wwPDB X-ray Structure Validation Summary Report (i)

May 29, 2020 – 05:43 am BST

PDB ID	:	1H29
Title	:	Sulfate respiration in Desulfovibrio vulgaris Hildenborough: Structure of the 16-heme Cytochrome c HmcA at 2.5 A resolution and a view of its role in transmembrane electron transfer
Authors	:	Matias, P.M.; Coelho, A.V.; Valente, F.M.A.; Placido, D.; Legall, J.; Xavier, A.V.; Pereira, I.A.C.; Carrondo, M.A.
Deposited on	:	2002-08-01
Resolution	:	2.51 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

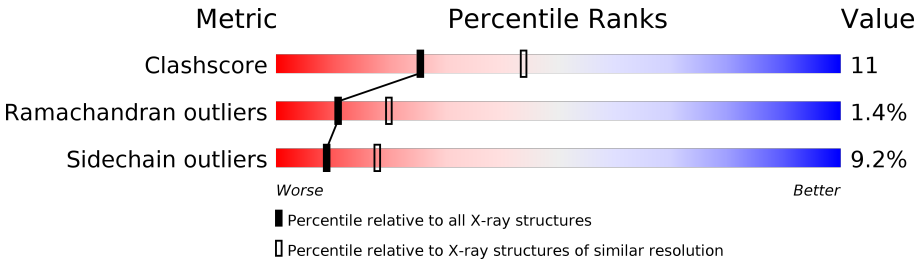
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.51 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	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)

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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	514	74% 19%
1	B	514	75% 19%
1	C	514	74% 21%
1	D	514	69% 23%

2 Entry composition

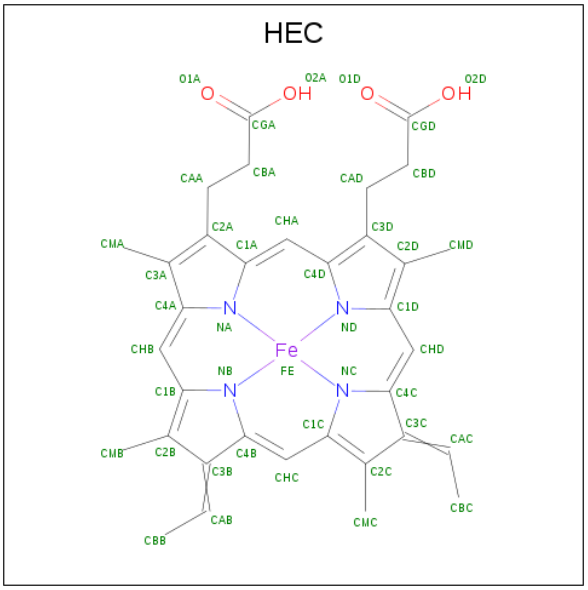
There are 3 unique types of molecules in this entry. The entry contains 18287 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 HIGH-MOLECULAR-WEIGHT CYTOCHROME C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	501	Total	C	N	O	S	38	0	0
			3783	2323	717	699	44			
1	B	499	Total	C	N	O	S	75	0	0
			3763	2312	712	695	44			
1	C	501	Total	C	N	O	S	90	0	0
			3777	2320	714	699	44			
1	D	492	Total	C	N	O	S	70	0	0
			3715	2284	699	688	44			

- Molecule 2 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C Fe N O 43 34 1 4 4	0	0
2	A	1	Total C Fe N O 43 34 1 4 4	0	0
2	A	1	Total C Fe N O 43 34 1 4 4	0	0
2	A	1	Total C Fe N O 43 34 1 4 4	0	0
2	A	1	Total C Fe N O 43 34 1 4 4	0	0
2	A	1	Total C Fe N O 43 34 1 4 4	0	0
2	A	1	Total C Fe N O 43 34 1 4 4	0	0
2	A	1	Total C Fe N O 43 34 1 4 4	0	0
2	A	1	Total C Fe N O 43 34 1 4 4	0	0
2	A	1	Total C Fe N O 43 34 1 4 4	0	0
2	A	1	Total C Fe N O 43 34 1 4 4	0	0
2	A	1	Total C Fe N O 43 34 1 4 4	0	0
2	A	1	Total C Fe N O 43 34 1 4 4	0	0
2	A	1	Total C Fe N O 43 34 1 4 4	0	0
2	B	1	Total C Fe N O 43 34 1 4 4	0	0
2	B	1	Total C Fe N O 43 34 1 4 4	0	0
2	B	1	Total C Fe N O 43 34 1 4 4	0	0
2	B	1	Total C Fe N O 43 34 1 4 4	0	0
2	B	1	Total C Fe N O 43 34 1 4 4	0	0
2	B	1	Total C Fe N O 43 34 1 4 4	0	0
2	B	1	Total C Fe N O 43 34 1 4 4	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total C Fe N O 43 34 1 4 4	0	0
2	B	1	Total C Fe N O 43 34 1 4 4	0	0
2	B	1	Total C Fe N O 43 34 1 4 4	0	0
2	B	1	Total C Fe N O 43 34 1 4 4	0	0
2	B	1	Total C Fe N O 43 34 1 4 4	0	0
2	B	1	Total C Fe N O 43 34 1 4 4	0	0
2	B	1	Total C Fe N O 43 34 1 4 4	0	0
2	B	1	Total C Fe N O 43 34 1 4 4	0	0
2	B	1	Total C Fe N O 43 34 1 4 4	0	0
2	C	1	Total C Fe N O 43 34 1 4 4	0	0
2	C	1	Total C Fe N O 43 34 1 4 4	0	0
2	C	1	Total C Fe N O 43 34 1 4 4	0	0
2	C	1	Total C Fe N O 43 34 1 4 4	0	0
2	C	1	Total C Fe N O 43 34 1 4 4	0	0
2	C	1	Total C Fe N O 43 34 1 4 4	0	0
2	C	1	Total C Fe N O 43 34 1 4 4	0	0
2	C	1	Total C Fe N O 43 34 1 4 4	0	0
2	C	1	Total C Fe N O 43 34 1 4 4	0	0
2	C	1	Total C Fe N O 43 34 1 4 4	0	0
2	C	1	Total C Fe N O 43 34 1 4 4	0	0
2	C	1	Total C Fe N O 43 34 1 4 4	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	1	Total C Fe N O 43 34 1 4 4	0	0
2	C	1	Total C Fe N O 43 34 1 4 4	0	0
2	C	1	Total C Fe N O 43 34 1 4 4	0	0
2	C	1	Total C Fe N O 43 34 1 4 4	0	0
2	D	1	Total C Fe N O 43 34 1 4 4	0	0
2	D	1	Total C Fe N O 43 34 1 4 4	0	0
2	D	1	Total C Fe N O 43 34 1 4 4	0	0
2	D	1	Total C Fe N O 43 34 1 4 4	0	0
2	D	1	Total C Fe N O 43 34 1 4 4	0	0
2	D	1	Total C Fe N O 43 34 1 4 4	0	0
2	D	1	Total C Fe N O 43 34 1 4 4	0	0
2	D	1	Total C Fe N O 43 34 1 4 4	0	0
2	D	1	Total C Fe N O 43 34 1 4 4	0	0
2	D	1	Total C Fe N O 43 34 1 4 4	0	0
2	D	1	Total C Fe N O 43 34 1 4 4	0	0
2	D	1	Total C Fe N O 43 34 1 4 4	0	0
2	D	1	Total C Fe N O 43 34 1 4 4	0	0
2	D	1	Total C Fe N O 43 34 1 4 4	0	0
2	D	1	Total C Fe N O 43 34 1 4 4	0	0
2	D	1	Total C Fe N O 43 34 1 4 4	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	123	Total O 123 123	0	0
3	B	126	Total O 126 126	0	0
3	C	136	Total O 136 136	0	0
3	D	112	Total O 112 112	0	0

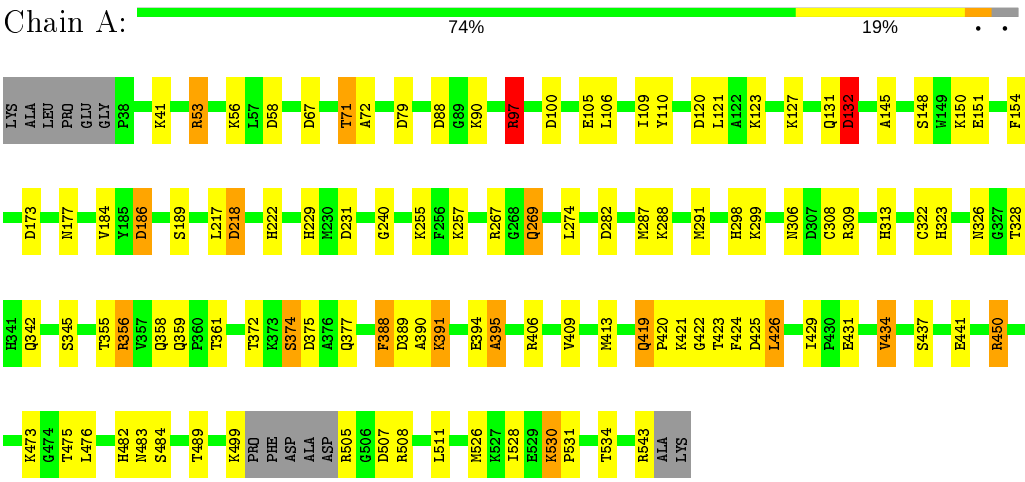
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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.

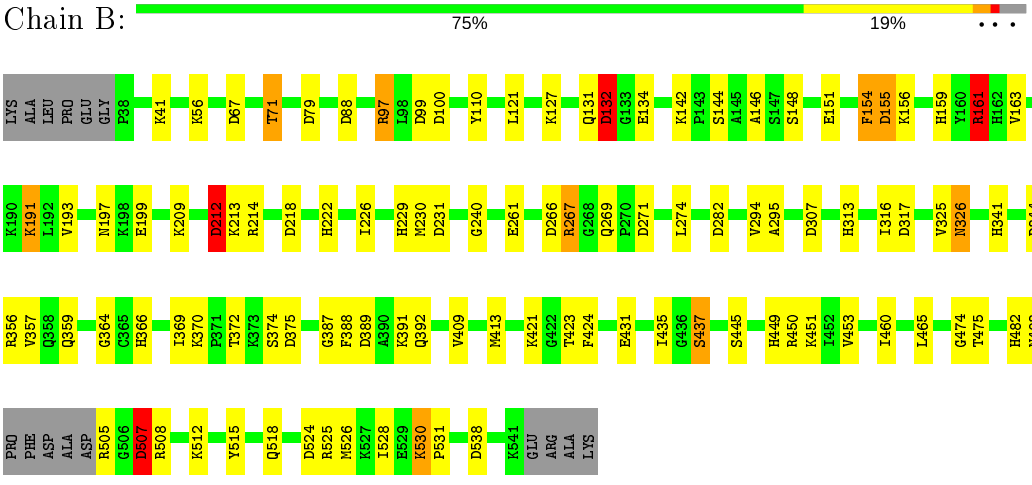
- Molecule 1: HIGH-MOLECULAR-WEIGHT CYTOCHROME C

Chain A:



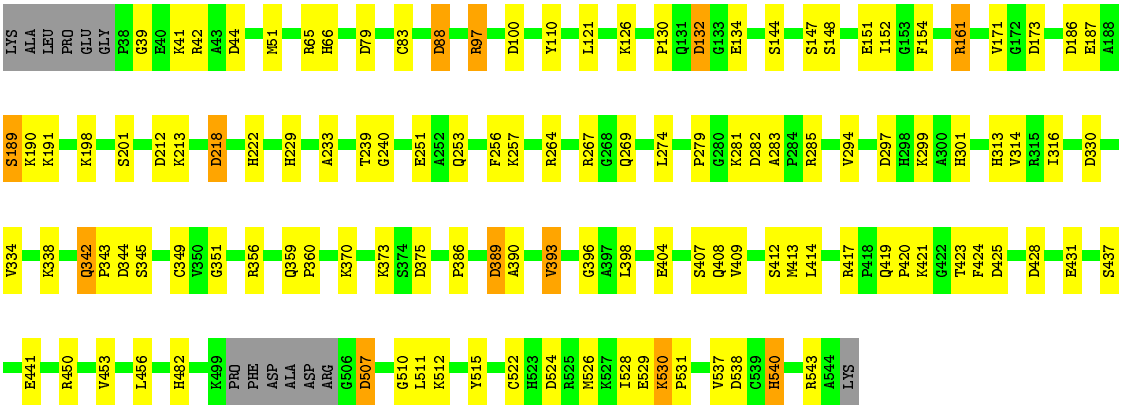
- Molecule 1: HIGH-MOLECULAR-WEIGHT CYTOCHROME C

Chain B:



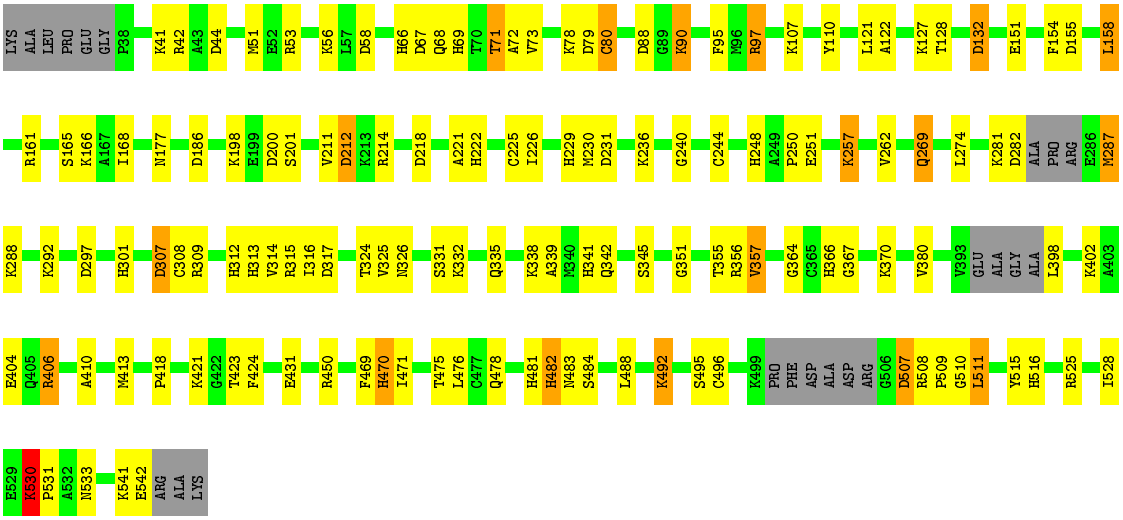
- Molecule 1: HIGH-MOLECULAR-WEIGHT CYTOCHROME C

Chain C:



- Molecule 1: HIGH-MOLECULAR-WEIGHT CYTOCHROME C

Chain D:



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 62	Depositor
Cell constants a, b, c, α, β, γ	220.39Å 220.39Å 102.64Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 2.51	Depositor
% Data completeness (in resolution range)	92.1 (30.00-2.51)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.192 , 0.258	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	18287	wwPDB-VP
Average B, all atoms (Å^2)	31.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: HEC

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).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.59	0/3864	0.83	17/5201 (0.3%)
1	B	0.59	1/3844 (0.0%)	0.83	21/5175 (0.4%)
1	C	0.57	0/3858	0.85	19/5194 (0.4%)
1	D	0.53	0/3793	0.83	15/5103 (0.3%)
All	All	0.57	1/15359 (0.0%)	0.84	72/20673 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	2
1	D	0	1
All	All	0	5

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	189	SER	CB-OG	7.80	1.52	1.42

The worst 5 of 72 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	218	ASP	CB-CG-OD2	10.44	127.69	118.30
1	A	132	ASP	CB-CG-OD2	8.26	125.73	118.30
1	D	79	ASP	CB-CG-OD2	8.20	125.68	118.30
1	C	97	ARG	NE-CZ-NH2	-7.42	116.59	120.30
1	C	428	ASP	CB-CG-OD2	7.37	124.93	118.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	131	GLN	Peptide
1	A	217	LEU	Peptide
1	B	131	GLN	Peptide
1	B	154	PHE	Peptide
1	D	470	HIS	Peptide

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	3783	0	3716	68	0
1	B	3763	0	3697	67	0
1	C	3777	0	3708	80	0
1	D	3715	0	3644	81	0
2	A	688	0	480	38	0
2	B	688	0	480	36	0
2	C	688	0	480	39	0
2	D	688	0	480	44	0
3	A	123	0	0	1	0
3	B	126	0	0	2	0
3	C	136	0	0	3	0
3	D	112	0	0	1	0
All	All	18287	0	16685	357	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 11.

The worst 5 of 357 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)
1:D:530:LYS:HB3	1:D:531:PRO:CD	1.85	1.07
1:B:530:LYS:HB2	1:B:531:PRO:HD3	1.34	1.06
1:D:530:LYS:HB3	1:D:531:PRO:HD3	1.29	1.06
1:C:522:CYS:SG	1:C:526:MET:HE2	1.97	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:530:LYS:CB	1:B:531:PRO:HD3	1.89	1.03

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	497/514 (97%)	463 (93%)	25 (5%)	9 (2%)	8 14
1	B	495/514 (96%)	460 (93%)	28 (6%)	7 (1%)	11 20
1	C	497/514 (97%)	468 (94%)	24 (5%)	5 (1%)	15 28
1	D	484/514 (94%)	451 (93%)	26 (5%)	7 (1%)	11 20
All	All	1973/2056 (96%)	1842 (93%)	103 (5%)	28 (1%)	11 20

5 of 28 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	132	ASP
1	A	218	ASP
1	A	390	ALA
1	A	395	ALA
1	B	132	ASP

5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	405/414 (98%)	363 (90%)	42 (10%)	7 13
1	B	403/414 (97%)	368 (91%)	35 (9%)	10 20
1	C	404/414 (98%)	374 (93%)	30 (7%)	13 27
1	D	400/414 (97%)	359 (90%)	41 (10%)	7 14
All	All	1612/1656 (97%)	1464 (91%)	148 (9%)	9 18

5 of 148 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	392	GLN
1	C	161	ARG
1	D	398	LEU
1	B	437	SER
1	B	508	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 25 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	483	ASN
1	C	358	GLN
1	D	443	GLN
1	C	68	GLN
1	C	377	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

64 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	$\#\|Z\| > 2$
2	HEC	B	1107	1	26,50,50	2.55	5 (19%)	18,82,82	1.76	3 (16%)
2	HEC	C	1107	1	26,50,50	2.41	5 (19%)	18,82,82	1.86	5 (27%)
2	HEC	B	1105	1	26,50,50	2.69	9 (34%)	18,82,82	1.46	3 (16%)
2	HEC	D	1105	1	26,50,50	2.51	6 (23%)	18,82,82	1.77	4 (22%)
2	HEC	C	1114	1	26,50,50	2.67	6 (23%)	18,82,82	1.49	3 (16%)
2	HEC	B	1108	1	26,50,50	2.61	7 (26%)	18,82,82	1.48	4 (22%)
2	HEC	A	1113	1	26,50,50	2.58	5 (19%)	18,82,82	1.55	3 (16%)
2	HEC	B	1106	1	26,50,50	2.50	6 (23%)	18,82,82	1.91	6 (33%)
2	HEC	A	1111	1	26,50,50	2.72	6 (23%)	18,82,82	1.39	2 (11%)
2	HEC	D	1102	1	26,50,50	2.52	6 (23%)	18,82,82	1.82	5 (27%)
2	HEC	A	1102	1	26,50,50	2.47	7 (26%)	18,82,82	1.75	5 (27%)
2	HEC	D	1106	1	26,50,50	2.50	6 (23%)	18,82,82	1.71	6 (33%)
2	HEC	A	1105	1	26,50,50	2.67	6 (23%)	18,82,82	1.67	4 (22%)
2	HEC	C	1105	1	26,50,50	2.72	7 (26%)	18,82,82	1.56	5 (27%)
2	HEC	B	1103	1	26,50,50	2.55	7 (26%)	18,82,82	1.91	5 (27%)
2	HEC	A	1101	1	26,50,50	2.43	10 (38%)	18,82,82	1.69	5 (27%)
2	HEC	D	1107	1	26,50,50	2.52	5 (19%)	18,82,82	1.65	6 (33%)
2	HEC	C	1116	1	26,50,50	2.61	6 (23%)	18,82,82	2.25	7 (38%)
2	HEC	B	1104	1	26,50,50	2.35	6 (23%)	18,82,82	1.87	4 (22%)
2	HEC	D	1104	1	26,50,50	2.50	6 (23%)	18,82,82	1.95	6 (33%)
2	HEC	D	1108	1	26,50,50	2.72	5 (19%)	18,82,82	1.69	3 (16%)
2	HEC	A	1107	1	26,50,50	2.39	6 (23%)	18,82,82	2.33	8 (44%)
2	HEC	B	1101	1	26,50,50	2.42	6 (23%)	18,82,82	1.72	5 (27%)
2	HEC	A	1103	1	26,50,50	2.55	6 (23%)	18,82,82	2.23	5 (27%)
2	HEC	C	1102	1	26,50,50	2.69	7 (26%)	18,82,82	1.89	6 (33%)
2	HEC	B	1102	1	26,50,50	2.58	7 (26%)	18,82,82	1.71	6 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	HEC	D	1116	1	26,50,50	2.82	6 (23%)	18,82,82	1.88	3 (16%)
2	HEC	D	1114	1	26,50,50	2.57	6 (23%)	18,82,82	1.56	3 (16%)
2	HEC	A	1108	1	26,50,50	2.58	6 (23%)	18,82,82	1.98	9 (50%)
2	HEC	C	1106	1	26,50,50	2.53	7 (26%)	18,82,82	2.06	7 (38%)
2	HEC	C	1104	1	26,50,50	2.41	5 (19%)	18,82,82	1.76	5 (27%)
2	HEC	B	1110	1	26,50,50	2.43	7 (26%)	18,82,82	2.25	7 (38%)
2	HEC	C	1110	1	26,50,50	2.45	5 (19%)	18,82,82	1.85	6 (33%)
2	HEC	B	1112	1	26,50,50	2.57	6 (23%)	18,82,82	1.86	7 (38%)
2	HEC	D	1112	1	26,50,50	2.55	5 (19%)	18,82,82	1.59	4 (22%)
2	HEC	C	1103	1	26,50,50	2.57	6 (23%)	18,82,82	2.08	5 (27%)
2	HEC	A	1104	1	26,50,50	2.58	5 (19%)	18,82,82	1.50	1 (5%)
2	HEC	B	1111	1	26,50,50	2.79	5 (19%)	18,82,82	1.51	4 (22%)
2	HEC	A	1106	1	26,50,50	2.71	6 (23%)	18,82,82	1.66	5 (27%)
2	HEC	D	1115	1	26,50,50	2.48	6 (23%)	18,82,82	1.57	4 (22%)
2	HEC	A	1109	1	26,50,50	2.62	6 (23%)	18,82,82	1.62	3 (16%)
2	HEC	A	1115	1	26,50,50	2.48	7 (26%)	18,82,82	2.03	6 (33%)
2	HEC	D	1111	1	26,50,50	2.45	5 (19%)	18,82,82	1.68	5 (27%)
2	HEC	A	1112	1	26,50,50	2.61	5 (19%)	18,82,82	1.45	4 (22%)
2	HEC	C	1112	1	26,50,50	2.72	6 (23%)	18,82,82	1.31	3 (16%)
2	HEC	B	1114	1	26,50,50	2.59	8 (30%)	18,82,82	1.48	4 (22%)
2	HEC	A	1116	1	26,50,50	2.48	5 (19%)	18,82,82	2.05	4 (22%)
2	HEC	D	1110	1	26,50,50	2.56	7 (26%)	18,82,82	1.64	5 (27%)
2	HEC	C	1101	1	26,50,50	2.41	6 (23%)	18,82,82	1.59	4 (22%)
2	HEC	D	1109	1	26,50,50	2.62	6 (23%)	18,82,82	1.38	3 (16%)
2	HEC	B	1113	1	26,50,50	2.77	8 (30%)	18,82,82	1.95	3 (16%)
2	HEC	D	1113	1	26,50,50	2.68	6 (23%)	18,82,82	1.52	4 (22%)
2	HEC	A	1110	1	26,50,50	2.69	6 (23%)	18,82,82	1.66	3 (16%)
2	HEC	B	1116	1	26,50,50	2.67	5 (19%)	18,82,82	1.89	4 (22%)
2	HEC	A	1114	1	26,50,50	2.60	8 (30%)	18,82,82	1.30	1 (5%)
2	HEC	C	1115	1	26,50,50	2.70	7 (26%)	18,82,82	2.01	7 (38%)
2	HEC	B	1115	1	26,50,50	2.52	5 (19%)	18,82,82	1.57	4 (22%)
2	HEC	B	1109	1	26,50,50	2.79	8 (30%)	18,82,82	1.29	2 (11%)
2	HEC	C	1109	1	26,50,50	2.57	7 (26%)	18,82,82	1.77	4 (22%)
2	HEC	D	1101	1	26,50,50	2.54	7 (26%)	18,82,82	1.53	3 (16%)
2	HEC	D	1103	1	26,50,50	2.67	8 (30%)	18,82,82	2.05	6 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	HEC	C	1108	1	26,50,50	2.53	5 (19%)	18,82,82	1.70	6 (33%)
2	HEC	C	1111	1	26,50,50	2.59	6 (23%)	18,82,82	1.47	3 (16%)
2	HEC	C	1113	1	26,50,50	2.73	5 (19%)	18,82,82	1.97	7 (38%)

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
2	HEC	B	1107	1	-	4/6/54/54	-
2	HEC	C	1107	1	-	1/6/54/54	-
2	HEC	B	1105	1	-	0/6/54/54	-
2	HEC	D	1105	1	-	2/6/54/54	-
2	HEC	C	1114	1	-	0/6/54/54	-
2	HEC	B	1108	1	-	0/6/54/54	-
2	HEC	A	1113	1	-	0/6/54/54	-
2	HEC	B	1106	1	-	0/6/54/54	-
2	HEC	A	1111	1	-	1/6/54/54	-
2	HEC	D	1102	1	-	0/6/54/54	-
2	HEC	A	1102	1	-	0/6/54/54	-
2	HEC	D	1106	1	-	0/6/54/54	-
2	HEC	A	1105	1	-	2/6/54/54	-
2	HEC	C	1105	1	-	3/6/54/54	-
2	HEC	B	1103	1	-	0/6/54/54	-
2	HEC	A	1101	1	-	1/6/54/54	-
2	HEC	D	1107	1	-	0/6/54/54	-
2	HEC	C	1116	1	-	0/6/54/54	-
2	HEC	B	1104	1	-	0/6/54/54	-
2	HEC	D	1104	1	-	0/6/54/54	-
2	HEC	D	1108	1	-	0/6/54/54	-
2	HEC	A	1107	1	-	2/6/54/54	-
2	HEC	B	1101	1	-	1/6/54/54	-
2	HEC	A	1103	1	-	0/6/54/54	-
2	HEC	C	1102	1	-	0/6/54/54	-
2	HEC	B	1102	1	-	0/6/54/54	-
2	HEC	D	1116	1	-	0/6/54/54	-
2	HEC	D	1114	1	-	0/6/54/54	-
2	HEC	A	1108	1	-	0/6/54/54	-
2	HEC	C	1106	1	-	0/6/54/54	-
2	HEC	C	1104	1	-	0/6/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEC	B	1110	1	-	0/6/54/54	-
2	HEC	C	1110	1	-	1/6/54/54	-
2	HEC	B	1112	1	-	0/6/54/54	-
2	HEC	D	1112	1	-	0/6/54/54	-
2	HEC	C	1103	1	-	0/6/54/54	-
2	HEC	A	1104	1	-	1/6/54/54	-
2	HEC	B	1111	1	-	0/6/54/54	-
2	HEC	A	1106	1	-	0/6/54/54	-
2	HEC	D	1115	1	-	0/6/54/54	-
2	HEC	A	1109	1	-	5/6/54/54	-
2	HEC	A	1115	1	-	0/6/54/54	-
2	HEC	D	1111	1	-	0/6/54/54	-
2	HEC	A	1112	1	-	0/6/54/54	-
2	HEC	C	1112	1	-	0/6/54/54	-
2	HEC	B	1114	1	-	0/6/54/54	-
2	HEC	A	1116	1	-	0/6/54/54	-
2	HEC	D	1110	1	-	2/6/54/54	-
2	HEC	C	1101	1	-	1/6/54/54	-
2	HEC	D	1109	1	-	5/6/54/54	-
2	HEC	B	1113	1	-	0/6/54/54	-
2	HEC	D	1113	1	-	0/6/54/54	-
2	HEC	A	1110	1	-	0/6/54/54	-
2	HEC	B	1116	1	-	0/6/54/54	-
2	HEC	A	1114	1	-	0/6/54/54	-
2	HEC	C	1115	1	-	0/6/54/54	-
2	HEC	B	1115	1	-	0/6/54/54	-
2	HEC	B	1109	1	-	0/6/54/54	-
2	HEC	C	1109	1	-	0/6/54/54	-
2	HEC	D	1101	1	-	1/6/54/54	-
2	HEC	D	1103	1	-	0/6/54/54	-
2	HEC	C	1108	1	-	0/6/54/54	-
2	HEC	C	1111	1	-	2/6/54/54	-
2	HEC	C	1113	1	-	0/6/54/54	-

The worst 5 of 397 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1112	HEC	C3B-C2B	-8.05	1.32	1.40
2	D	1108	HEC	C3B-C2B	-7.94	1.32	1.40
2	D	1113	HEC	C3C-C2C	-7.85	1.32	1.40
2	C	1113	HEC	C3C-C2C	-7.79	1.32	1.40
2	B	1109	HEC	C3C-C2C	-7.62	1.32	1.40

The worst 5 of 292 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1103	HEC	CBD-CAD-C3D	-7.00	99.57	112.49
2	C	1103	HEC	CBD-CAD-C3D	-6.29	100.89	112.49
2	B	1113	HEC	CBD-CAD-C3D	-5.65	102.07	112.49
2	A	1116	HEC	CBD-CAD-C3D	-5.65	102.07	112.49
2	C	1116	HEC	CBD-CAD-C3D	-5.47	102.40	112.49

There are no chirality outliers.

5 of 35 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1107	HEC	C1A-C2A-CAA-CBA
2	B	1107	HEC	C3A-C2A-CAA-CBA
2	D	1105	HEC	C1A-C2A-CAA-CBA
2	D	1105	HEC	C3A-C2A-CAA-CBA
2	A	1105	HEC	C1A-C2A-CAA-CBA

There are no ring outliers.

56 monomers are involved in 157 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1107	HEC	2	0
2	C	1107	HEC	3	0
2	B	1105	HEC	1	0
2	C	1114	HEC	1	0
2	B	1108	HEC	1	0
2	A	1113	HEC	5	0
2	B	1106	HEC	3	0
2	A	1111	HEC	2	0
2	D	1102	HEC	6	0
2	A	1102	HEC	5	0
2	D	1106	HEC	4	0
2	C	1105	HEC	2	0
2	A	1101	HEC	1	0
2	D	1107	HEC	2	0
2	B	1104	HEC	2	0
2	D	1104	HEC	6	0
2	D	1108	HEC	4	0
2	B	1101	HEC	1	0
2	A	1103	HEC	1	0
2	C	1102	HEC	4	0
2	B	1102	HEC	5	0

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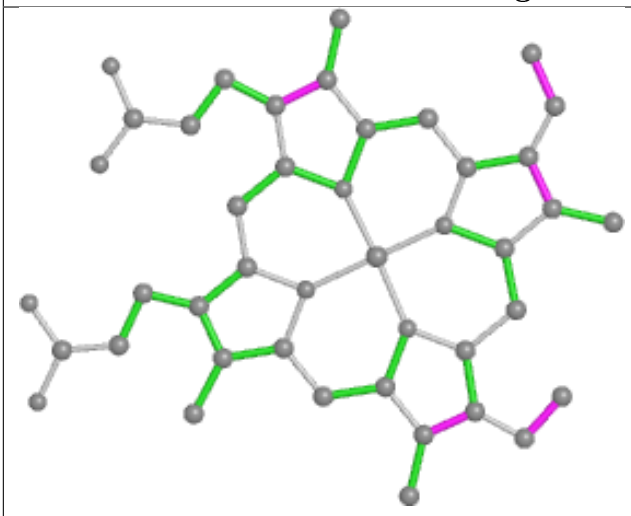
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1114	HEC	2	0
2	A	1108	HEC	3	0
2	C	1106	HEC	2	0
2	C	1104	HEC	1	0
2	B	1110	HEC	2	0
2	C	1110	HEC	5	0
2	B	1112	HEC	3	0
2	D	1112	HEC	3	0
2	C	1103	HEC	2	0
2	A	1104	HEC	4	0
2	B	1111	HEC	4	0
2	A	1106	HEC	1	0
2	D	1115	HEC	1	0
2	A	1109	HEC	3	0
2	A	1115	HEC	3	0
2	D	1111	HEC	3	0
2	A	1112	HEC	5	0
2	C	1112	HEC	1	0
2	B	1114	HEC	2	0
2	D	1110	HEC	7	0
2	C	1101	HEC	3	0
2	D	1109	HEC	4	0
2	B	1113	HEC	2	0
2	D	1113	HEC	2	0
2	A	1110	HEC	4	0
2	B	1116	HEC	1	0
2	A	1114	HEC	1	0
2	C	1115	HEC	5	0
2	B	1115	HEC	6	0
2	B	1109	HEC	1	0
2	C	1109	HEC	4	0
2	D	1101	HEC	6	0
2	C	1108	HEC	3	0
2	C	1111	HEC	4	0
2	C	1113	HEC	1	0

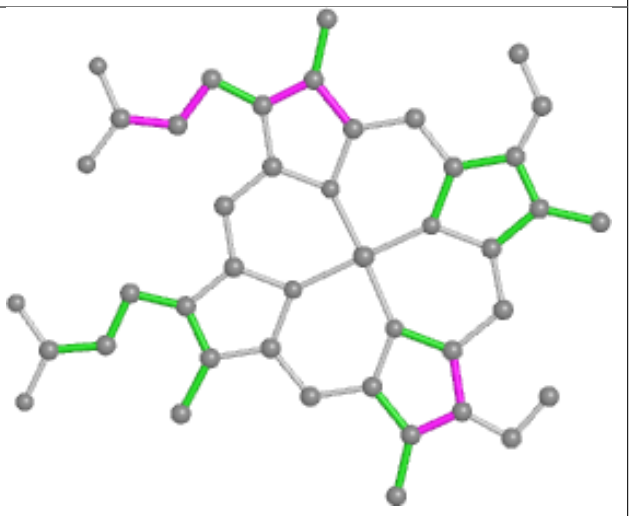
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring

in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

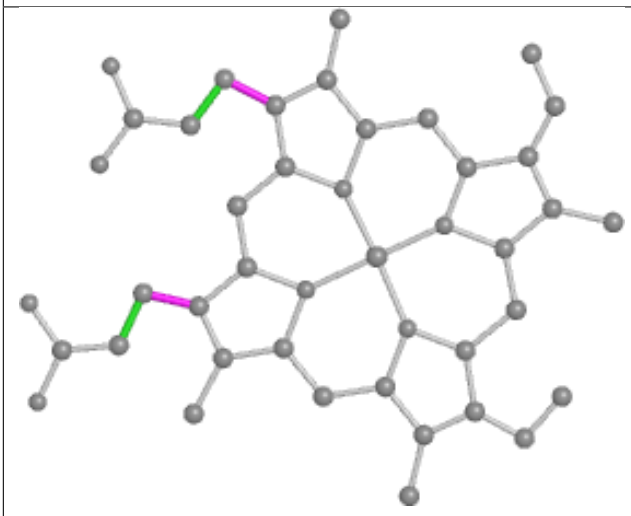
Ligand HEC B 1107



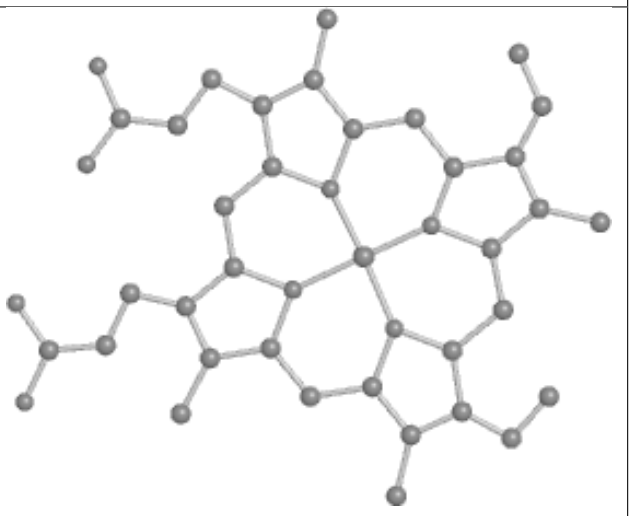
Bond lengths



Bond angles

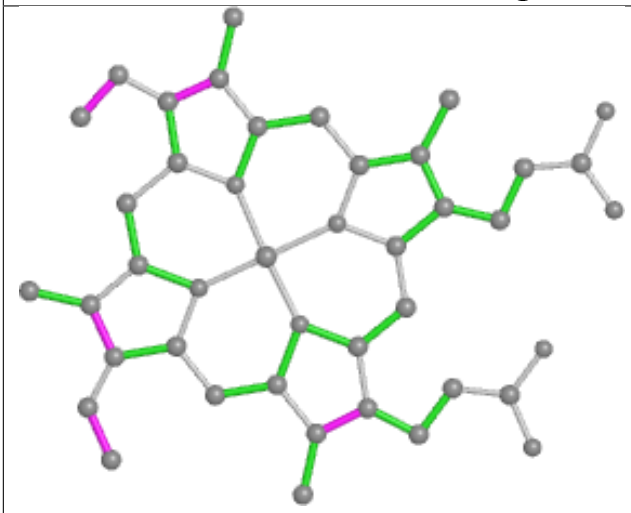


Torsions

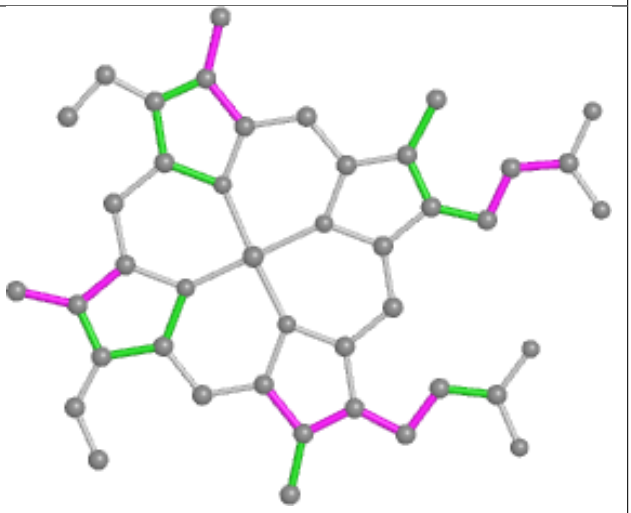


Rings

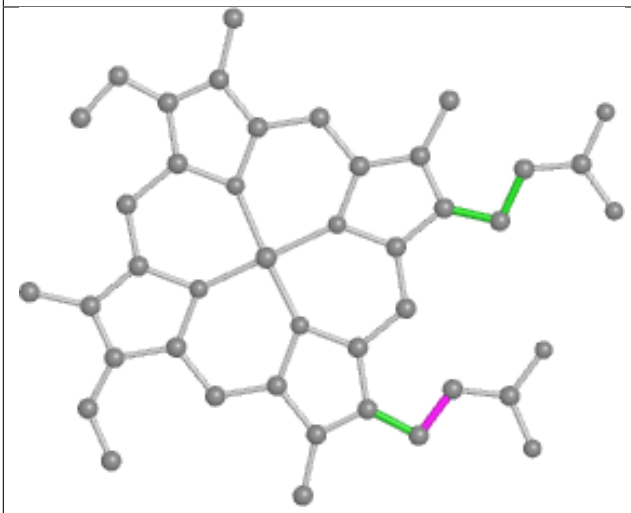
Ligand HEC C 1107



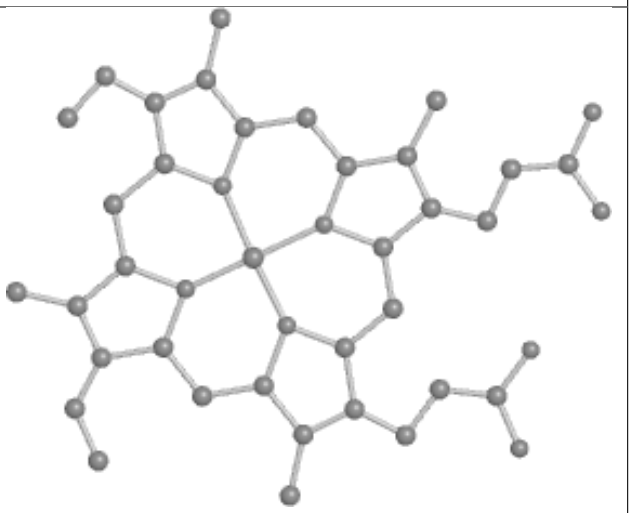
Bond lengths



Bond angles

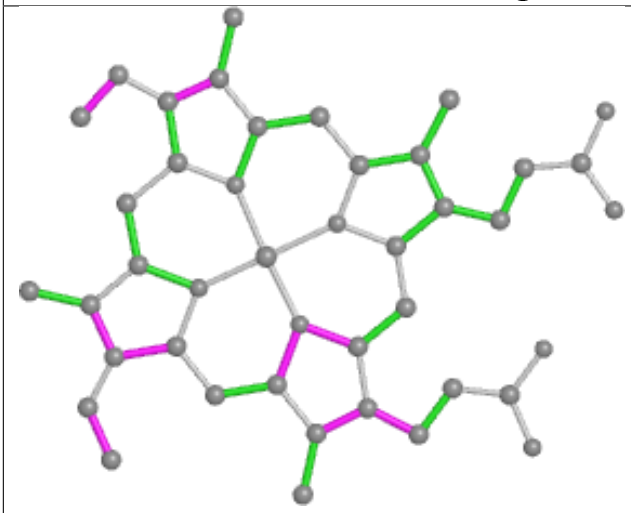


Torsions

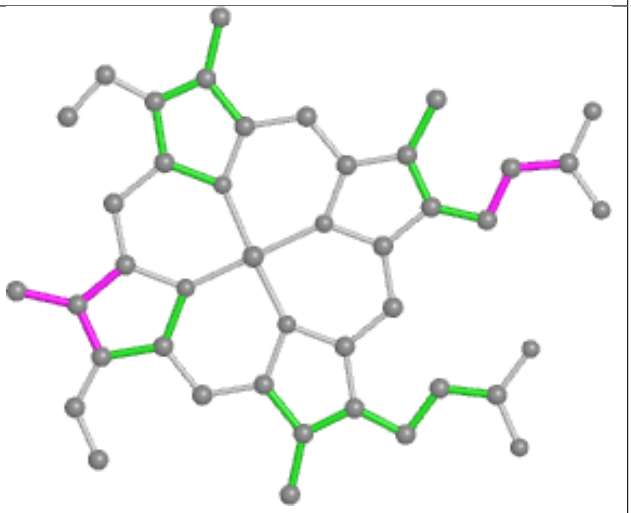


Rings

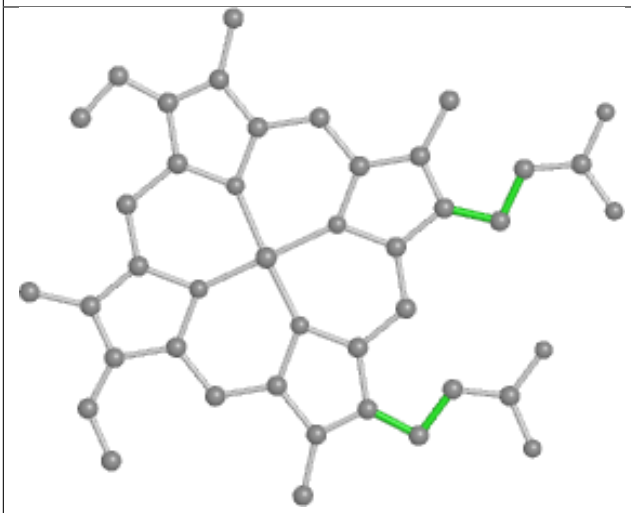
Ligand HEC B 1105



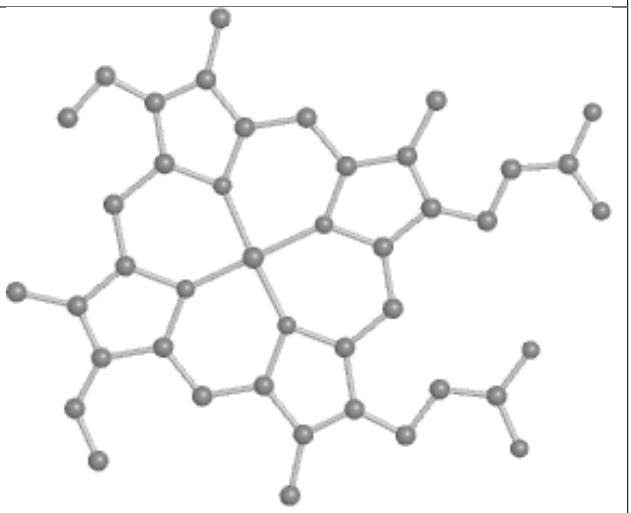
Bond lengths



Bond angles

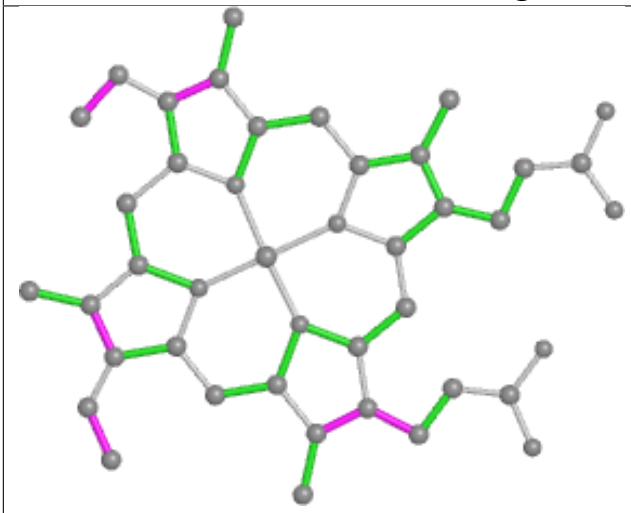


Torsions

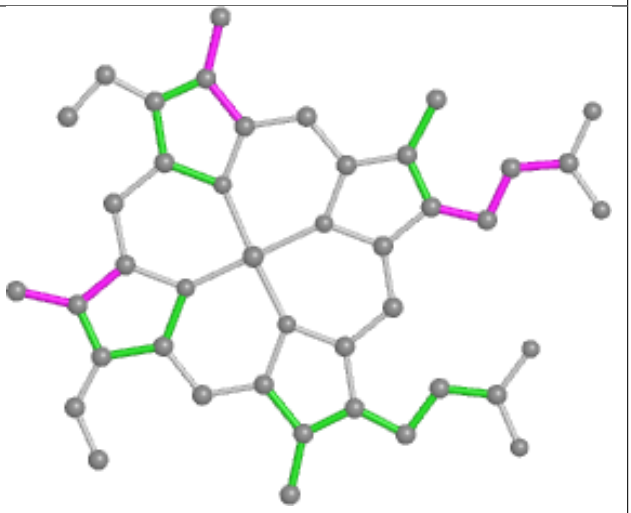


Rings

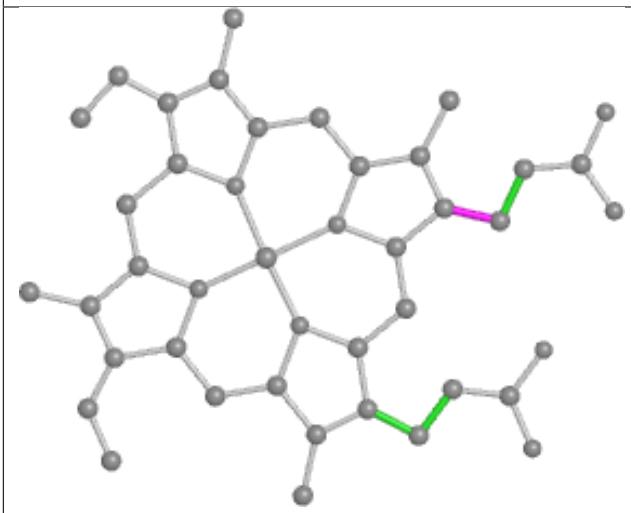
Ligand HEC D 1105



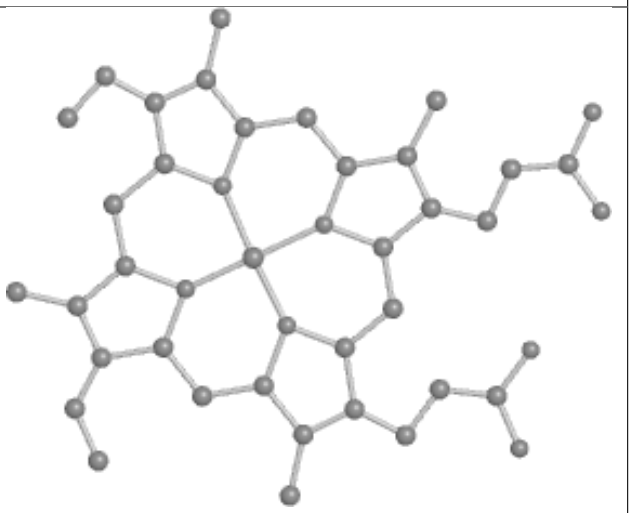
Bond lengths



Bond angles

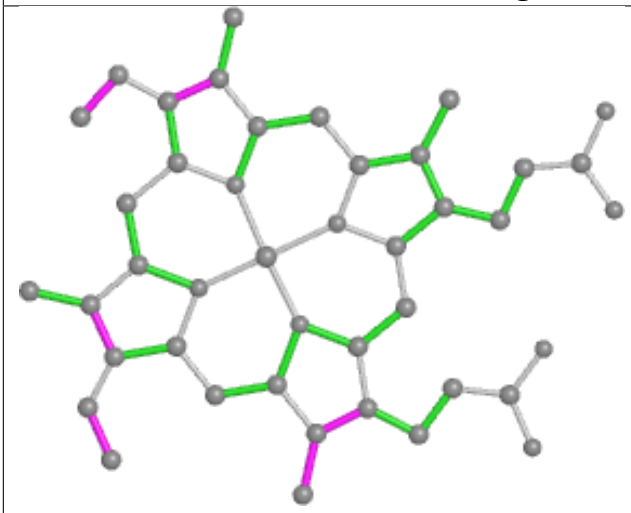


Torsions

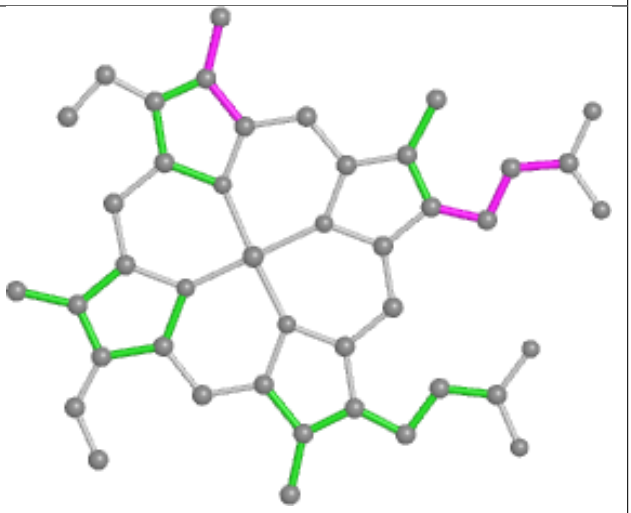


Rings

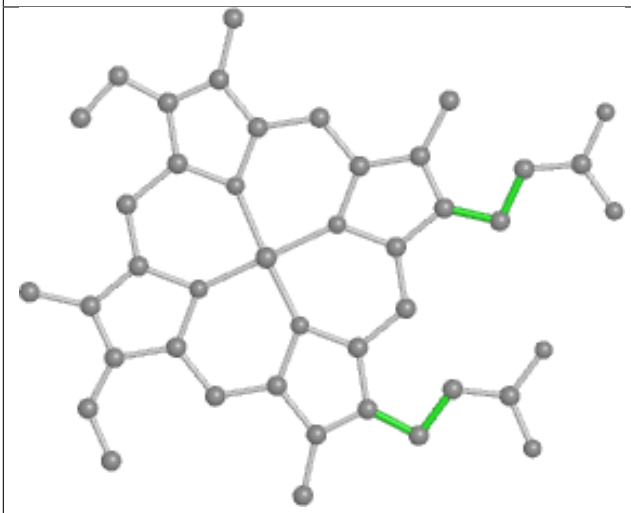
Ligand HEC C 1114



Bond lengths



Bond angles



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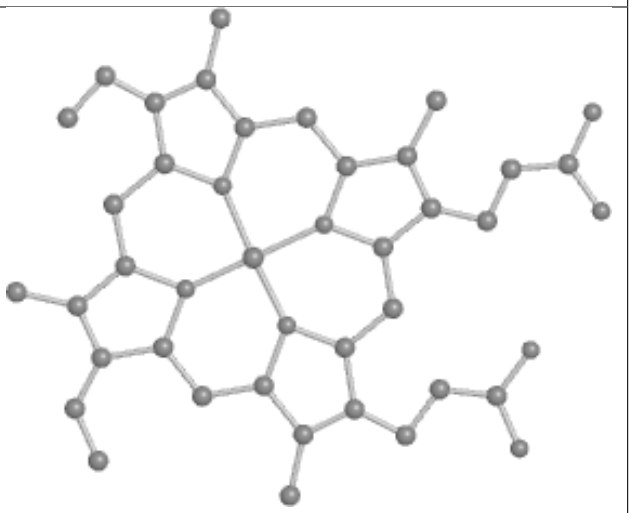
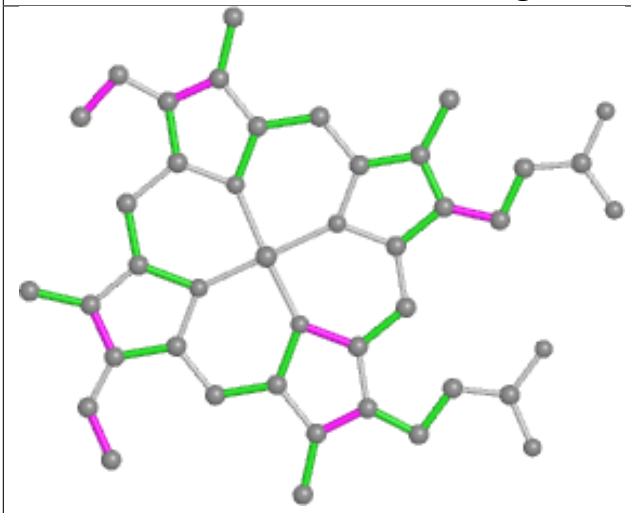
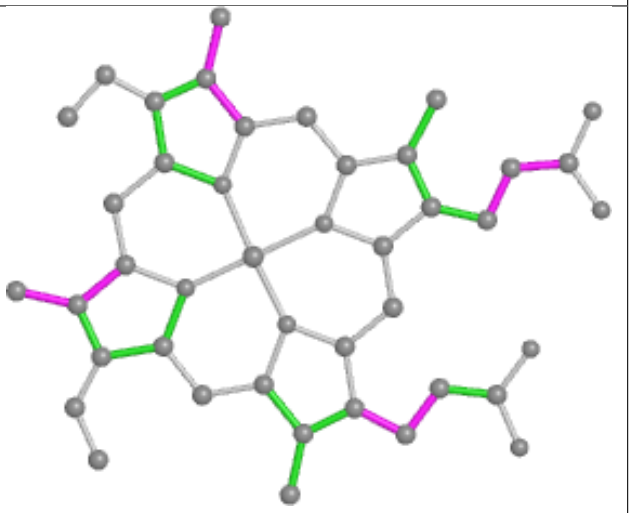


Rings

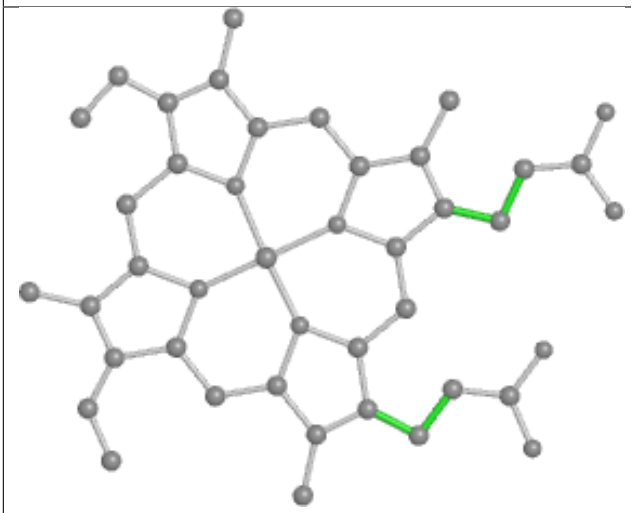
Ligand HEC B 1108



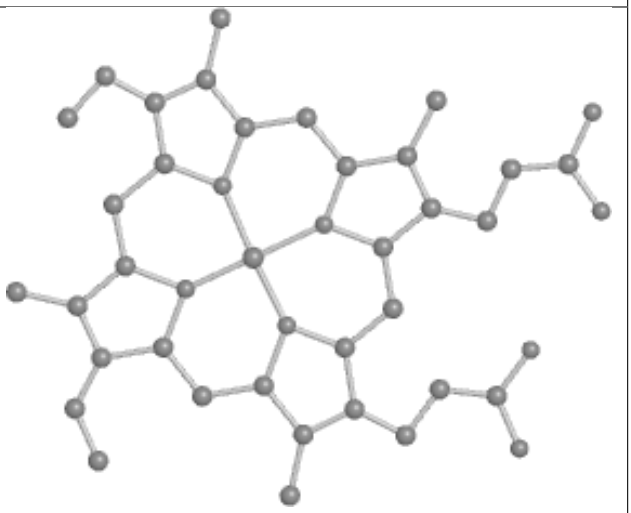
Bond lengths



Bond angles

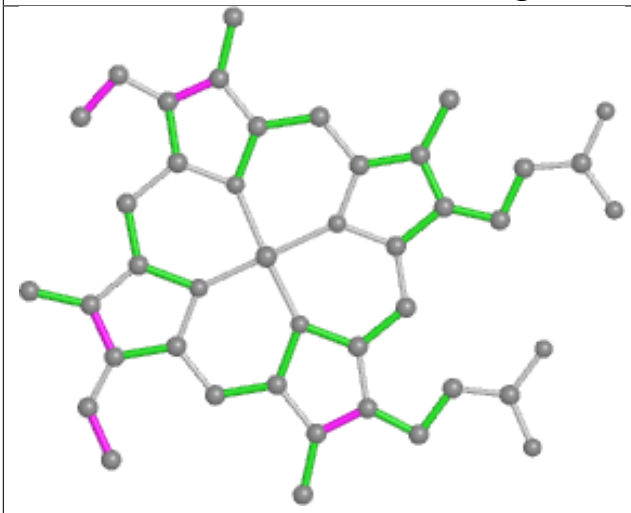


Torsions

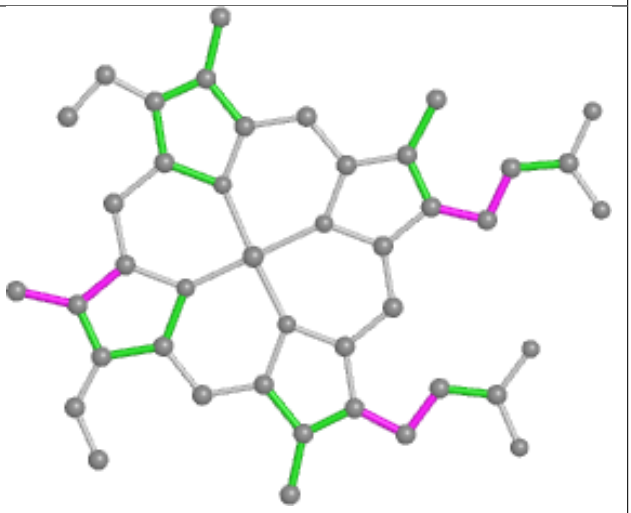


Rings

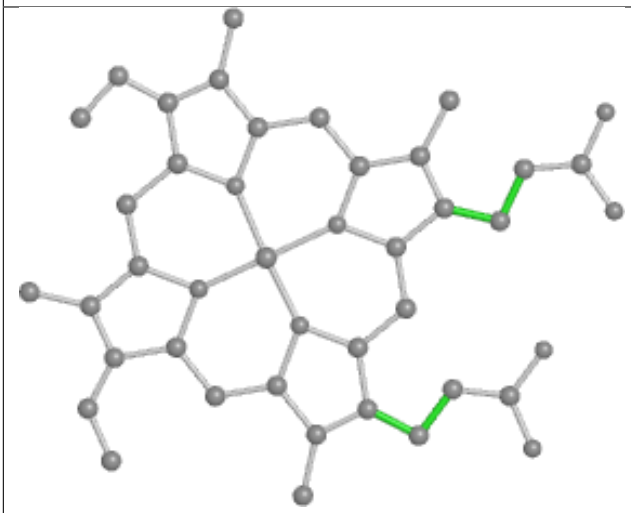
Ligand HEC A 1113



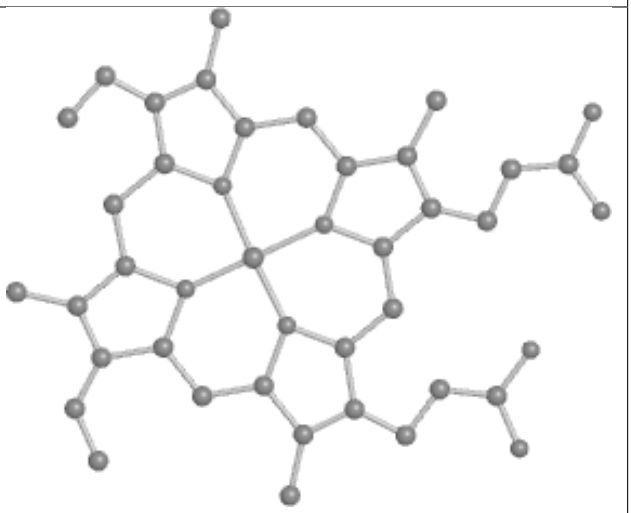
Bond lengths



Bond angles

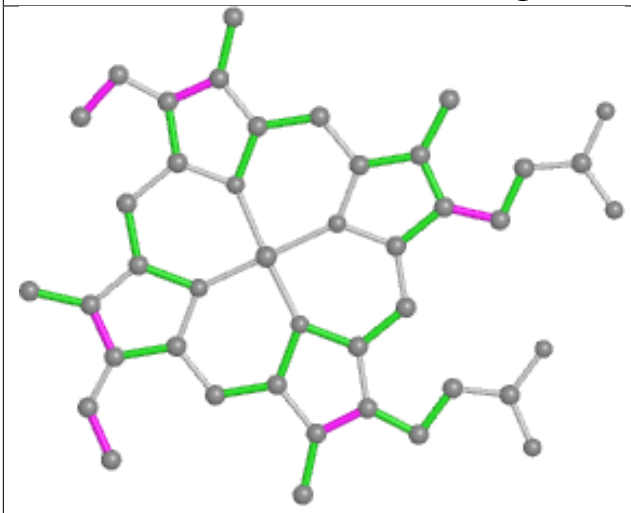


Torsions



Rings

Ligand HEC B 1106



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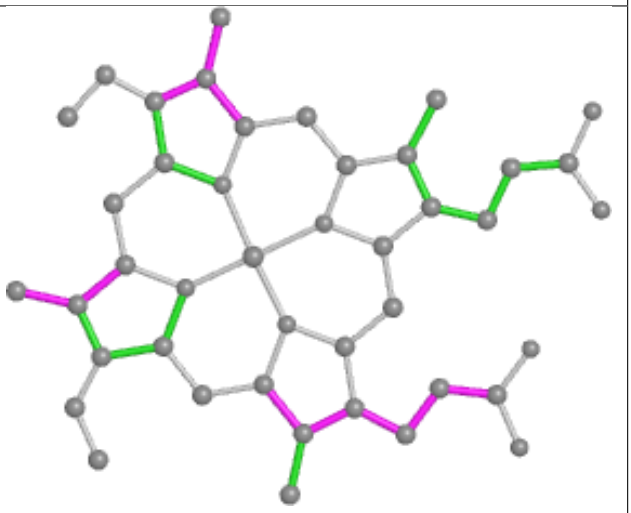
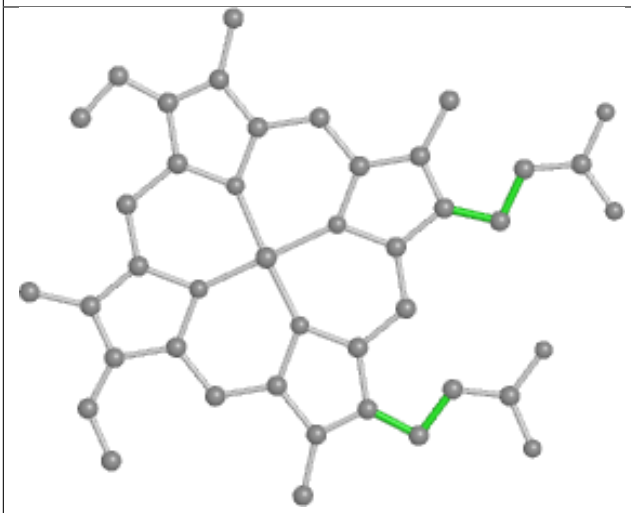


Bond angles



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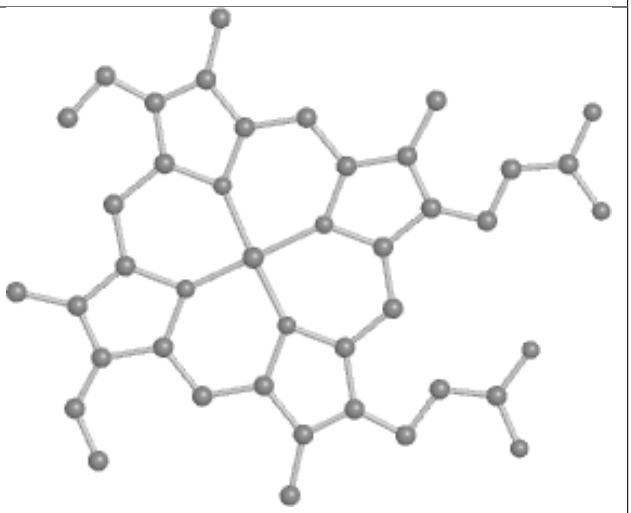
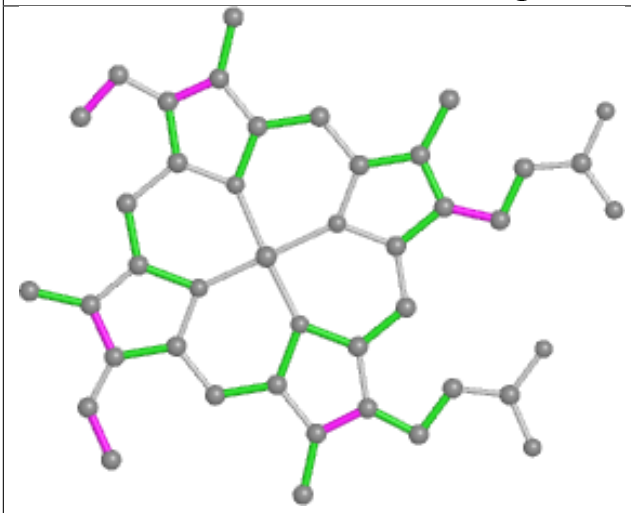
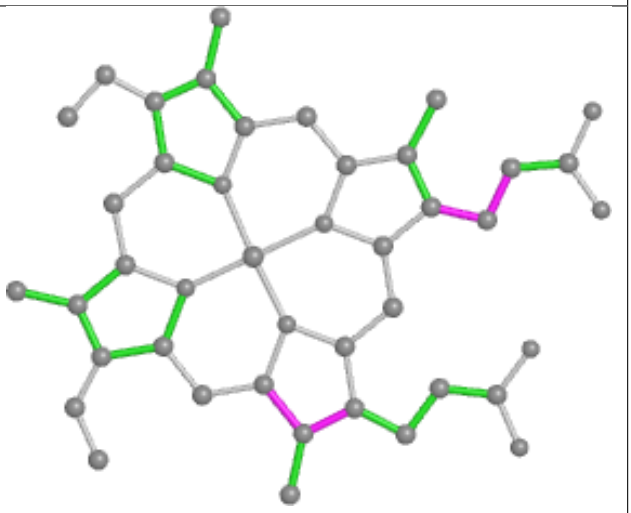


Rings

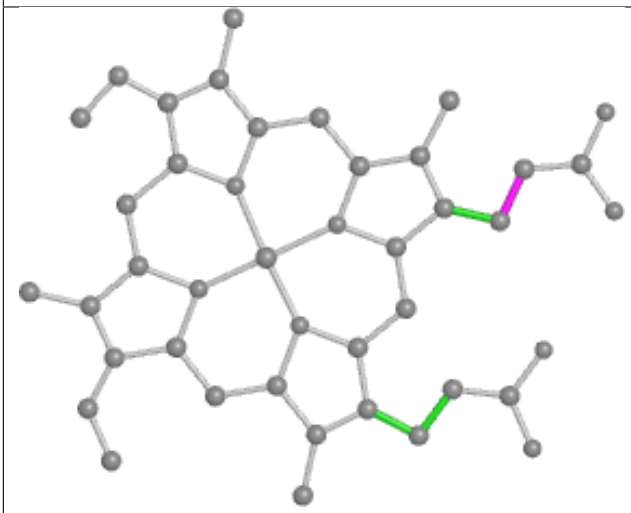
Ligand HEC A 1111



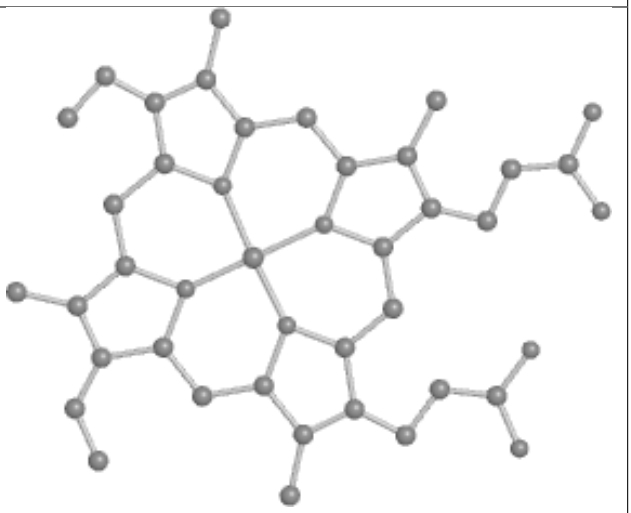
Bond lengths



Bond angles

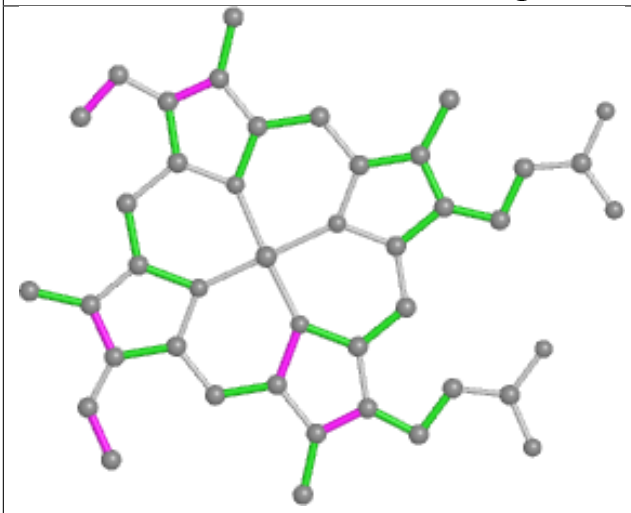


Torsions

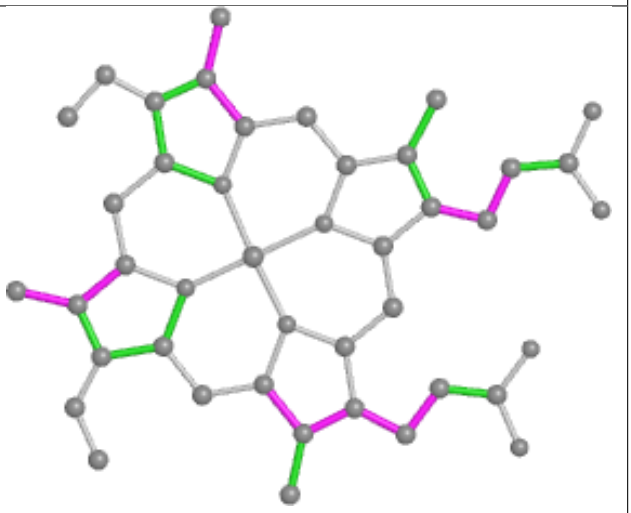


Rings

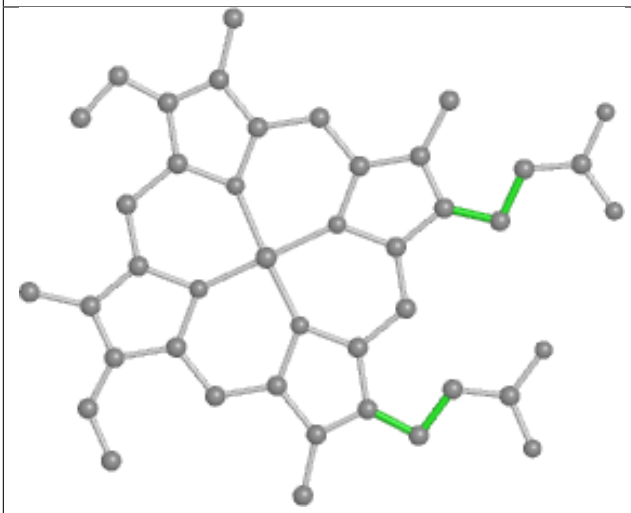
Ligand HEC D 1102



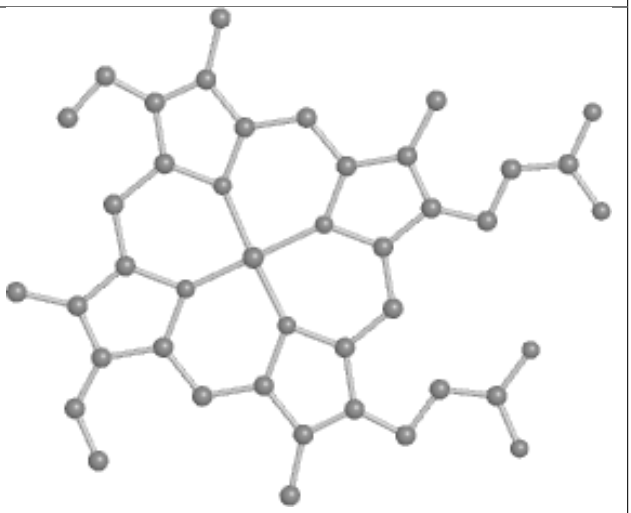
Bond lengths



Bond angles

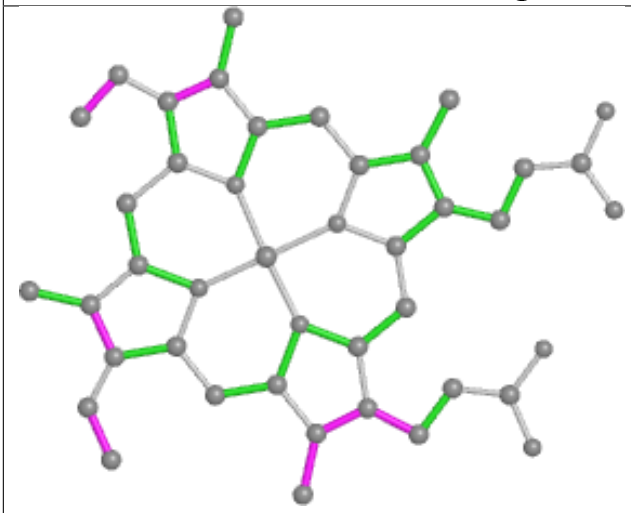


Torsions



Rings

Ligand HEC A 1102



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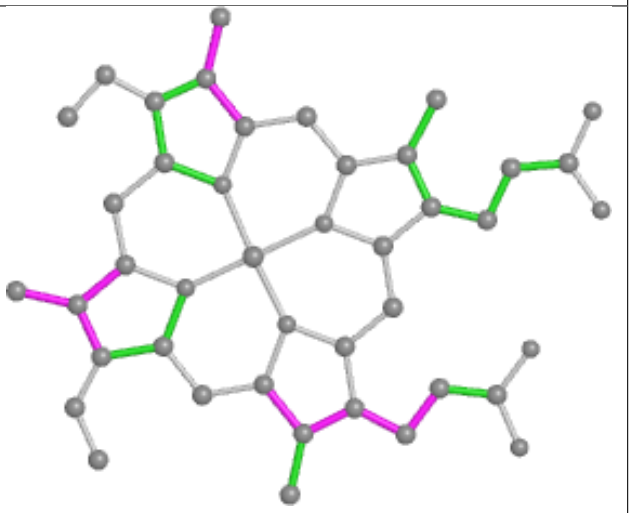
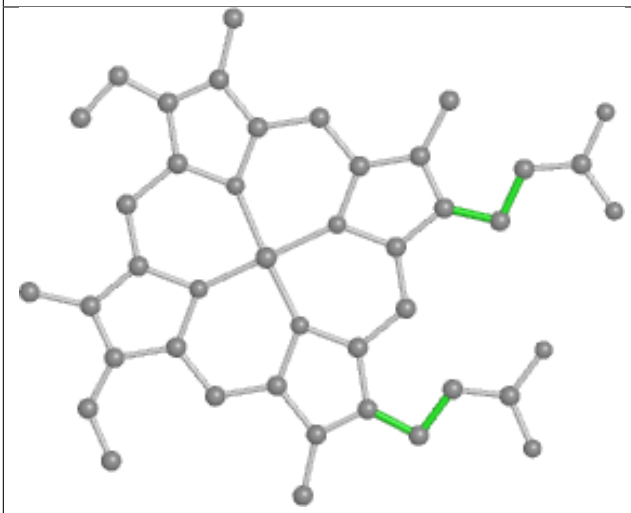


Bond angles



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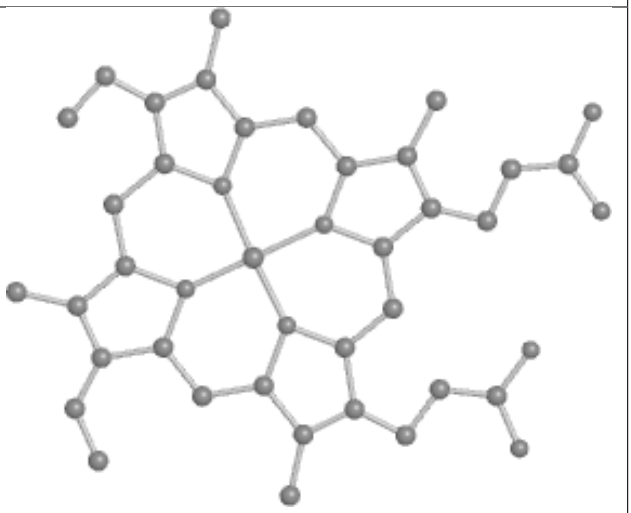
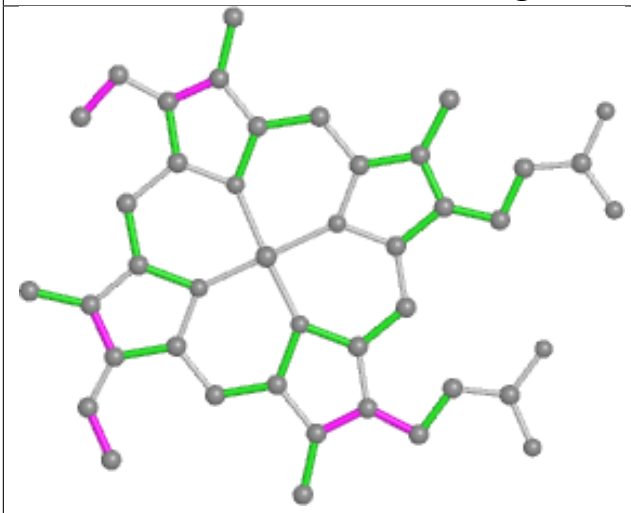


Rings

Ligand HEC D 1106



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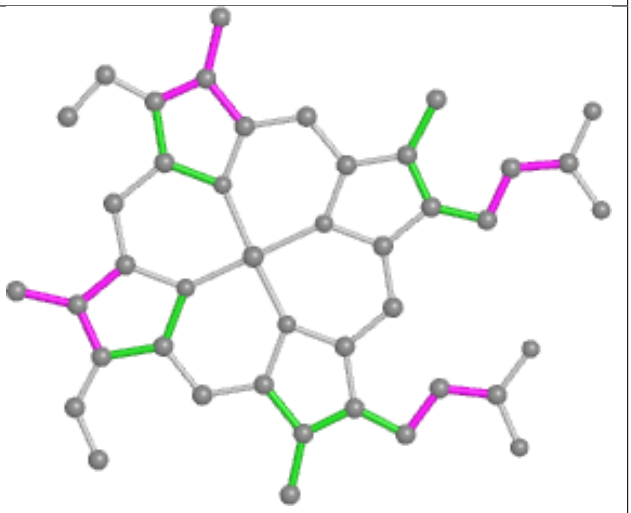
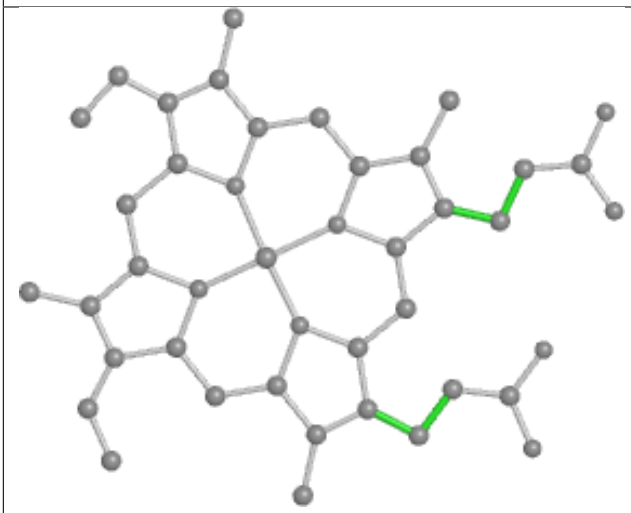


Bond angles



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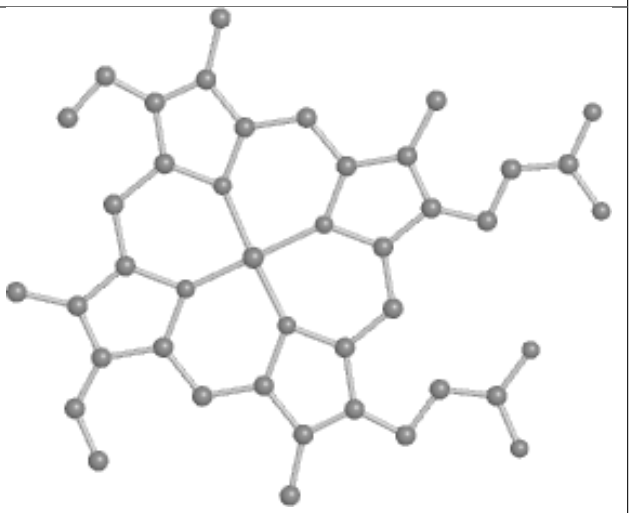
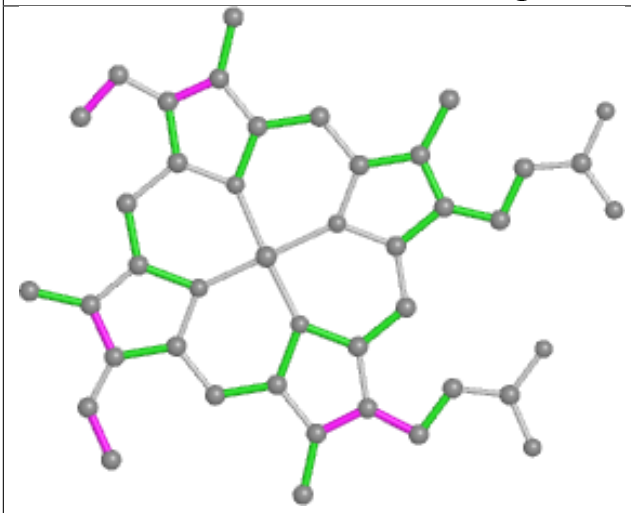


Rings

Ligand HEC A 1105



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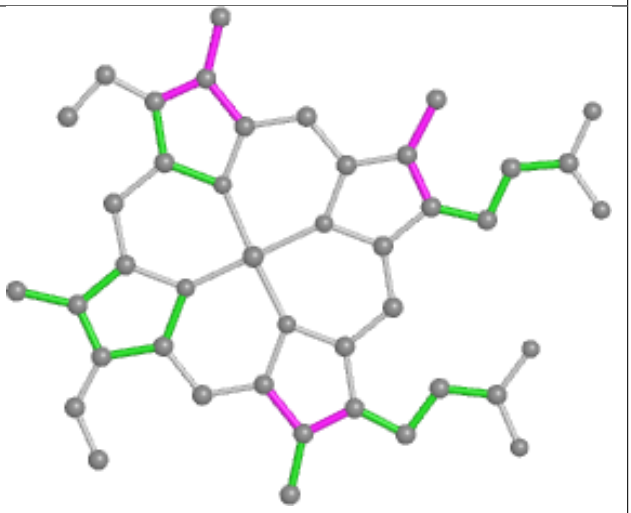
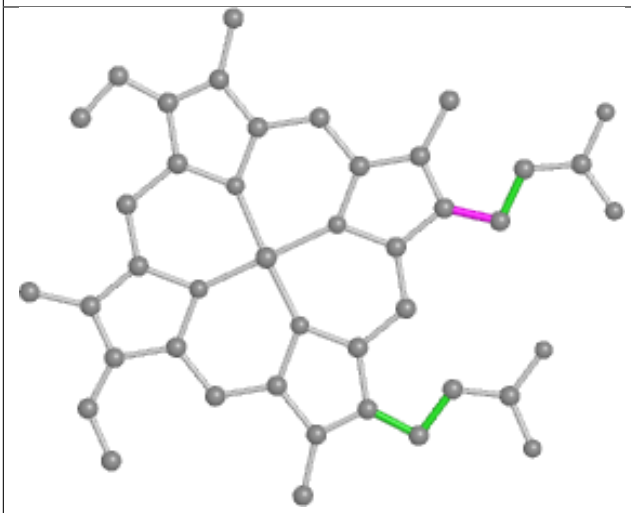


Bond angles



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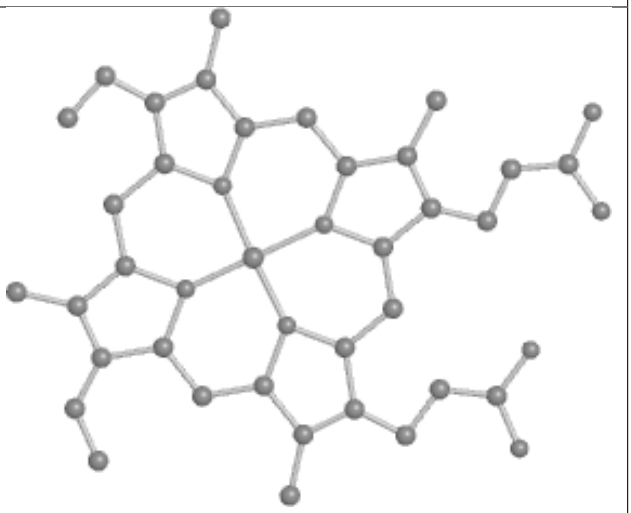
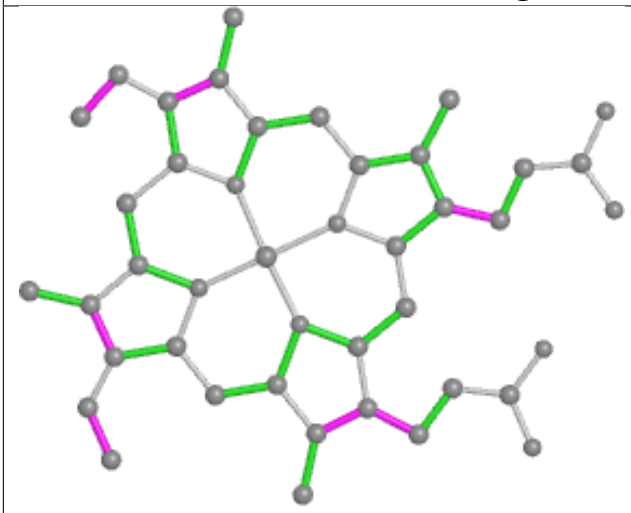
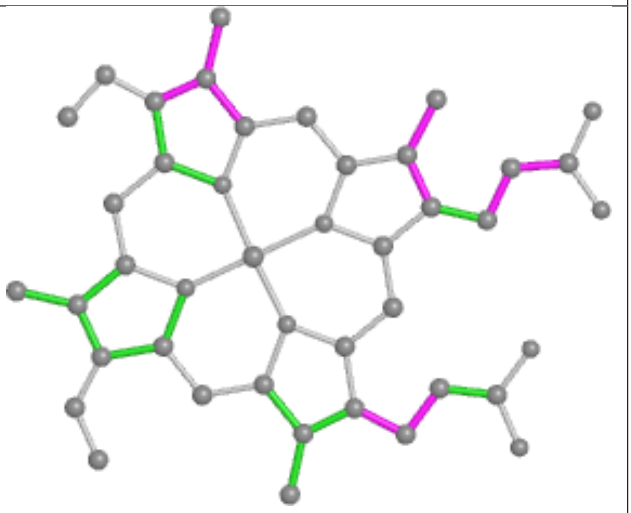


Rings

Ligand HEC C 1105



Bond lengths



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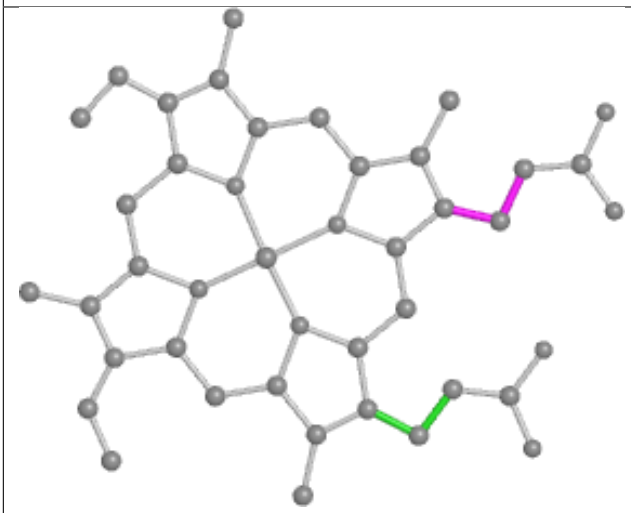

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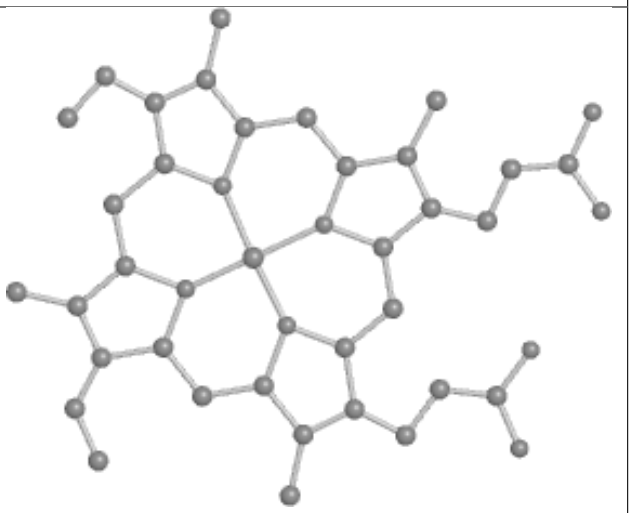
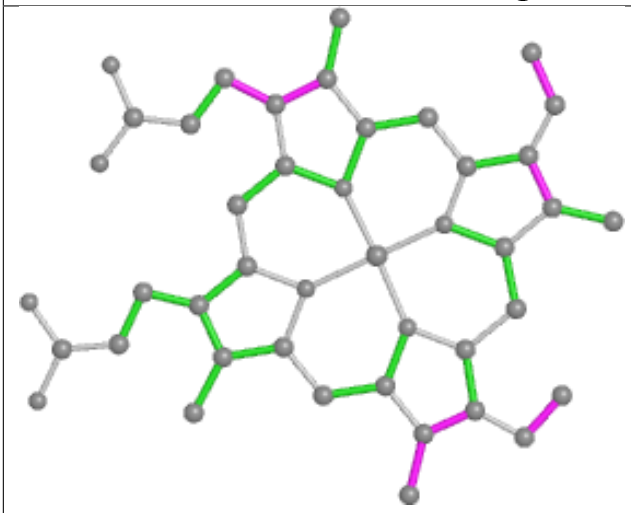


Rings

Ligand HEC B 1103



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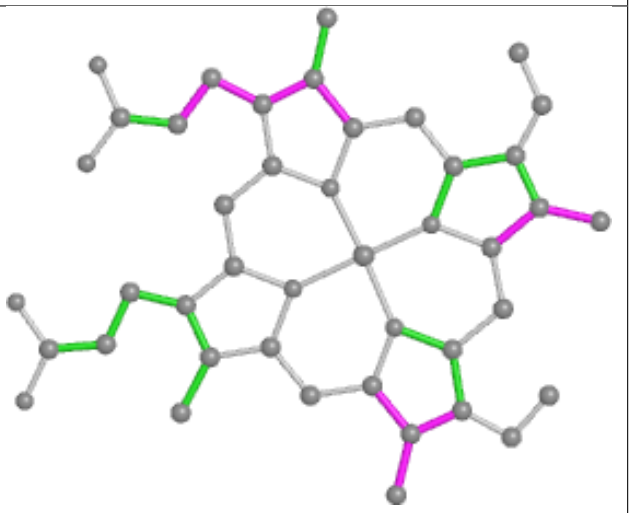
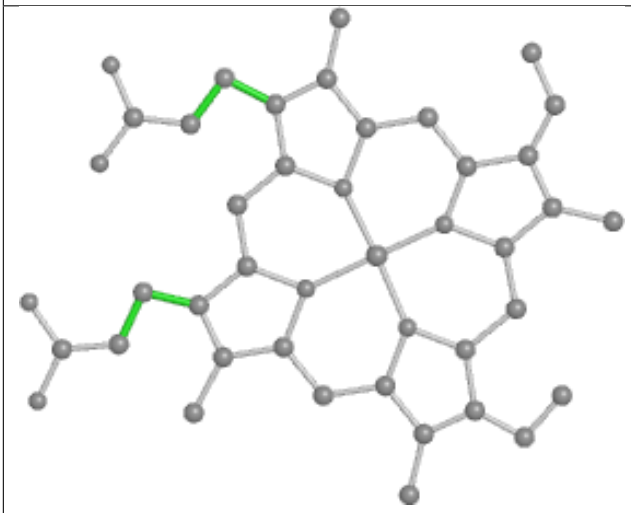
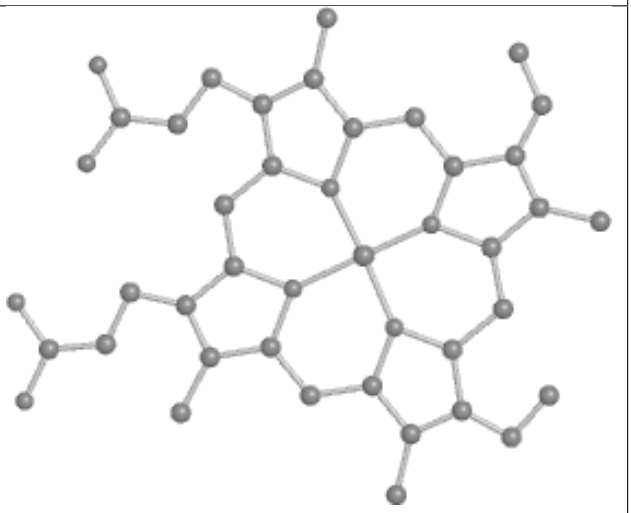


Bond angles

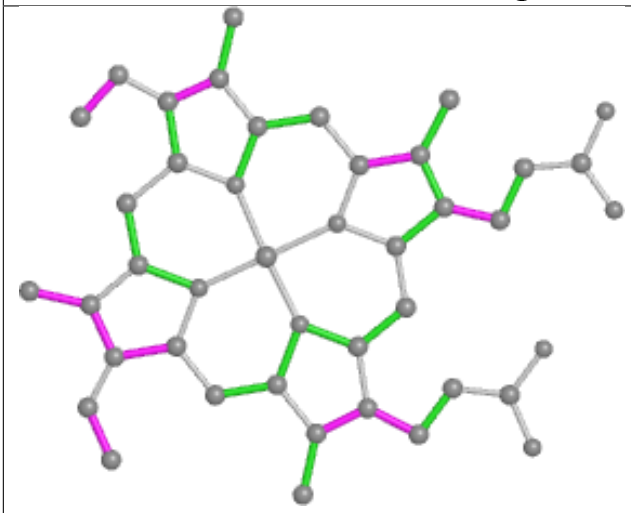


Torsions

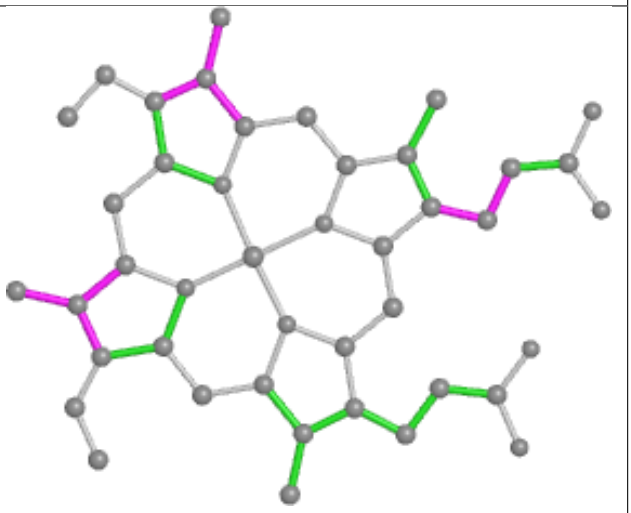


Rings

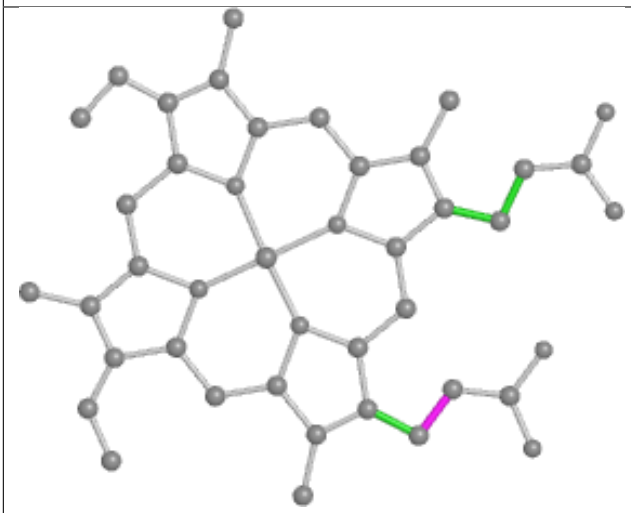
Ligand HEC A 1101



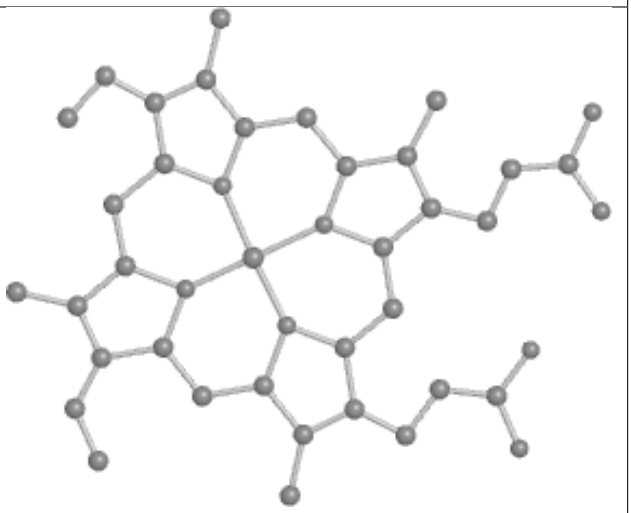
Bond lengths



Bond angles

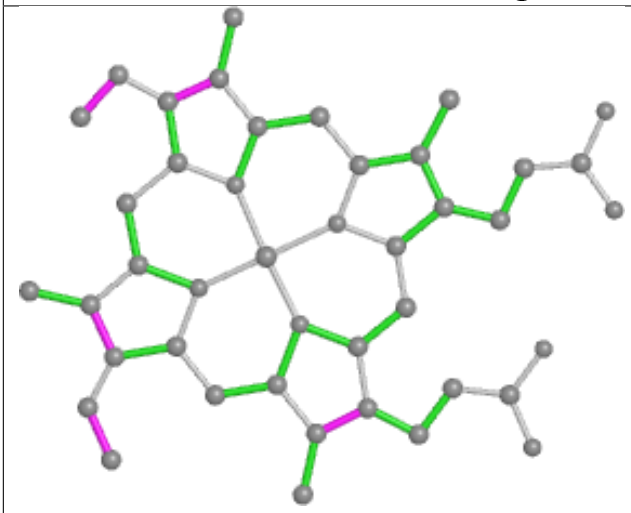


Torsions

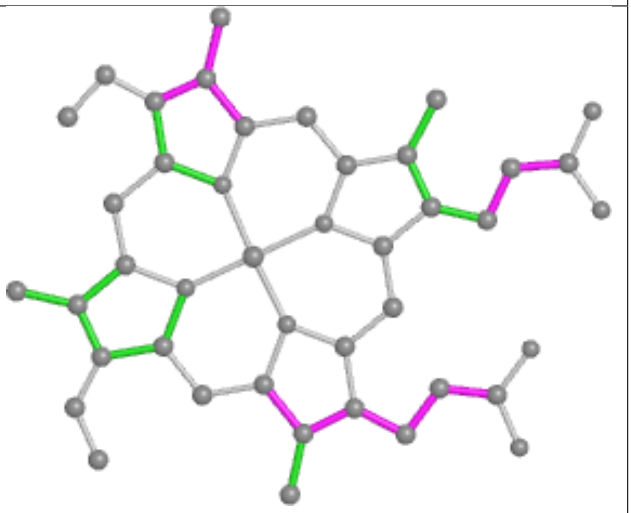


Rings

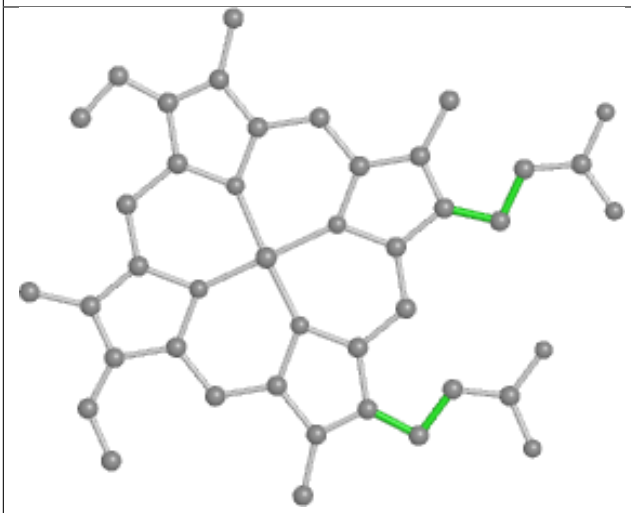
Ligand HEC D 1107



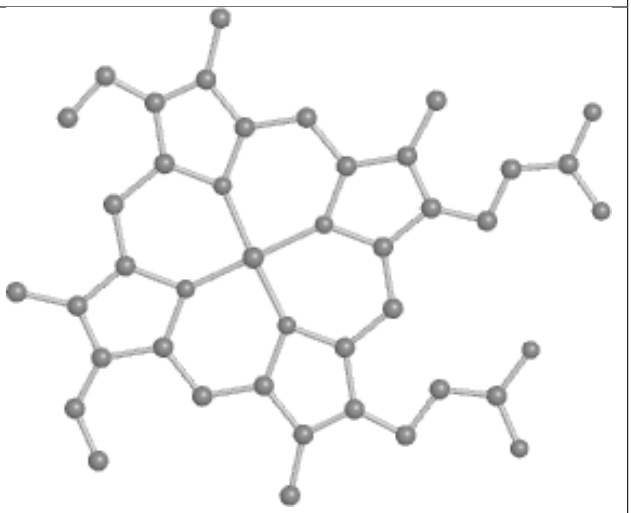
Bond lengths



Bond angles

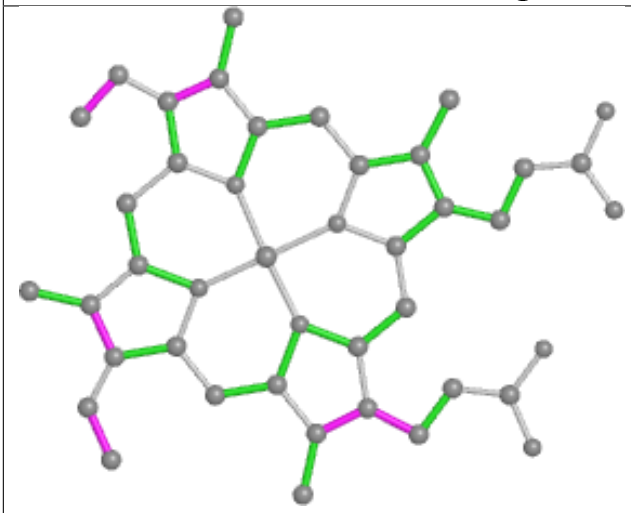


Torsions



Rings

Ligand HEC C 1116



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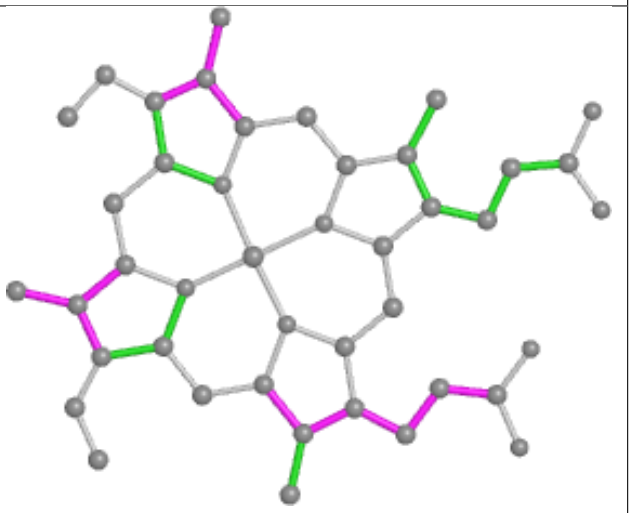
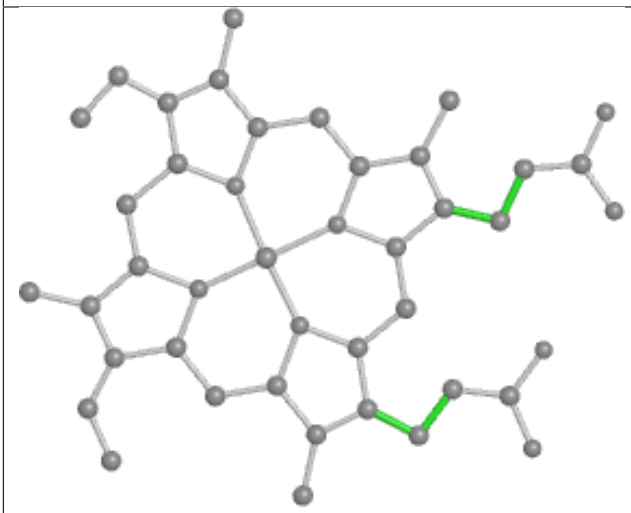


Bond angles



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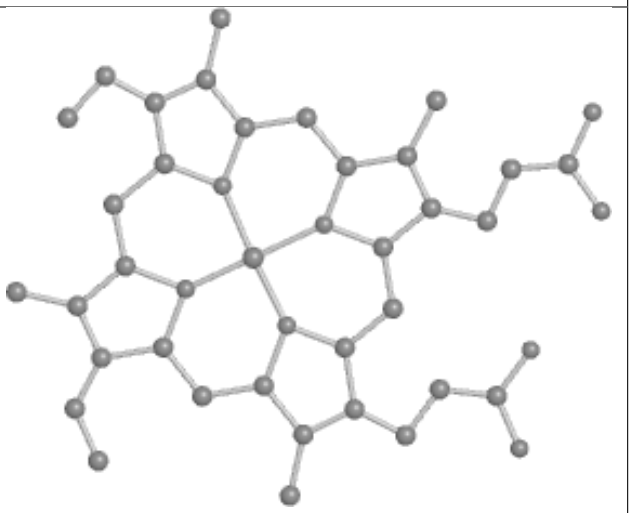
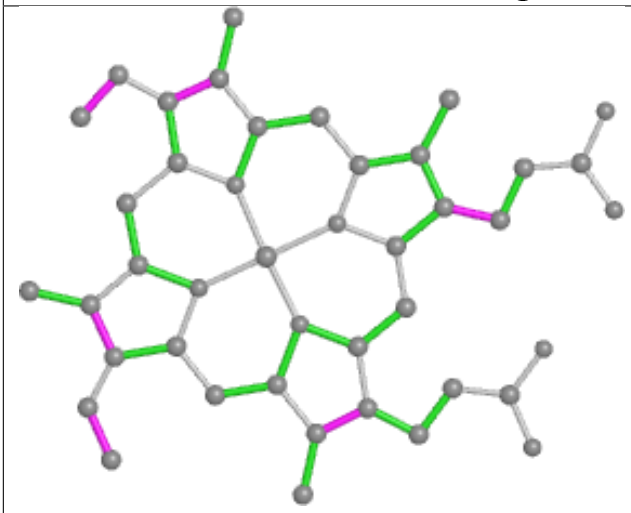
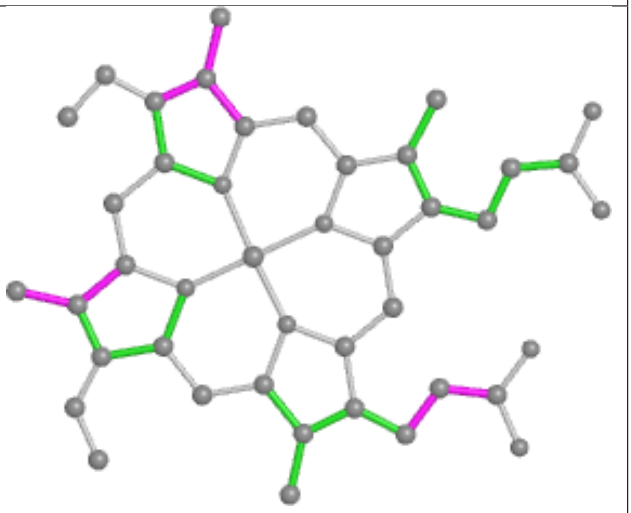


Rings

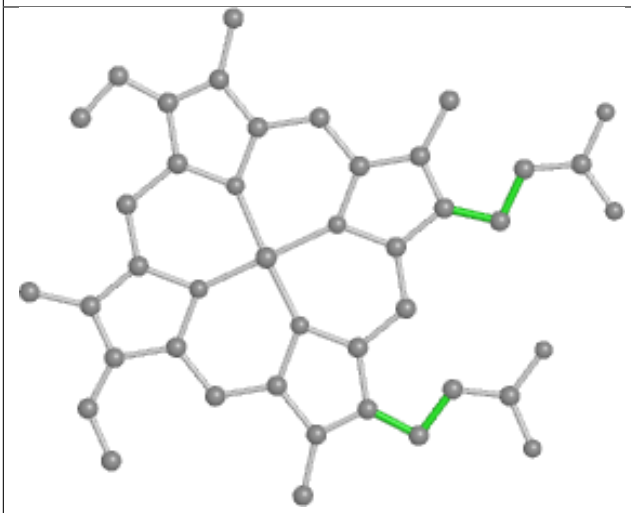
Ligand HEC B 1104



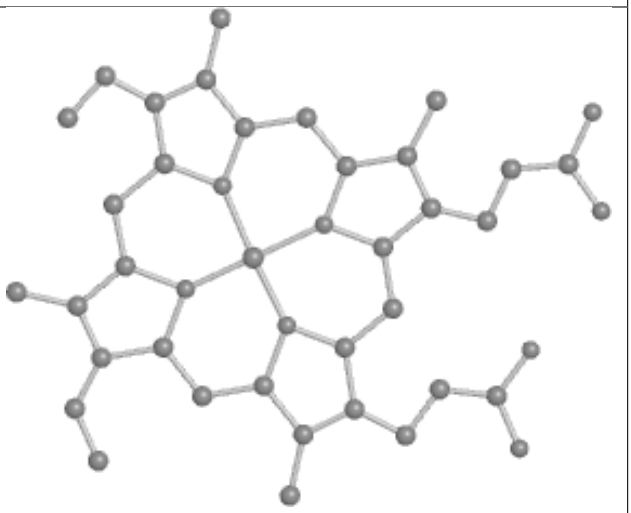
Bond lengths



Bond angles

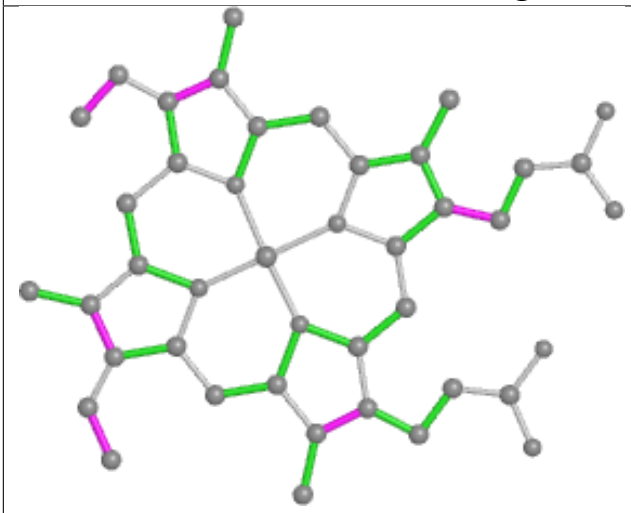


Torsions

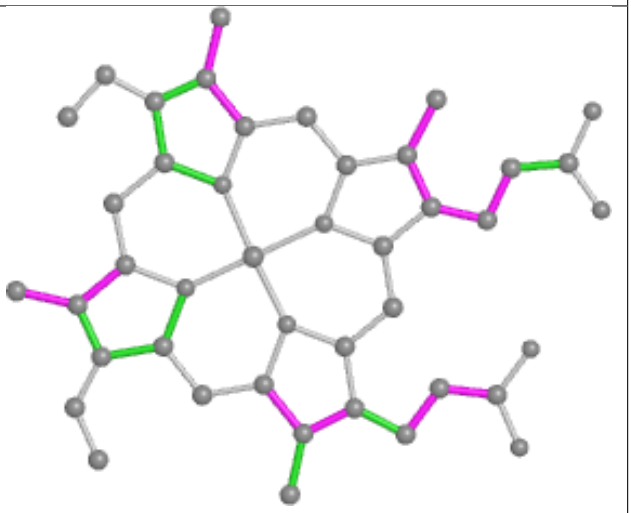


Rings

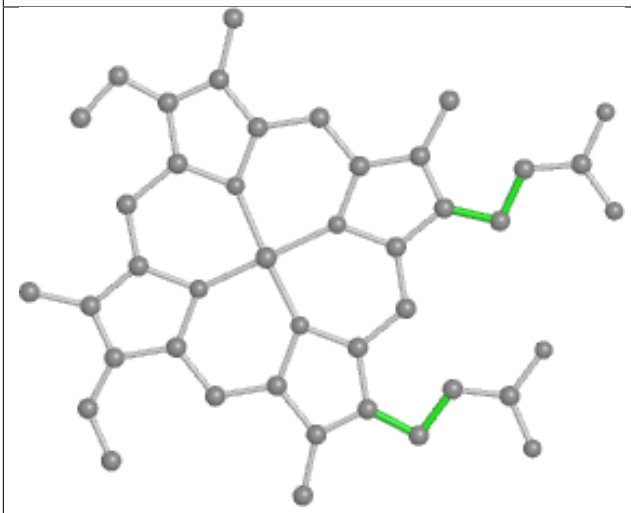
Ligand HEC D 1104



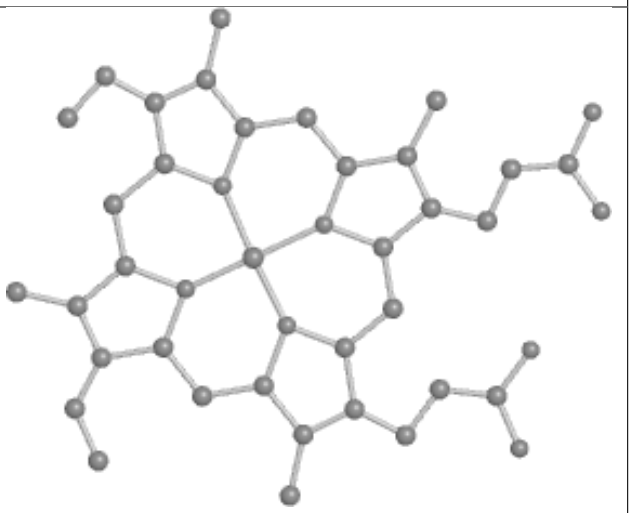
Bond lengths



Bond angles

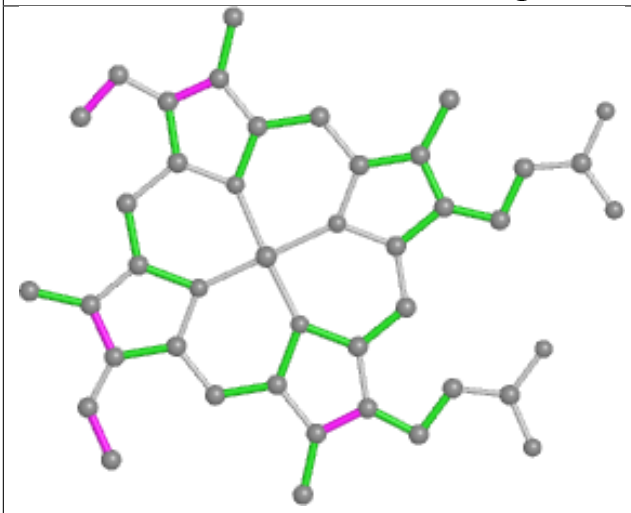


Torsions

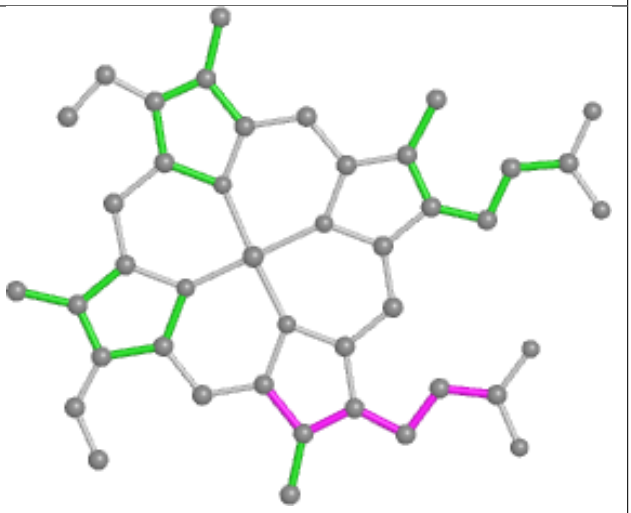


Rings

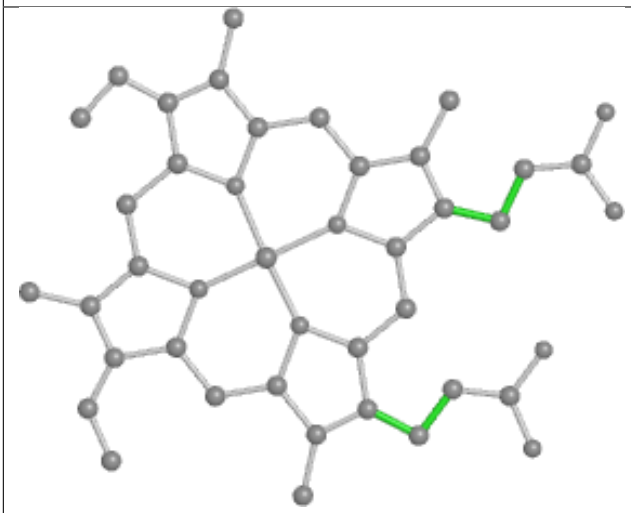
Ligand HEC D 1108



Bond lengths



Bond angles



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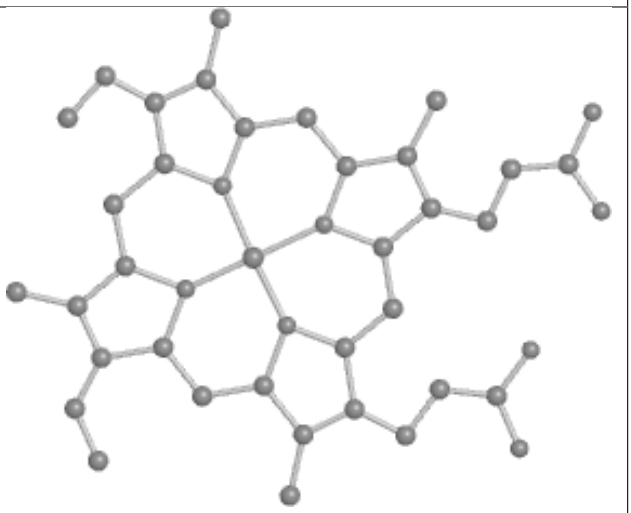
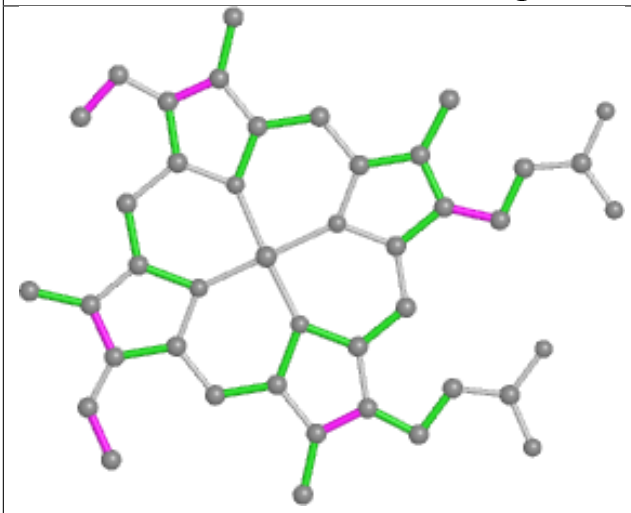
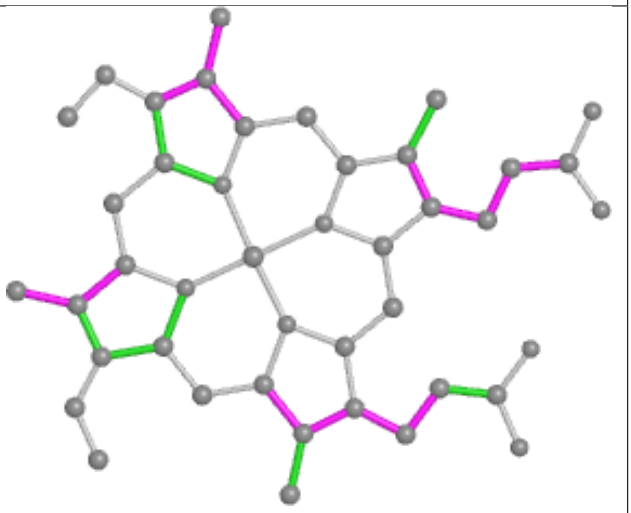


Rings

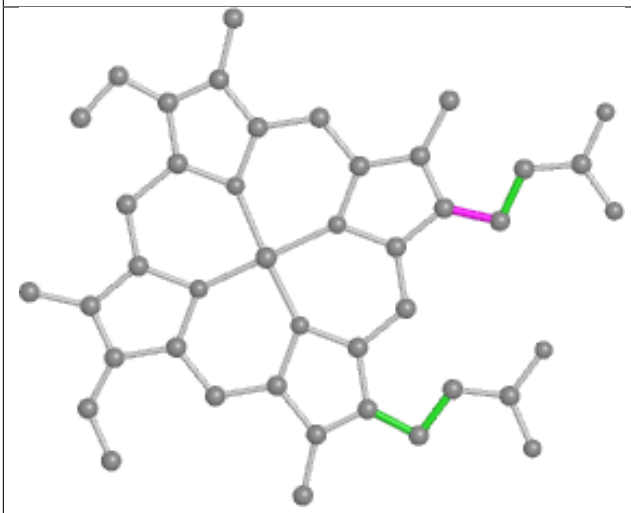
Ligand HEC A 1107



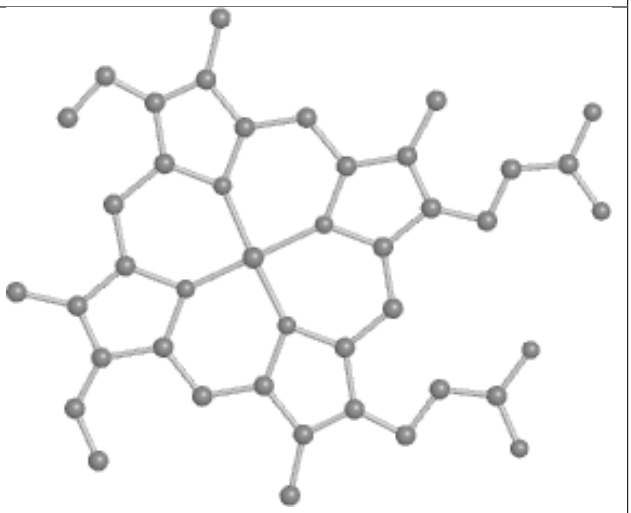
Bond lengths



Bond angles

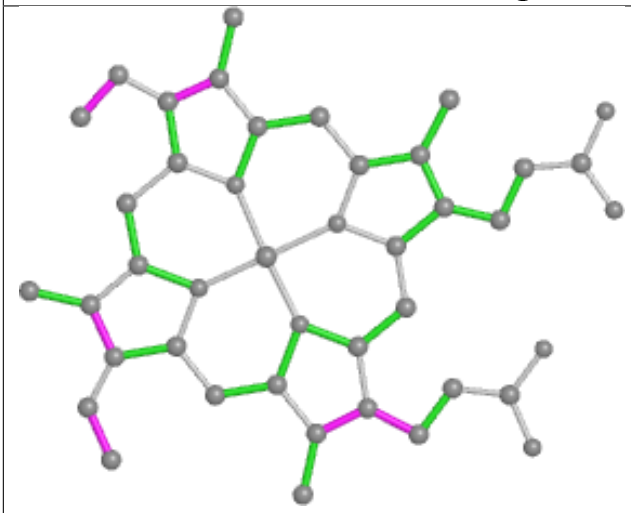


Torsions

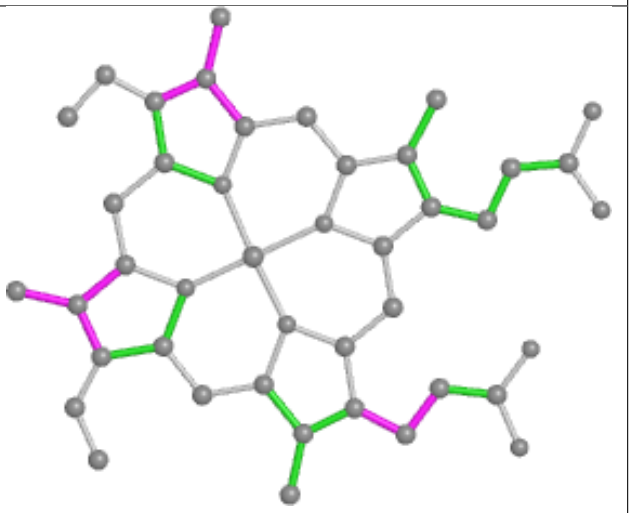


Rings

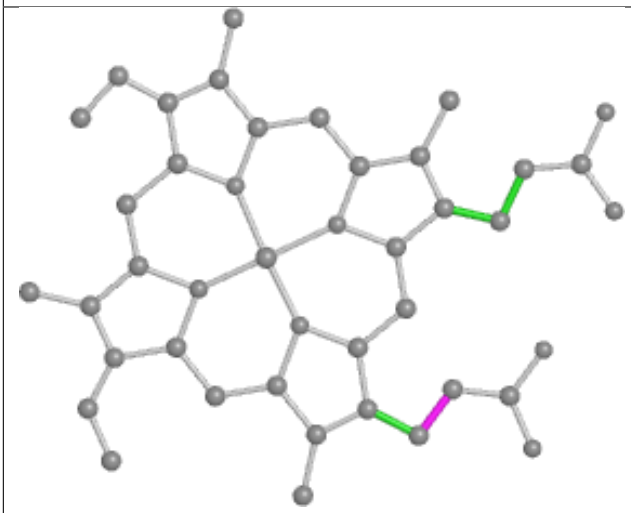
Ligand HEC B 1101



Bond lengths



Bond angles



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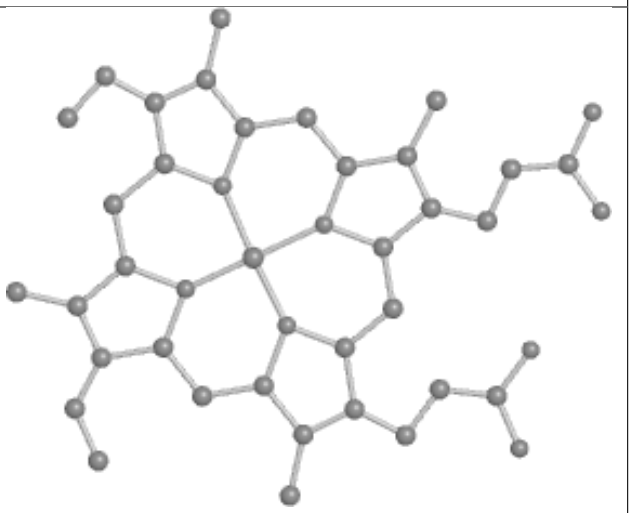
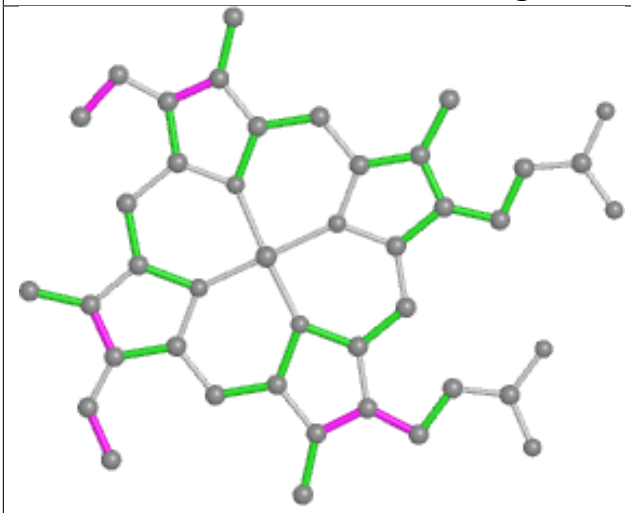


Rings

Ligand HEC A 1103



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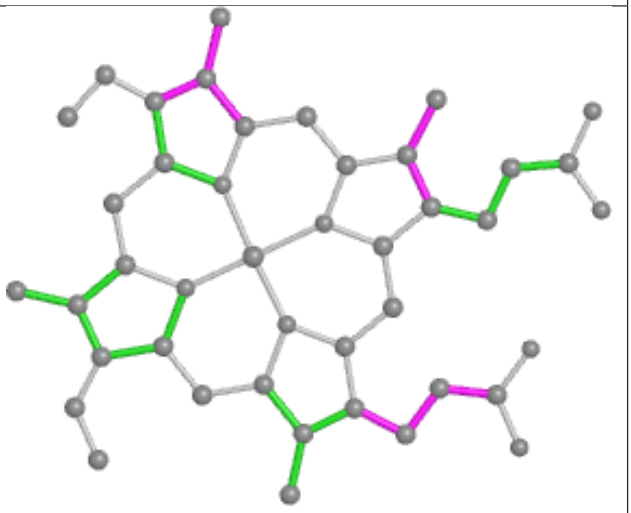
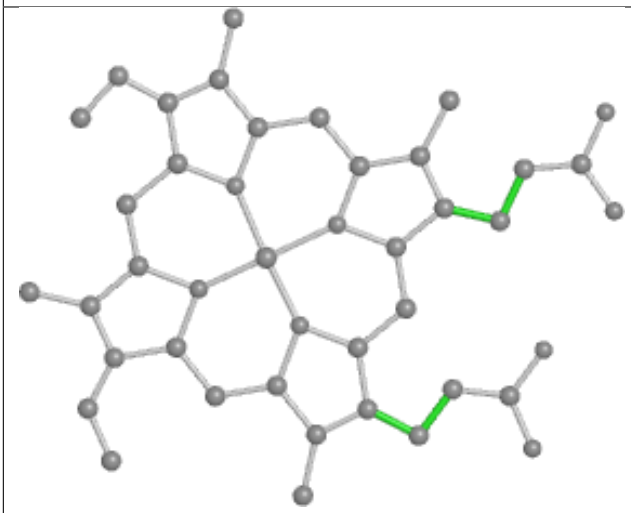


Bond angles



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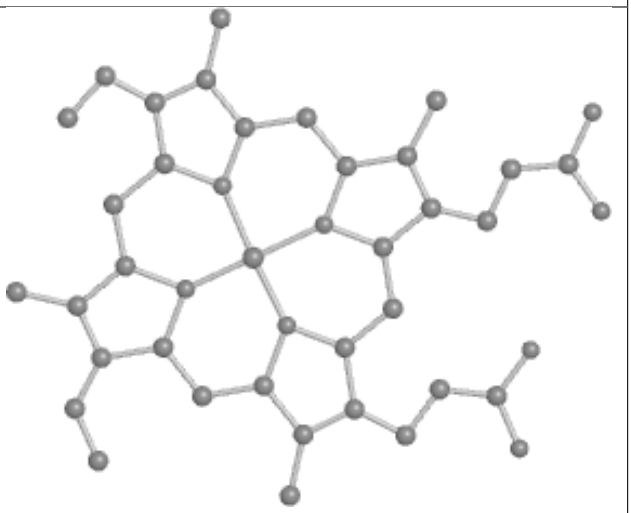
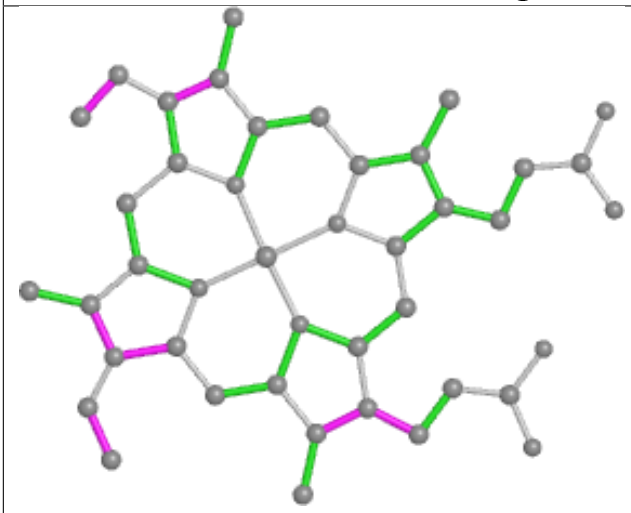


Rings

Ligand HEC C 1102



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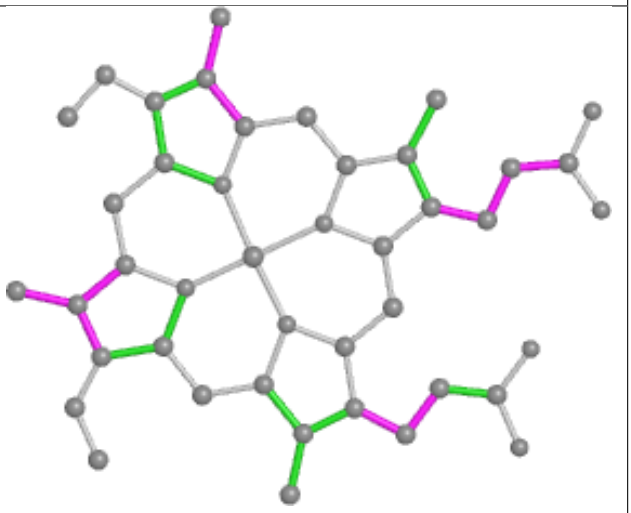
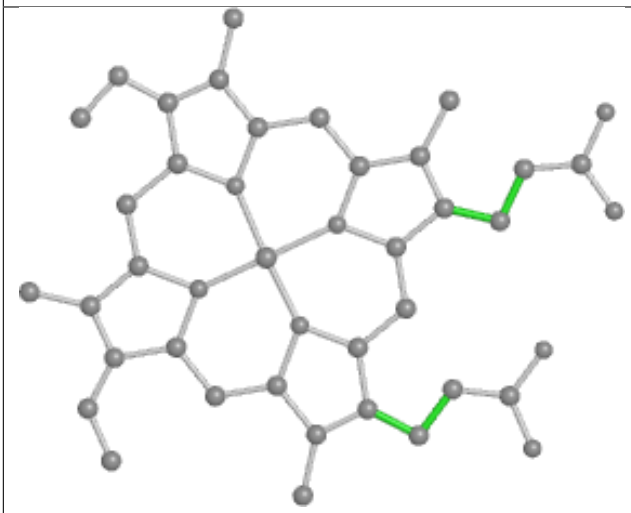


Bond angles



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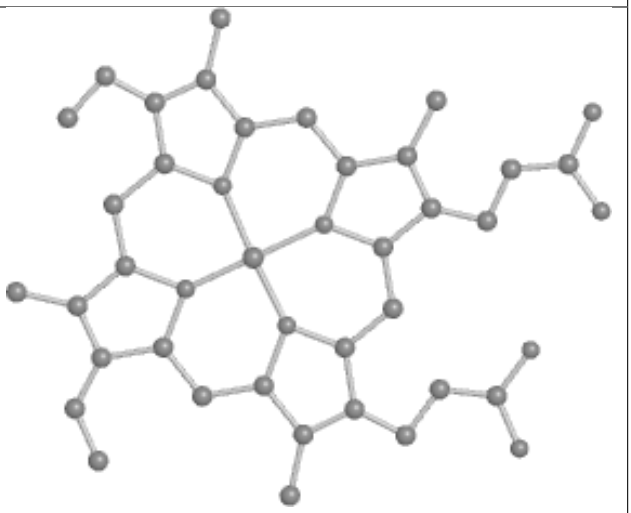
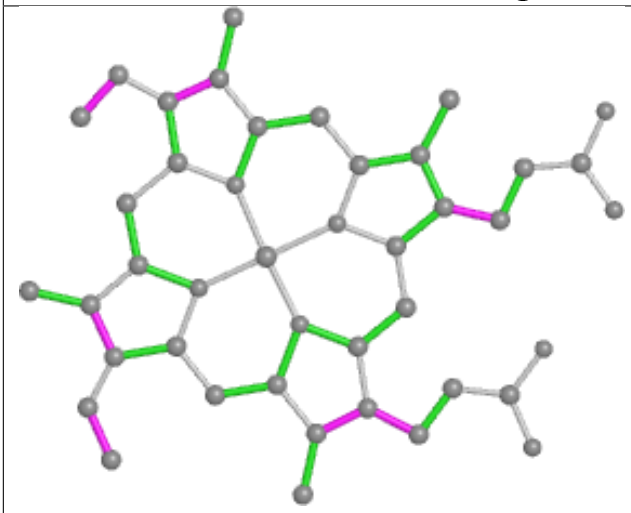


Rings

Ligand HEC B 1102



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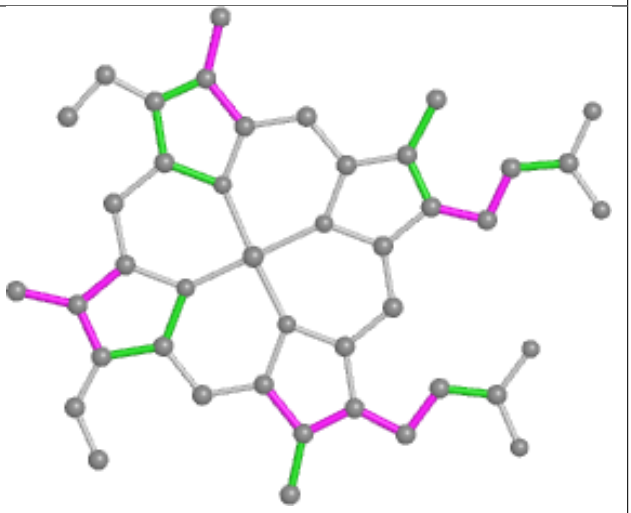

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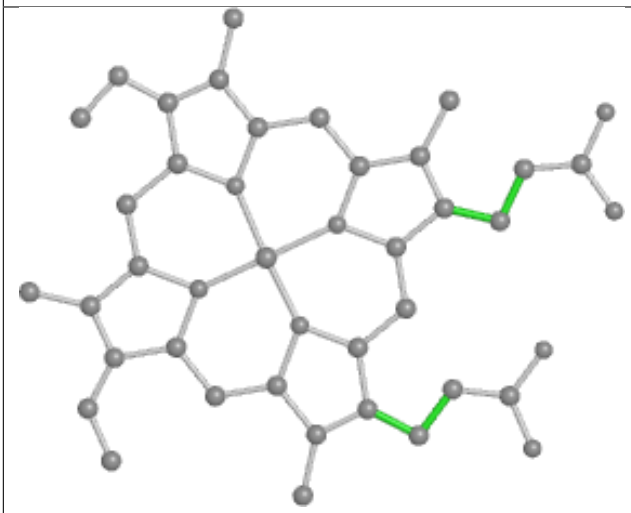

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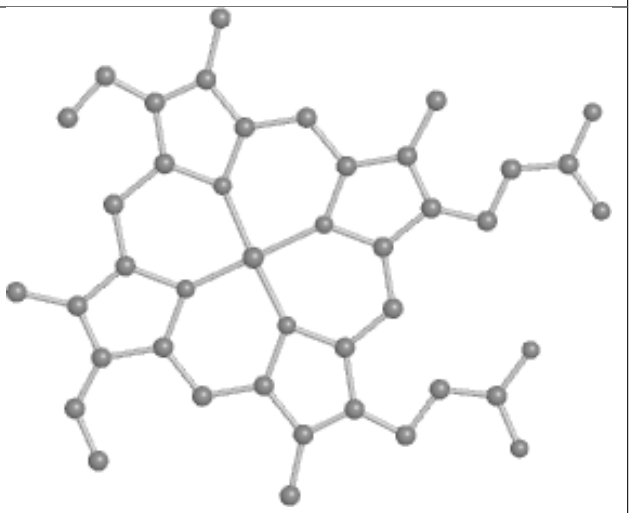
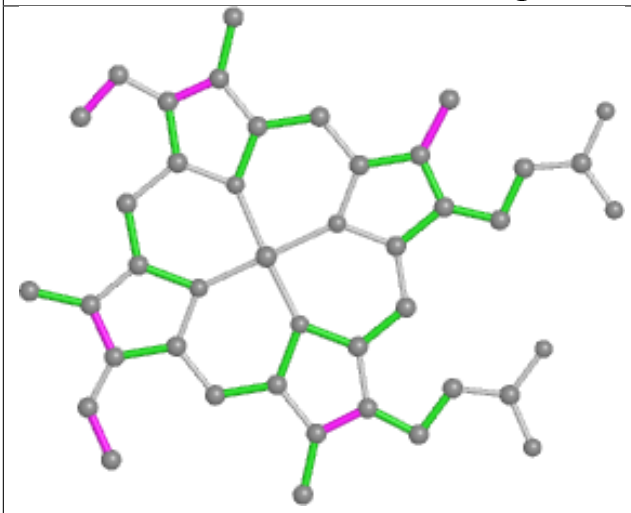


Rings

Ligand HEC D 1116



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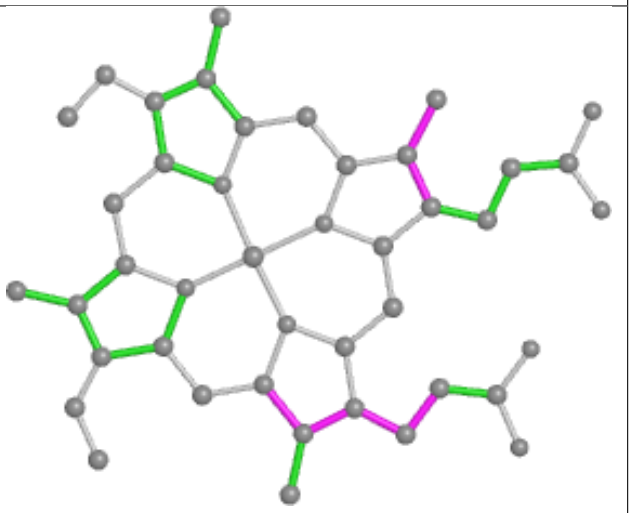
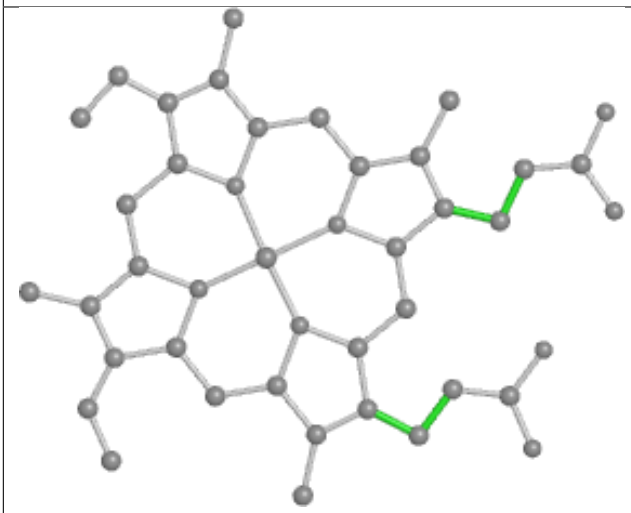


Bond angles



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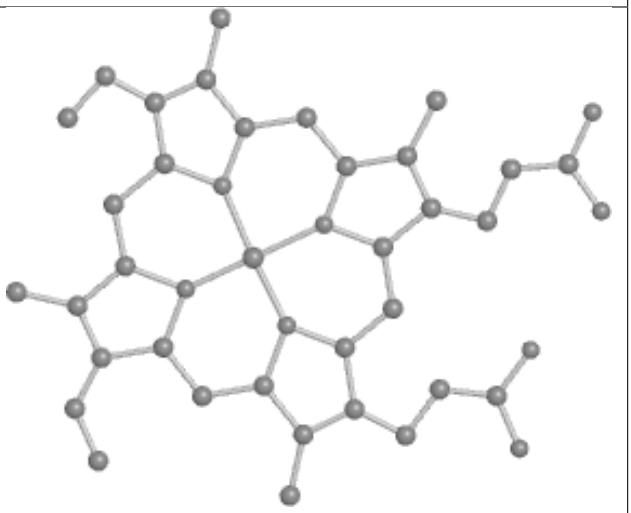
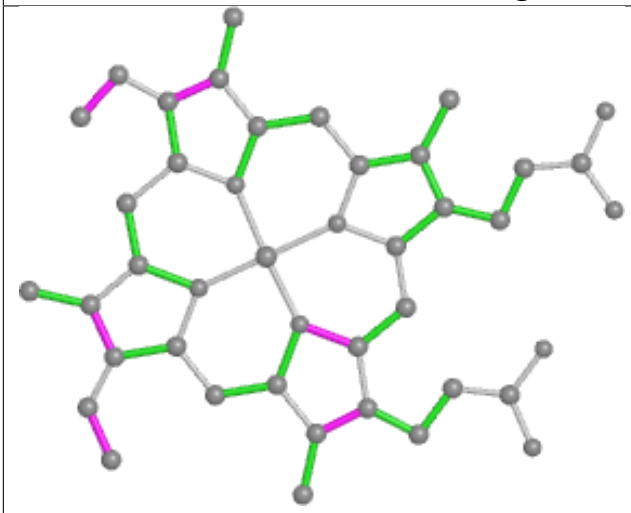


Rings

Ligand HEC D 1114



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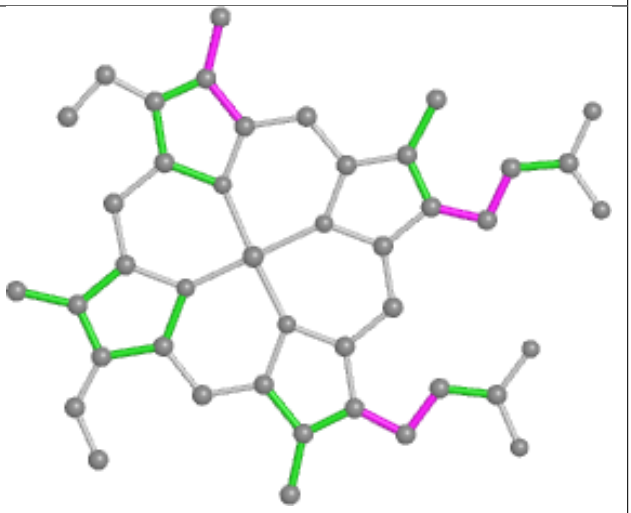
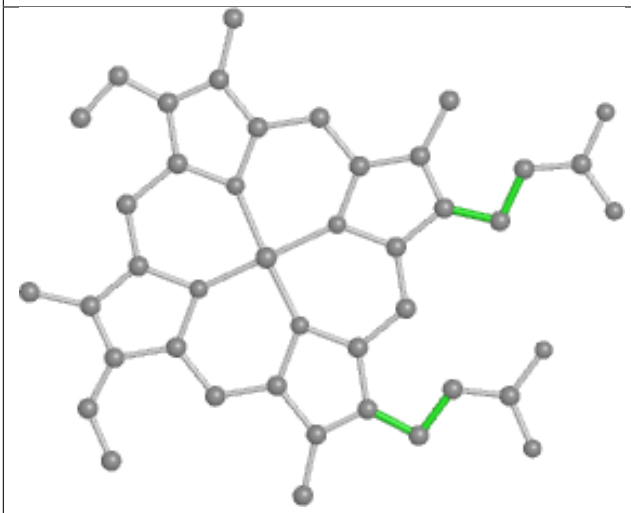


Bond angles



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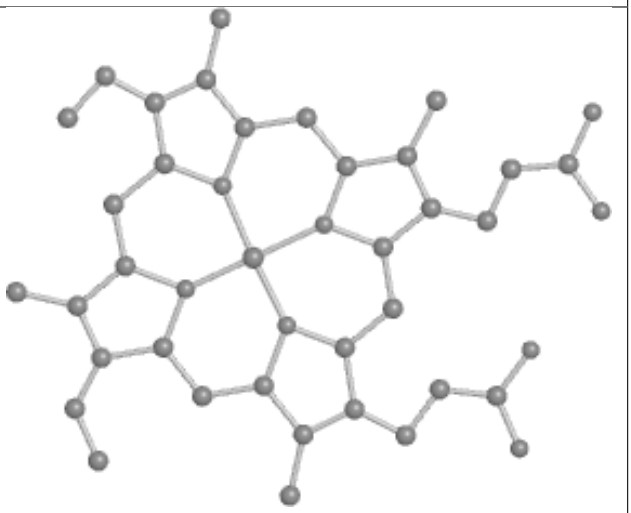
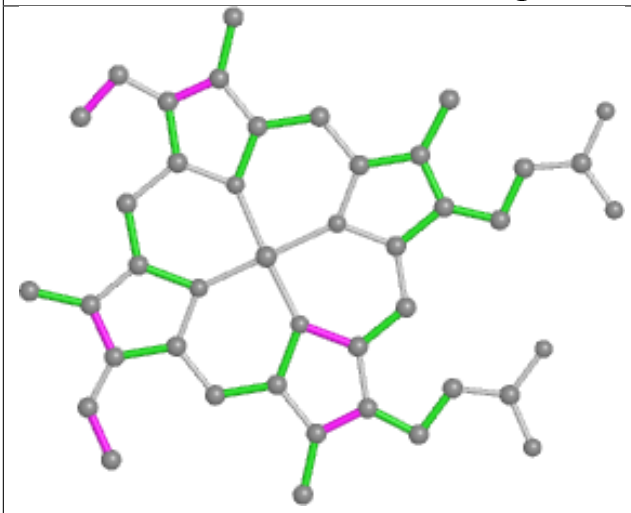


Rings

Ligand HEC A 1108



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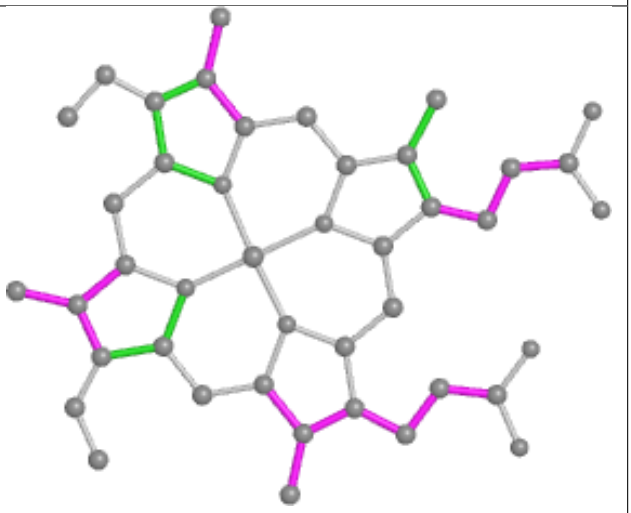
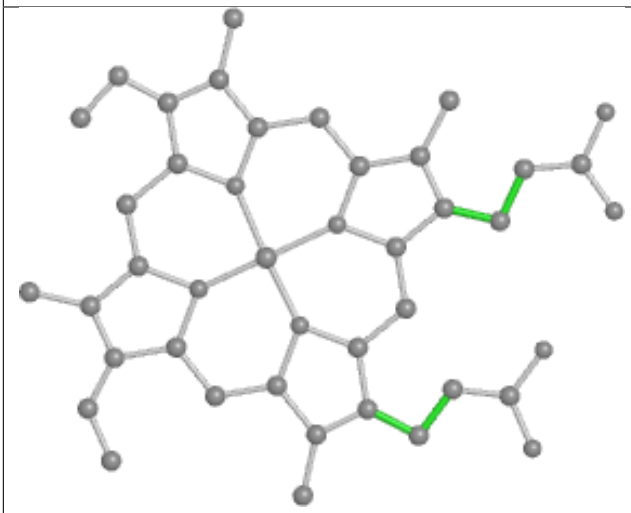


Bond angles



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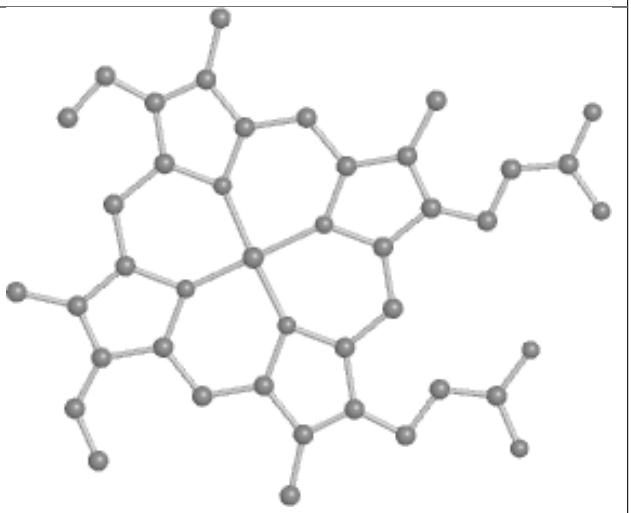
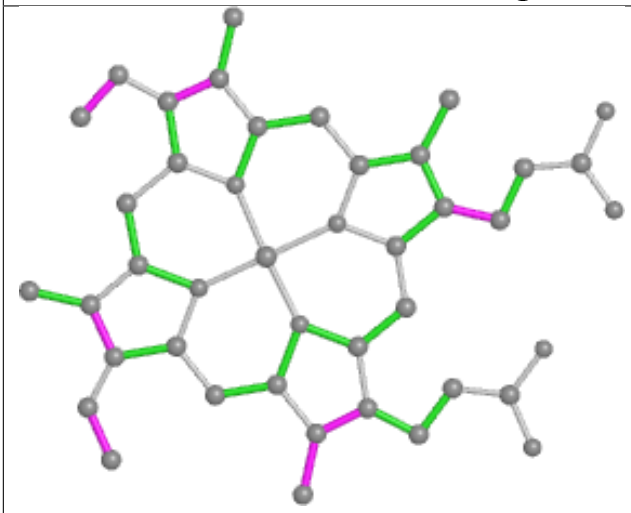


Rings

Ligand HEC C 1106



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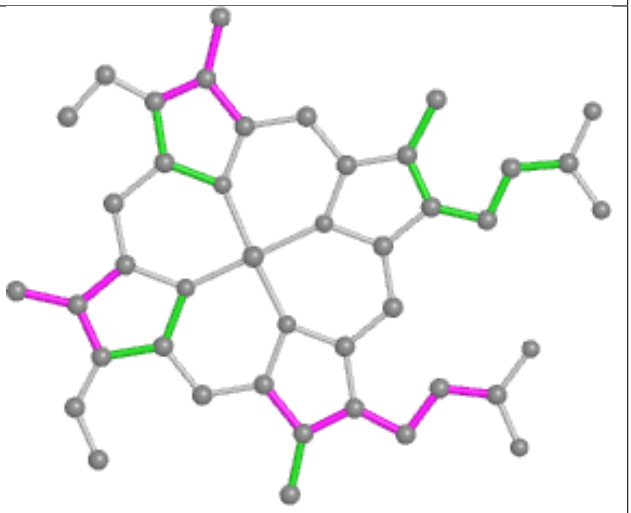
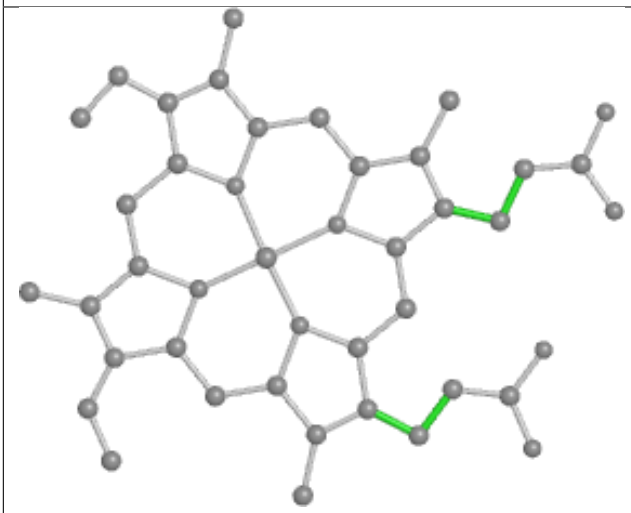
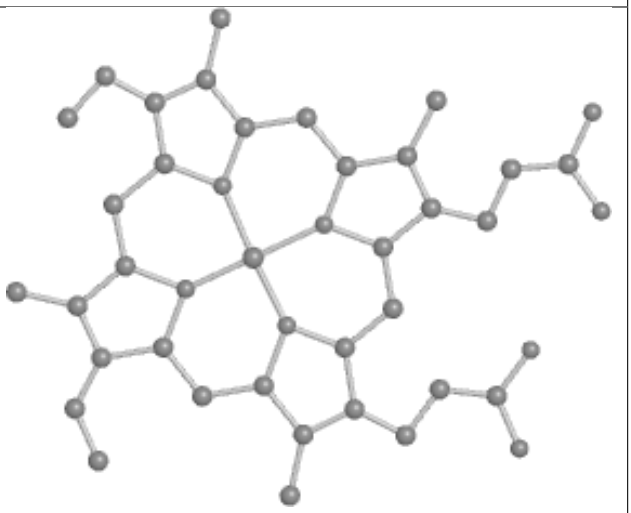


Bond angles

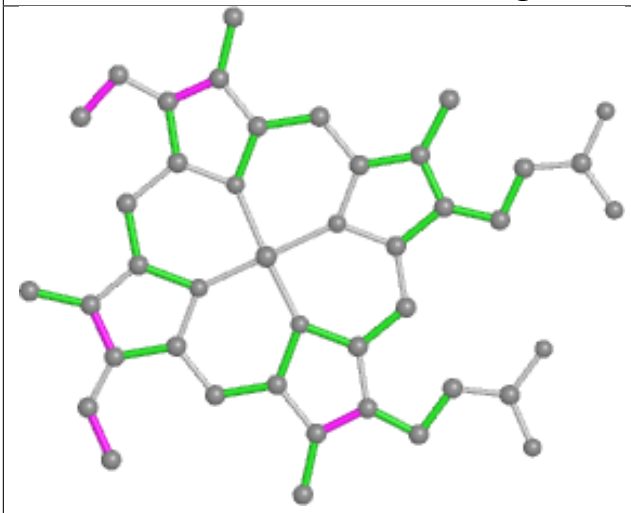


Torsions



Rings

Ligand HEC C 1104



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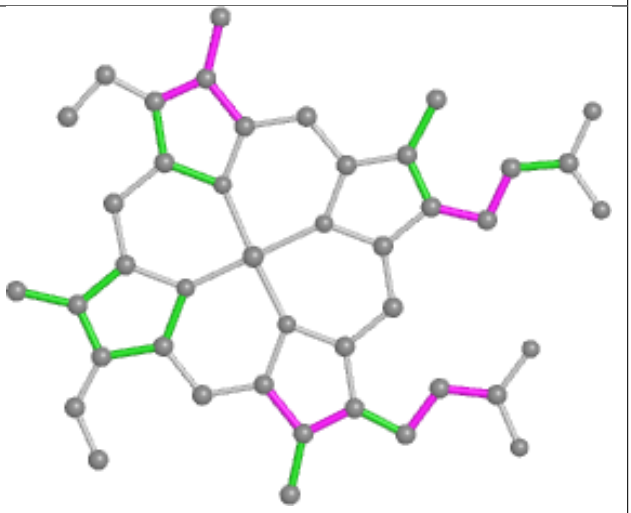
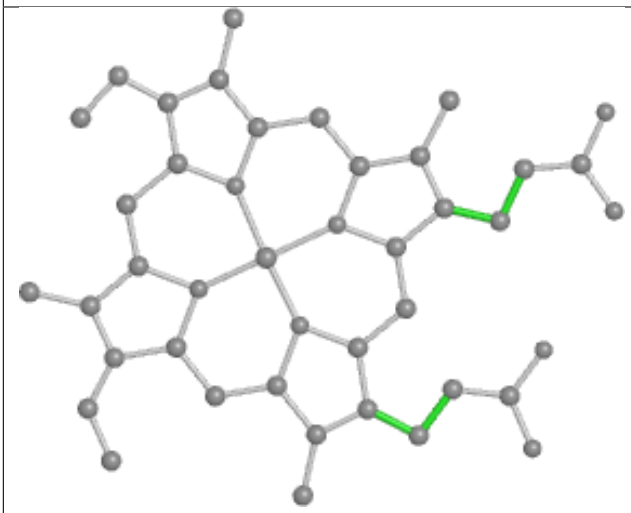
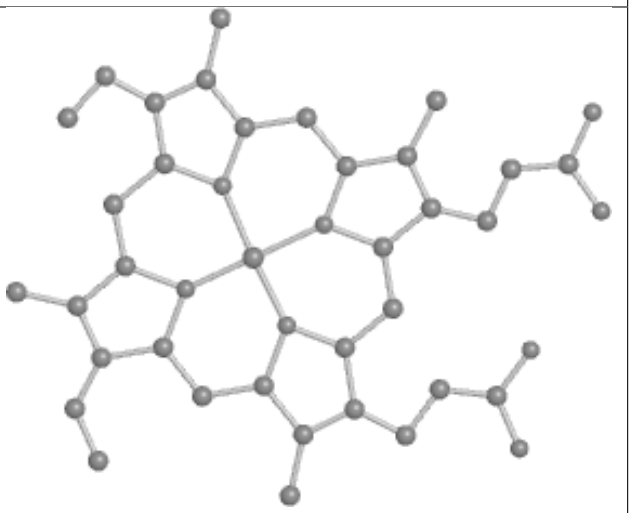


Bond angles

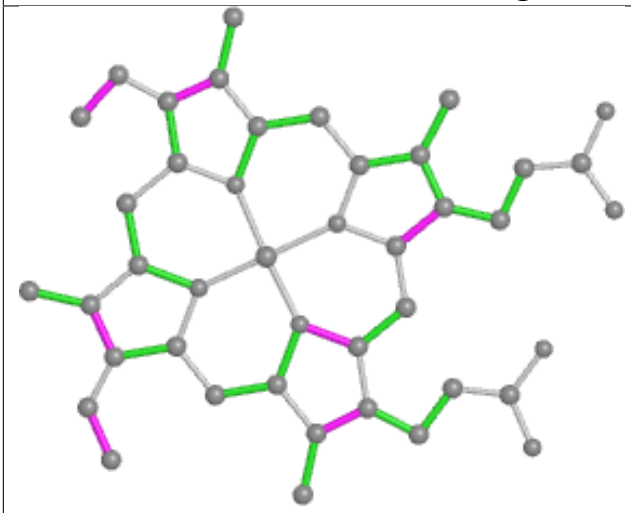


Torsions



Rings

Ligand HEC B 1110



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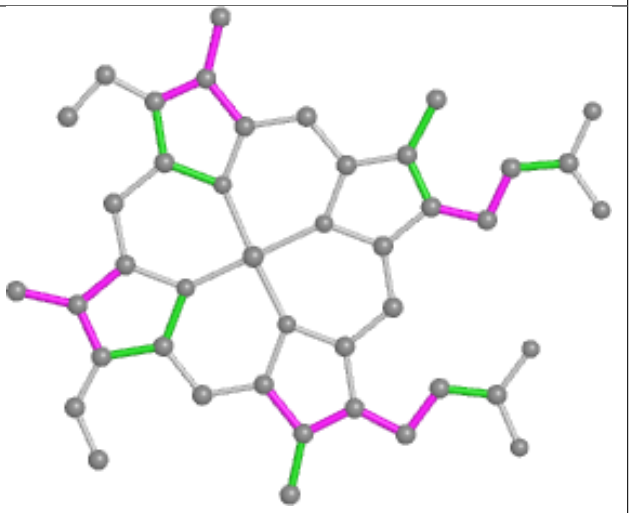
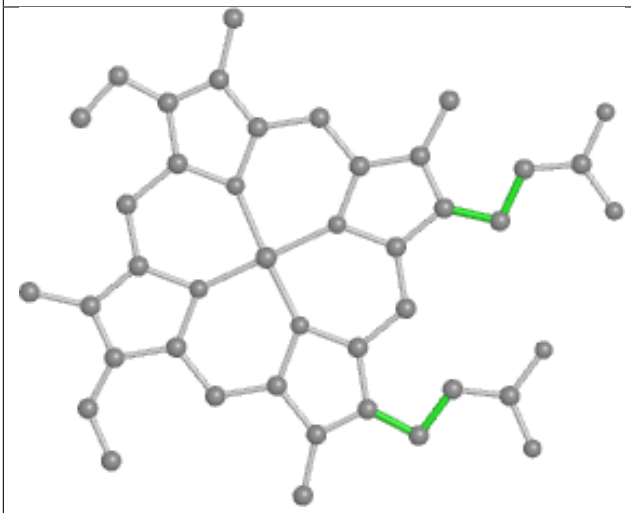
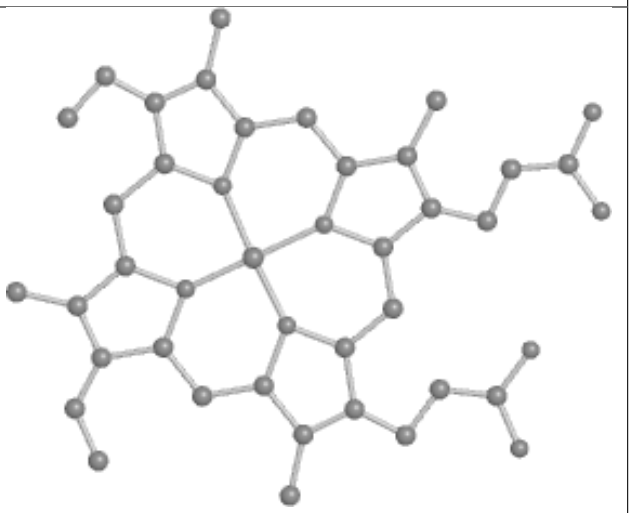


Bond angles

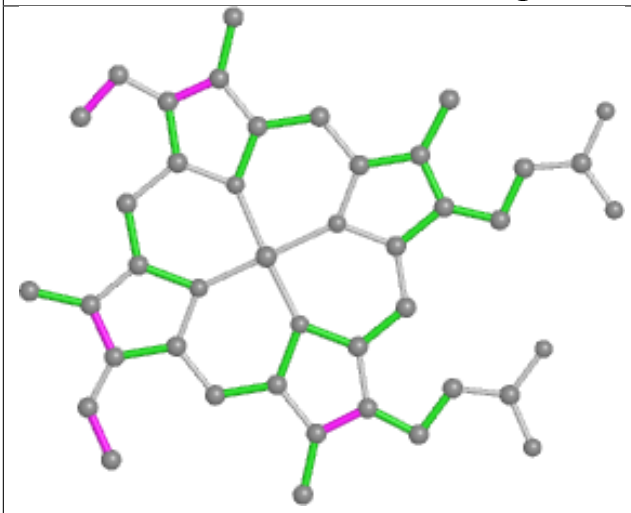


Torsions



Rings

Ligand HEC C 1110



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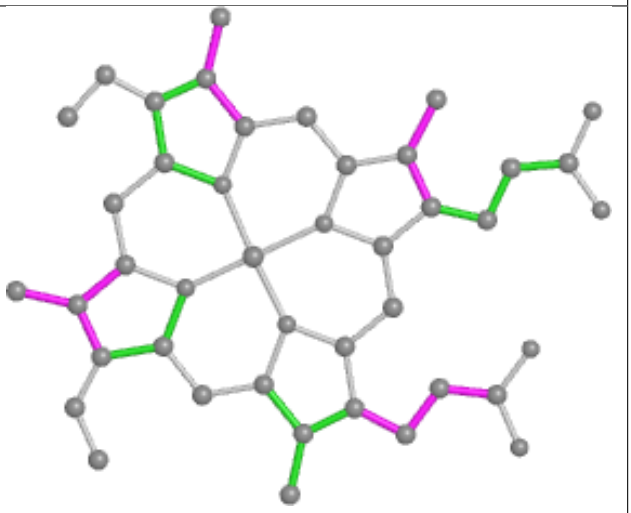

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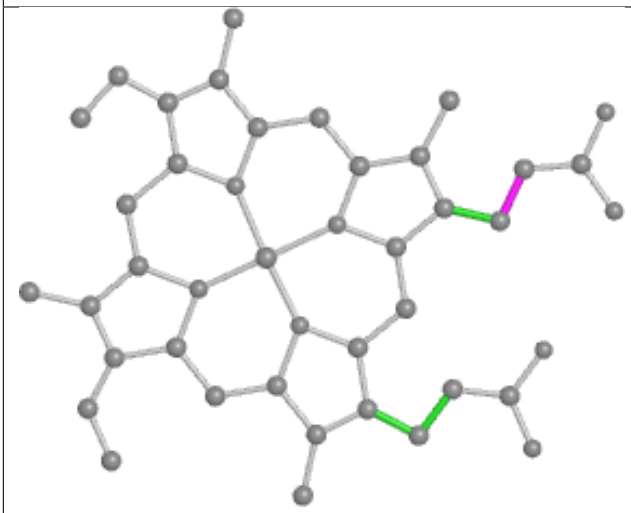

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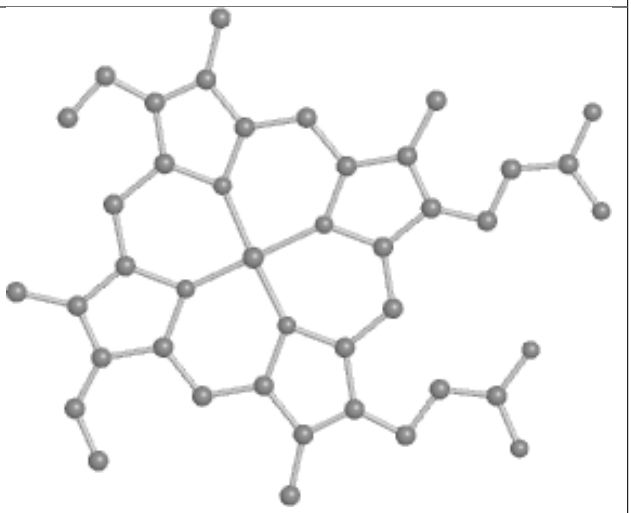
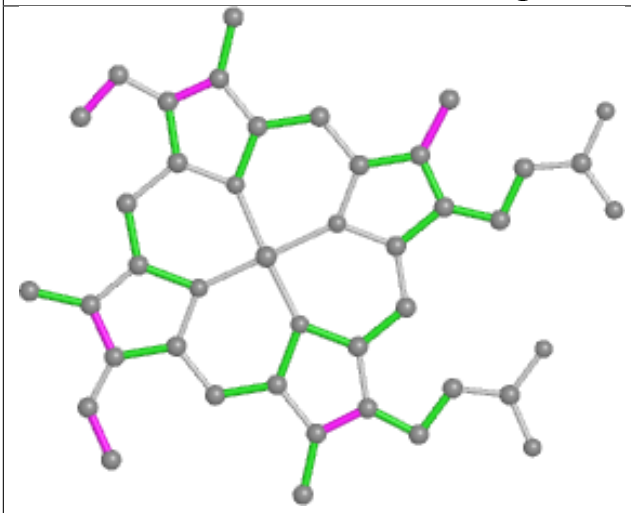
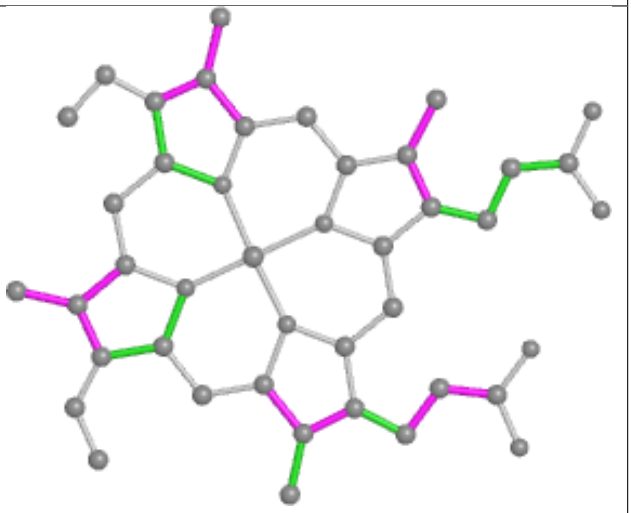


Rings

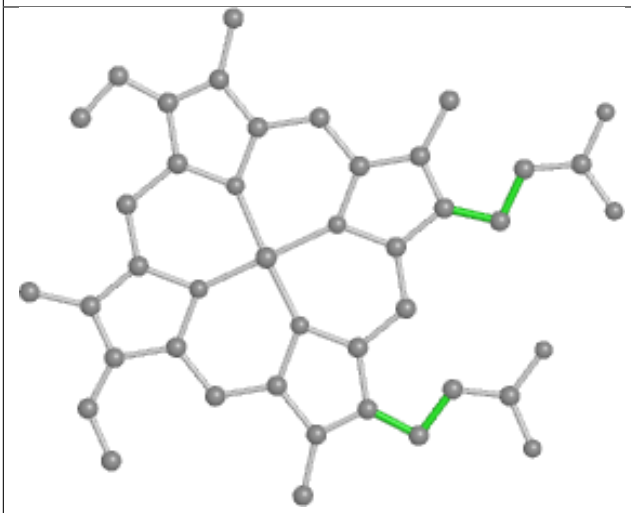
Ligand HEC B 1112



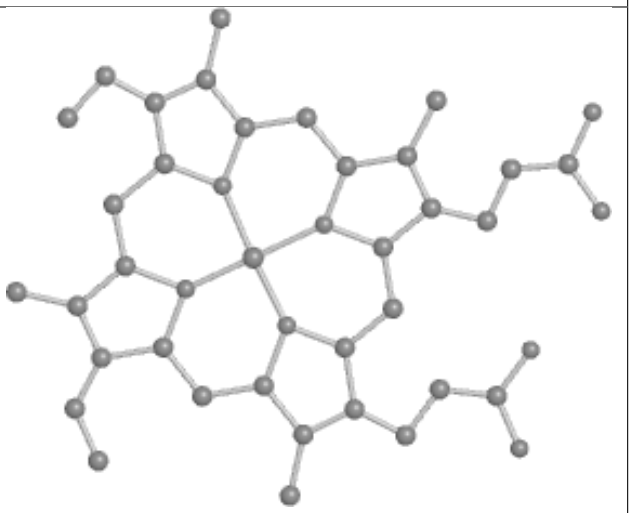
Bond lengths



Bond angles

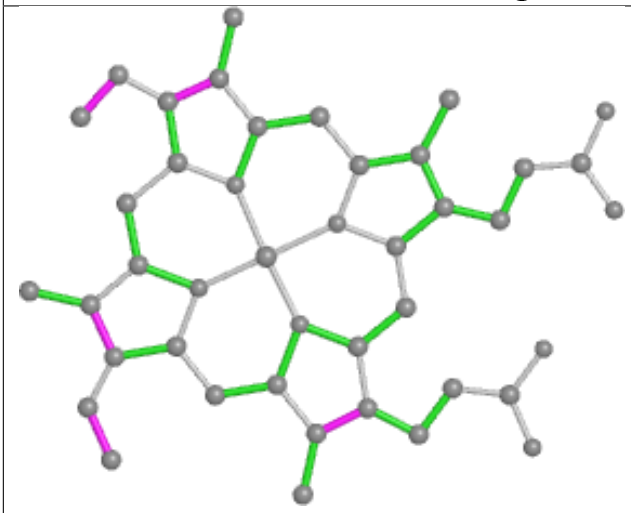


Torsions

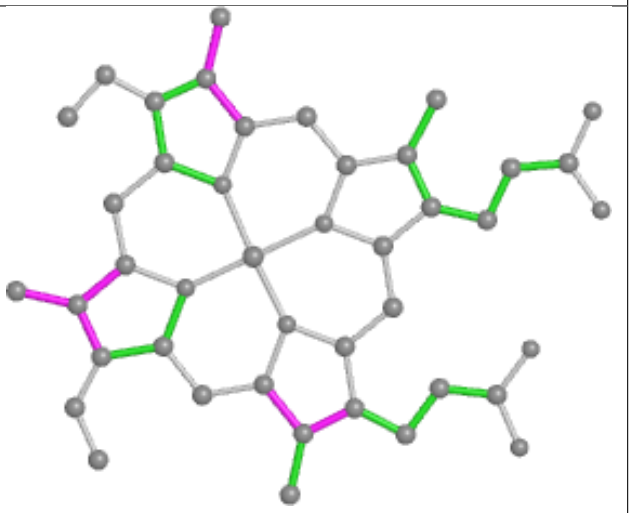


Rings

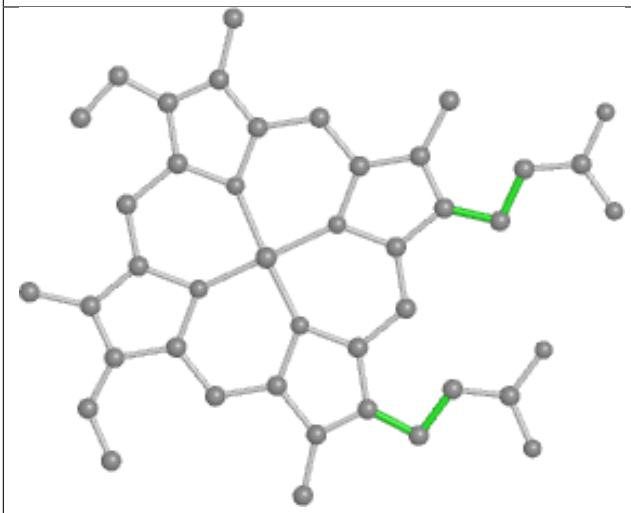
Ligand HEC D 1112



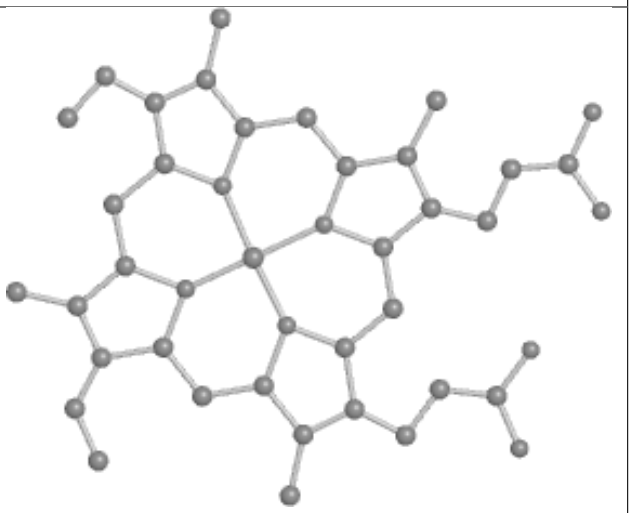
Bond lengths



Bond angles

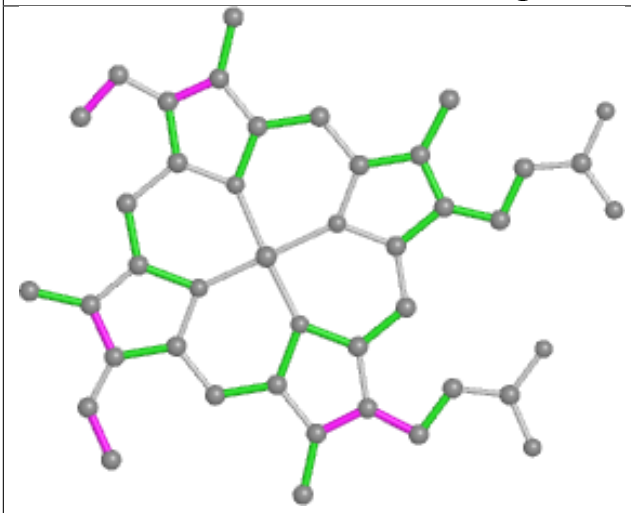


Torsions

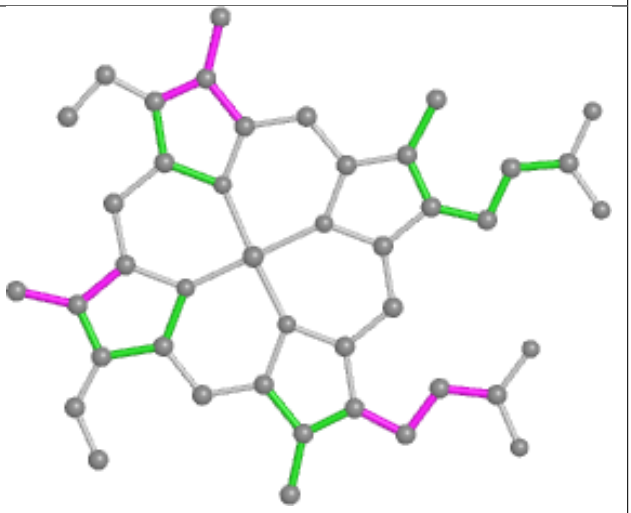


Rings

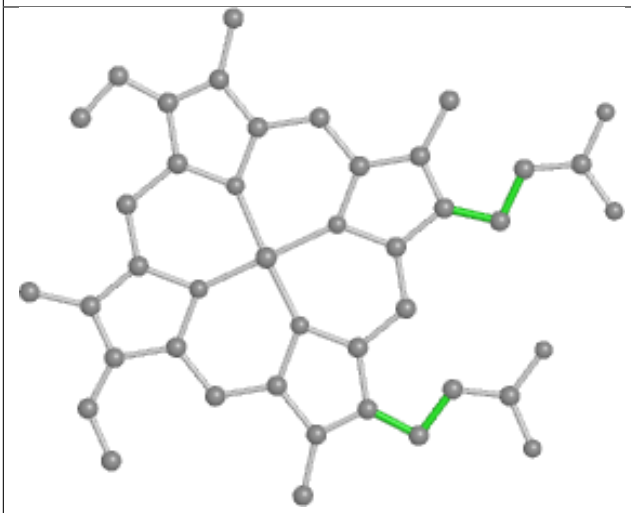
Ligand HEC C 1103



Bond lengths



Bond angles



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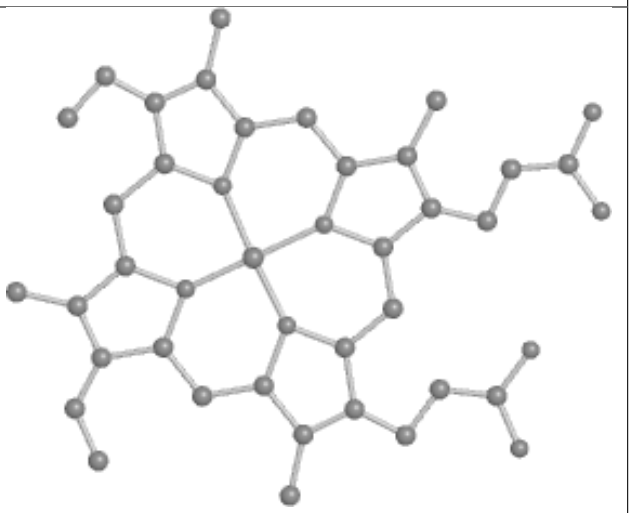
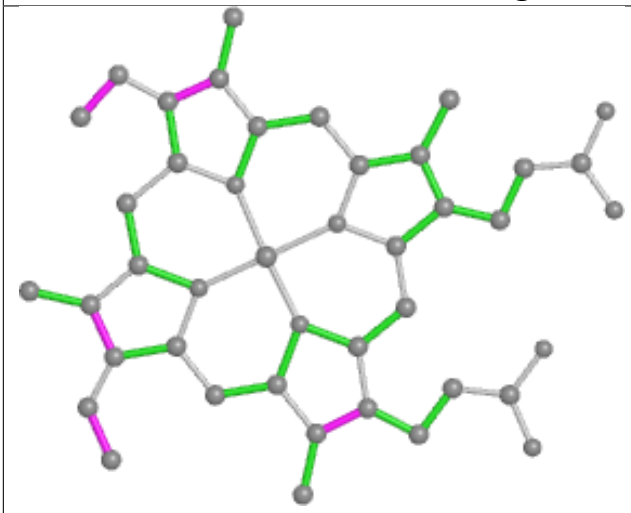
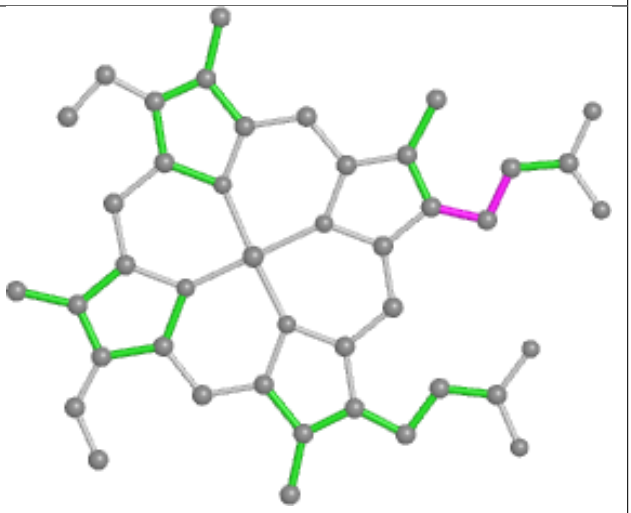


Rings

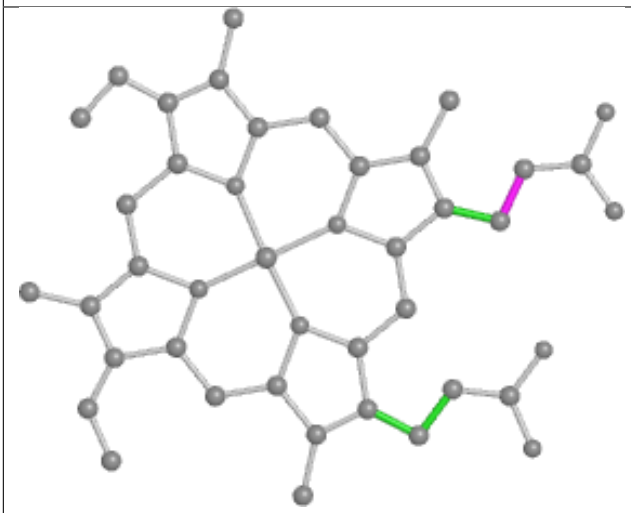
Ligand HEC A 1104



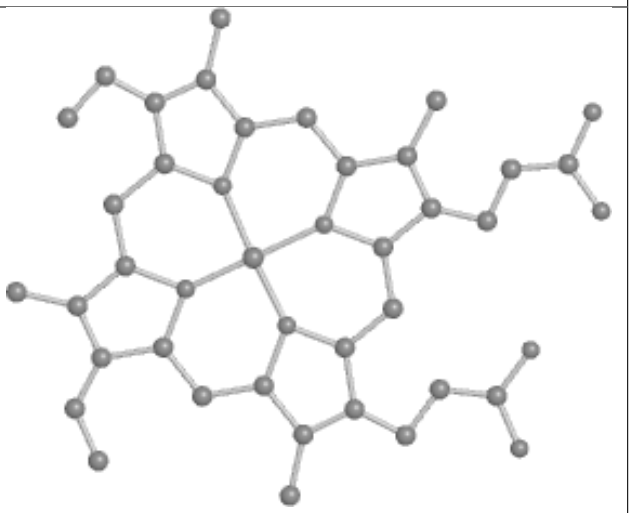
Bond lengths



Bond angles

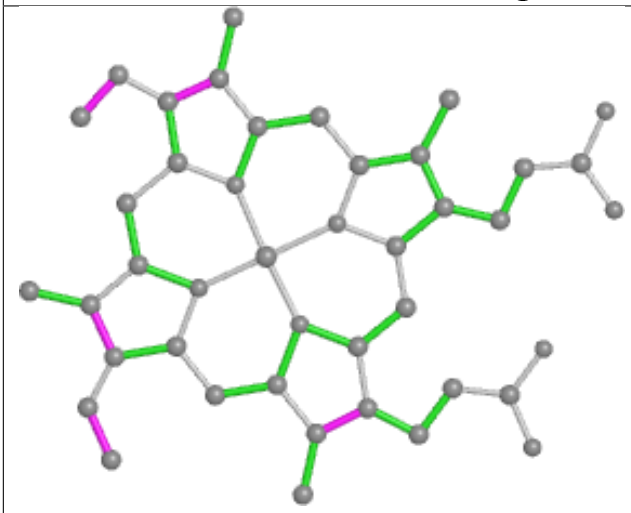


Torsions



Rings

Ligand HEC B 1111



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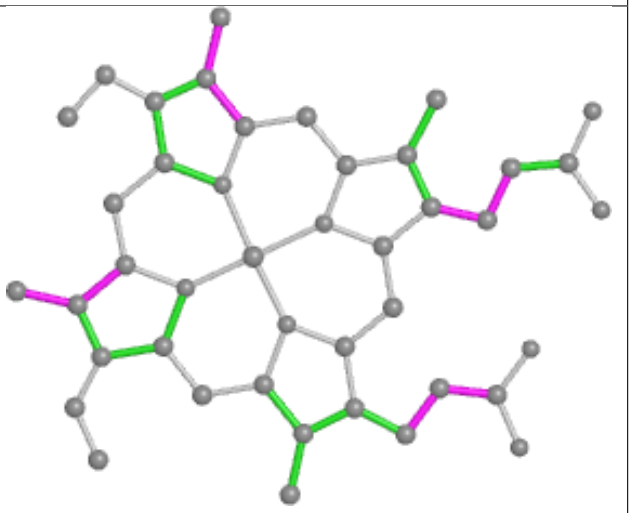

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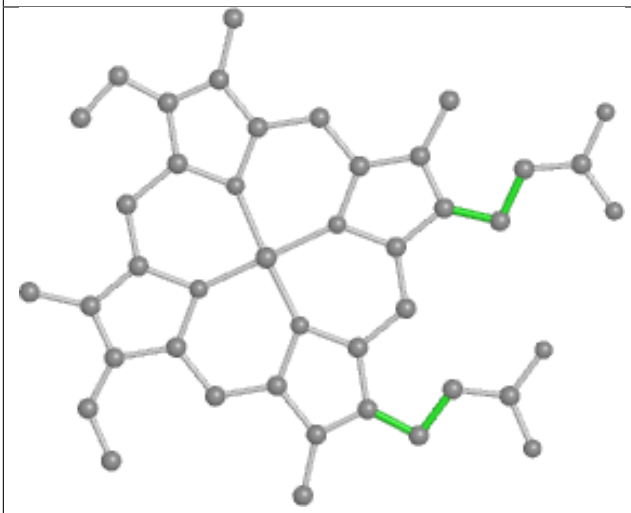

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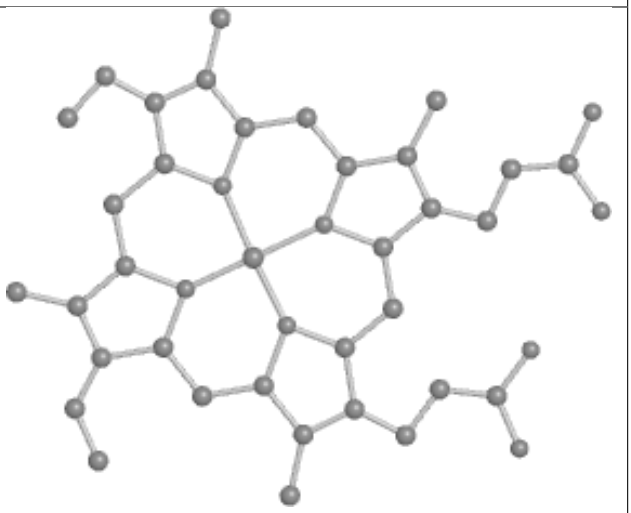
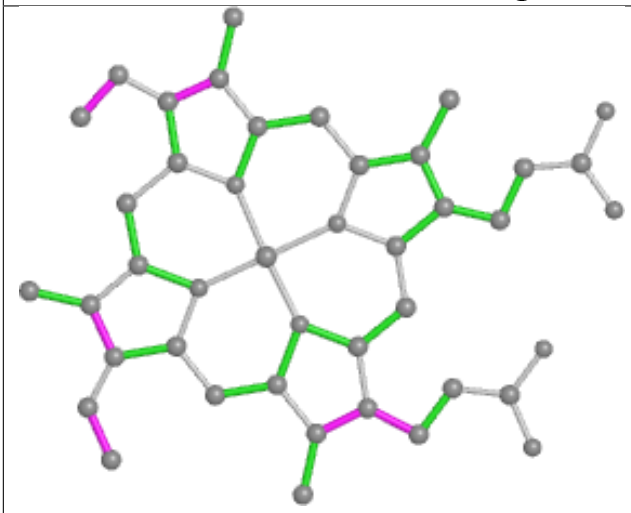


Rings

Ligand HEC A 1106



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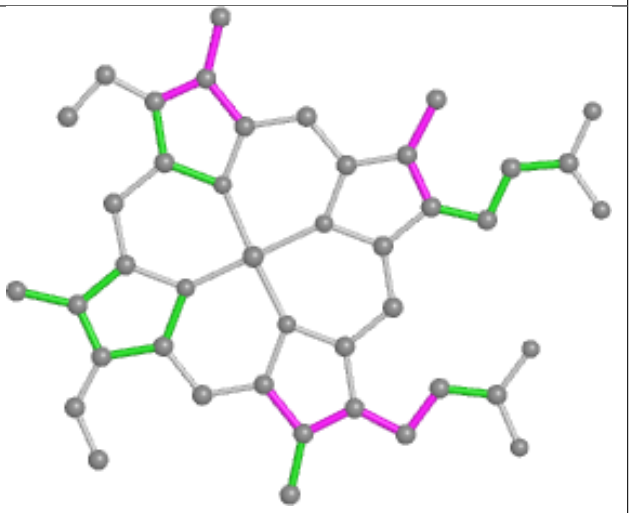

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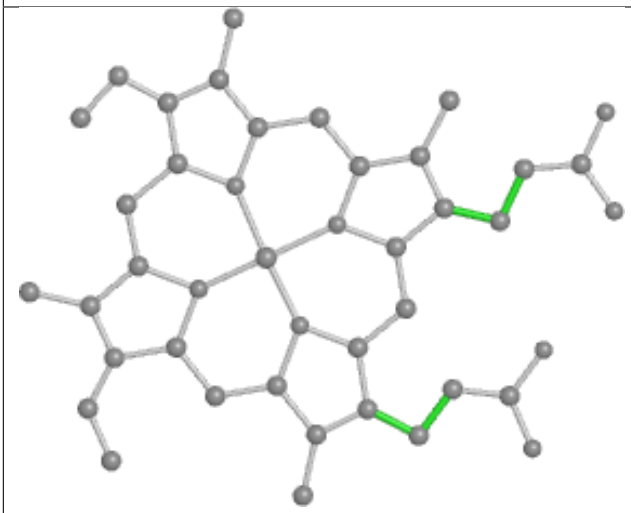

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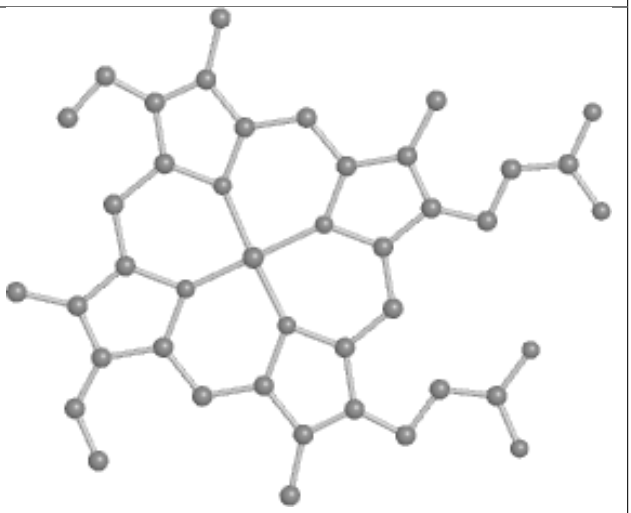
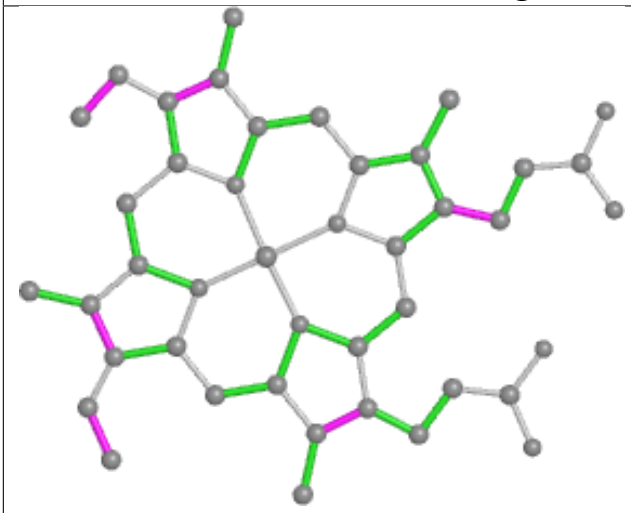


Rings

Ligand HEC D 1115



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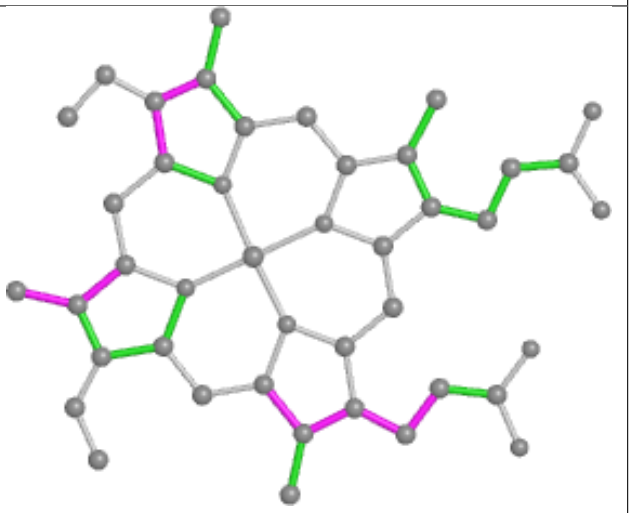
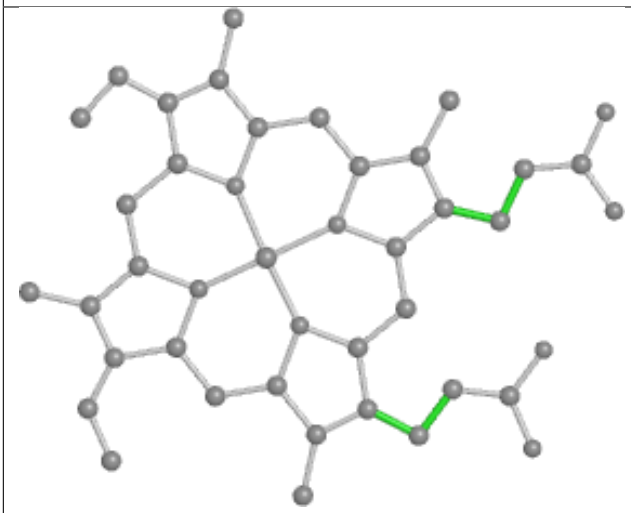


Bond angles



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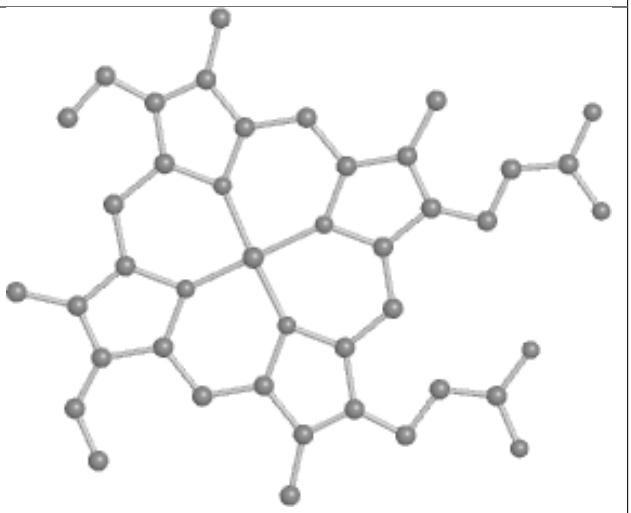
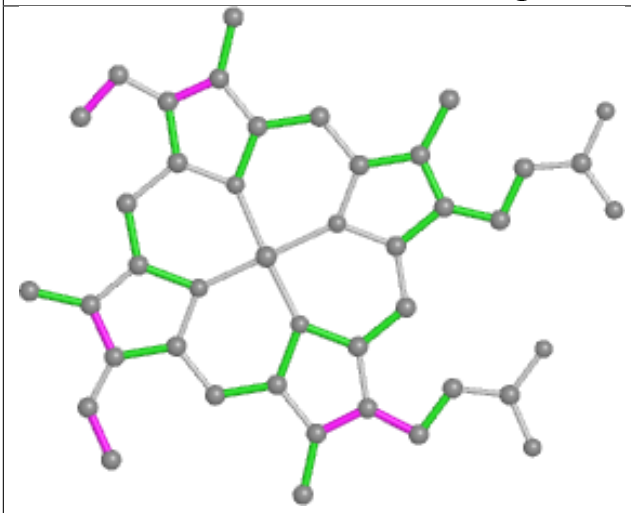


Rings

Ligand HEC A 1109



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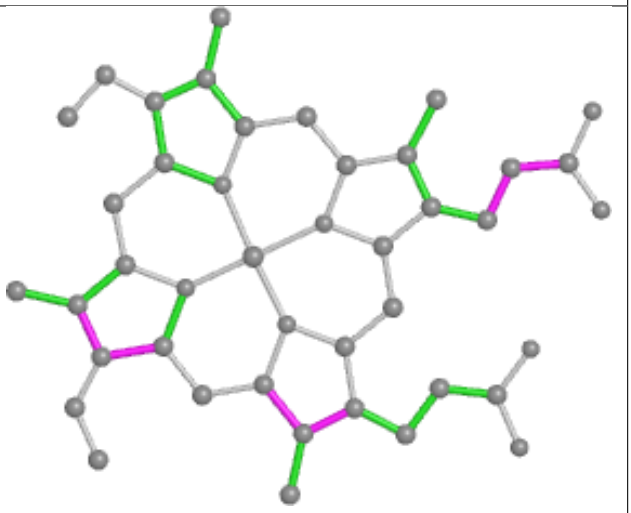

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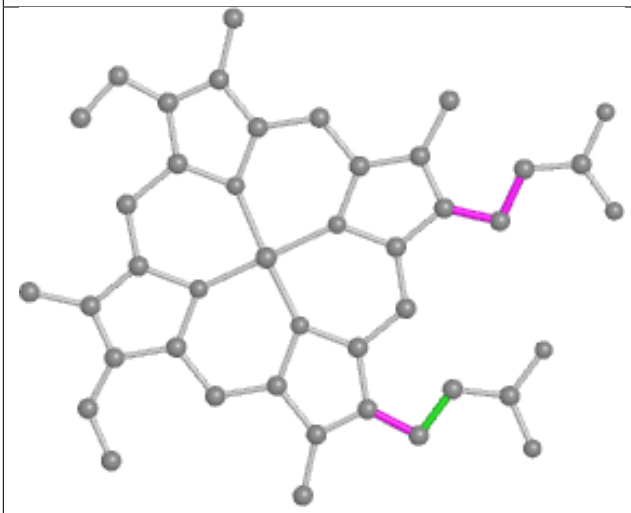

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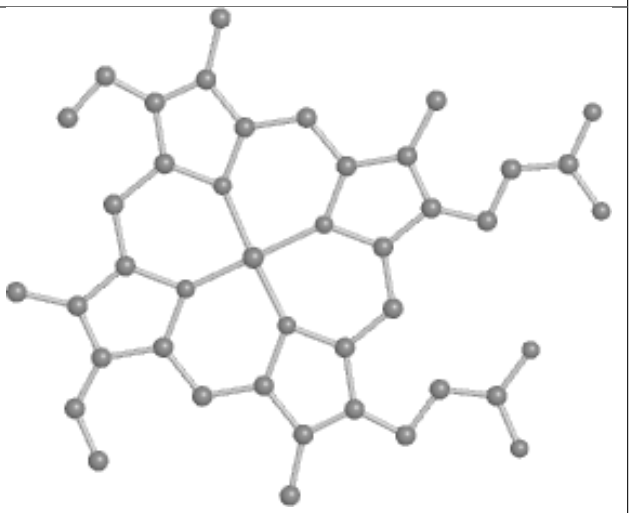
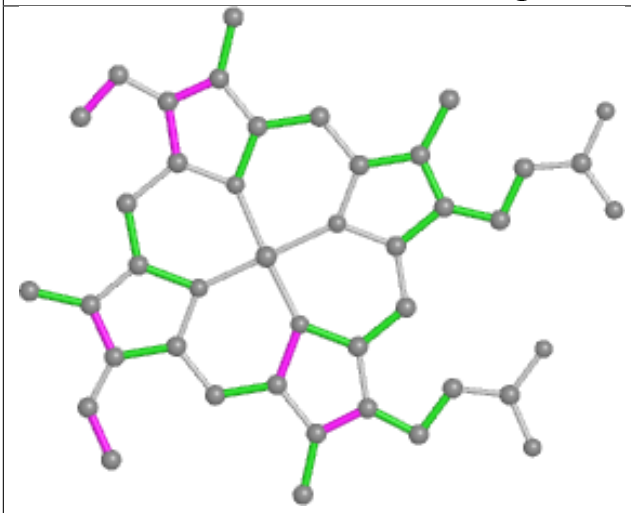


Rings

Ligand HEC A 1115



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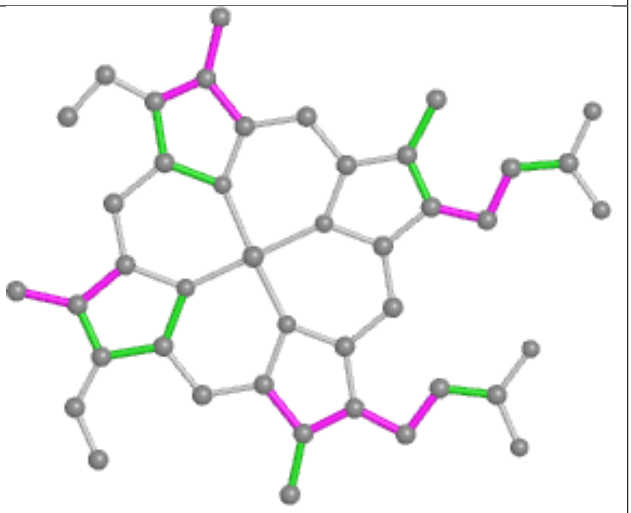

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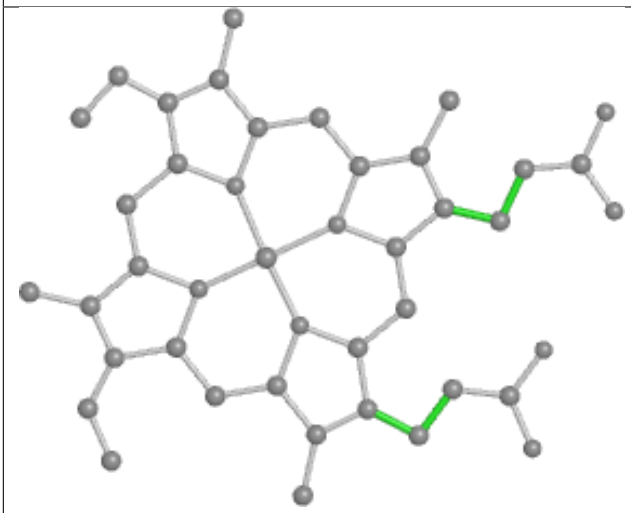

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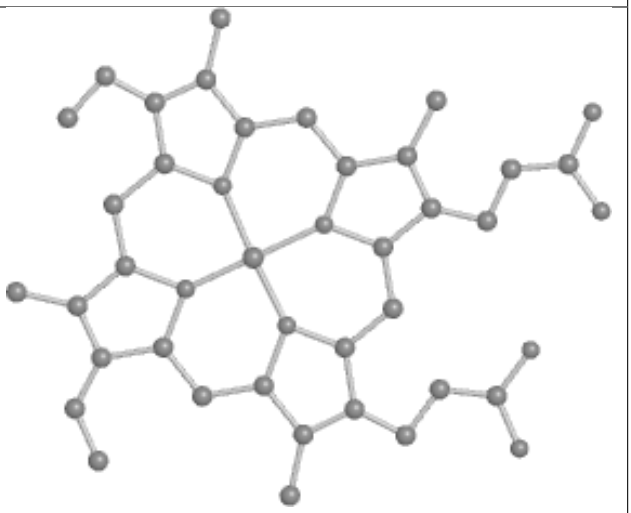
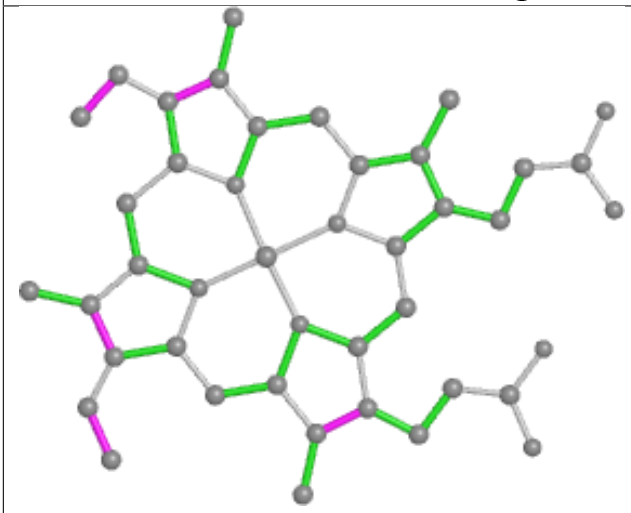


Rings

Ligand HEC D 1111



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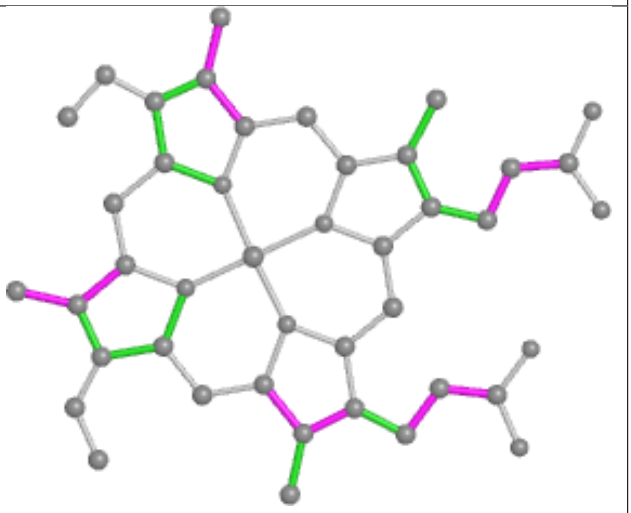
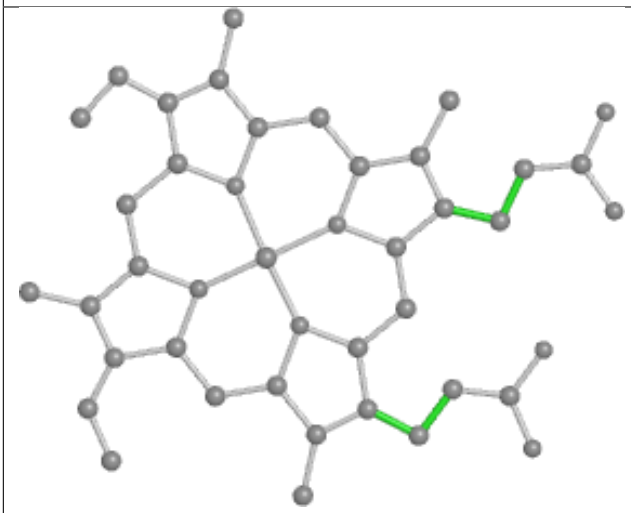


Bond angles



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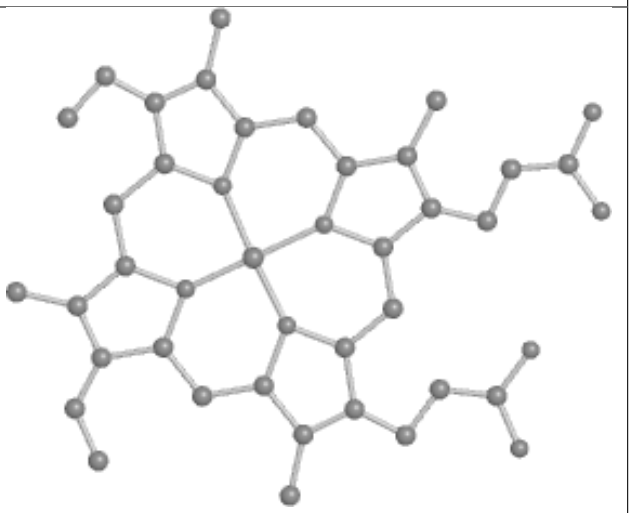
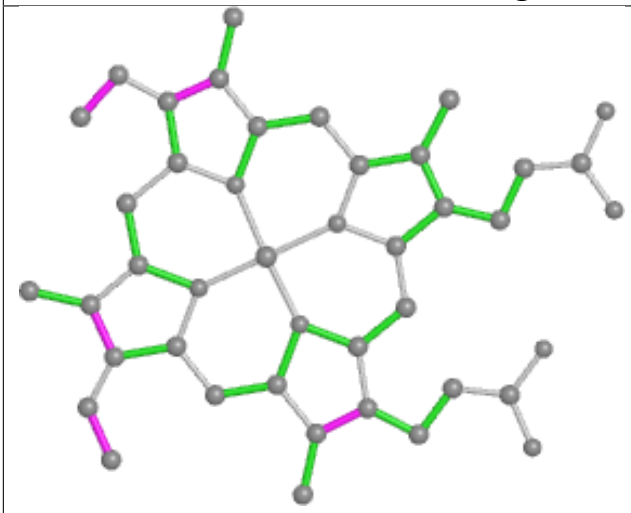


Rings

Ligand HEC A 1112



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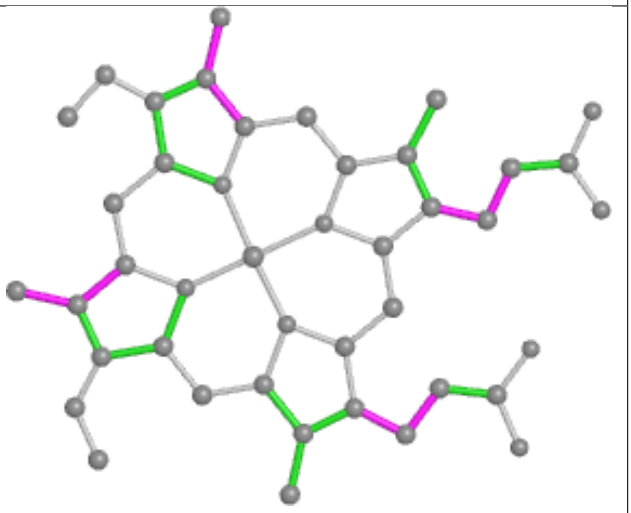

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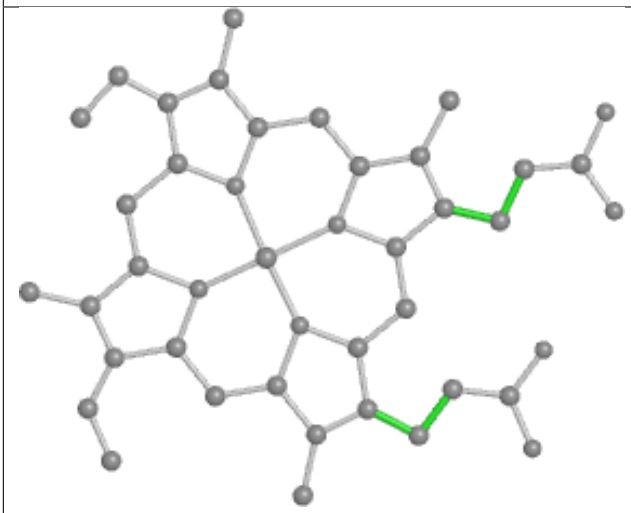

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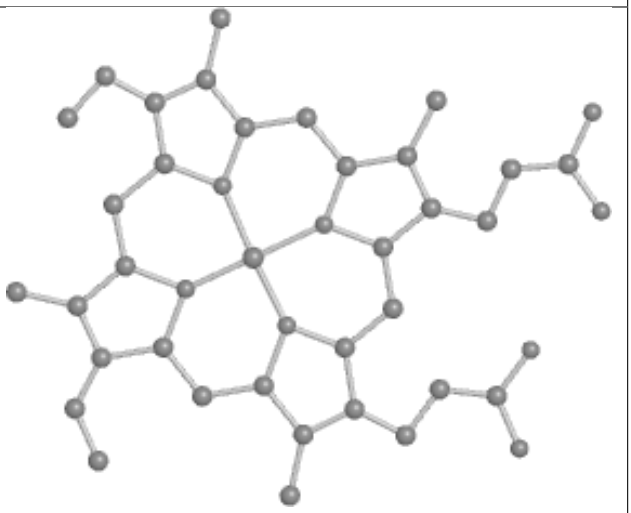
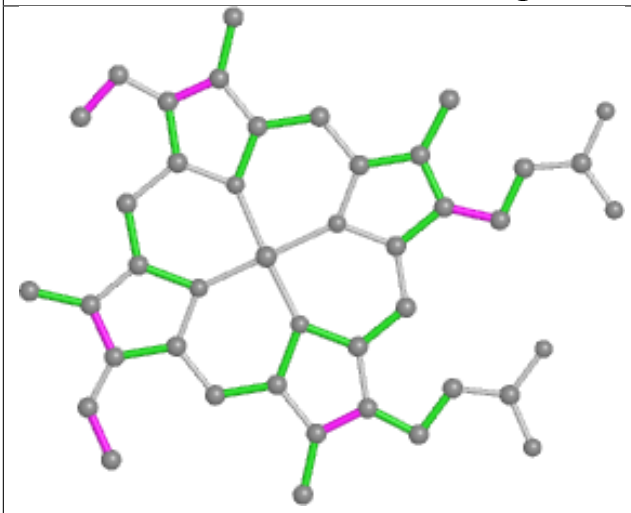


Rings

Ligand HEC C 1112



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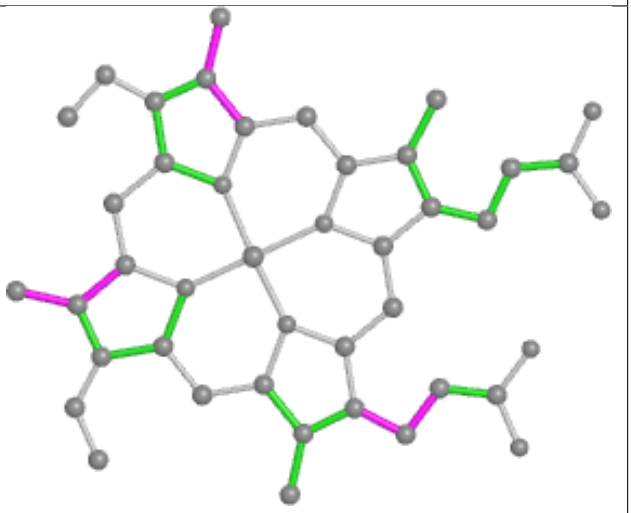
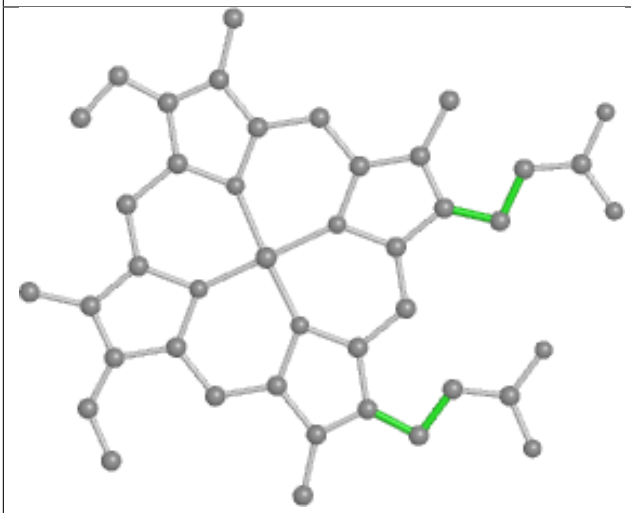


Bond angles



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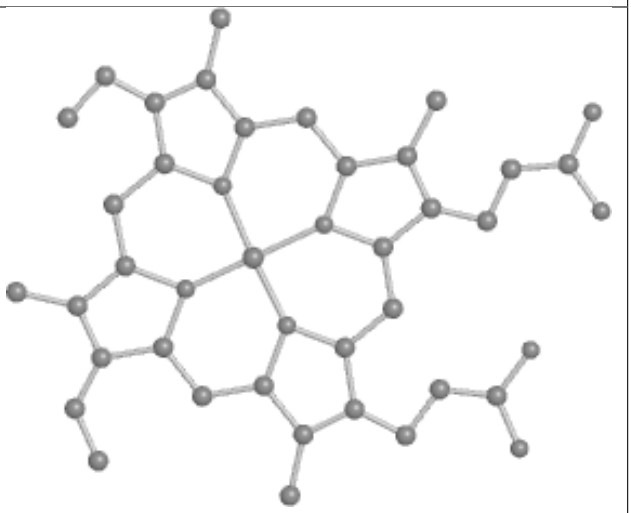
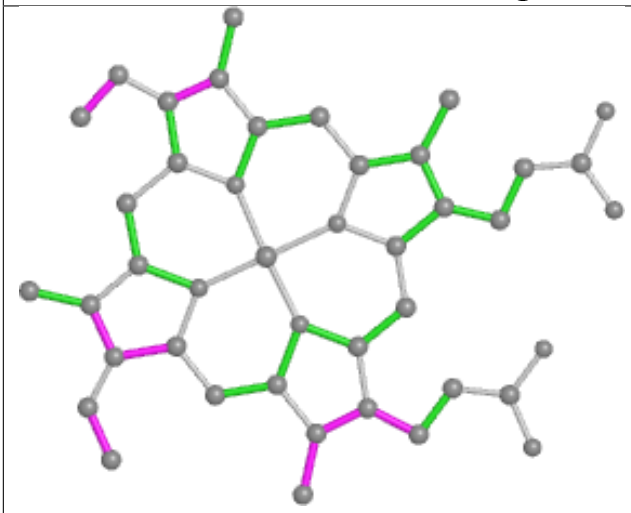


Rings

Ligand HEC B 1114



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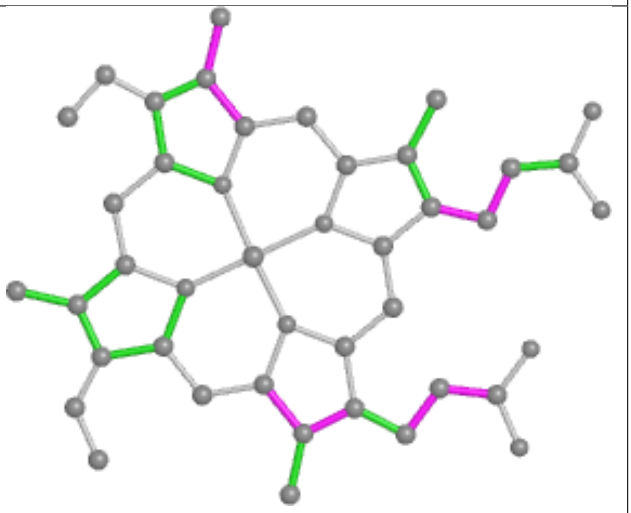

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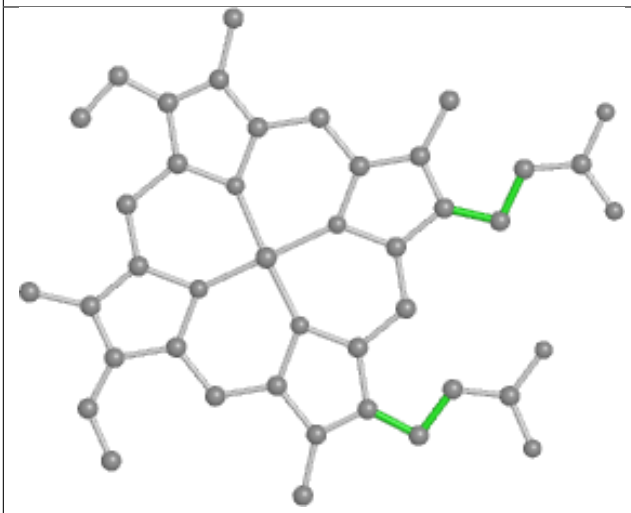
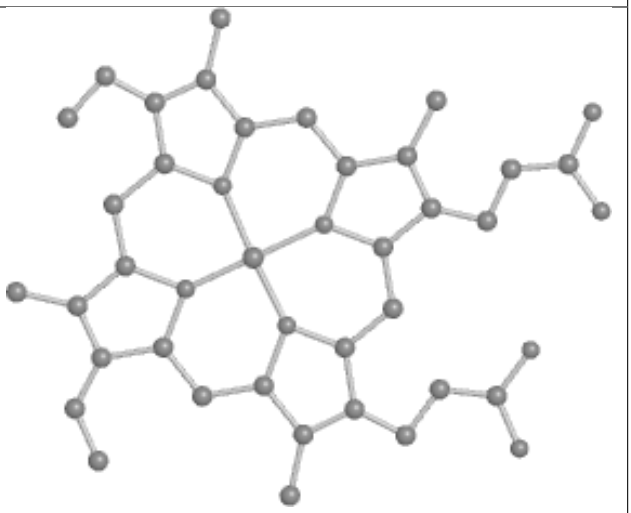
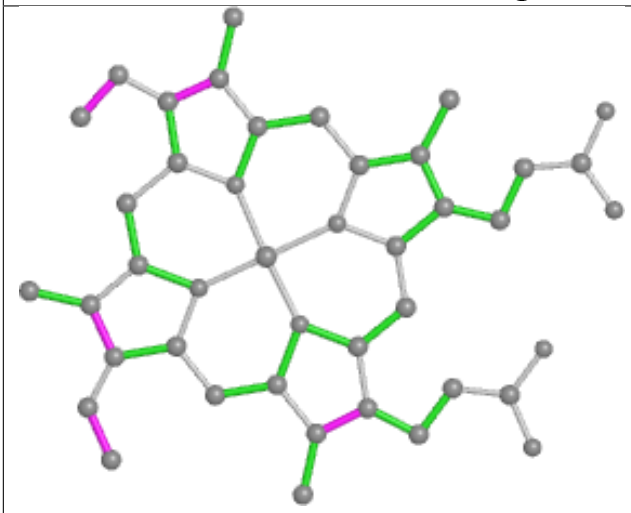


Torsions



Rings

Ligand HEC A 1116



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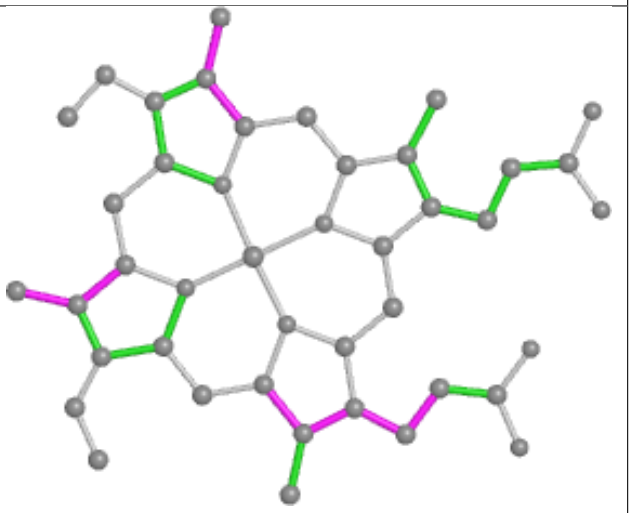

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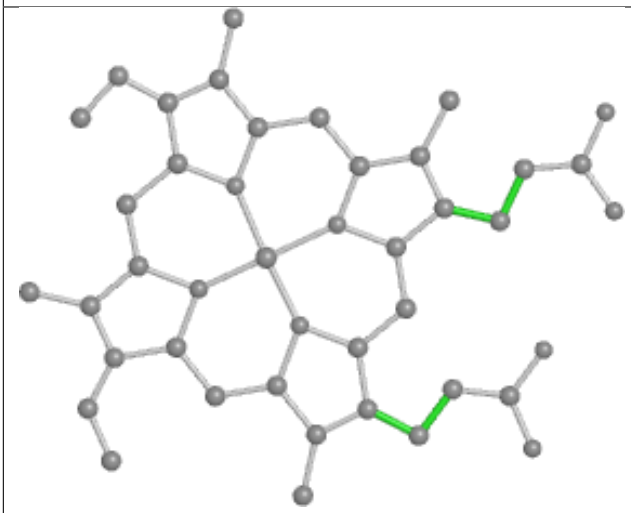
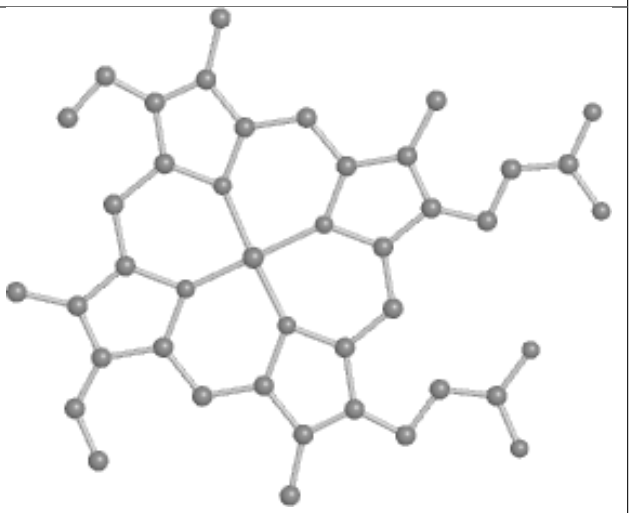
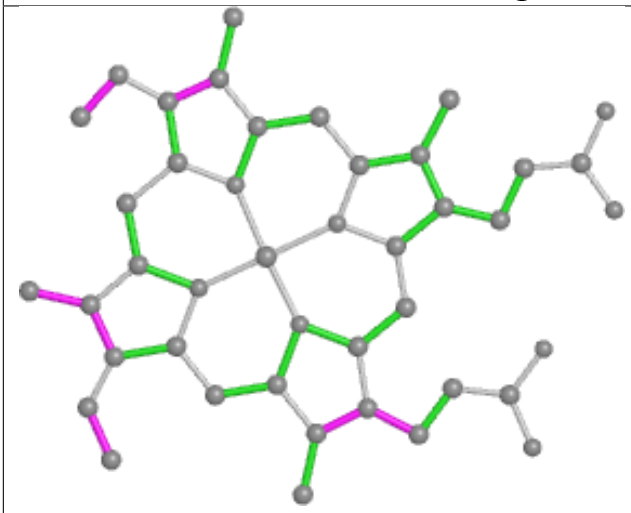


Torsions



Rings

Ligand HEC D 1110



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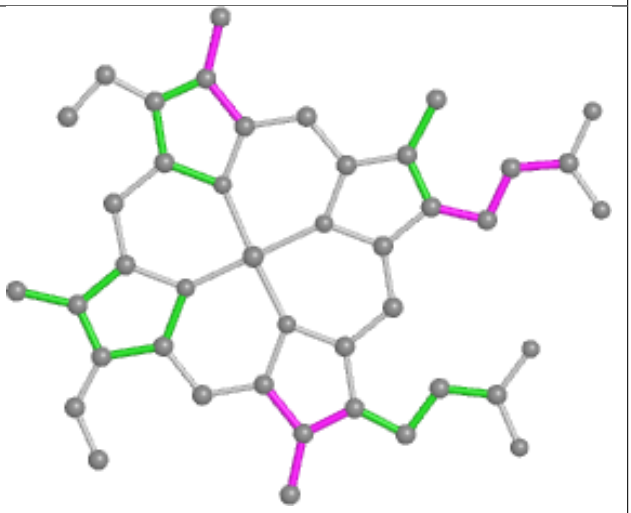
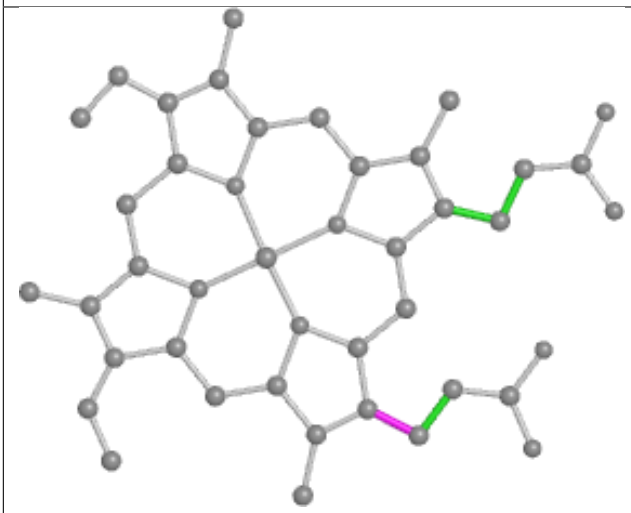


Bond angles



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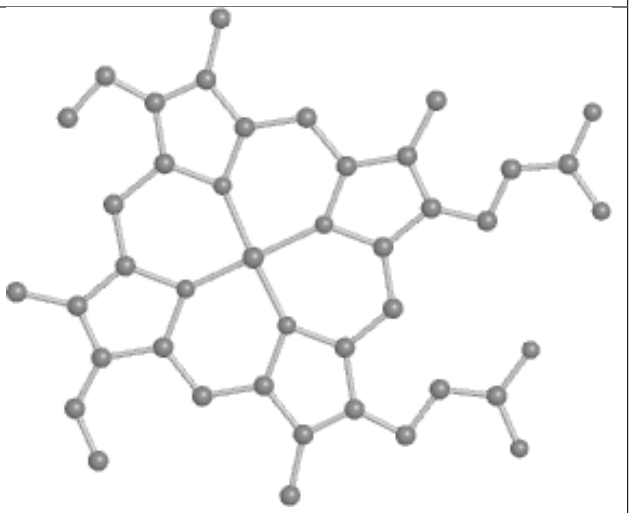
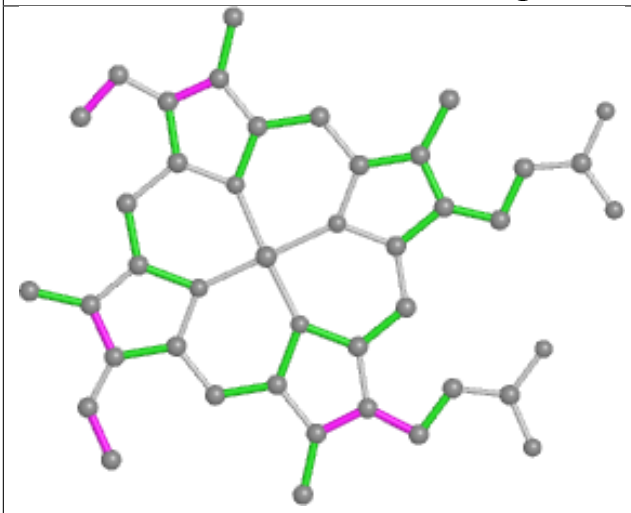
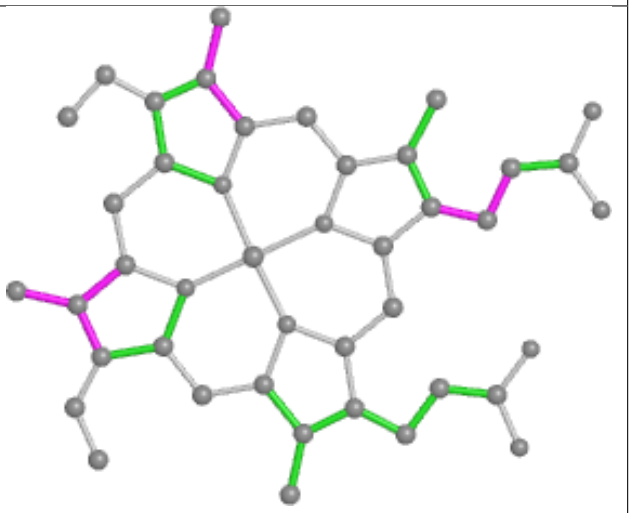


Rings

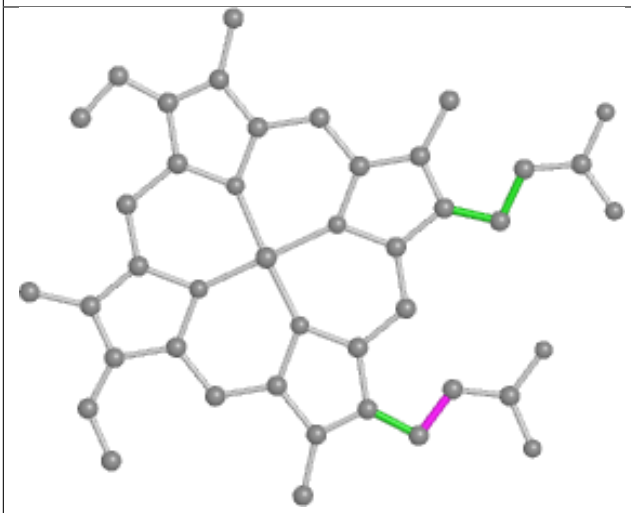
Ligand HEC C 1101



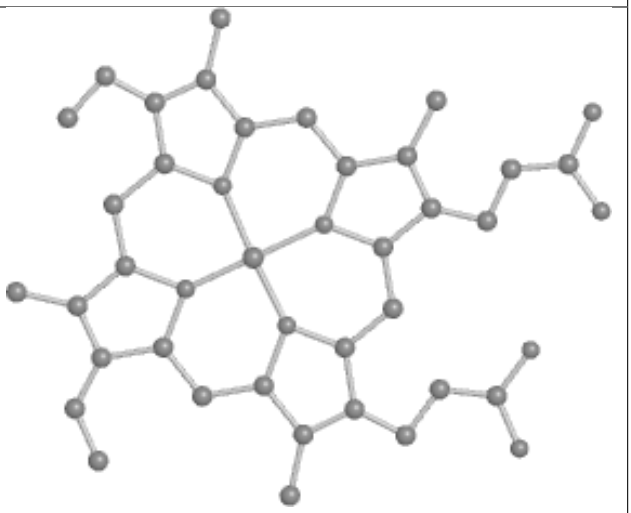
Bond lengths



Bond angles

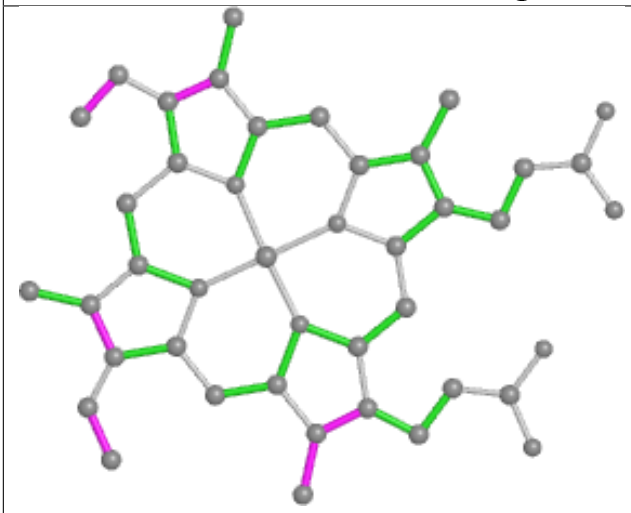


Torsions

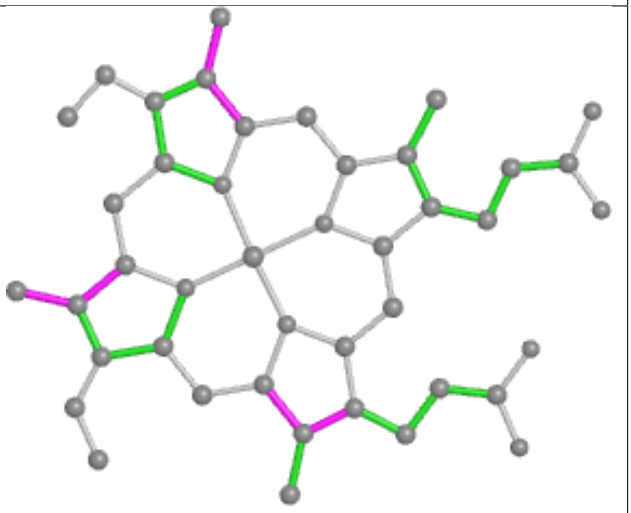


Rings

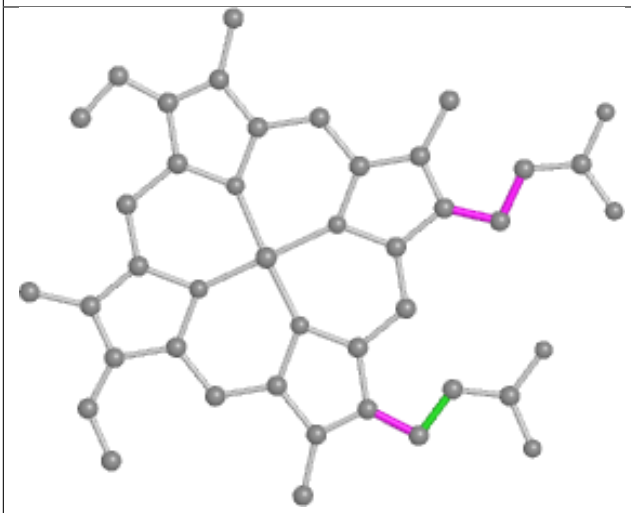
Ligand HEC D 1109



Bond lengths



Bond angles



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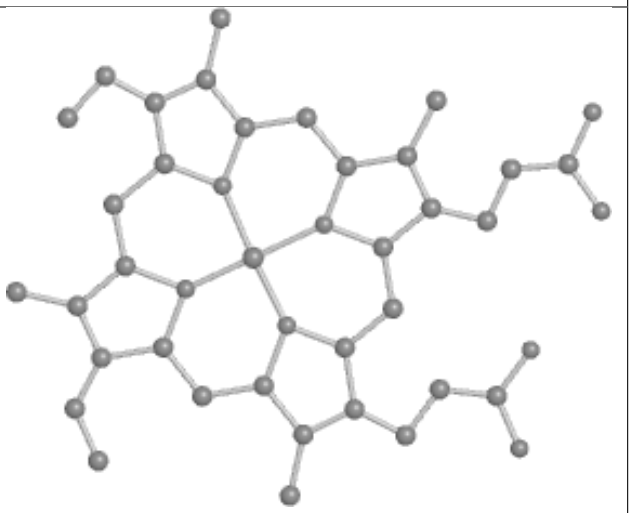
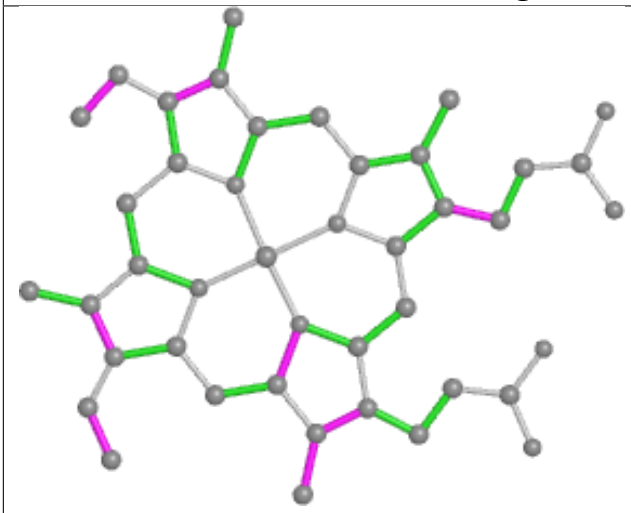
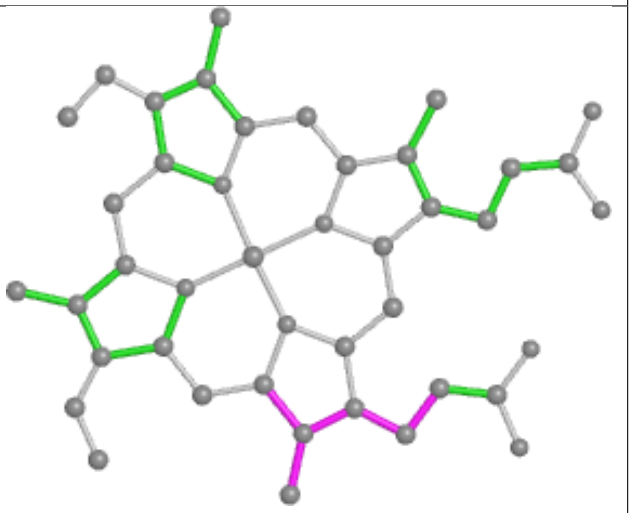


Rings

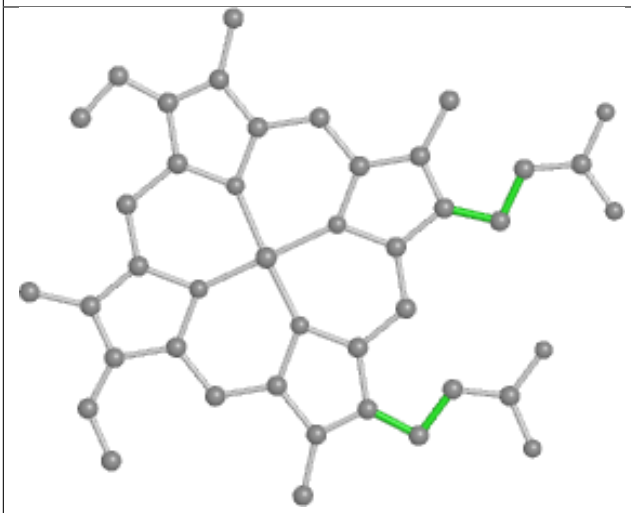
Ligand HEC B 1113



Bond lengths



Bond angles



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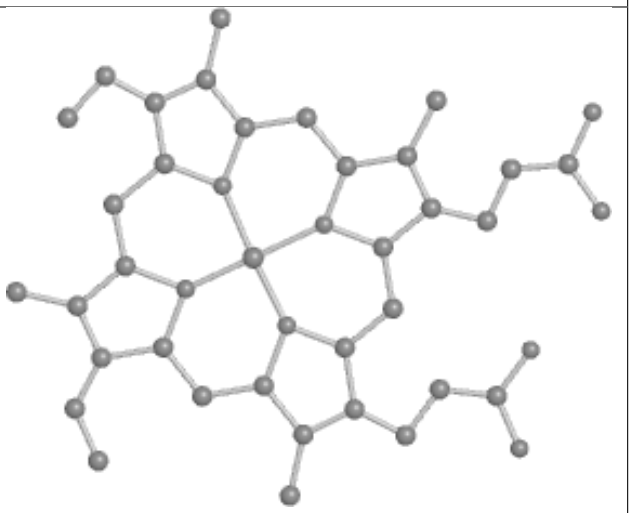
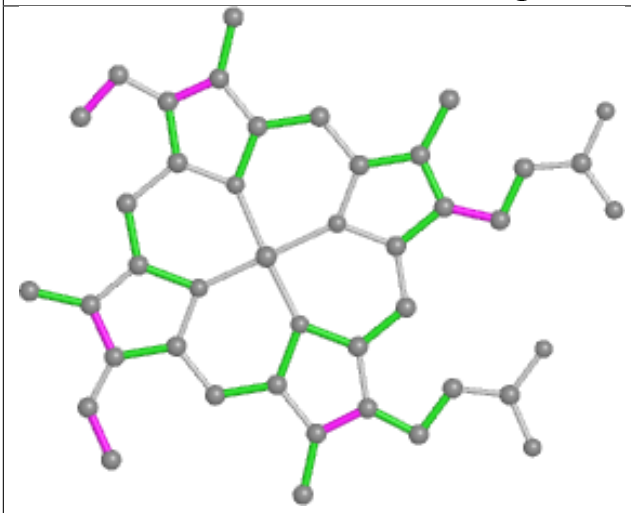
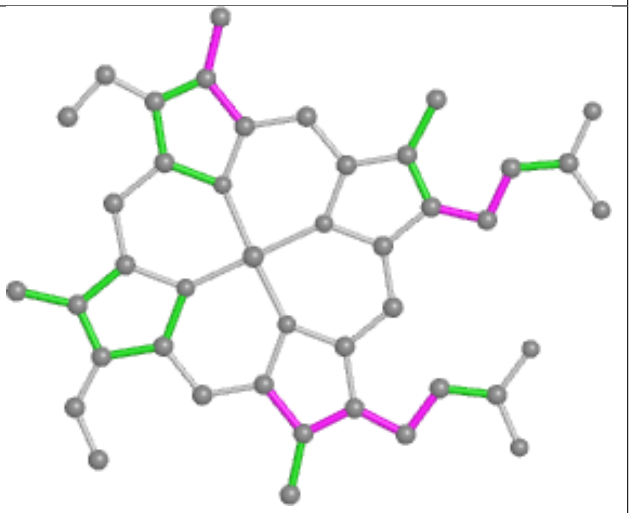


Rings

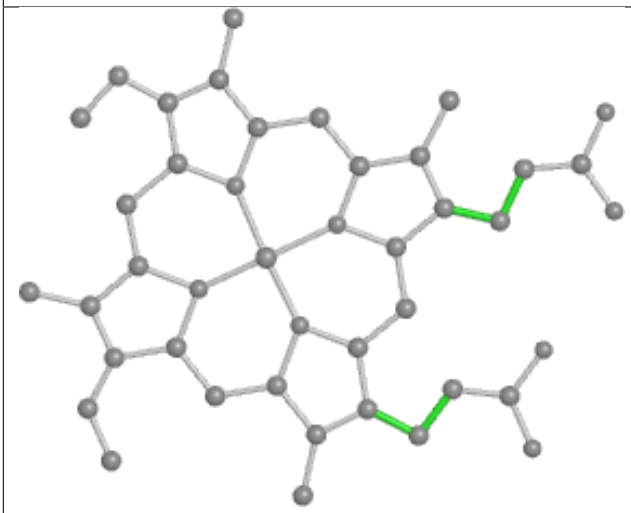
Ligand HEC D 1113



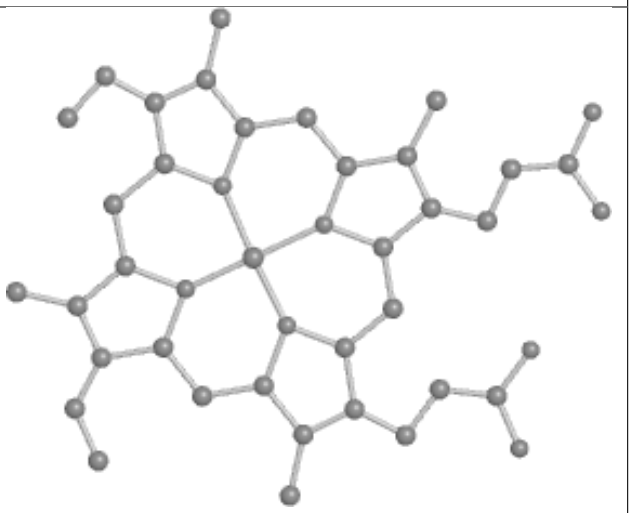
Bond lengths



Bond angles

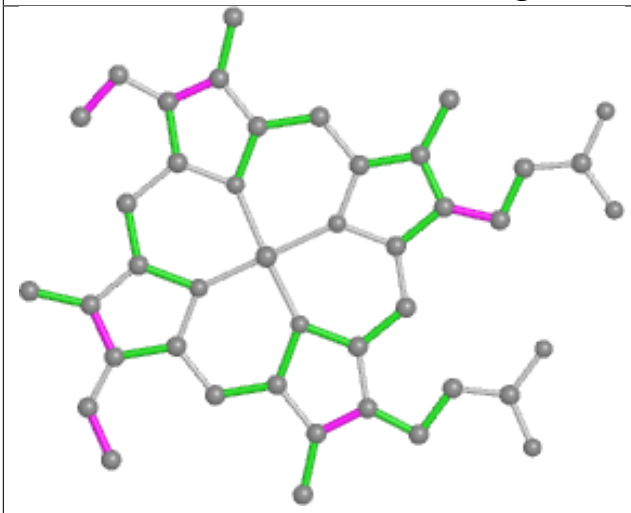


Torsions

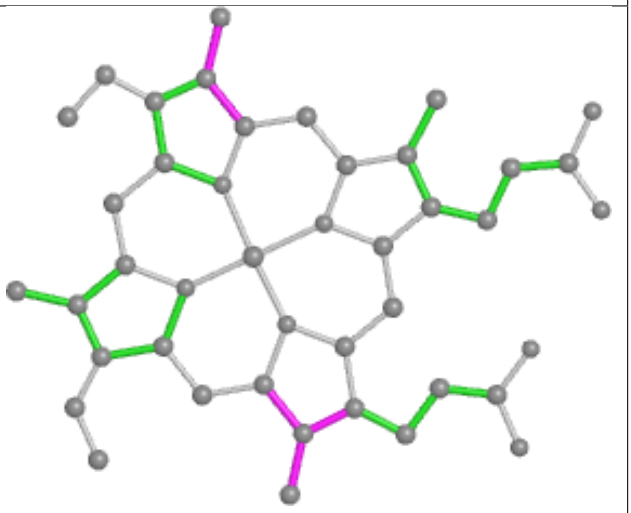


Rings

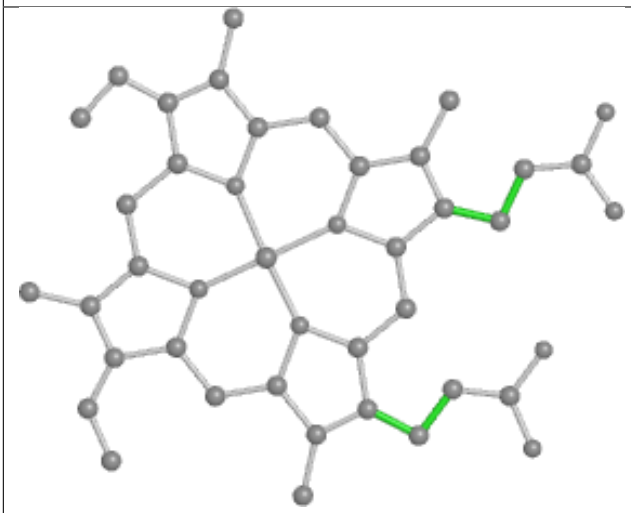
Ligand HEC A 1110



Bond lengths



Bond angles



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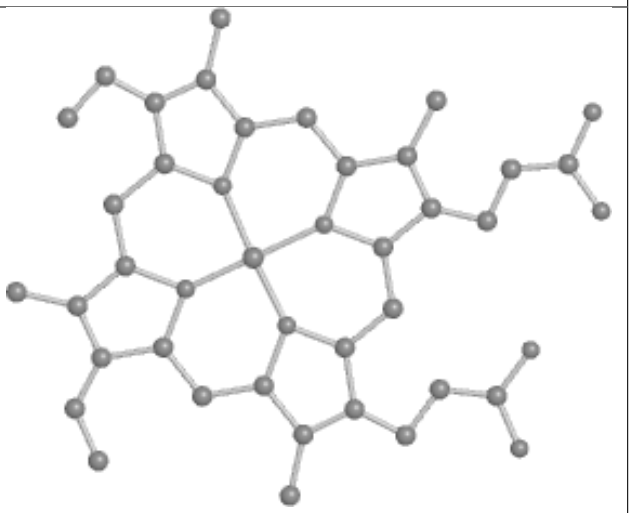
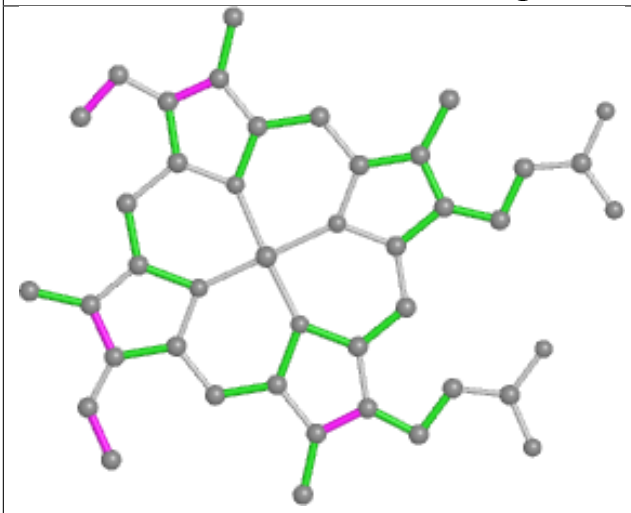
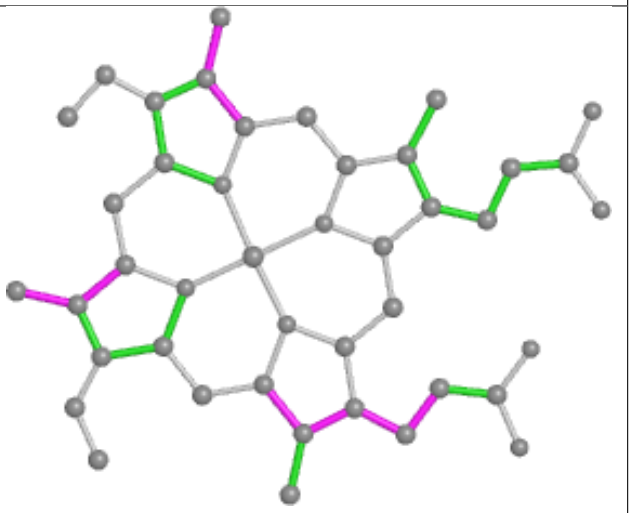


Rings

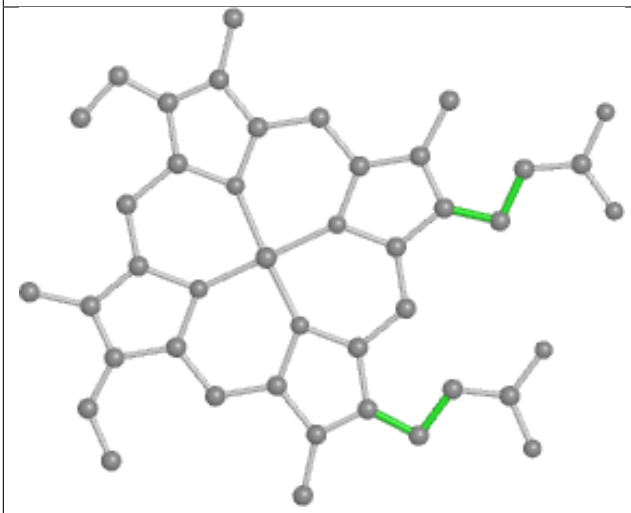
Ligand HEC B 1116



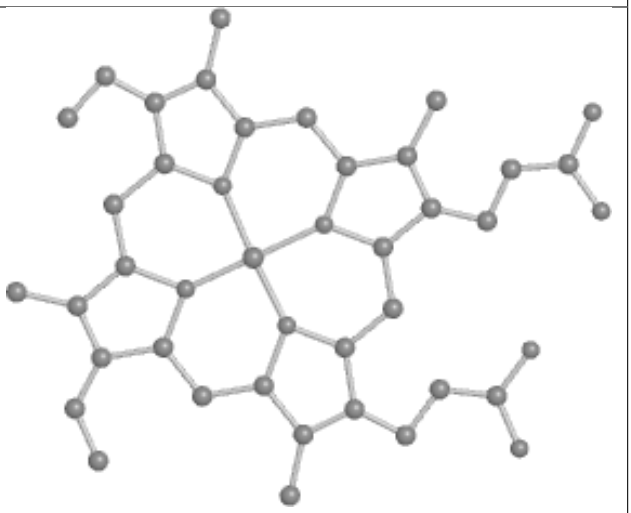
Bond lengths



Bond angles

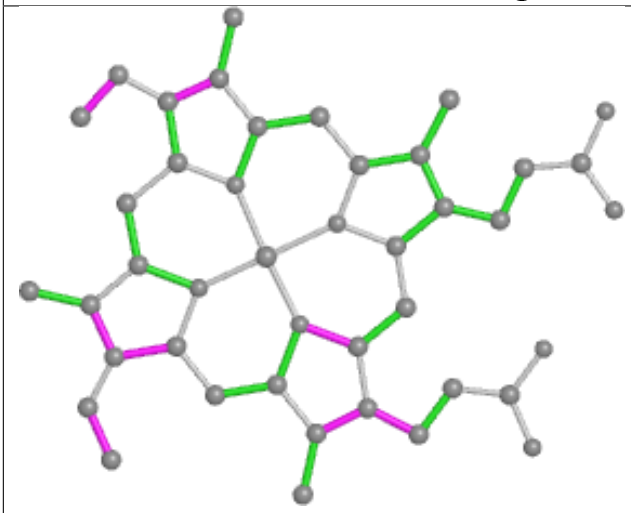


Torsions

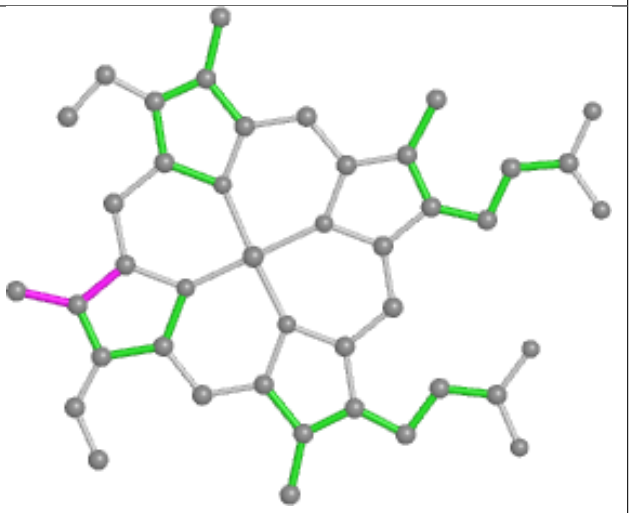


Rings

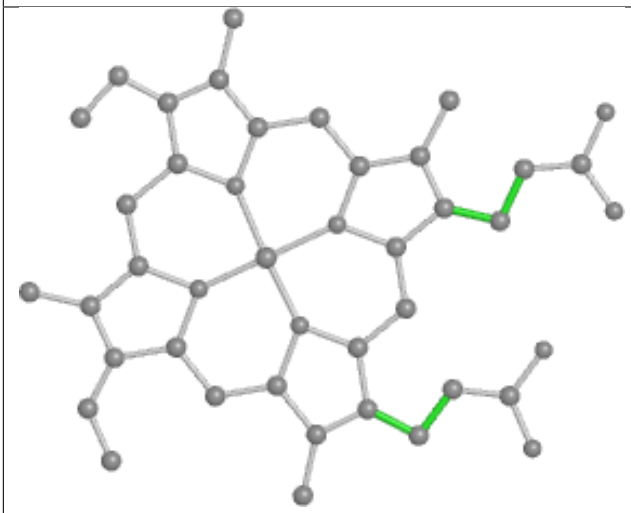
Ligand HEC A 1114



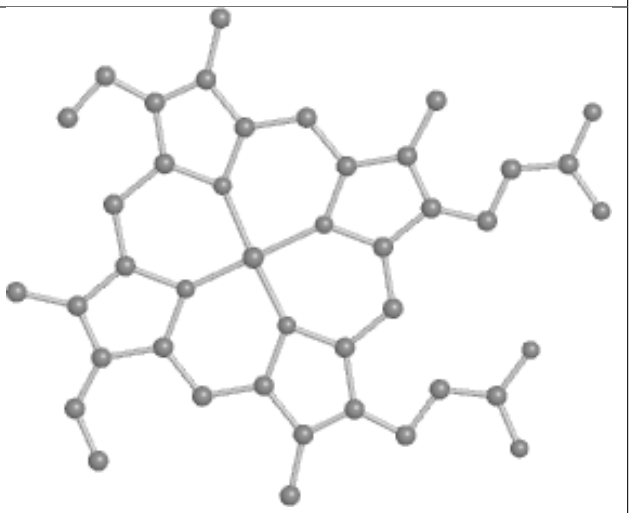
Bond lengths



Bond angles

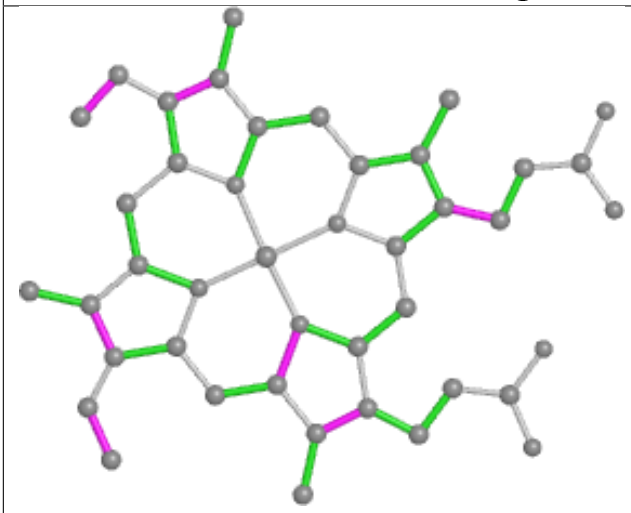


Torsions

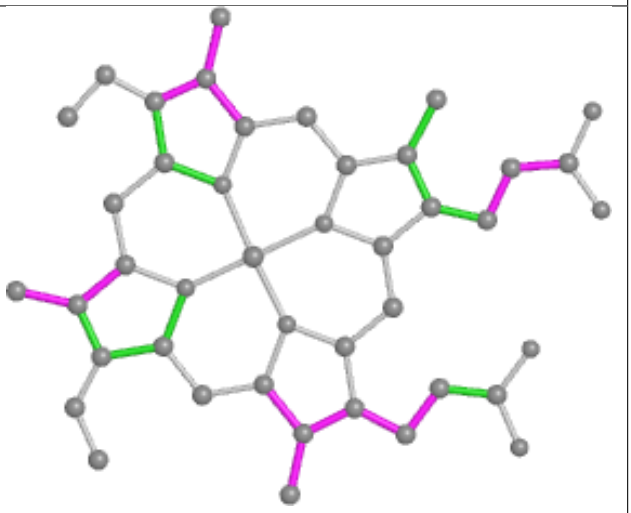


Rings

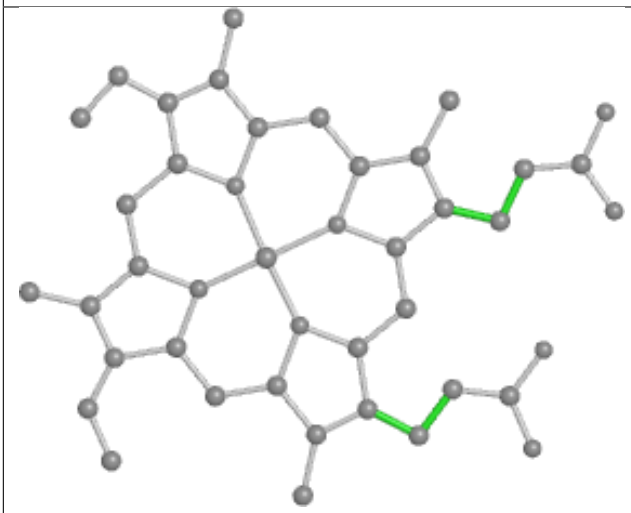
Ligand HEC C 1115



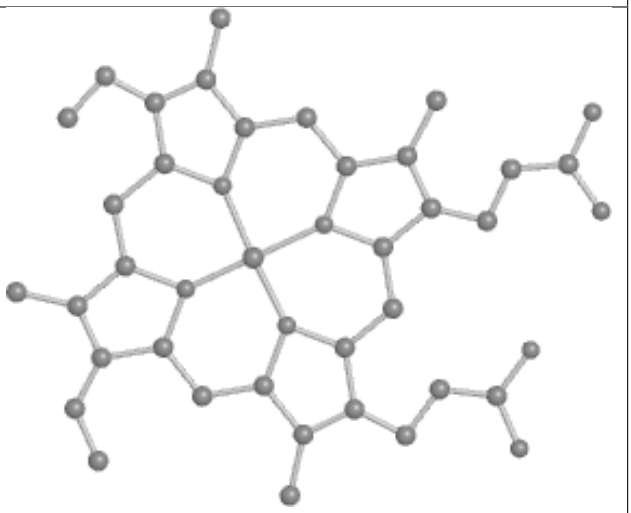
Bond lengths



Bond angles

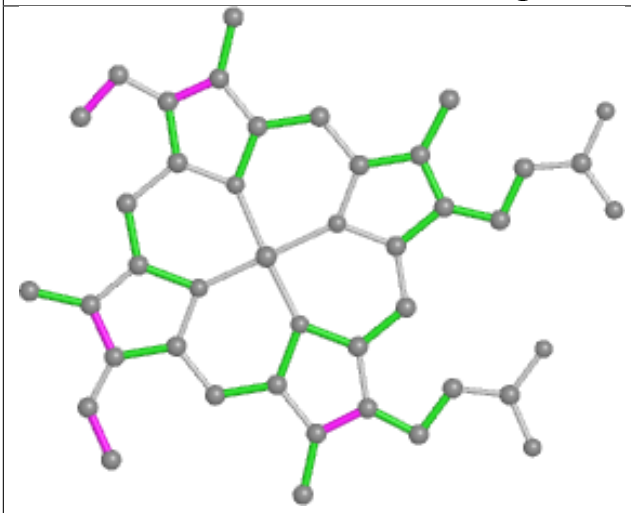


Torsions



Rings

Ligand HEC B 1115



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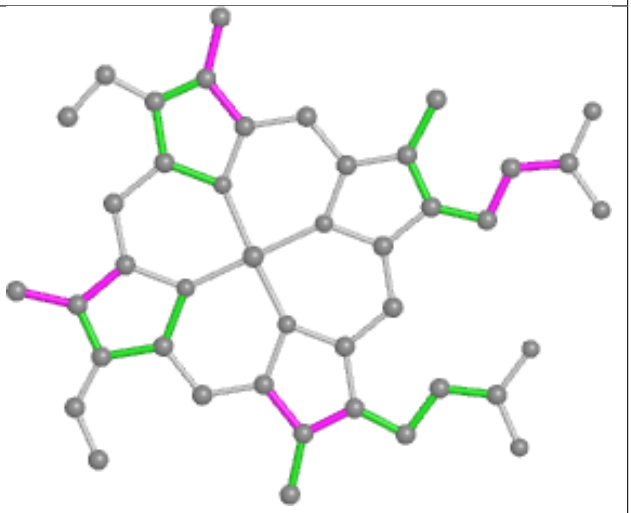
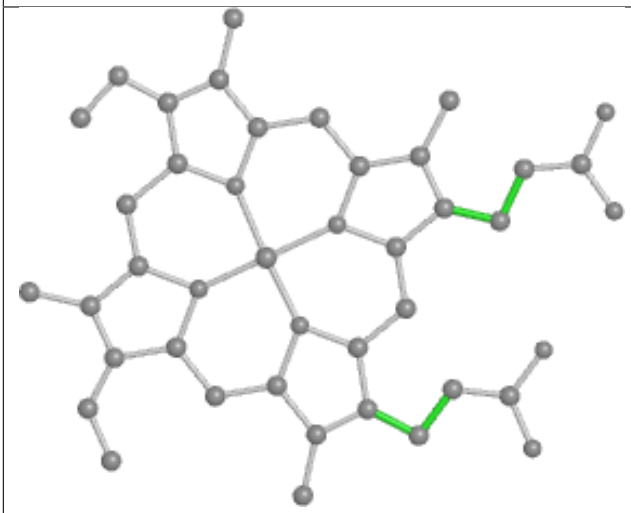
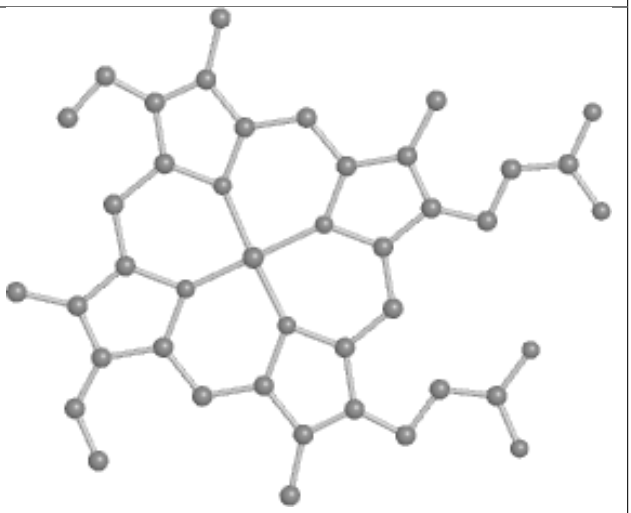


Bond angles

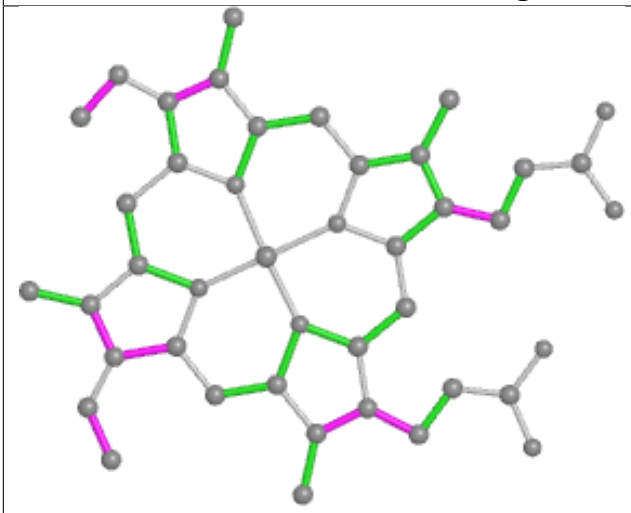


Torsions

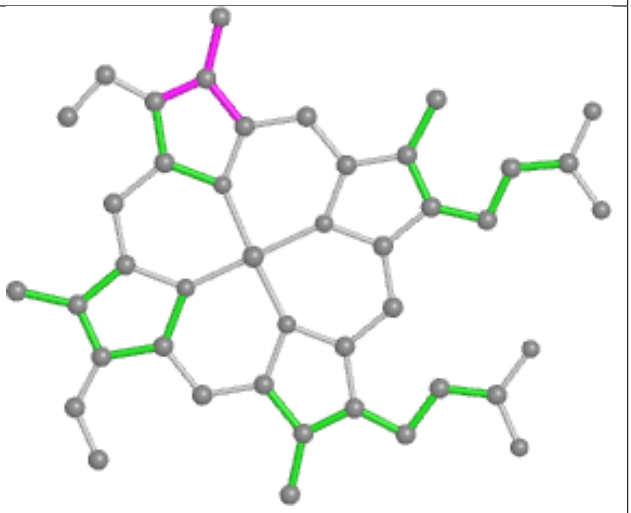


Rings

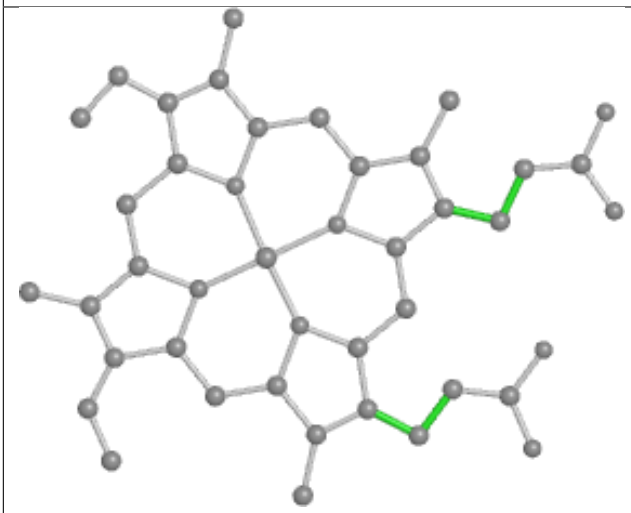
Ligand HEC B 1109



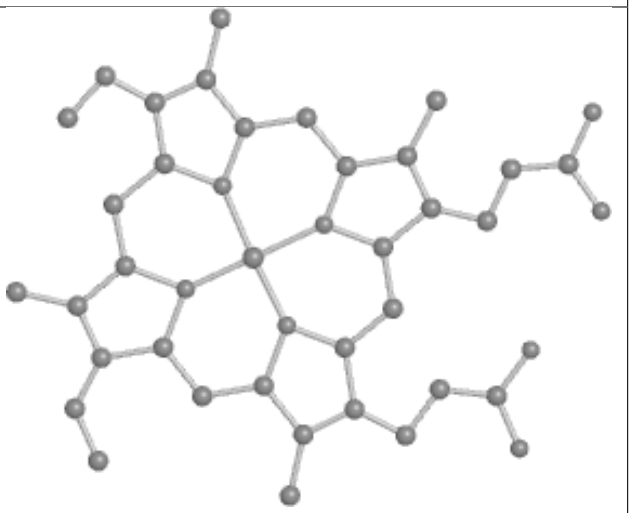
Bond lengths



Bond angles

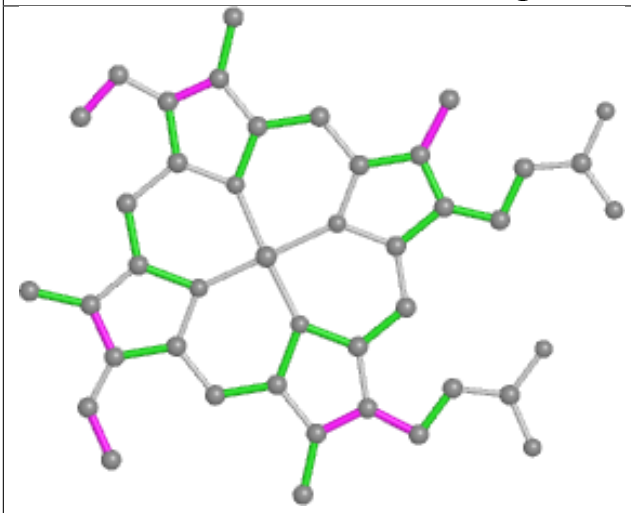


Torsions

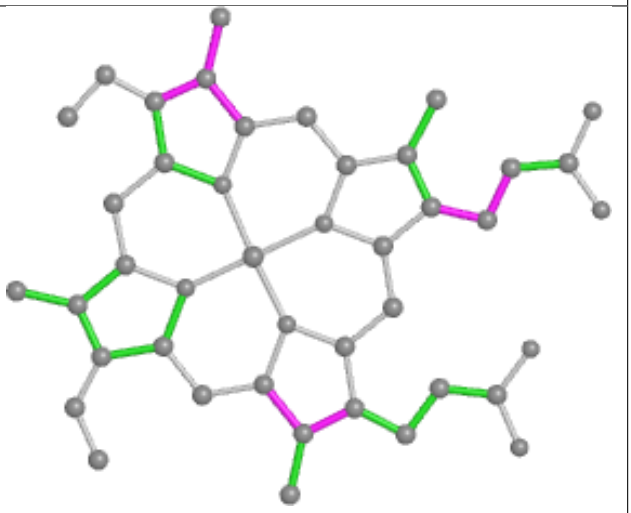


Rings

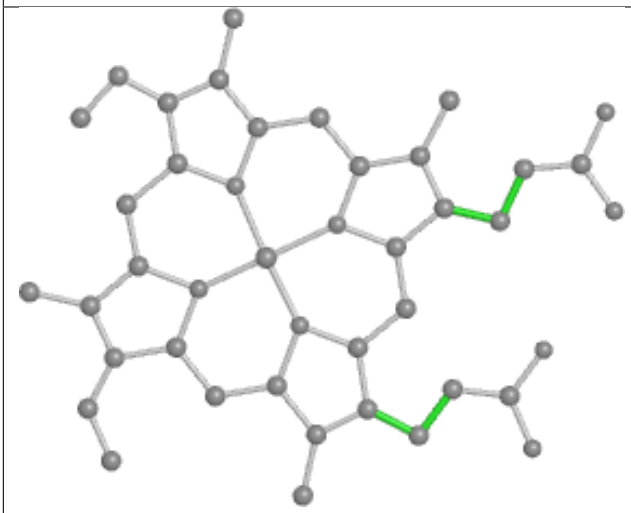
Ligand HEC C 1109



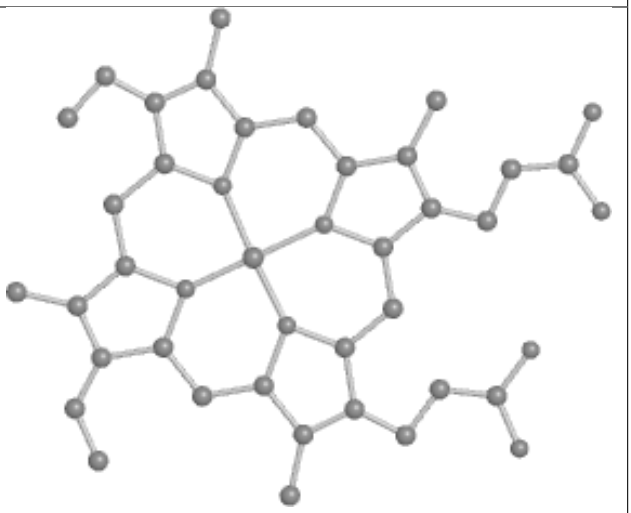
Bond lengths



Bond angles

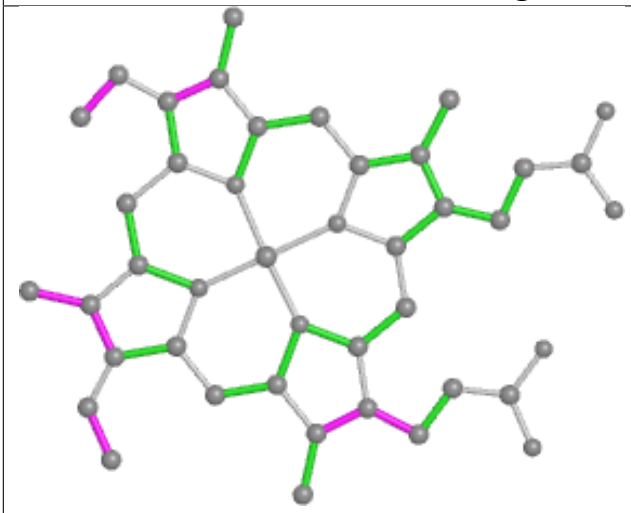


Torsions

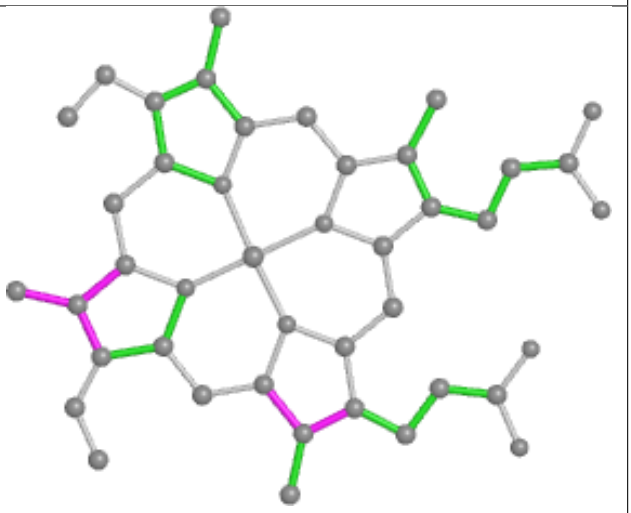


Rings

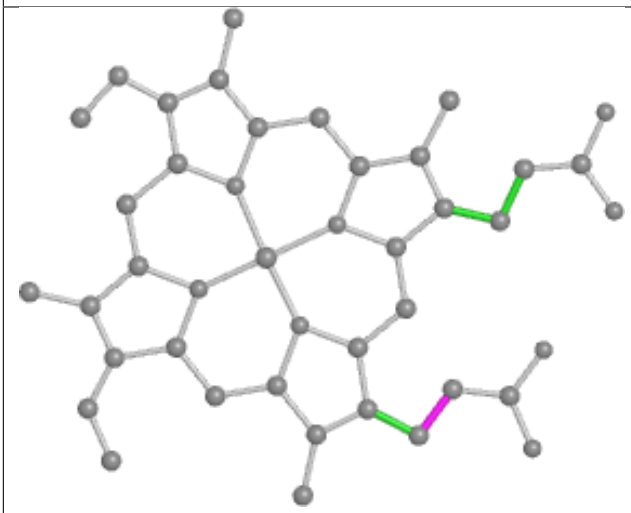
Ligand HEC D 1101



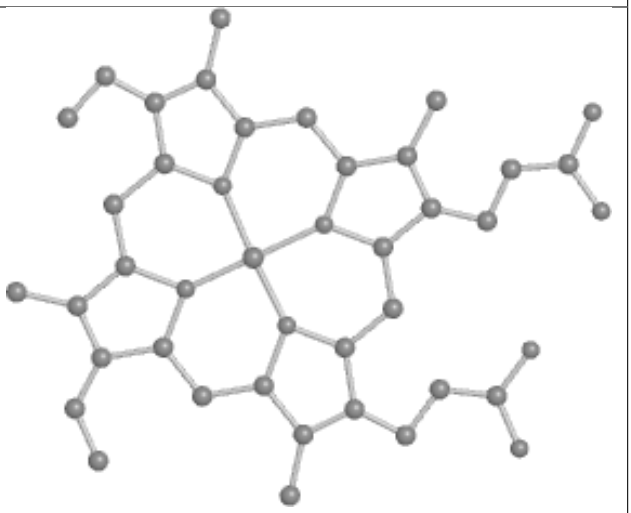
Bond lengths



Bond angles

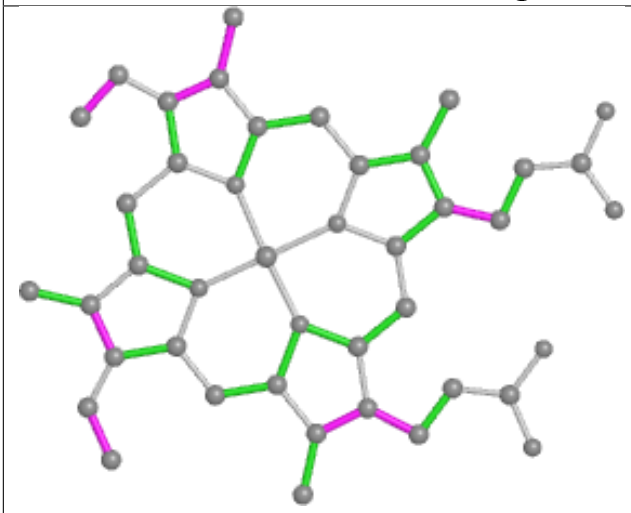


Torsions

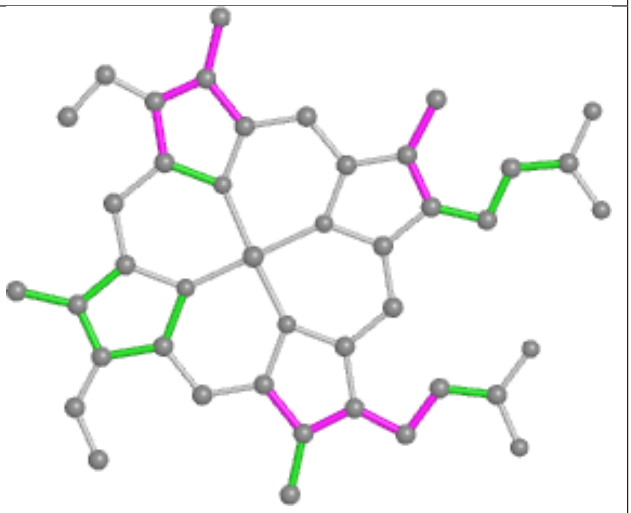


Rings

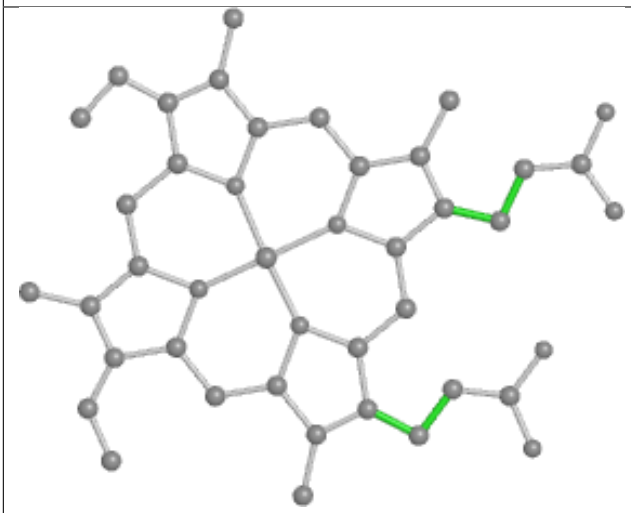
Ligand HEC D 1103



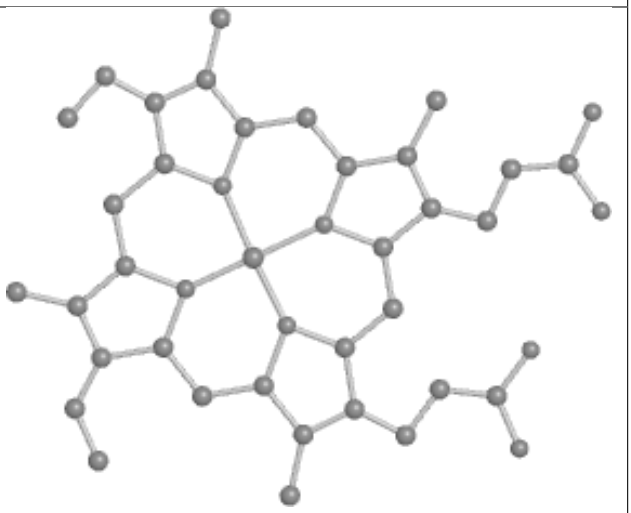
Bond lengths



Bond angles

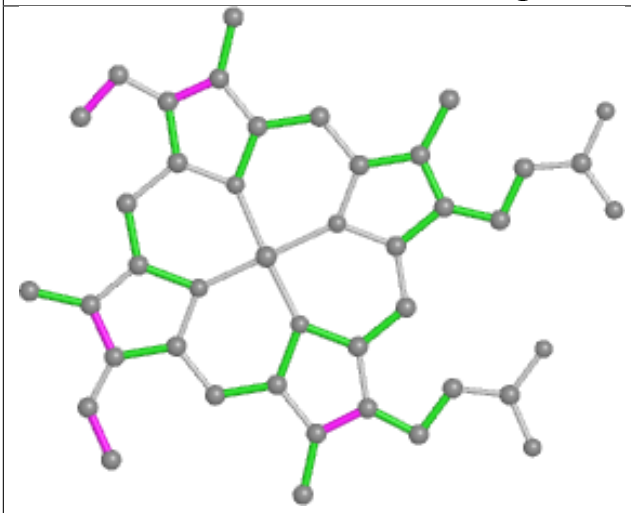


Torsions

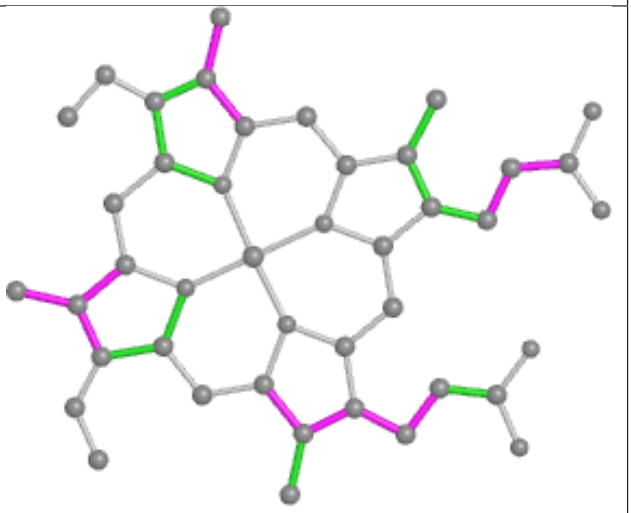


Rings

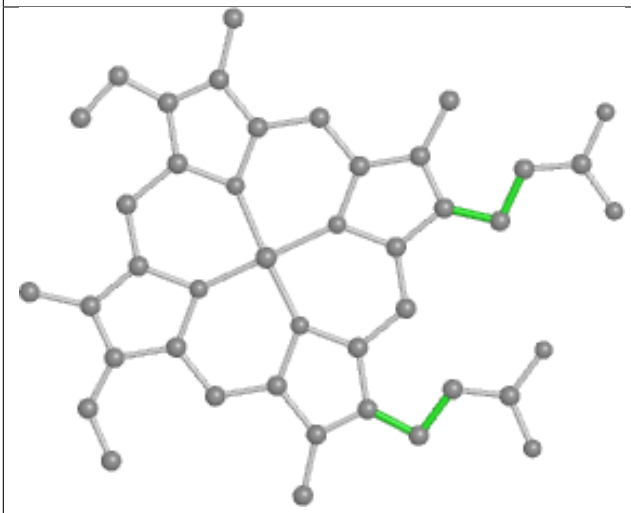
Ligand HEC C 1108



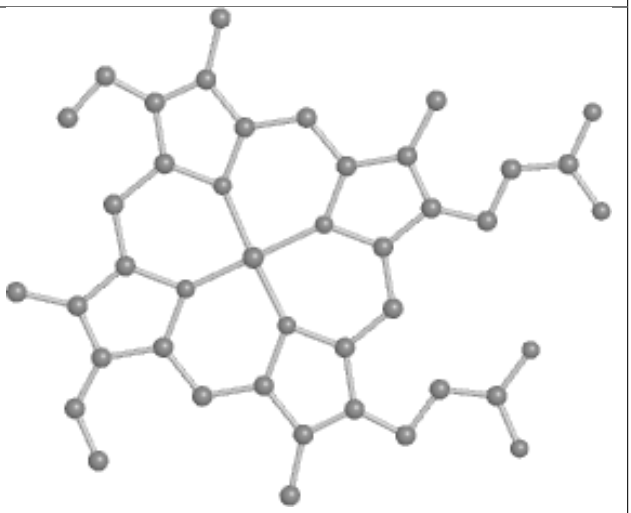
Bond lengths



Bond angles

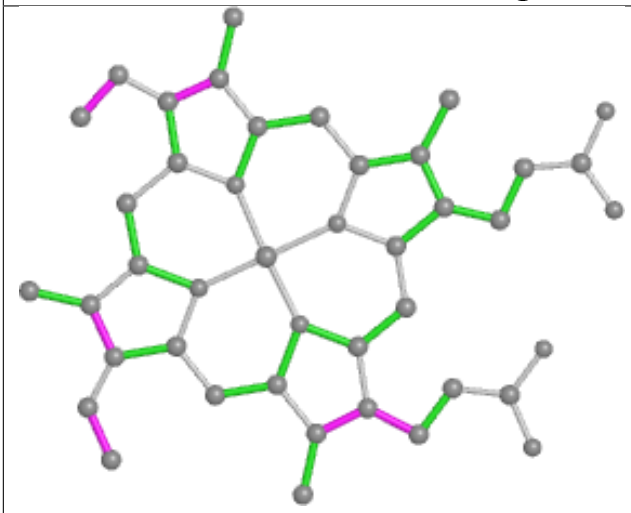


Torsions

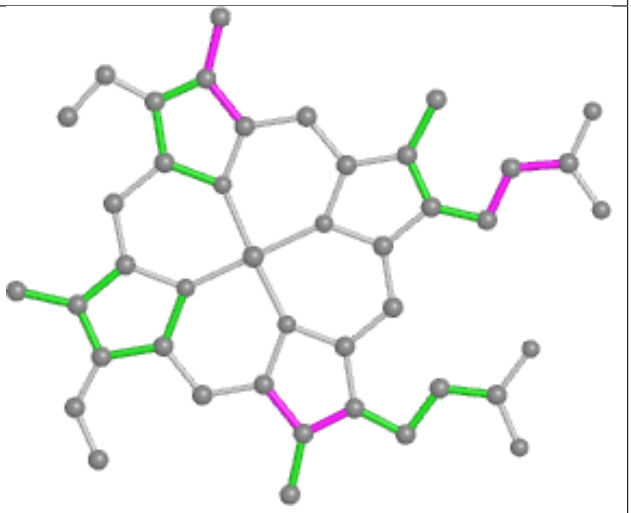


Rings

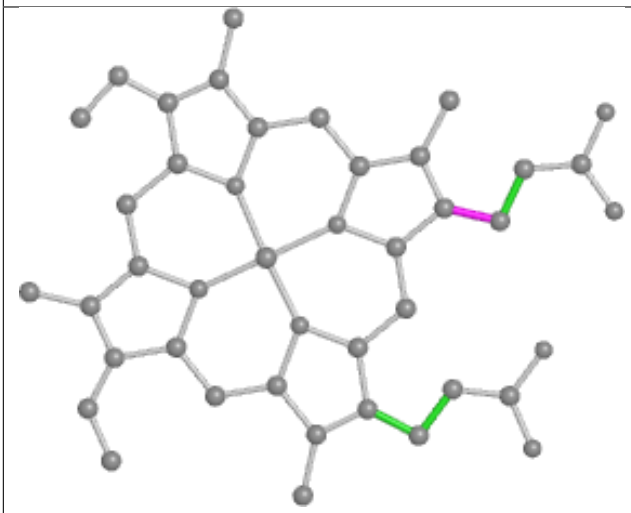
Ligand HEC C 1111



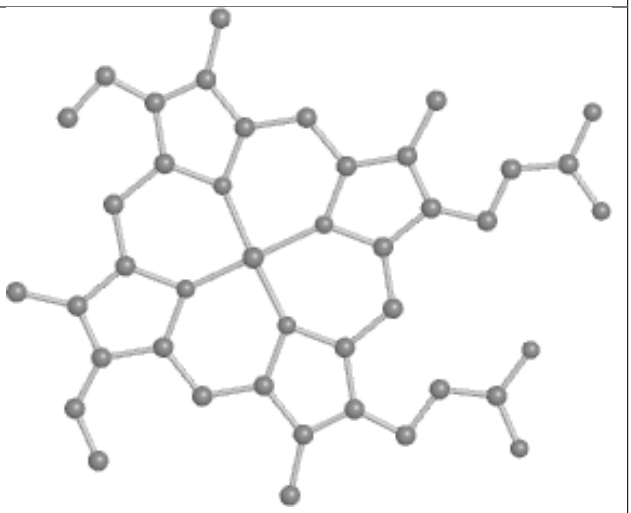
Bond lengths



Bond angles

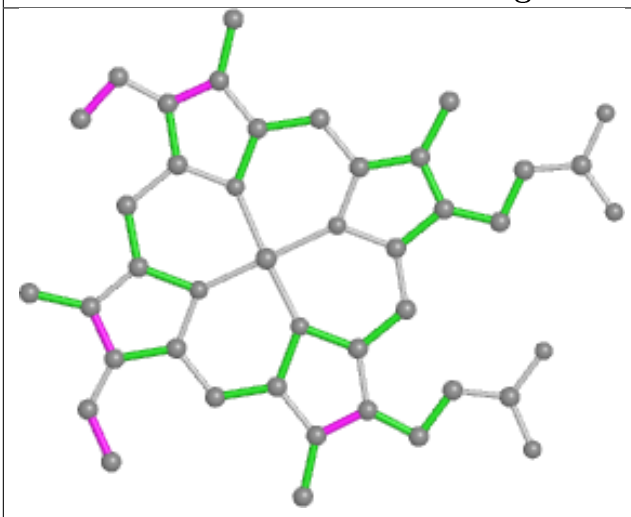


Torsions

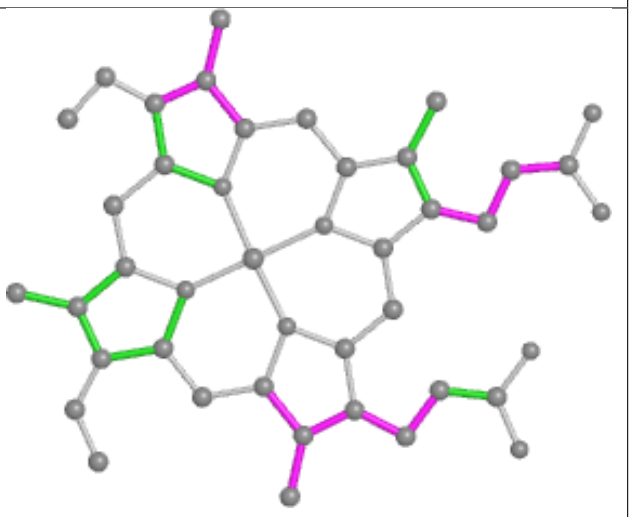


Rings

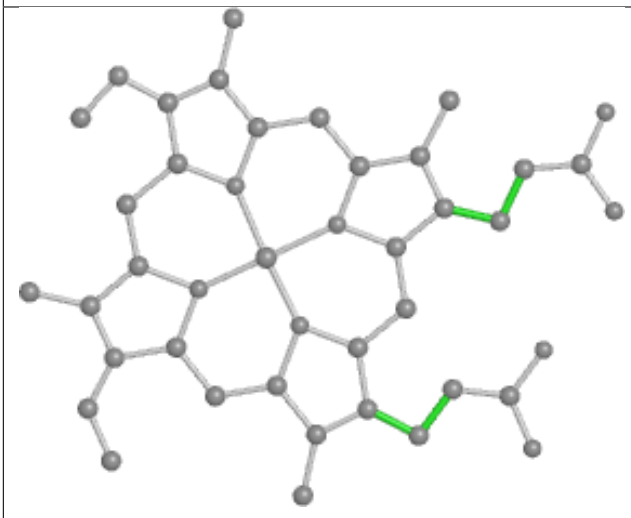
Ligand HEC C 1113



Bond lengths



Bond angles



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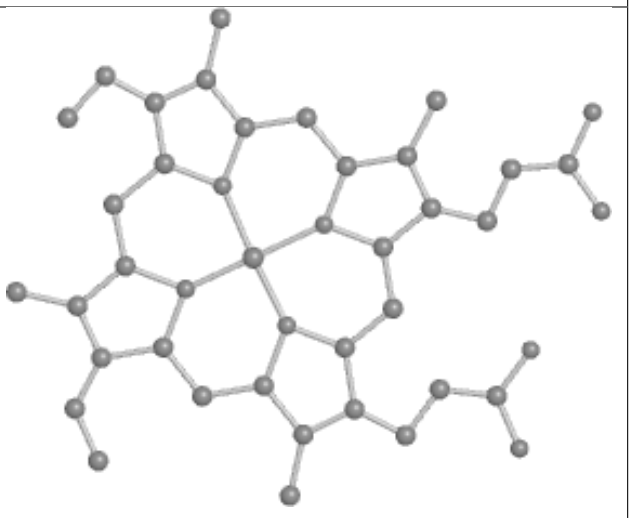

Rings

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

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.