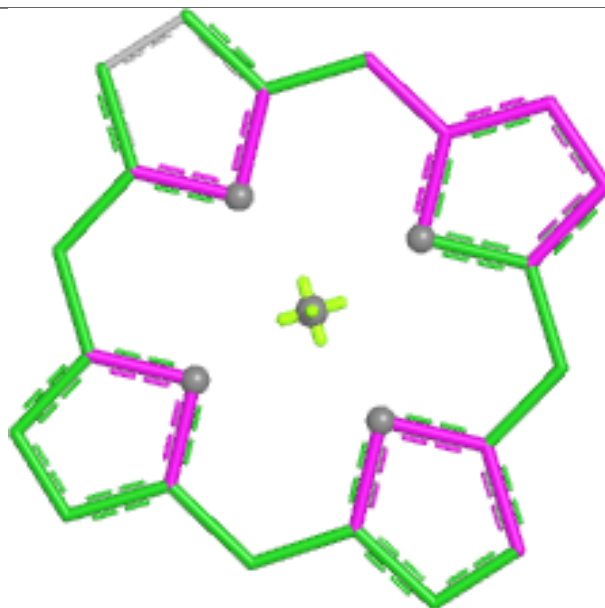


Rings

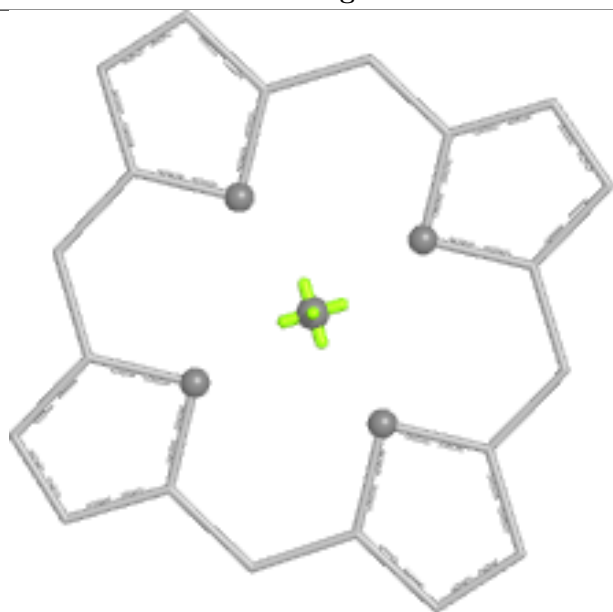
Ligand CLA U 5229



Bond lengths



Bond angles

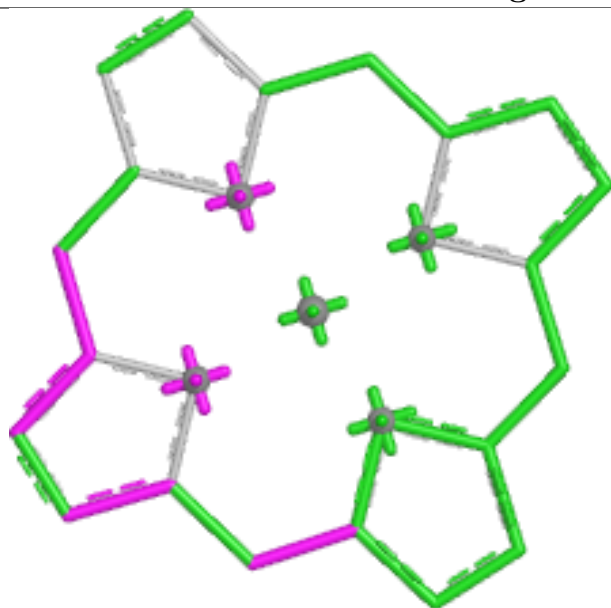


Torsions



Rings

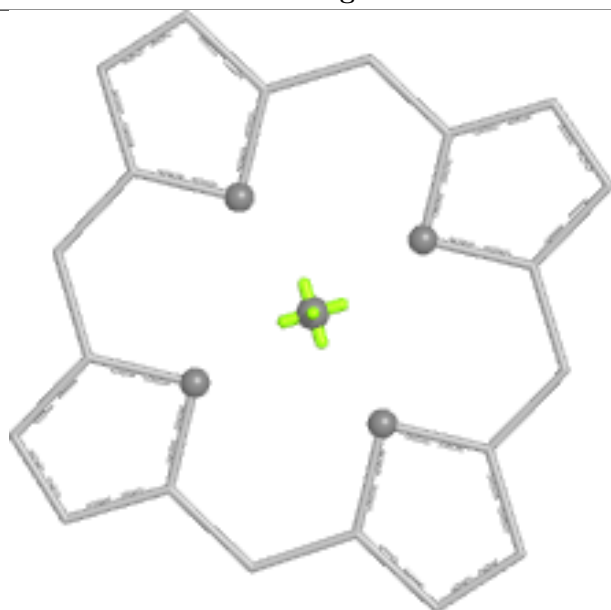
Ligand CLA 3 1041



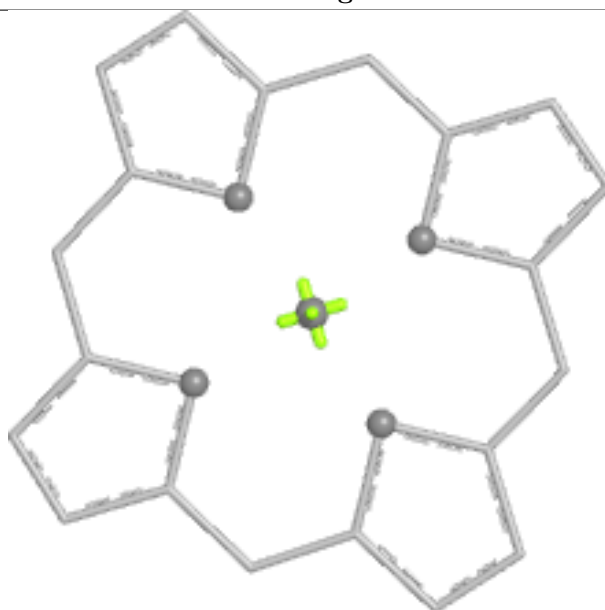
Bond lengths



Bond angles

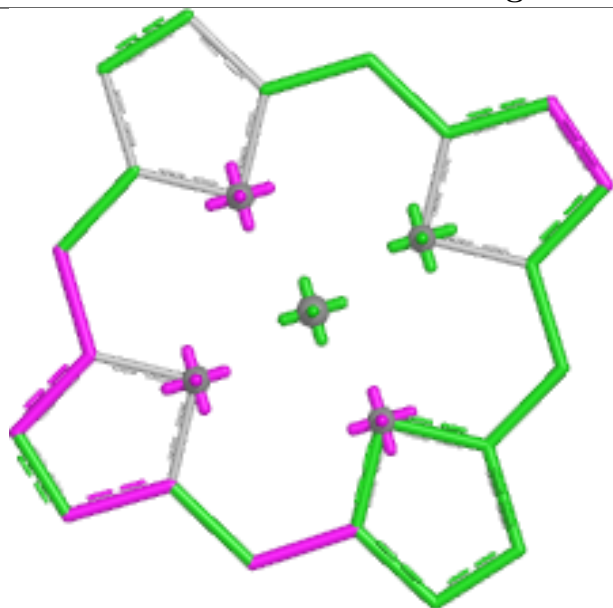


Torsions

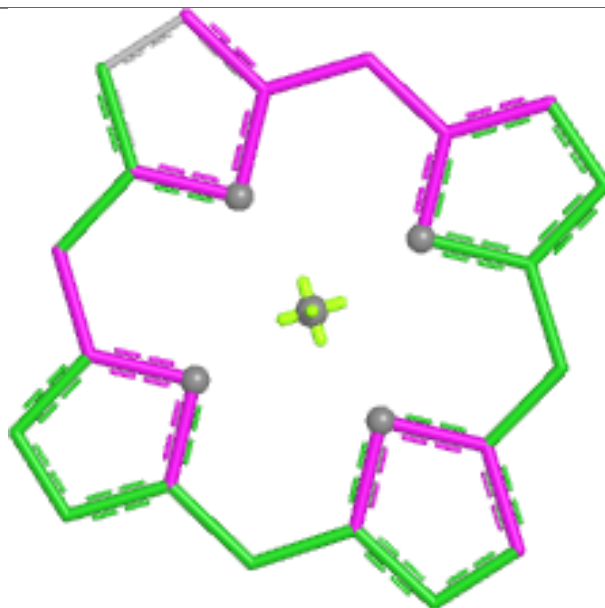


Rings

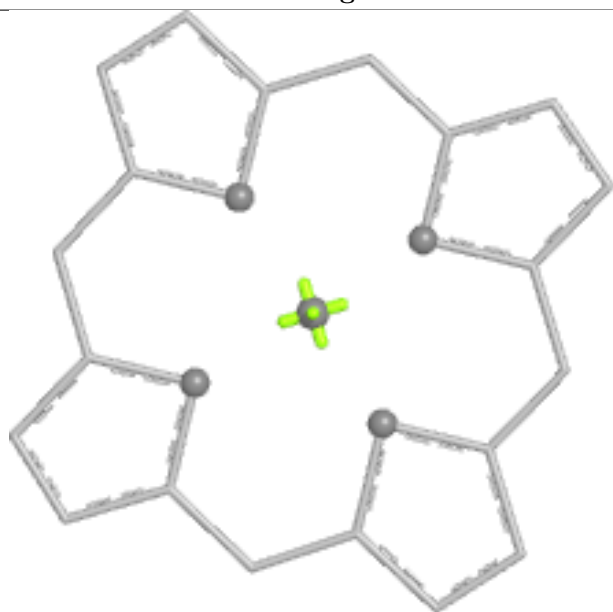
Ligand CLA P 5112



Bond lengths



Bond angles

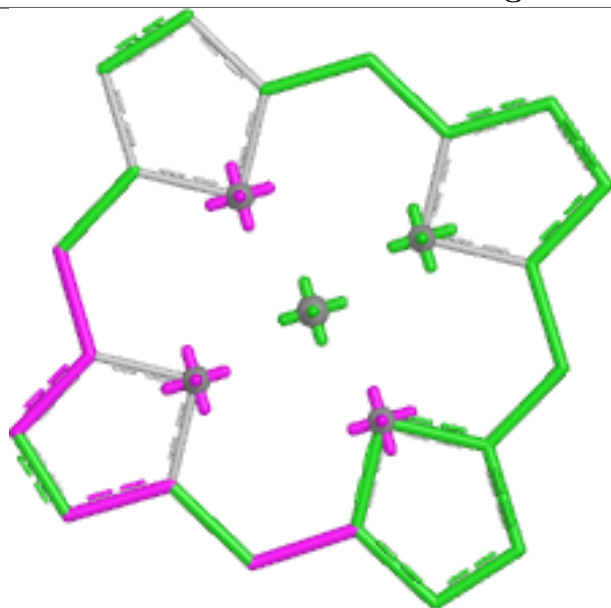


Torsions

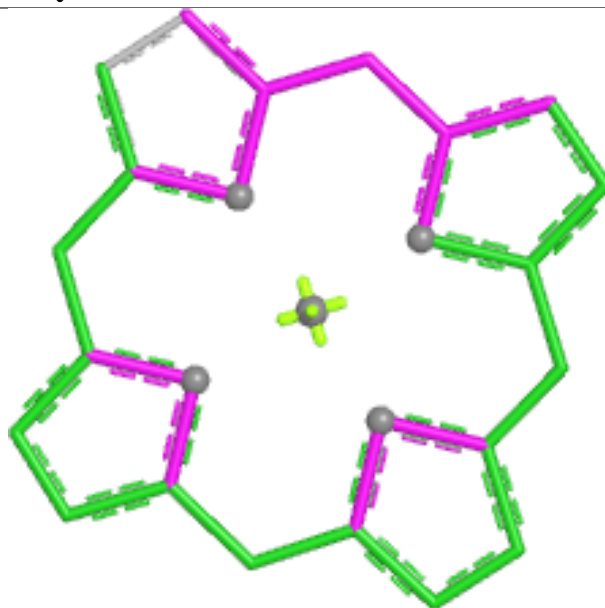


Rings

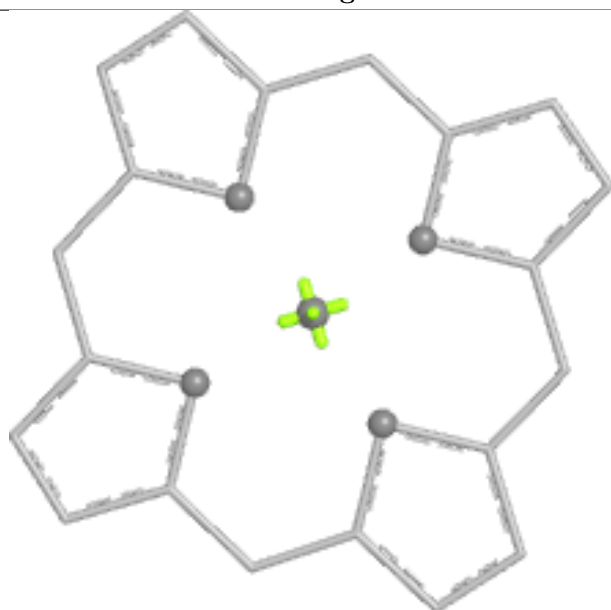
Ligand CLA Q 5205



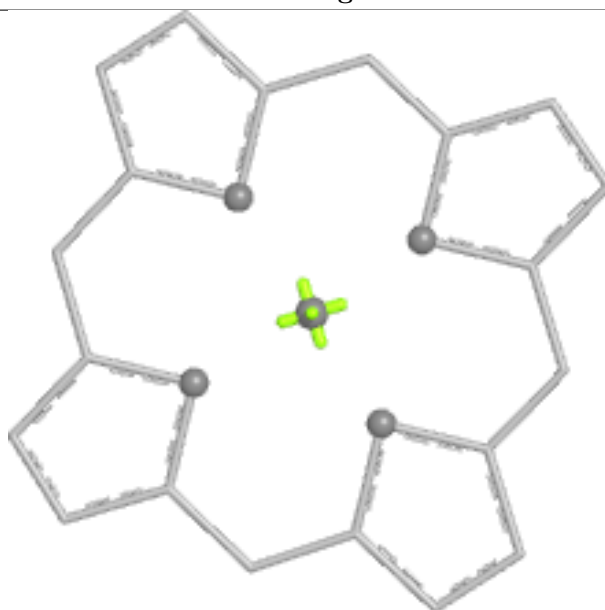
Bond lengths



Bond angles

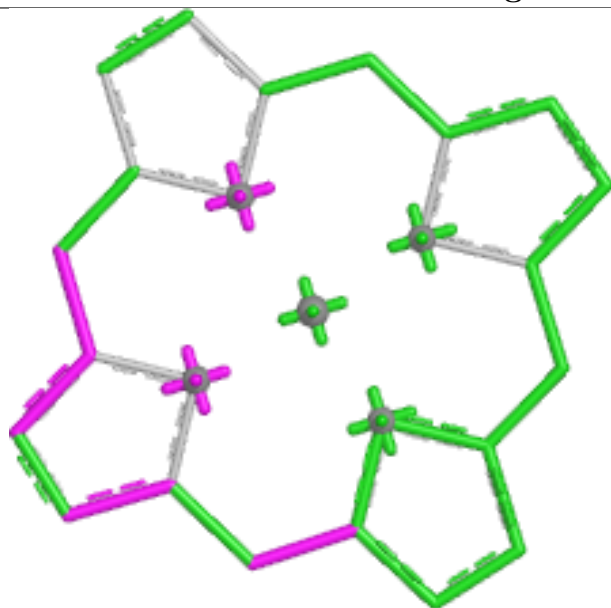


Torsions

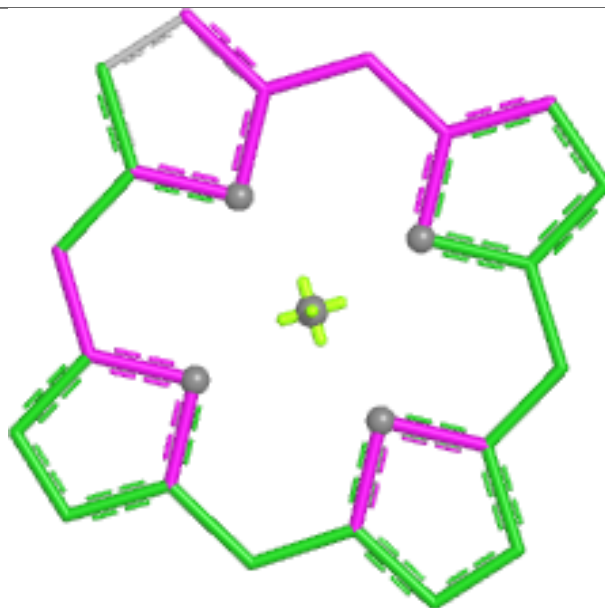


Rings

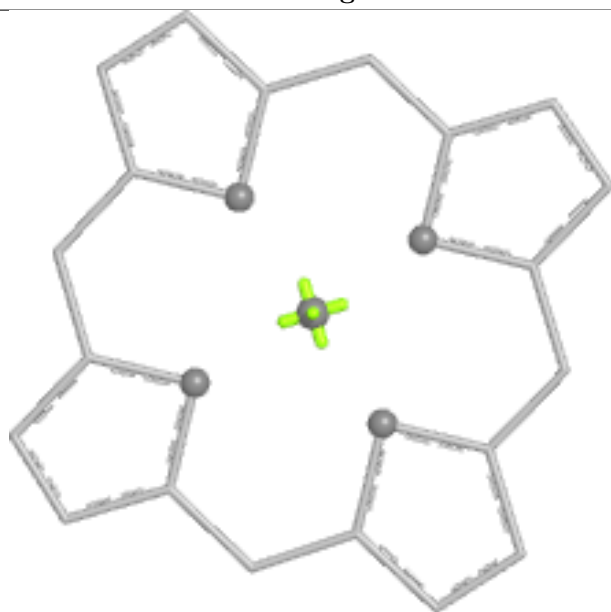
Ligand CLA A 4009



Bond lengths



Bond angles

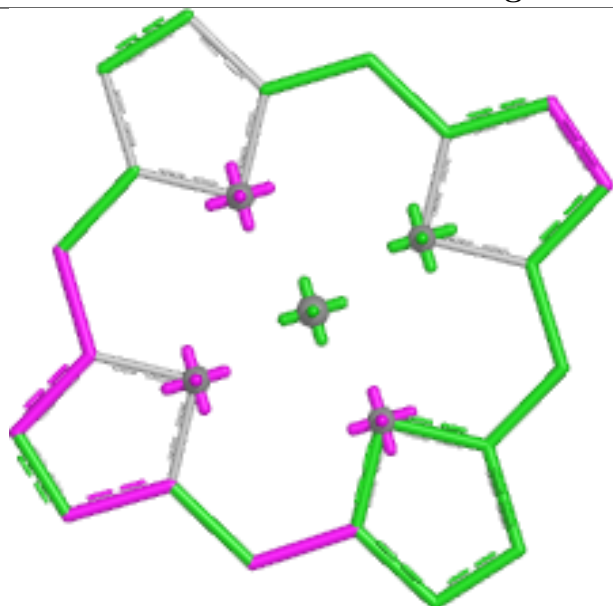


Torsions

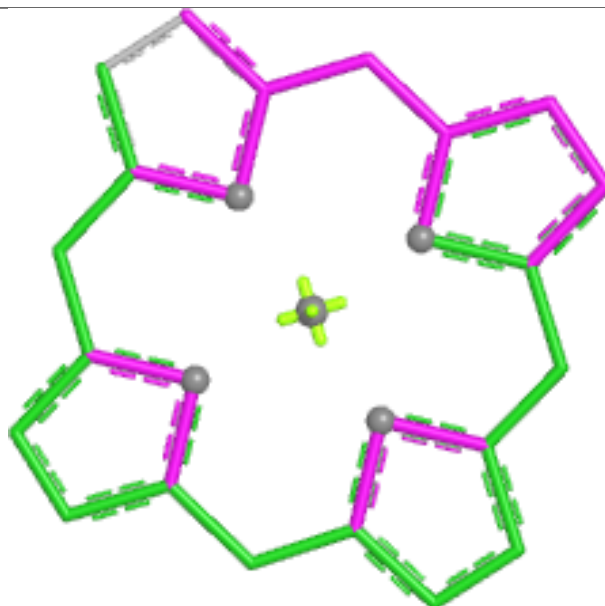


Rings

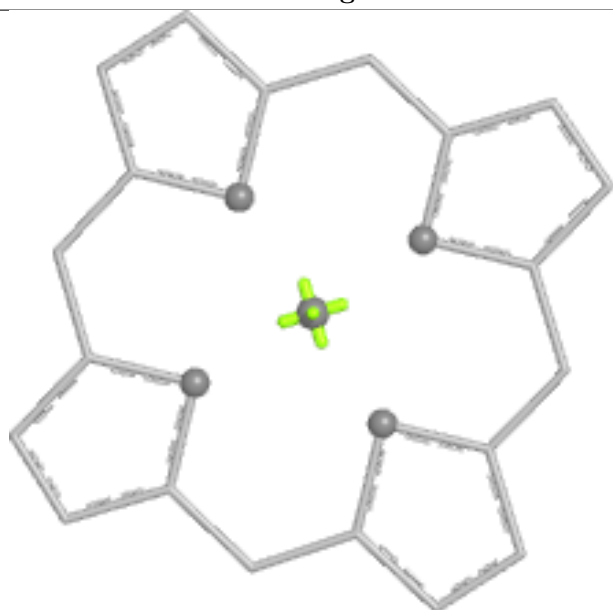
Ligand CLA A 1120



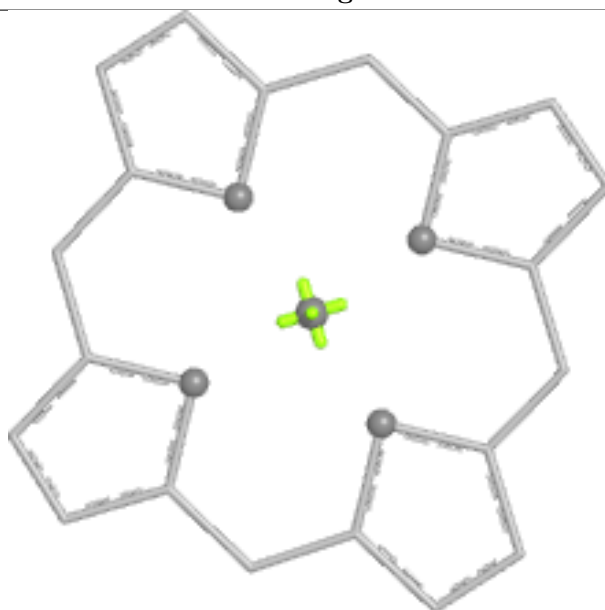
Bond lengths



Bond angles

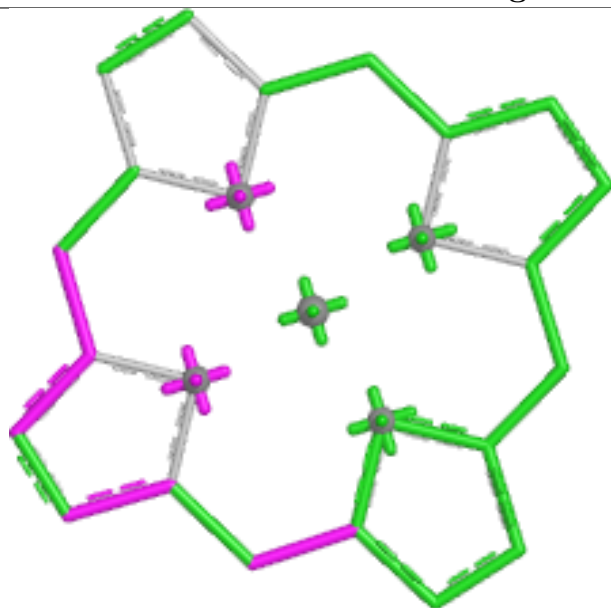


Torsions

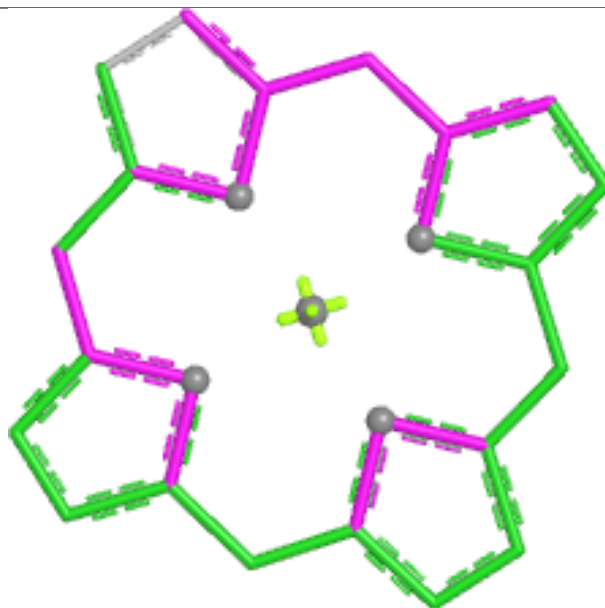


Rings

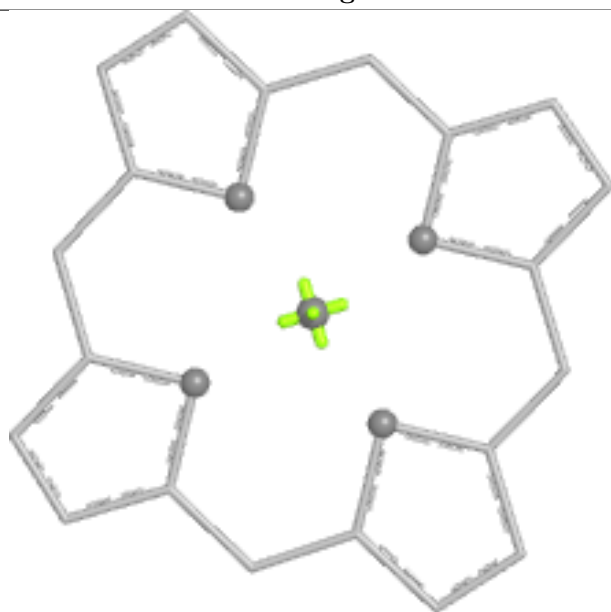
Ligand CLA J 1101



Bond lengths



Bond angles

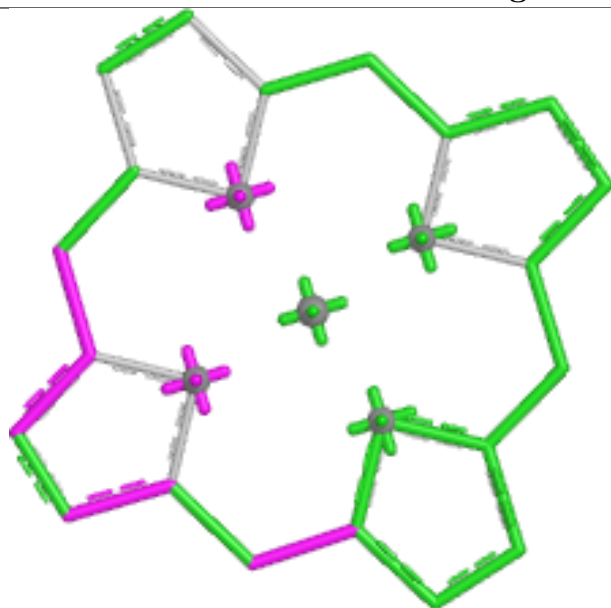


Torsions

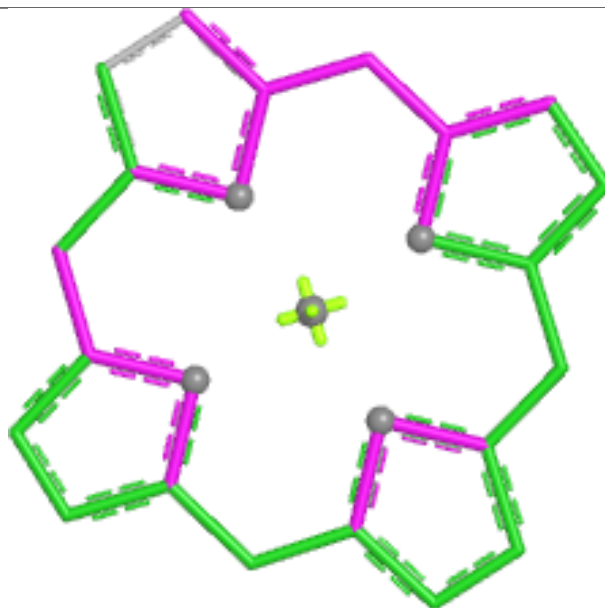


Rings

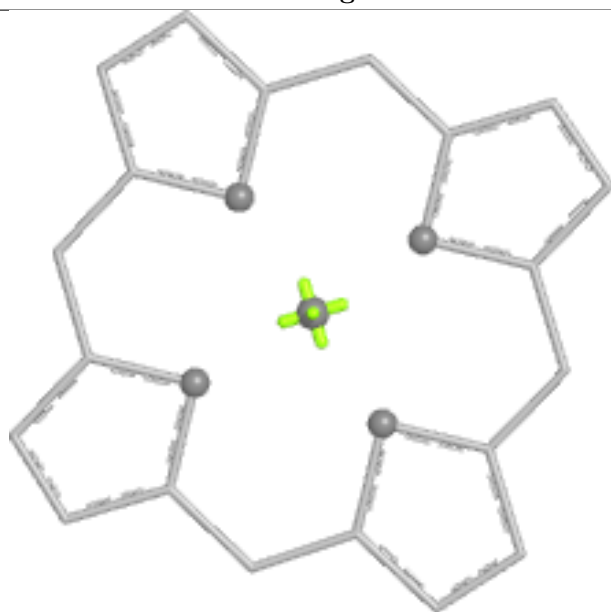
Ligand CLA 1 1022



Bond lengths



Bond angles

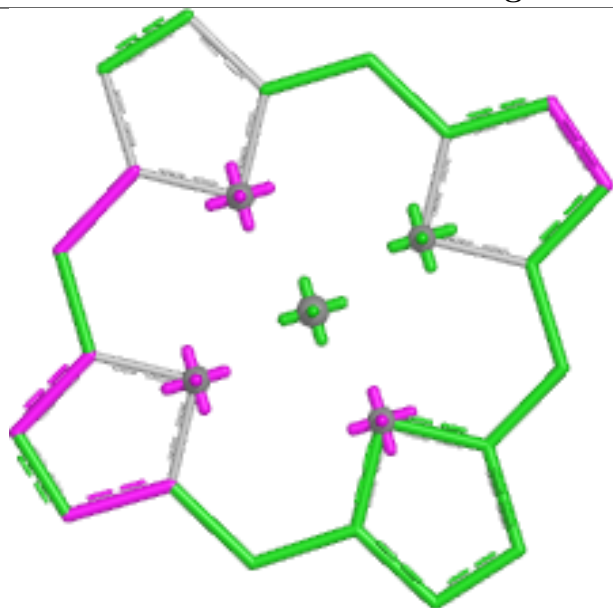


Torsions

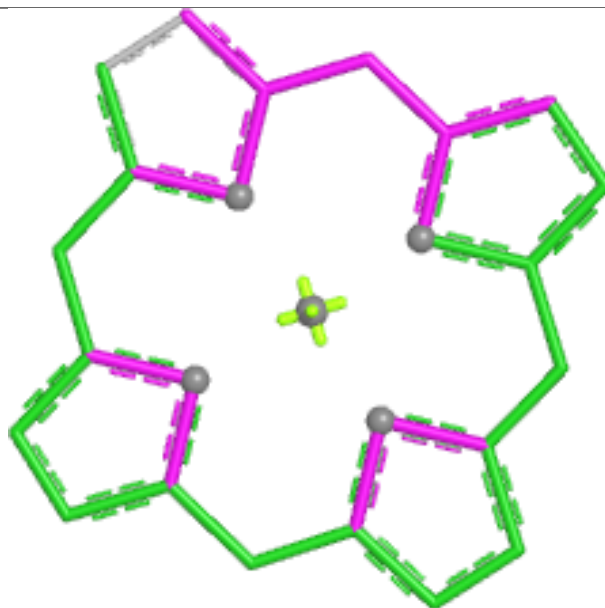


Rings

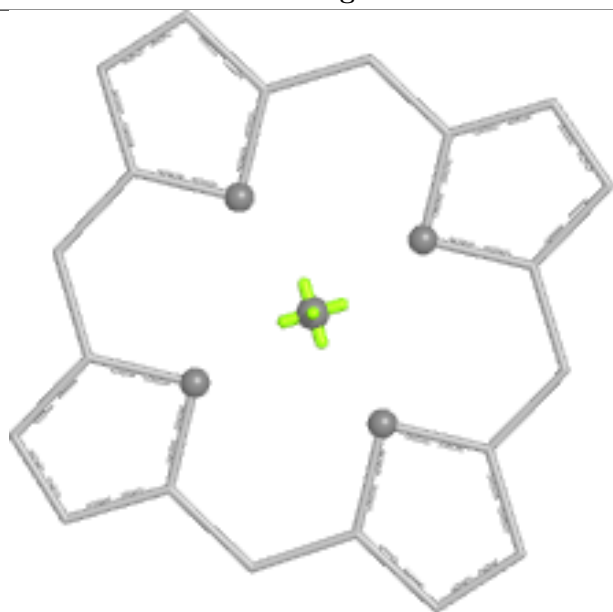
Ligand CLA A 1402



Bond lengths



Bond angles

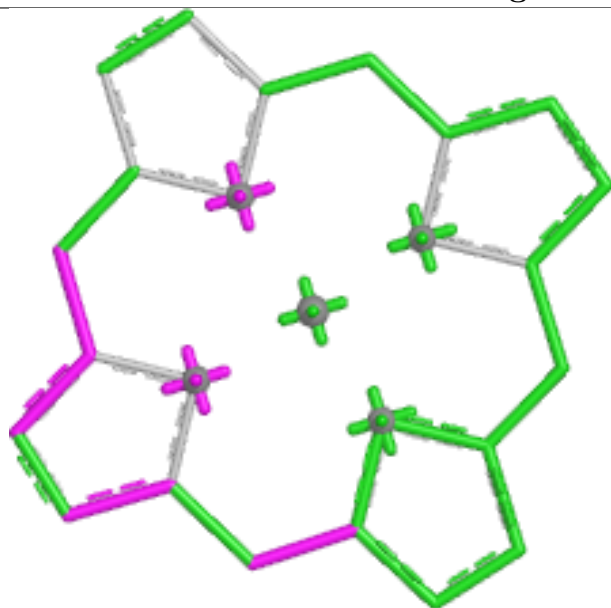


Torsions



Rings

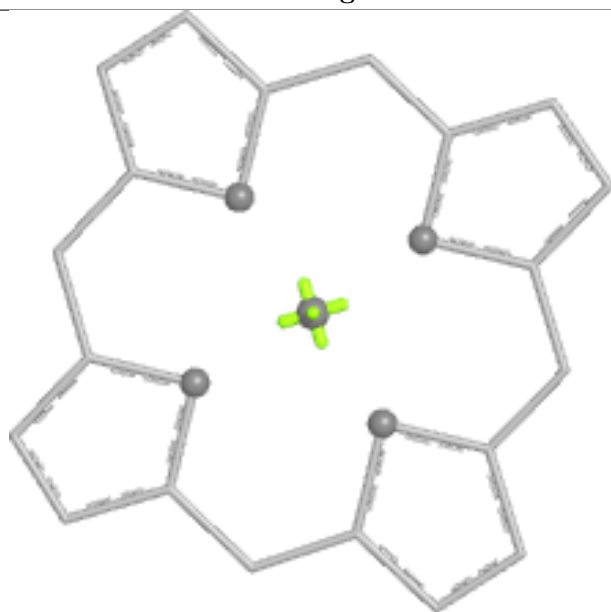
Ligand CLA 8 1016



Bond lengths



Bond angles

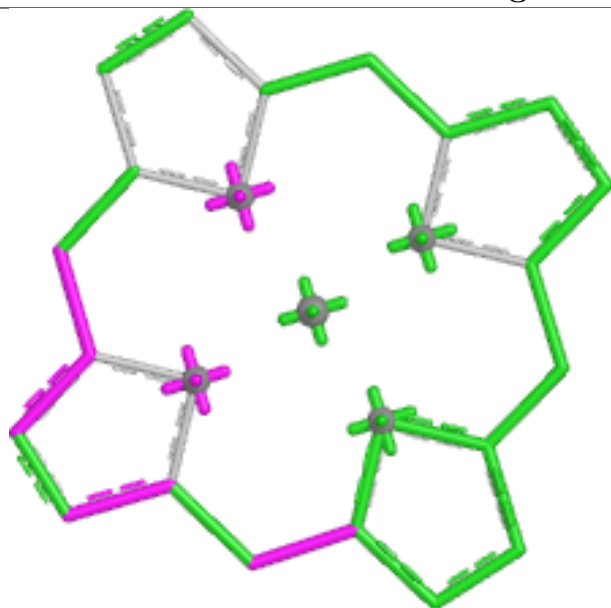


Torsions

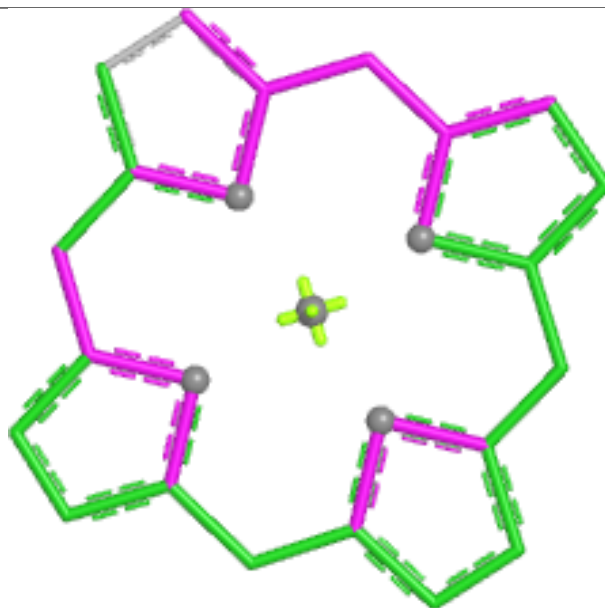


Rings

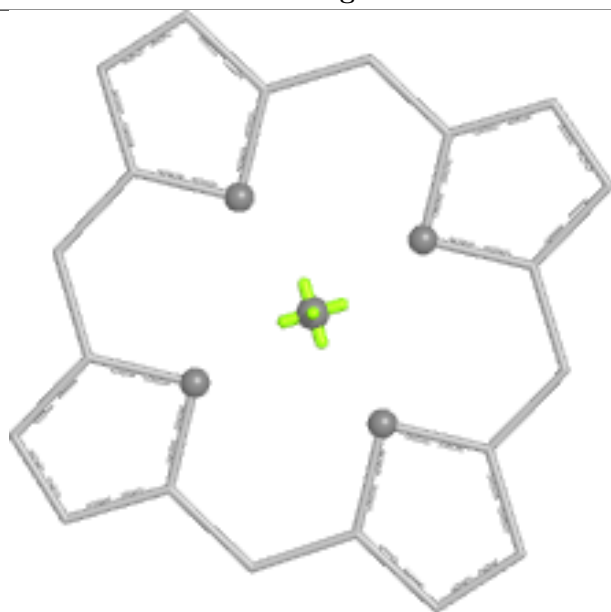
Ligand CLA 1 1017



Bond lengths



Bond angles

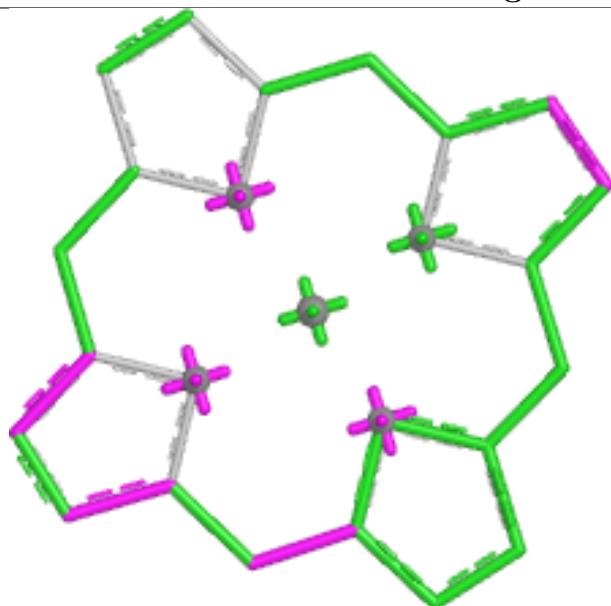


Torsions

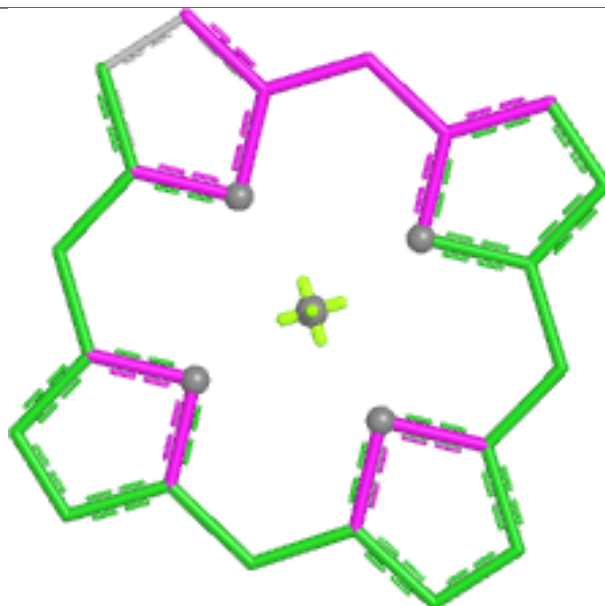


Rings

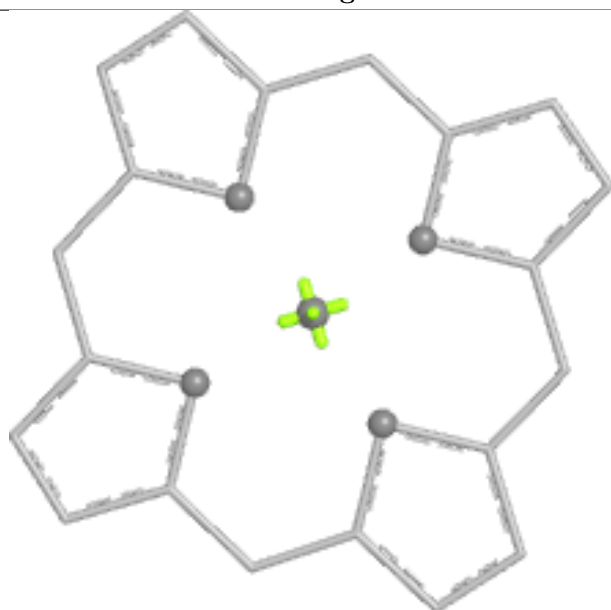
Ligand CLA U 5301



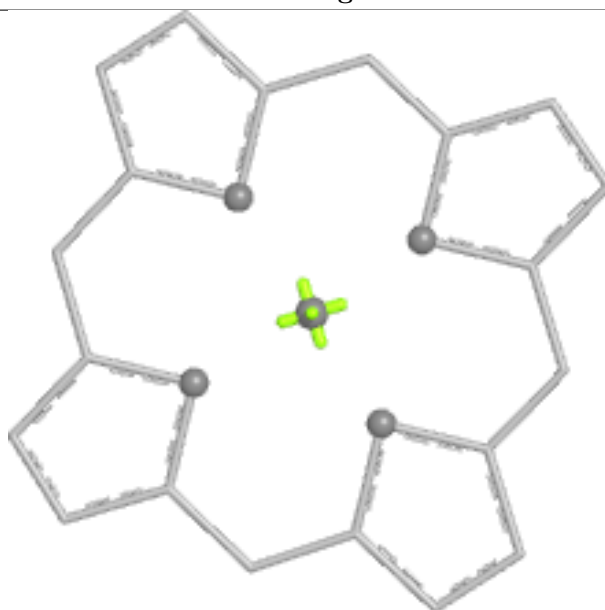
Bond lengths



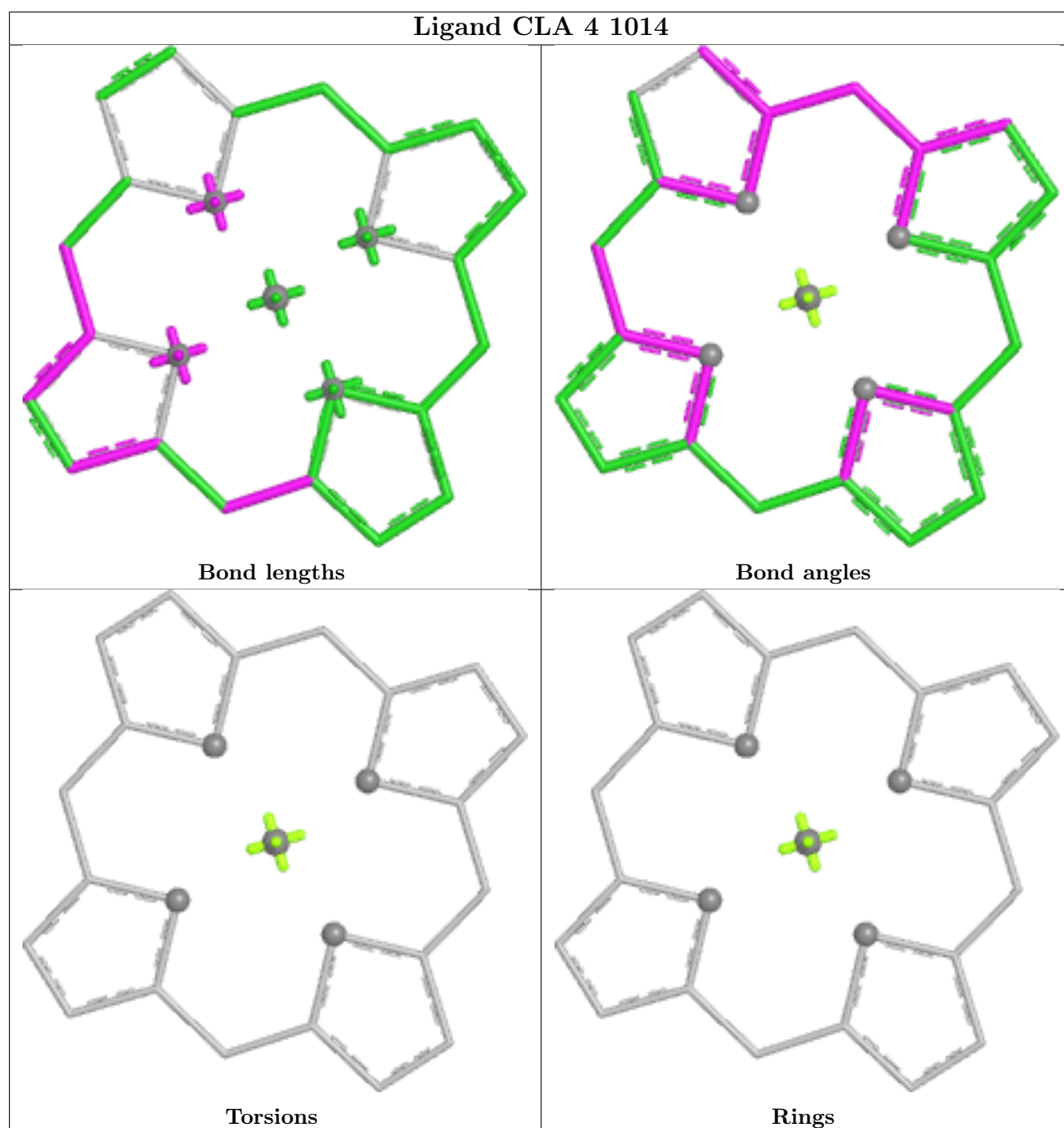
Bond angles



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.