



wwPDB X-ray Structure Validation Summary Report

Feb 4, 2024 – 11:06 AM EST

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

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the  symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtrriage (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) : 2.36

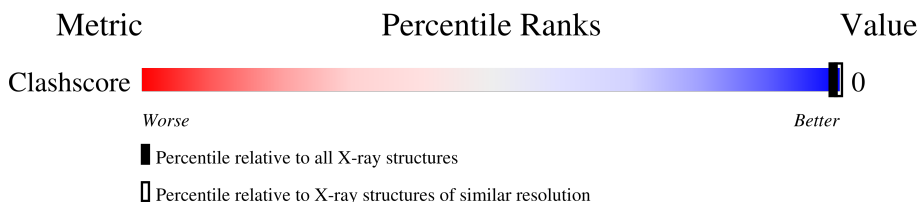
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.44 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	1116 (5.08-3.80)

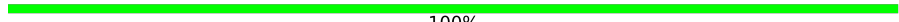









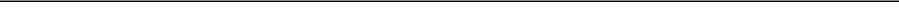

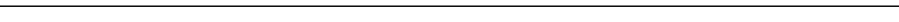


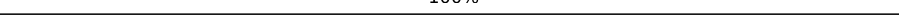
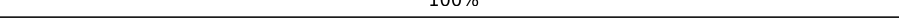
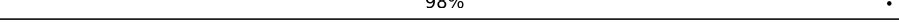
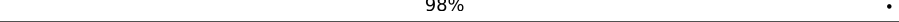
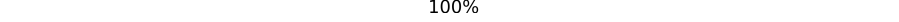
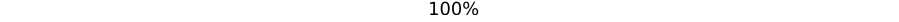
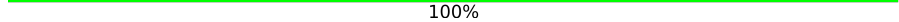
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively.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

Note EDS was not executed.

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

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

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

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

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

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

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

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

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

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

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

2 Entry composition [i](#)

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

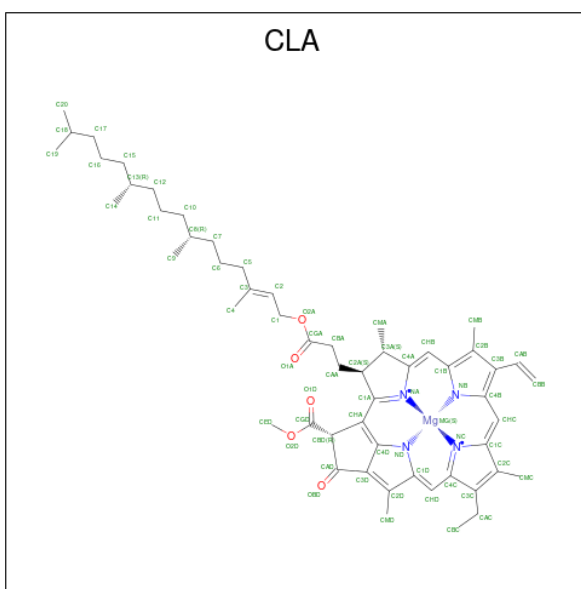
- Molecule 15 is a protein called PLANT LIGHT HARVESTING COMPLEX I(LHCI): SUB-UNIT LHCA3.

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

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

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

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



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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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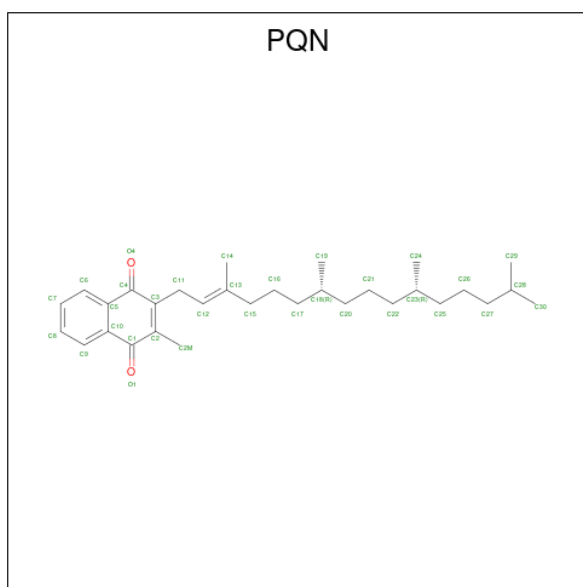
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
17	8	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	8	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	8	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	8	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	8	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	9	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	9	1	Total	C	Mg	N	0	0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

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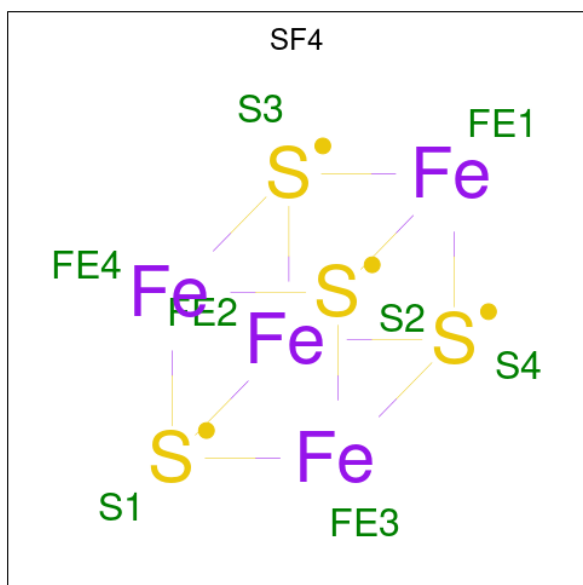
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
17	0	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	0	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	0	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	0	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	0	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	0	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	0	1	Total	C	Mg	N	0	0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

- Molecule 18 is PHYLLOQUINONE (three-letter code: PQN) (formula: C₃₁H₄₆O₂).



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

- Molecule 19 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



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

3 Residue-property plots

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

Note EDS was not executed.

- Molecule 1: PLANT PHOTOSYSTEM I: SUBUNIT PSAA

Chain A:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: PLANT PHOTOSYSTEM I: SUBUNIT PSAA

Chain P:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: PLANT PHOTOSYSTEM I: SUBUNIT PSAB

Chain B:  100%



- Molecule 2: PLANT PHOTOSYSTEM I: SUBUNIT PSAB

Chain Q:  100%



- Molecule 3: PLANT PHOTOSYSTEM I: SUBUNIT PSAC

Chain C:  100%

There are no outlier residues recorded for this chain.

- Molecule 3: PLANT PHOTOSYSTEM I: SUBUNIT PSAC

Chain R:  100%

There are no outlier residues recorded for this chain.

- Molecule 4: PLANT PHOTOSYSTEM I: SUBUNIT PSAD

Chain D:  100%

There are no outlier residues recorded for this chain.

- Molecule 4: PLANT PHOTOSYSTEM I: SUBUNIT PSAD

Chain S:  100%

There are no outlier residues recorded for this chain.

- Molecule 5: PLANT PHOTOSYSTEM I: SUBUNIT PSAE

Chain E:  100%

There are no outlier residues recorded for this chain.

- Molecule 5: PLANT PHOTOSYSTEM I: SUBUNIT PSAE

Chain T:  100%

There are no outlier residues recorded for this chain.

- Molecule 6: PLANT PHOTOSYSTEM I: SUBUNIT PSAF

Chain F:  100%

There are no outlier residues recorded for this chain.

- Molecule 6: PLANT PHOTOSYSTEM I: SUBUNIT PSAF

Chain U:  100%

There are no outlier residues recorded for this chain.

- Molecule 7: PLANT PHOTOSYSTEM I: SUBUNIT PSAG

Chain G:  100%

There are no outlier residues recorded for this chain.

- Molecule 7: PLANT PHOTOSYSTEM I: SUBUNIT PSAG

Chain V:  100%

There are no outlier residues recorded for this chain.

- Molecule 8: PLANT PHOTOSYSTEM I: SUBUNIT PSAH

Chain H:  100%

There are no outlier residues recorded for this chain.

- Molecule 8: PLANT PHOTOSYSTEM I: SUBUNIT PSAH

Chain W:  100%

There are no outlier residues recorded for this chain.

- Molecule 9: PLANT PHOTOSYSTEM I: SUBUNIT PSAI

Chain I:  100%

There are no outlier residues recorded for this chain.

- Molecule 9: PLANT PHOTOSYSTEM I: SUBUNIT PSAI

Chain Y:  100%

There are no outlier residues recorded for this chain.

- Molecule 10: PLANT PHOTOSYSTEM I: SUBUNIT PSAJ

Chain J:  100%

There are no outlier residues recorded for this chain.

- Molecule 10: PLANT PHOTOSYSTEM I: SUBUNIT PSAJ

Chain Z:  100%

There are no outlier residues recorded for this chain.

- Molecule 11: PLANT PHOTOSYSTEM I: SUBUNIT PSAK

Chain K:  100%

There are no outlier residues recorded for this chain.

- Molecule 11: PLANT PHOTOSYSTEM I: SUBUNIT PSAK

Chain 5:  100%

There are no outlier residues recorded for this chain.

- Molecule 12: PLANT PHOTOSYSTEM I: SUBUNIT PSAL

Chain L:  100%

There are no outlier residues recorded for this chain.

- Molecule 12: PLANT PHOTOSYSTEM I: SUBUNIT PSAL

Chain 6:  100%

There are no outlier residues recorded for this chain.

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

Chain 1:  100%

There are no outlier residues recorded for this chain.

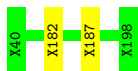
- Molecule 13: PLANT LIGHT HARVESTING COMPLEX I(LHCI): SUBUNIT LHCA1

Chain 7:  100%

There are no outlier residues recorded for this chain.

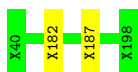
- Molecule 14: PLANT LIGHT HARVESTING COMPLEX I(LHCI): SUBUNIT LHCA2

Chain 2:  98%



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

Chain 8:  98%



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

Chain 3:  100%

There are no outlier residues recorded for this chain.

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

Chain 9:  100%

There are no outlier residues recorded for this chain.

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

Chain 4:  100%

There are no outlier residues recorded for this chain.

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

Chain 0:  100%

There are no outlier residues recorded for this chain.

4 Data and refinement statistics

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

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

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

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

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

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

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

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

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

5.3.2 Protein sidechains [i](#)

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

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

344 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	CLA	A	1139	-	27,32,73	2.92	8 (29%)	30,54,113	3.14	6 (20%)
17	CLA	P	5137	-	27,32,73	3.06	10 (37%)	30,54,113	4.13	11 (36%)
17	CLA	B	1021	-	27,32,73	2.94	9 (33%)	30,54,113	3.28	5 (16%)
17	CLA	A	1107	-	27,32,73	2.68	9 (33%)	30,54,113	3.28	7 (23%)
17	CLA	P	5134	-	27,32,73	2.89	9 (33%)	30,54,113	3.31	8 (26%)
17	CLA	0	1014	-	27,32,73	2.71	8 (29%)	30,54,113	3.32	8 (26%)
17	CLA	P	5132	-	27,32,73	2.38	9 (33%)	30,54,113	3.19	6 (20%)
17	CLA	Q	5230	-	27,32,73	2.90	9 (33%)	30,54,113	3.20	7 (23%)
17	CLA	A	1120	-	27,32,73	2.72	8 (29%)	30,54,113	3.29	8 (26%)
17	CLA	A	1136	-	27,32,73	2.67	9 (33%)	30,54,113	3.03	7 (23%)
17	CLA	B	1218	-	27,32,73	2.88	9 (33%)	30,54,113	3.37	9 (30%)
17	CLA	8	1013	-	27,32,73	2.70	8 (29%)	30,54,113	3.32	8 (26%)
17	CLA	2	1014	-	27,32,73	2.69	7 (25%)	30,54,113	3.32	8 (26%)
17	CLA	7	1025	-	27,32,73	2.71	7 (25%)	30,54,113	3.32	8 (26%)
17	CLA	9	1016	-	27,32,73	2.69	7 (25%)	30,54,113	3.31	8 (26%)
17	CLA	P	5109	-	27,32,73	2.64	8 (29%)	30,54,113	3.12	7 (23%)
17	CLA	4	1012	-	27,32,73	2.74	7 (25%)	30,54,113	3.34	8 (26%)
17	CLA	A	1108	-	27,32,73	2.81	7 (25%)	30,54,113	4.01	11 (36%)
17	CLA	Q	5211	-	27,32,73	2.65	9 (33%)	30,54,113	3.25	8 (26%)
17	CLA	J	4008	-	27,32,73	2.71	7 (25%)	30,54,113	3.33	8 (26%)
17	CLA	B	1214	-	27,32,73	2.61	9 (33%)	30,54,113	3.26	7 (23%)
17	CLA	2	1025	-	27,32,73	2.72	7 (25%)	30,54,113	3.31	8 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	CLA	0	1023	-	27,32,73	2.68	7 (25%)	30,54,113	3.31	8 (26%)
17	CLA	9	1032	-	27,32,73	2.72	8 (29%)	30,54,113	3.34	8 (26%)
17	CLA	B	1208	-	27,32,73	2.60	9 (33%)	30,54,113	3.16	7 (23%)
17	CLA	2	1015	-	27,32,73	2.71	7 (25%)	30,54,113	3.31	8 (26%)
17	CLA	4	1032	-	27,32,73	2.69	7 (25%)	30,54,113	3.34	8 (26%)
17	CLA	8	1025	-	27,32,73	2.73	7 (25%)	30,54,113	3.30	8 (26%)
17	CLA	1	1022	-	27,32,73	2.69	8 (29%)	30,54,113	3.33	8 (26%)
17	CLA	0	1016	-	27,32,73	2.70	7 (25%)	30,54,113	3.32	8 (26%)
17	CLA	1	1025	-	27,32,73	2.71	7 (25%)	30,54,113	3.33	8 (26%)
17	CLA	P	5129	-	27,32,73	2.57	9 (33%)	30,54,113	3.36	9 (30%)
17	CLA	Q	5241	-	27,32,73	2.70	7 (25%)	30,54,113	3.33	8 (26%)
17	CLA	8	8007	-	27,32,73	2.71	8 (29%)	30,54,113	3.33	8 (26%)
17	CLA	B	4001	-	27,32,73	2.71	8 (29%)	30,54,113	3.32	8 (26%)
17	CLA	B	1242	-	27,32,73	2.70	7 (25%)	30,54,113	3.30	8 (26%)
17	CLA	3	1017	-	27,32,73	2.71	7 (25%)	30,54,113	3.32	8 (26%)
17	CLA	Q	5210	-	27,32,73	2.79	9 (33%)	30,54,113	3.26	7 (23%)
17	CLA	0	1025	-	27,32,73	2.70	8 (29%)	30,54,113	3.29	8 (26%)
17	CLA	A	1011	-	27,32,73	2.98	11 (40%)	30,54,113	3.47	5 (16%)
17	CLA	3	1025	-	27,32,73	2.70	7 (25%)	30,54,113	3.32	8 (26%)
17	CLA	Z	8008	-	27,32,73	2.71	7 (25%)	30,54,113	3.33	8 (26%)
19	SF4	R	7002	-	0,12,12	-	-	-	-	-
17	CLA	L	1503	-	27,32,73	2.79	10 (37%)	30,54,113	3.11	7 (23%)
17	CLA	Q	8001	-	27,32,73	2.71	8 (29%)	30,54,113	3.32	8 (26%)
17	CLA	P	5102	-	27,32,73	2.67	9 (33%)	30,54,113	3.28	6 (20%)
17	CLA	1	1013	-	27,32,73	2.72	7 (25%)	30,54,113	3.31	8 (26%)
17	CLA	F	4004	-	27,32,73	2.71	7 (25%)	30,54,113	3.33	8 (26%)
17	CLA	0	1026	-	27,32,73	2.71	7 (25%)	30,54,113	3.32	8 (26%)
17	CLA	3	1012	-	27,32,73	2.69	7 (25%)	30,54,113	3.33	8 (26%)
17	CLA	Q	5226	-	27,32,73	2.81	8 (29%)	30,54,113	3.02	6 (20%)
17	CLA	Q	5240	-	27,32,73	2.71	7 (25%)	30,54,113	3.31	8 (26%)
17	CLA	P	5012	-	27,32,73	2.90	8 (29%)	30,54,113	3.39	7 (23%)
17	CLA	P	5127	-	27,32,73	2.98	9 (33%)	30,54,113	3.16	6 (20%)
17	CLA	A	1103	-	27,32,73	2.65	8 (29%)	30,54,113	3.49	9 (30%)
17	CLA	P	5121	-	27,32,73	2.82	11 (40%)	30,54,113	3.10	5 (16%)
17	CLA	Q	5216	-	27,32,73	2.63	8 (29%)	30,54,113	3.09	6 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	CLA	4	1014	-	27,32,73	2.70	8 (29%)	30,54,113	3.32	8 (26%)
17	CLA	9	1017	-	27,32,73	2.71	8 (29%)	30,54,113	3.31	8 (26%)
17	CLA	1	1017	-	27,32,73	2.70	7 (25%)	30,54,113	3.33	8 (26%)
17	CLA	9	1026	-	27,32,73	2.71	7 (25%)	30,54,113	3.33	8 (26%)
17	CLA	4	1017	-	27,32,73	2.72	7 (25%)	30,54,113	3.32	8 (26%)
17	CLA	0	1013	-	27,32,73	2.71	7 (25%)	30,54,113	3.30	8 (26%)
19	SF4	A	3001	-	0,12,12	-	-	-	-	-
17	CLA	A	1110	-	27,32,73	2.79	9 (33%)	30,54,113	3.40	9 (30%)
17	CLA	V	5701	-	27,32,73	2.71	7 (25%)	30,54,113	3.33	8 (26%)
17	CLA	G	1701	-	27,32,73	2.71	7 (25%)	30,54,113	3.33	8 (26%)
17	CLA	P	5108	-	27,32,73	2.80	7 (25%)	30,54,113	4.00	11 (36%)
17	CLA	0	1021	-	27,32,73	2.69	8 (29%)	30,54,113	3.29	7 (23%)
17	CLA	0	1017	-	27,32,73	2.71	7 (25%)	30,54,113	3.32	8 (26%)
17	CLA	A	1126	-	27,32,73	2.57	7 (25%)	30,54,113	3.22	7 (23%)
17	CLA	2	1013	-	27,32,73	2.70	8 (29%)	30,54,113	3.32	8 (26%)
17	CLA	7	1016	-	27,32,73	2.71	7 (25%)	30,54,113	3.30	8 (26%)
17	CLA	6	5503	-	27,32,73	2.80	10 (37%)	30,54,113	3.11	6 (20%)
17	CLA	L	1504	-	27,32,73	2.70	7 (25%)	30,54,113	3.32	8 (26%)
17	CLA	Q	5204	-	27,32,73	2.83	10 (37%)	30,54,113	3.53	8 (26%)
17	CLA	A	1128	-	27,32,73	2.83	11 (40%)	30,54,113	3.07	8 (26%)
17	CLA	U	8004	-	27,32,73	2.71	7 (25%)	30,54,113	3.32	8 (26%)
17	CLA	3	1031	-	27,32,73	2.71	7 (25%)	30,54,113	3.32	8 (26%)
17	CLA	B	1240	-	27,32,73	2.70	7 (25%)	30,54,113	3.32	8 (26%)
17	CLA	P	5133	-	27,32,73	2.65	7 (25%)	30,54,113	3.23	8 (26%)
17	CLA	P	5112	-	27,32,73	2.79	9 (33%)	30,54,113	3.18	9 (30%)
17	CLA	U	5229	-	27,32,73	2.60	9 (33%)	30,54,113	3.30	8 (26%)
17	CLA	4	4002	-	27,32,73	2.70	7 (25%)	30,54,113	3.35	8 (26%)
17	CLA	Q	5022	-	27,32,73	2.82	10 (37%)	30,54,113	3.36	7 (23%)
17	CLA	9	1015	-	27,32,73	2.70	7 (25%)	30,54,113	3.32	8 (26%)
17	CLA	4	1015	-	27,32,73	2.73	7 (25%)	30,54,113	3.33	8 (26%)
17	CLA	Q	5220	-	27,32,73	2.82	8 (29%)	30,54,113	3.21	7 (23%)
17	CLA	1	1011	-	27,32,73	2.72	7 (25%)	30,54,113	3.34	7 (23%)
17	CLA	Q	5227	-	27,32,73	2.65	8 (29%)	30,54,113	3.35	9 (30%)
17	CLA	A	1109	-	27,32,73	2.64	8 (29%)	30,54,113	3.11	7 (23%)
17	CLA	1	1031	-	27,32,73	2.70	7 (25%)	30,54,113	3.32	8 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	CLA	8	1011	-	27,32,73	2.69	7 (25%)	30,54,113	3.32	8 (26%)
17	CLA	Q	5214	-	27,32,73	2.60	9 (33%)	30,54,113	3.27	7 (23%)
17	CLA	A	1111	-	27,32,73	2.72	9 (33%)	30,54,113	3.43	9 (30%)
17	CLA	B	1203	-	27,32,73	2.69	10 (37%)	30,54,113	3.18	7 (23%)
17	CLA	F	1301	-	27,32,73	2.97	9 (33%)	30,54,113	3.21	6 (20%)
17	CLA	P	5111	-	27,32,73	2.72	9 (33%)	30,54,113	3.44	9 (30%)
17	CLA	P	5117	-	27,32,73	2.46	9 (33%)	30,54,113	3.12	8 (26%)
17	CLA	A	1125	-	27,32,73	2.88	8 (29%)	30,54,113	3.42	7 (23%)
17	CLA	B	1227	-	27,32,73	2.64	8 (29%)	30,54,113	3.35	9 (30%)
17	CLA	0	1011	-	27,32,73	2.69	7 (25%)	30,54,113	3.33	8 (26%)
17	CLA	3	1015	-	27,32,73	2.70	7 (25%)	30,54,113	3.33	8 (26%)
17	CLA	8	1015	-	27,32,73	2.70	7 (25%)	30,54,113	3.31	8 (26%)
17	CLA	8	1021	-	27,32,73	2.71	7 (25%)	30,54,113	3.30	8 (26%)
17	CLA	Q	5207	-	27,32,73	2.96	9 (33%)	30,54,113	3.30	7 (23%)
17	CLA	4	1025	-	27,32,73	2.70	7 (25%)	30,54,113	3.30	8 (26%)
17	CLA	3	1032	-	27,32,73	2.71	8 (29%)	30,54,113	3.35	8 (26%)
17	CLA	Q	5021	-	27,32,73	2.93	9 (33%)	30,54,113	3.28	6 (20%)
17	CLA	B	1231	-	27,32,73	2.90	10 (37%)	30,54,113	3.39	8 (26%)
17	CLA	Q	5238	-	27,32,73	2.53	10 (37%)	30,54,113	3.12	7 (23%)
17	CLA	A	1133	-	27,32,73	2.66	7 (25%)	30,54,113	3.24	8 (26%)
17	CLA	B	1223	-	27,32,73	3.07	8 (29%)	30,54,113	3.37	8 (26%)
17	CLA	B	1130	-	27,32,73	2.85	8 (29%)	30,54,113	3.36	6 (20%)
17	CLA	Q	5023	-	27,32,73	2.70	12 (44%)	30,54,113	3.32	8 (26%)
17	CLA	Z	5101	-	27,32,73	2.70	7 (25%)	30,54,113	3.32	8 (26%)
17	CLA	7	1031	-	27,32,73	2.69	7 (25%)	30,54,113	3.31	8 (26%)
17	CLA	Q	5130	-	27,32,73	2.86	8 (29%)	30,54,113	3.38	6 (20%)
17	CLA	7	1013	-	27,32,73	2.72	7 (25%)	30,54,113	3.31	8 (26%)
17	CLA	B	1239	-	27,32,73	2.61	7 (25%)	30,54,113	3.20	5 (16%)
17	CLA	0	1032	-	27,32,73	2.68	7 (25%)	30,54,113	3.35	8 (26%)
17	CLA	Q	5202	-	27,32,73	2.71	9 (33%)	30,54,113	3.19	5 (16%)
17	CLA	P	5106	-	27,32,73	2.62	7 (25%)	30,54,113	3.23	7 (23%)
17	CLA	P	5139	-	27,32,73	2.92	8 (29%)	30,54,113	3.14	6 (20%)
17	CLA	K	1401	-	27,32,73	2.77	9 (33%)	30,54,113	3.17	7 (23%)
17	CLA	Q	5213	-	27,32,73	2.74	8 (29%)	30,54,113	3.12	7 (23%)
17	CLA	Q	5225	-	27,32,73	2.80	9 (33%)	30,54,113	2.88	7 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	CLA	7	1017	-	27,32,73	2.70	8 (29%)	30,54,113	3.34	8 (26%)
17	CLA	7	1026	-	27,32,73	2.70	7 (25%)	30,54,113	3.33	8 (26%)
17	CLA	F	4003	-	27,32,73	2.70	7 (25%)	30,54,113	3.33	8 (26%)
17	CLA	1	1015	-	27,32,73	2.70	8 (29%)	30,54,113	3.33	8 (26%)
17	CLA	P	8009	-	27,32,73	2.73	7 (25%)	30,54,113	3.32	8 (26%)
17	CLA	2	1022	-	27,32,73	2.71	7 (25%)	30,54,113	3.31	8 (26%)
17	CLA	Q	5205	-	27,32,73	2.51	9 (33%)	30,54,113	2.99	6 (20%)
17	CLA	P	5013	-	27,32,73	2.71	8 (29%)	30,54,113	3.04	7 (23%)
17	CLA	B	1222	-	27,32,73	2.65	9 (33%)	30,54,113	3.26	7 (23%)
17	CLA	Q	5228	-	27,32,73	2.61	8 (29%)	30,54,113	3.38	9 (30%)
17	CLA	W	5801	-	27,32,73	2.71	7 (25%)	30,54,113	3.32	8 (26%)
17	CLA	B	1204	-	27,32,73	2.82	10 (37%)	30,54,113	3.52	8 (26%)
17	CLA	A	1129	-	27,32,73	2.57	9 (33%)	30,54,113	3.37	8 (26%)
17	CLA	2	1021	-	27,32,73	2.70	7 (25%)	30,54,113	3.29	8 (26%)
17	CLA	A	1106	-	27,32,73	2.61	6 (22%)	30,54,113	3.22	8 (26%)
17	CLA	2	1033	-	27,32,73	2.72	7 (25%)	30,54,113	3.30	8 (26%)
17	CLA	P	5105	-	27,32,73	2.91	8 (29%)	30,54,113	3.10	6 (20%)
17	CLA	B	1206	-	27,32,73	2.67	9 (33%)	30,54,113	3.30	8 (26%)
17	CLA	A	1127	-	27,32,73	2.99	9 (33%)	30,54,113	3.15	6 (20%)
17	CLA	F	1229	-	27,32,73	2.58	9 (33%)	30,54,113	3.28	8 (26%)
17	CLA	B	1207	-	27,32,73	2.96	9 (33%)	30,54,113	3.29	7 (23%)
17	CLA	P	5107	-	27,32,73	2.68	9 (33%)	30,54,113	3.27	7 (23%)
17	CLA	B	1213	-	27,32,73	2.74	8 (29%)	30,54,113	3.13	7 (23%)
17	CLA	9	1022	-	27,32,73	2.70	7 (25%)	30,54,113	3.35	8 (26%)
17	CLA	4	1022	-	27,32,73	2.72	7 (25%)	30,54,113	3.33	8 (26%)
17	CLA	J	1101	-	27,32,73	2.71	7 (25%)	30,54,113	3.33	8 (26%)
17	CLA	Q	5234	-	27,32,73	2.91	8 (29%)	30,54,113	3.25	7 (23%)
17	CLA	4	1033	-	27,32,73	2.72	7 (25%)	30,54,113	3.32	8 (26%)
17	CLA	F	4005	-	27,32,73	2.70	7 (25%)	30,54,113	3.33	8 (26%)
17	CLA	U	8005	-	27,32,73	2.71	7 (25%)	30,54,113	3.34	8 (26%)
17	CLA	B	1238	-	27,32,73	2.54	9 (33%)	30,54,113	3.11	7 (23%)
17	CLA	8	1031	-	27,32,73	2.71	7 (25%)	30,54,113	3.31	8 (26%)
17	CLA	Q	5222	-	27,32,73	2.67	9 (33%)	30,54,113	3.25	7 (23%)
17	CLA	Q	5212	-	27,32,73	2.67	8 (29%)	30,54,113	3.19	7 (23%)
17	CLA	9	1031	-	27,32,73	2.71	7 (25%)	30,54,113	3.32	8 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	CLA	0	1022	-	27,32,73	2.71	7 (25%)	30,54,113	3.34	8 (26%)
17	CLA	P	5122	-	27,32,73	2.66	9 (33%)	30,54,113	3.28	8 (26%)
17	CLA	2	4007	-	27,32,73	2.71	7 (25%)	30,54,113	3.31	8 (26%)
17	CLA	P	5103	-	27,32,73	2.65	8 (29%)	30,54,113	3.50	9 (30%)
17	CLA	P	5115	-	27,32,73	2.76	9 (33%)	30,54,113	2.96	6 (20%)
17	CLA	B	1232	-	27,32,73	2.75	8 (29%)	30,54,113	3.25	9 (30%)
17	CLA	P	5402	-	27,32,73	2.96	9 (33%)	30,54,113	3.33	6 (20%)
17	CLA	5	5401	-	27,32,73	2.77	9 (33%)	30,54,113	3.17	7 (23%)
19	SF4	C	3002	-	0,12,12	-	-	-	-	-
17	CLA	3	1033	-	27,32,73	2.70	7 (25%)	30,54,113	3.33	8 (26%)
17	CLA	8	1017	-	27,32,73	2.71	7 (25%)	30,54,113	3.31	8 (26%)
17	CLA	8	1026	-	27,32,73	2.70	7 (25%)	30,54,113	3.33	8 (26%)
17	CLA	P	5135	-	27,32,73	3.12	9 (33%)	30,54,113	3.29	6 (20%)
17	CLA	0	1031	-	27,32,73	2.71	8 (29%)	30,54,113	3.34	8 (26%)
17	CLA	Q	5215	-	27,32,73	2.61	9 (33%)	30,54,113	3.27	7 (23%)
17	CLA	7	1014	-	27,32,73	2.70	7 (25%)	30,54,113	3.29	8 (26%)
17	CLA	2	1016	-	27,32,73	2.70	7 (25%)	30,54,113	3.34	8 (26%)
17	CLA	Q	5231	-	27,32,73	2.89	10 (37%)	30,54,113	3.37	8 (26%)
17	CLA	A	1122	-	27,32,73	2.66	9 (33%)	30,54,113	3.28	8 (26%)
17	CLA	B	1230	-	27,32,73	2.90	9 (33%)	30,54,113	3.20	7 (23%)
17	CLA	P	5110	-	27,32,73	2.79	9 (33%)	30,54,113	3.42	9 (30%)
17	CLA	B	1205	-	27,32,73	2.52	9 (33%)	30,54,113	2.98	6 (20%)
17	CLA	A	1132	-	27,32,73	2.39	9 (33%)	30,54,113	3.19	6 (20%)
17	CLA	Q	5242	-	27,32,73	2.68	7 (25%)	30,54,113	3.30	8 (26%)
17	CLA	Q	5236	-	27,32,73	2.62	10 (37%)	30,54,113	3.16	6 (20%)
17	CLA	P	5116	-	27,32,73	2.78	9 (33%)	30,54,113	3.31	7 (23%)
17	CLA	Q	5201	-	27,32,73	2.59	9 (33%)	30,54,113	3.28	8 (26%)
17	CLA	B	1237	-	27,32,73	2.58	10 (37%)	30,54,113	3.20	8 (26%)
17	CLA	9	1012	-	27,32,73	2.69	7 (25%)	30,54,113	3.33	8 (26%)
17	CLA	1	1012	-	27,32,73	2.70	7 (25%)	30,54,113	3.32	8 (26%)
17	CLA	A	1116	-	27,32,73	2.79	9 (33%)	30,54,113	3.32	7 (23%)
18	PQN	Q	6002	-	14,14,34	4.31	12 (85%)	20,20,45	1.02	1 (5%)
17	CLA	A	1138	-	27,32,73	2.67	8 (29%)	30,54,113	3.21	9 (30%)
17	CLA	2	1011	-	27,32,73	2.70	7 (25%)	30,54,113	3.34	8 (26%)
17	CLA	B	1226	-	27,32,73	2.80	8 (29%)	30,54,113	3.03	6 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	CLA	Q	5232	-	27,32,73	2.74	8 (29%)	30,54,113	3.24	8 (26%)
17	CLA	3	1016	-	27,32,73	2.68	7 (25%)	30,54,113	3.31	8 (26%)
17	CLA	4	1023	-	27,32,73	2.69	7 (25%)	30,54,113	3.30	8 (26%)
17	CLA	3	1014	-	27,32,73	2.69	7 (25%)	30,54,113	3.32	8 (26%)
17	CLA	P	5114	-	27,32,73	2.66	9 (33%)	30,54,113	3.26	7 (23%)
17	CLA	A	1137	-	27,32,73	3.07	10 (37%)	30,54,113	4.12	11 (36%)
17	CLA	B	1215	-	27,32,73	2.59	9 (33%)	30,54,113	3.26	7 (23%)
17	CLA	G	1233	-	27,32,73	2.95	9 (33%)	30,54,113	3.33	7 (23%)
17	CLA	Q	5209	-	27,32,73	2.98	10 (37%)	30,54,113	3.29	9 (30%)
17	CLA	9	1021	-	27,32,73	2.71	7 (25%)	30,54,113	3.32	8 (26%)
17	CLA	K	1403	-	27,32,73	2.71	7 (25%)	30,54,113	3.32	8 (26%)
17	CLA	7	1011	-	27,32,73	2.71	7 (25%)	30,54,113	3.34	7 (23%)
17	CLA	A	1114	-	27,32,73	2.65	9 (33%)	30,54,113	3.26	7 (23%)
19	SF4	C	3003	-	0,12,12	-	-	-	-	-
17	CLA	P	5113	-	27,32,73	2.99	8 (29%)	30,54,113	4.27	11 (36%)
17	CLA	B	1211	-	27,32,73	2.65	9 (33%)	30,54,113	3.25	8 (26%)
17	CLA	J	1302	-	27,32,73	3.12	9 (33%)	30,54,113	4.45	9 (30%)
17	CLA	2	1026	-	27,32,73	2.70	7 (25%)	30,54,113	3.33	8 (26%)
17	CLA	6	5501	-	27,32,73	3.02	11 (40%)	30,54,113	3.05	8 (26%)
17	CLA	2	1031	-	27,32,73	2.71	7 (25%)	30,54,113	3.31	8 (26%)
17	CLA	1	1014	-	27,32,73	2.69	7 (25%)	30,54,113	3.32	8 (26%)
17	CLA	F	4006	-	27,32,73	2.71	7 (25%)	30,54,113	3.33	8 (26%)
17	CLA	Q	5221	-	27,32,73	2.79	10 (37%)	30,54,113	3.44	7 (23%)
17	CLA	P	5131	-	27,32,73	2.62	8 (29%)	30,54,113	3.23	8 (26%)
17	CLA	U	5301	-	27,32,73	2.95	9 (33%)	30,54,113	3.21	6 (20%)
17	CLA	A	1012	-	27,32,73	2.91	8 (29%)	30,54,113	3.38	7 (23%)
17	CLA	7	1022	-	27,32,73	2.69	8 (29%)	30,54,113	3.32	8 (26%)
18	PQN	B	2002	-	14,14,34	4.31	12 (85%)	20,20,45	1.02	1 (5%)
17	CLA	L	1502	-	27,32,73	2.58	11 (40%)	30,54,113	3.19	6 (20%)
17	CLA	A	4010	-	27,32,73	2.72	7 (25%)	30,54,113	3.33	8 (26%)
17	CLA	4	1016	-	27,32,73	2.70	7 (25%)	30,54,113	3.33	8 (26%)
17	CLA	Q	5218	-	27,32,73	2.87	9 (33%)	30,54,113	3.35	9 (30%)
17	CLA	B	1209	-	27,32,73	2.99	10 (37%)	30,54,113	3.29	9 (30%)
17	CLA	B	1212	-	27,32,73	2.66	8 (29%)	30,54,113	3.18	7 (23%)
17	CLA	P	5126	-	27,32,73	2.57	7 (25%)	30,54,113	3.22	7 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	CLA	B	1225	-	27,32,73	2.78	9 (33%)	30,54,113	2.88	7 (23%)
17	CLA	A	1134	-	27,32,73	2.88	9 (33%)	30,54,113	3.32	8 (26%)
17	CLA	B	1217	-	27,32,73	2.94	9 (33%)	30,54,113	3.39	8 (26%)
17	CLA	B	1224	-	27,32,73	2.82	8 (29%)	30,54,113	3.22	8 (26%)
17	CLA	Q	5219	-	27,32,73	2.93	8 (29%)	30,54,113	4.21	9 (30%)
17	CLA	P	5136	-	27,32,73	2.67	9 (33%)	30,54,113	3.03	7 (23%)
17	CLA	0	1015	-	27,32,73	2.73	7 (25%)	30,54,113	3.33	8 (26%)
17	CLA	6	5502	-	27,32,73	2.58	11 (40%)	30,54,113	3.21	6 (20%)
17	CLA	4	1026	-	27,32,73	2.71	7 (25%)	30,54,113	3.33	8 (26%)
17	CLA	A	4009	-	27,32,73	2.72	7 (25%)	30,54,113	3.33	8 (26%)
17	CLA	B	1228	-	27,32,73	2.60	8 (29%)	30,54,113	3.37	9 (30%)
17	CLA	3	1011	-	27,32,73	2.73	7 (25%)	30,54,113	3.32	8 (26%)
18	PQN	P	6001	-	14,14,34	4.44	13 (92%)	20,20,45	0.97	1 (5%)
17	CLA	4	1013	-	27,32,73	2.70	8 (29%)	30,54,113	3.31	8 (26%)
17	CLA	3	1022	-	27,32,73	2.70	7 (25%)	30,54,113	3.35	8 (26%)
17	CLA	Z	5302	-	27,32,73	3.12	9 (33%)	30,54,113	4.45	9 (30%)
17	CLA	1	1016	-	27,32,73	2.70	7 (25%)	30,54,113	3.31	8 (26%)
17	CLA	8	1012	-	27,32,73	2.71	7 (25%)	30,54,113	3.34	8 (26%)
17	CLA	5	5403	-	27,32,73	2.72	7 (25%)	30,54,113	3.32	8 (26%)
17	CLA	A	1105	-	27,32,73	2.90	8 (29%)	30,54,113	3.11	6 (20%)
17	CLA	5	5404	-	27,32,73	2.69	7 (25%)	30,54,113	3.34	8 (26%)
17	CLA	A	1117	-	27,32,73	2.46	9 (33%)	30,54,113	3.13	8 (26%)
19	SF4	P	7001	-	0,12,12	-	-	-	-	-
17	CLA	A	1115	-	27,32,73	2.76	9 (33%)	30,54,113	2.96	6 (20%)
17	CLA	H	1801	-	27,32,73	2.71	7 (25%)	30,54,113	3.32	8 (26%)
17	CLA	A	1102	-	27,32,73	2.66	9 (33%)	30,54,113	3.29	6 (20%)
17	CLA	P	5138	-	27,32,73	2.67	8 (29%)	30,54,113	3.22	9 (30%)
17	CLA	3	1021	-	27,32,73	2.71	7 (25%)	30,54,113	3.31	8 (26%)
17	CLA	1	1021	-	27,32,73	3.12	8 (29%)	30,54,113	3.33	8 (26%)
17	CLA	4	1021	-	27,32,73	2.69	8 (29%)	30,54,113	3.30	8 (26%)
17	CLA	B	1221	-	27,32,73	2.80	10 (37%)	30,54,113	3.45	7 (23%)
19	SF4	R	7003	-	0,12,12	-	-	-	-	-
17	CLA	P	5011	-	27,32,73	2.99	10 (37%)	30,54,113	3.48	5 (16%)
17	CLA	P	5901	-	27,32,73	2.81	10 (37%)	30,54,113	4.53	10 (33%)
17	CLA	Q	5217	-	27,32,73	2.94	9 (33%)	30,54,113	3.38	9 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	CLA	L	1501	-	27,32,73	3.00	11 (40%)	30,54,113	3.04	8 (26%)
17	CLA	A	1104	-	27,32,73	2.87	11 (40%)	30,54,113	3.32	7 (23%)
17	CLA	8	1033	-	27,32,73	2.72	7 (25%)	30,54,113	3.31	8 (26%)
17	CLA	P	8010	-	27,32,73	2.72	7 (25%)	30,54,113	3.33	8 (26%)
17	CLA	B	1216	-	27,32,73	2.63	8 (29%)	30,54,113	3.09	6 (20%)
17	CLA	7	1015	-	27,32,73	2.71	8 (29%)	30,54,113	3.33	8 (26%)
17	CLA	P	5118	-	27,32,73	2.85	8 (29%)	30,54,113	3.52	9 (30%)
17	CLA	A	1123	-	27,32,73	2.88	8 (29%)	30,54,113	3.40	8 (26%)
17	CLA	9	1011	-	27,32,73	2.74	7 (25%)	30,54,113	3.34	8 (26%)
17	CLA	4	1011	-	27,32,73	2.70	7 (25%)	30,54,113	3.34	8 (26%)
17	CLA	8	1014	-	27,32,73	2.70	8 (29%)	30,54,113	3.33	8 (26%)
17	CLA	7	1012	-	27,32,73	2.71	7 (25%)	30,54,113	3.31	8 (26%)
17	CLA	Q	5239	-	27,32,73	2.60	7 (25%)	30,54,113	3.20	5 (16%)
17	CLA	9	1025	-	27,32,73	2.71	7 (25%)	30,54,113	3.32	7 (23%)
17	CLA	B	1202	-	27,32,73	2.71	9 (33%)	30,54,113	3.19	5 (16%)
17	CLA	B	1220	-	27,32,73	2.82	8 (29%)	30,54,113	3.20	7 (23%)
17	CLA	Q	5224	-	27,32,73	2.83	8 (29%)	30,54,113	3.21	8 (26%)
17	CLA	U	8003	-	27,32,73	2.71	7 (25%)	30,54,113	3.32	8 (26%)
17	CLA	P	5125	-	27,32,73	2.89	8 (29%)	30,54,113	3.42	7 (23%)
17	CLA	8	1022	-	27,32,73	2.71	7 (25%)	30,54,113	3.31	8 (26%)
17	CLA	P	5119	-	27,32,73	2.55	9 (33%)	30,54,113	3.20	7 (23%)
17	CLA	9	1033	-	27,32,73	2.69	7 (25%)	30,54,113	3.33	8 (26%)
17	CLA	A	1112	-	27,32,73	2.77	9 (33%)	30,54,113	3.19	9 (30%)
17	CLA	A	1119	-	27,32,73	2.55	9 (33%)	30,54,113	3.21	7 (23%)
17	CLA	P	5140	-	27,32,73	2.66	8 (29%)	30,54,113	3.26	7 (23%)
17	CLA	7	1023	-	27,32,73	2.70	7 (25%)	30,54,113	3.31	8 (26%)
17	CLA	2	1023	-	27,32,73	2.71	7 (25%)	30,54,113	3.31	8 (26%)
17	CLA	Q	5208	-	27,32,73	2.60	9 (33%)	30,54,113	3.15	7 (23%)
17	CLA	A	1131	-	27,32,73	2.63	7 (25%)	30,54,113	3.24	8 (26%)
17	CLA	B	1241	-	27,32,73	2.71	7 (25%)	30,54,113	3.31	8 (26%)
17	CLA	Q	5237	-	27,32,73	2.57	10 (37%)	30,54,113	3.21	8 (26%)
17	CLA	8	1023	-	27,32,73	2.71	7 (25%)	30,54,113	3.32	8 (26%)
17	CLA	A	1118	-	27,32,73	2.85	8 (29%)	30,54,113	3.51	8 (26%)
17	CLA	B	1023	-	27,32,73	2.70	12 (44%)	30,54,113	3.31	8 (26%)
17	CLA	2	1017	-	27,32,73	2.70	7 (25%)	30,54,113	3.31	8 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	CLA	8	1016	-	27,32,73	2.69	7 (25%)	30,54,113	3.33	8 (26%)
17	CLA	4	1031	-	27,32,73	2.70	8 (29%)	30,54,113	3.34	8 (26%)
17	CLA	B	1219	-	27,32,73	2.92	7 (25%)	30,54,113	4.22	10 (33%)
17	CLA	Q	5235	-	27,32,73	2.75	9 (33%)	30,54,113	3.22	9 (30%)
17	CLA	3	1041	-	27,32,73	2.71	7 (25%)	30,54,113	3.33	8 (26%)
17	CLA	A	1113	-	27,32,73	2.97	8 (29%)	30,54,113	4.27	11 (36%)
17	CLA	0	8002	-	27,32,73	2.70	8 (29%)	30,54,113	3.37	8 (26%)
17	CLA	2	1012	-	27,32,73	2.71	7 (25%)	30,54,113	3.33	8 (26%)
17	CLA	Q	5223	-	27,32,73	3.08	8 (29%)	30,54,113	3.37	8 (26%)
18	PQN	A	2001	-	14,14,34	4.45	13 (92%)	20,20,45	0.97	1 (5%)
17	CLA	1	1026	-	27,32,73	2.70	7 (25%)	30,54,113	3.32	8 (26%)
17	CLA	P	5120	-	27,32,73	2.72	8 (29%)	30,54,113	3.30	8 (26%)
17	CLA	K	1404	-	27,32,73	2.71	7 (25%)	30,54,113	3.33	8 (26%)
17	CLA	A	1124	-	27,32,73	2.51	7 (25%)	30,54,113	3.10	6 (20%)
17	CLA	P	5128	-	27,32,73	2.81	11 (40%)	30,54,113	3.08	8 (26%)
17	CLA	B	1234	-	27,32,73	2.92	8 (29%)	30,54,113	3.25	7 (23%)
17	CLA	A	1901	-	27,32,73	2.81	10 (37%)	30,54,113	4.55	10 (33%)
17	CLA	P	5123	-	27,32,73	2.87	8 (29%)	30,54,113	3.41	8 (26%)
17	CLA	B	1236	-	27,32,73	2.63	10 (37%)	30,54,113	3.15	6 (20%)
17	CLA	A	1140	-	27,32,73	2.64	8 (29%)	30,54,113	3.27	7 (23%)
17	CLA	A	1121	-	27,32,73	2.82	11 (40%)	30,54,113	3.09	5 (16%)
17	CLA	A	1402	-	27,32,73	2.96	9 (33%)	30,54,113	3.34	6 (20%)
17	CLA	Q	5203	-	27,32,73	2.70	10 (37%)	30,54,113	3.19	7 (23%)
17	CLA	0	1012	-	27,32,73	2.73	7 (25%)	30,54,113	3.33	8 (26%)
17	CLA	A	1013	-	27,32,73	2.71	8 (29%)	30,54,113	3.05	7 (23%)
17	CLA	U	8006	-	27,32,73	2.70	7 (25%)	30,54,113	3.33	8 (26%)
17	CLA	6	5504	-	27,32,73	2.70	7 (25%)	30,54,113	3.32	8 (26%)
17	CLA	B	1201	-	27,32,73	2.60	9 (33%)	30,54,113	3.27	8 (26%)
17	CLA	A	1135	-	27,32,73	3.11	9 (33%)	30,54,113	3.30	6 (20%)
17	CLA	P	5124	-	27,32,73	2.51	7 (25%)	30,54,113	3.11	6 (20%)
17	CLA	B	1235	-	27,32,73	2.76	9 (33%)	30,54,113	3.22	9 (30%)
17	CLA	3	1026	-	27,32,73	2.70	8 (29%)	30,54,113	3.33	8 (26%)
17	CLA	B	1210	-	27,32,73	2.79	9 (33%)	30,54,113	3.27	7 (23%)
17	CLA	1	1023	-	27,32,73	2.71	7 (25%)	30,54,113	3.31	8 (26%)
17	CLA	9	1041	-	27,32,73	2.72	7 (25%)	30,54,113	3.31	8 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	CLA	9	1014	-	27,32,73	2.68	7 (25%)	30,54,113	3.32	8 (26%)
17	CLA	0	1033	-	27,32,73	2.72	7 (25%)	30,54,113	3.32	8 (26%)
17	CLA	V	5233	-	27,32,73	2.95	9 (33%)	30,54,113	3.32	8 (26%)
17	CLA	B	1022	-	27,32,73	2.82	10 (37%)	30,54,113	3.37	7 (23%)
17	CLA	7	1021	-	27,32,73	3.12	8 (29%)	30,54,113	3.32	8 (26%)
17	CLA	P	5104	-	27,32,73	2.87	11 (40%)	30,54,113	3.31	7 (23%)
17	CLA	Q	5206	-	27,32,73	2.68	9 (33%)	30,54,113	3.30	8 (26%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	A	1139	-	1/1/4/20	-	-
17	CLA	P	5137	-	1/1/4/20	-	-
17	CLA	B	1021	-	1/1/4/20	-	-
17	CLA	A	1107	-	1/1/4/20	-	-
17	CLA	P	5134	-	1/1/4/20	-	-
17	CLA	0	1014	-	1/1/4/20	-	-
17	CLA	P	5132	-	1/1/4/20	-	-
17	CLA	Q	5230	-	1/1/4/20	-	-
17	CLA	A	1120	-	1/1/4/20	-	-
17	CLA	A	1136	-	1/1/4/20	-	-
17	CLA	B	1218	-	1/1/4/20	-	-
17	CLA	8	1013	-	1/1/4/20	-	-
17	CLA	2	1014	-	1/1/4/20	-	-
17	CLA	7	1025	-	1/1/4/20	-	-
17	CLA	9	1016	-	1/1/4/20	-	-
17	CLA	P	5109	-	1/1/4/20	-	-
17	CLA	4	1012	-	1/1/4/20	-	-
17	CLA	A	1108	-	1/1/4/20	-	-
17	CLA	Q	5211	-	1/1/4/20	-	-
17	CLA	J	4008	-	1/1/4/20	-	-
17	CLA	B	1214	-	1/1/4/20	-	-
17	CLA	2	1025	-	1/1/4/20	-	-
17	CLA	0	1023	-	1/1/4/20	-	-
17	CLA	9	1032	-	1/1/4/20	-	-
17	CLA	B	1208	-	1/1/4/20	-	-
17	CLA	2	1015	-	1/1/4/20	-	-
17	CLA	4	1032	-	1/1/4/20	-	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	8	1025	-	1/1/4/20	-	-
17	CLA	1	1022	-	1/1/4/20	-	-
17	CLA	0	1016	-	1/1/4/20	-	-
17	CLA	1	1025	-	1/1/4/20	-	-
17	CLA	P	5129	-	1/1/4/20	-	-
17	CLA	Q	5241	-	1/1/4/20	-	-
17	CLA	8	8007	-	1/1/4/20	-	-
17	CLA	B	4001	-	1/1/4/20	-	-
17	CLA	B	1242	-	1/1/4/20	-	-
17	CLA	3	1017	-	1/1/4/20	-	-
17	CLA	Q	5210	-	1/1/4/20	-	-
17	CLA	0	1025	-	1/1/4/20	-	-
17	CLA	A	1011	-	1/1/4/20	-	-
17	CLA	3	1025	-	1/1/4/20	-	-
17	CLA	Z	8008	-	1/1/4/20	-	-
19	SF4	R	7002	-	-	-	0/6/5/5
17	CLA	L	1503	-	1/1/4/20	-	-
17	CLA	Q	8001	-	1/1/4/20	-	-
17	CLA	P	5102	-	1/1/4/20	-	-
17	CLA	1	1013	-	1/1/4/20	-	-
17	CLA	F	4004	-	1/1/4/20	-	-
17	CLA	0	1026	-	1/1/4/20	-	-
17	CLA	3	1012	-	1/1/4/20	-	-
17	CLA	Q	5226	-	1/1/4/20	-	-
17	CLA	Q	5240	-	1/1/4/20	-	-
17	CLA	P	5012	-	1/1/4/20	-	-
17	CLA	P	5127	-	1/1/4/20	-	-
17	CLA	A	1103	-	1/1/4/20	-	-
17	CLA	P	5121	-	1/1/4/20	-	-
17	CLA	Q	5216	-	1/1/4/20	-	-
17	CLA	4	1014	-	1/1/4/20	-	-
17	CLA	9	1017	-	1/1/4/20	-	-
17	CLA	1	1017	-	1/1/4/20	-	-
17	CLA	9	1026	-	1/1/4/20	-	-
17	CLA	4	1017	-	1/1/4/20	-	-
17	CLA	0	1013	-	1/1/4/20	-	-
19	SF4	A	3001	-	-	-	0/6/5/5
17	CLA	A	1110	-	1/1/4/20	-	-
17	CLA	V	5701	-	1/1/4/20	-	-
17	CLA	G	1701	-	1/1/4/20	-	-
17	CLA	P	5108	-	1/1/4/20	-	-
17	CLA	0	1021	-	1/1/4/20	-	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	0	1017	-	1/1/4/20	-	-
17	CLA	A	1126	-	1/1/4/20	-	-
17	CLA	2	1013	-	1/1/4/20	-	-
17	CLA	7	1016	-	1/1/4/20	-	-
17	CLA	6	5503	-	1/1/4/20	-	-
17	CLA	L	1504	-	1/1/4/20	-	-
17	CLA	Q	5204	-	1/1/4/20	-	-
17	CLA	A	1128	-	1/1/4/20	-	-
17	CLA	U	8004	-	1/1/4/20	-	-
17	CLA	3	1031	-	1/1/4/20	-	-
17	CLA	B	1240	-	1/1/4/20	-	-
17	CLA	P	5133	-	1/1/4/20	-	-
17	CLA	P	5112	-	1/1/4/20	-	-
17	CLA	U	5229	-	1/1/4/20	-	-
17	CLA	4	4002	-	1/1/4/20	-	-
17	CLA	Q	5022	-	1/1/4/20	-	-
17	CLA	9	1015	-	1/1/4/20	-	-
17	CLA	4	1015	-	1/1/4/20	-	-
17	CLA	Q	5220	-	1/1/4/20	-	-
17	CLA	1	1011	-	1/1/4/20	-	-
17	CLA	Q	5227	-	1/1/4/20	-	-
17	CLA	A	1109	-	1/1/4/20	-	-
17	CLA	1	1031	-	1/1/4/20	-	-
17	CLA	8	1011	-	1/1/4/20	-	-
17	CLA	Q	5214	-	1/1/4/20	-	-
17	CLA	A	1111	-	1/1/4/20	-	-
17	CLA	B	1203	-	1/1/4/20	-	-
17	CLA	F	1301	-	1/1/4/20	-	-
17	CLA	P	5111	-	1/1/4/20	-	-
17	CLA	P	5117	-	1/1/4/20	-	-
17	CLA	A	1125	-	1/1/4/20	-	-
17	CLA	B	1227	-	1/1/4/20	-	-
17	CLA	0	1011	-	1/1/4/20	-	-
17	CLA	3	1015	-	1/1/4/20	-	-
17	CLA	8	1015	-	1/1/4/20	-	-
17	CLA	8	1021	-	1/1/4/20	-	-
17	CLA	Q	5207	-	1/1/4/20	-	-
17	CLA	4	1025	-	1/1/4/20	-	-
17	CLA	3	1032	-	1/1/4/20	-	-
17	CLA	Q	5021	-	1/1/4/20	-	-
17	CLA	B	1231	-	1/1/4/20	-	-
17	CLA	Q	5238	-	1/1/4/20	-	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	A	1133	-	1/1/4/20	-	-
17	CLA	B	1223	-	1/1/4/20	-	-
17	CLA	B	1130	-	1/1/4/20	-	-
17	CLA	Q	5023	-	1/1/4/20	-	-
17	CLA	Z	5101	-	1/1/4/20	-	-
17	CLA	7	1031	-	1/1/4/20	-	-
17	CLA	Q	5130	-	1/1/4/20	-	-
17	CLA	7	1013	-	1/1/4/20	-	-
17	CLA	B	1239	-	1/1/4/20	-	-
17	CLA	0	1032	-	1/1/4/20	-	-
17	CLA	Q	5202	-	1/1/4/20	-	-
17	CLA	P	5106	-	1/1/4/20	-	-
17	CLA	P	5139	-	1/1/4/20	-	-
17	CLA	K	1401	-	1/1/4/20	-	-
17	CLA	Q	5213	-	1/1/4/20	-	-
17	CLA	Q	5225	-	1/1/4/20	-	-
17	CLA	7	1017	-	1/1/4/20	-	-
17	CLA	7	1026	-	1/1/4/20	-	-
17	CLA	F	4003	-	1/1/4/20	-	-
17	CLA	1	1015	-	1/1/4/20	-	-
17	CLA	P	8009	-	1/1/4/20	-	-
17	CLA	2	1022	-	1/1/4/20	-	-
17	CLA	Q	5205	-	1/1/4/20	-	-
17	CLA	P	5013	-	1/1/4/20	-	-
17	CLA	B	1222	-	1/1/4/20	-	-
17	CLA	Q	5228	-	1/1/4/20	-	-
17	CLA	W	5801	-	1/1/4/20	-	-
17	CLA	B	1204	-	1/1/4/20	-	-
17	CLA	A	1129	-	1/1/4/20	-	-
17	CLA	2	1021	-	1/1/4/20	-	-
17	CLA	A	1106	-	1/1/4/20	-	-
17	CLA	2	1033	-	1/1/4/20	-	-
17	CLA	P	5105	-	1/1/4/20	-	-
17	CLA	B	1206	-	1/1/4/20	-	-
17	CLA	A	1127	-	1/1/4/20	-	-
17	CLA	F	1229	-	1/1/4/20	-	-
17	CLA	B	1207	-	1/1/4/20	-	-
17	CLA	P	5107	-	1/1/4/20	-	-
17	CLA	B	1213	-	1/1/4/20	-	-
17	CLA	9	1022	-	1/1/4/20	-	-
17	CLA	4	1022	-	1/1/4/20	-	-
17	CLA	J	1101	-	1/1/4/20	-	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	Q	5234	-	1/1/4/20	-	-
17	CLA	4	1033	-	1/1/4/20	-	-
17	CLA	F	4005	-	1/1/4/20	-	-
17	CLA	U	8005	-	1/1/4/20	-	-
17	CLA	B	1238	-	1/1/4/20	-	-
17	CLA	8	1031	-	1/1/4/20	-	-
17	CLA	Q	5222	-	1/1/4/20	-	-
17	CLA	Q	5212	-	1/1/4/20	-	-
17	CLA	9	1031	-	1/1/4/20	-	-
17	CLA	0	1022	-	1/1/4/20	-	-
17	CLA	P	5122	-	1/1/4/20	-	-
17	CLA	2	4007	-	1/1/4/20	-	-
17	CLA	P	5103	-	1/1/4/20	-	-
17	CLA	P	5115	-	1/1/4/20	-	-
17	CLA	B	1232	-	1/1/4/20	-	-
17	CLA	P	5402	-	1/1/4/20	-	-
17	CLA	5	5401	-	1/1/4/20	-	-
19	SF4	C	3002	-	-	-	0/6/5/5
17	CLA	3	1033	-	1/1/4/20	-	-
17	CLA	8	1017	-	1/1/4/20	-	-
17	CLA	8	1026	-	1/1/4/20	-	-
17	CLA	P	5135	-	1/1/4/20	-	-
17	CLA	0	1031	-	1/1/4/20	-	-
17	CLA	Q	5215	-	1/1/4/20	-	-
17	CLA	7	1014	-	1/1/4/20	-	-
17	CLA	2	1016	-	1/1/4/20	-	-
17	CLA	Q	5231	-	1/1/4/20	-	-
17	CLA	A	1122	-	1/1/4/20	-	-
17	CLA	B	1230	-	1/1/4/20	-	-
17	CLA	P	5110	-	1/1/4/20	-	-
17	CLA	B	1205	-	1/1/4/20	-	-
17	CLA	A	1132	-	1/1/4/20	-	-
17	CLA	Q	5242	-	1/1/4/20	-	-
17	CLA	Q	5236	-	1/1/4/20	-	-
17	CLA	P	5116	-	1/1/4/20	-	-
17	CLA	Q	5201	-	1/1/4/20	-	-
17	CLA	B	1237	-	1/1/4/20	-	-
17	CLA	9	1012	-	1/1/4/20	-	-
17	CLA	1	1012	-	1/1/4/20	-	-
17	CLA	A	1116	-	1/1/4/20	-	-
18	PQN	Q	6002	-	-	-	0/2/2/2
17	CLA	A	1138	-	1/1/4/20	-	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	2	1011	-	1/1/4/20	-	-
17	CLA	B	1226	-	1/1/4/20	-	-
17	CLA	Q	5232	-	1/1/4/20	-	-
17	CLA	3	1016	-	1/1/4/20	-	-
17	CLA	4	1023	-	1/1/4/20	-	-
17	CLA	3	1014	-	1/1/4/20	-	-
17	CLA	P	5114	-	1/1/4/20	-	-
17	CLA	A	1137	-	1/1/4/20	-	-
17	CLA	B	1215	-	1/1/4/20	-	-
17	CLA	G	1233	-	1/1/4/20	-	-
17	CLA	Q	5209	-	1/1/4/20	-	-
17	CLA	9	1021	-	1/1/4/20	-	-
17	CLA	K	1403	-	1/1/4/20	-	-
17	CLA	7	1011	-	1/1/4/20	-	-
17	CLA	A	1114	-	1/1/4/20	-	-
19	SF4	C	3003	-	-	-	0/6/5/5
17	CLA	P	5113	-	1/1/4/20	-	-
17	CLA	B	1211	-	1/1/4/20	-	-
17	CLA	J	1302	-	1/1/4/20	-	-
17	CLA	2	1026	-	1/1/4/20	-	-
17	CLA	6	5501	-	1/1/4/20	-	-
17	CLA	2	1031	-	1/1/4/20	-	-
17	CLA	1	1014	-	1/1/4/20	-	-
17	CLA	F	4006	-	1/1/4/20	-	-
17	CLA	Q	5221	-	1/1/4/20	-	-
17	CLA	P	5131	-	1/1/4/20	-	-
17	CLA	U	5301	-	1/1/4/20	-	-
17	CLA	A	1012	-	1/1/4/20	-	-
17	CLA	7	1022	-	1/1/4/20	-	-
18	PQN	B	2002	-	-	-	0/2/2/2
17	CLA	A	4010	-	1/1/4/20	-	-
17	CLA	4	1016	-	1/1/4/20	-	-
17	CLA	Q	5218	-	1/1/4/20	-	-
17	CLA	B	1209	-	1/1/4/20	-	-
17	CLA	B	1212	-	1/1/4/20	-	-
17	CLA	P	5126	-	1/1/4/20	-	-
17	CLA	B	1225	-	1/1/4/20	-	-
17	CLA	A	1134	-	1/1/4/20	-	-
17	CLA	B	1217	-	1/1/4/20	-	-
17	CLA	B	1224	-	1/1/4/20	-	-
17	CLA	Q	5219	-	1/1/4/20	-	-
17	CLA	P	5136	-	1/1/4/20	-	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	0	1015	-	1/1/4/20	-	-
17	CLA	4	1026	-	1/1/4/20	-	-
17	CLA	A	4009	-	1/1/4/20	-	-
17	CLA	B	1228	-	1/1/4/20	-	-
17	CLA	3	1011	-	1/1/4/20	-	-
18	PQN	P	6001	-	-	-	0/2/2/2
17	CLA	4	1013	-	1/1/4/20	-	-
17	CLA	3	1022	-	1/1/4/20	-	-
17	CLA	Z	5302	-	1/1/4/20	-	-
17	CLA	1	1016	-	1/1/4/20	-	-
17	CLA	8	1012	-	1/1/4/20	-	-
17	CLA	5	5403	-	1/1/4/20	-	-
17	CLA	A	1105	-	1/1/4/20	-	-
17	CLA	5	5404	-	1/1/4/20	-	-
17	CLA	A	1117	-	1/1/4/20	-	-
19	SF4	P	7001	-	-	-	0/6/5/5
17	CLA	A	1115	-	1/1/4/20	-	-
17	CLA	H	1801	-	1/1/4/20	-	-
17	CLA	A	1102	-	1/1/4/20	-	-
17	CLA	P	5138	-	1/1/4/20	-	-
17	CLA	3	1021	-	1/1/4/20	-	-
17	CLA	1	1021	-	1/1/4/20	-	-
17	CLA	4	1021	-	1/1/4/20	-	-
17	CLA	B	1221	-	1/1/4/20	-	-
19	SF4	R	7003	-	-	-	0/6/5/5
17	CLA	P	5011	-	1/1/4/20	-	-
17	CLA	P	5901	-	1/1/4/20	-	-
17	CLA	Q	5217	-	1/1/4/20	-	-
17	CLA	L	1501	-	1/1/4/20	-	-
17	CLA	A	1104	-	1/1/4/20	-	-
17	CLA	8	1033	-	1/1/4/20	-	-
17	CLA	P	8010	-	1/1/4/20	-	-
17	CLA	B	1216	-	1/1/4/20	-	-
17	CLA	7	1015	-	1/1/4/20	-	-
17	CLA	P	5118	-	1/1/4/20	-	-
17	CLA	A	1123	-	1/1/4/20	-	-
17	CLA	9	1011	-	1/1/4/20	-	-
17	CLA	4	1011	-	1/1/4/20	-	-
17	CLA	8	1014	-	1/1/4/20	-	-
17	CLA	7	1012	-	1/1/4/20	-	-
17	CLA	Q	5239	-	1/1/4/20	-	-
17	CLA	9	1025	-	1/1/4/20	-	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	B	1202	-	1/1/4/20	-	-
17	CLA	B	1220	-	1/1/4/20	-	-
17	CLA	Q	5224	-	1/1/4/20	-	-
17	CLA	U	8003	-	1/1/4/20	-	-
17	CLA	P	5125	-	1/1/4/20	-	-
17	CLA	8	1022	-	1/1/4/20	-	-
17	CLA	P	5119	-	1/1/4/20	-	-
17	CLA	9	1033	-	1/1/4/20	-	-
17	CLA	A	1112	-	1/1/4/20	-	-
17	CLA	A	1119	-	1/1/4/20	-	-
17	CLA	P	5140	-	1/1/4/20	-	-
17	CLA	7	1023	-	1/1/4/20	-	-
17	CLA	2	1023	-	1/1/4/20	-	-
17	CLA	Q	5208	-	1/1/4/20	-	-
17	CLA	A	1131	-	1/1/4/20	-	-
17	CLA	B	1241	-	1/1/4/20	-	-
17	CLA	Q	5237	-	1/1/4/20	-	-
17	CLA	8	1023	-	1/1/4/20	-	-
17	CLA	A	1118	-	1/1/4/20	-	-
17	CLA	B	1023	-	1/1/4/20	-	-
17	CLA	2	1017	-	1/1/4/20	-	-
17	CLA	8	1016	-	1/1/4/20	-	-
17	CLA	4	1031	-	1/1/4/20	-	-
17	CLA	B	1219	-	1/1/4/20	-	-
17	CLA	Q	5235	-	1/1/4/20	-	-
17	CLA	3	1041	-	1/1/4/20	-	-
17	CLA	A	1113	-	1/1/4/20	-	-
17	CLA	0	8002	-	1/1/4/20	-	-
17	CLA	2	1012	-	1/1/4/20	-	-
17	CLA	Q	5223	-	1/1/4/20	-	-
18	PQN	A	2001	-	-	-	0/2/2/2
17	CLA	1	1026	-	1/1/4/20	-	-
17	CLA	P	5120	-	1/1/4/20	-	-
17	CLA	K	1404	-	1/1/4/20	-	-
17	CLA	A	1124	-	1/1/4/20	-	-
17	CLA	P	5128	-	1/1/4/20	-	-
17	CLA	B	1234	-	1/1/4/20	-	-
17	CLA	A	1901	-	1/1/4/20	-	-
17	CLA	P	5123	-	1/1/4/20	-	-
17	CLA	B	1236	-	1/1/4/20	-	-
17	CLA	A	1140	-	1/1/4/20	-	-
17	CLA	A	1121	-	1/1/4/20	-	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	A	1402	-	1/1/4/20	-	-
17	CLA	Q	5203	-	1/1/4/20	-	-
17	CLA	0	1012	-	1/1/4/20	-	-
17	CLA	A	1013	-	1/1/4/20	-	-
17	CLA	U	8006	-	1/1/4/20	-	-
17	CLA	6	5504	-	1/1/4/20	-	-
17	CLA	B	1201	-	1/1/4/20	-	-
17	CLA	A	1135	-	1/1/4/20	-	-
17	CLA	P	5124	-	1/1/4/20	-	-
17	CLA	B	1235	-	1/1/4/20	-	-
17	CLA	3	1026	-	1/1/4/20	-	-
17	CLA	B	1210	-	1/1/4/20	-	-
17	CLA	1	1023	-	1/1/4/20	-	-
17	CLA	9	1041	-	1/1/4/20	-	-
17	CLA	9	1014	-	1/1/4/20	-	-
17	CLA	0	1033	-	1/1/4/20	-	-
17	CLA	V	5233	-	1/1/4/20	-	-
17	CLA	B	1022	-	1/1/4/20	-	-
17	CLA	7	1021	-	1/1/4/20	-	-
17	CLA	P	5104	-	1/1/4/20	-	-
17	CLA	Q	5206	-	1/1/4/20	-	-

The worst 5 of 2753 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	P	5135	CLA	CHB-C4A	11.11	1.43	1.34
17	A	1135	CLA	CHB-C4A	11.01	1.43	1.34
17	Q	5223	CLA	CHB-C4A	10.54	1.42	1.34
17	Q	5230	CLA	CHB-C4A	10.51	1.42	1.34
17	B	1230	CLA	CHB-C4A	10.48	1.42	1.34

The worst 5 of 2567 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	Z	5302	CLA	C4A-NA-C1A	16.75	114.24	106.71
17	J	1302	CLA	C4A-NA-C1A	16.70	114.22	106.71
17	A	1901	CLA	C4A-NA-C1A	16.34	114.05	106.71
17	P	5901	CLA	C4A-NA-C1A	16.30	114.03	106.71
17	A	1113	CLA	C4A-NA-C1A	15.50	113.67	106.71

5 of 332 chirality outliers are listed below:

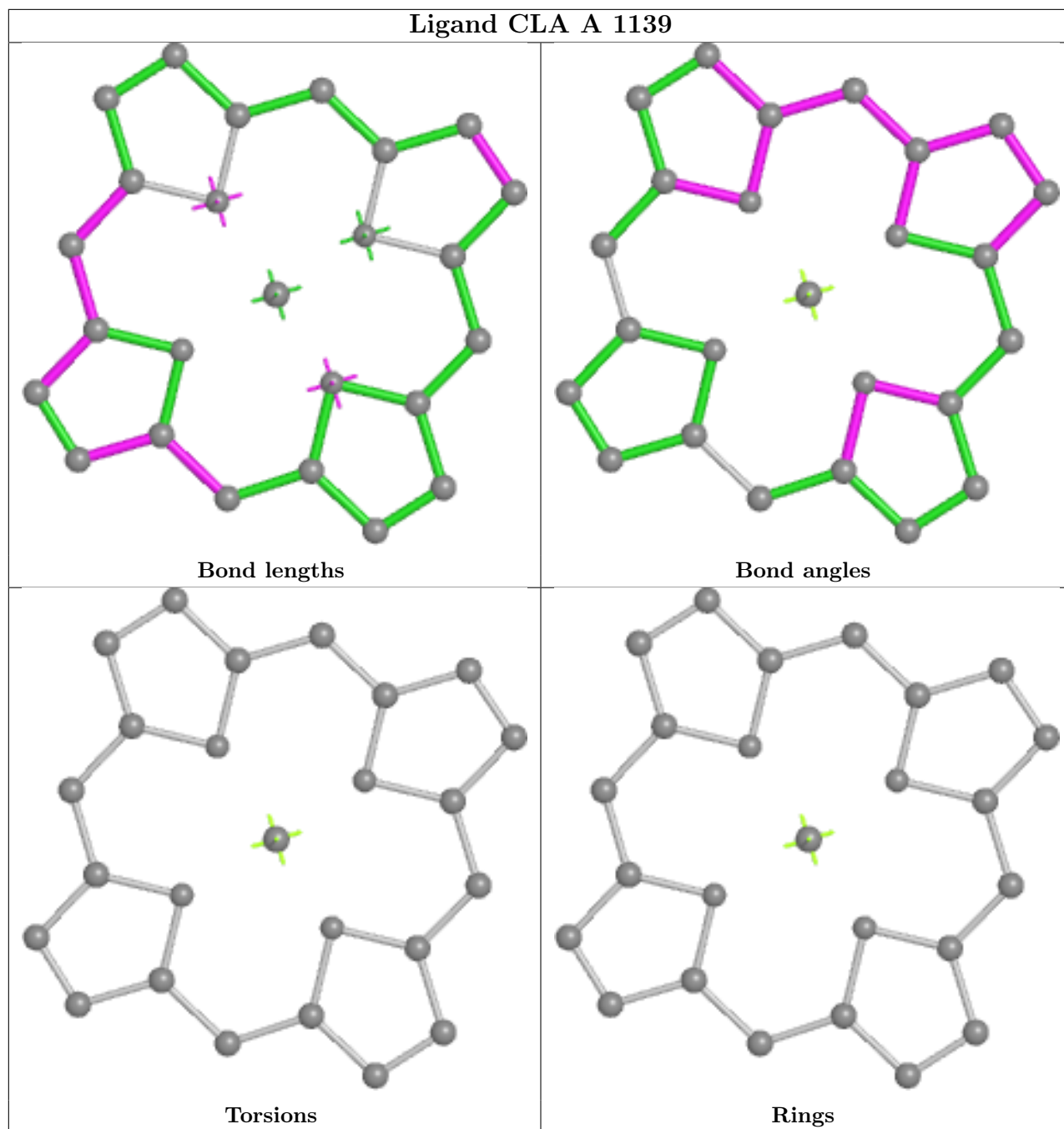
Mol	Chain	Res	Type	Atom
17	A	1011	CLA	ND
17	A	1012	CLA	ND
17	A	1013	CLA	ND
17	A	1102	CLA	ND
17	A	1103	CLA	ND

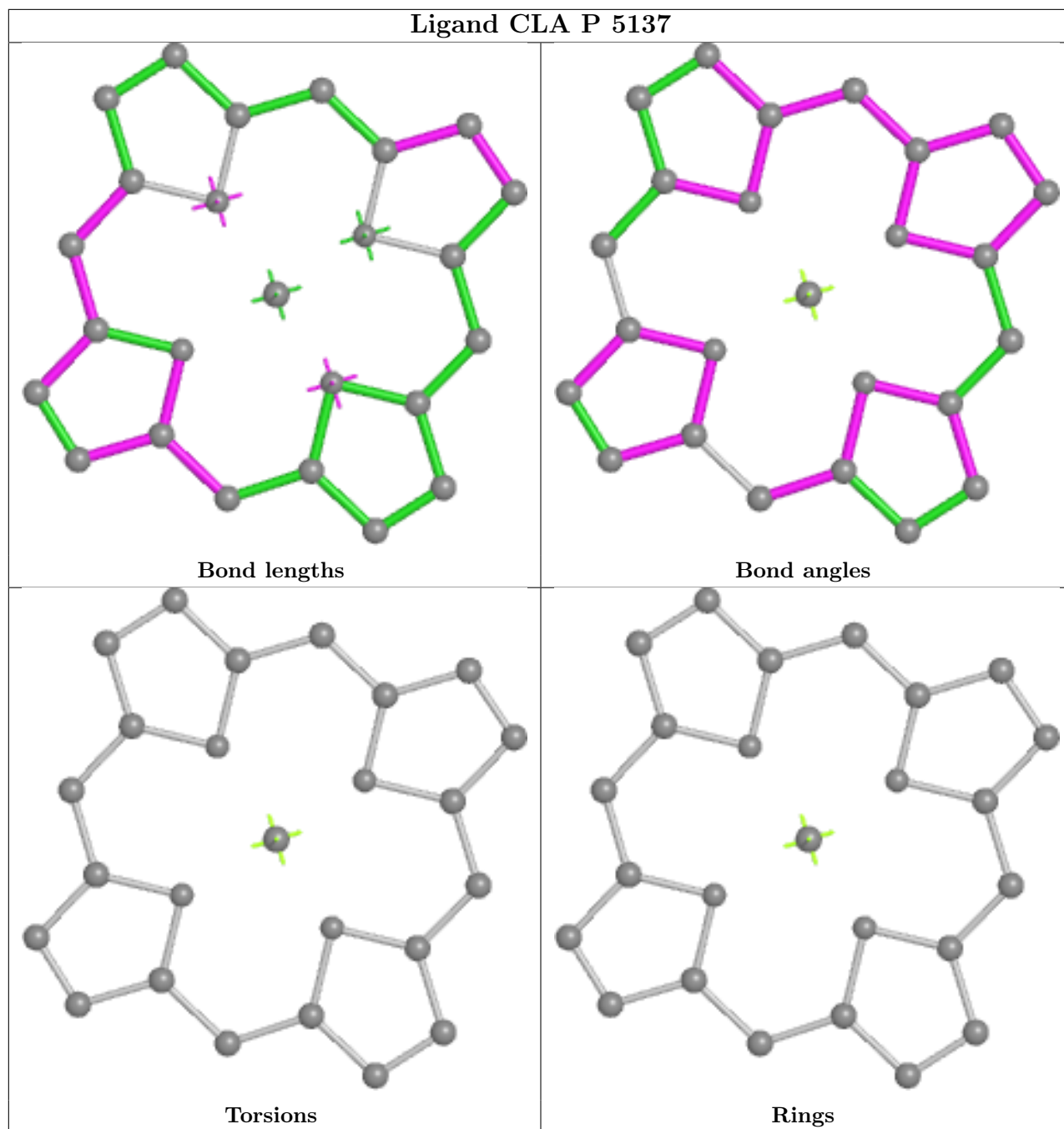
There are no torsion outliers.

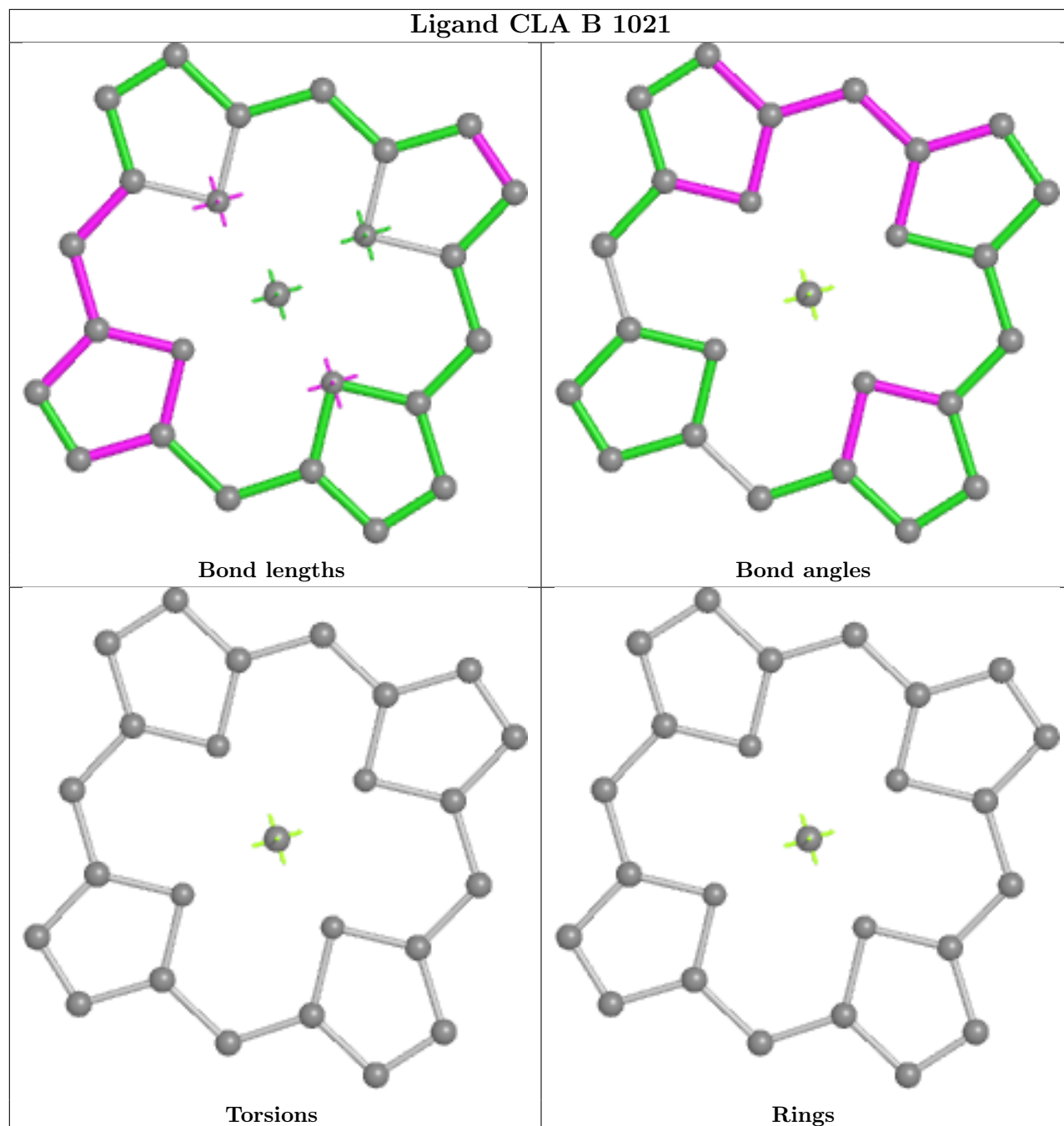
There are no ring outliers.

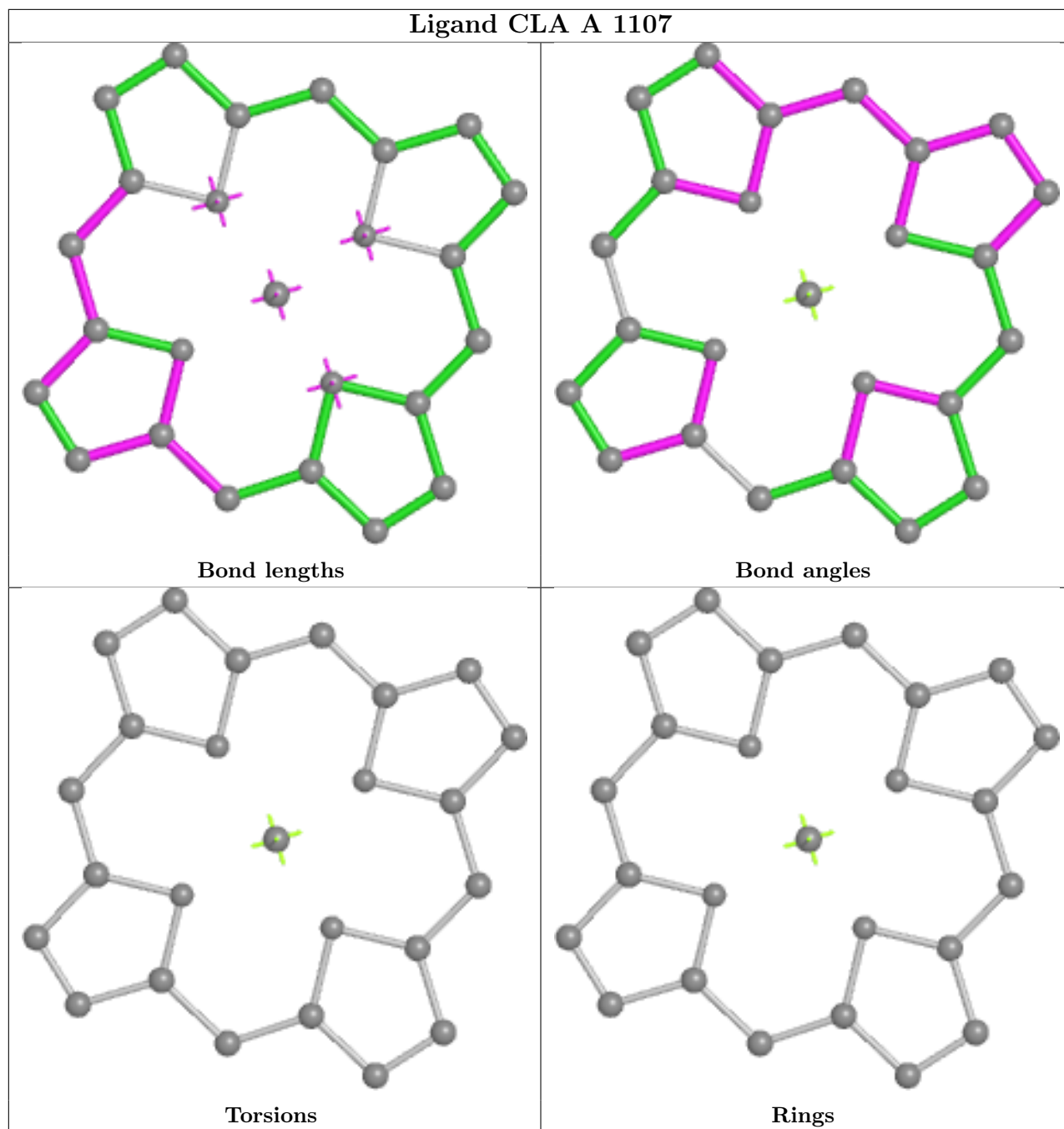
No monomer is involved in short contacts.

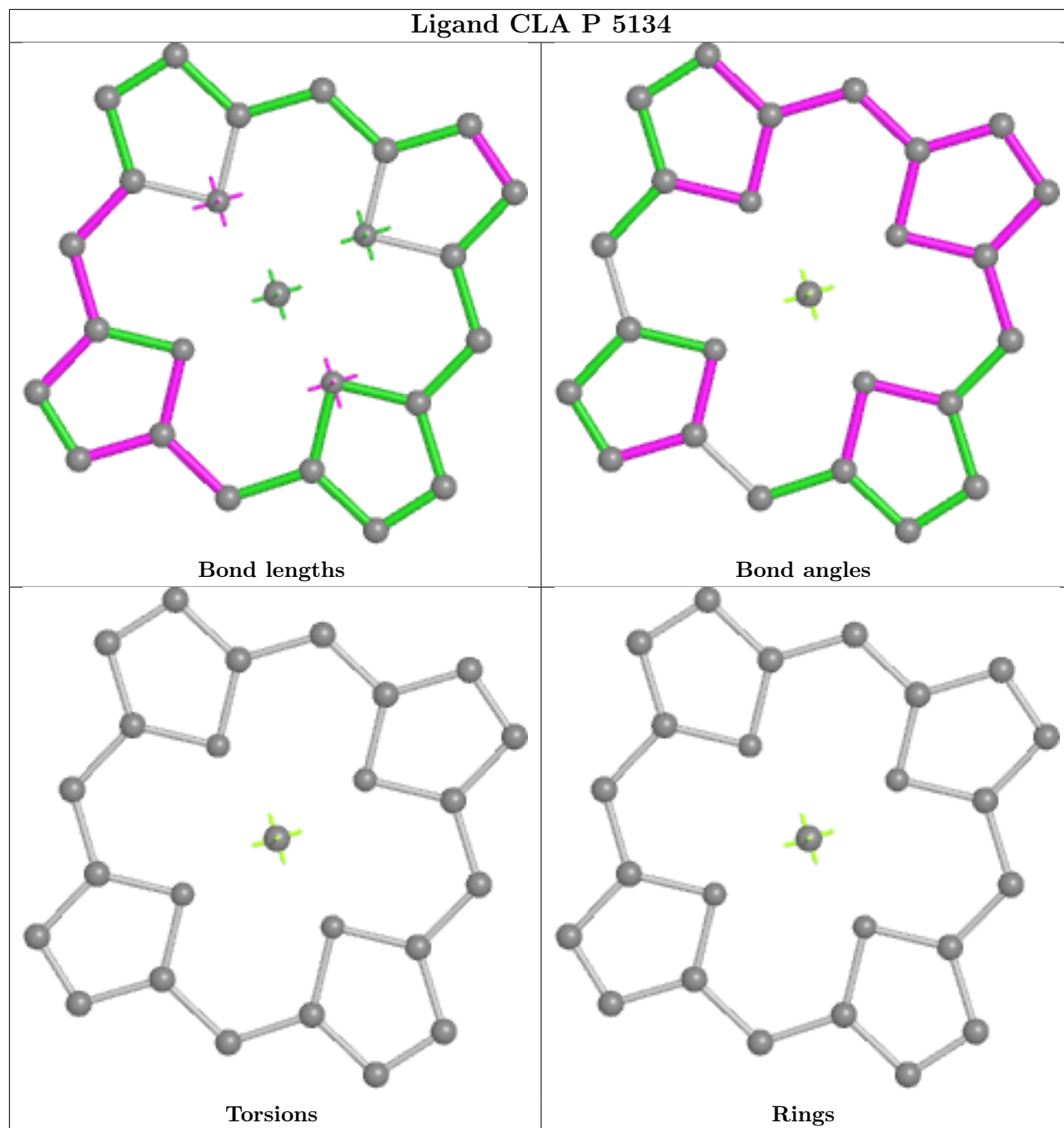
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

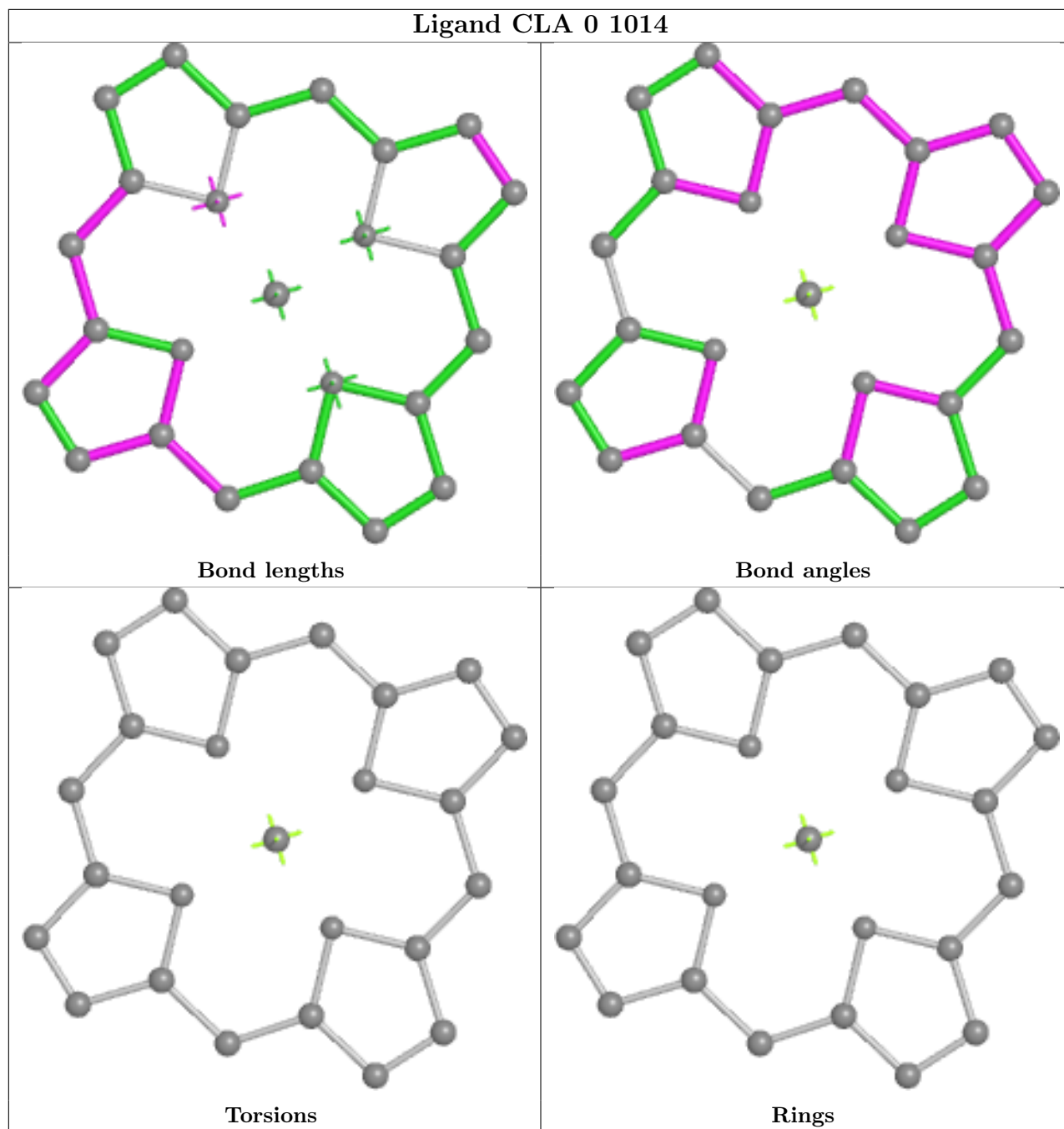


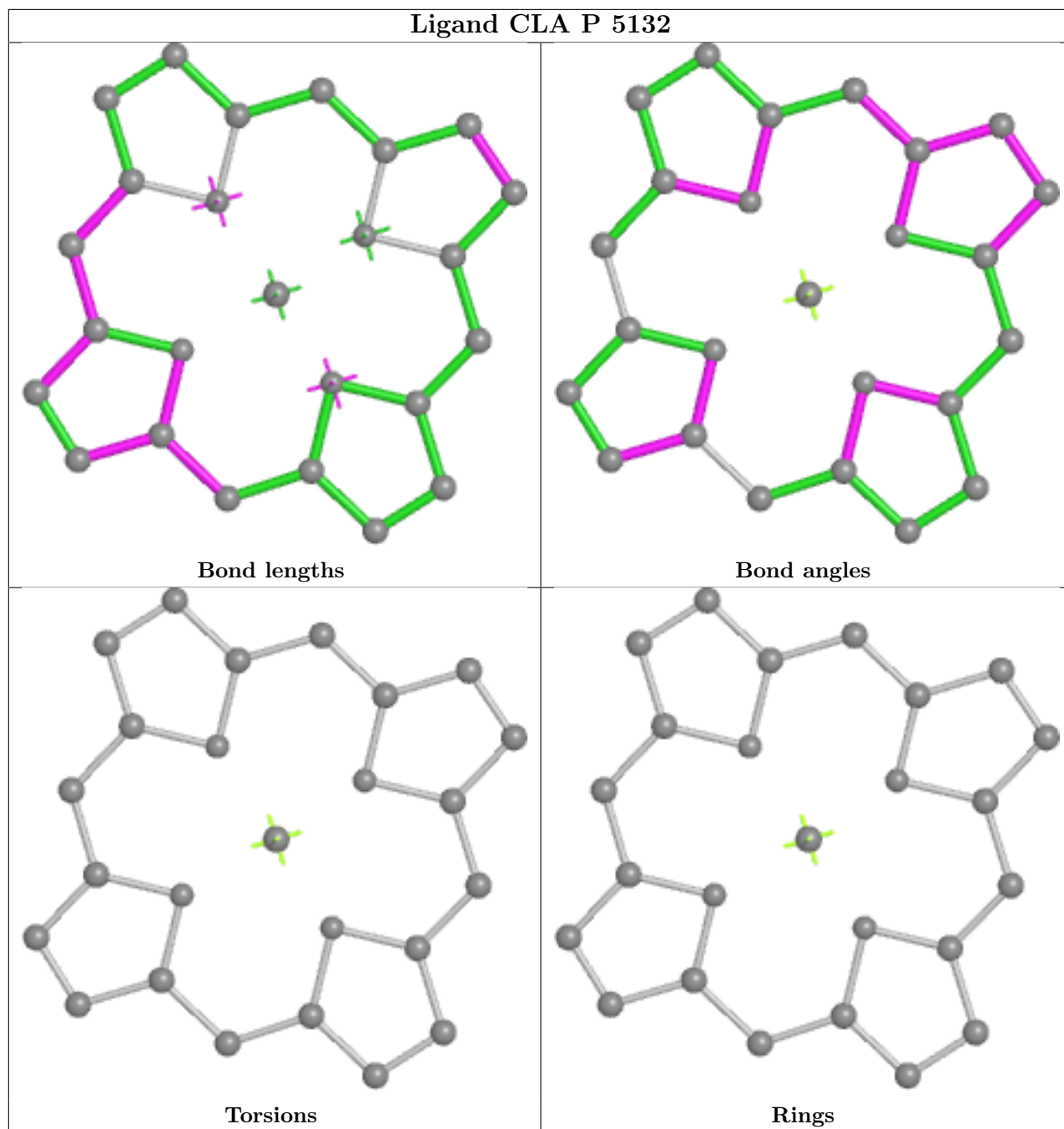


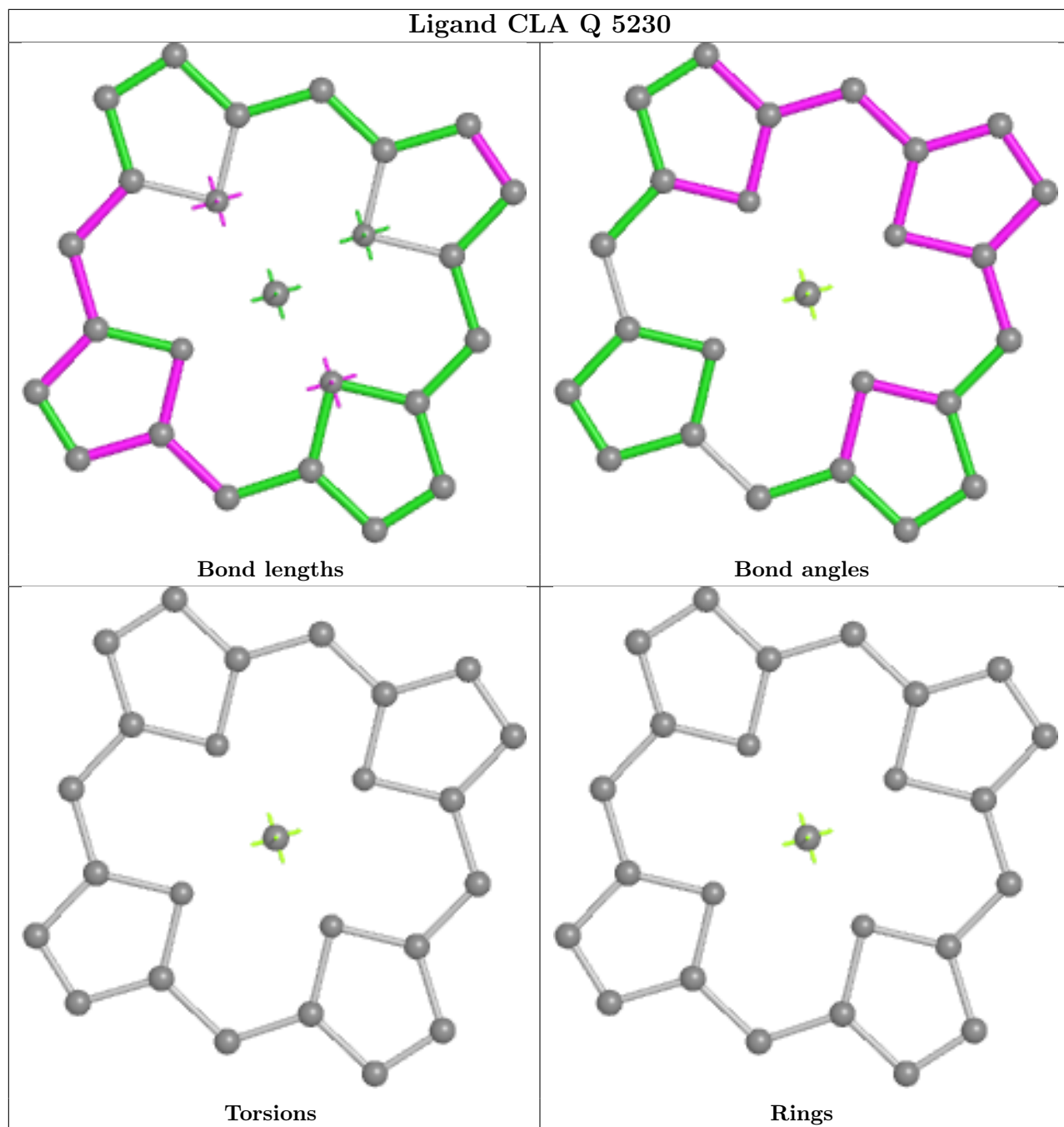


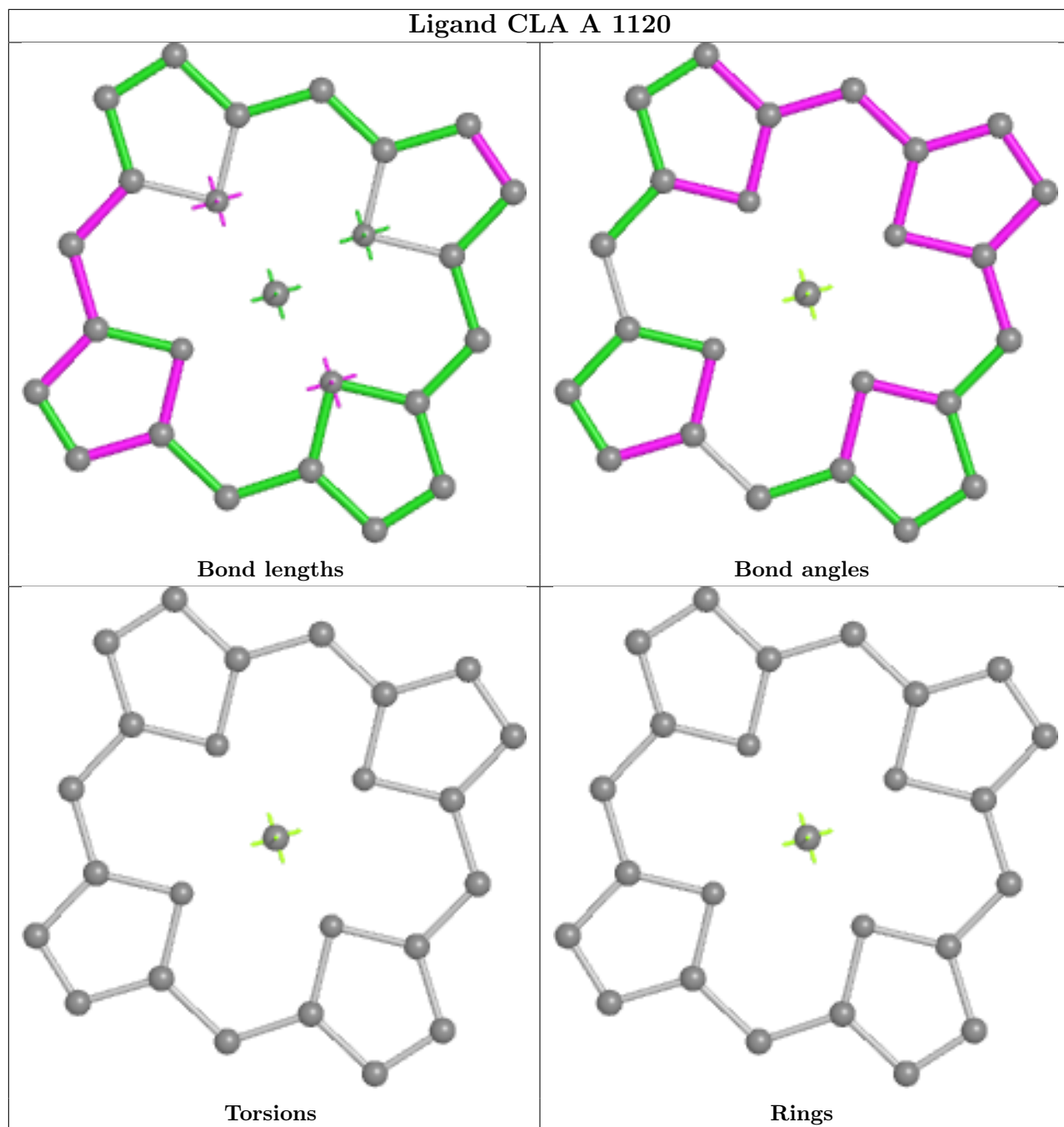


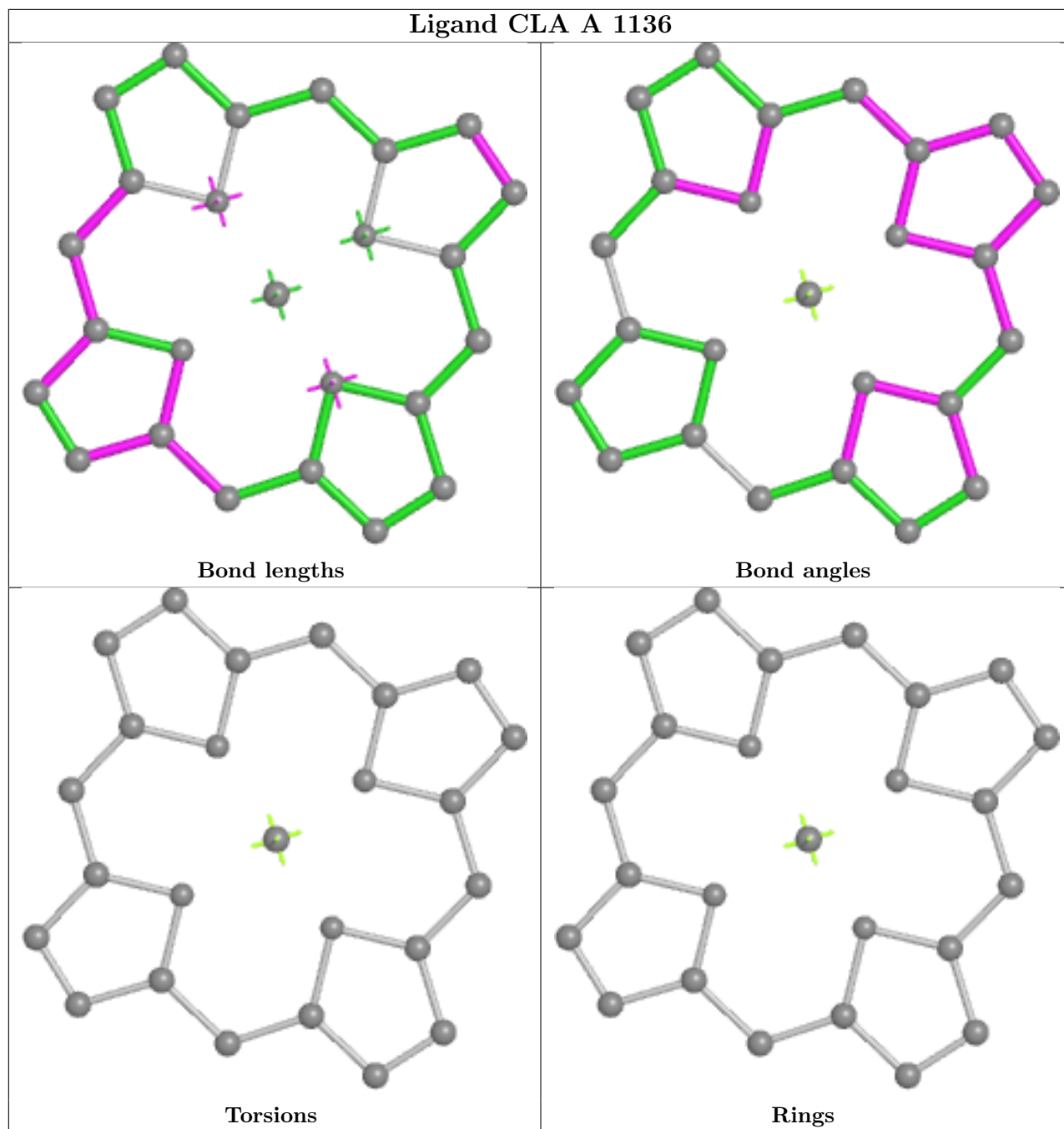


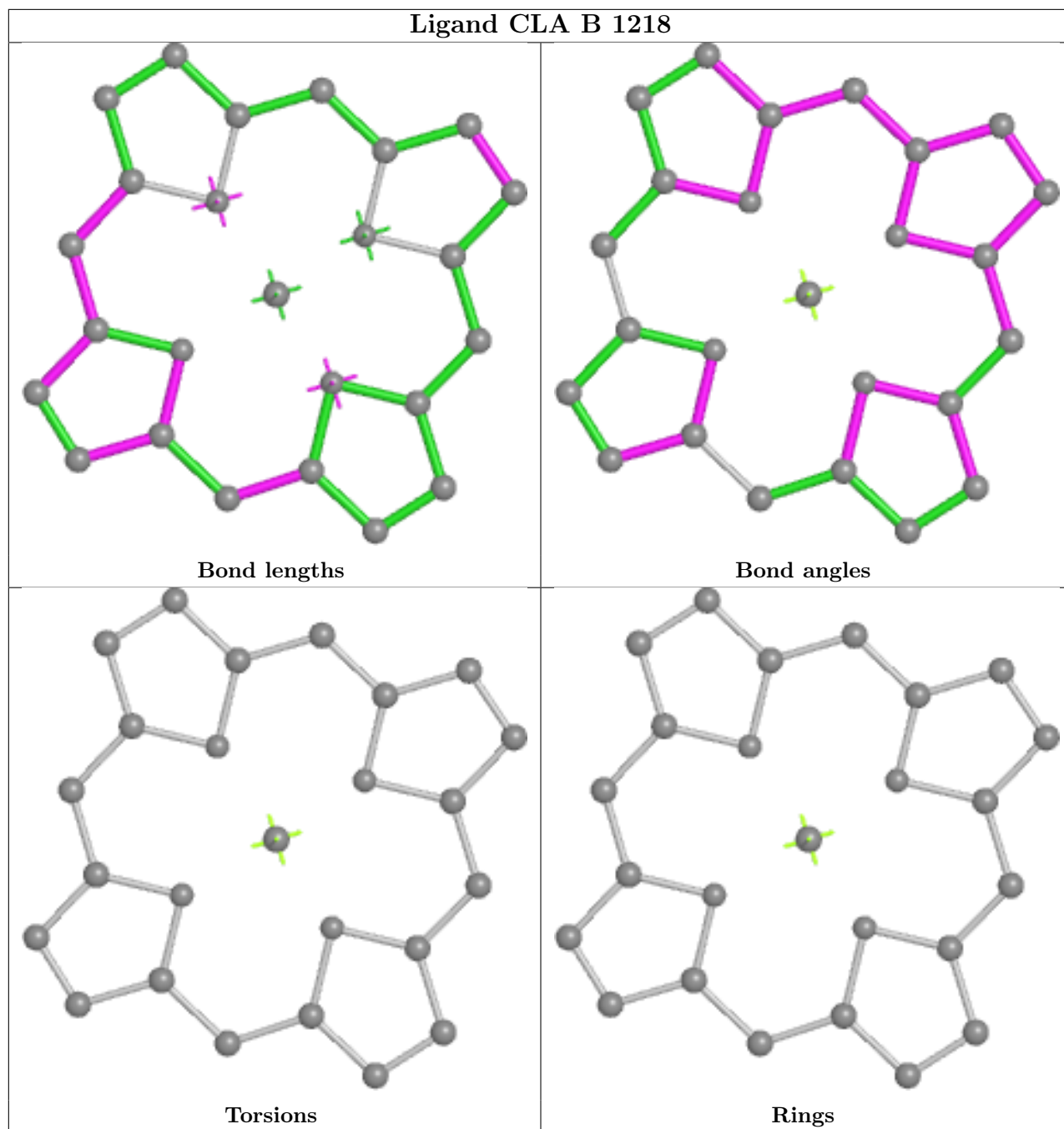


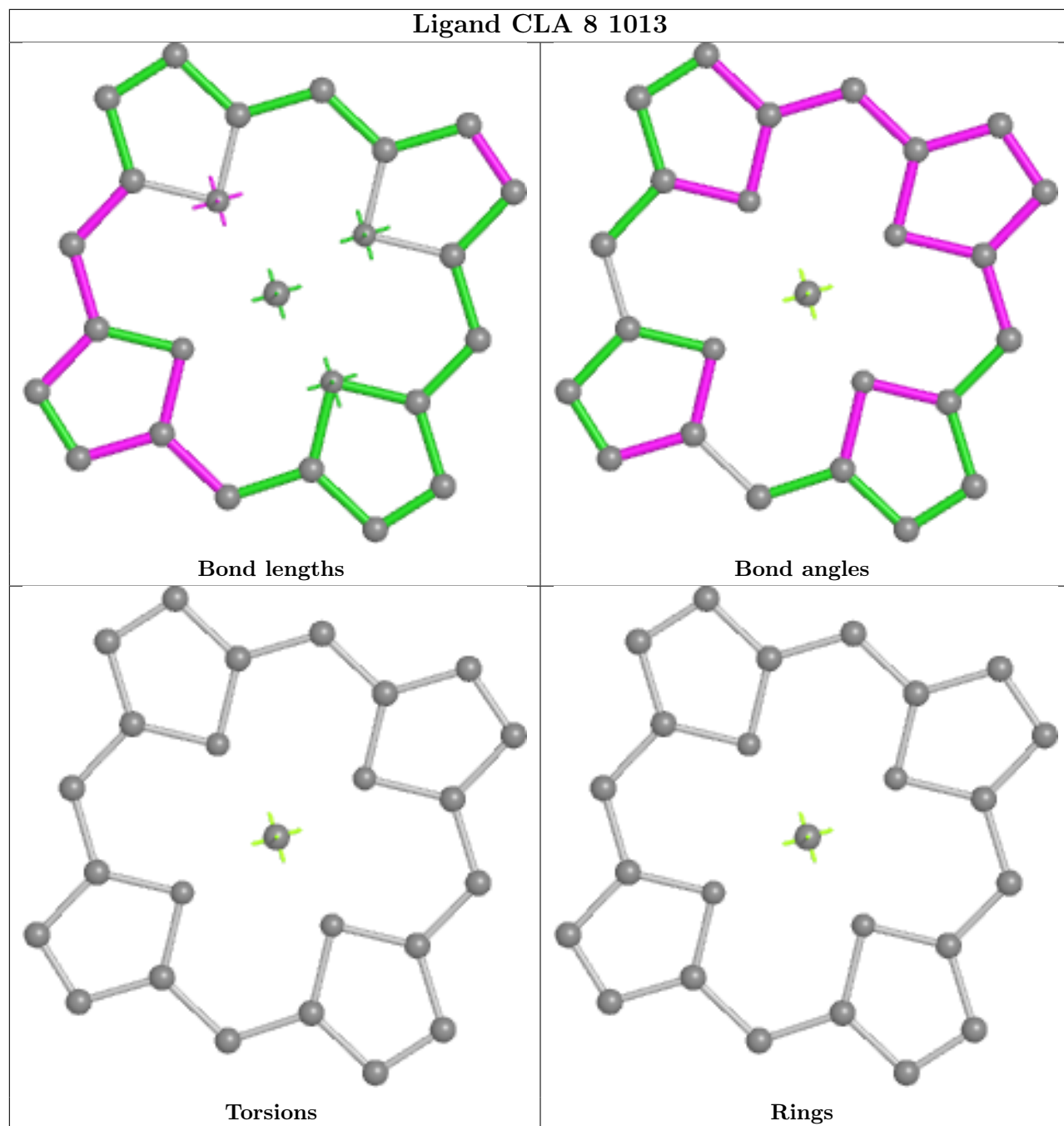


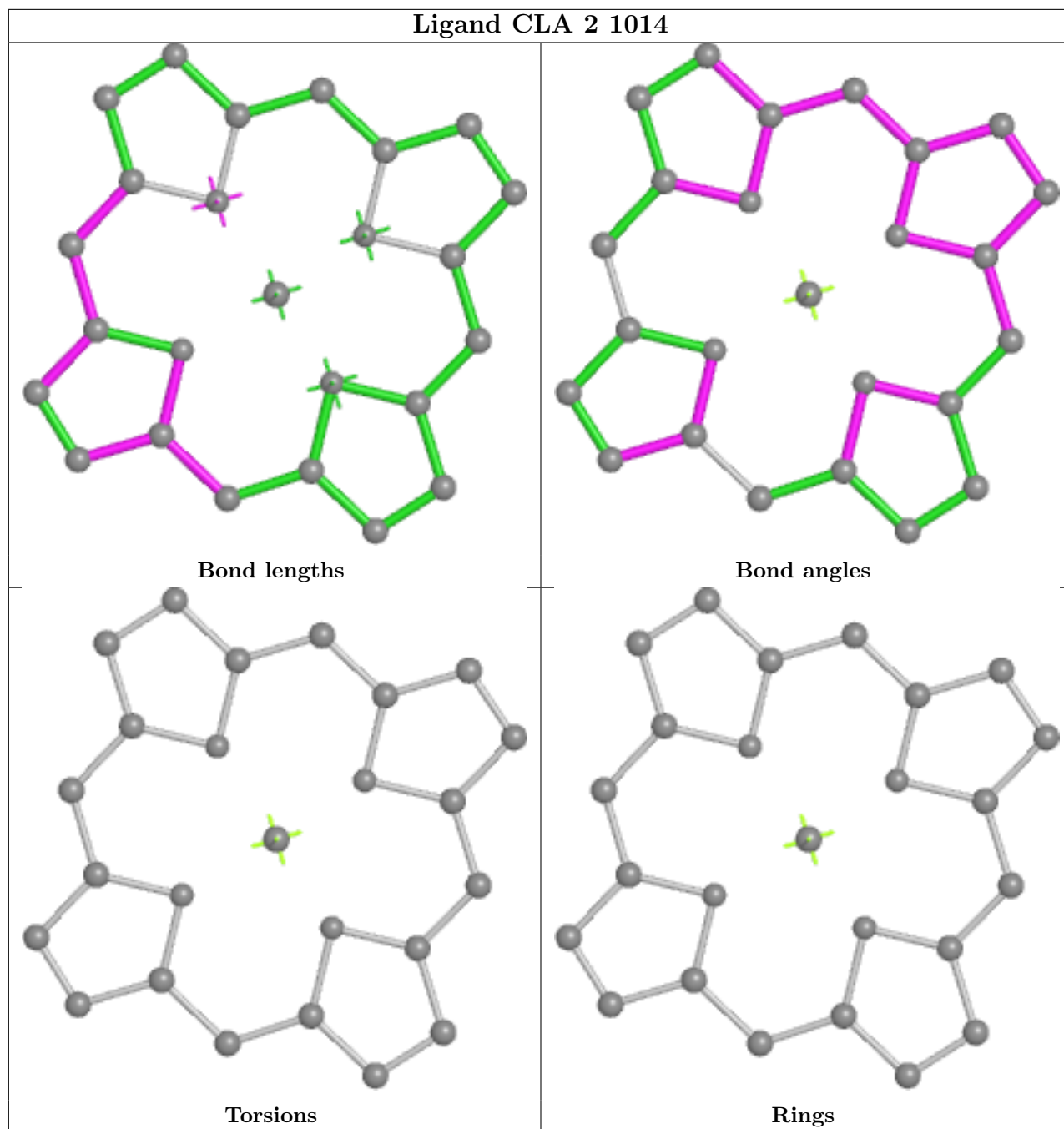


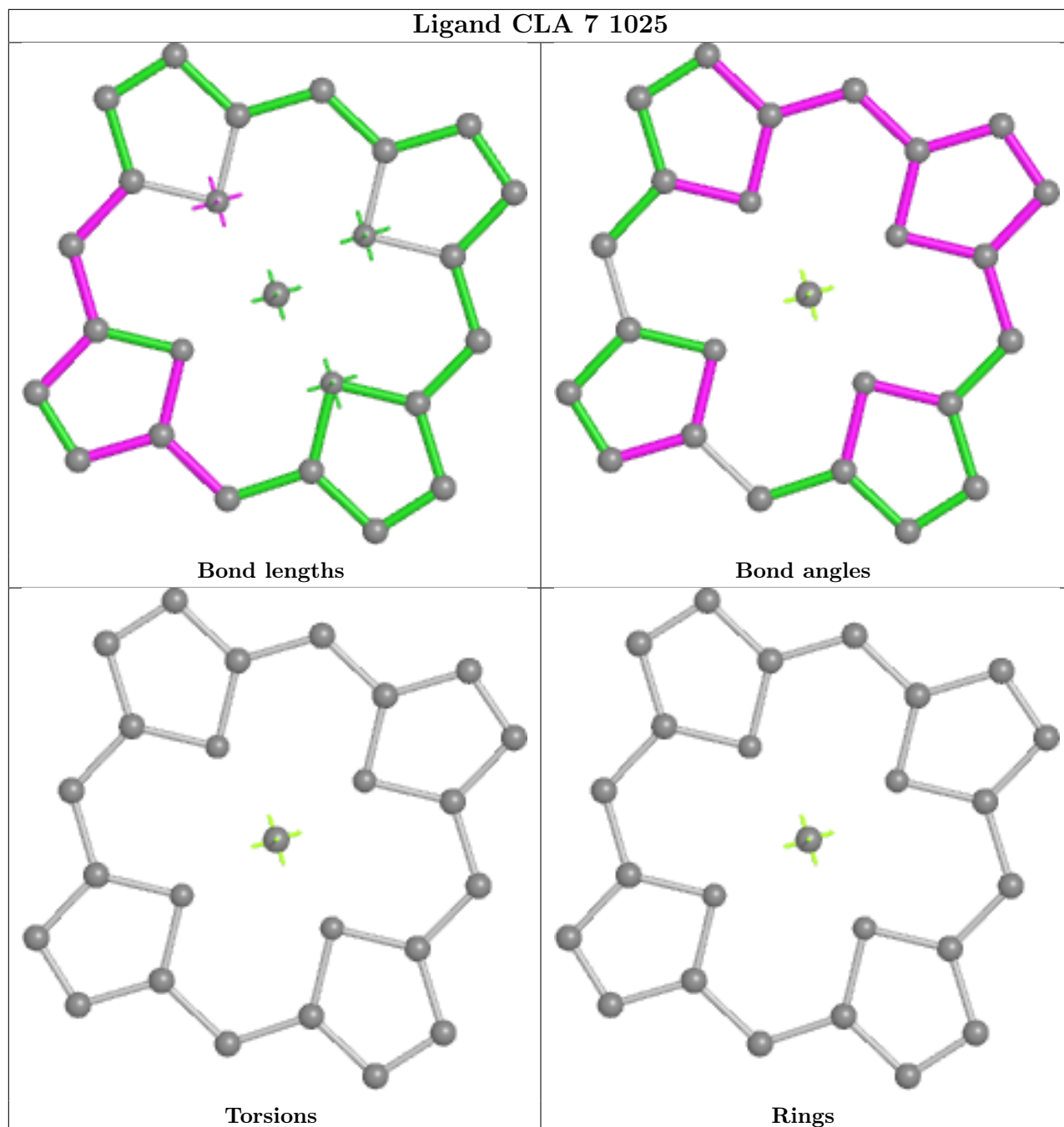


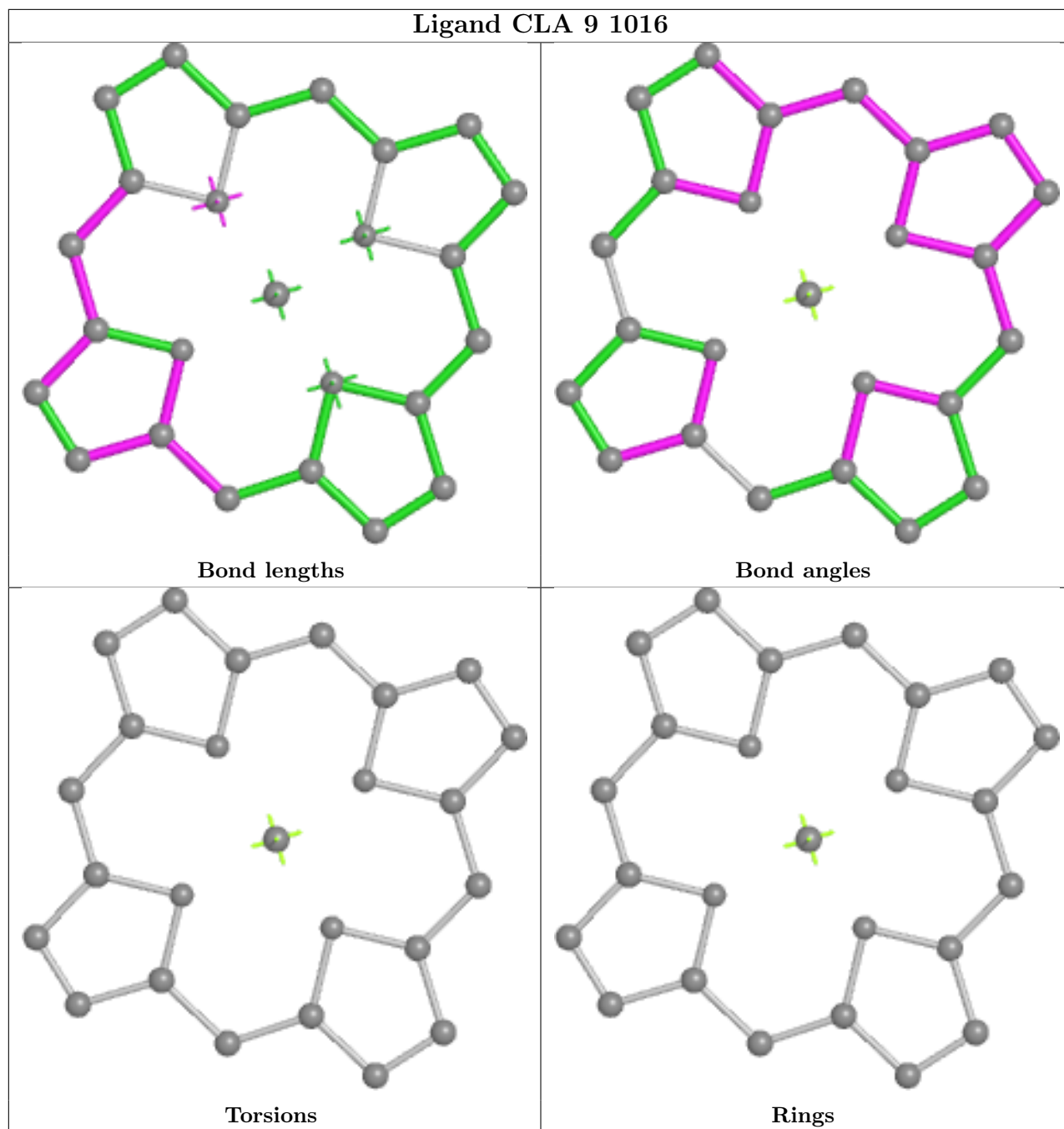


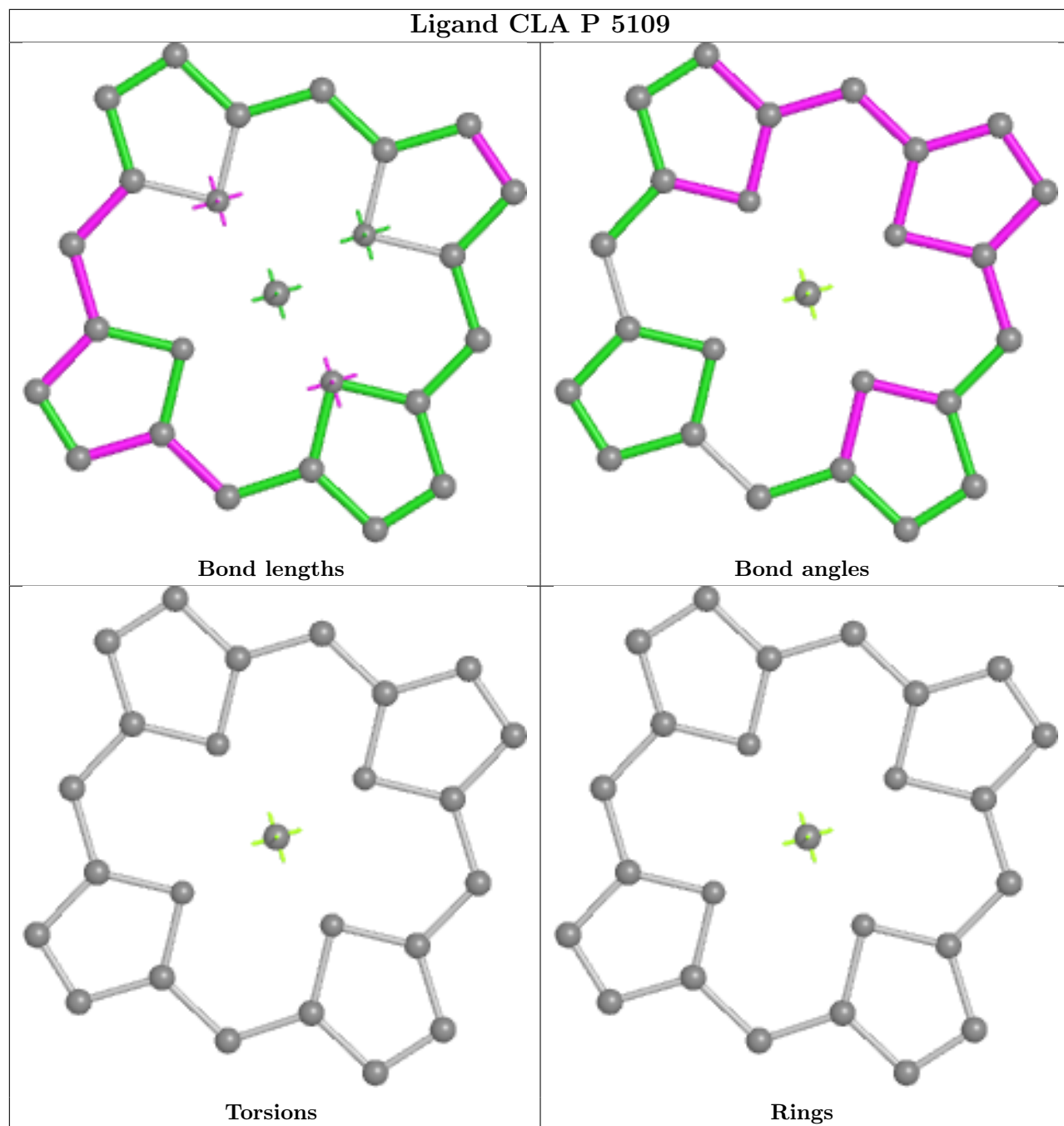


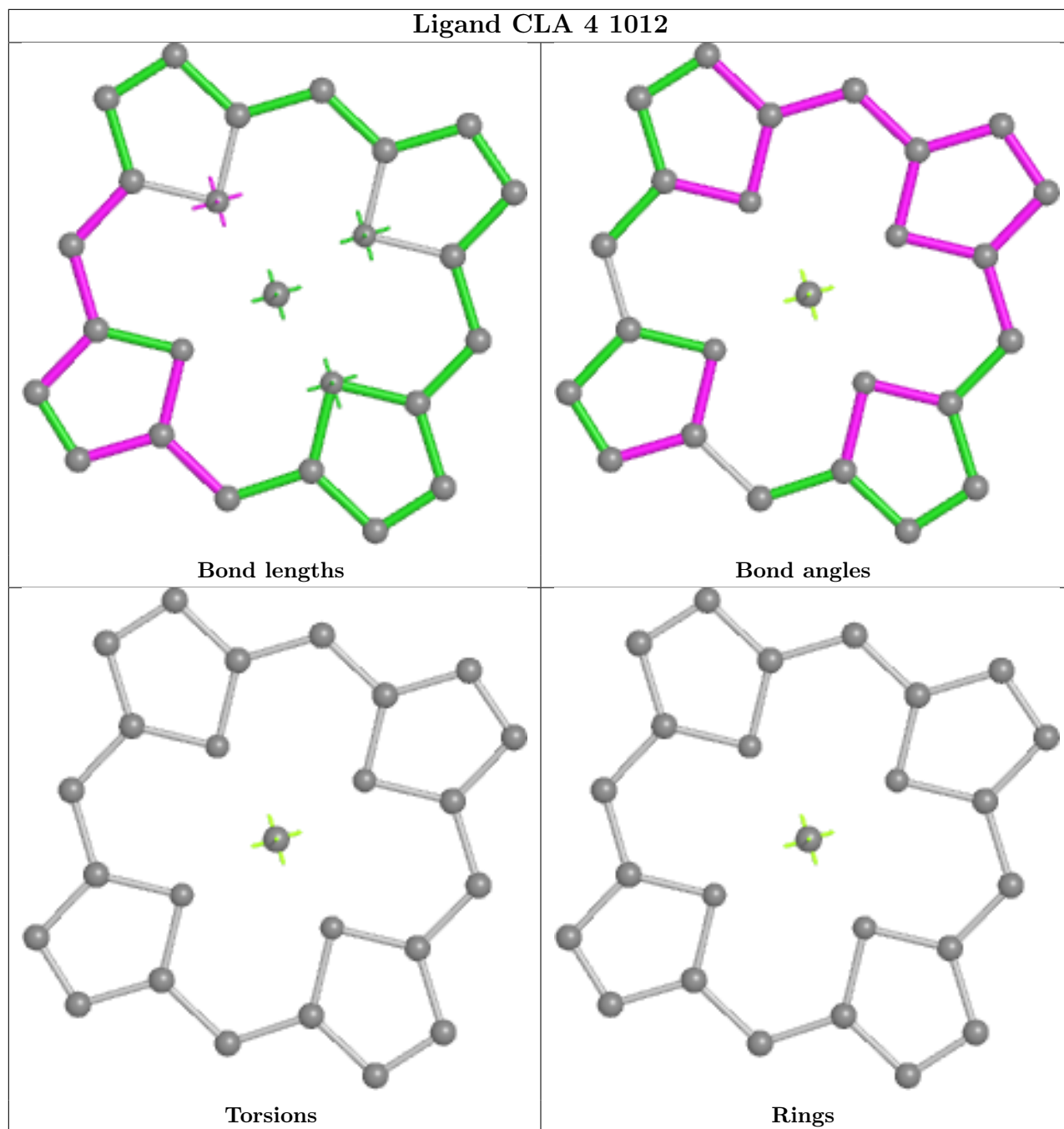


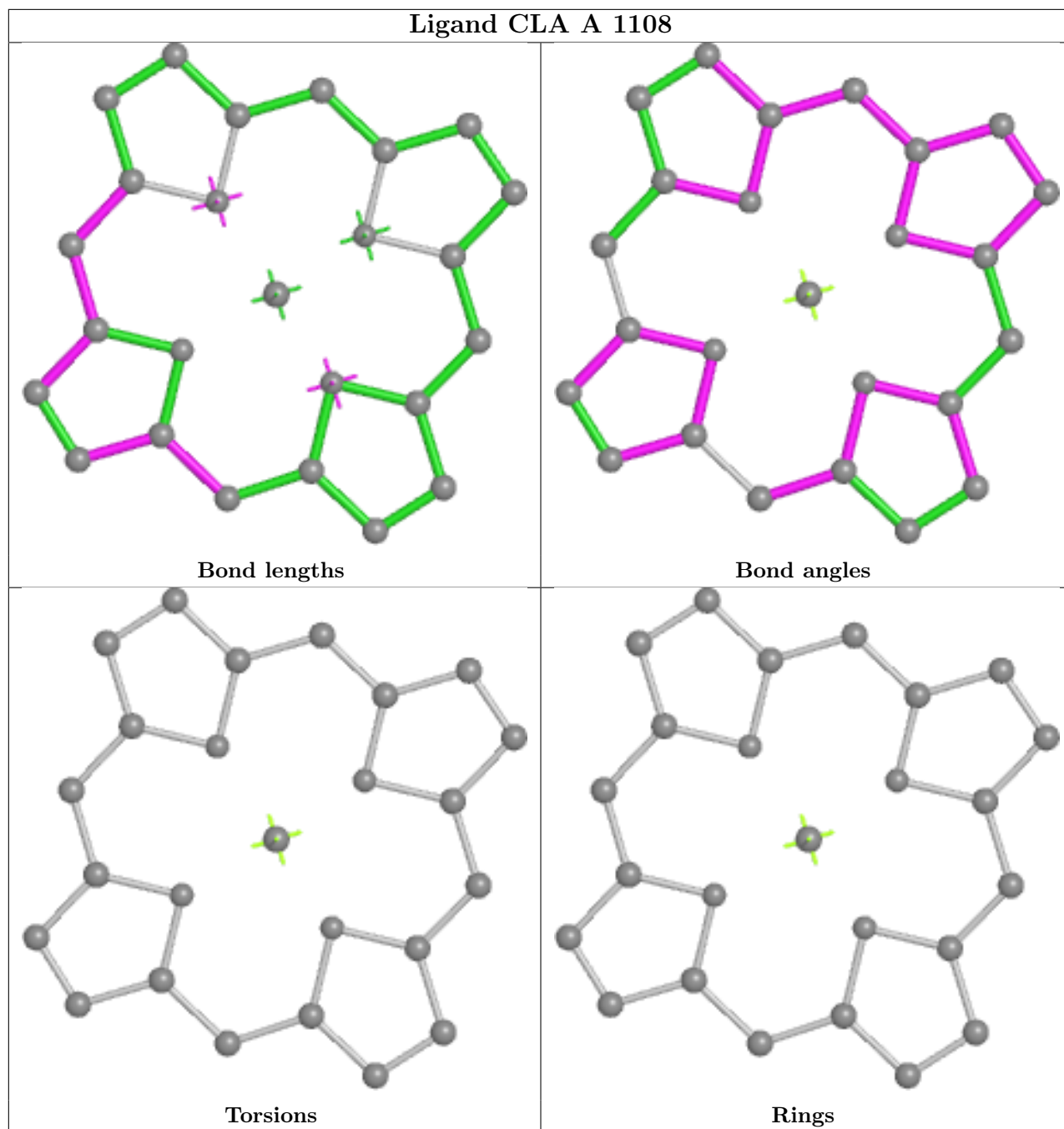


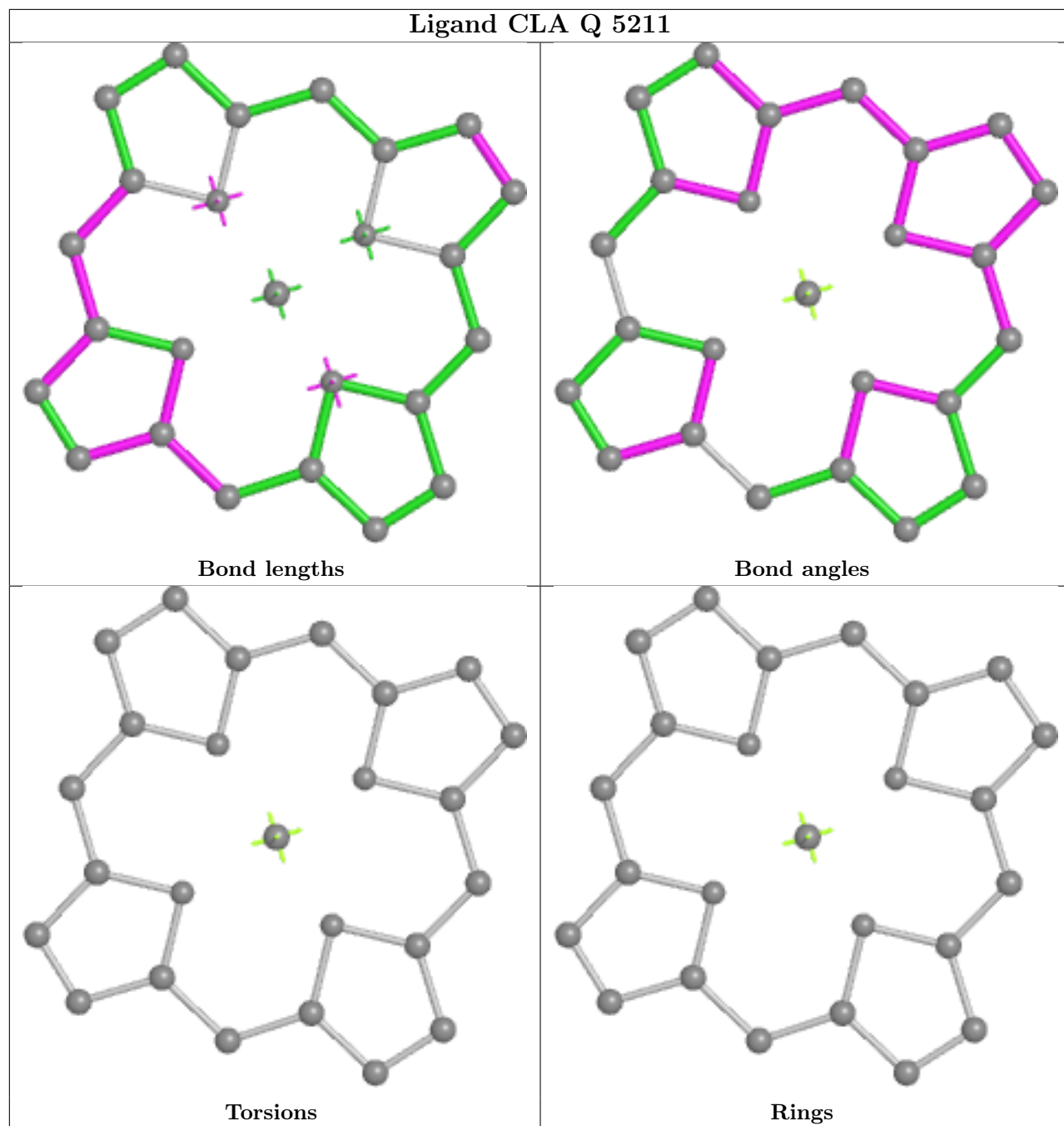


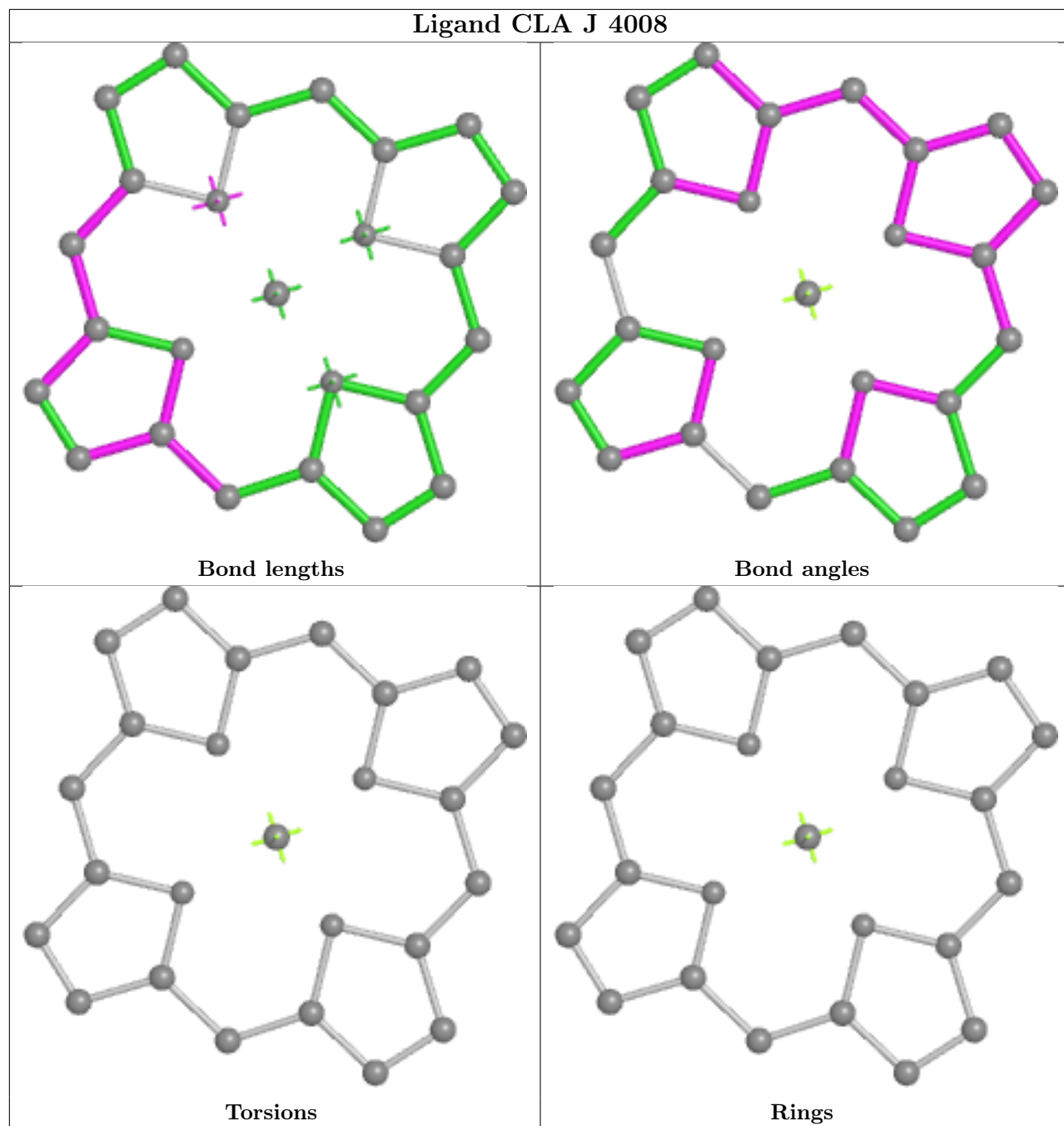


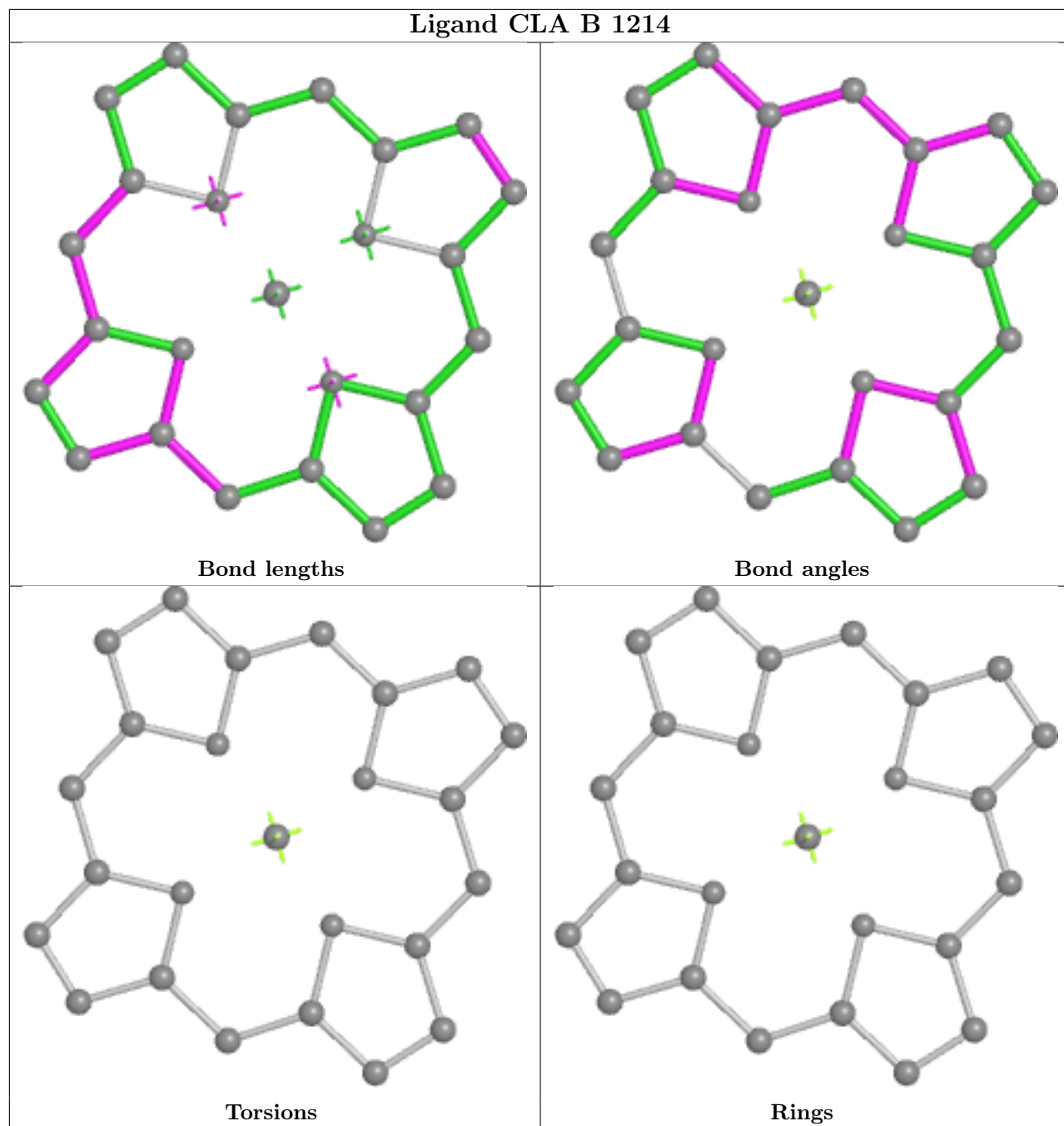


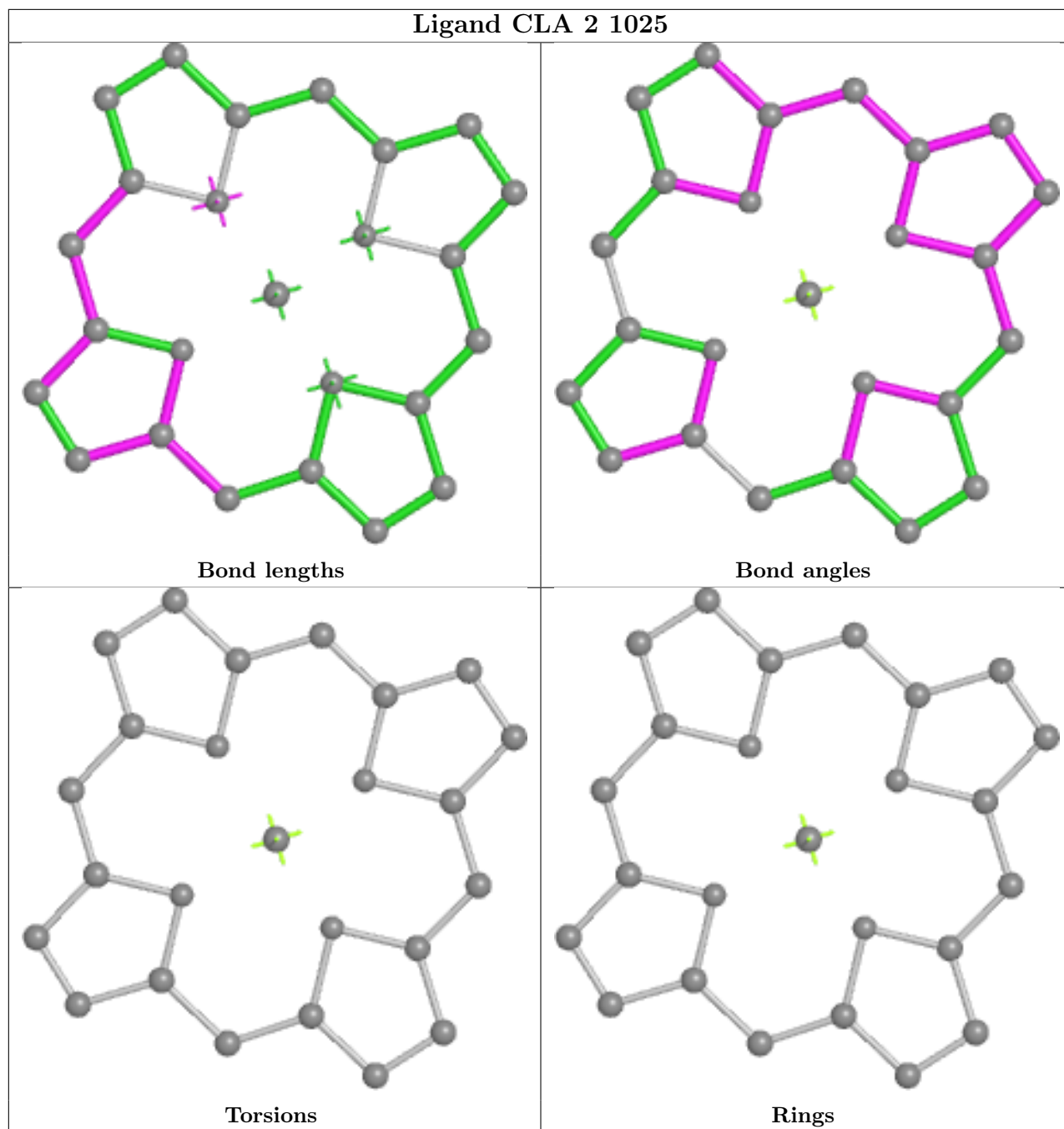


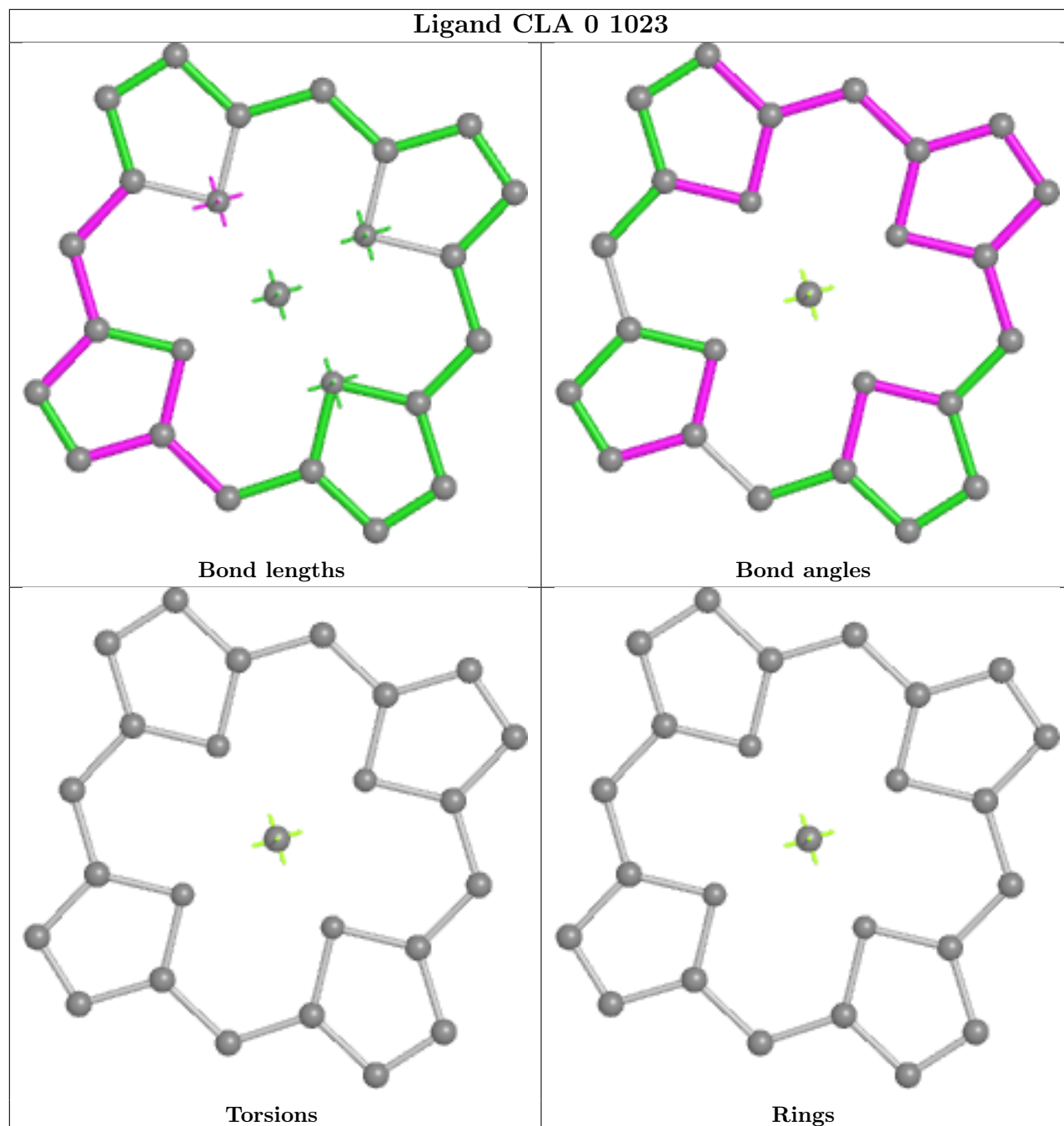


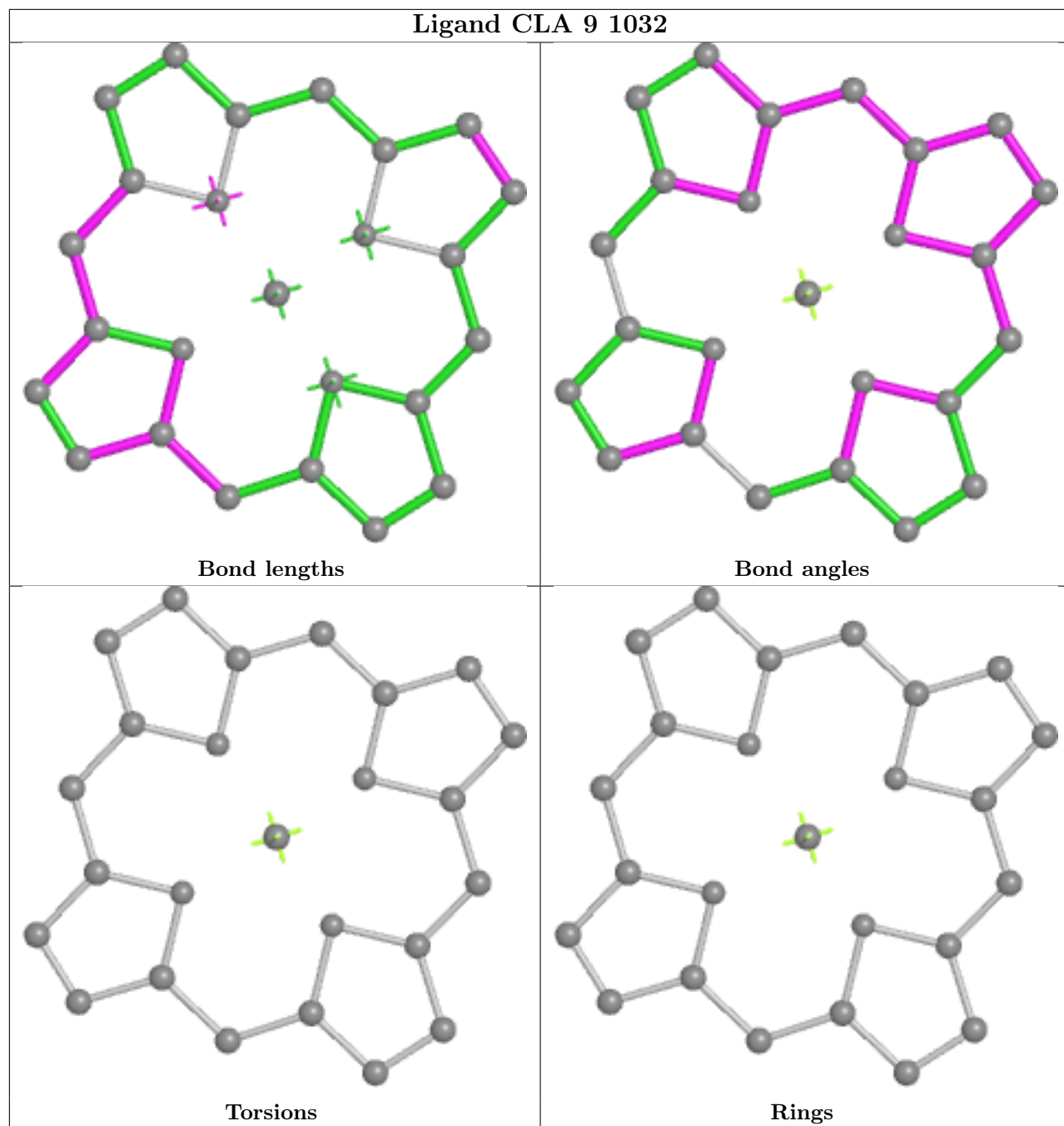


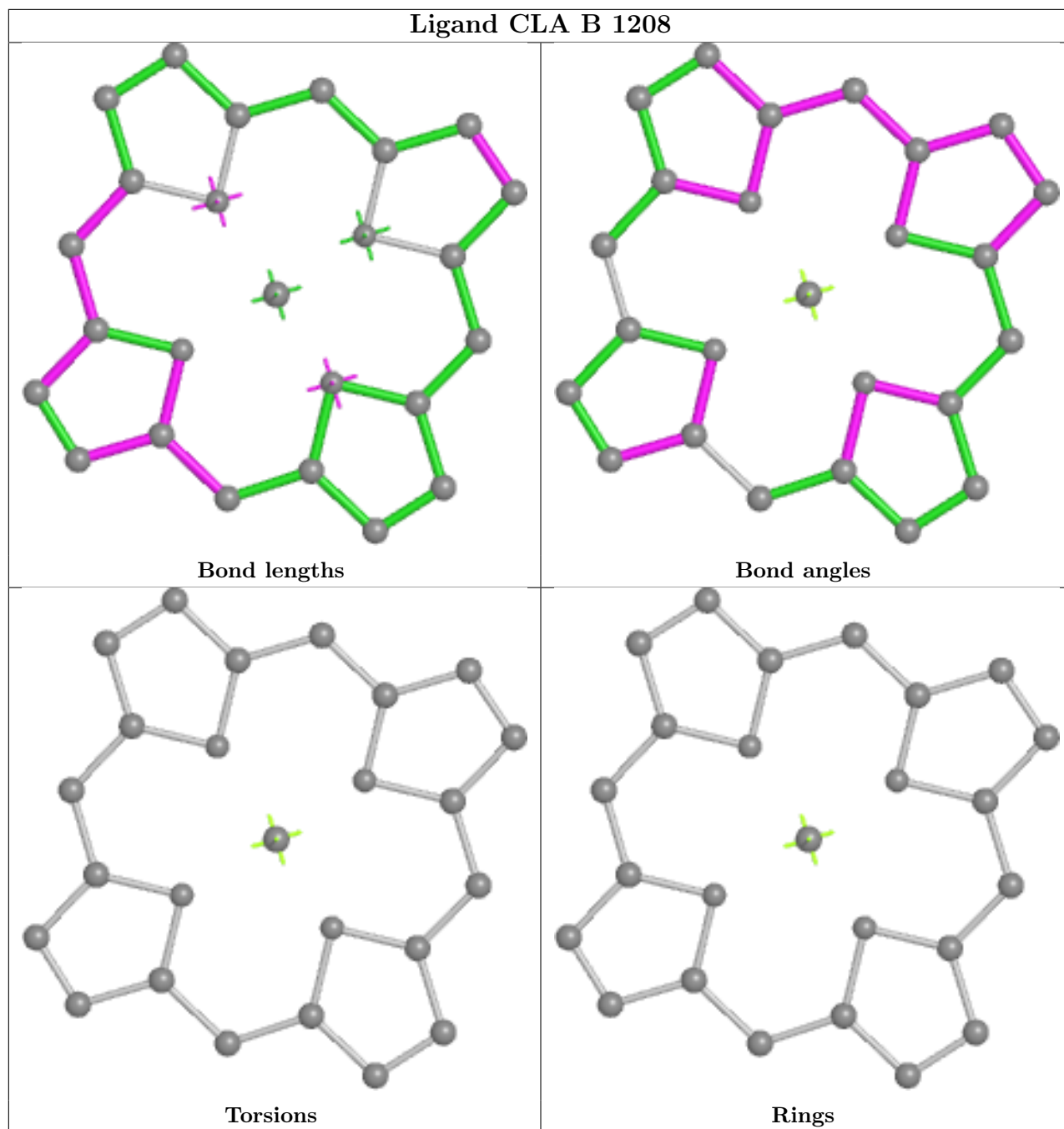


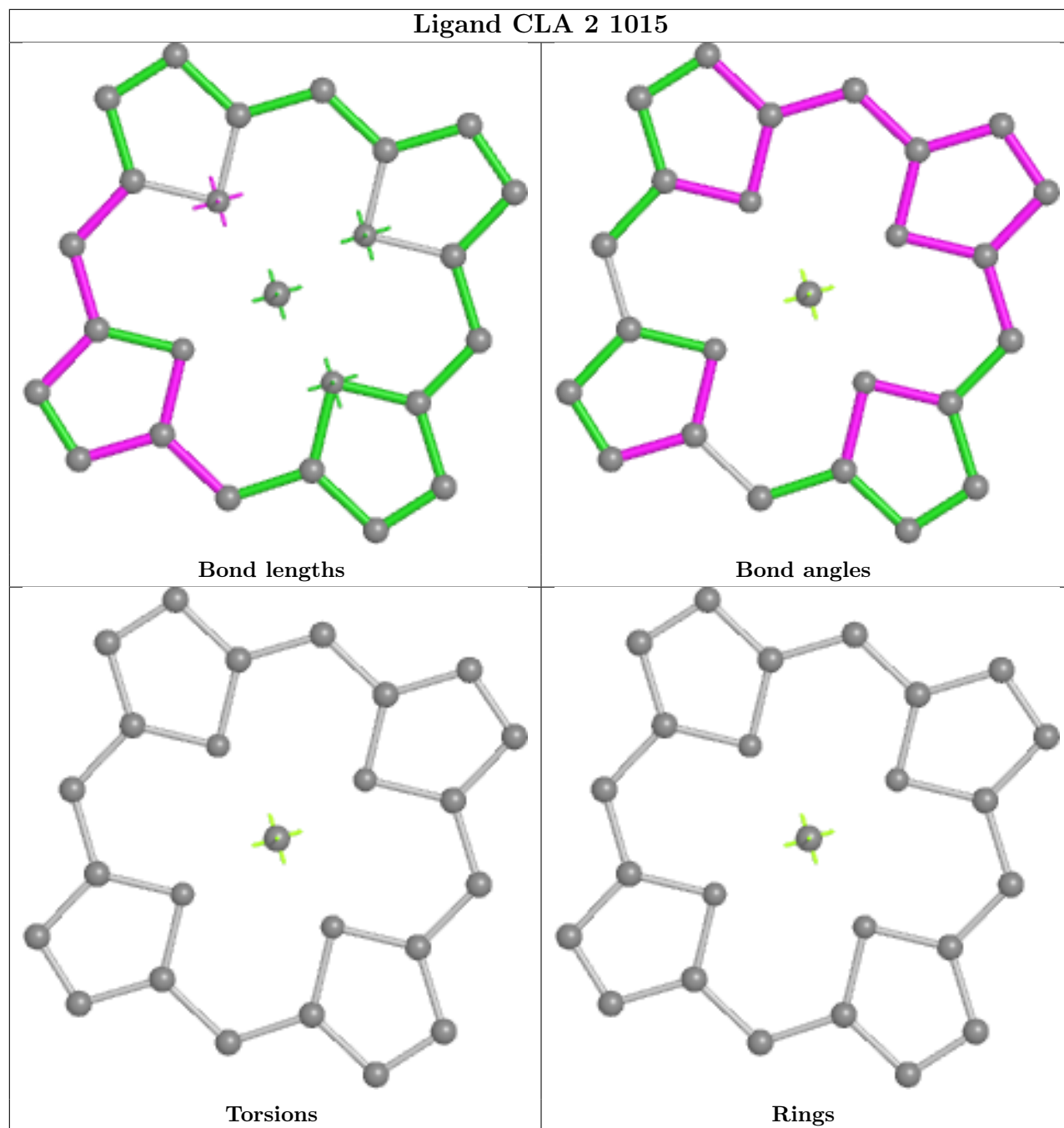


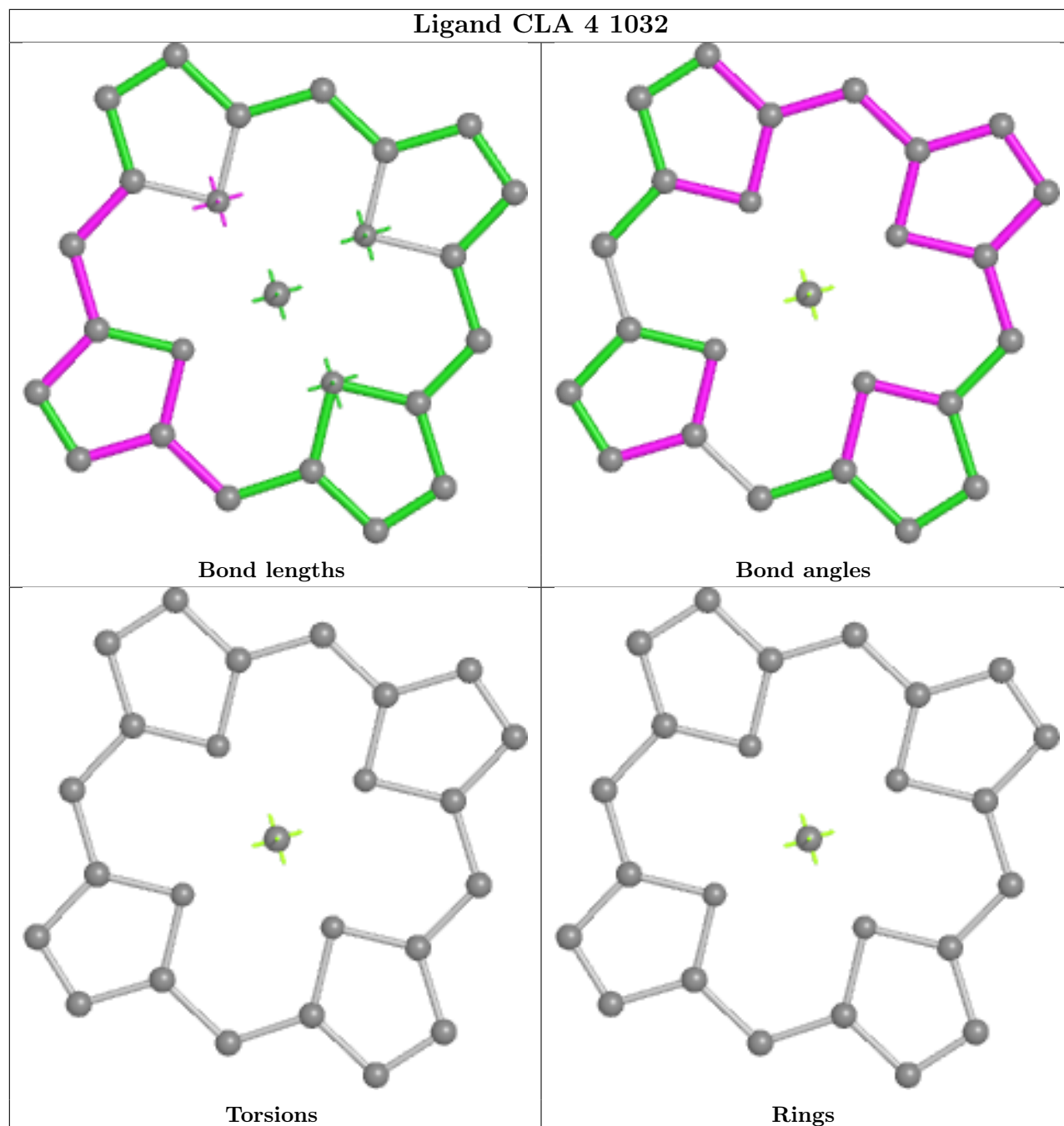


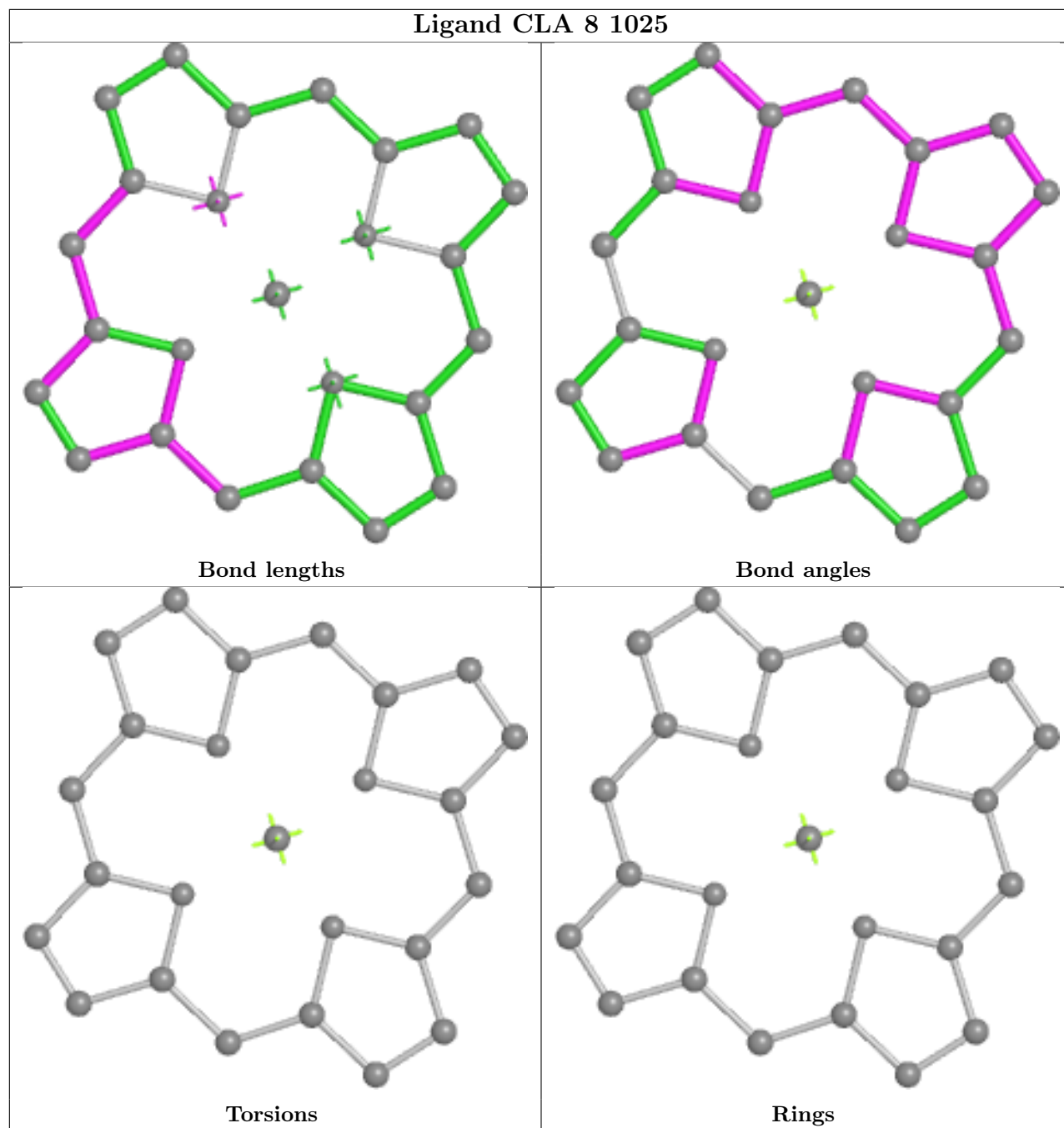


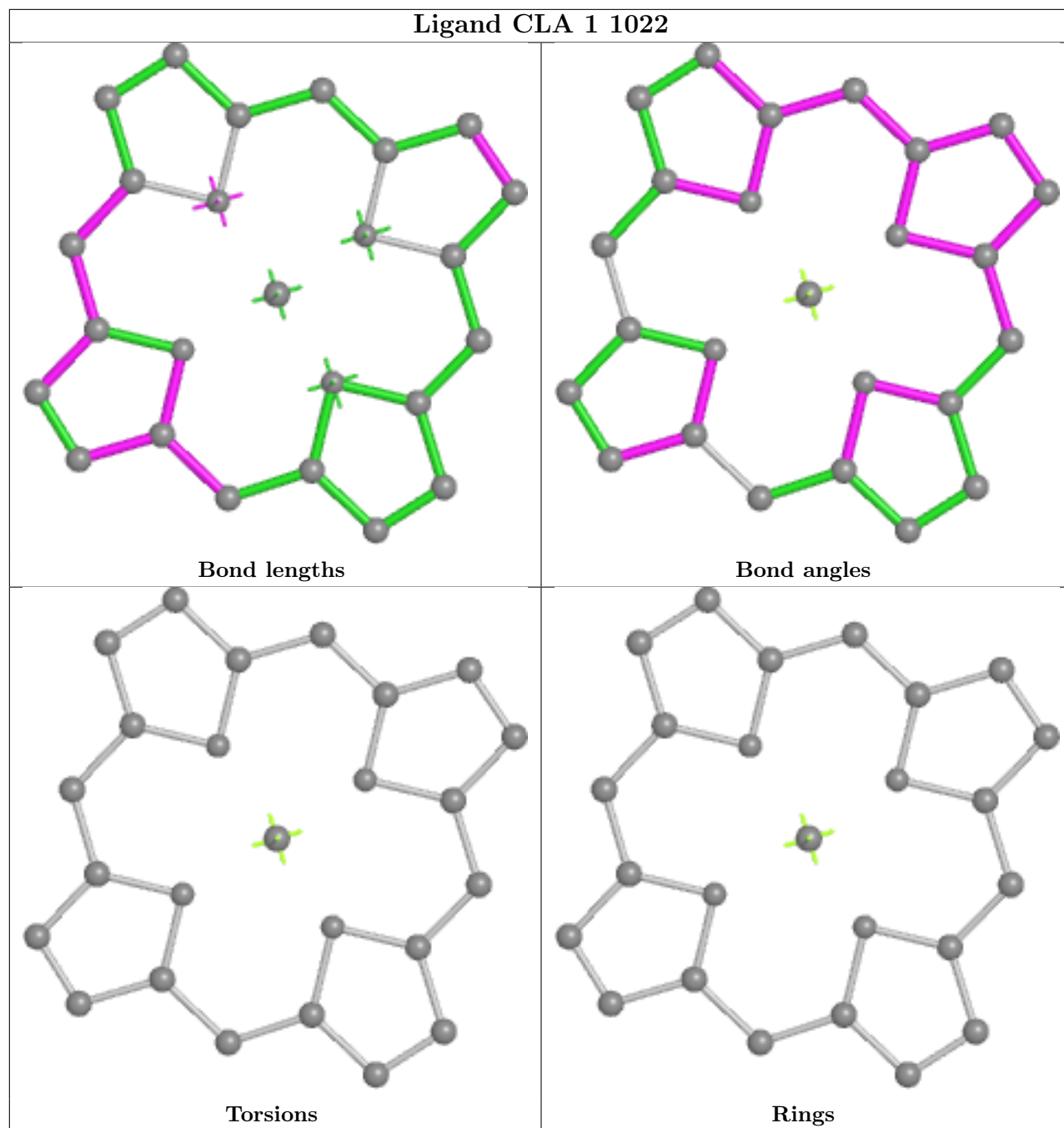


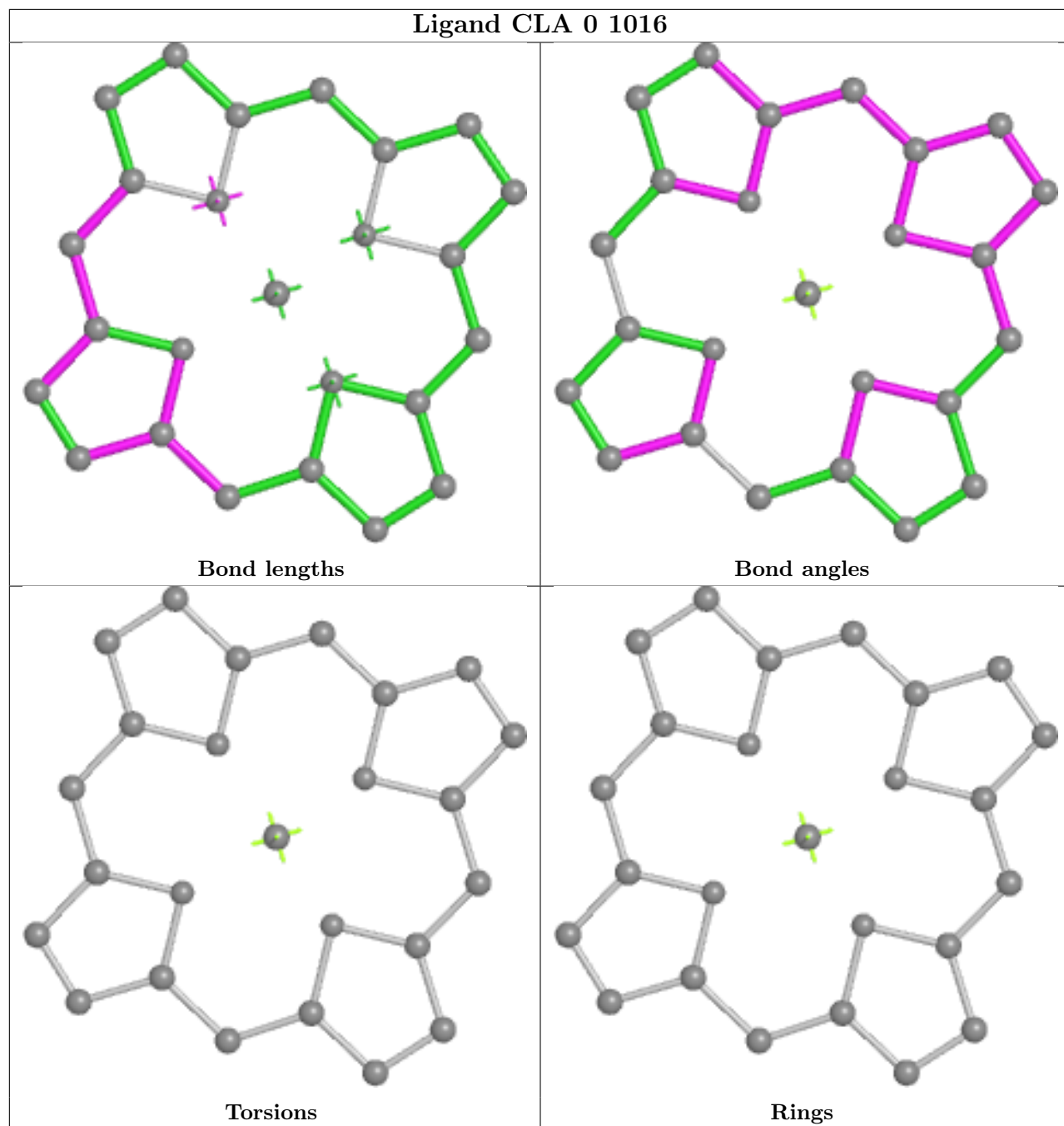


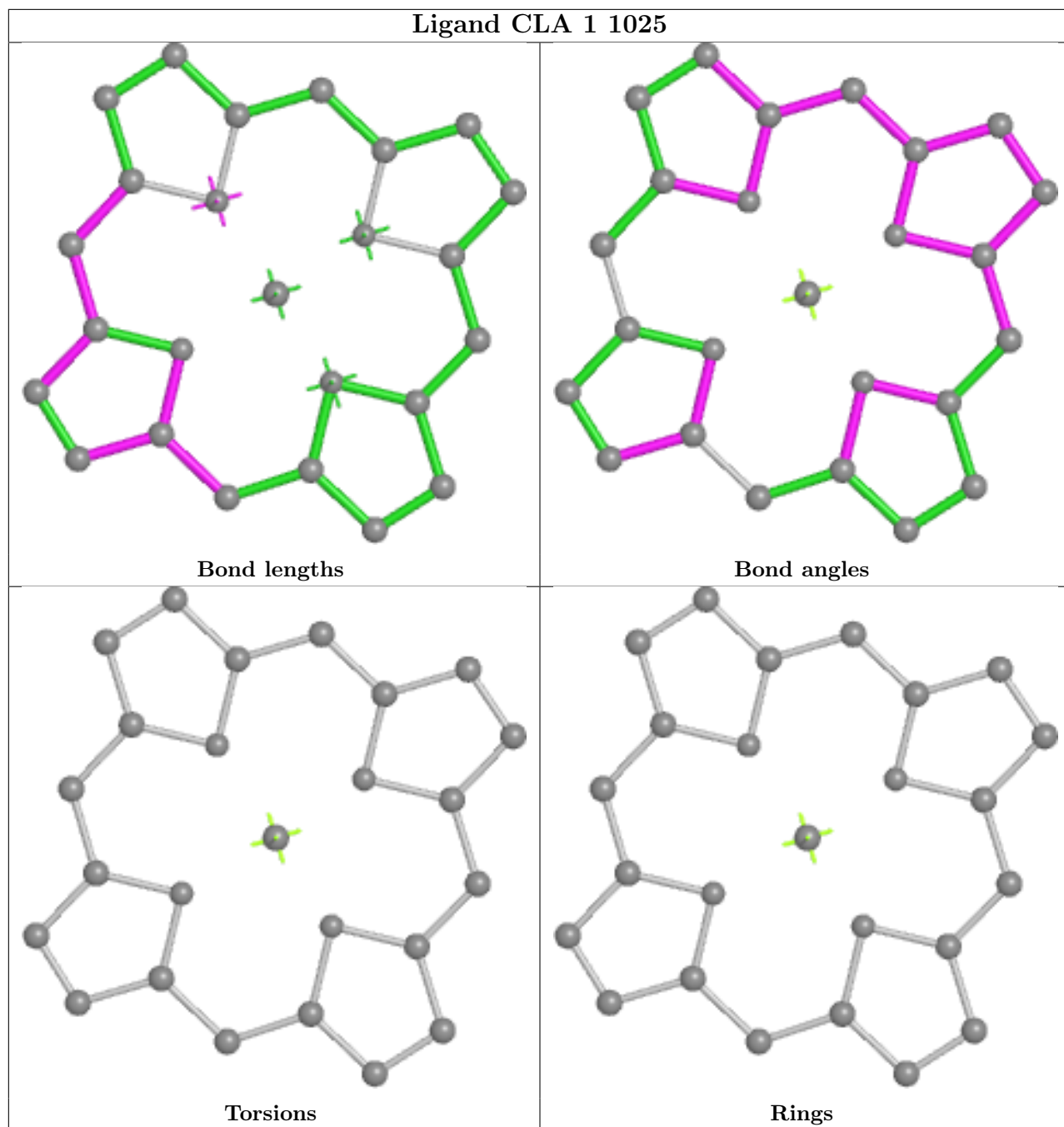


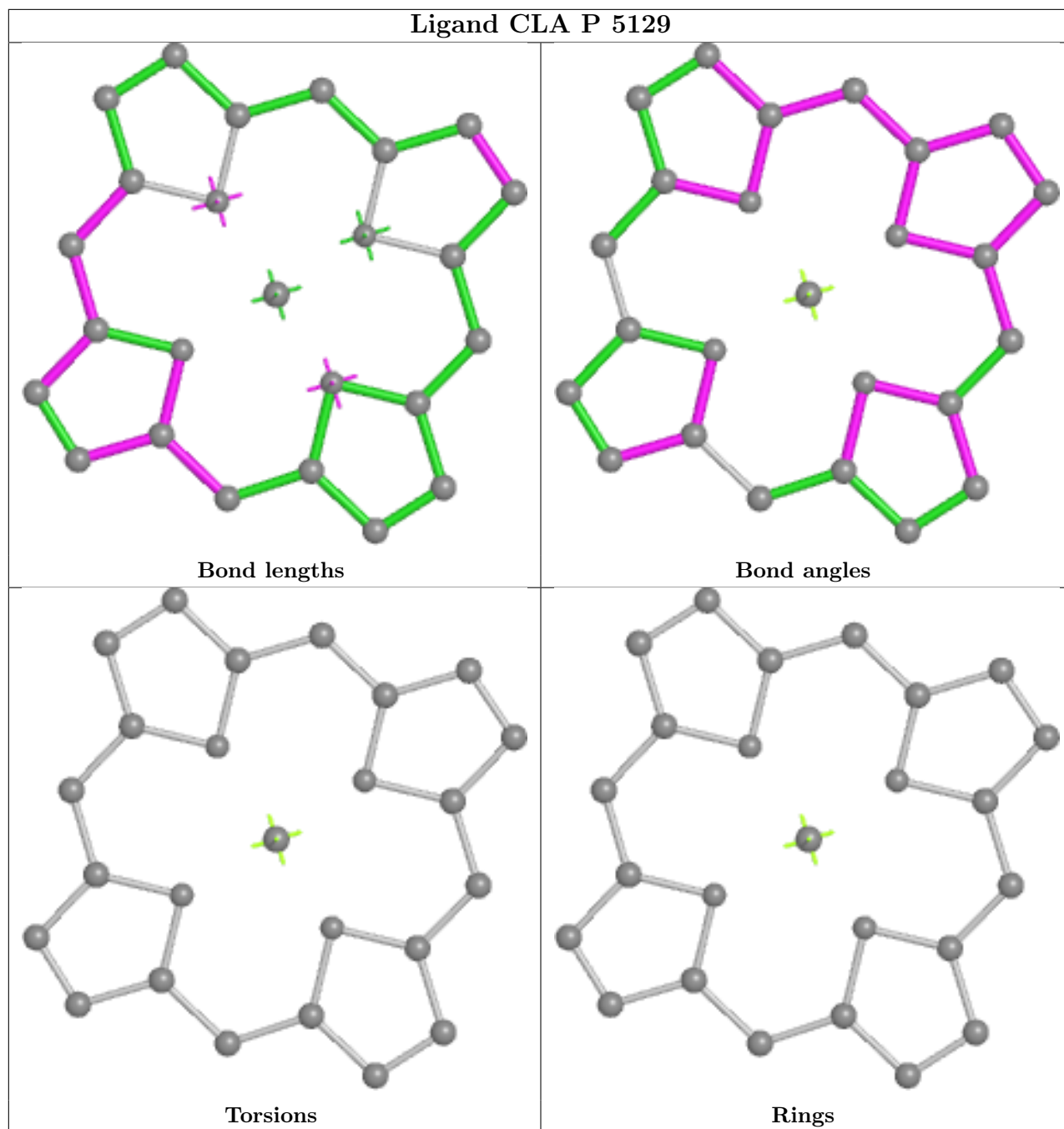


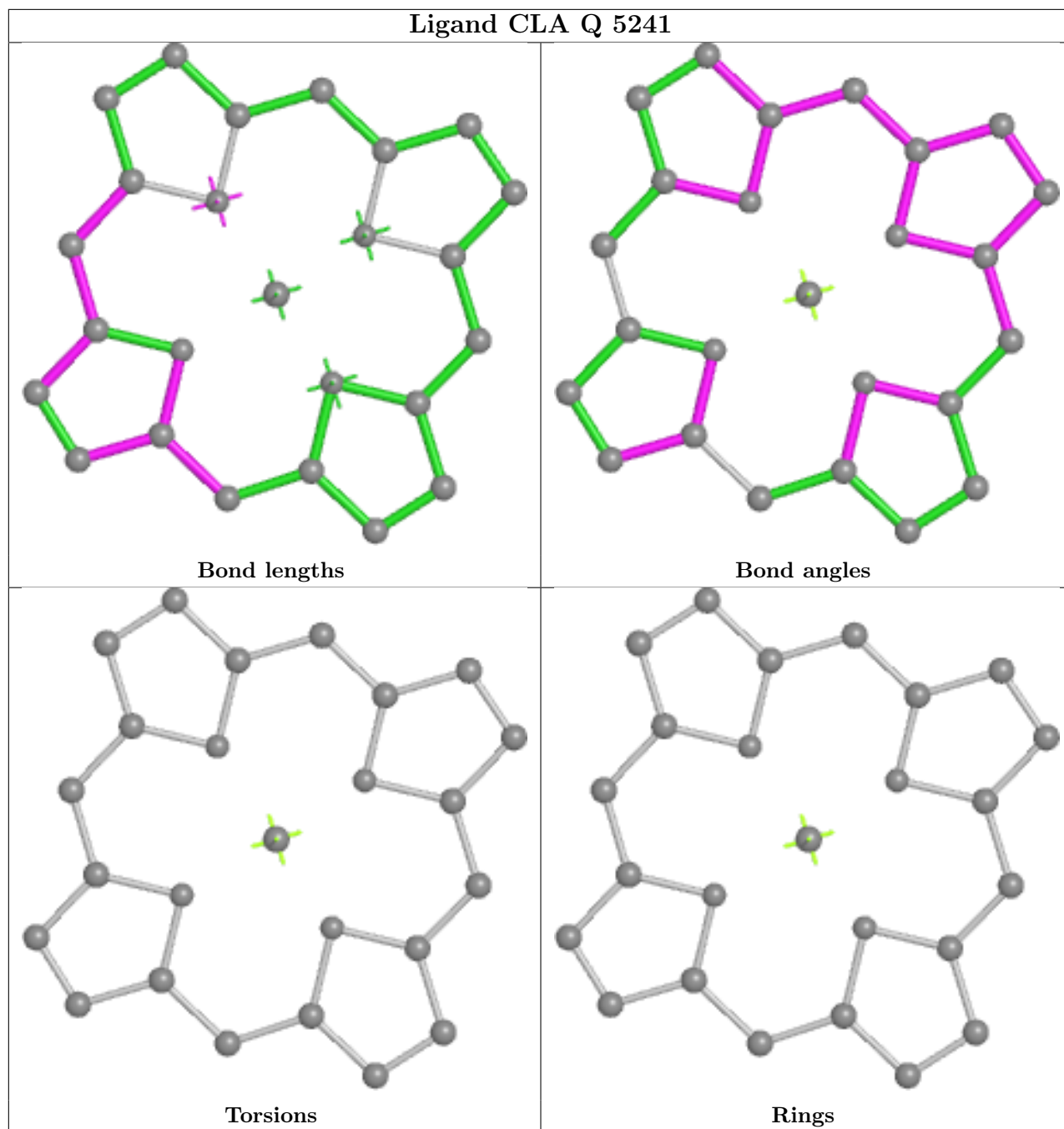


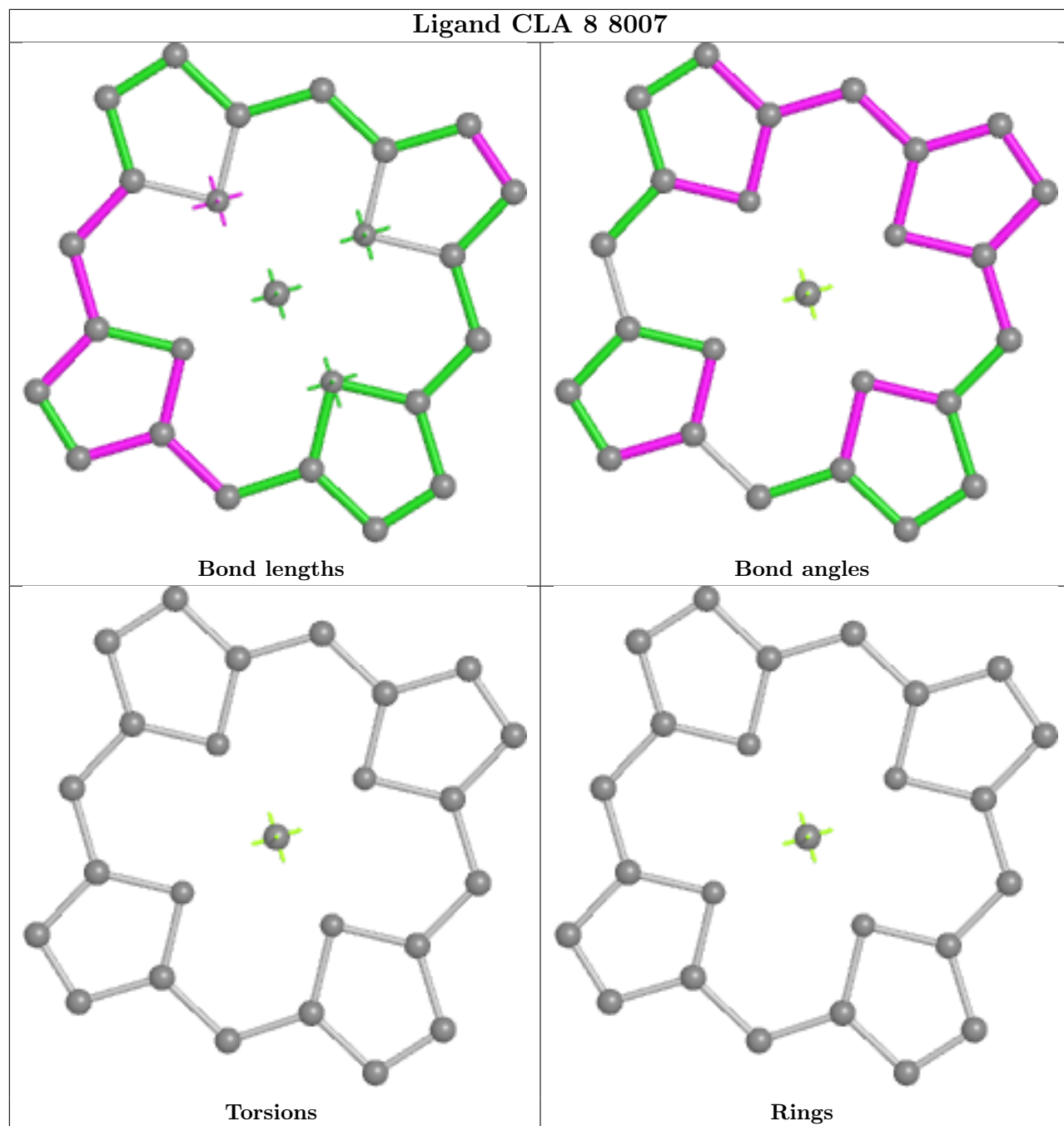


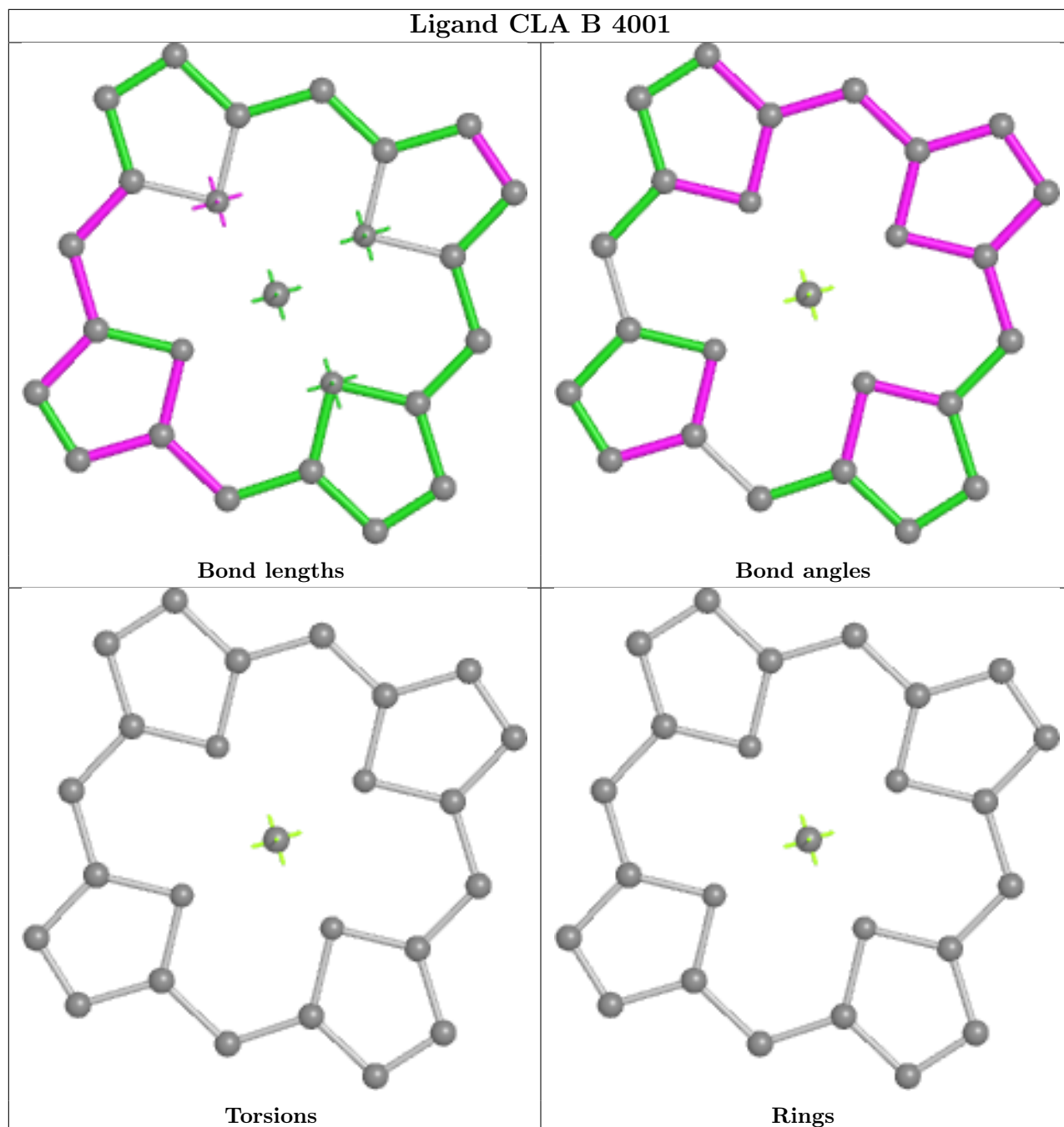


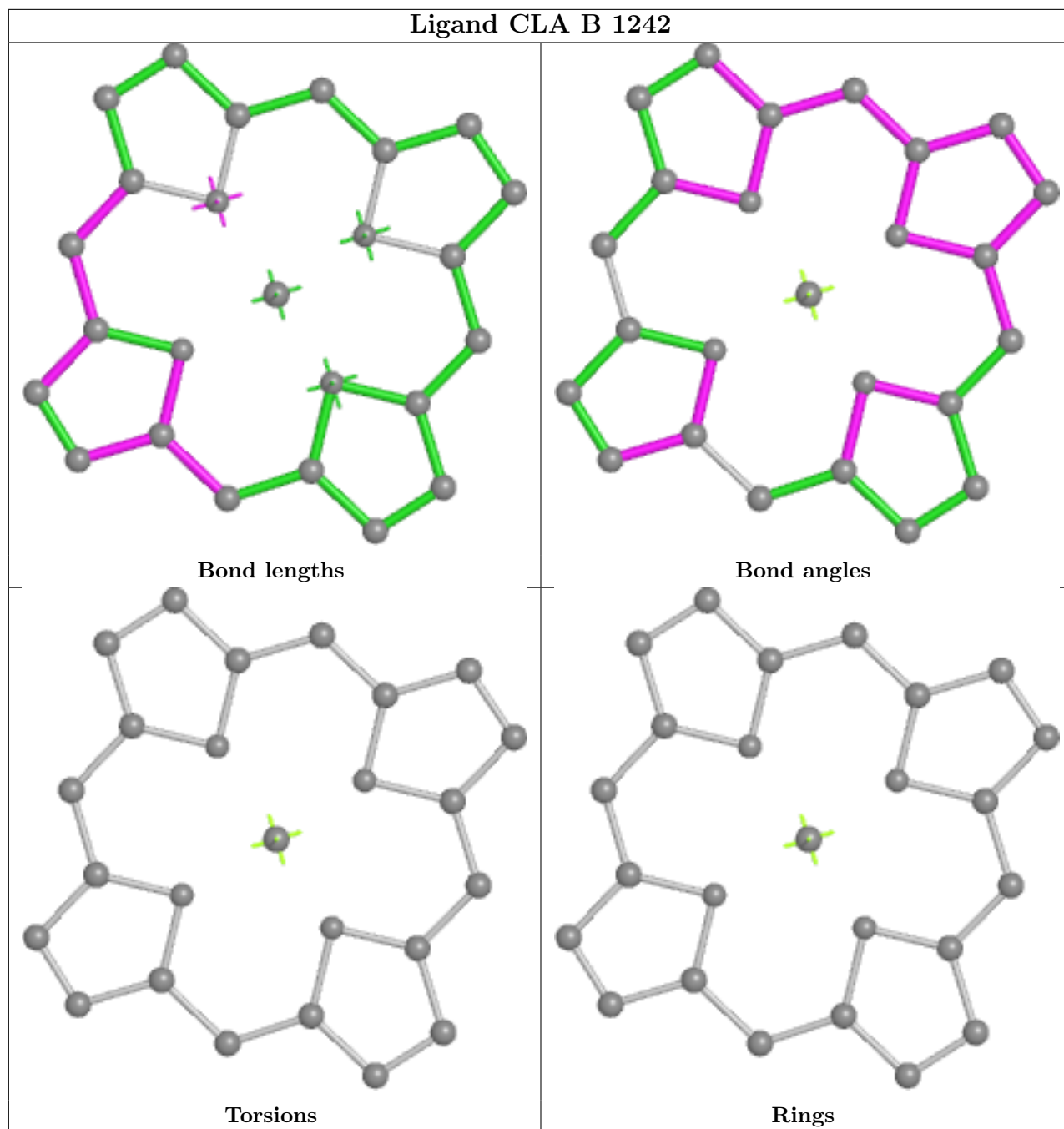


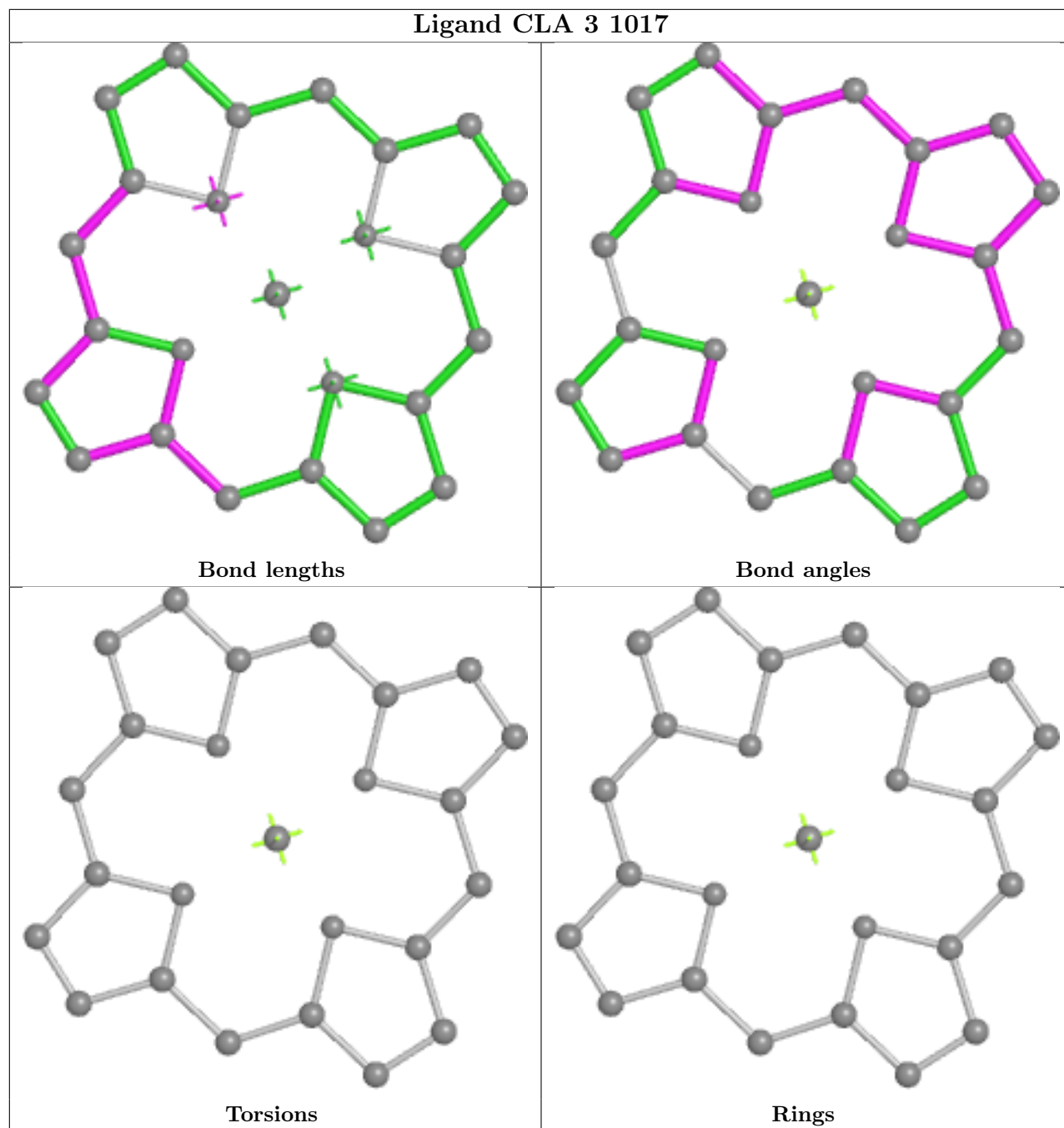


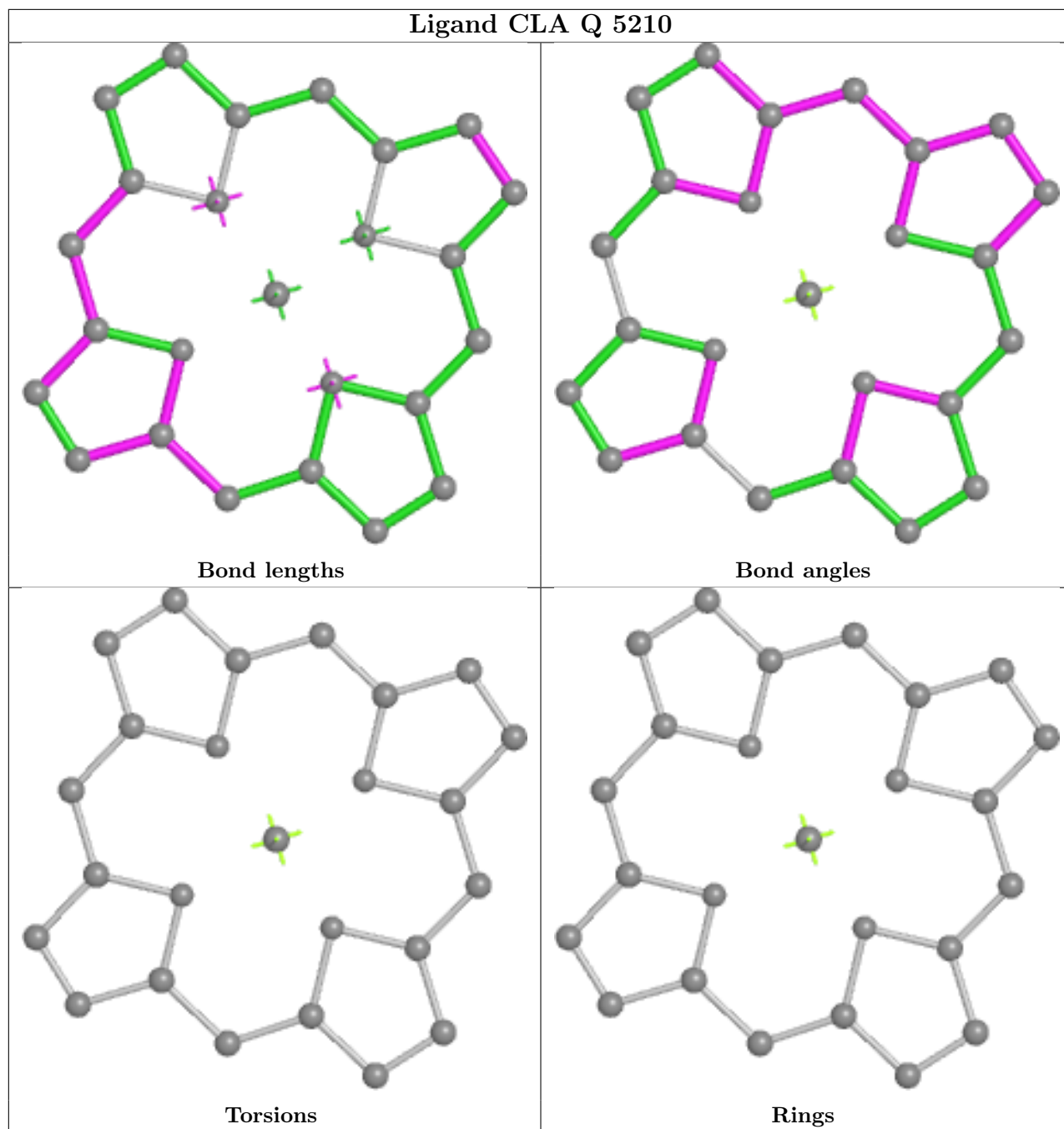


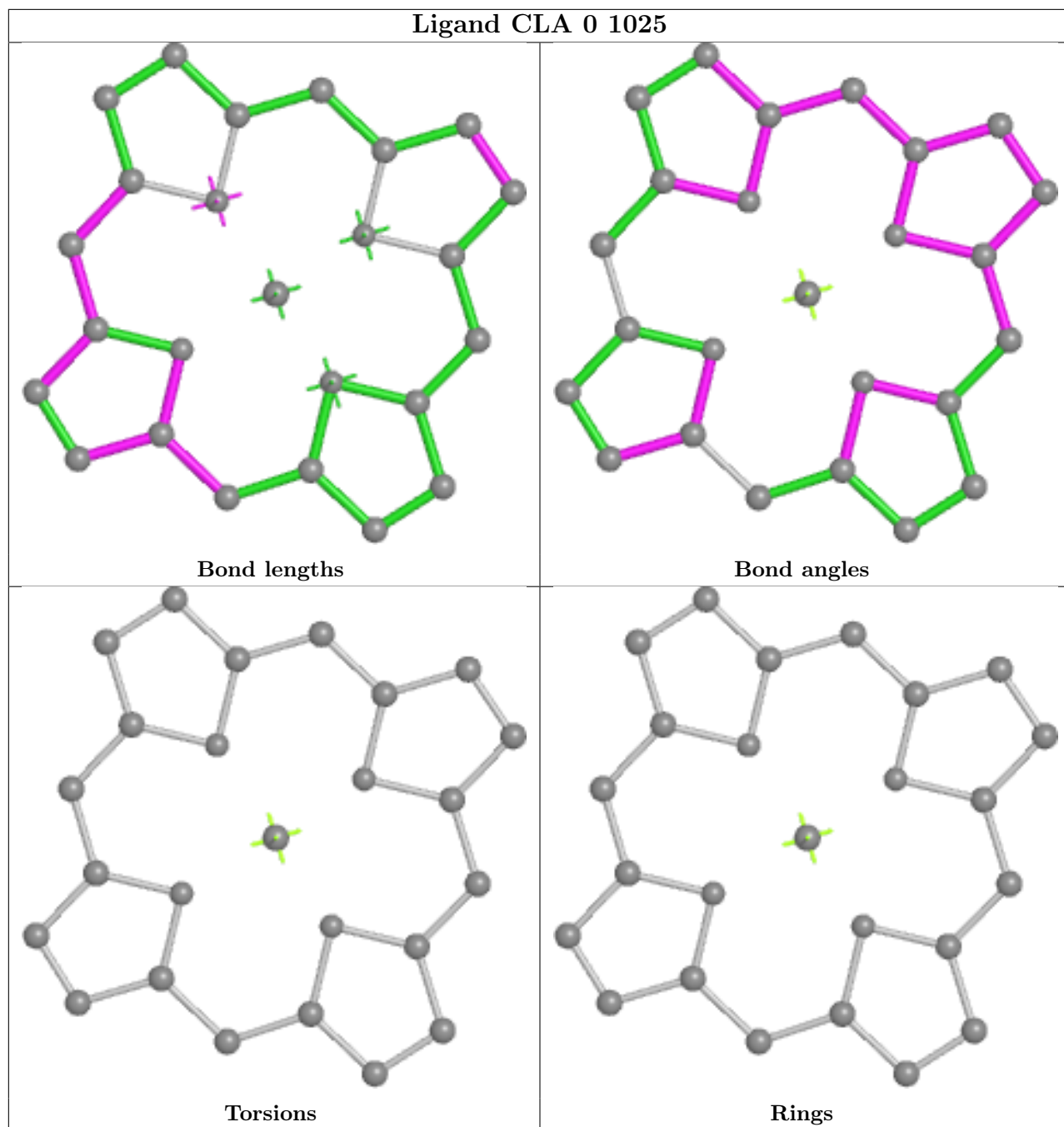


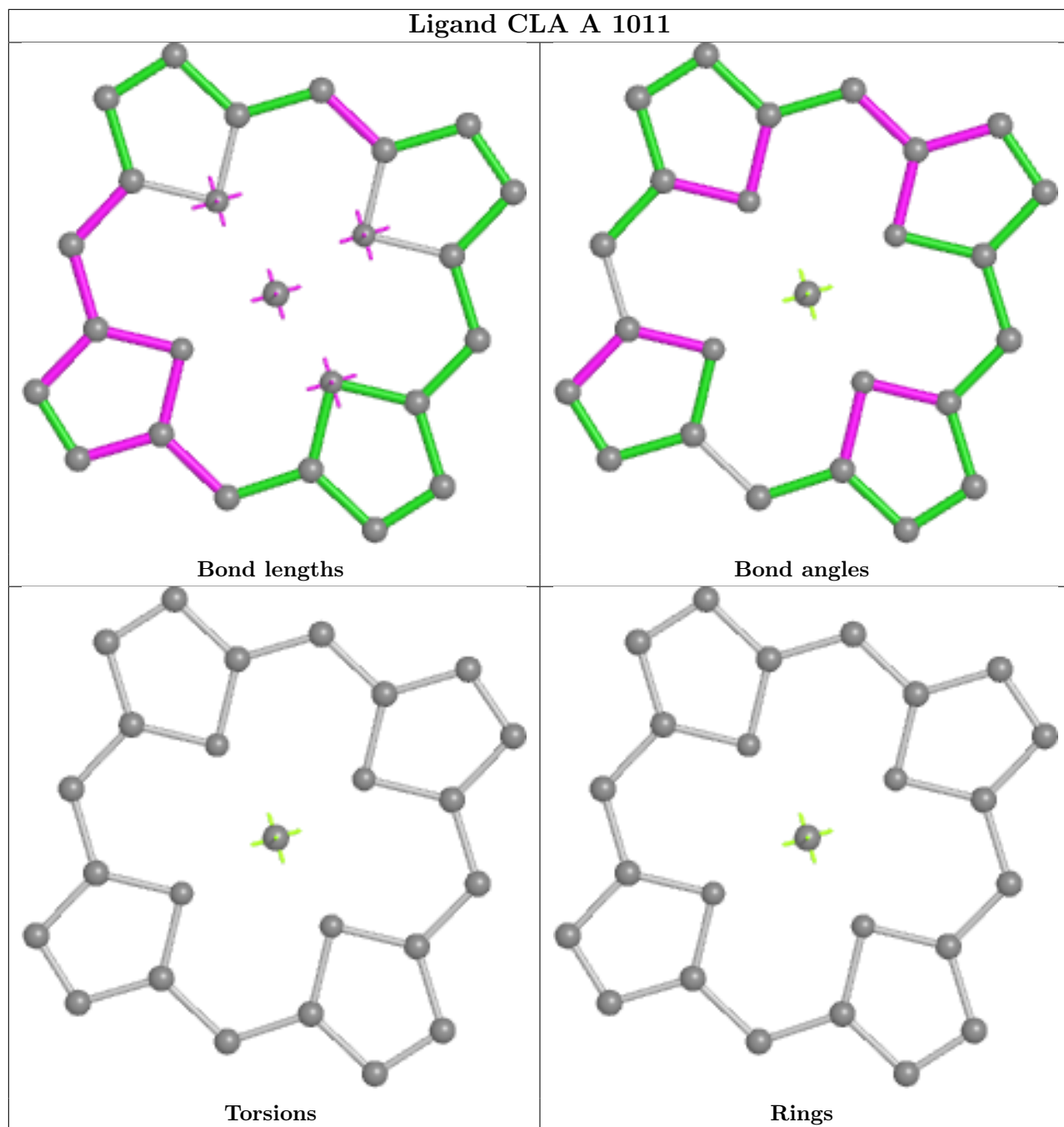


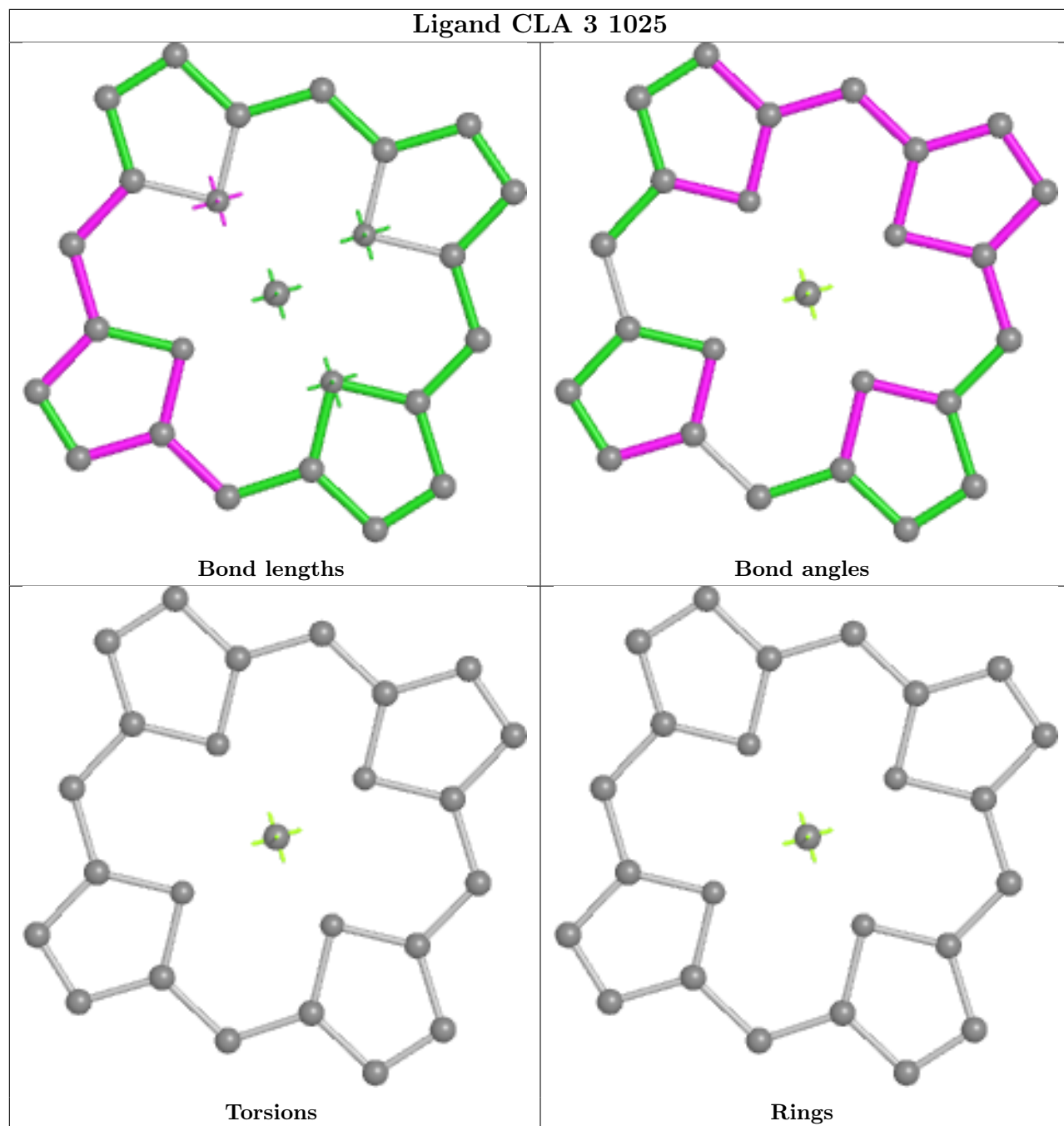


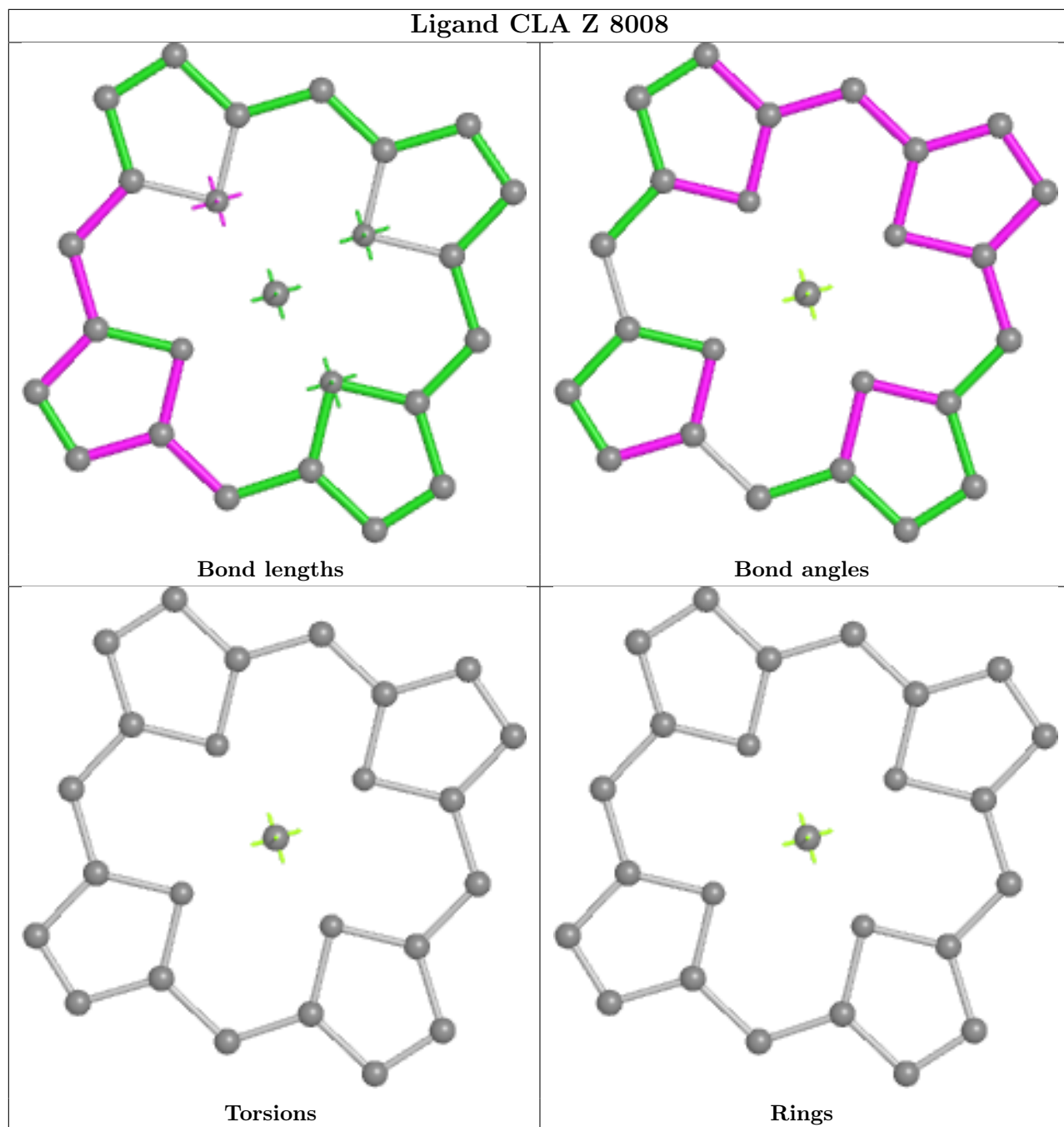


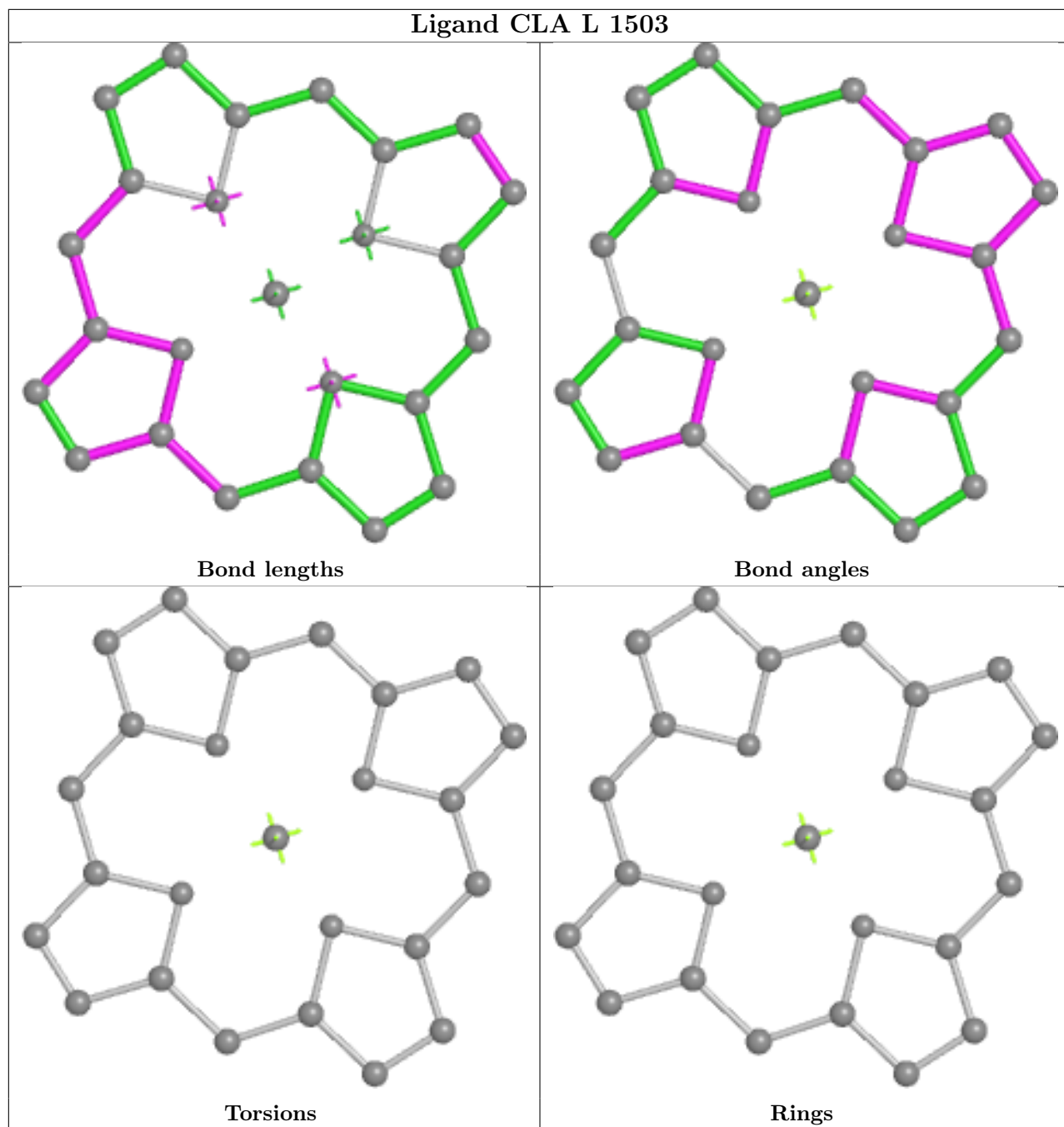


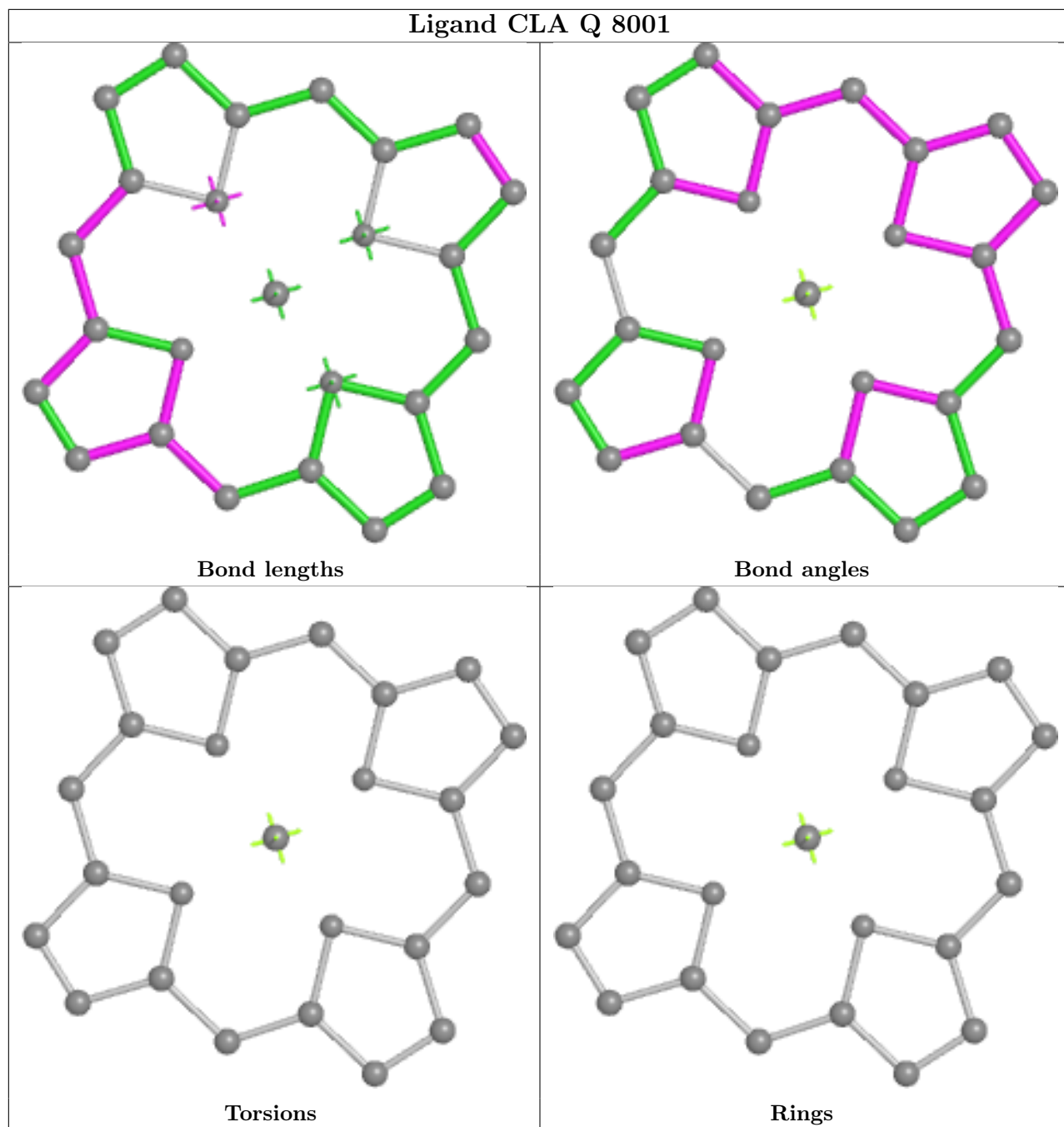


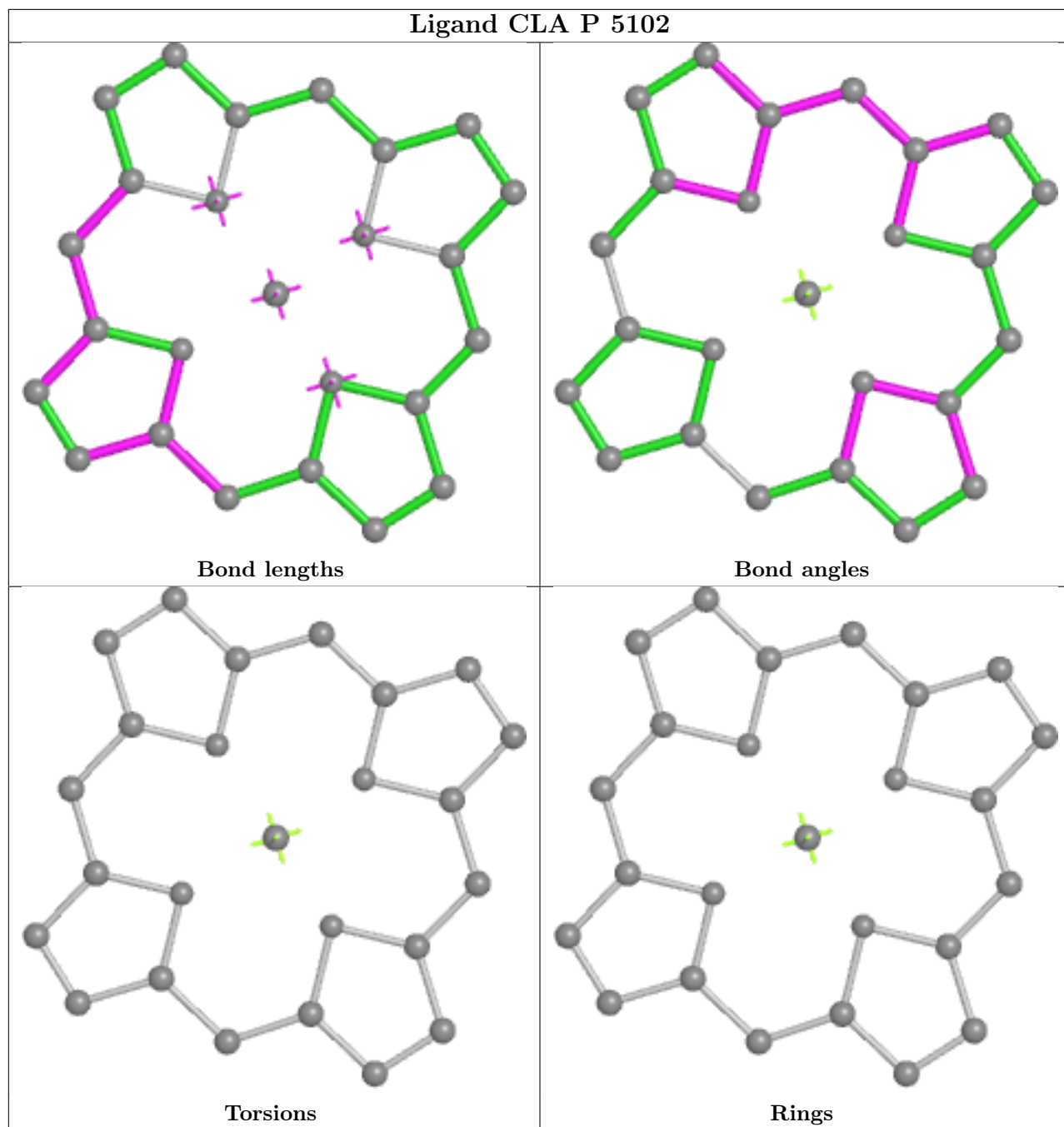


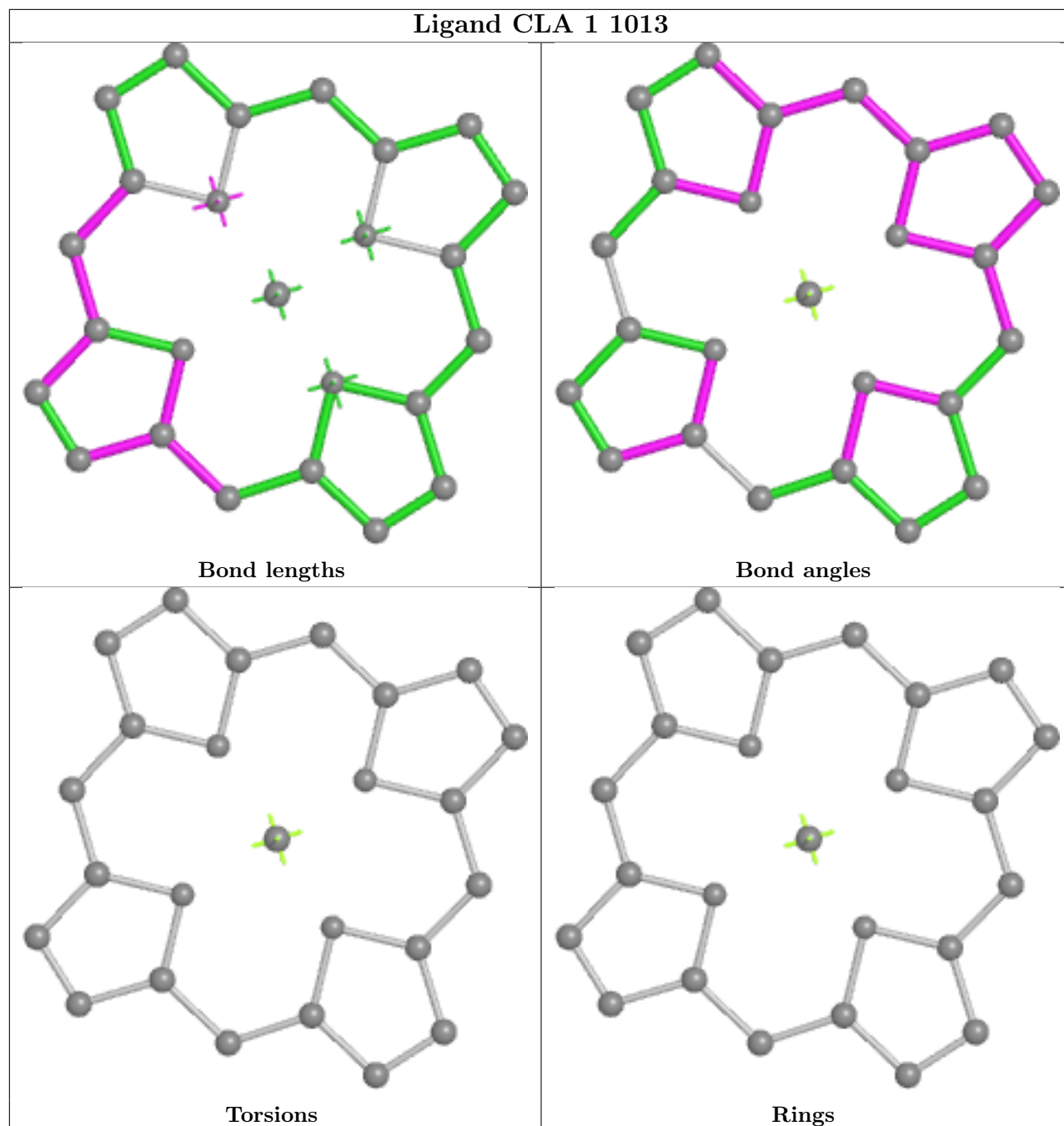


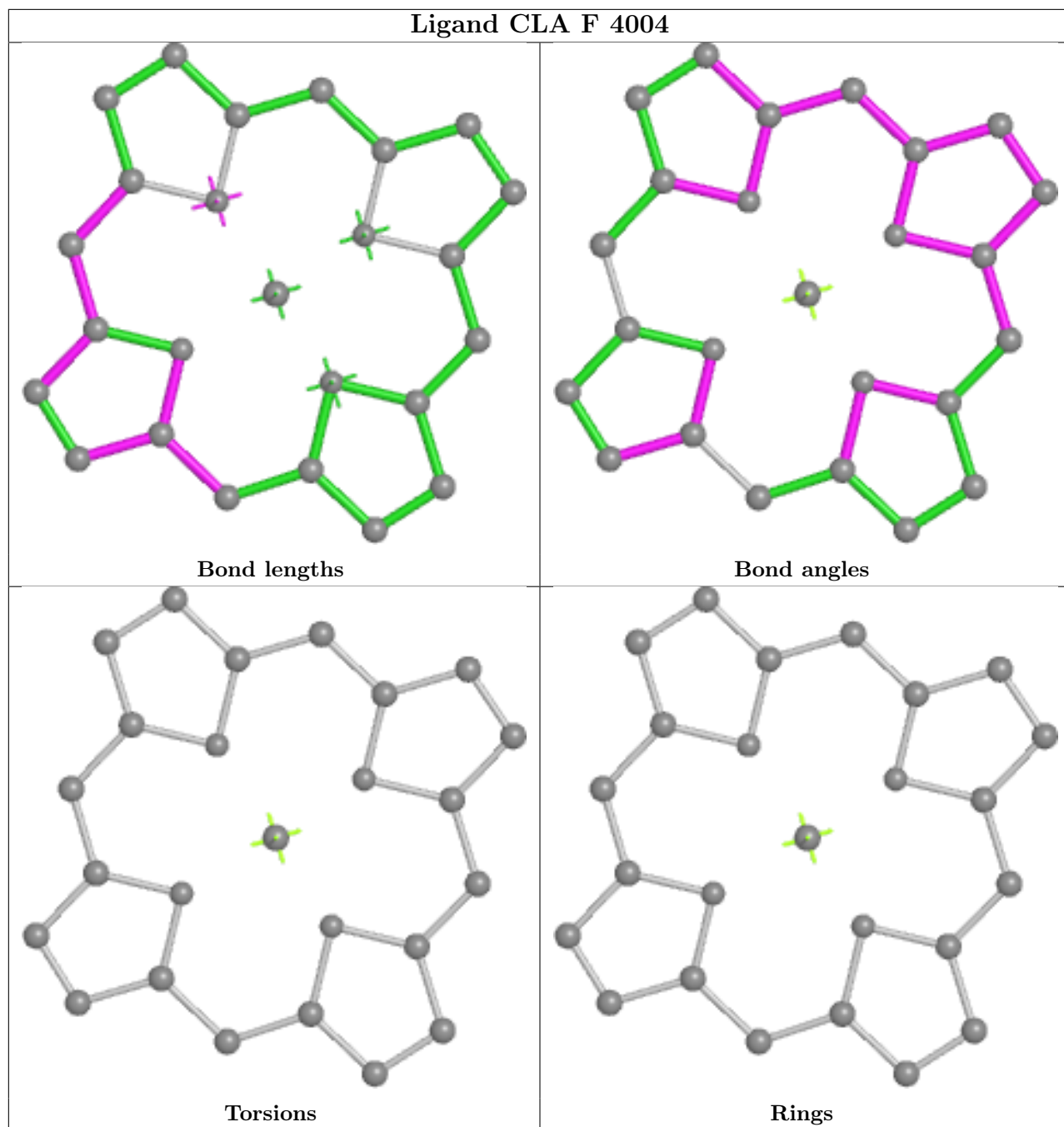


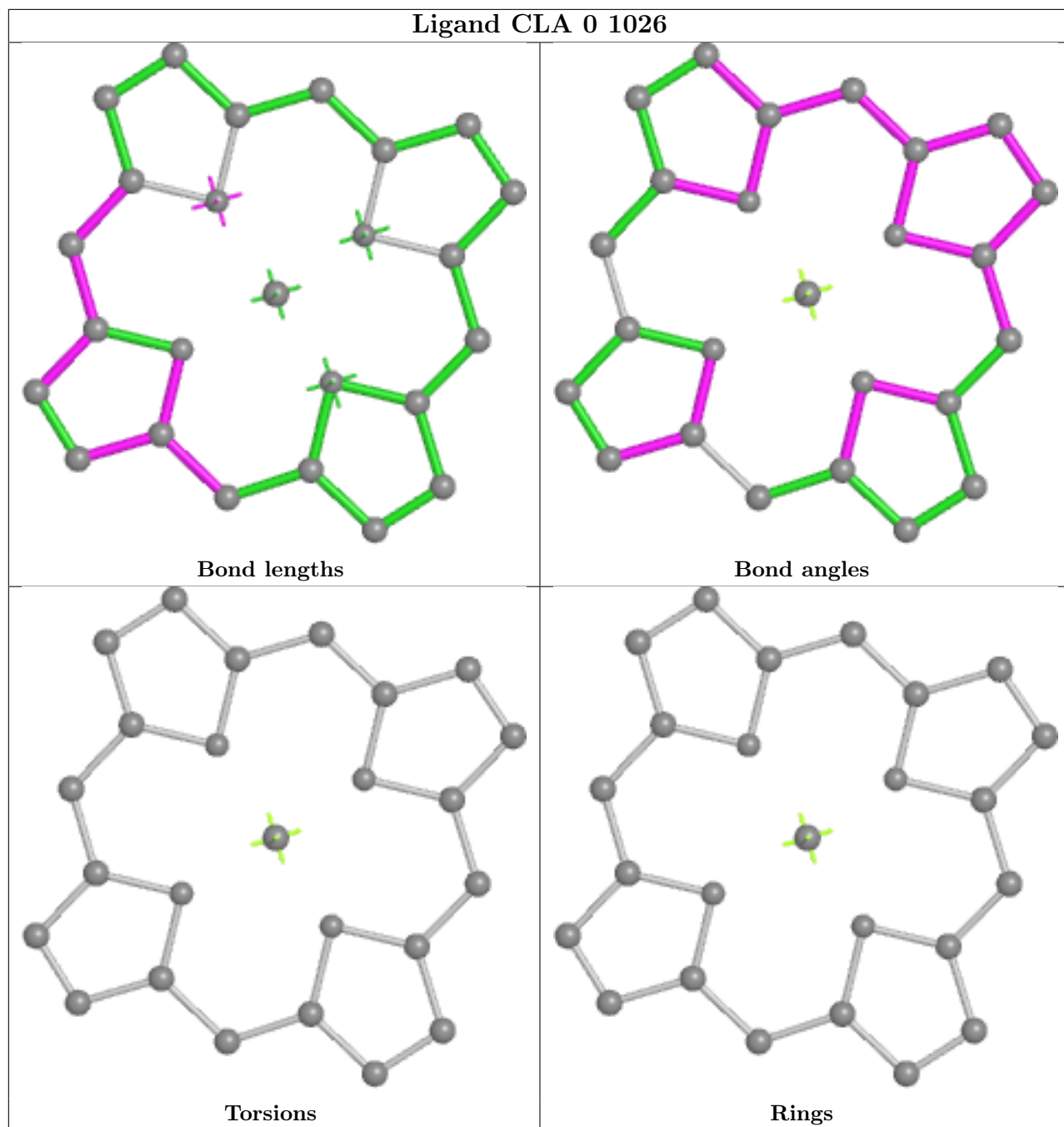


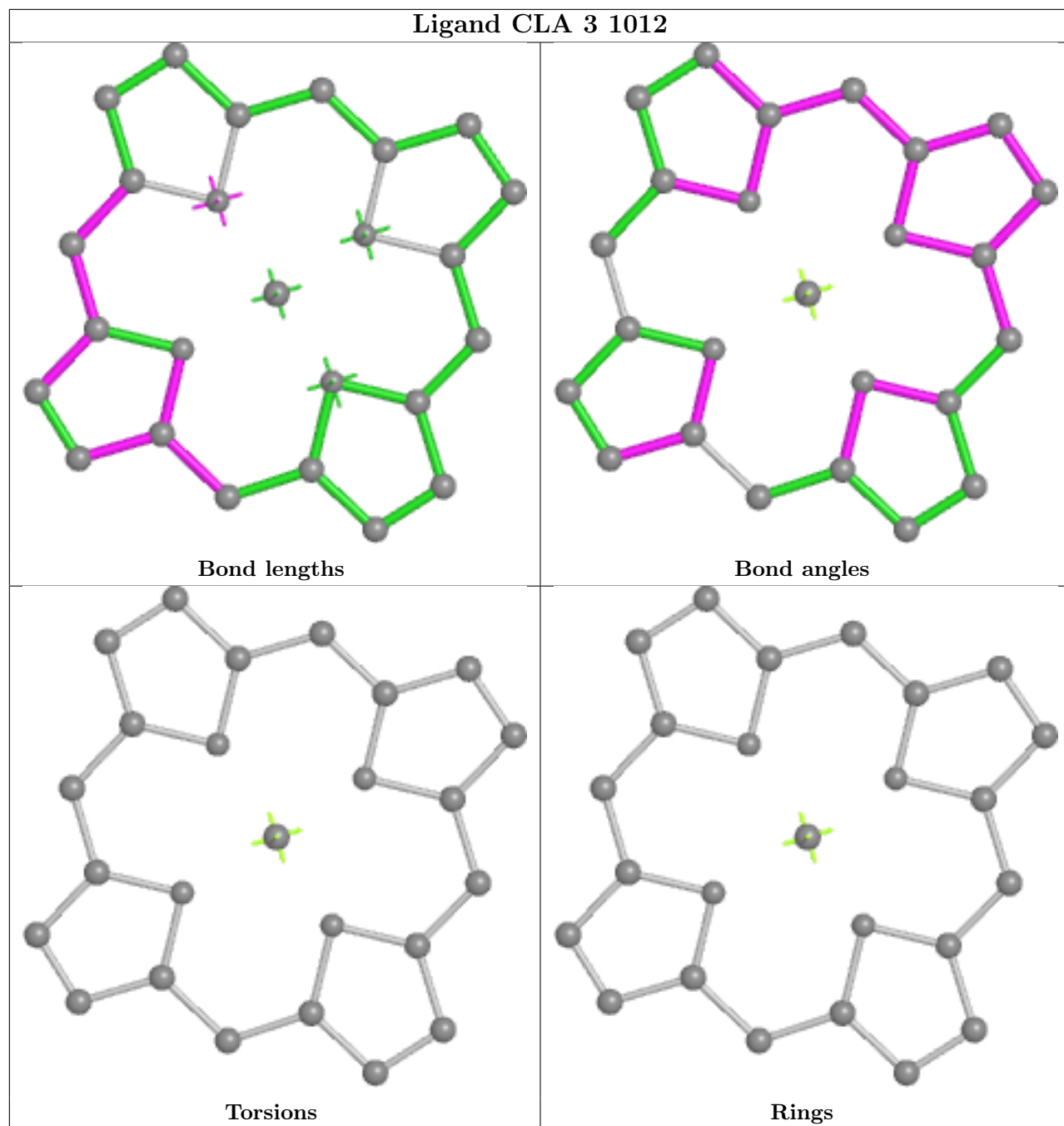


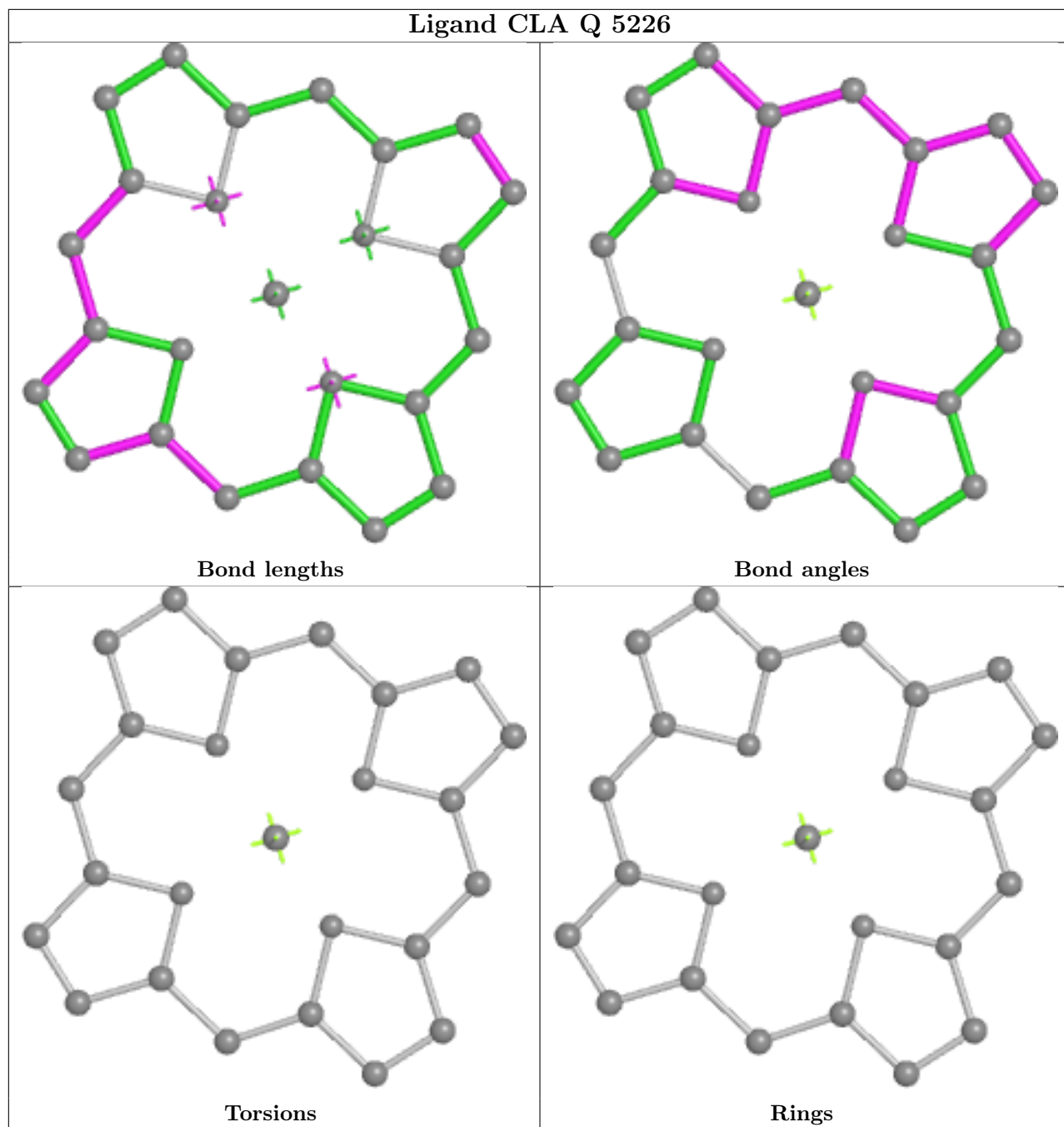


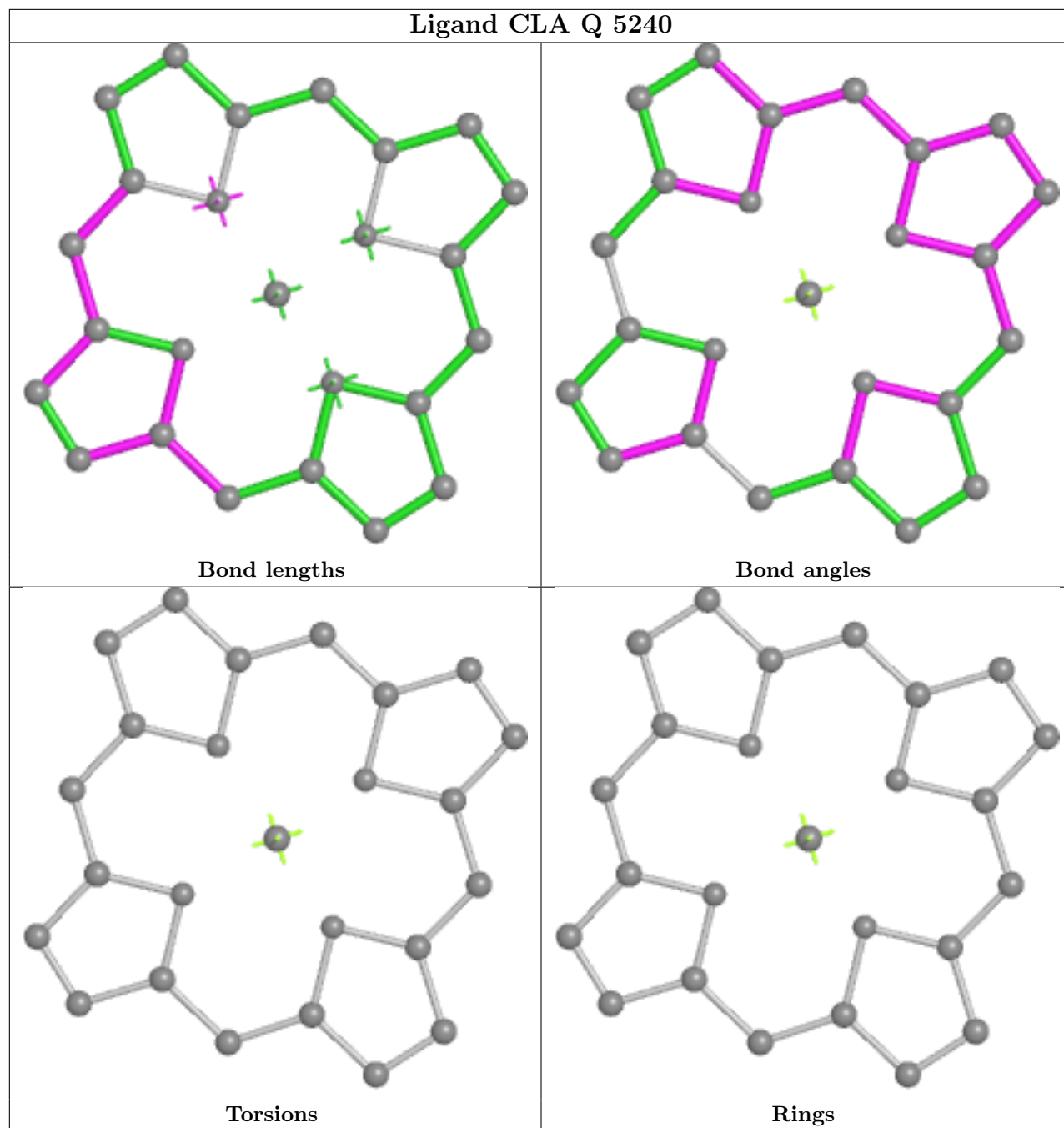


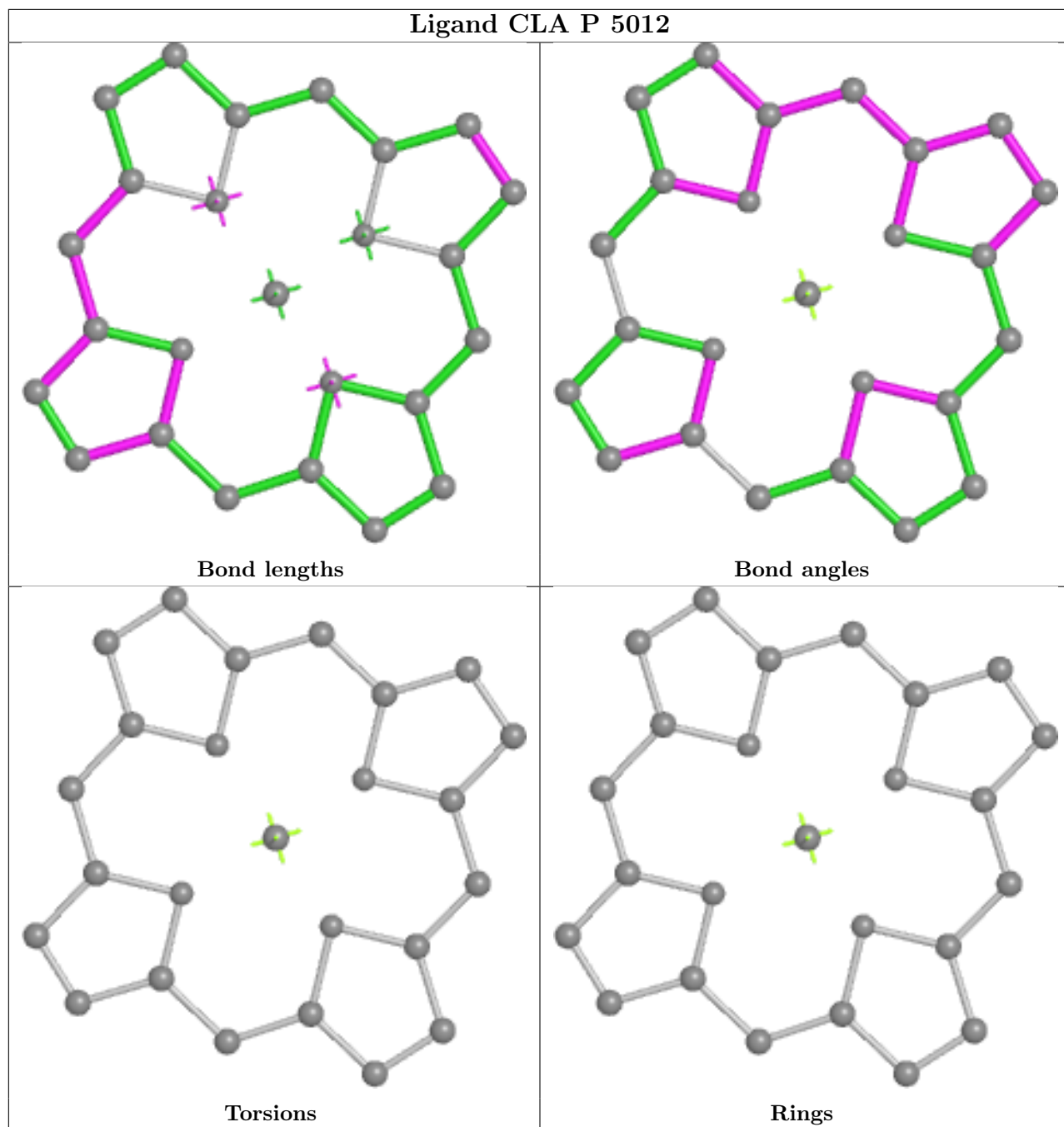


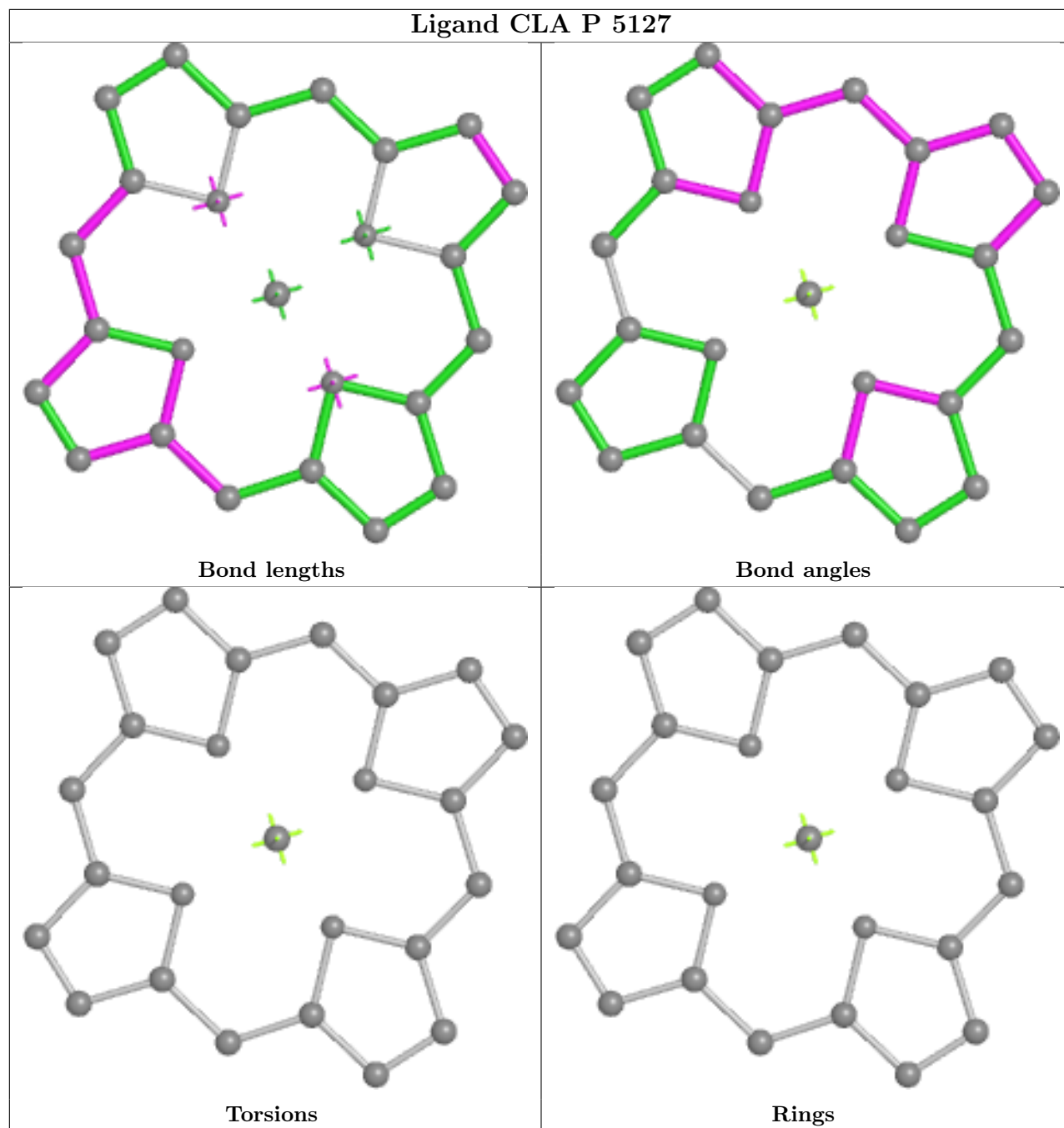


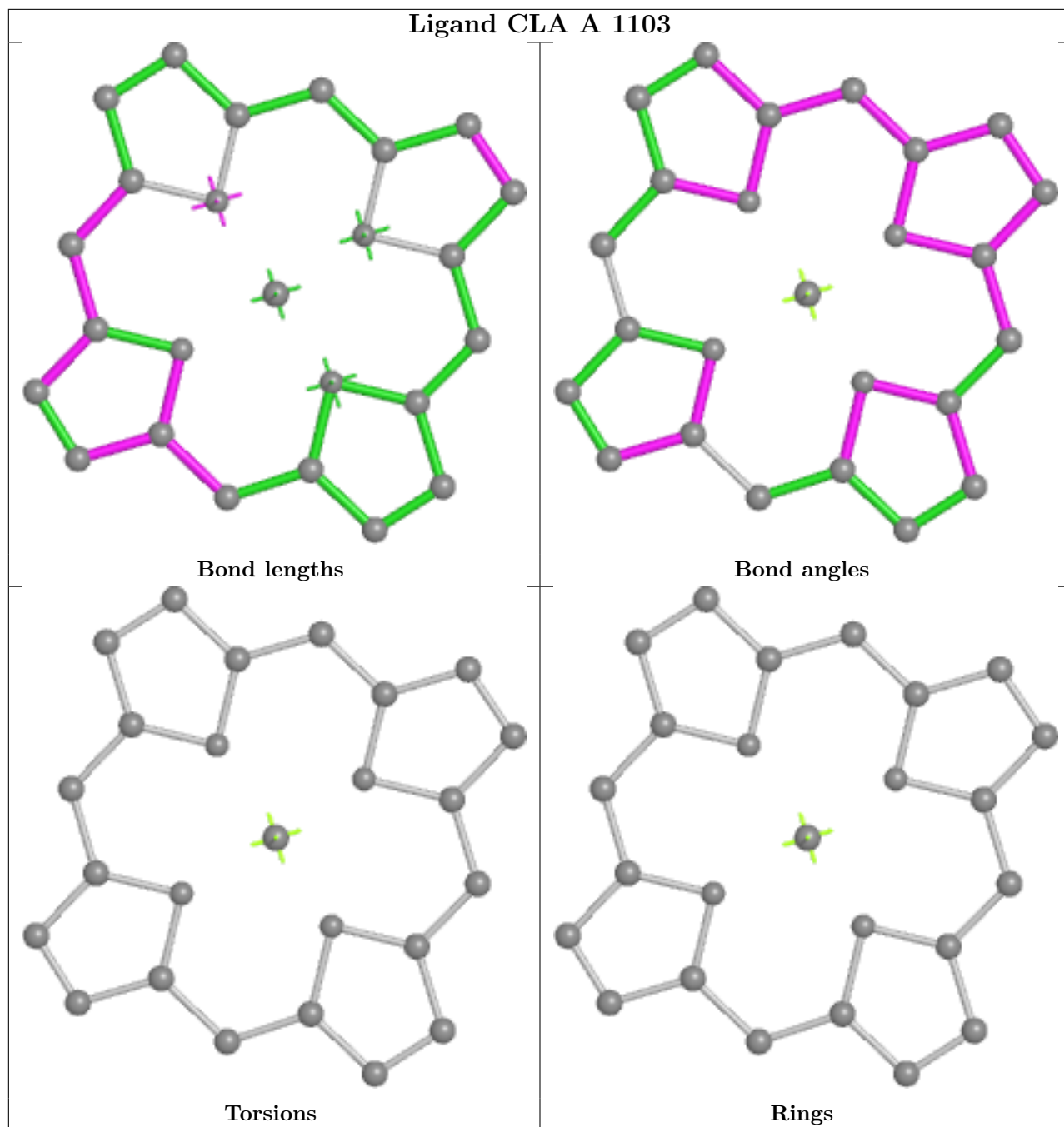


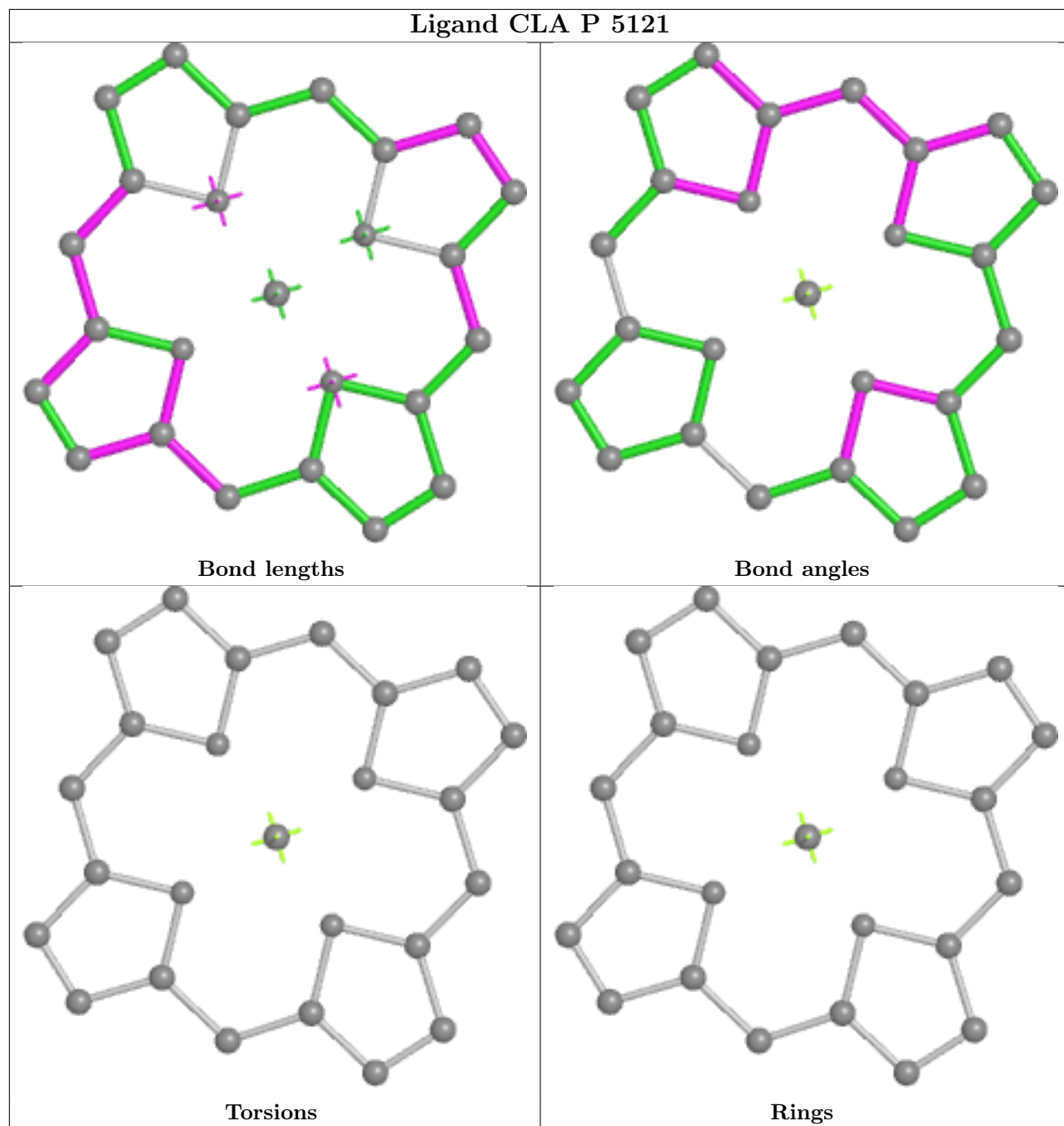


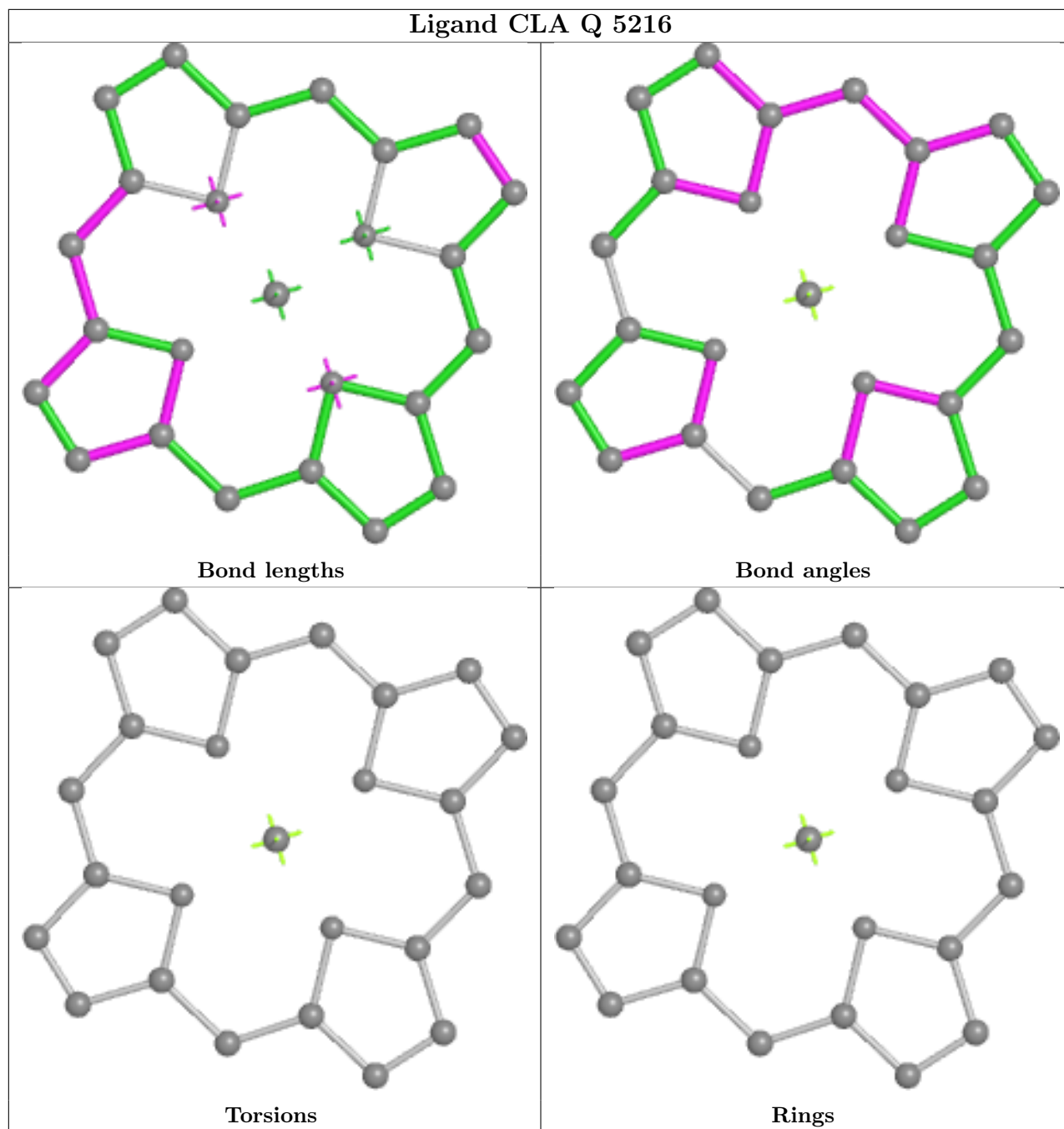


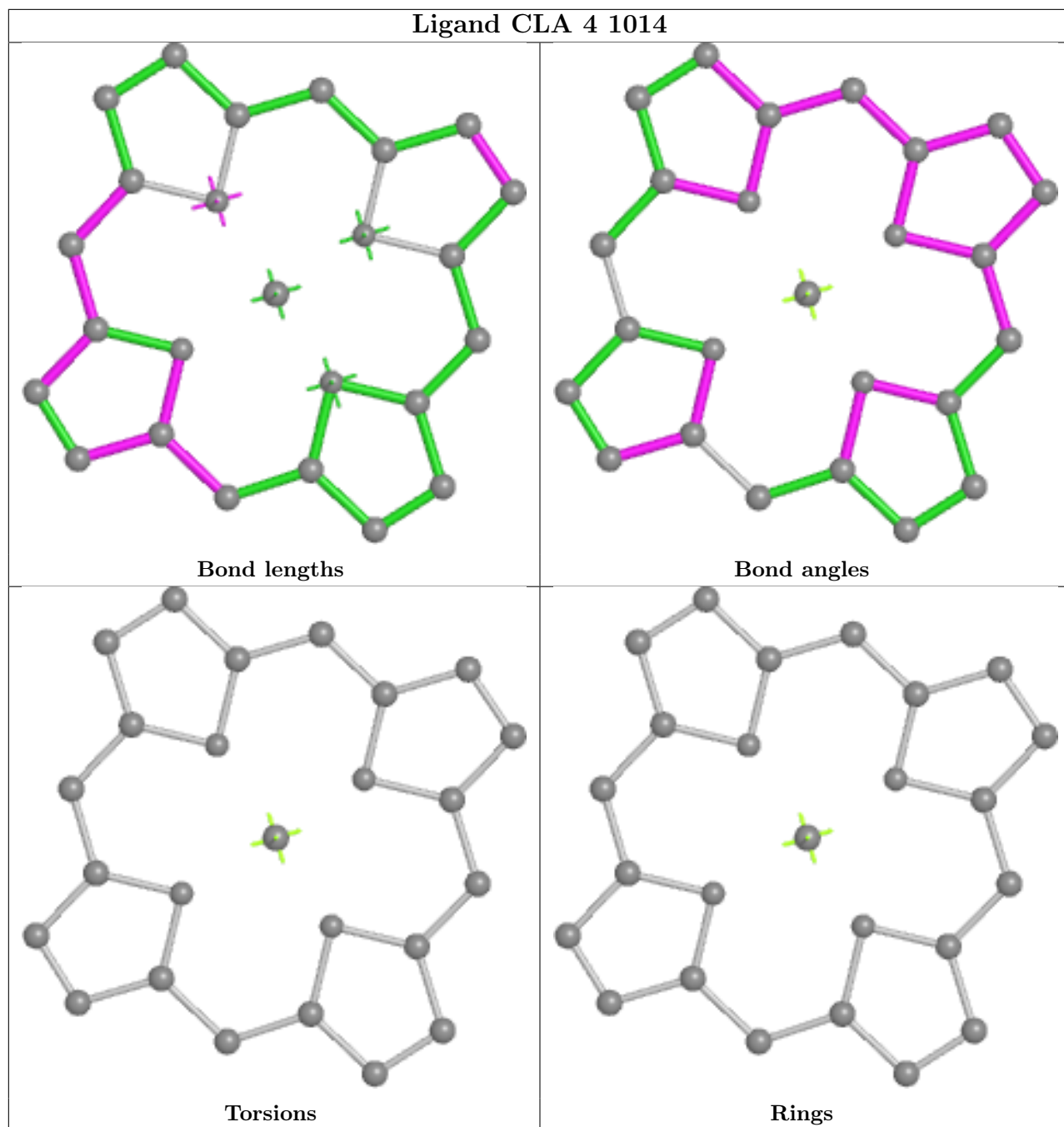


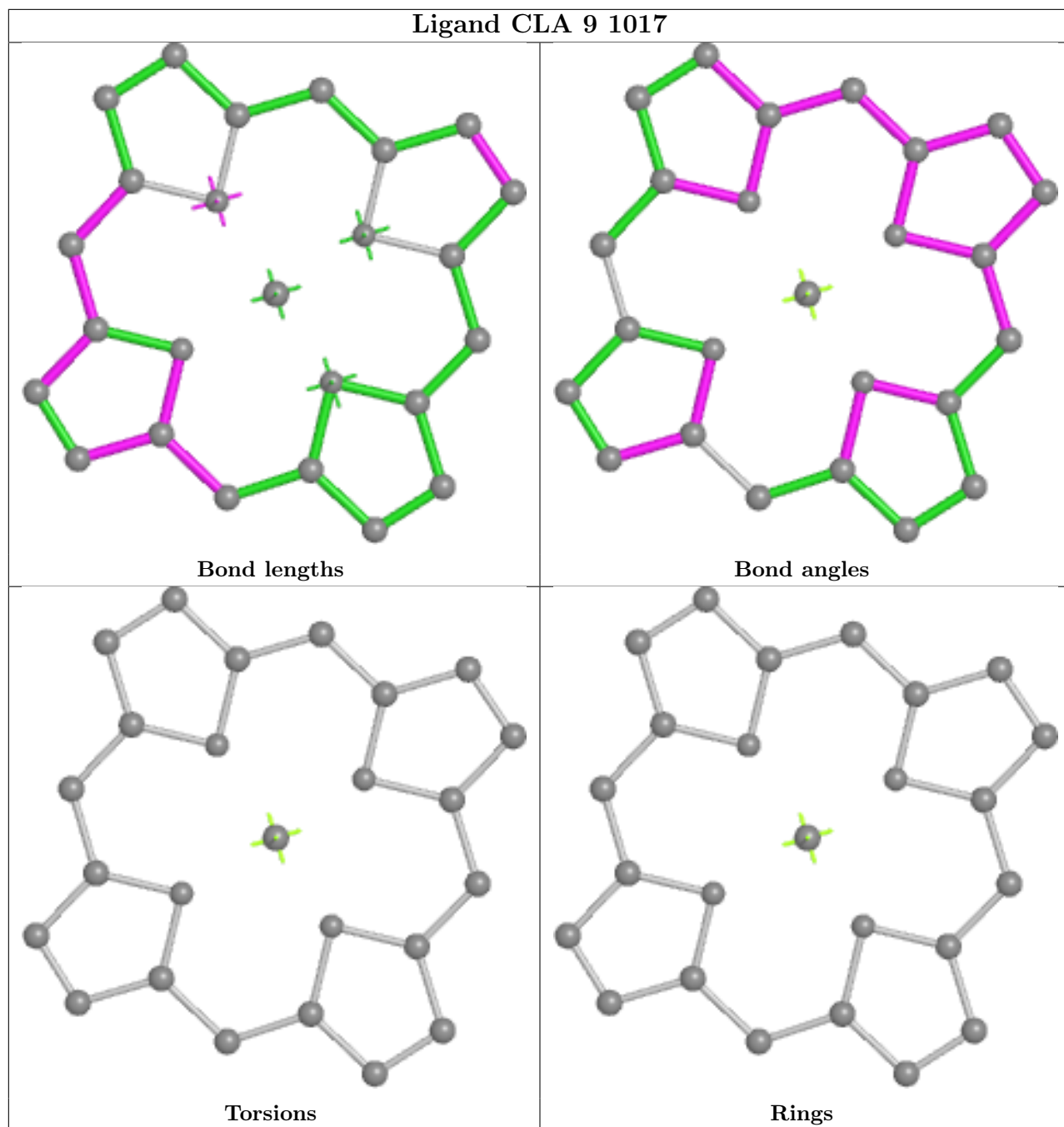


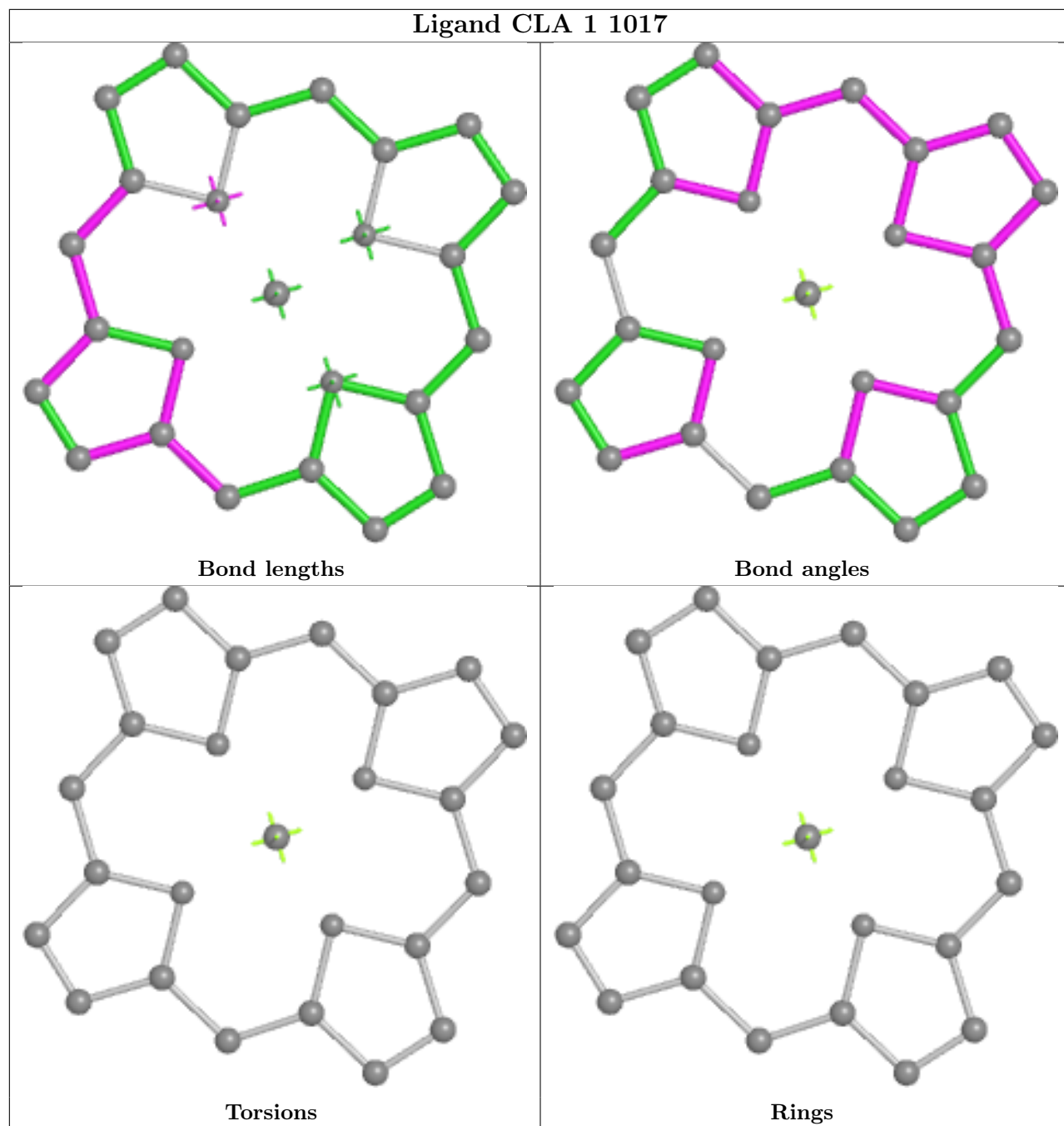


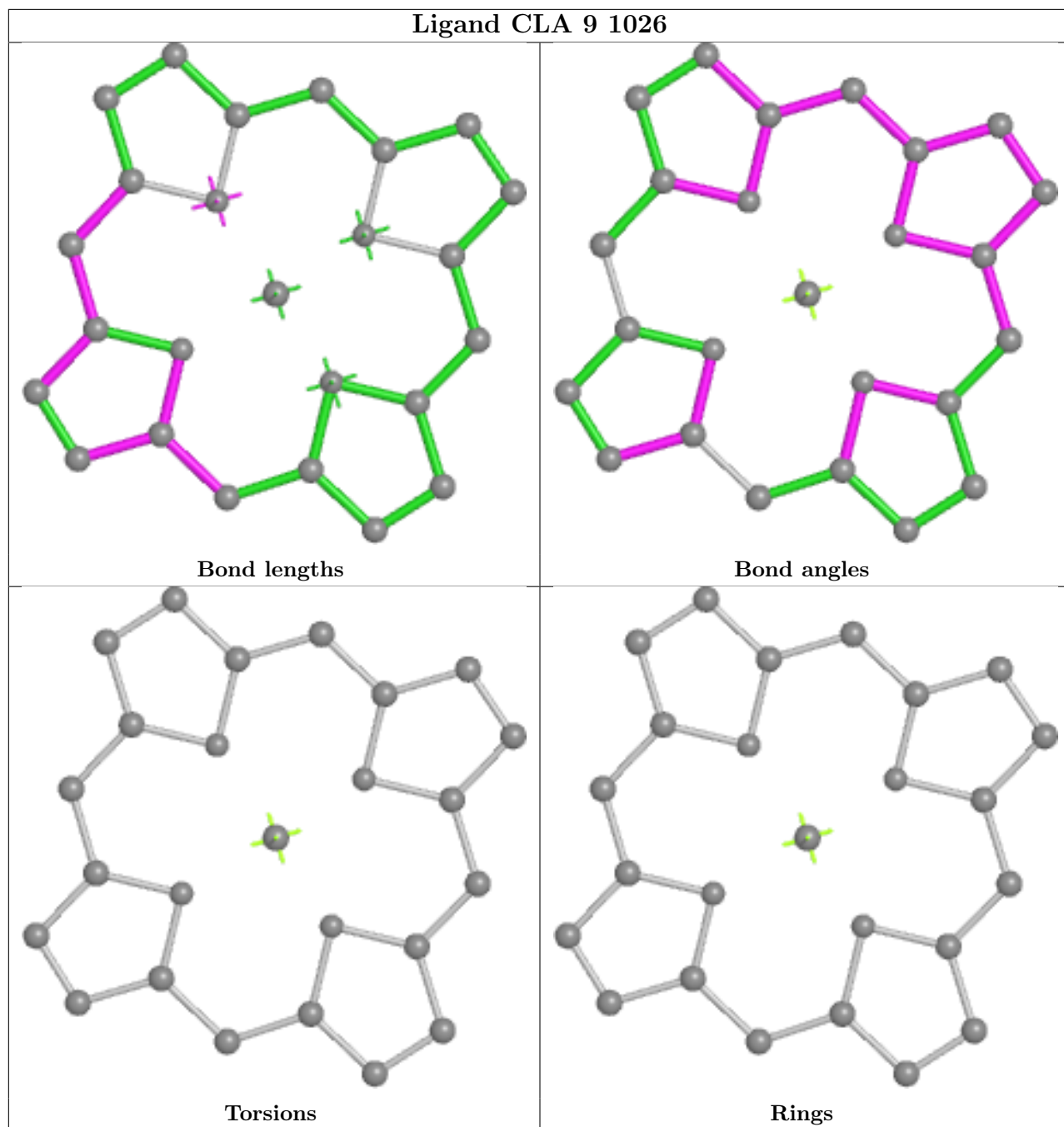


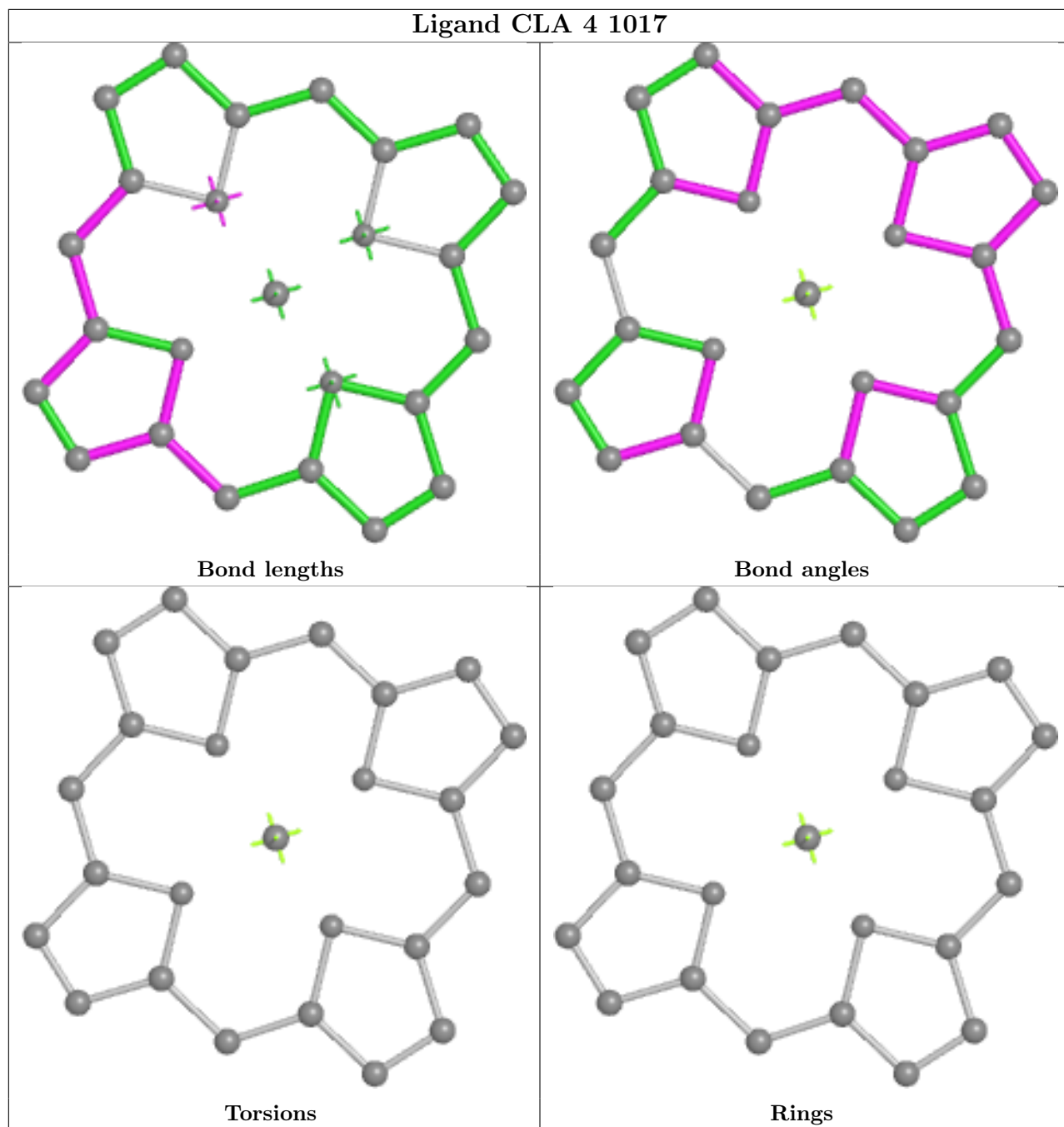


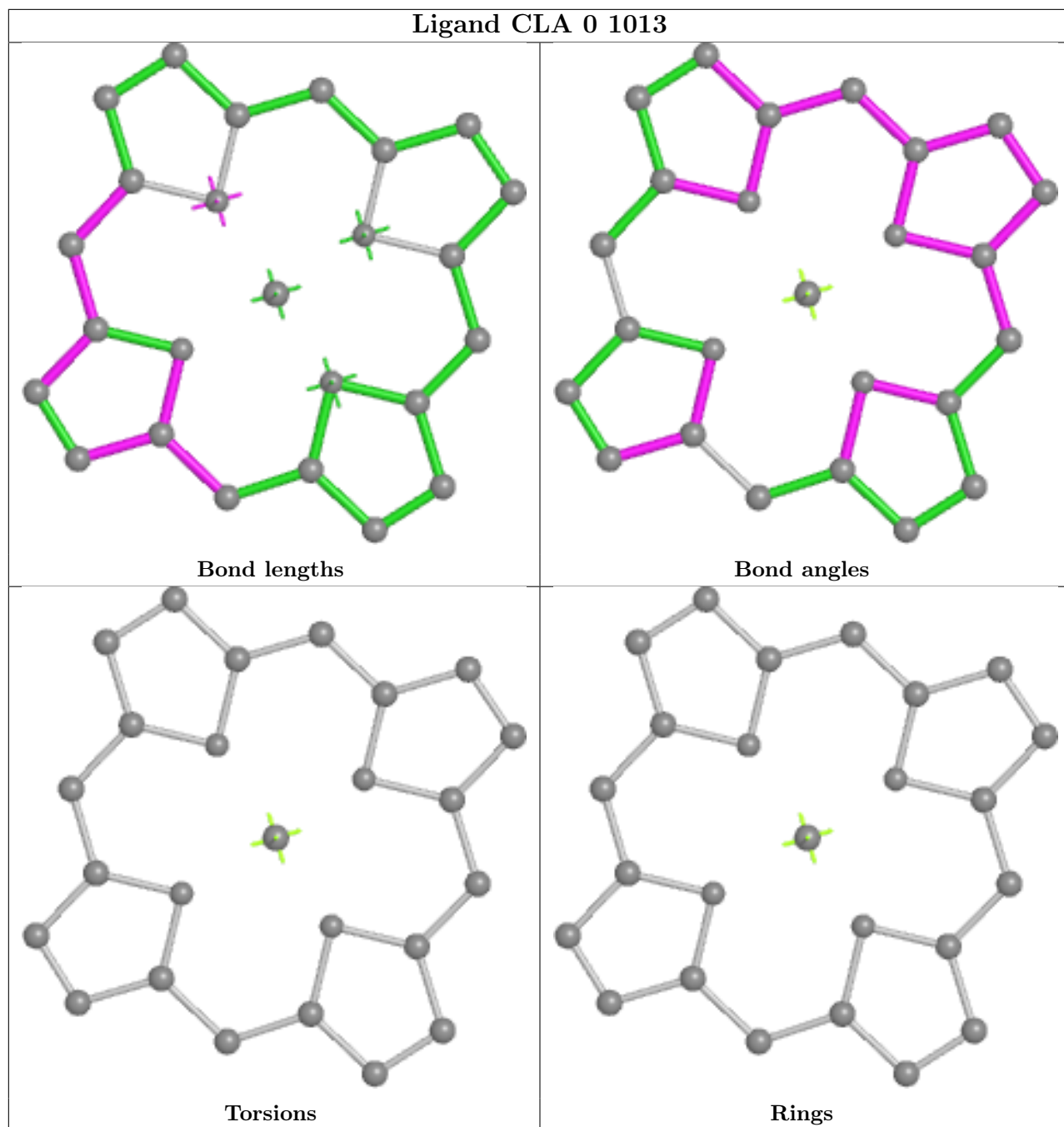


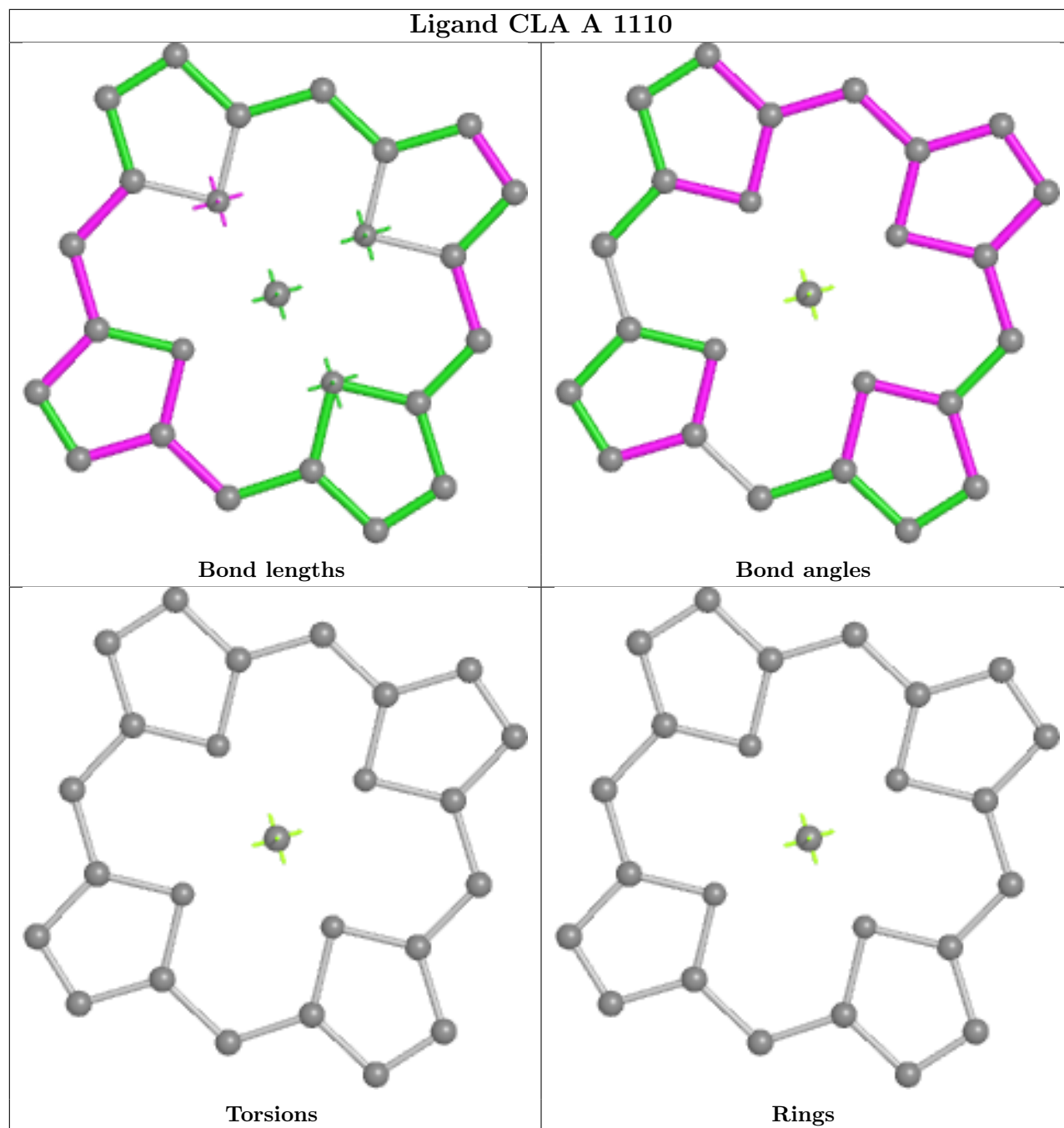


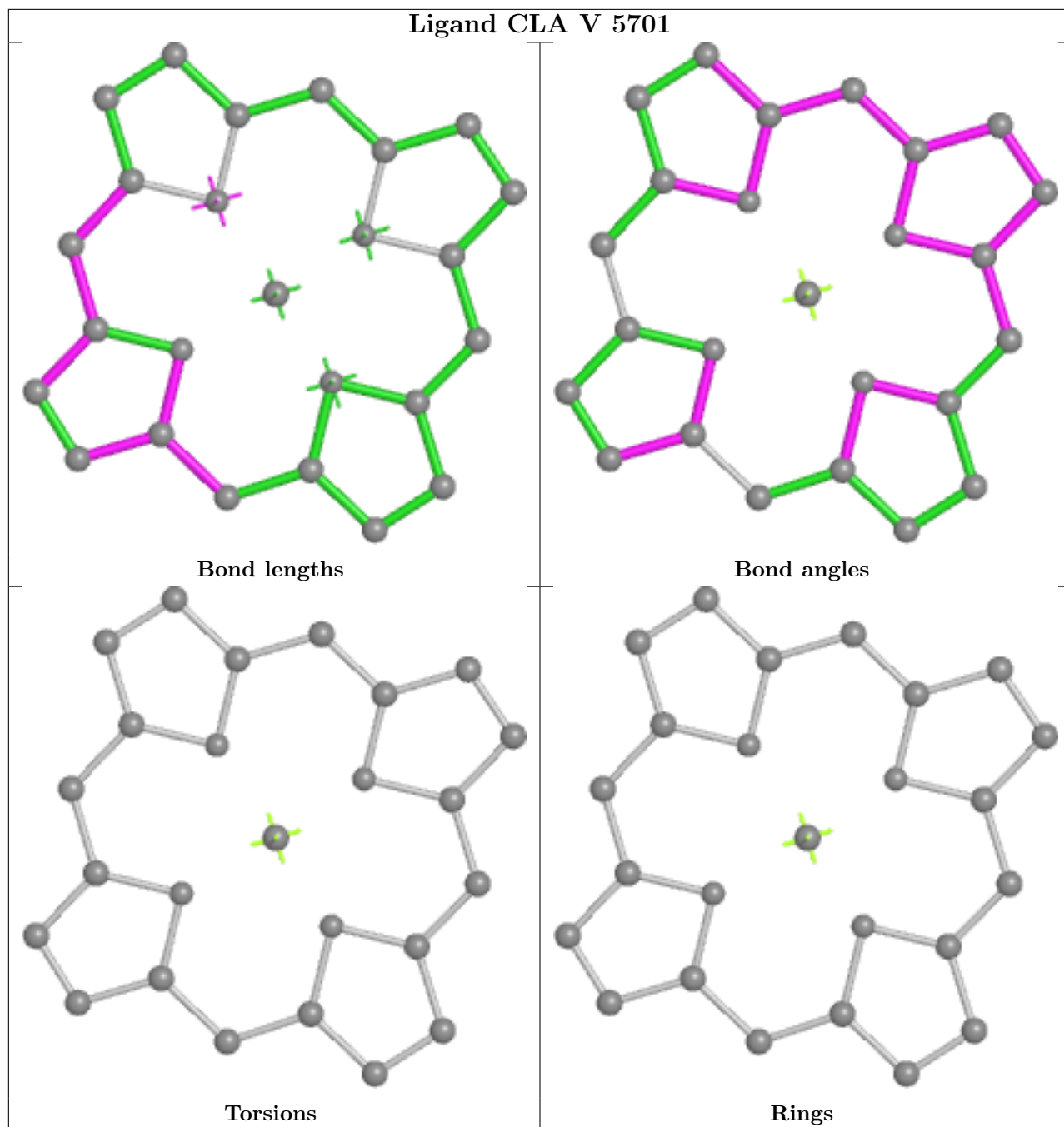


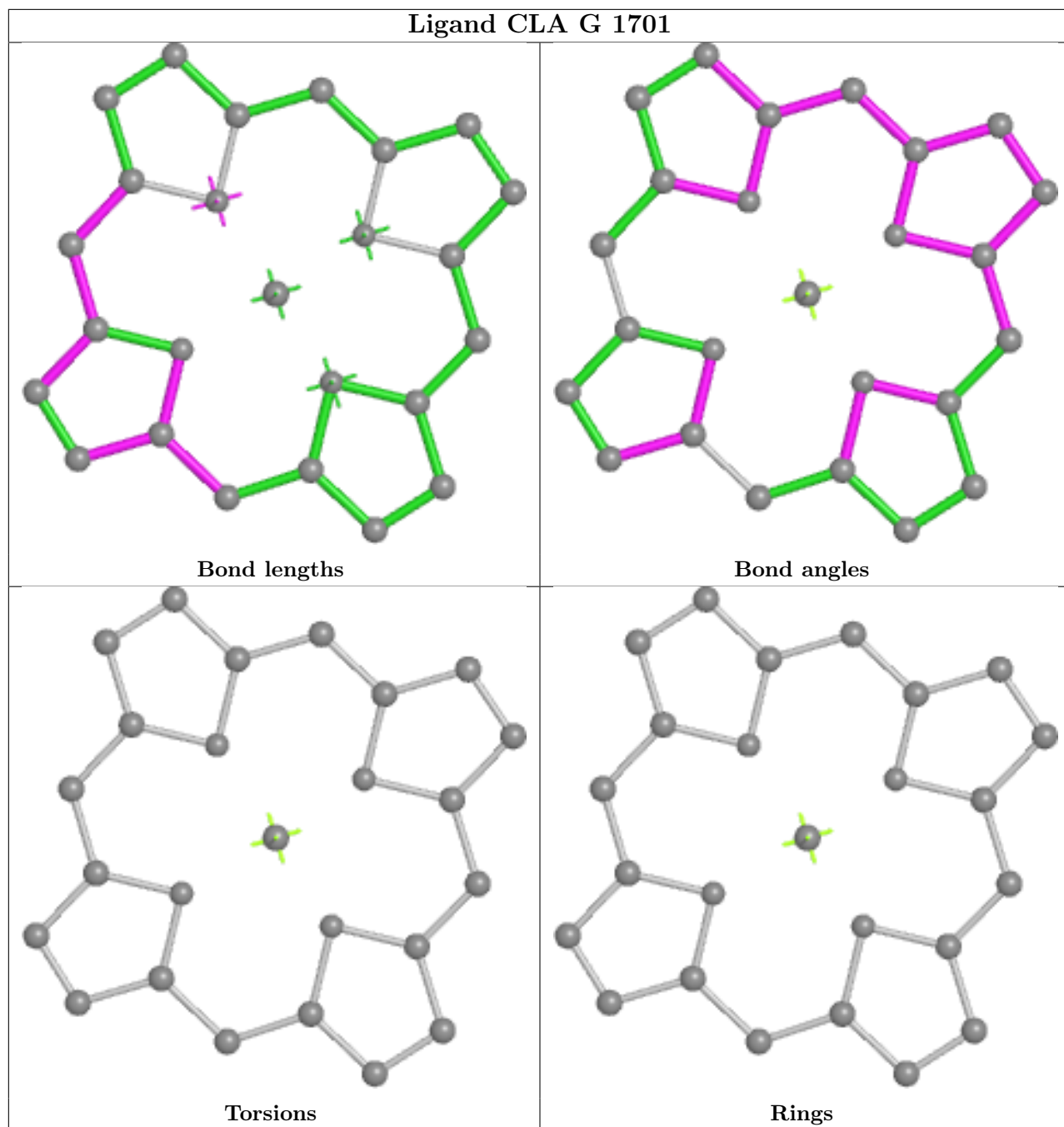


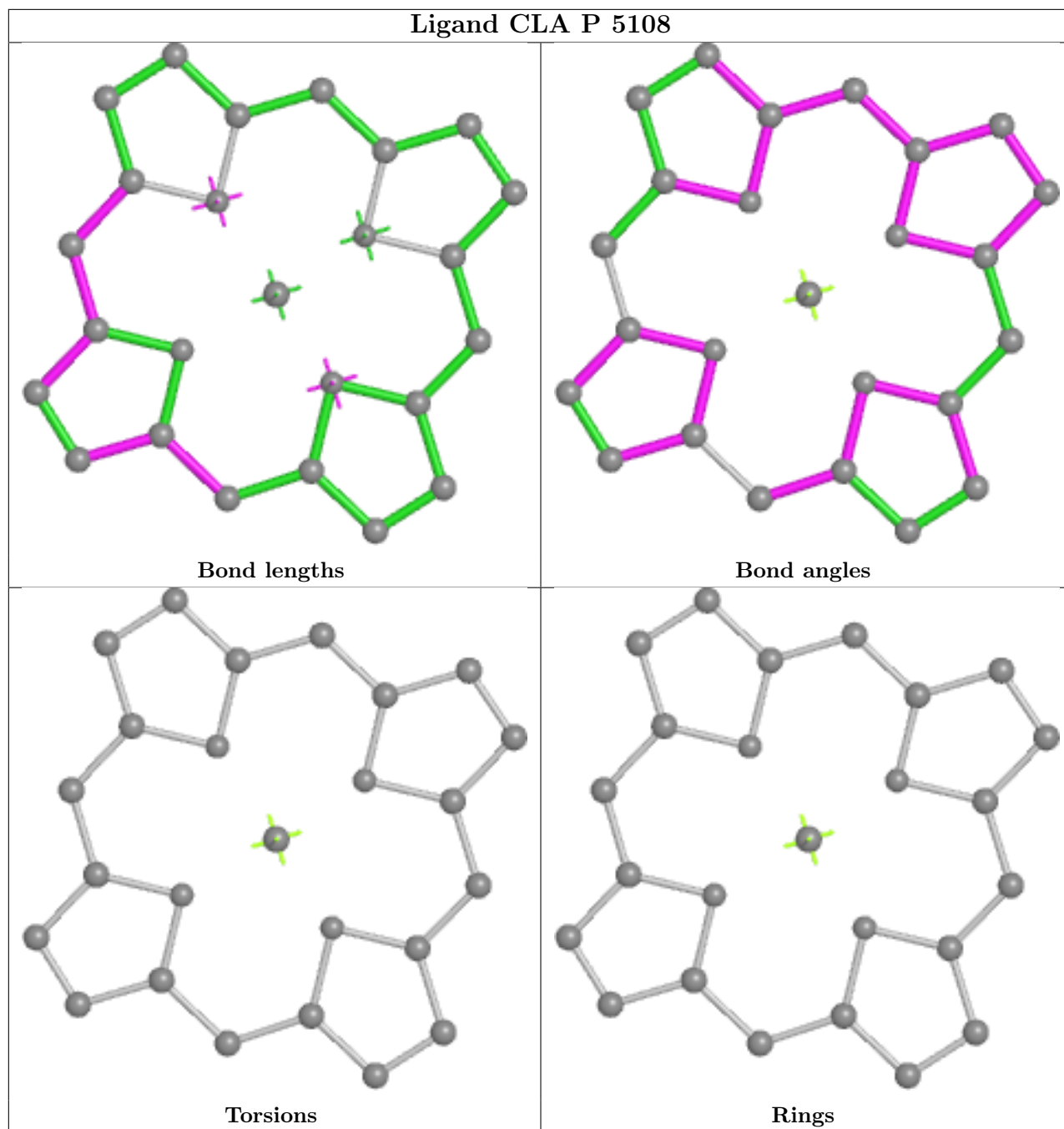


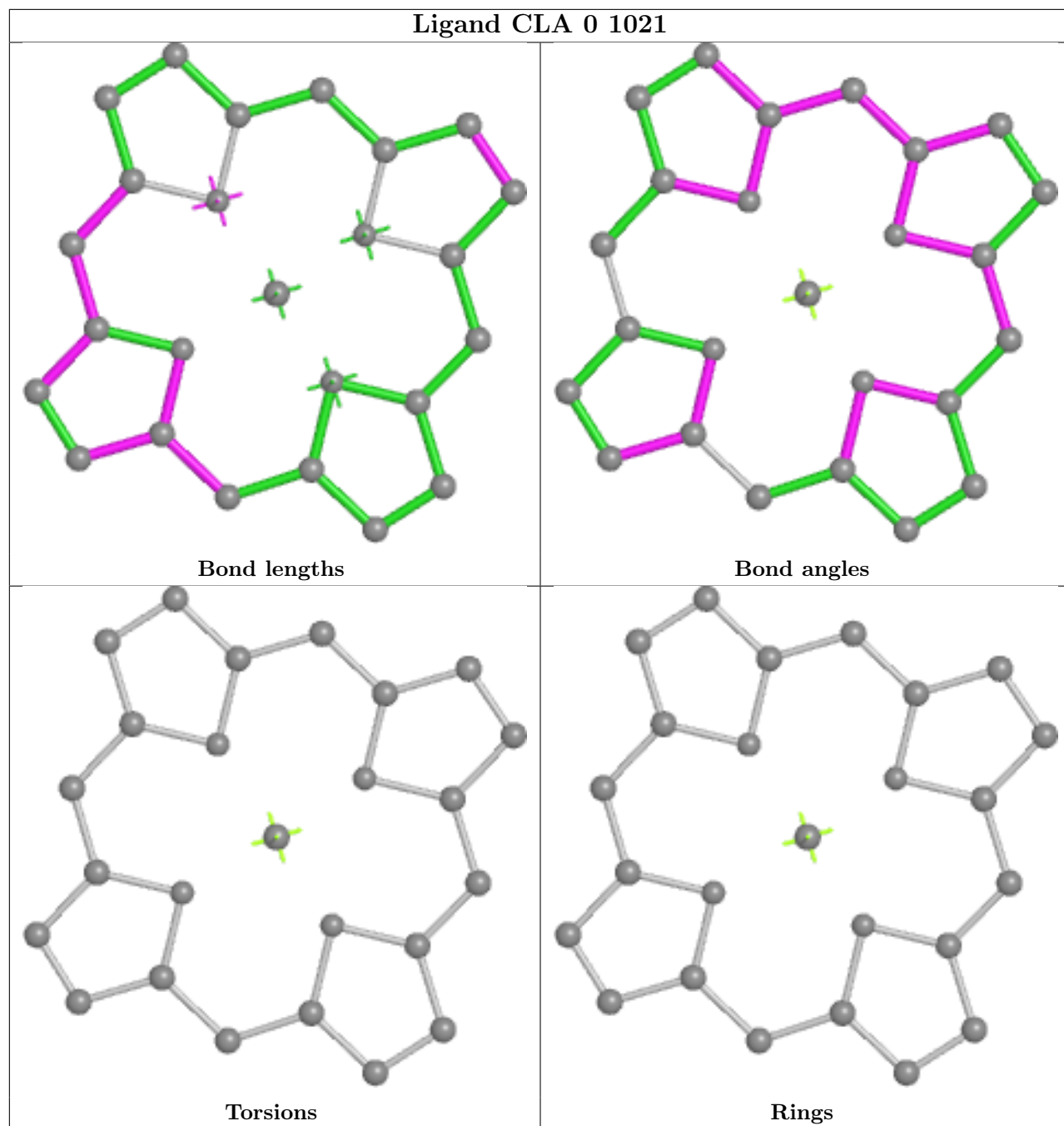


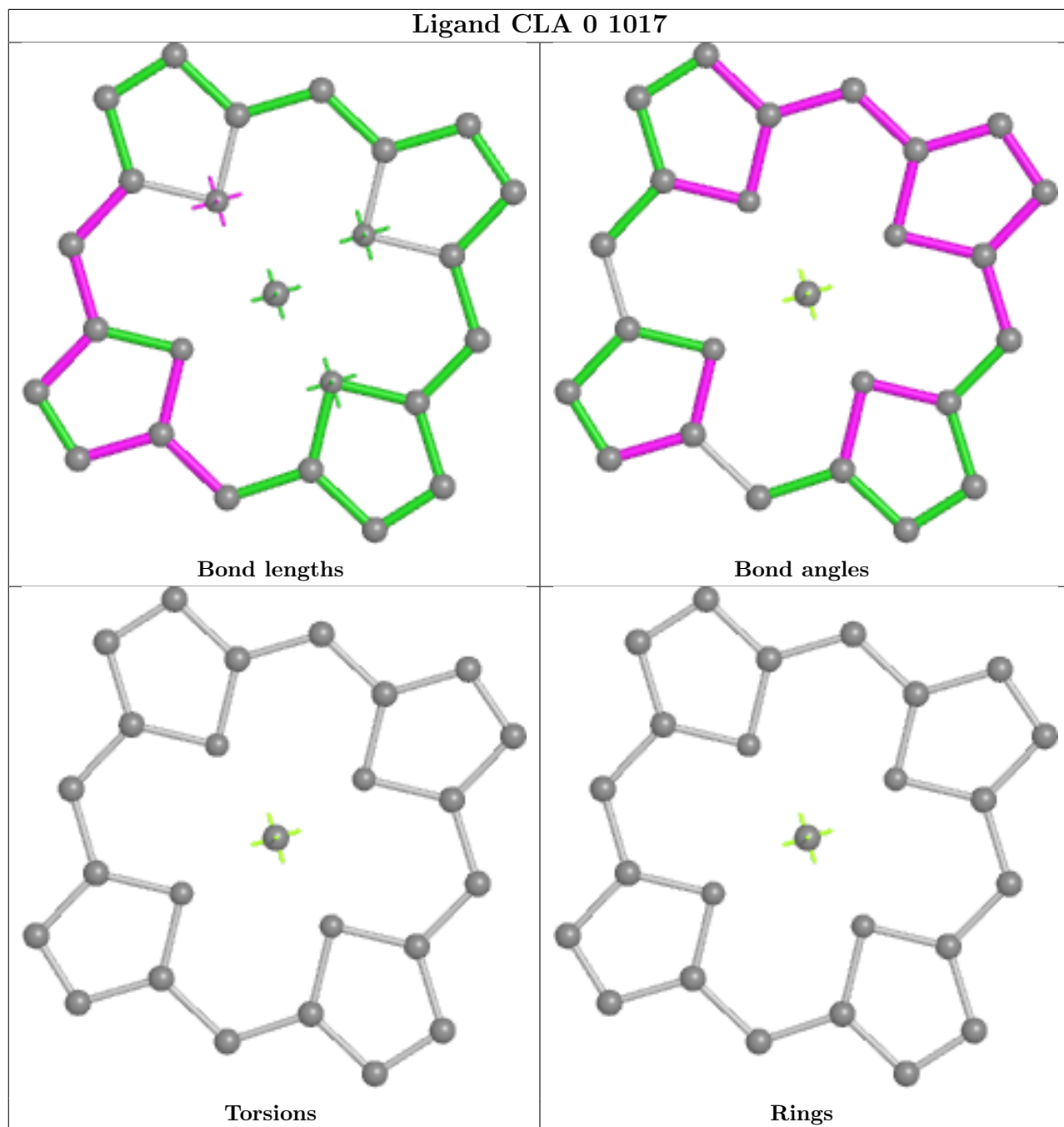


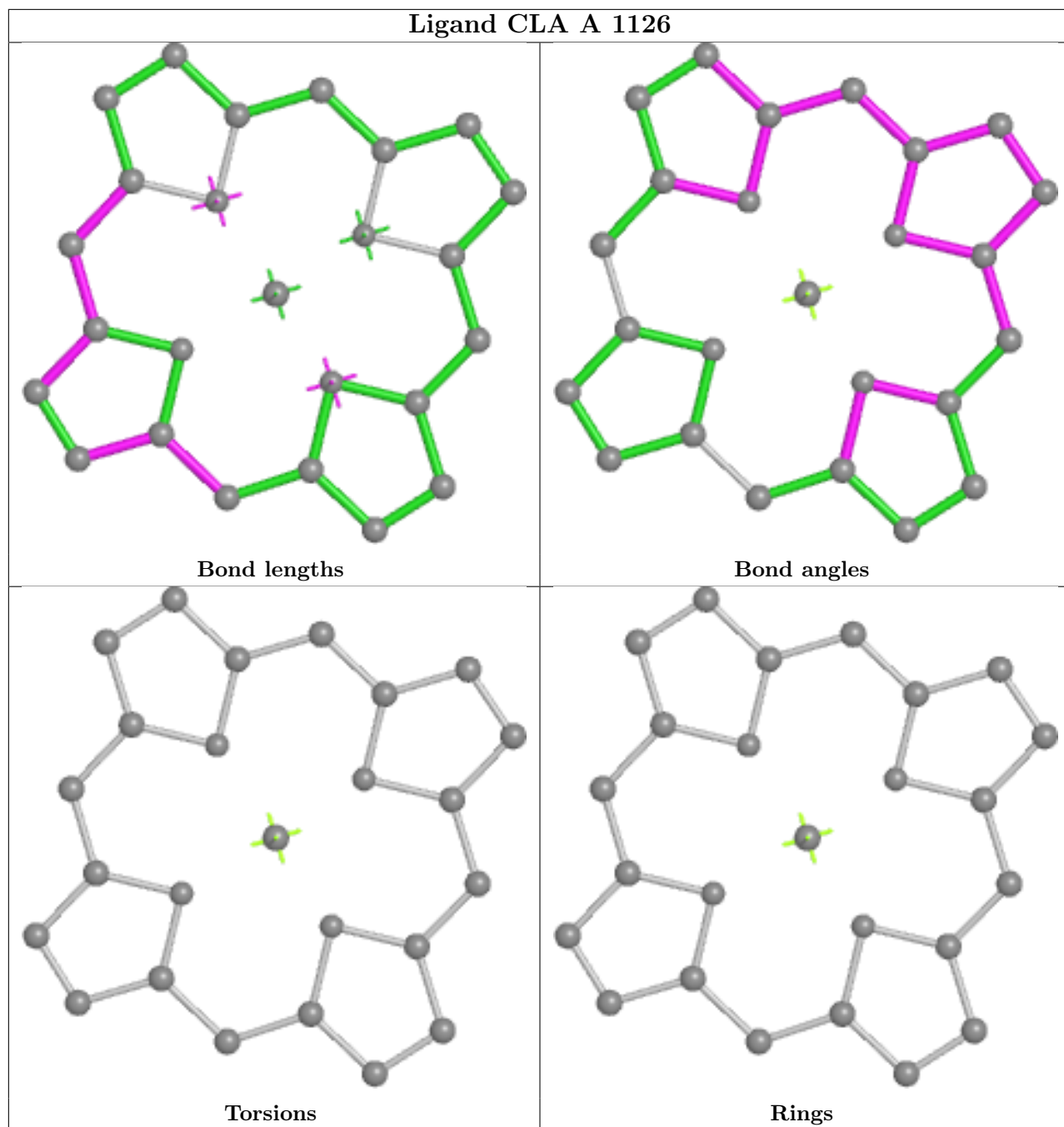


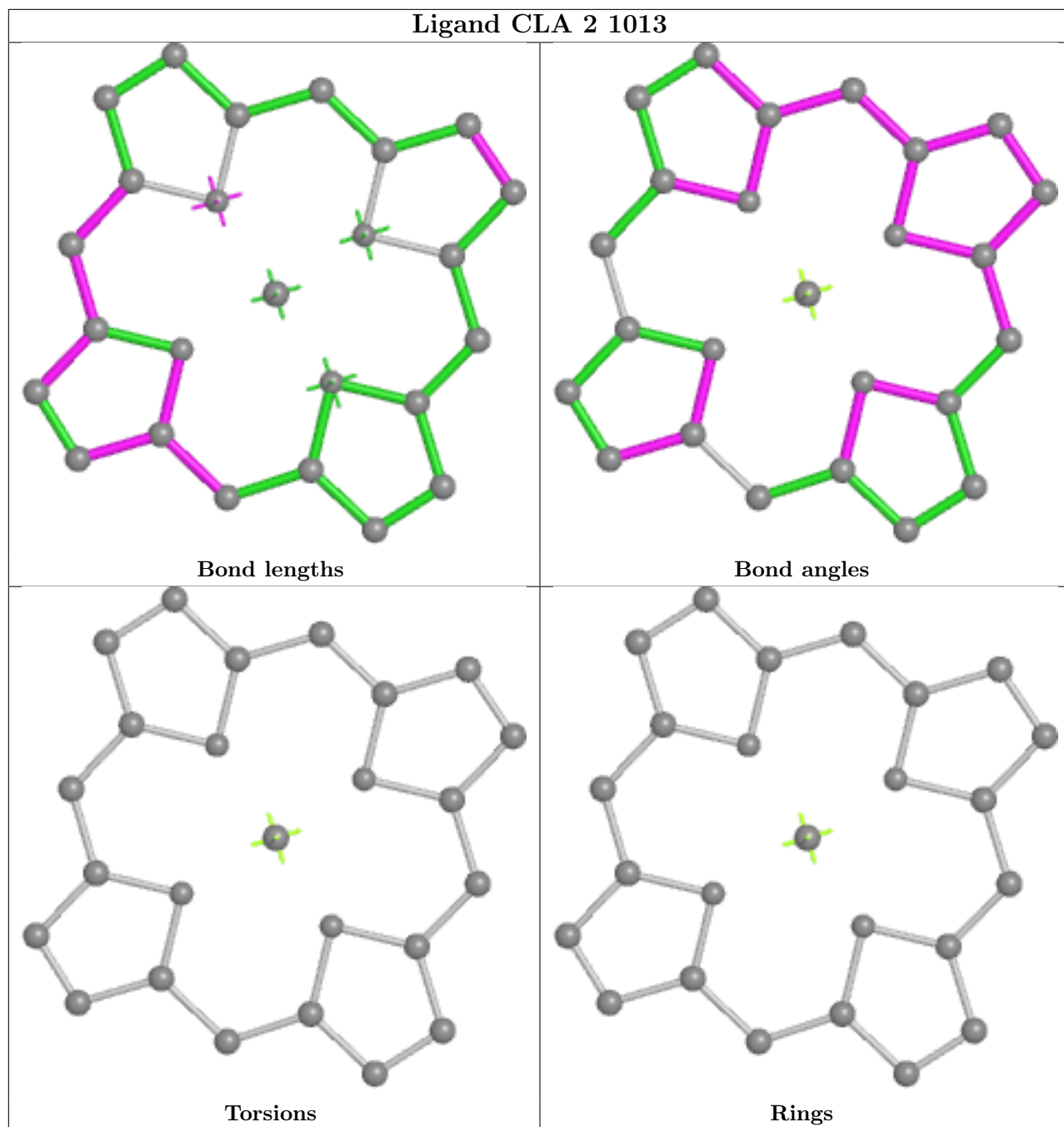


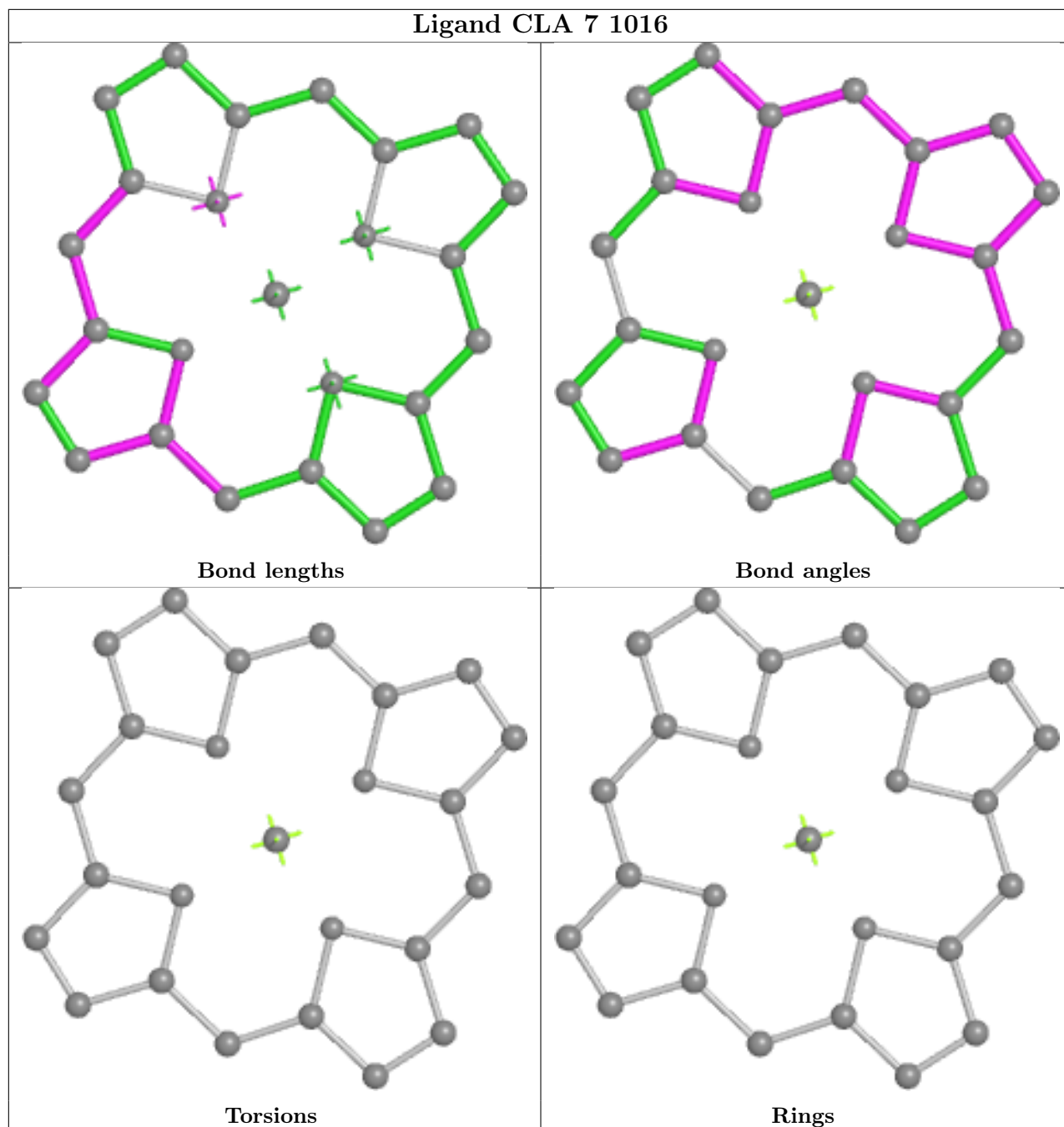


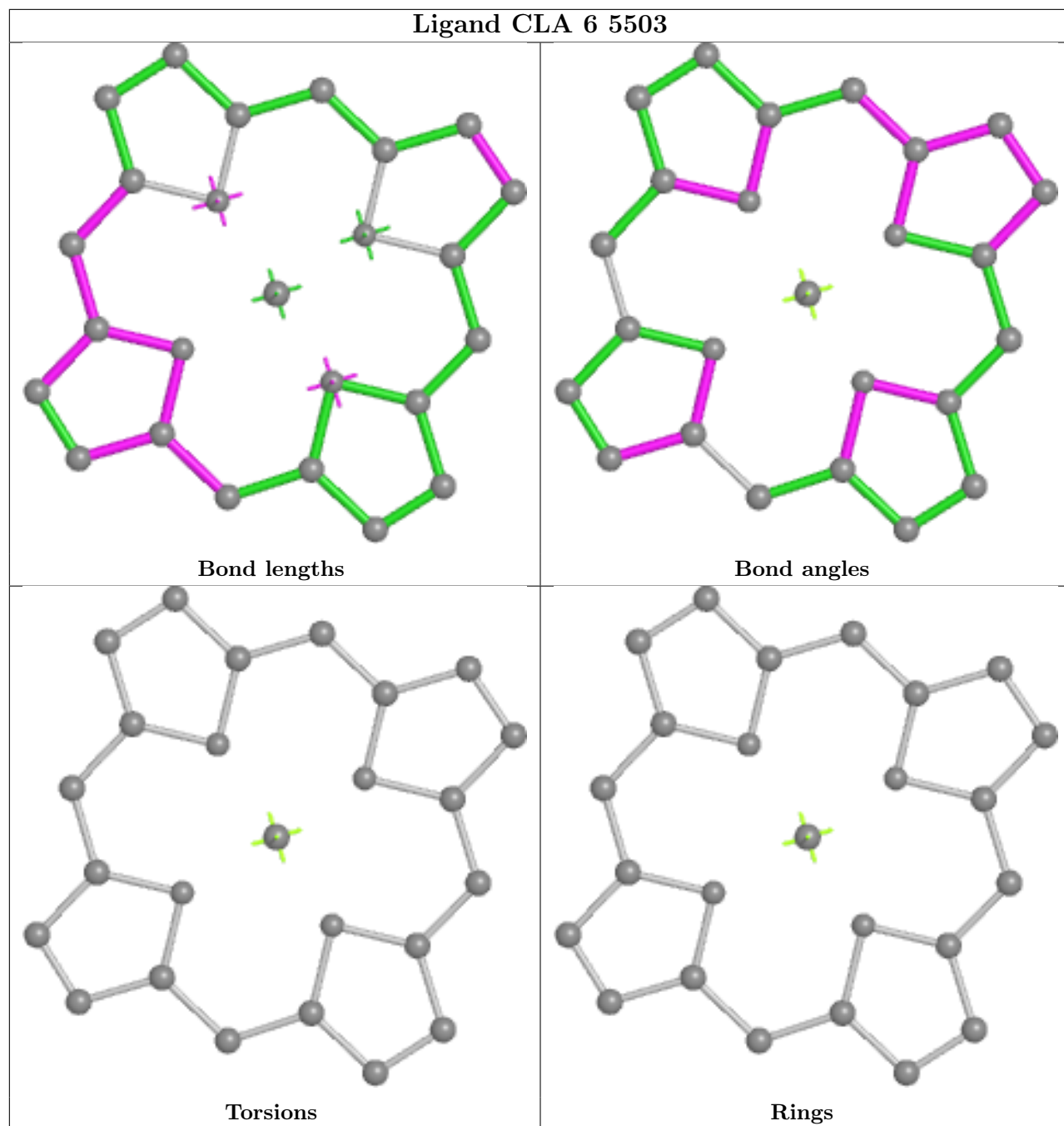


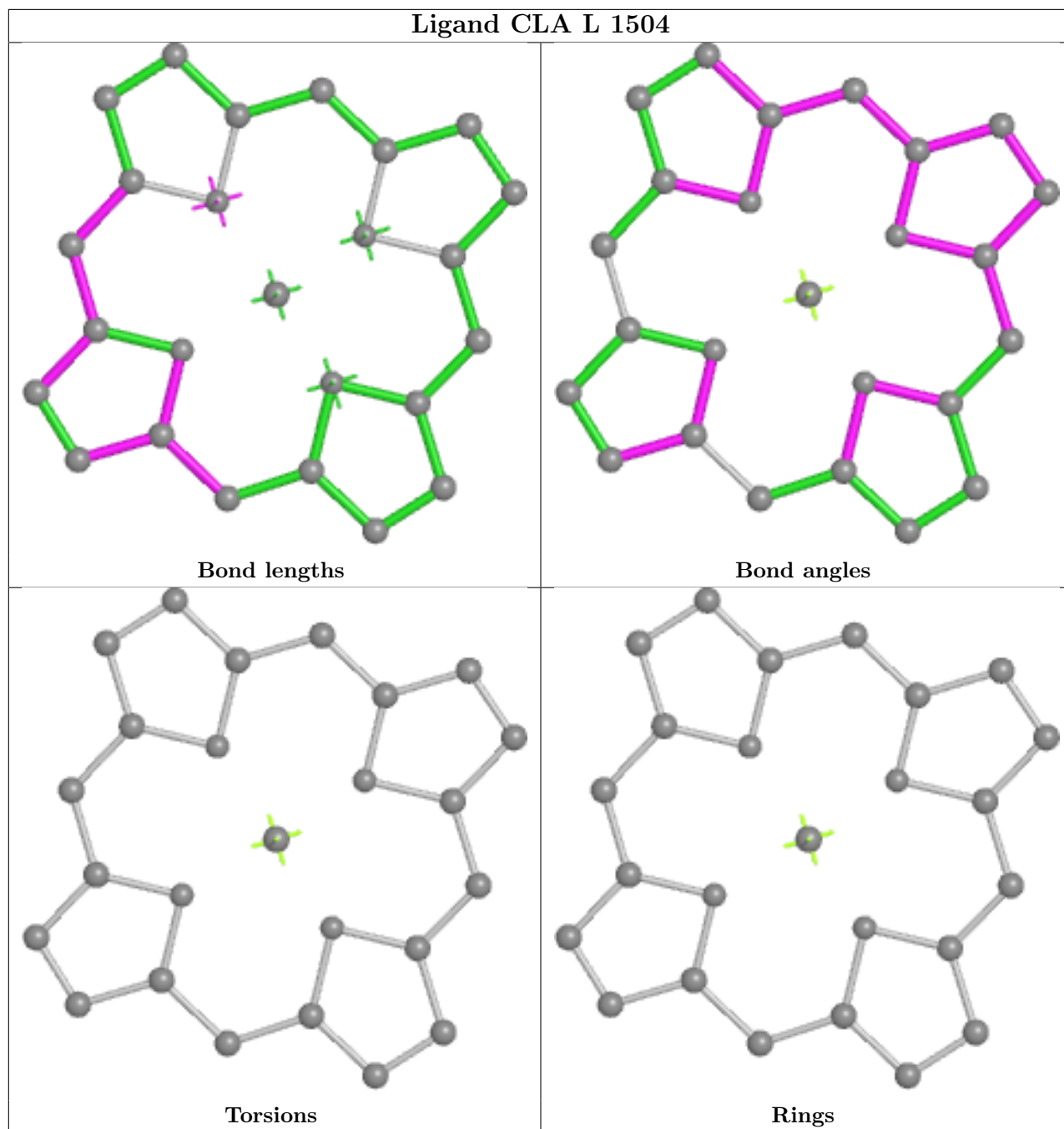


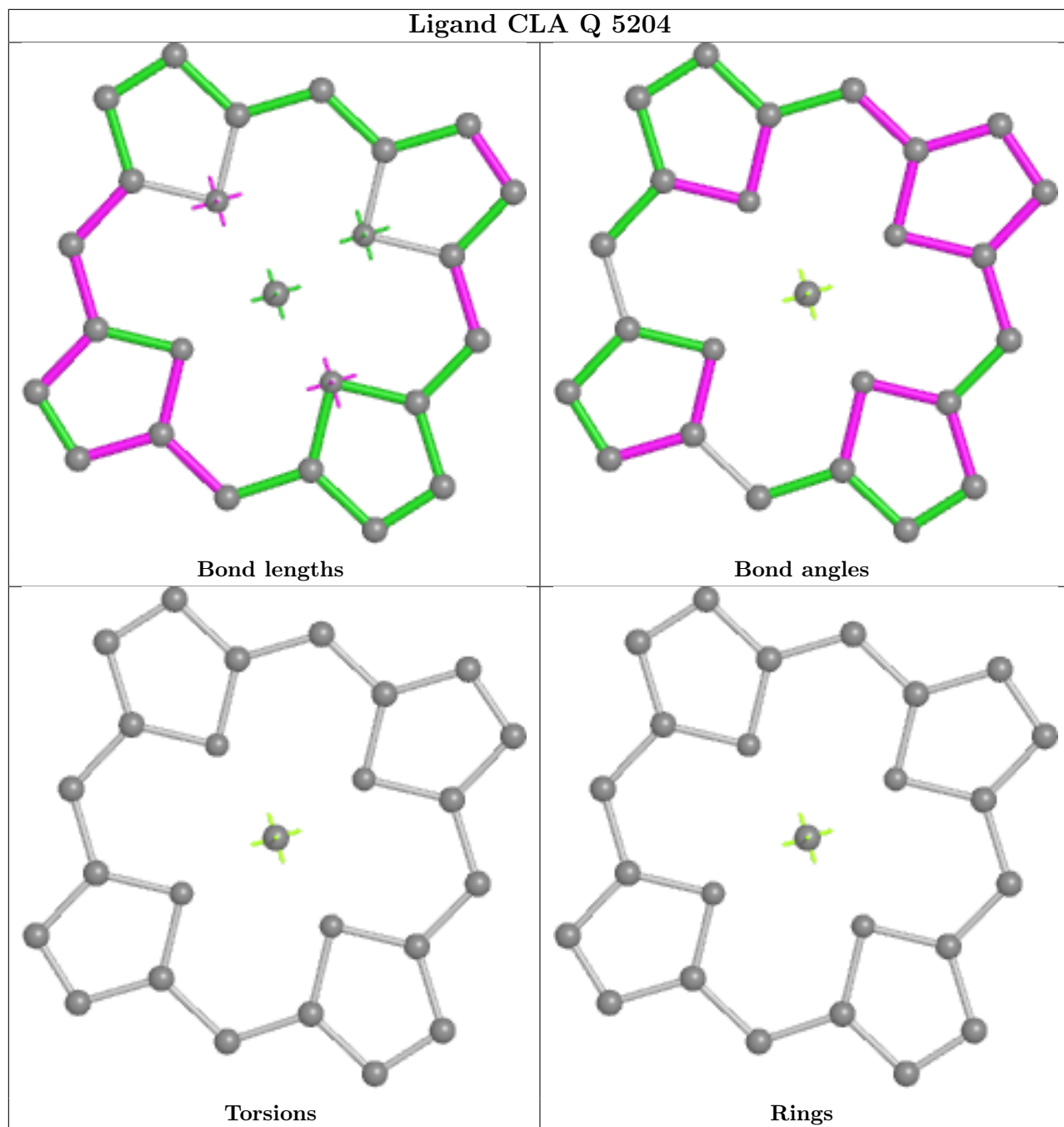


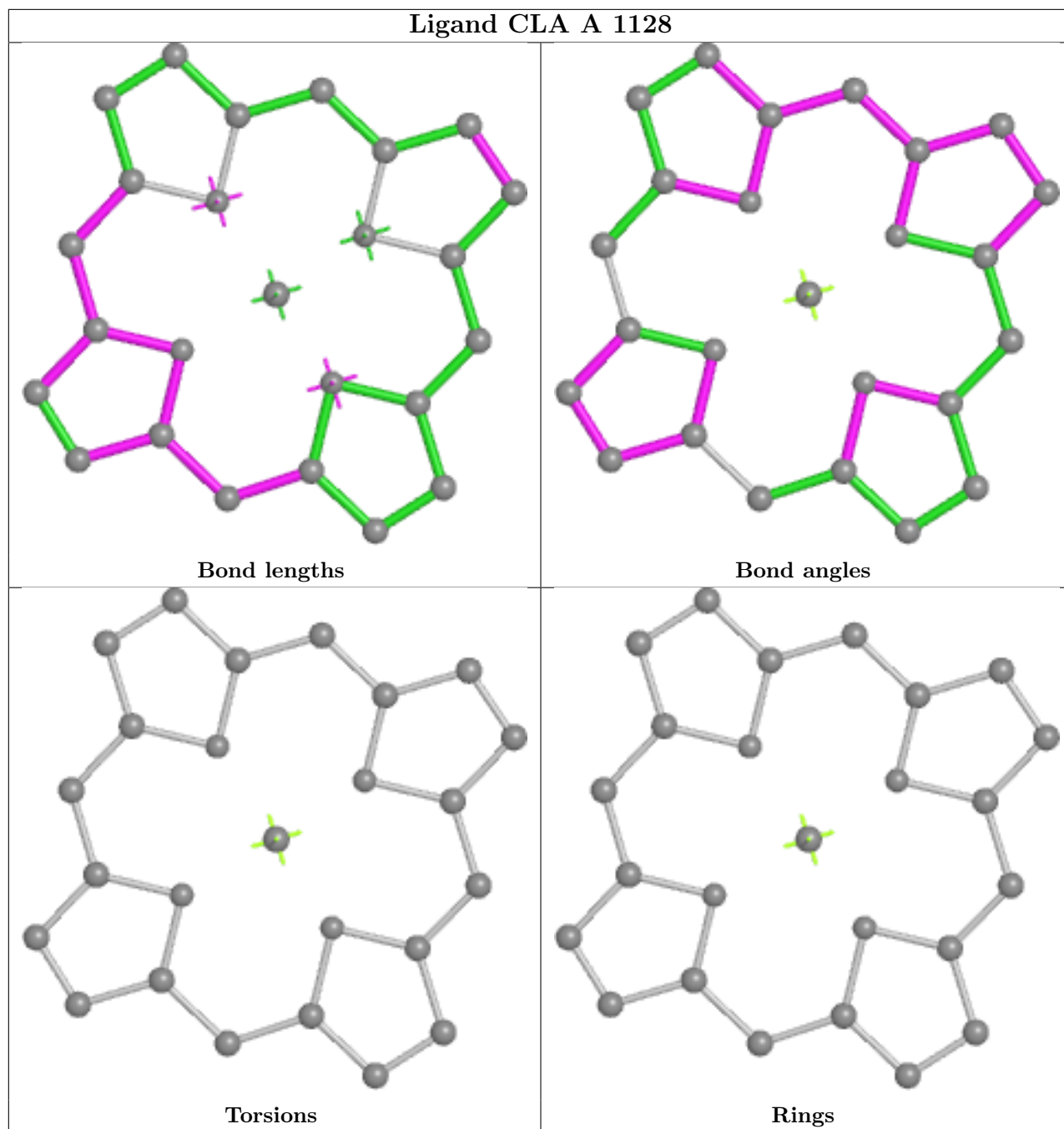


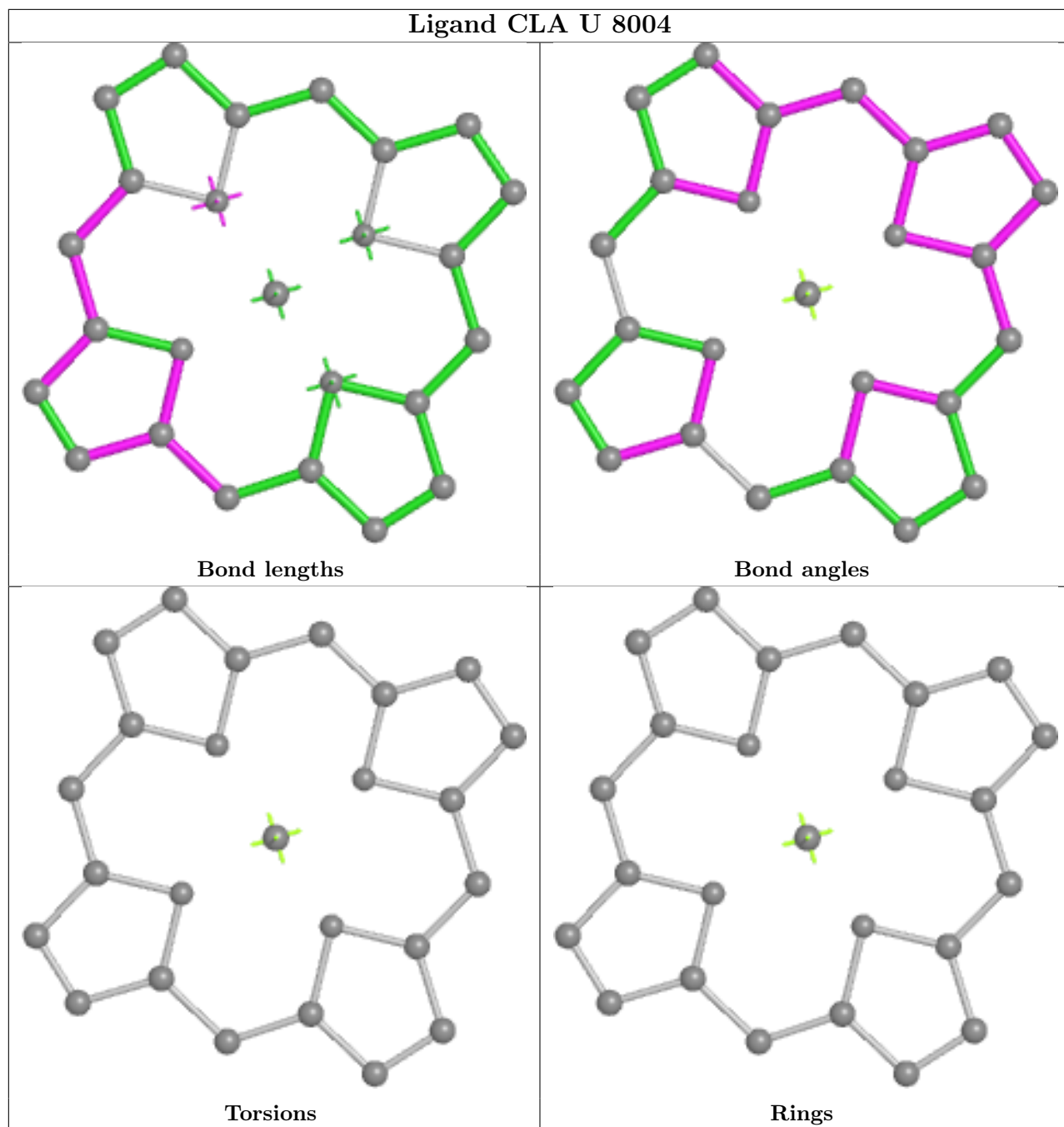


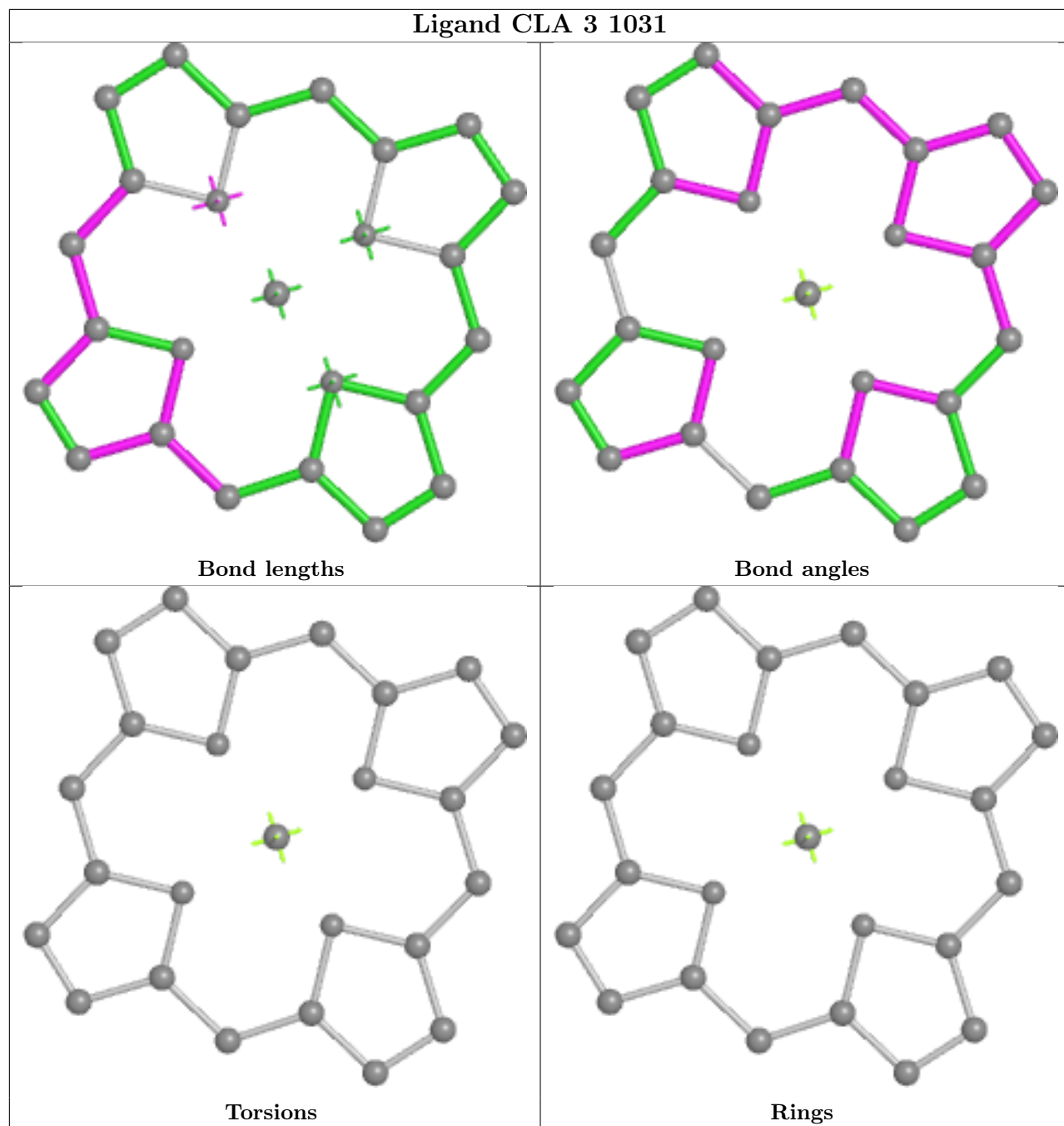


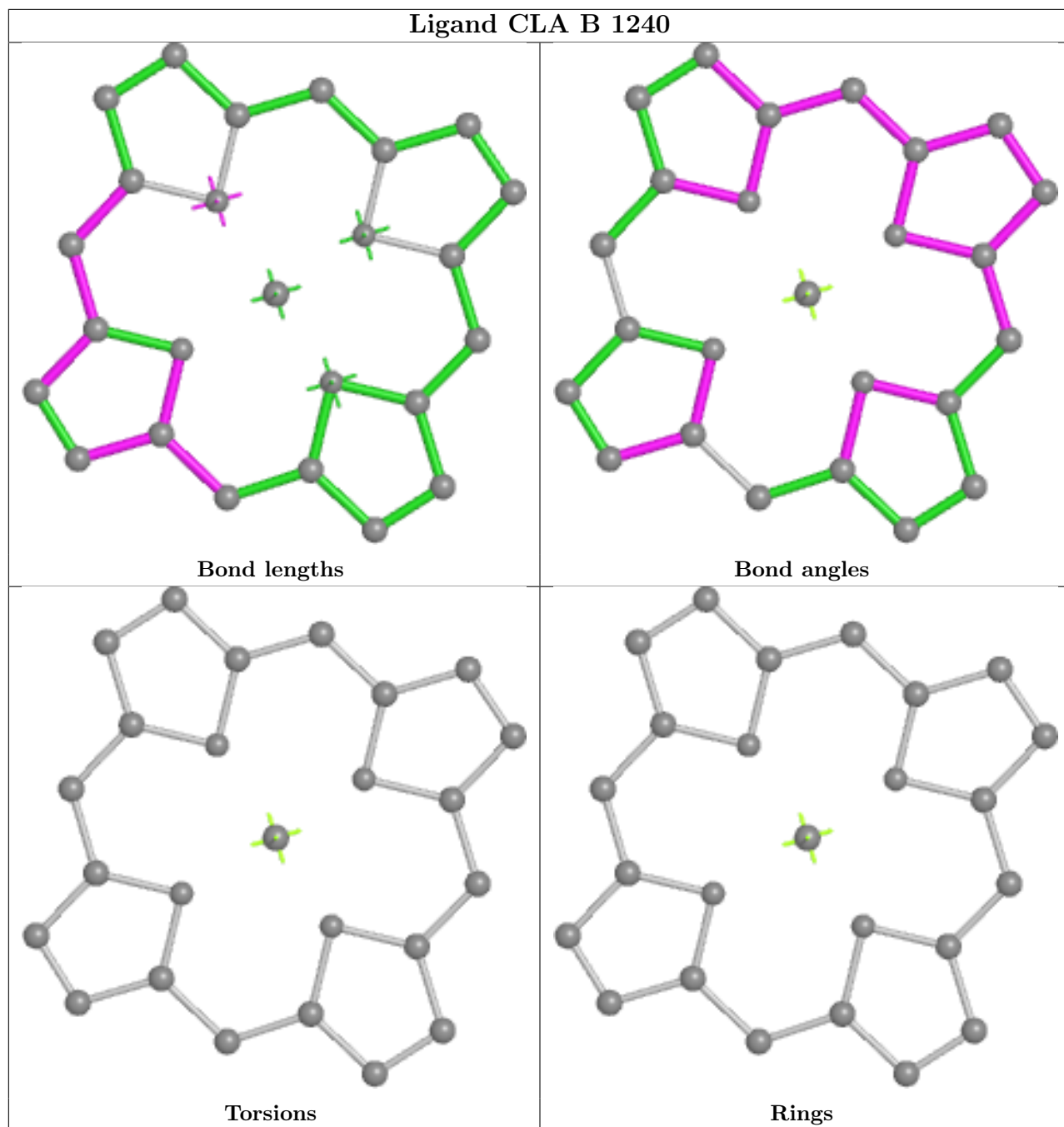


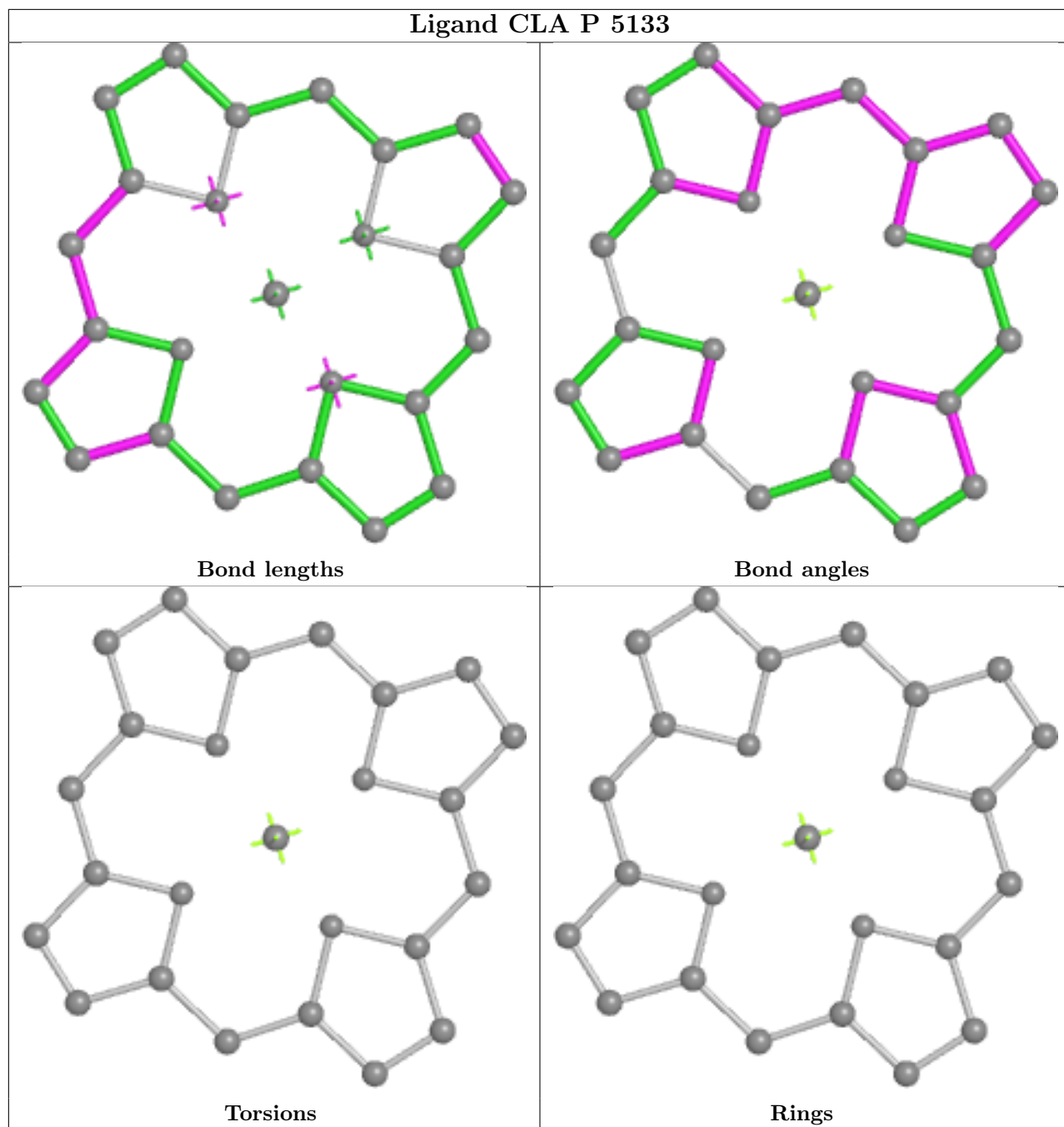


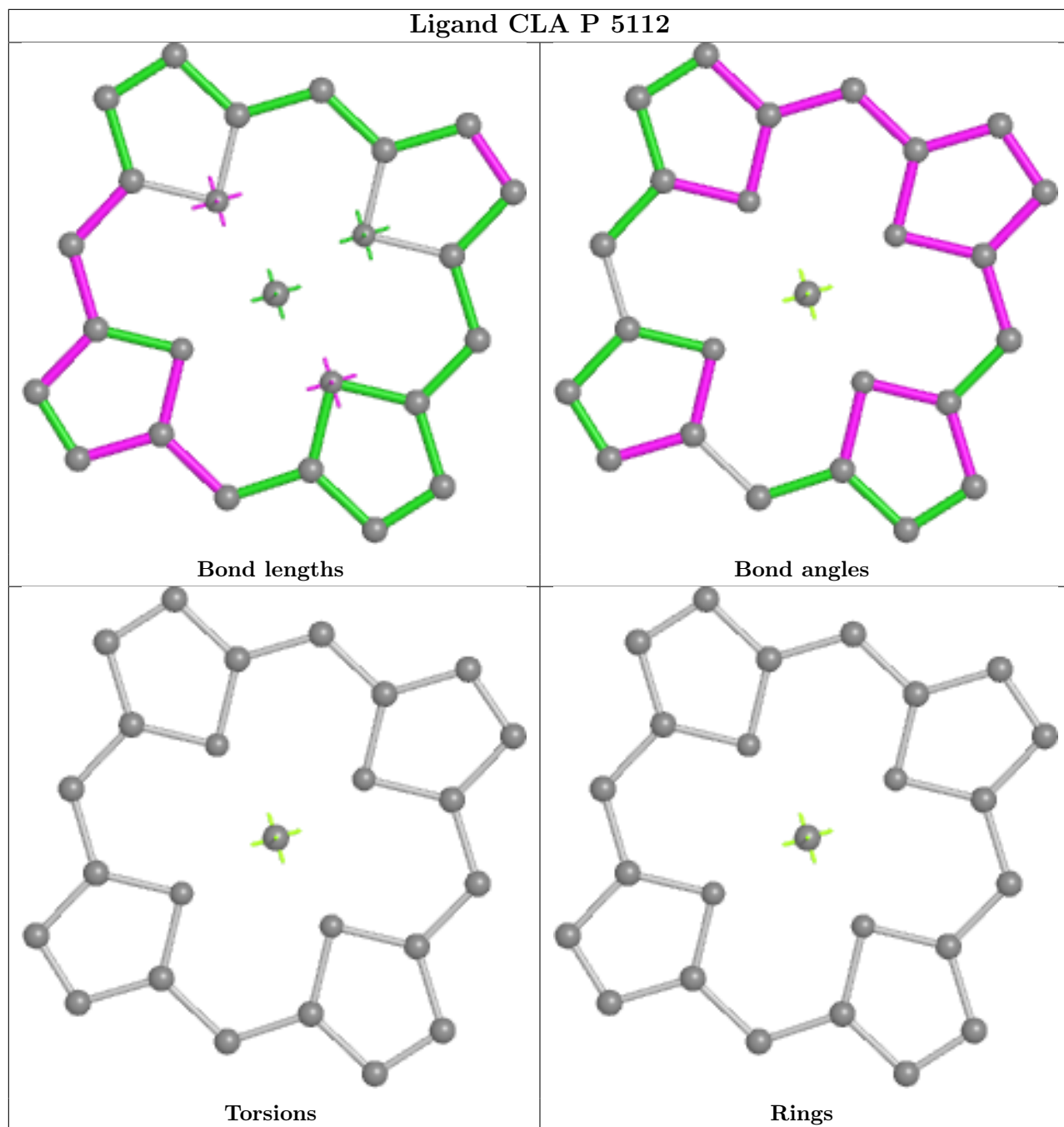


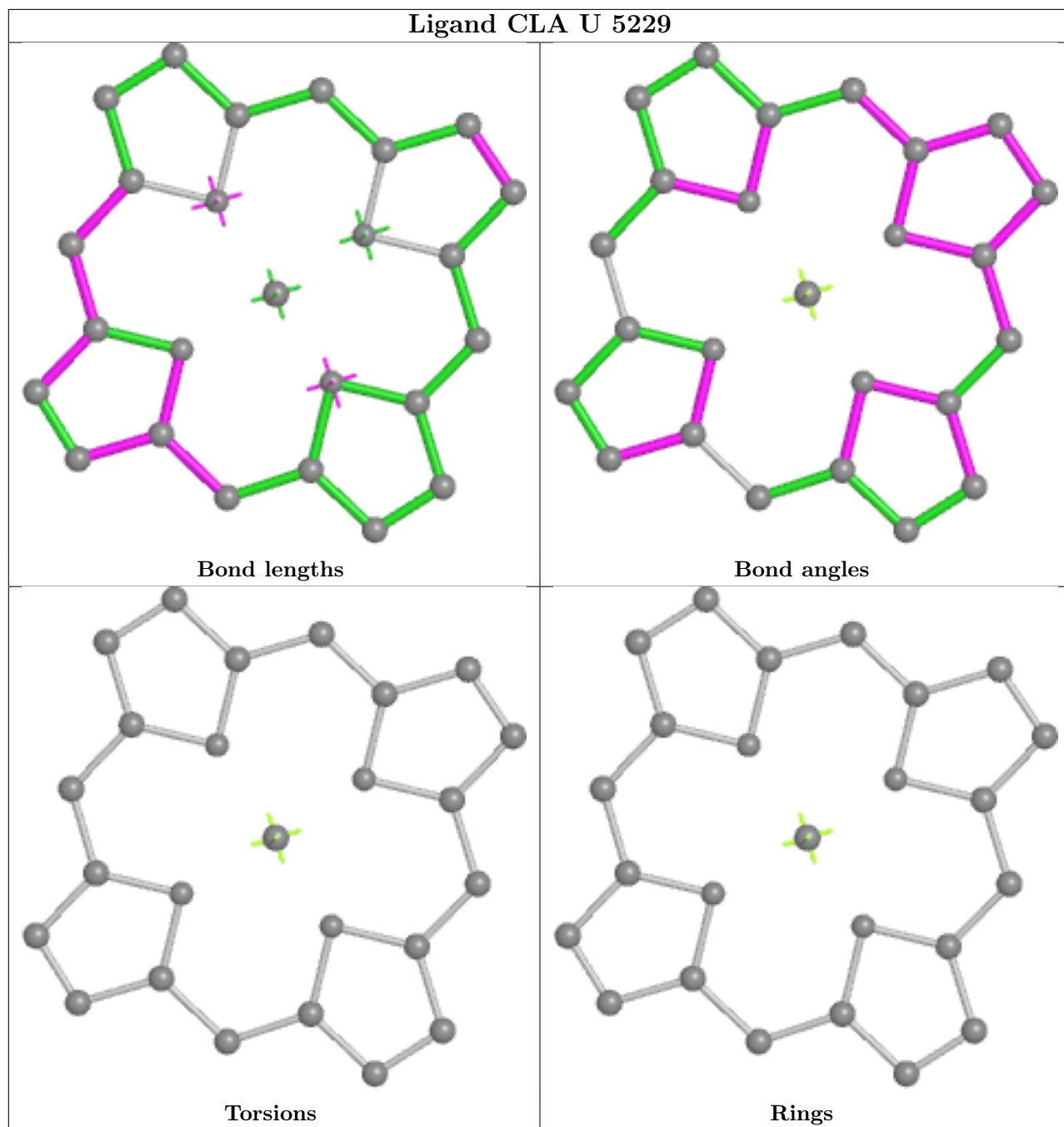


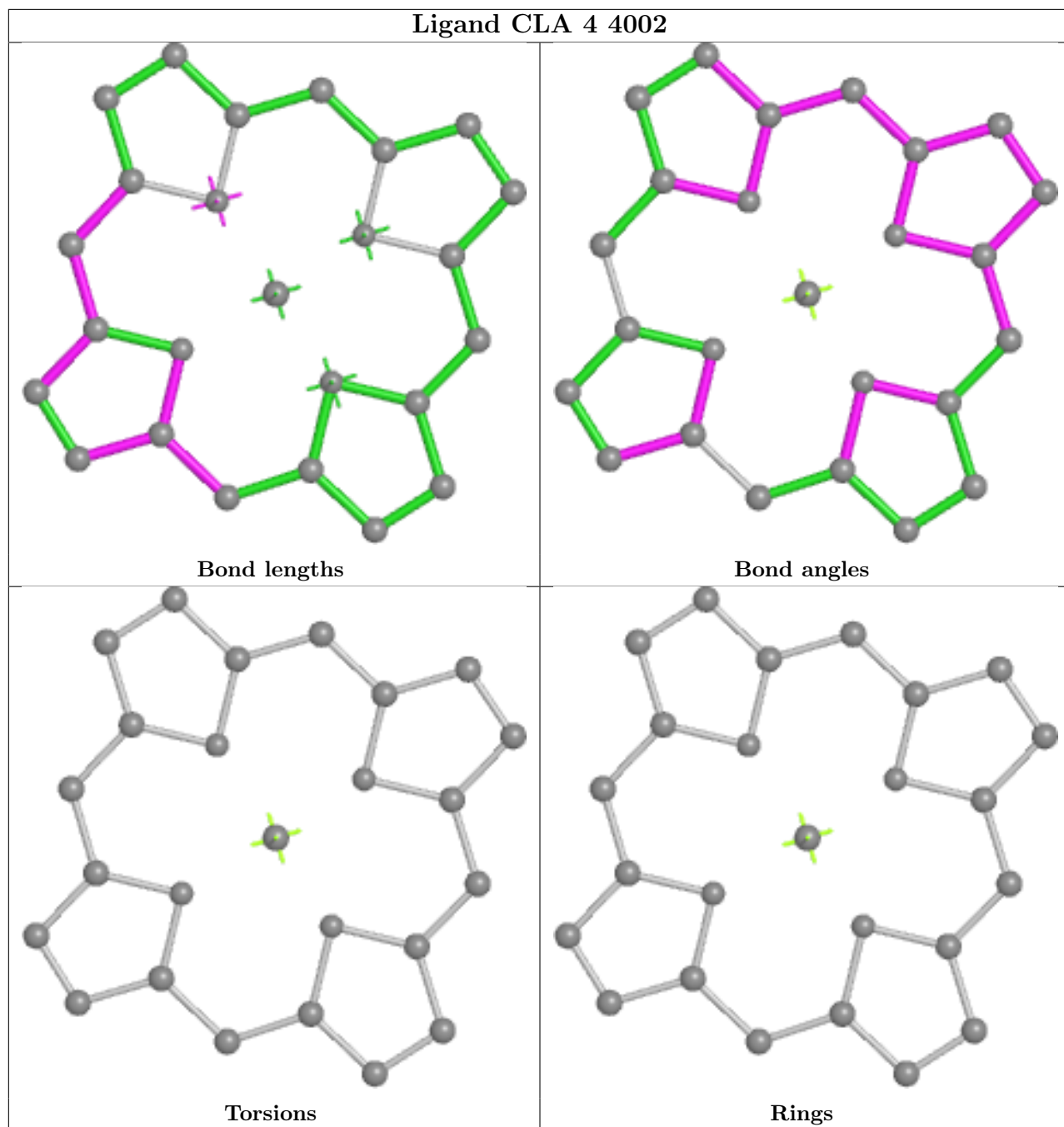


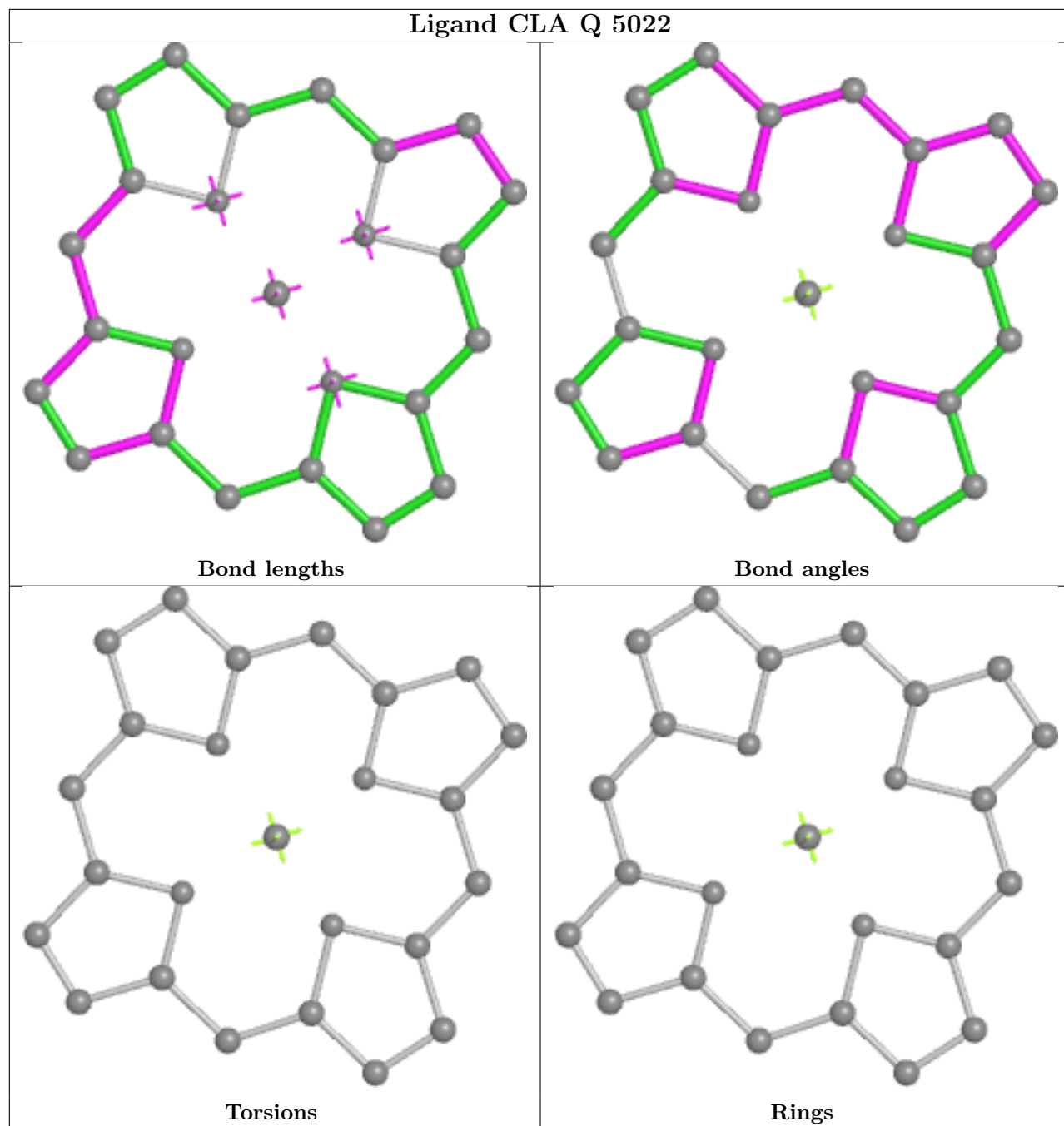


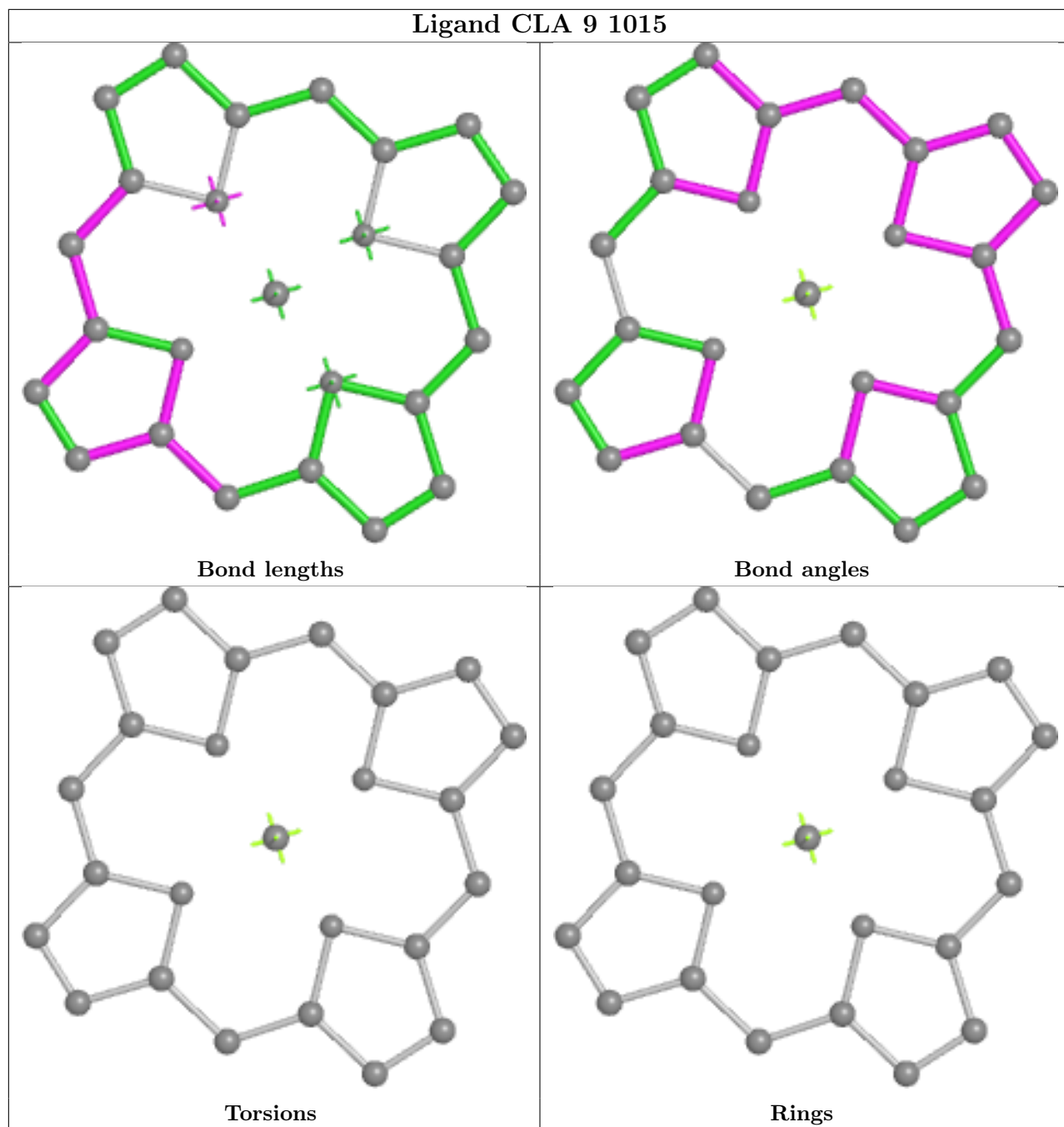


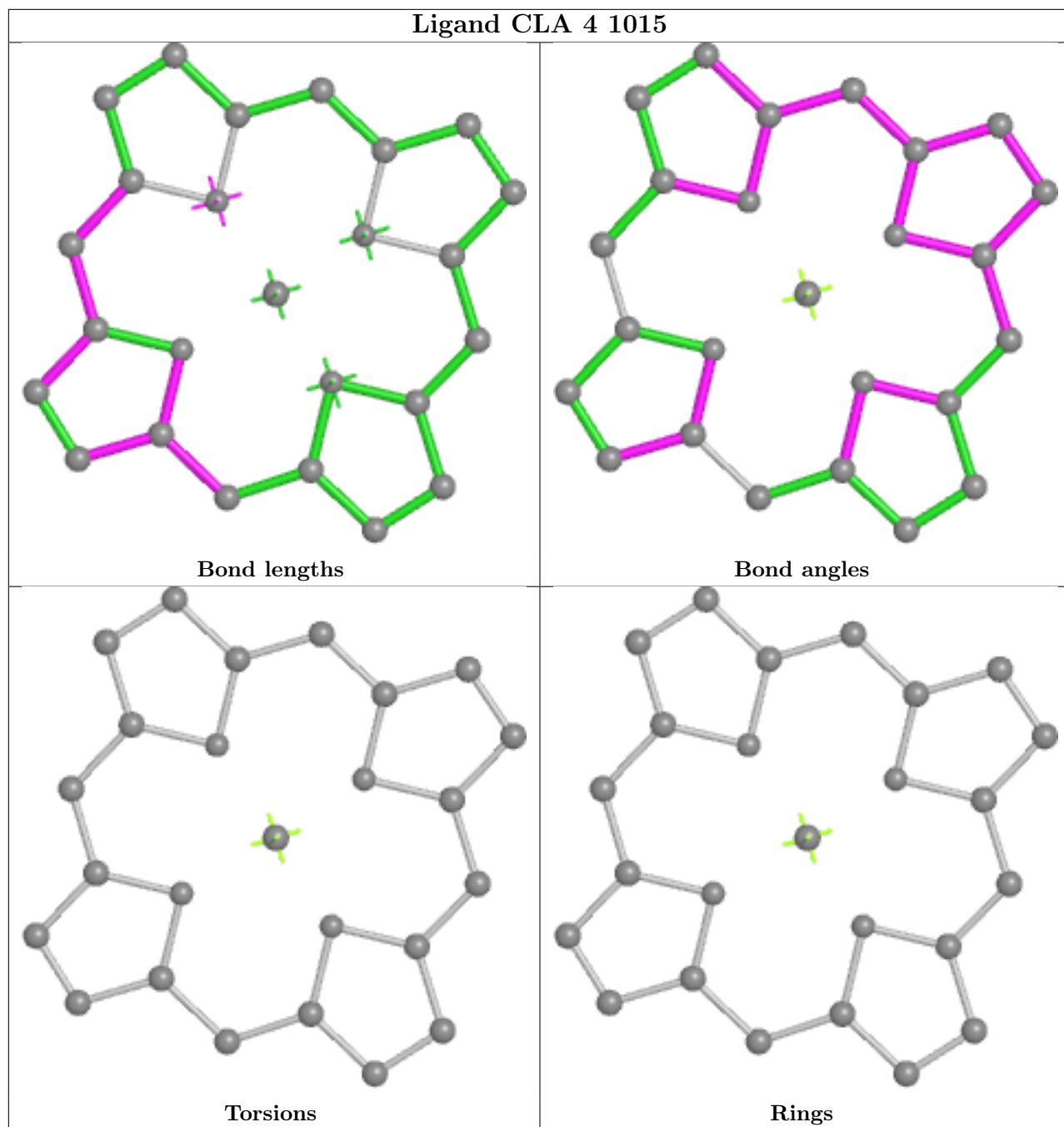


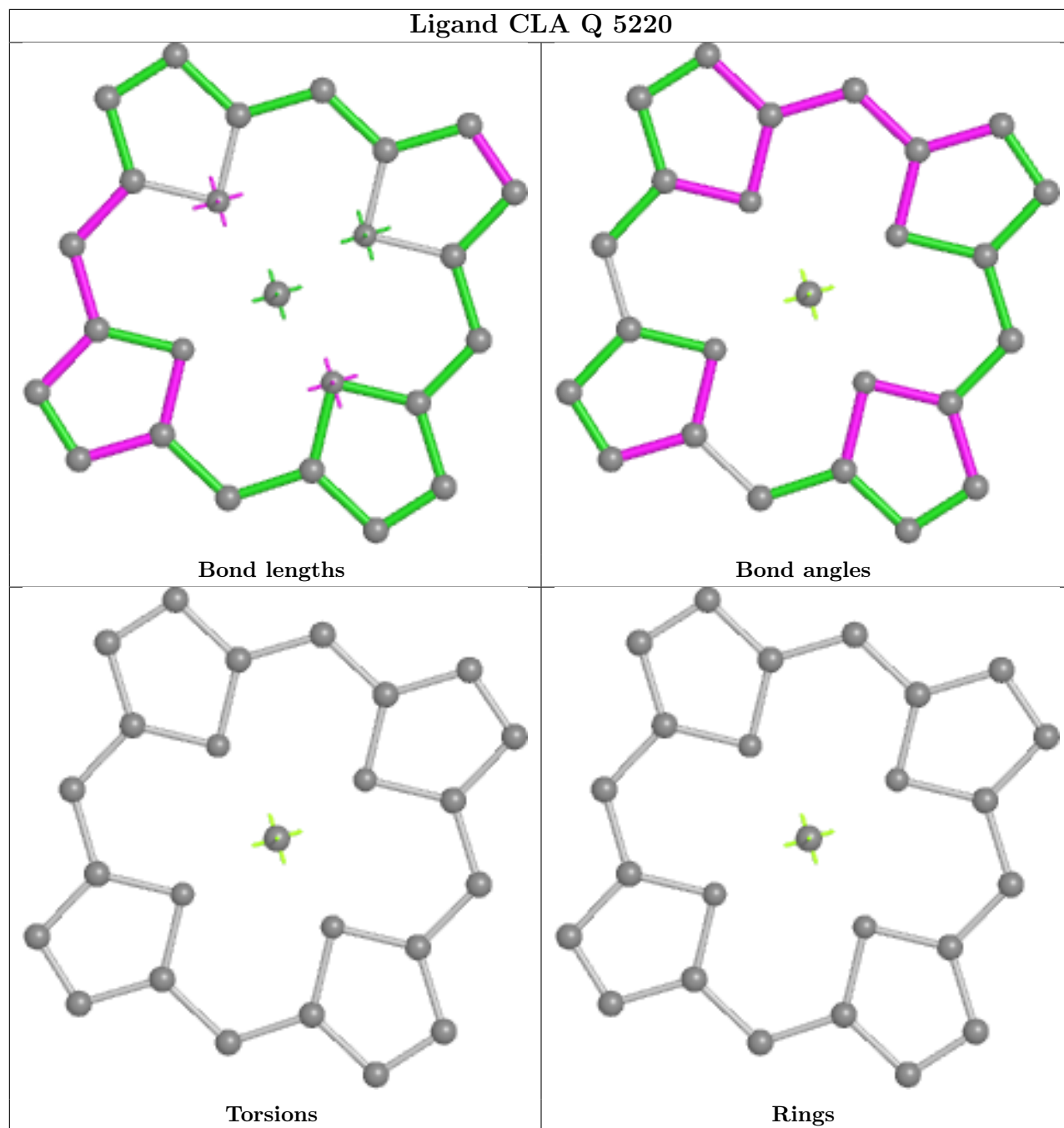


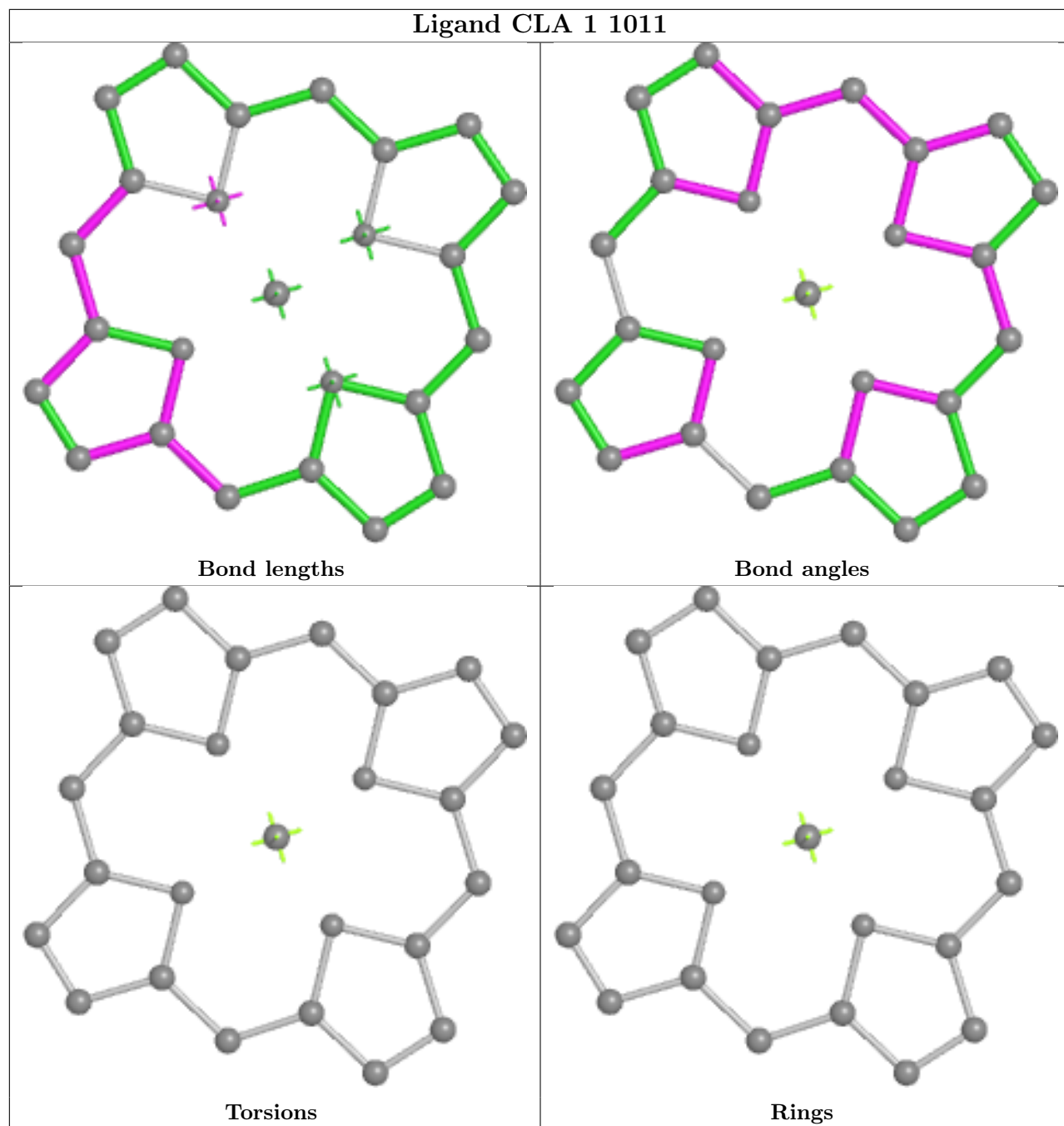


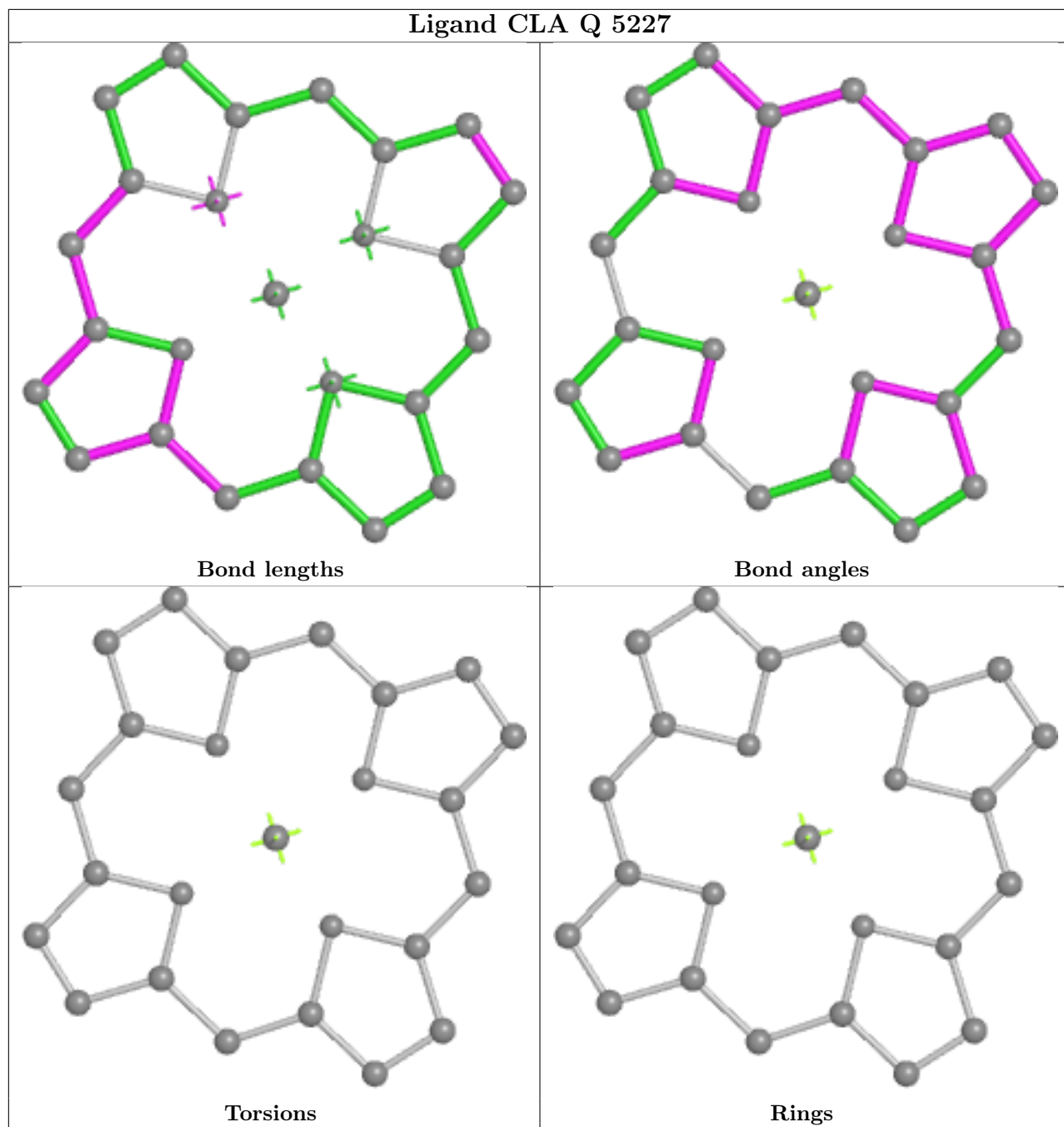


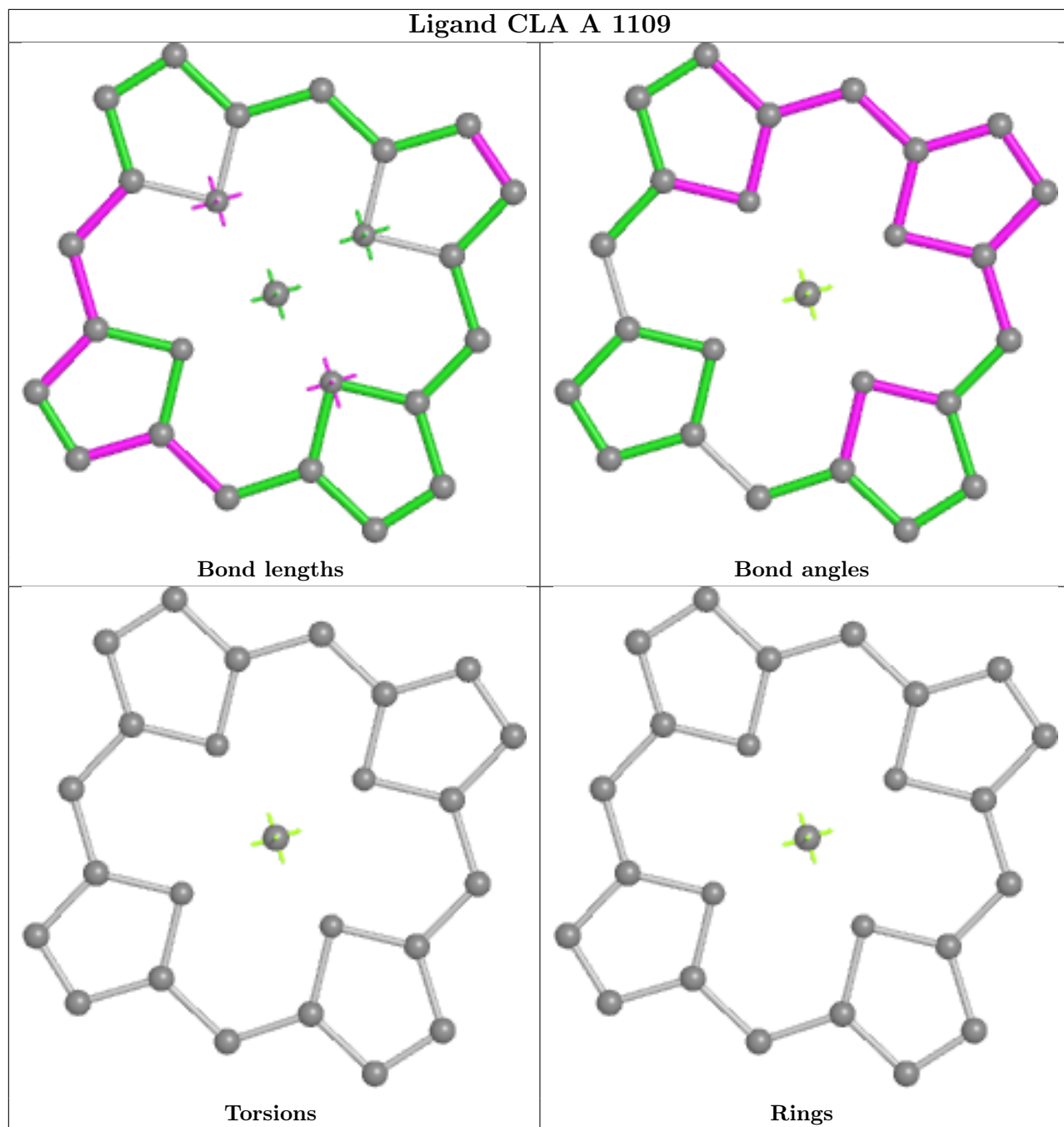


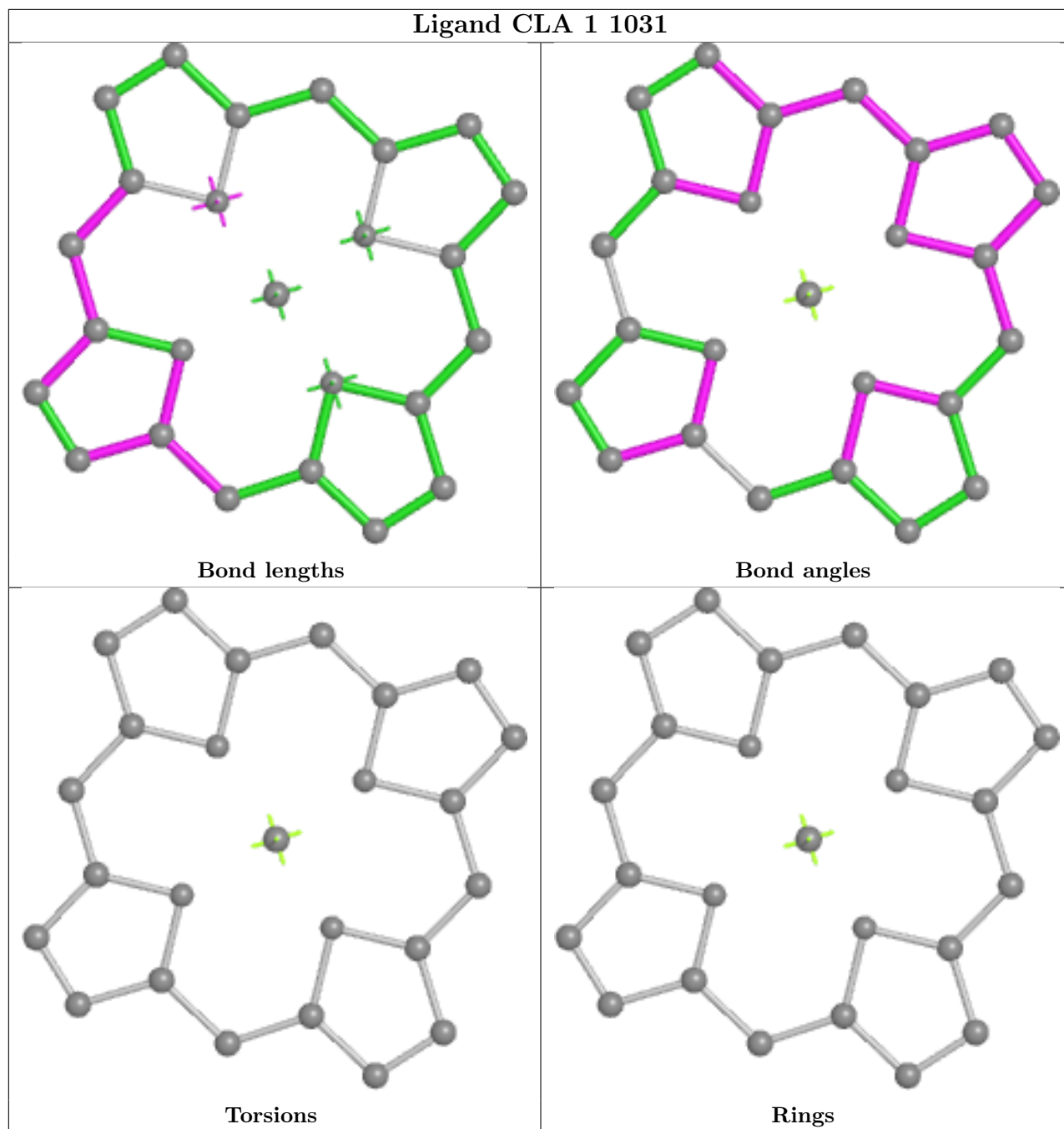


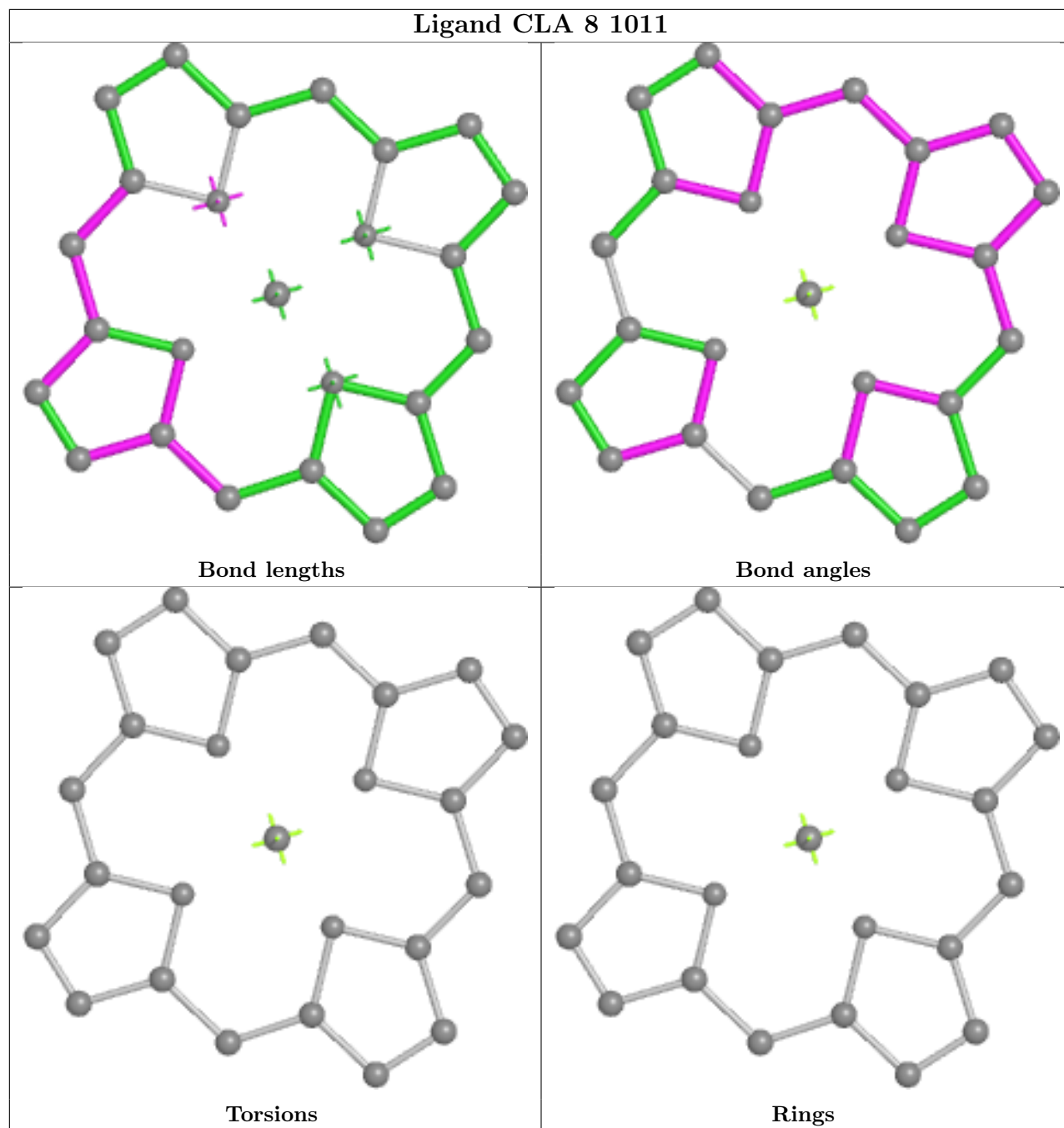


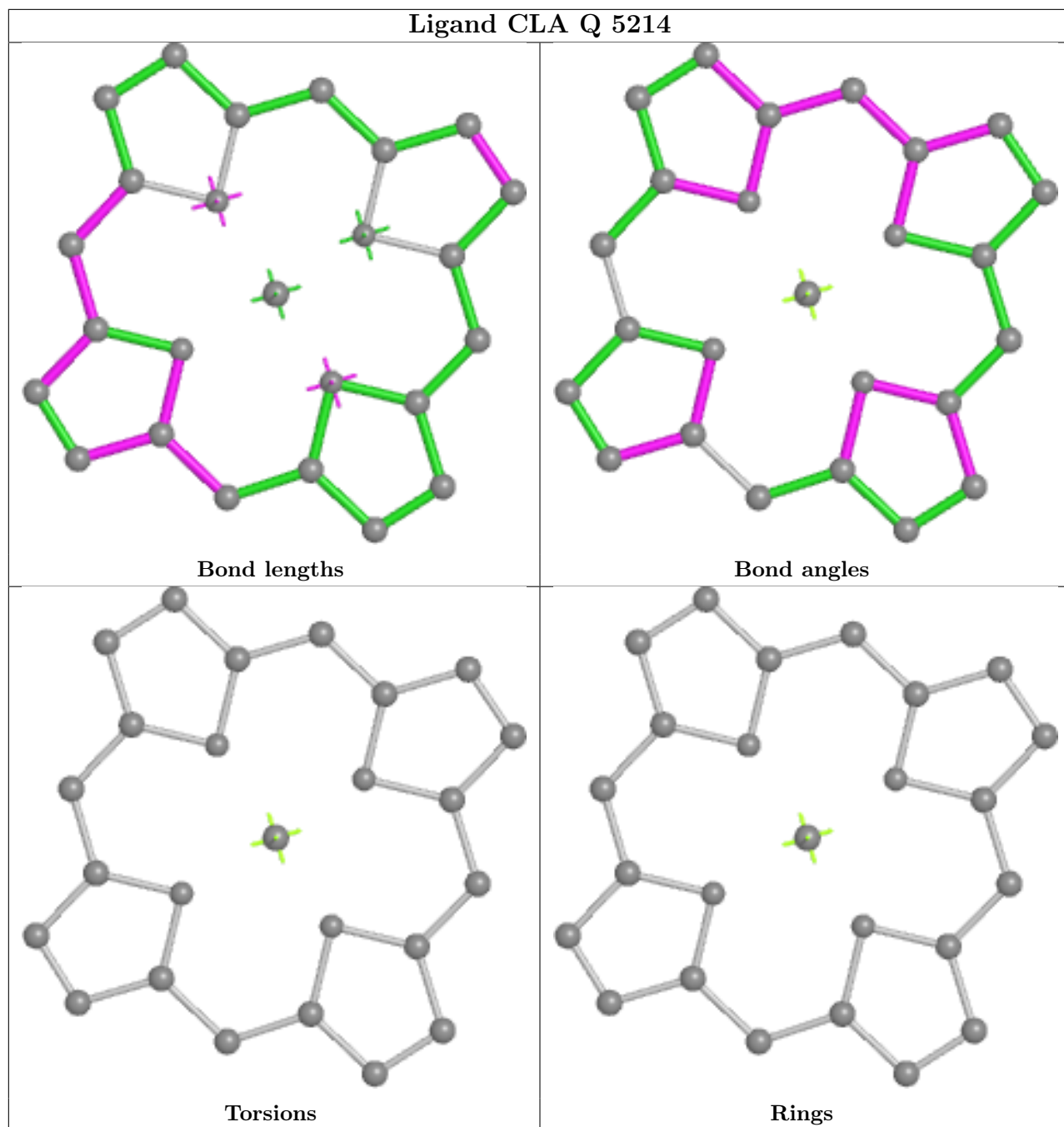


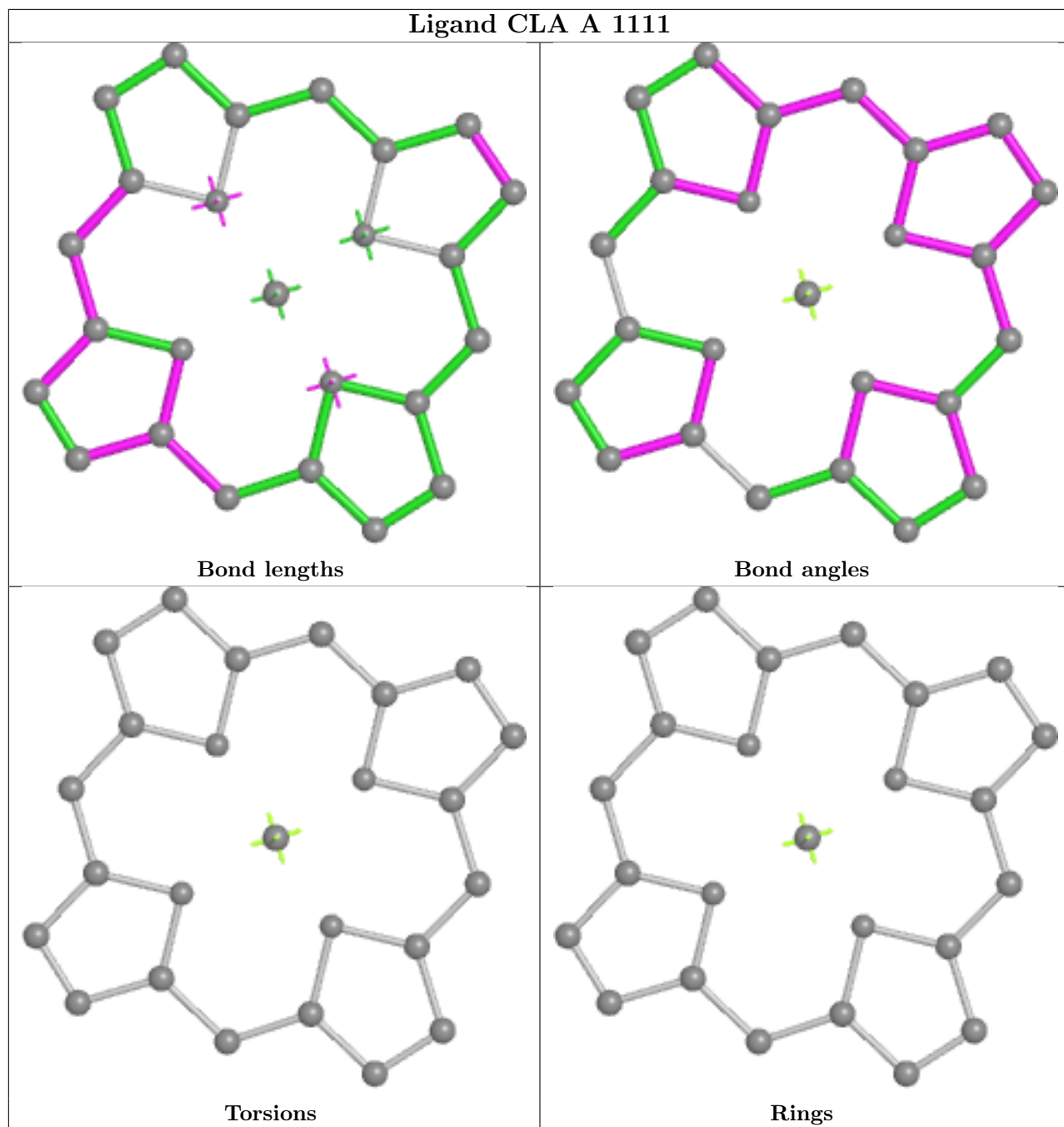


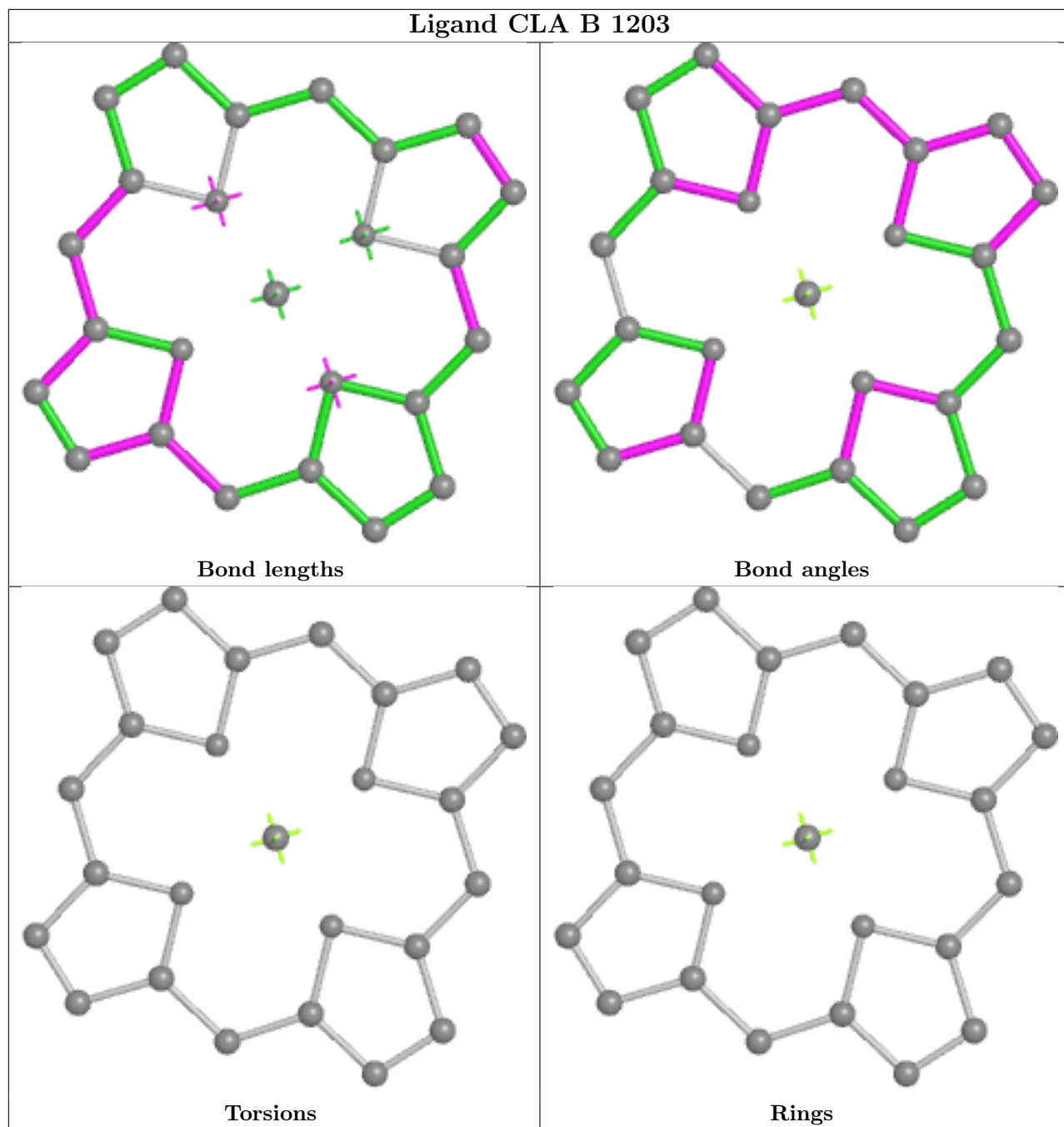


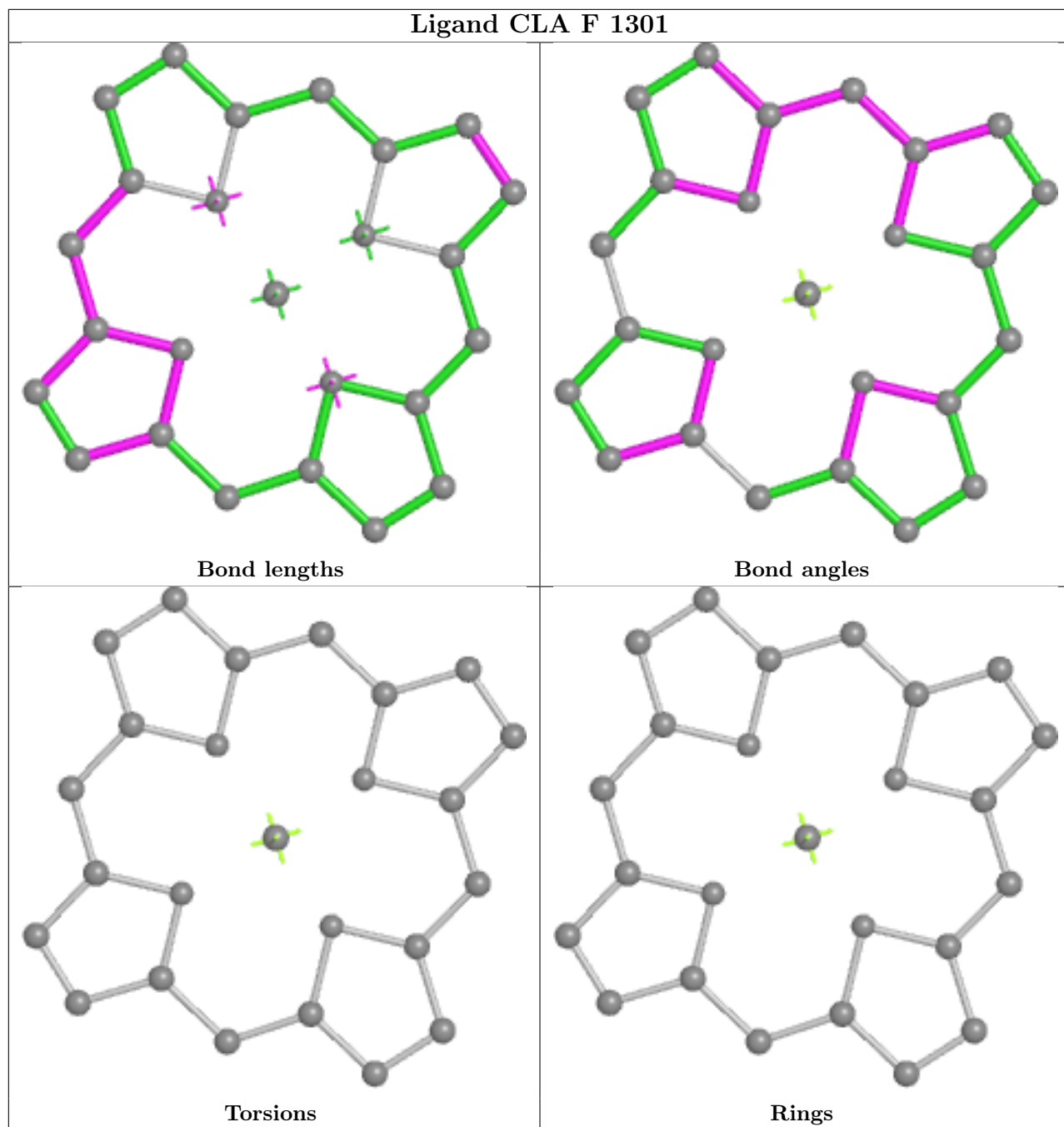


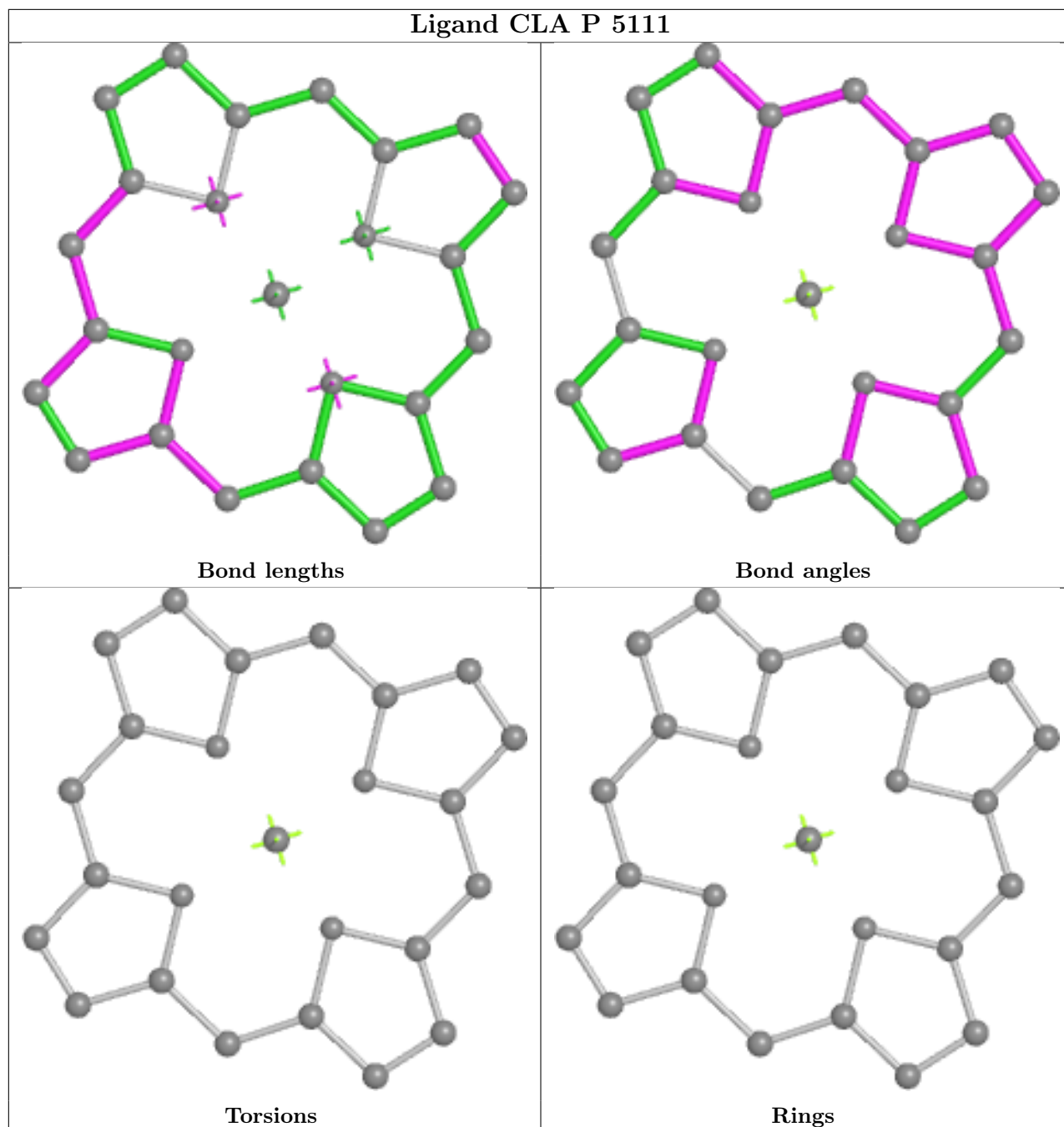


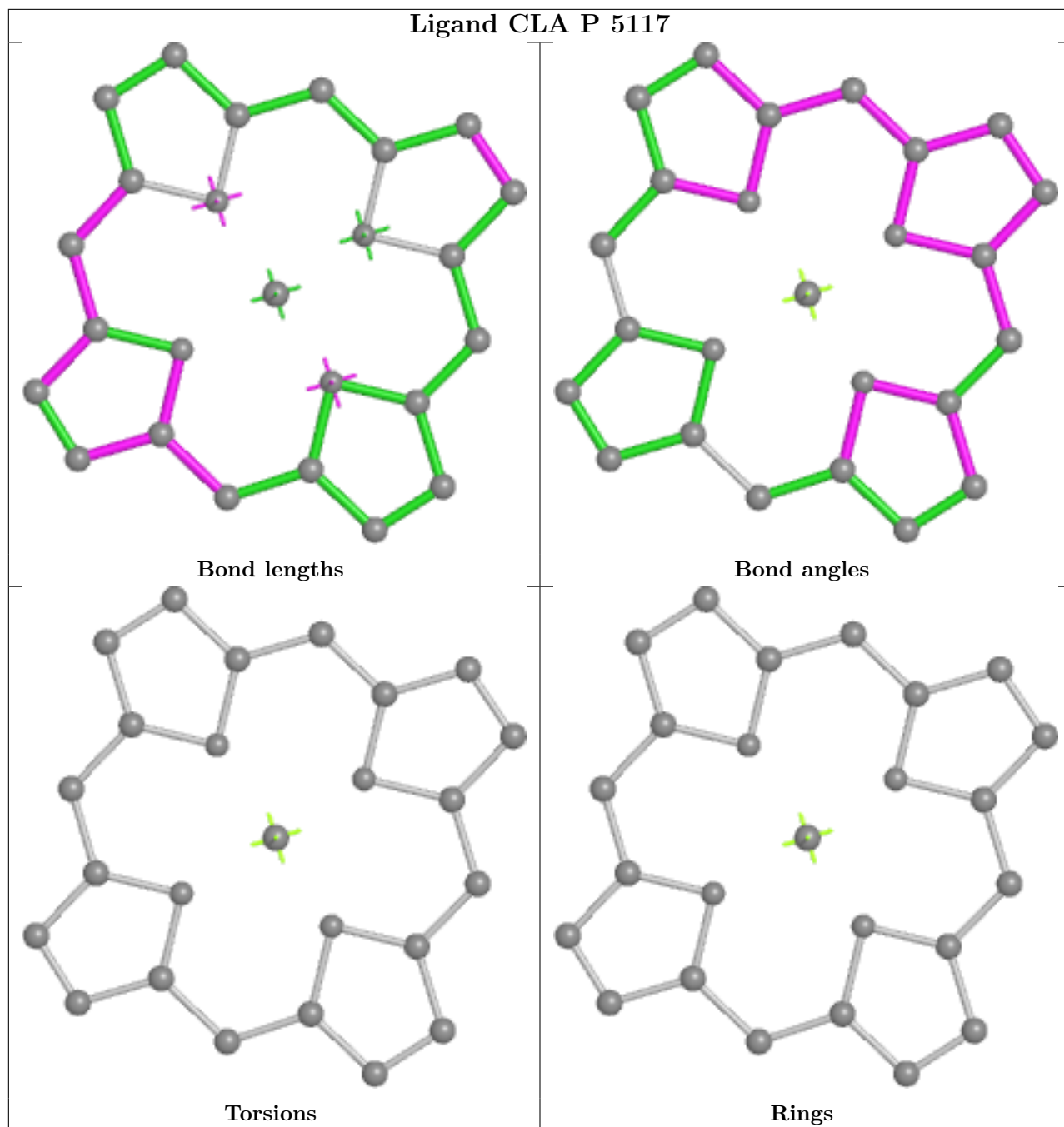


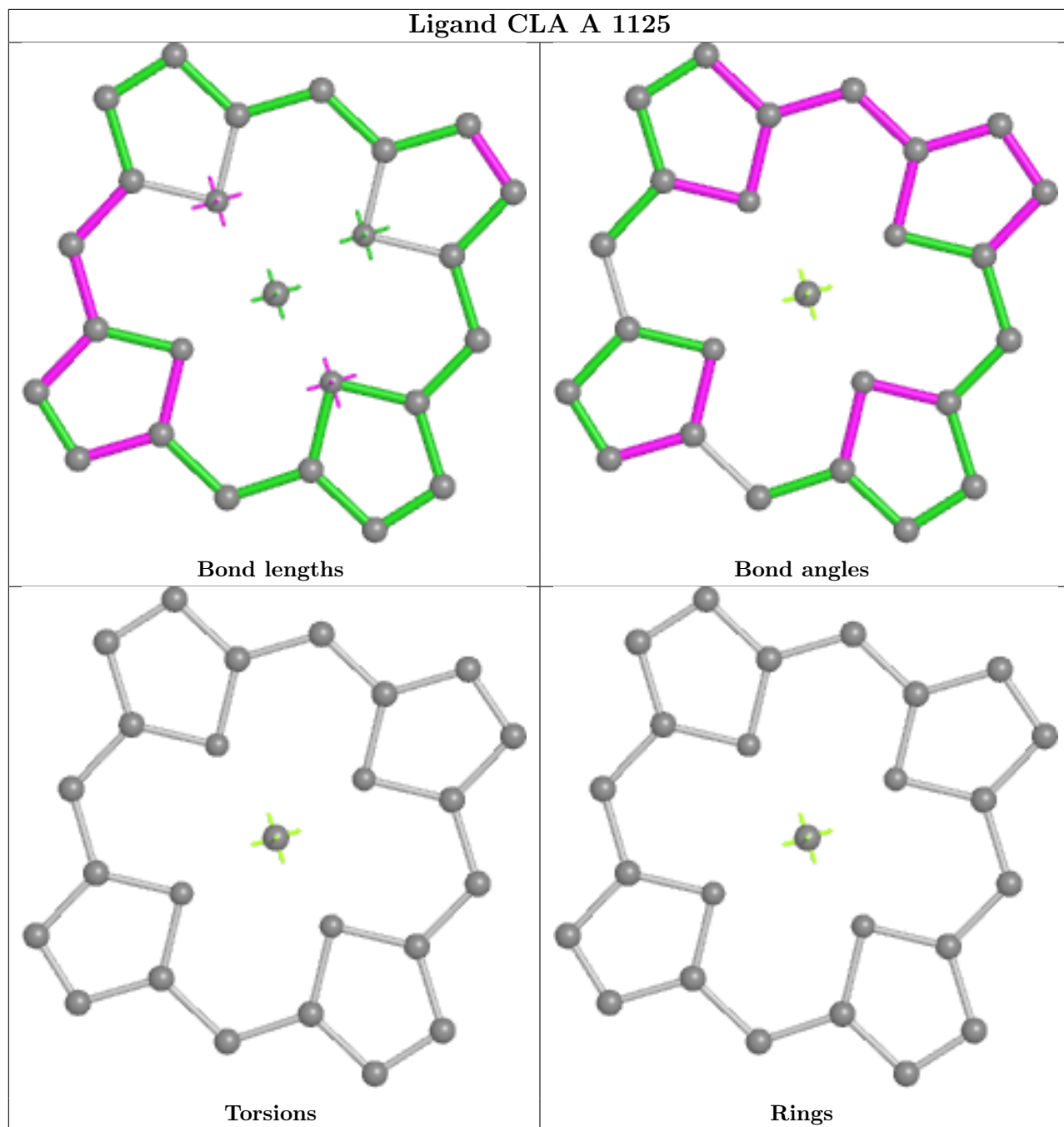


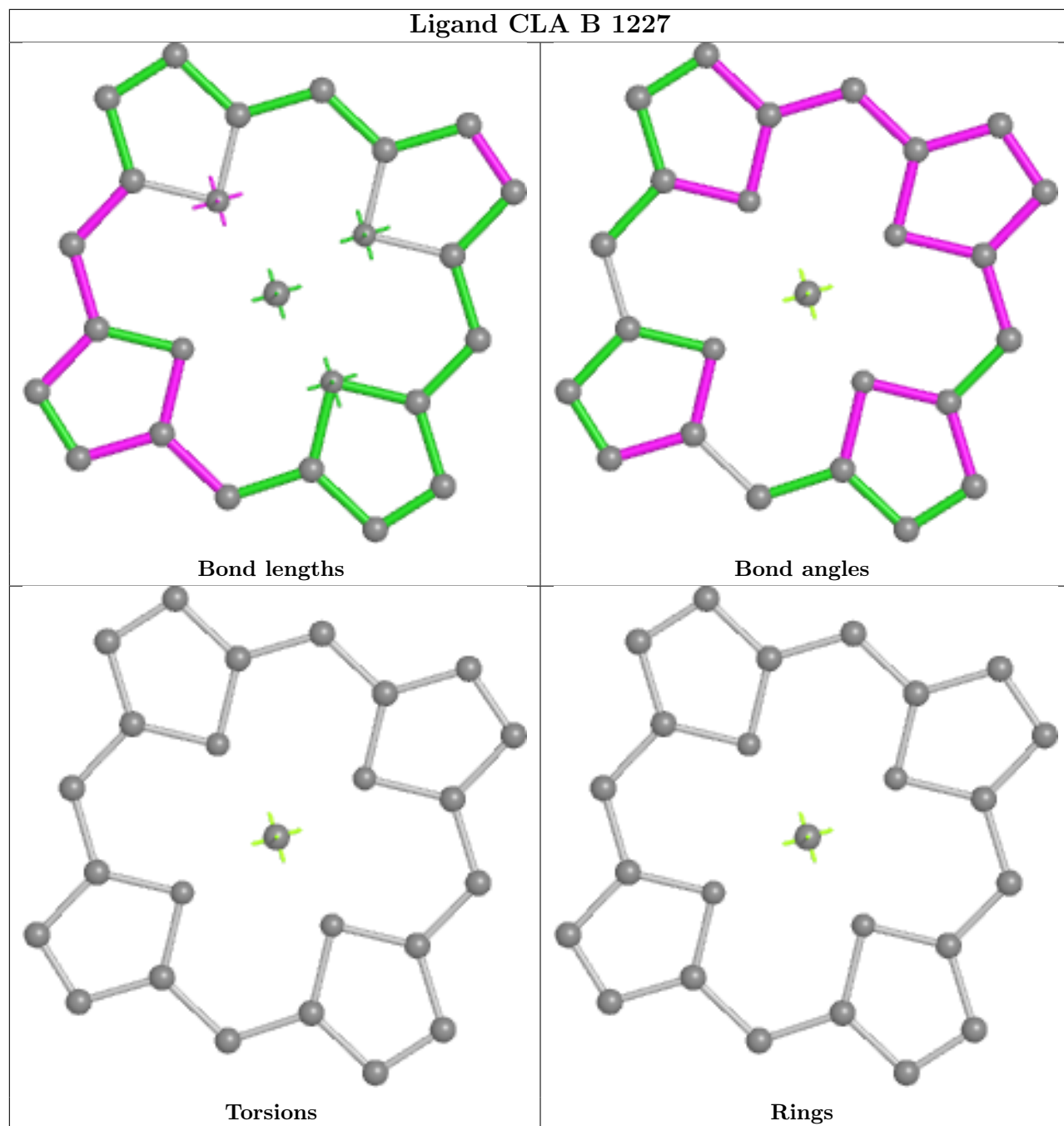


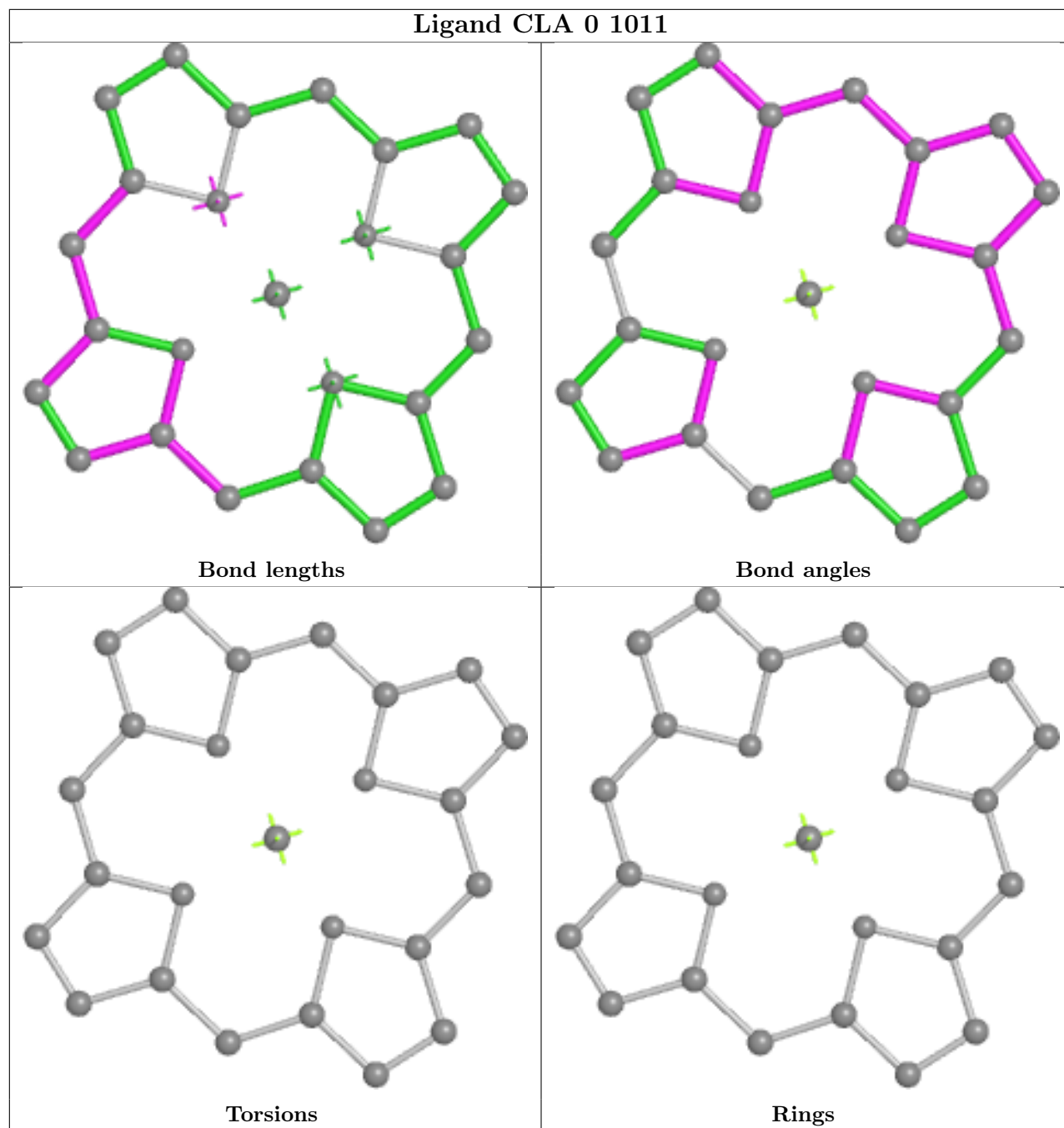


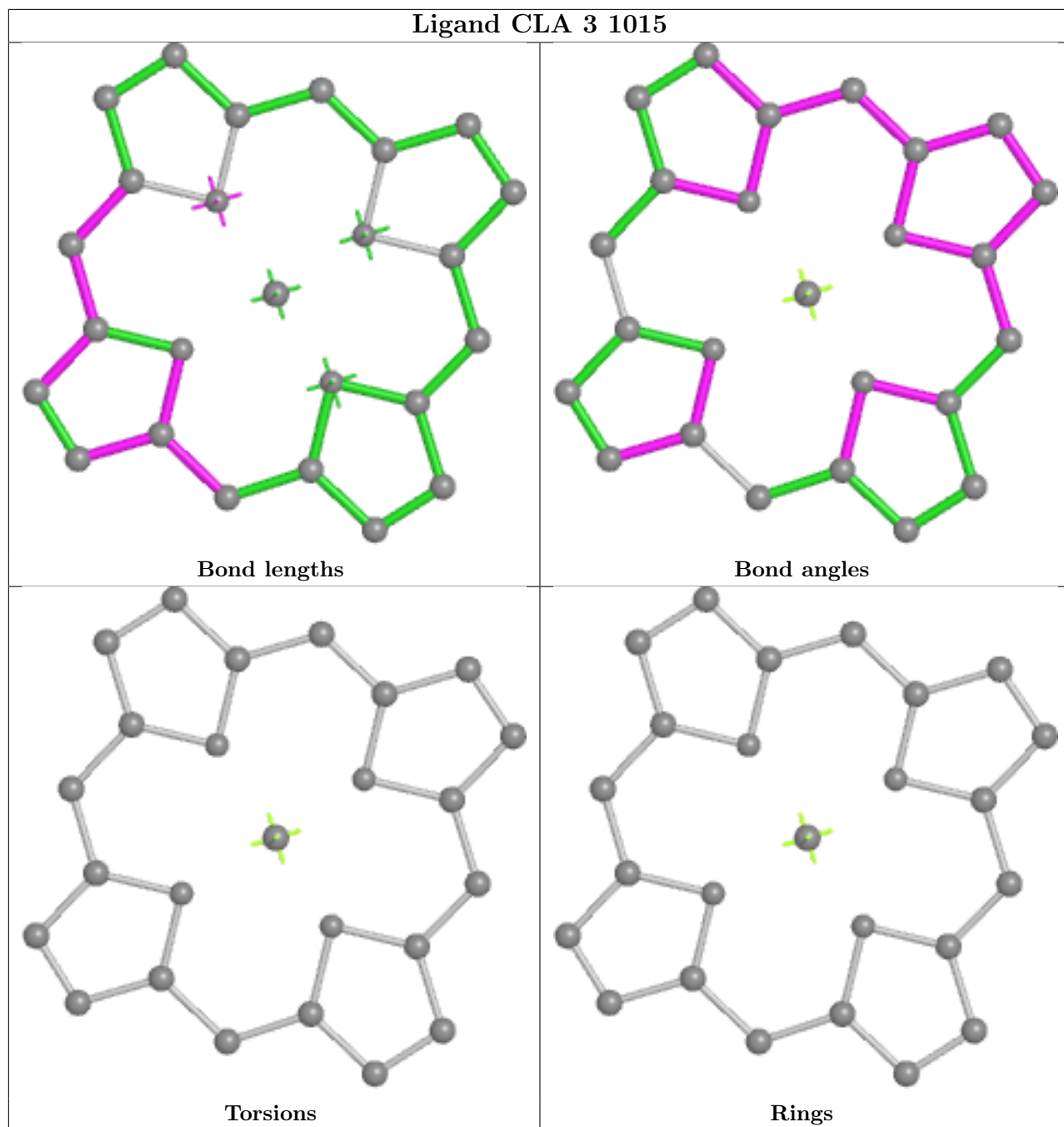


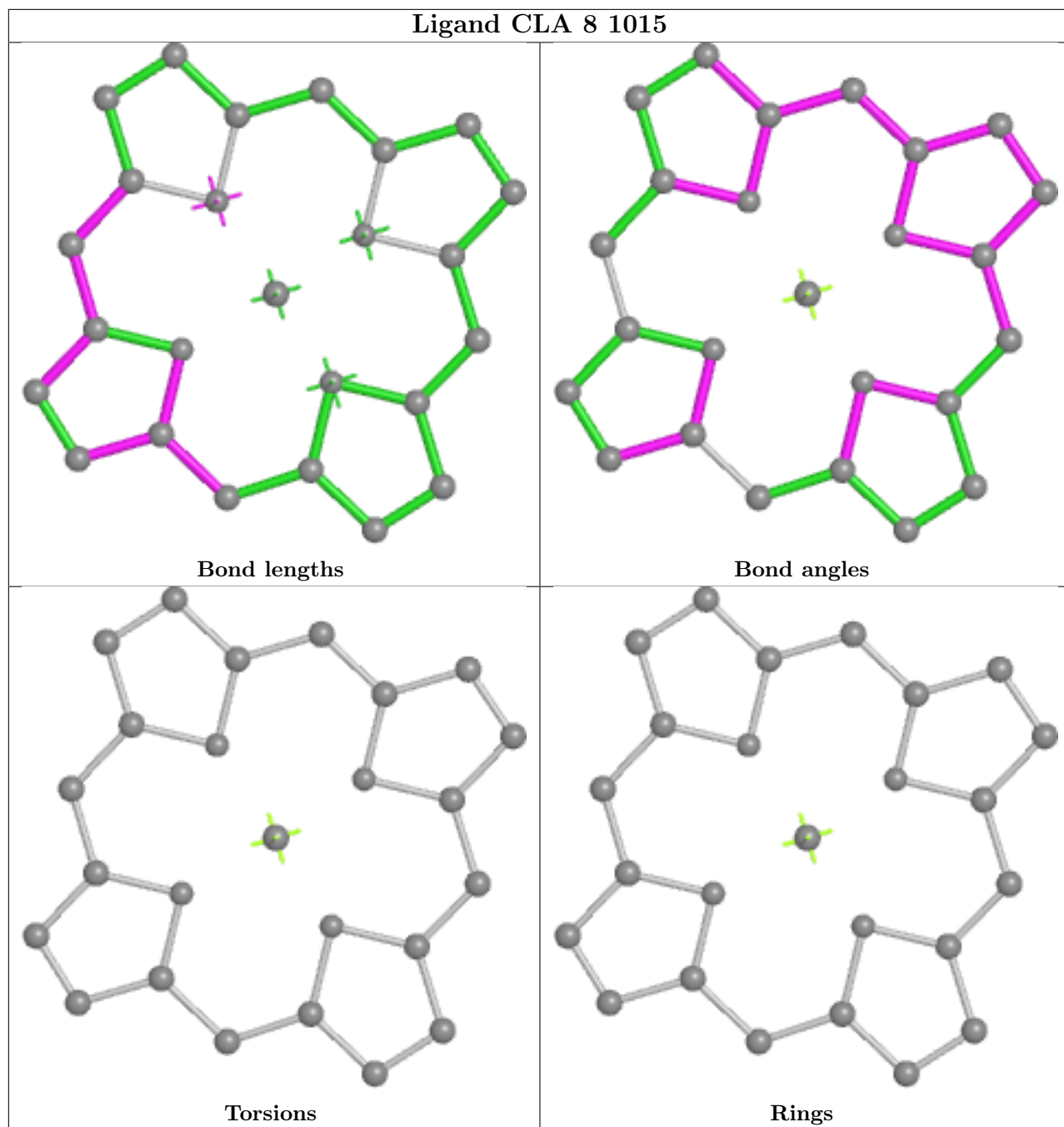


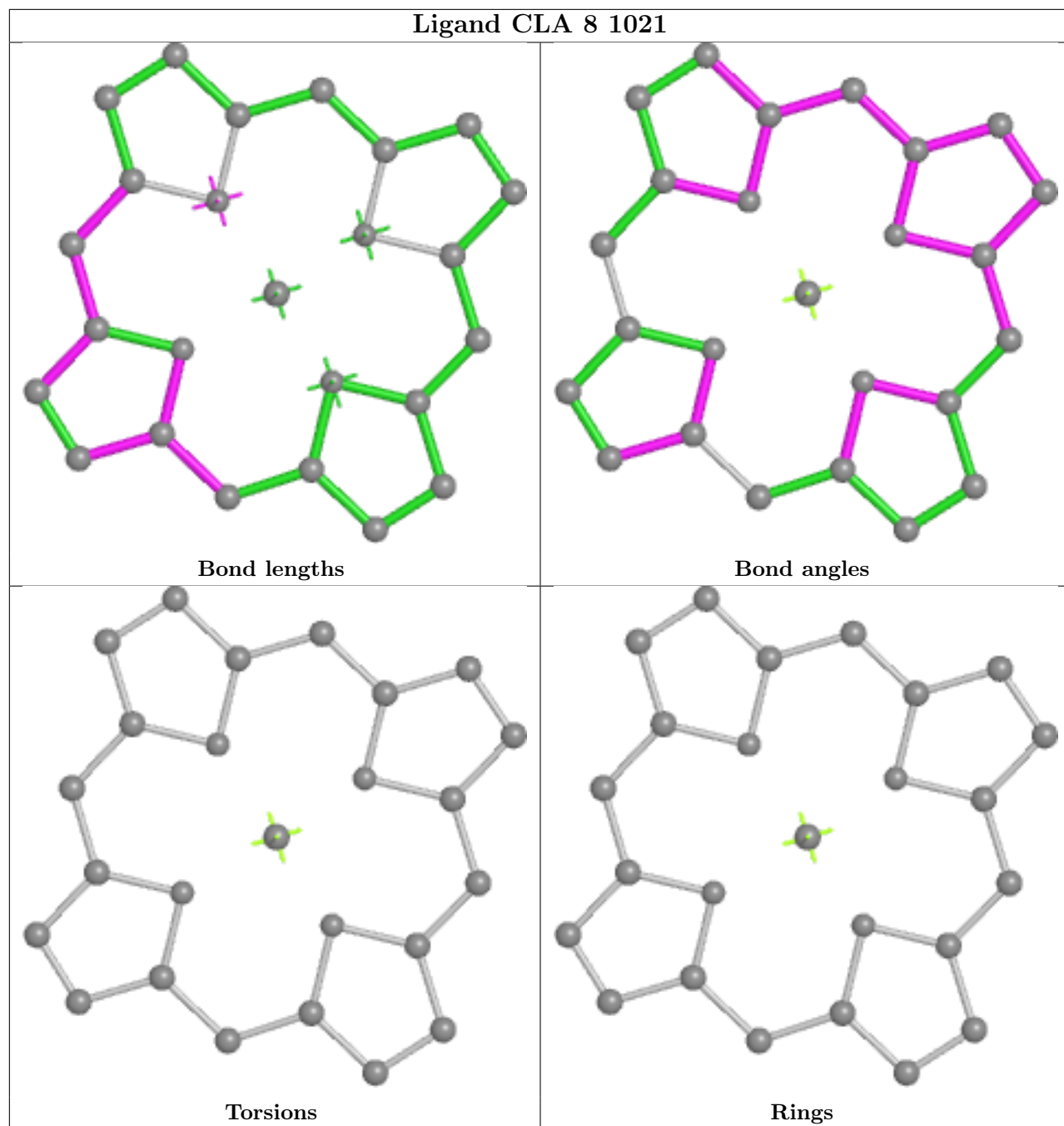


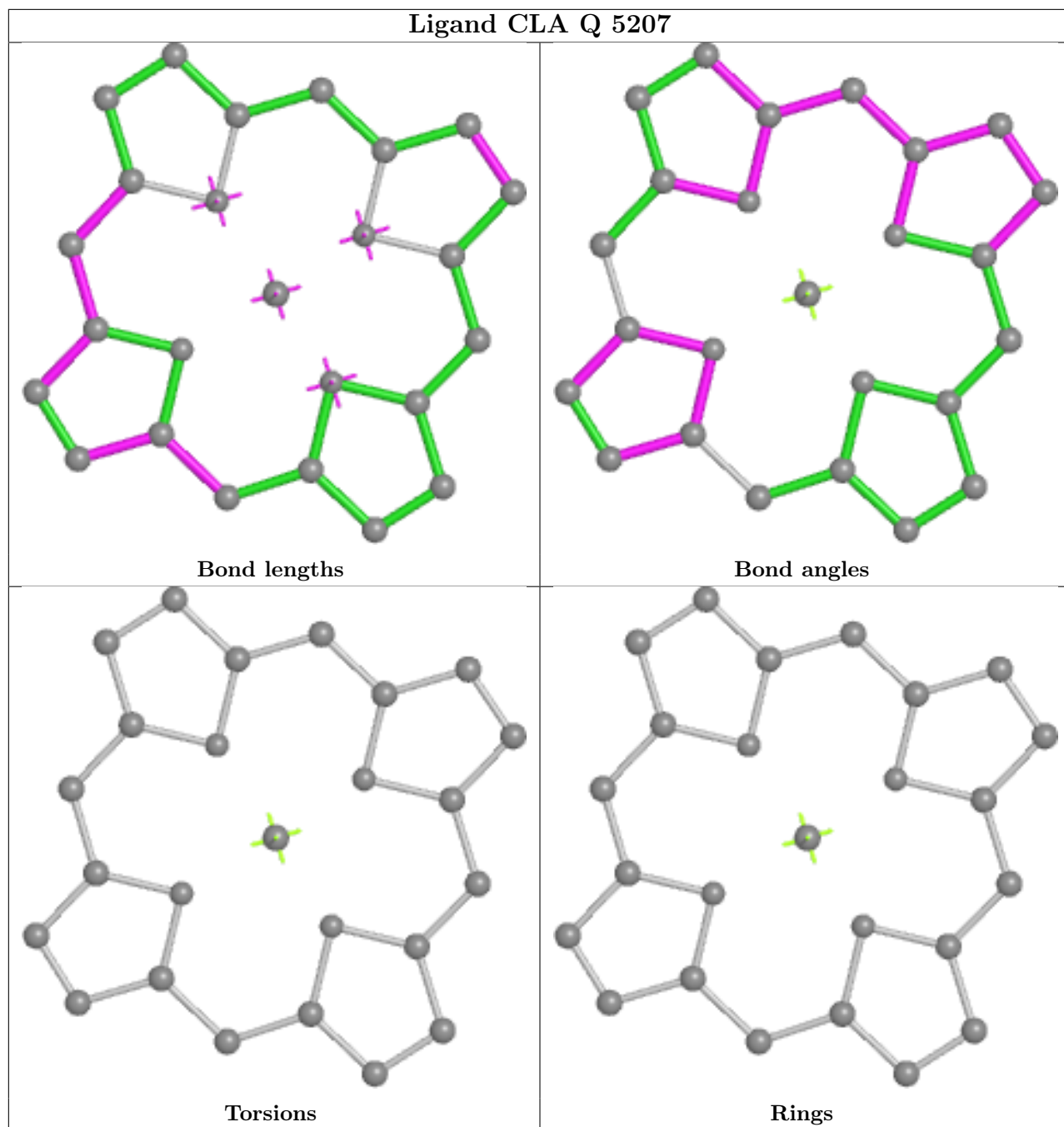


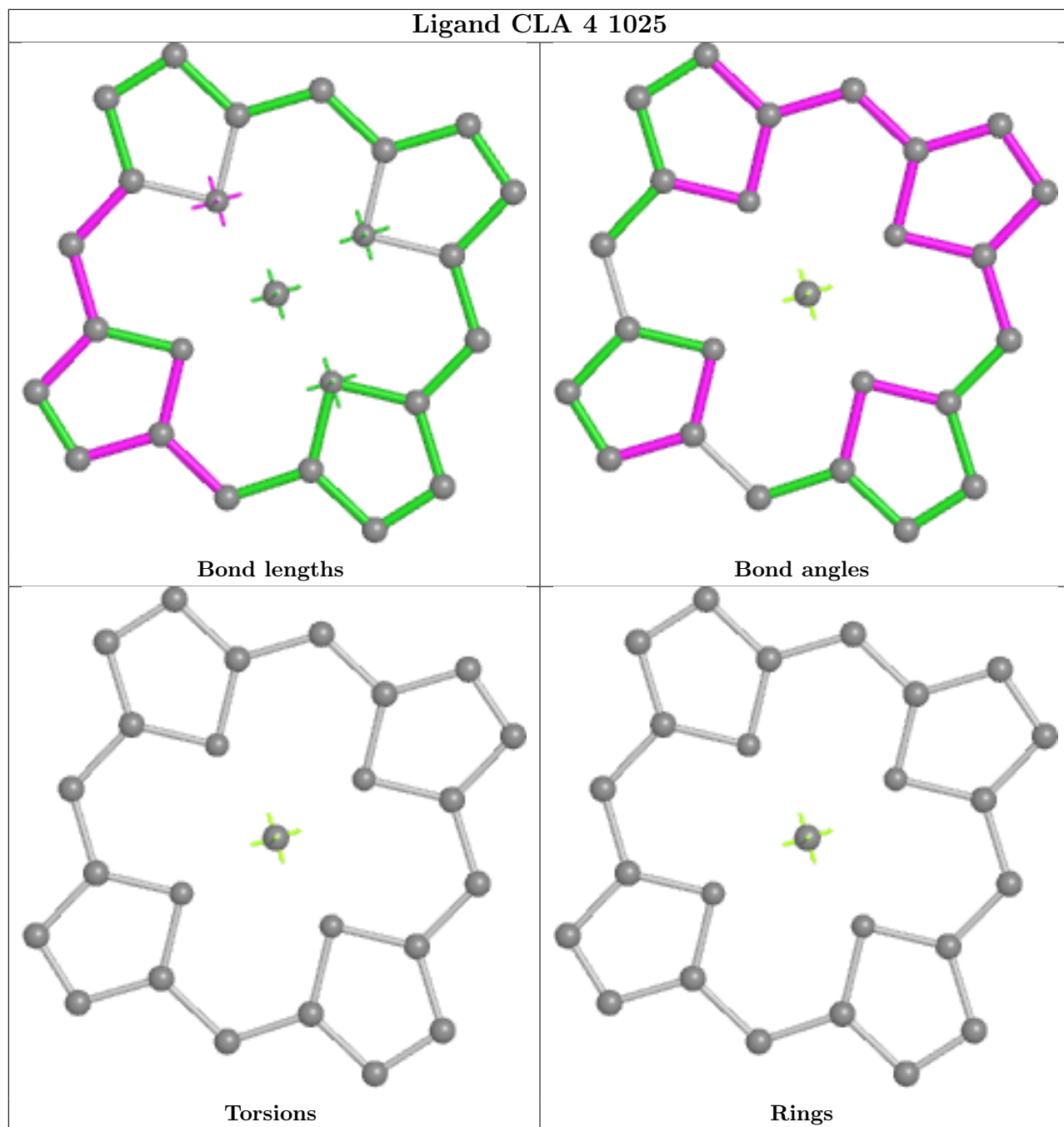


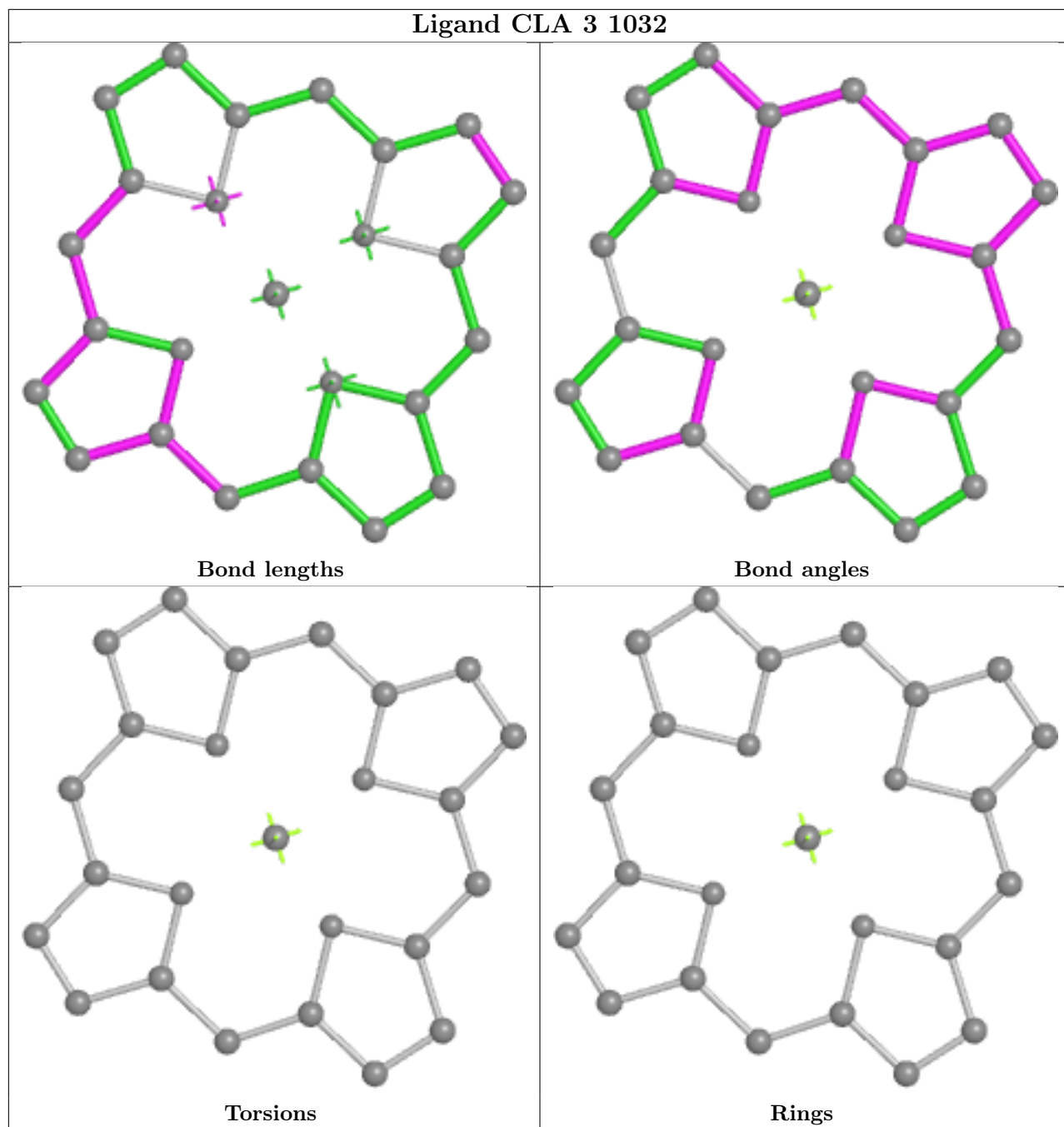


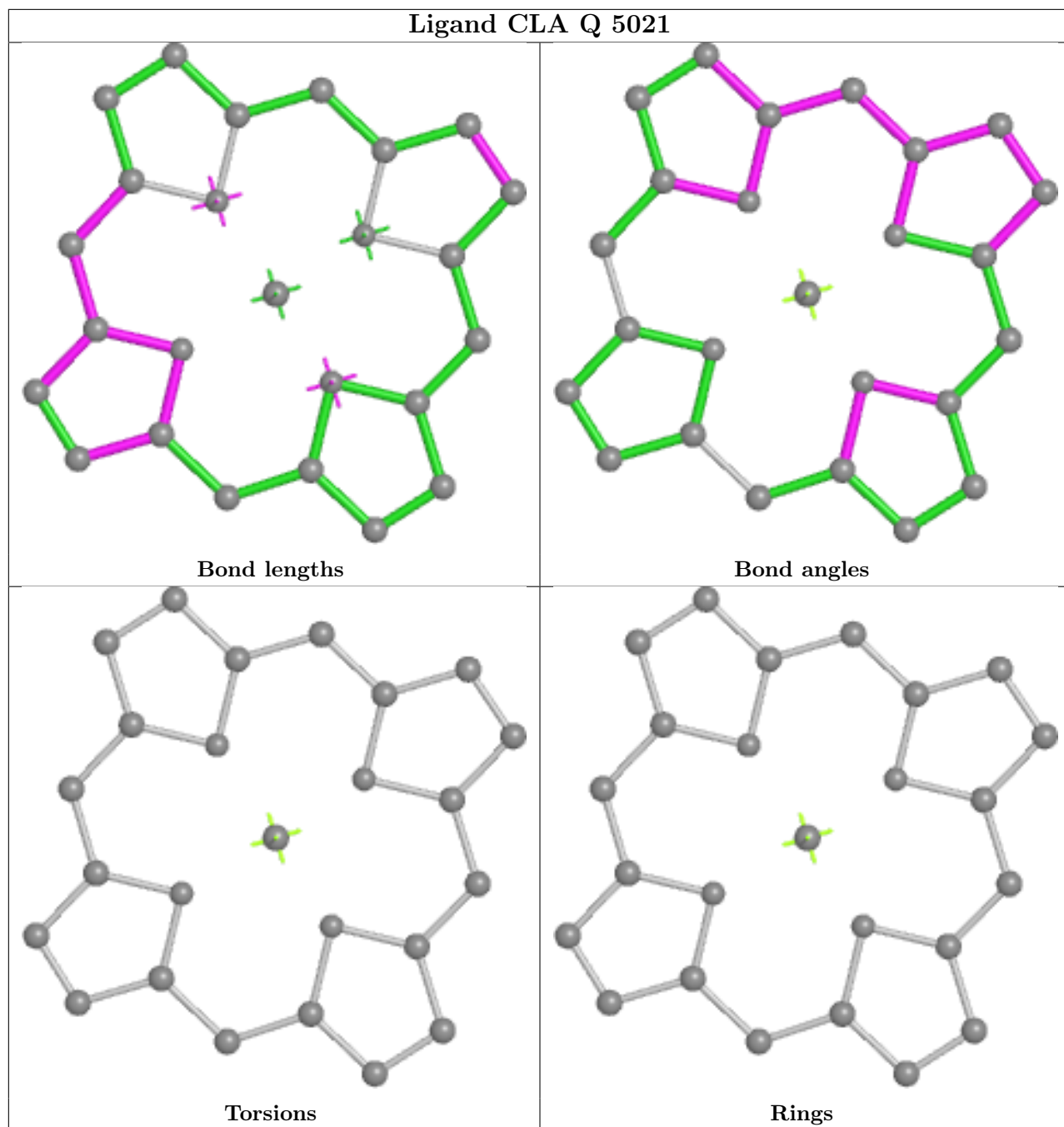


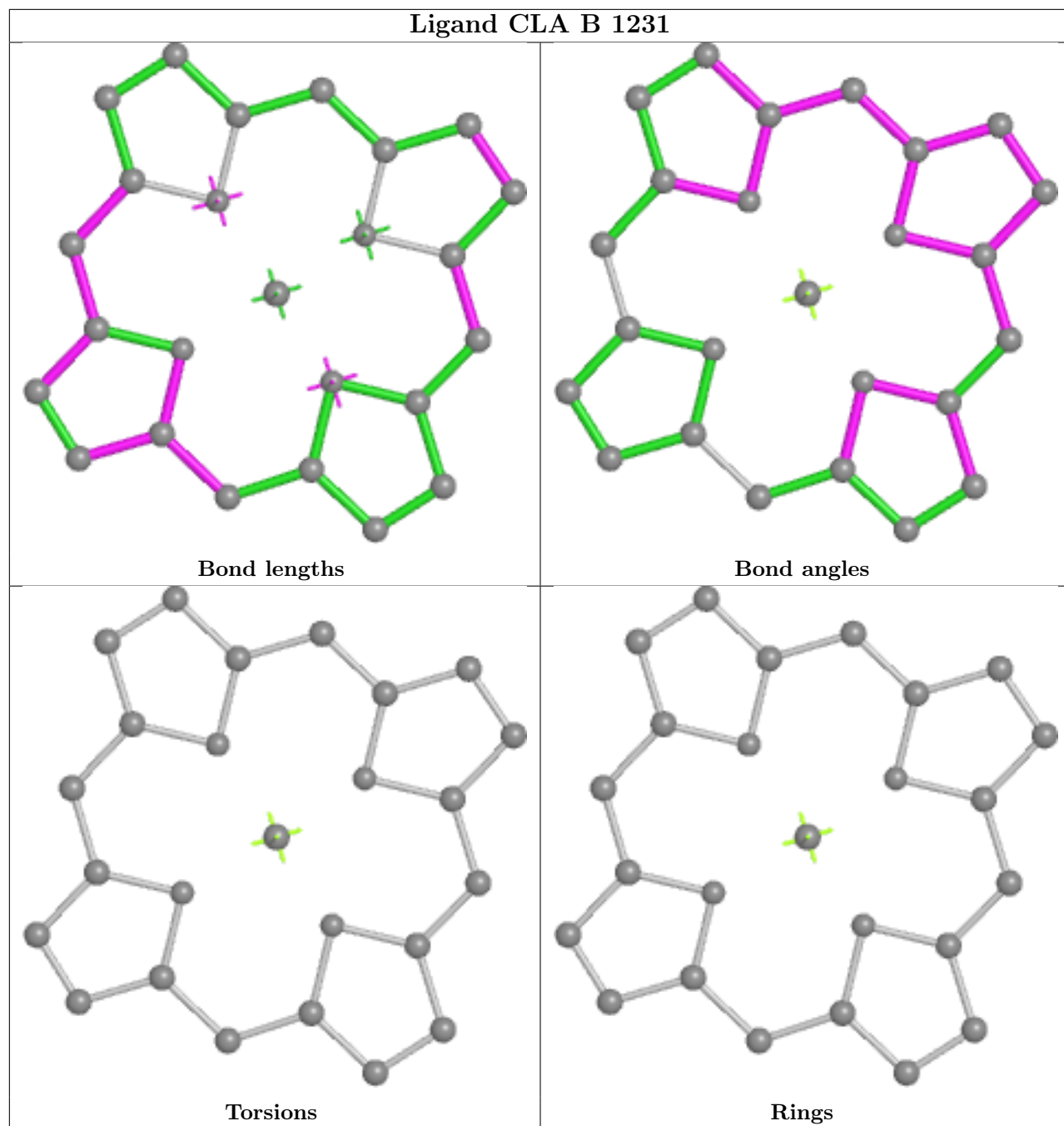


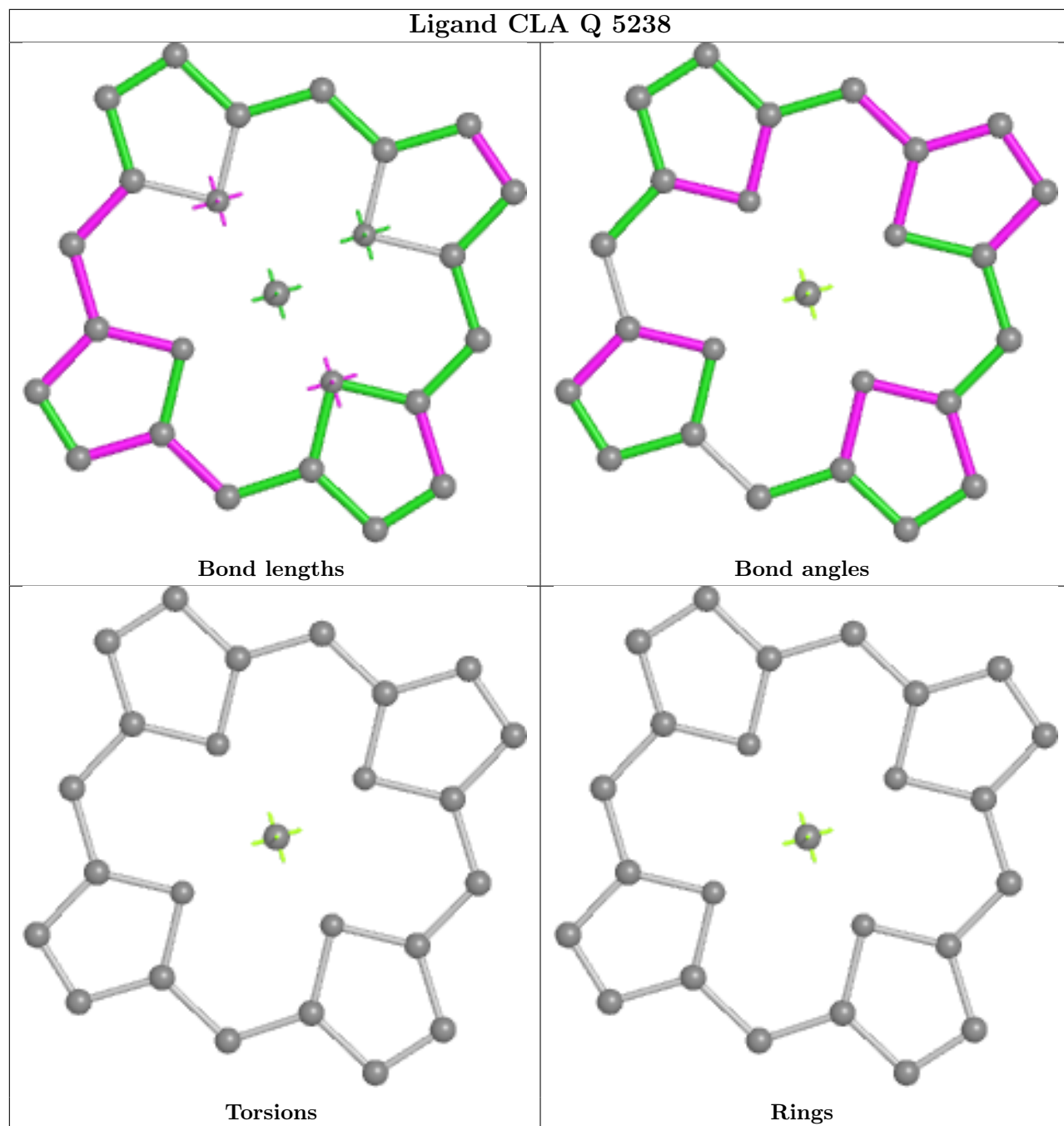


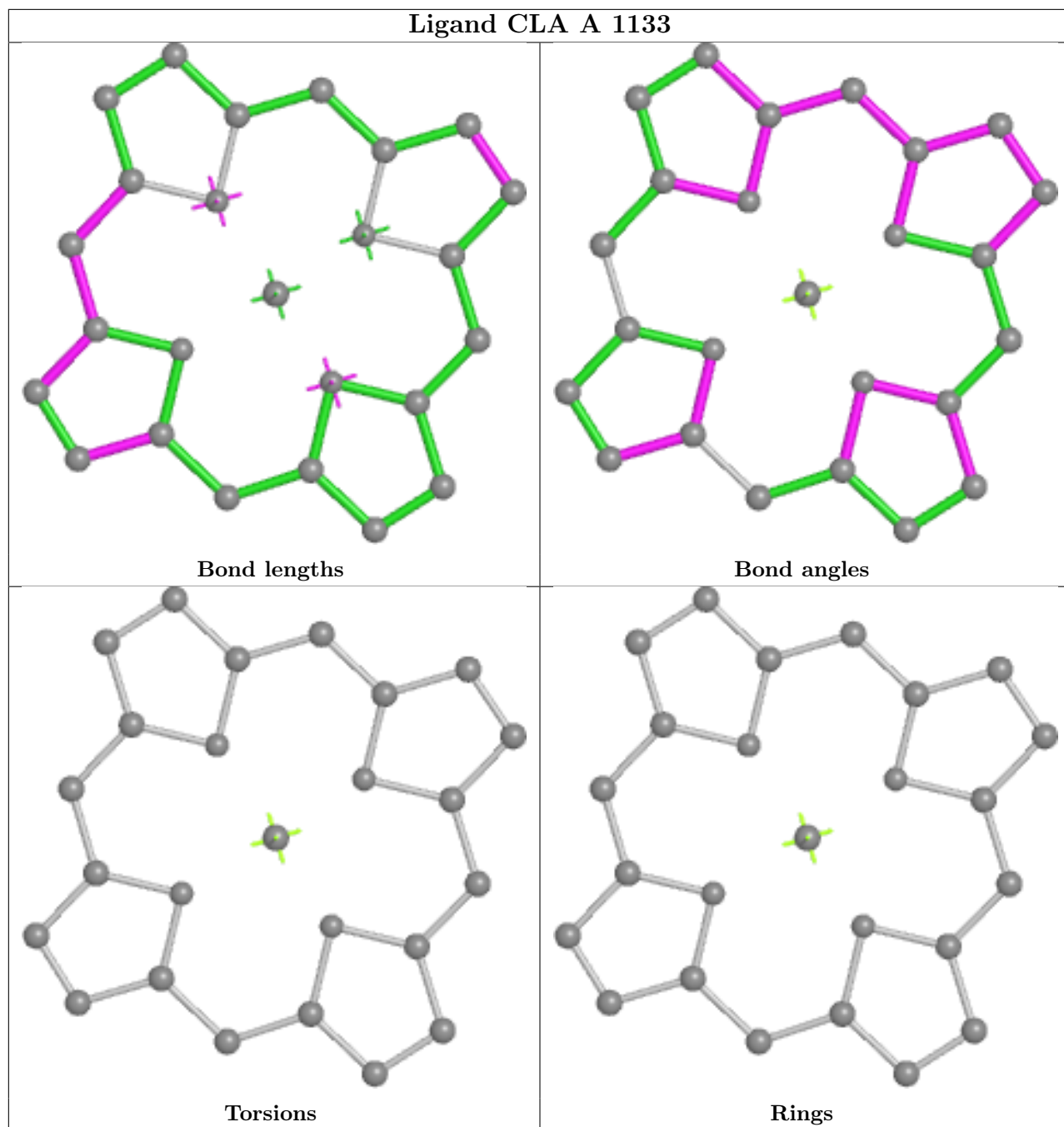


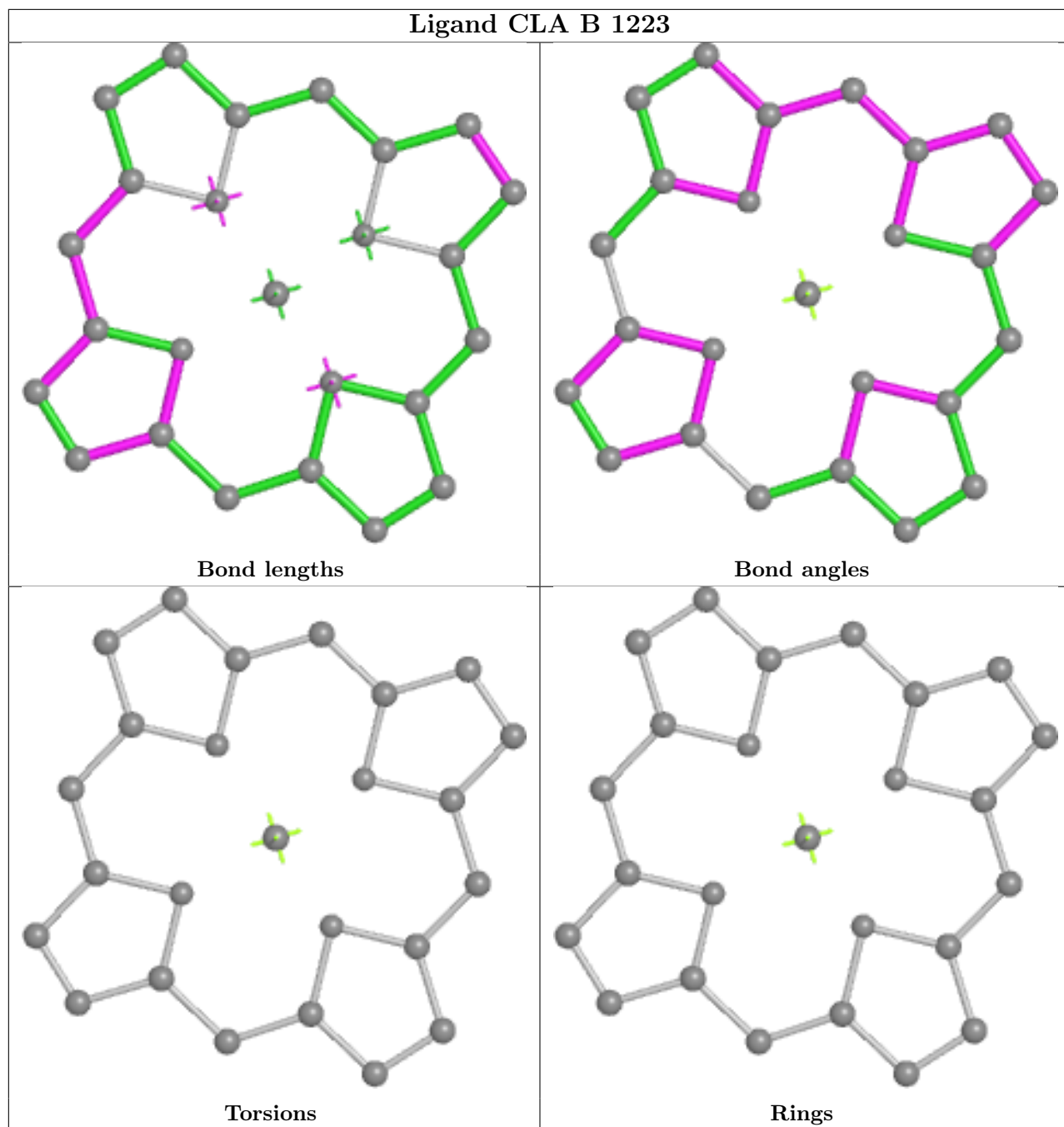


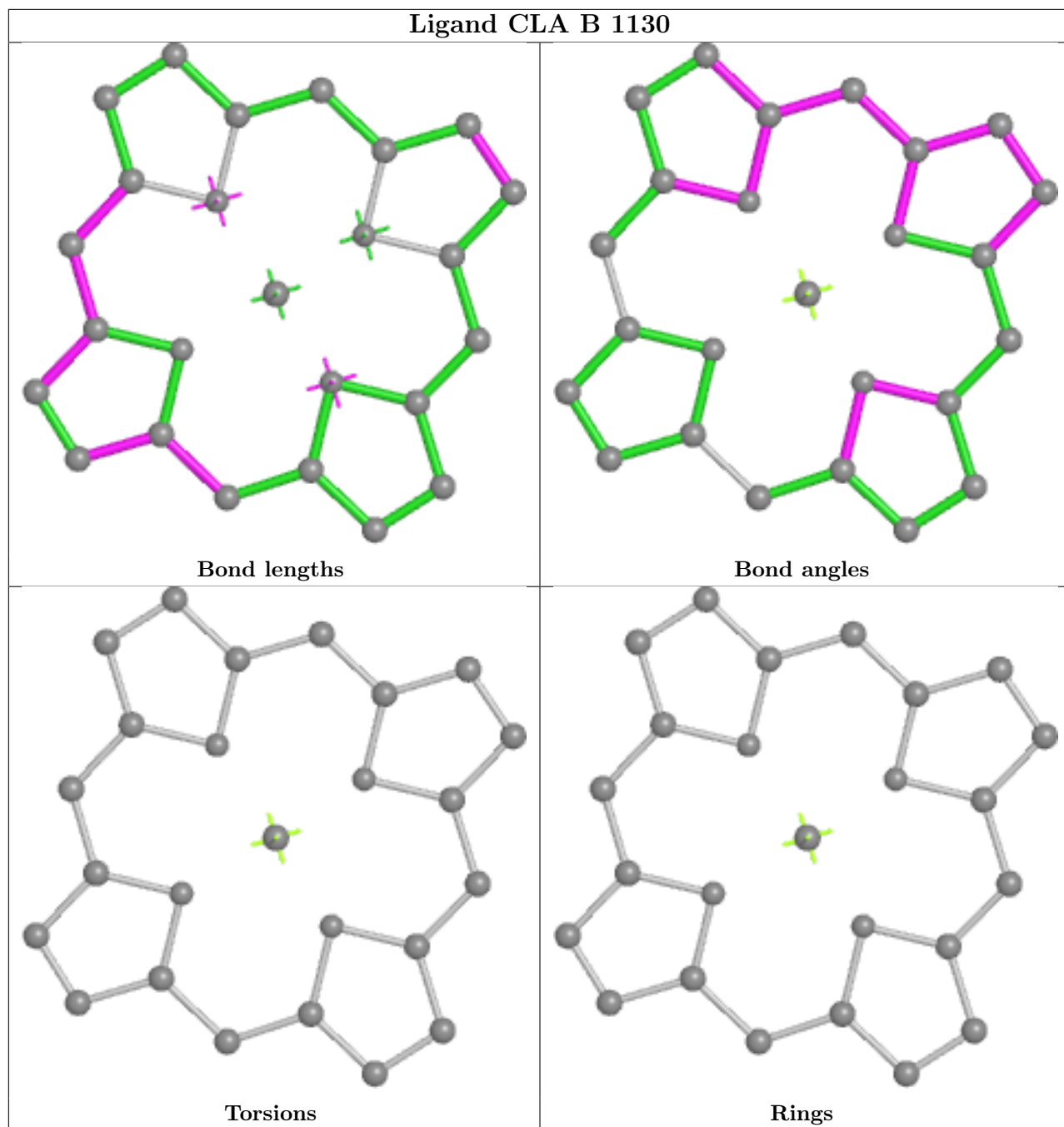


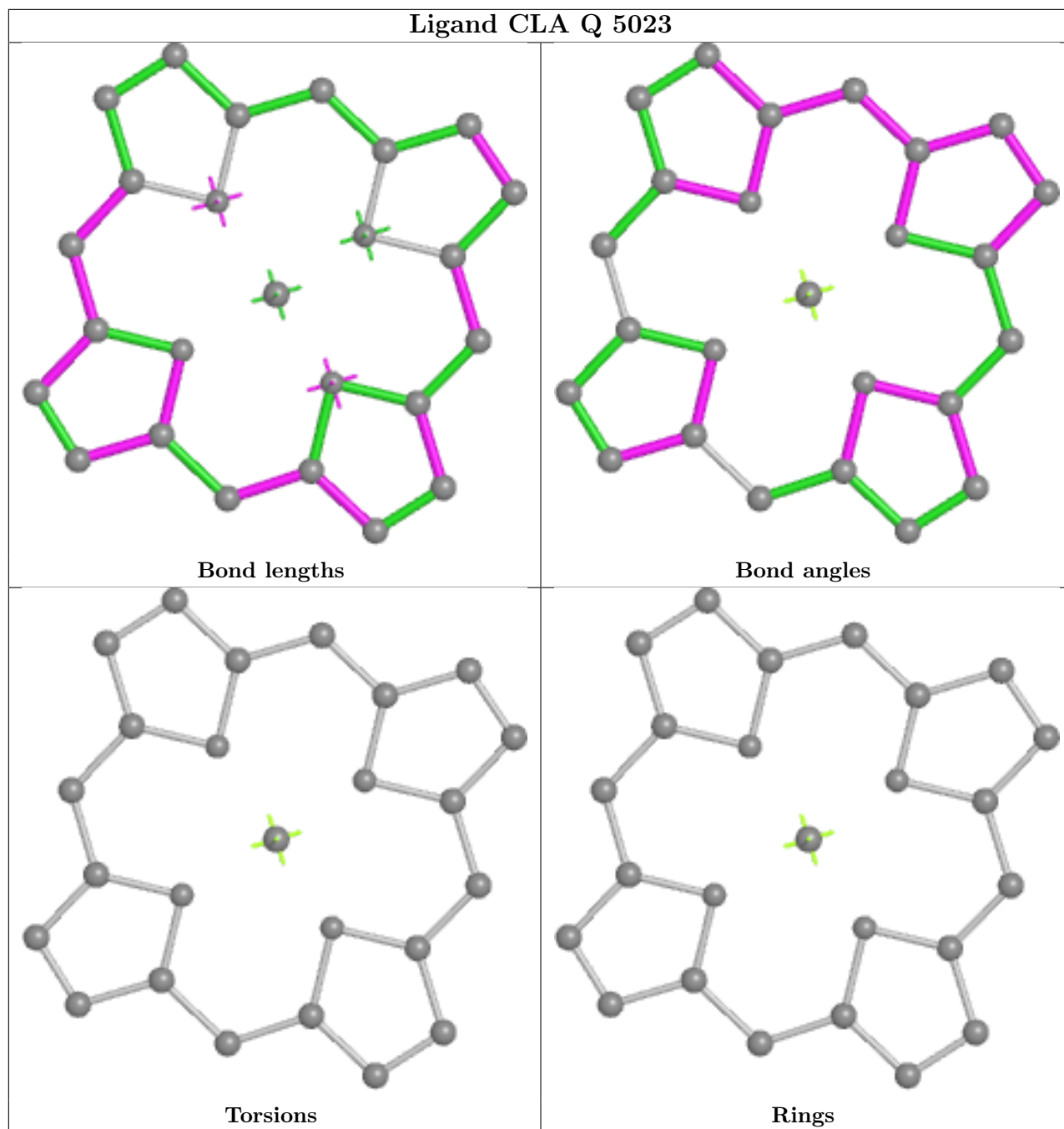


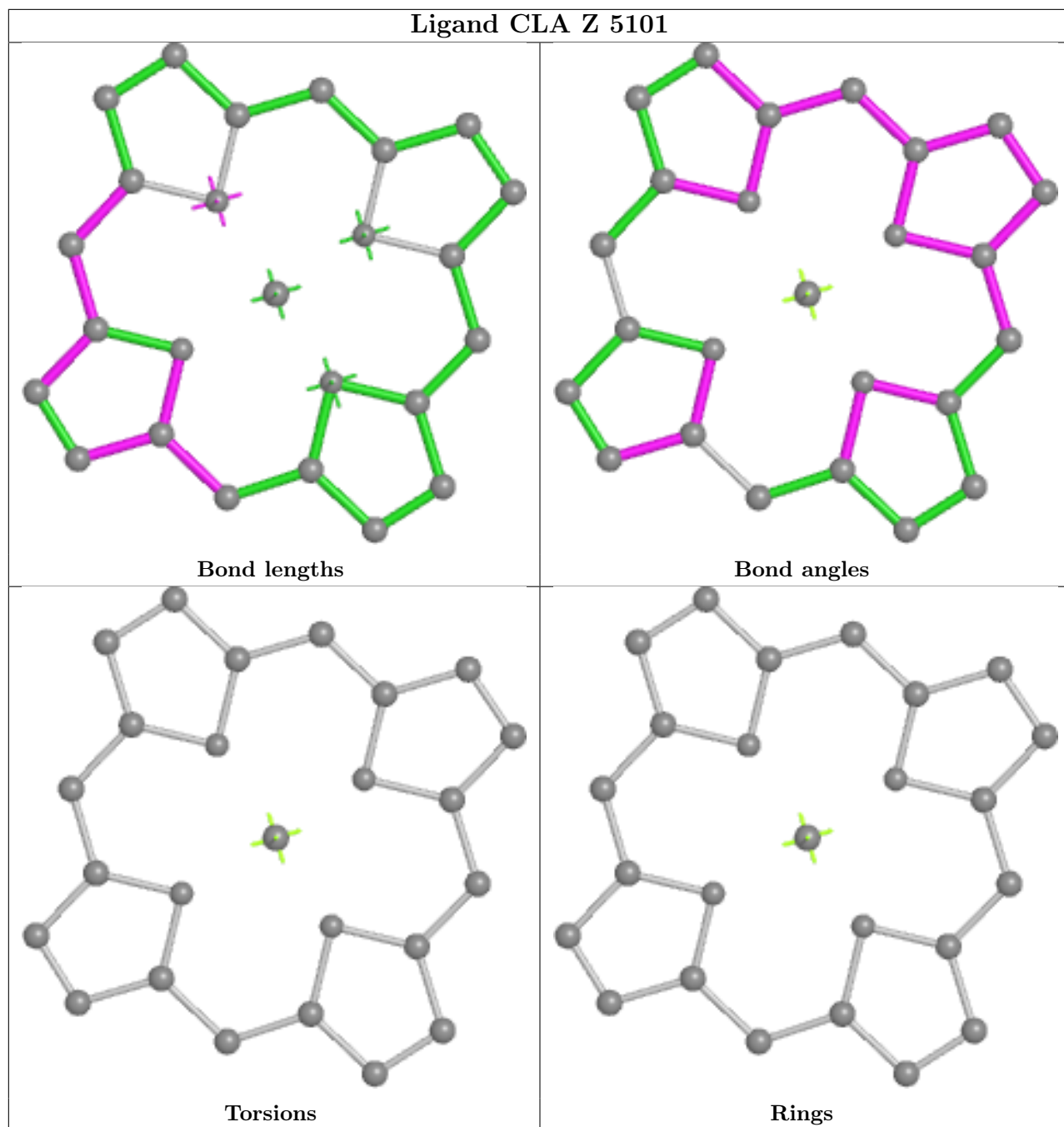


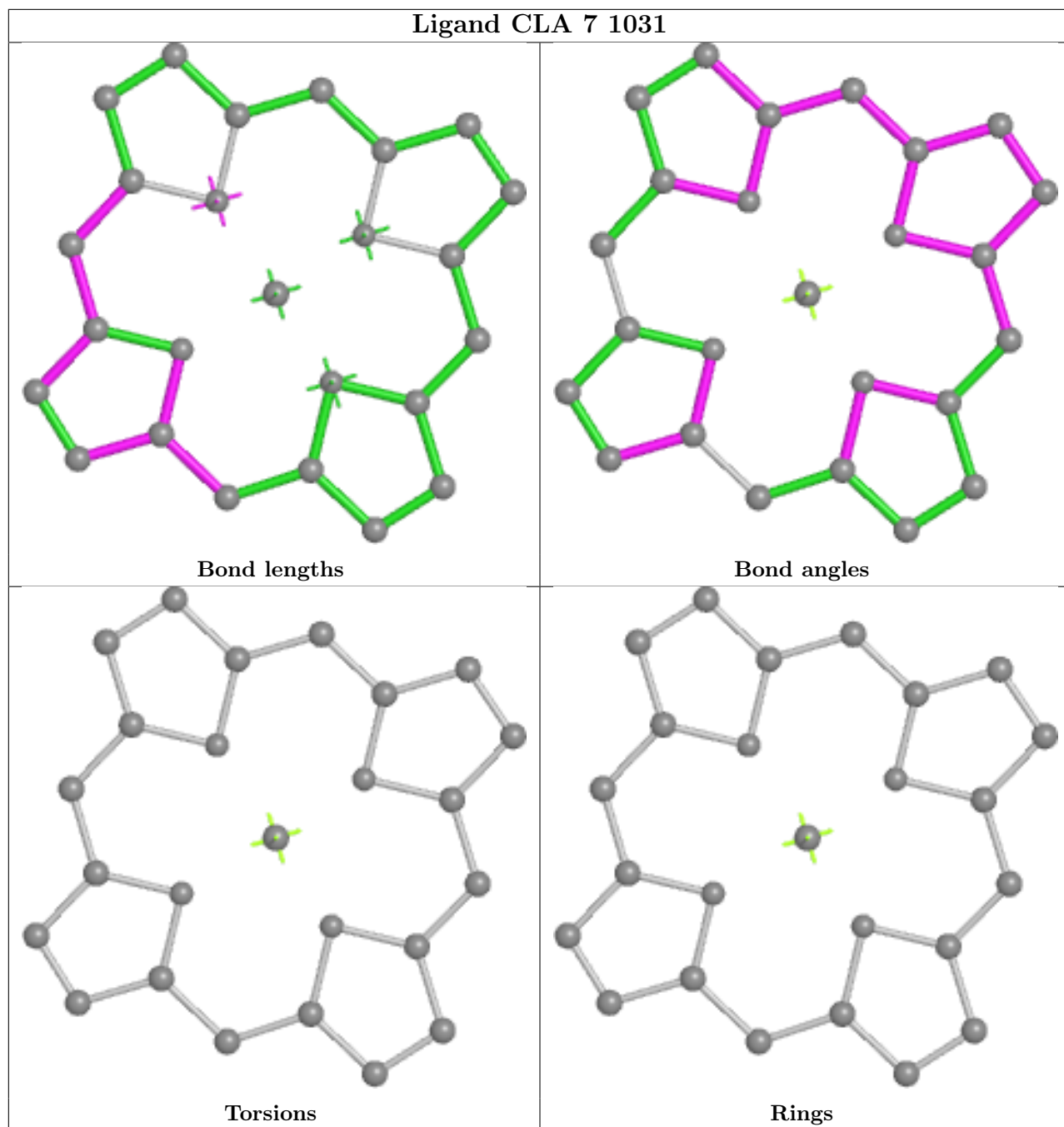


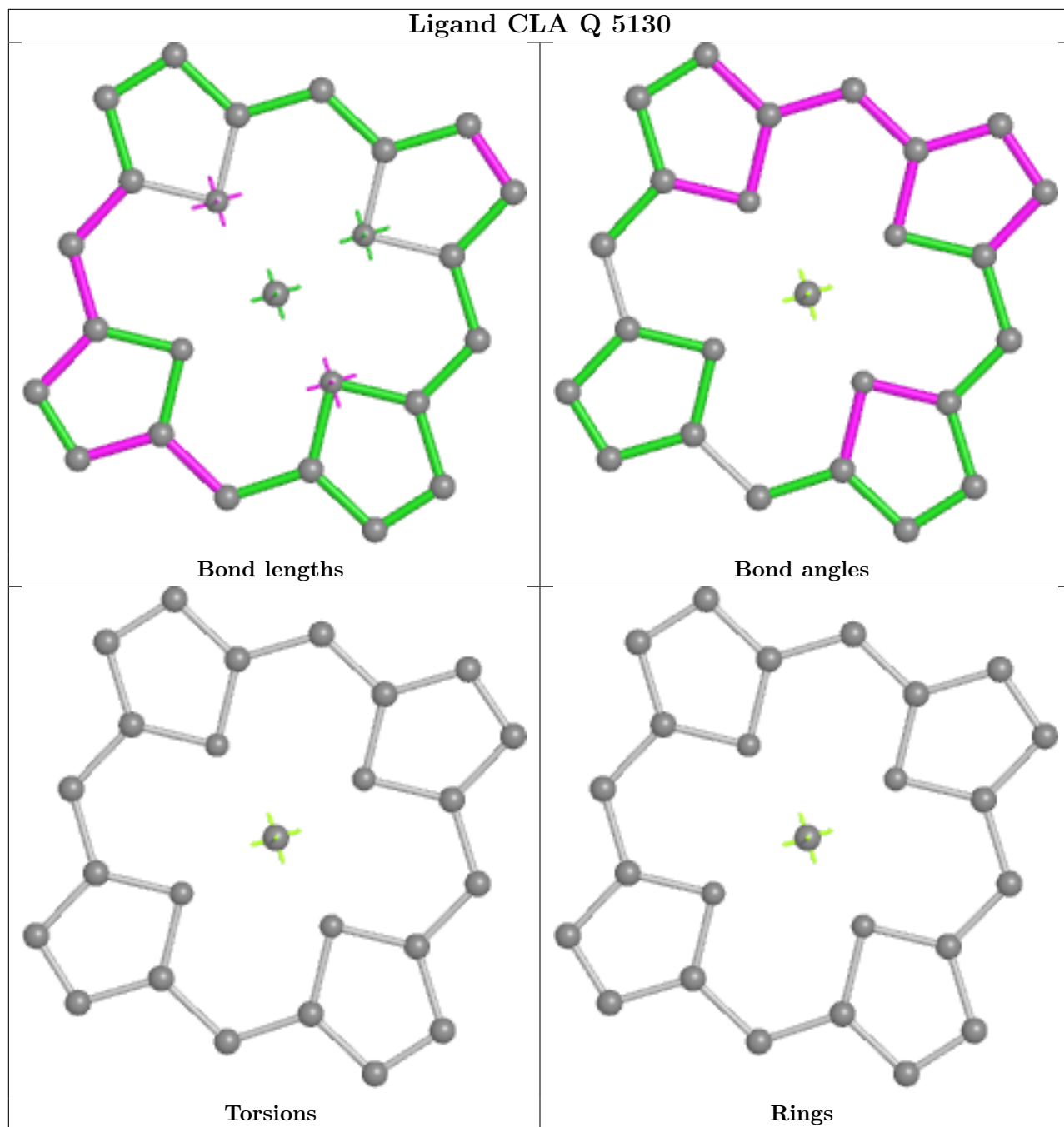


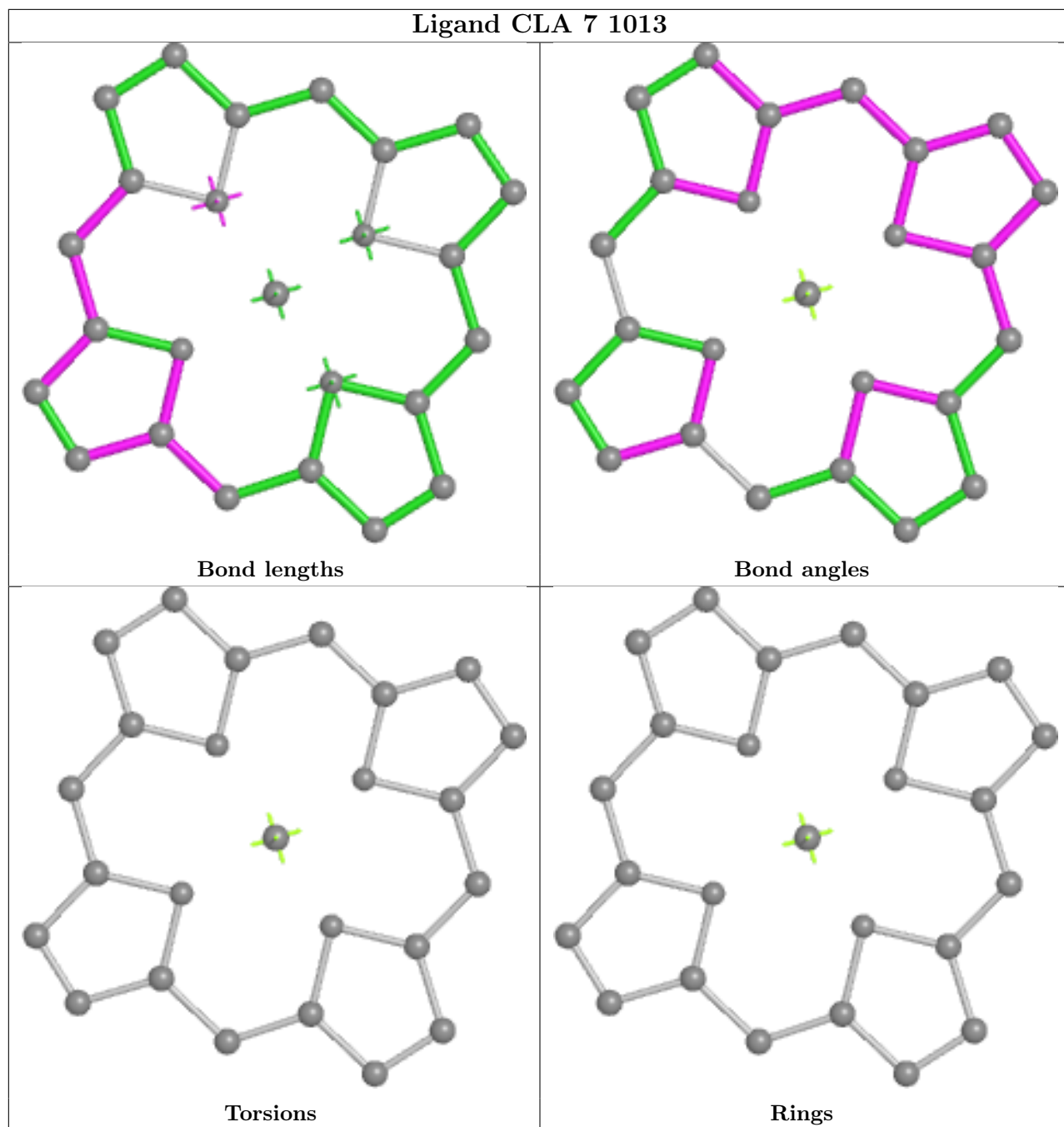


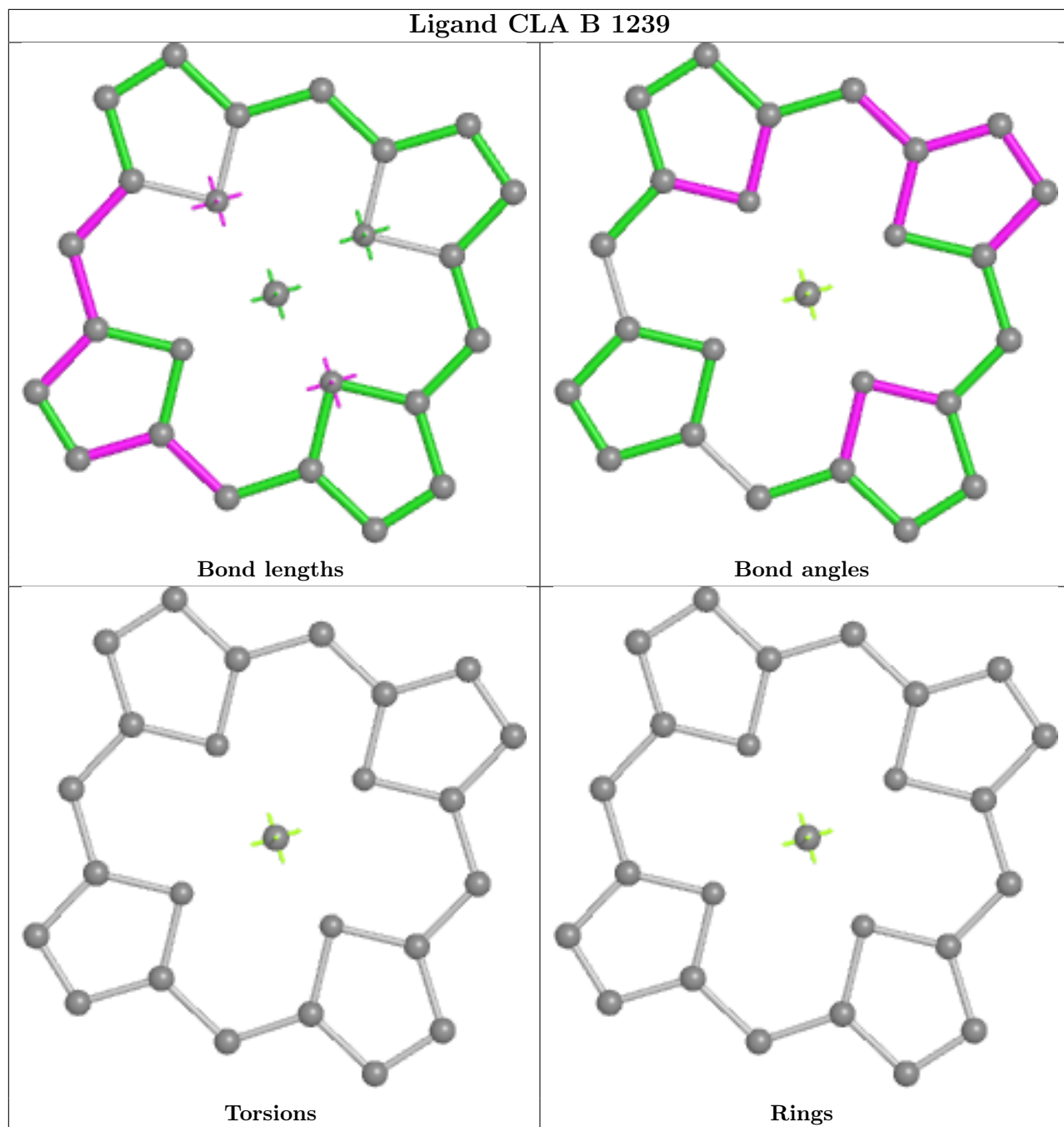


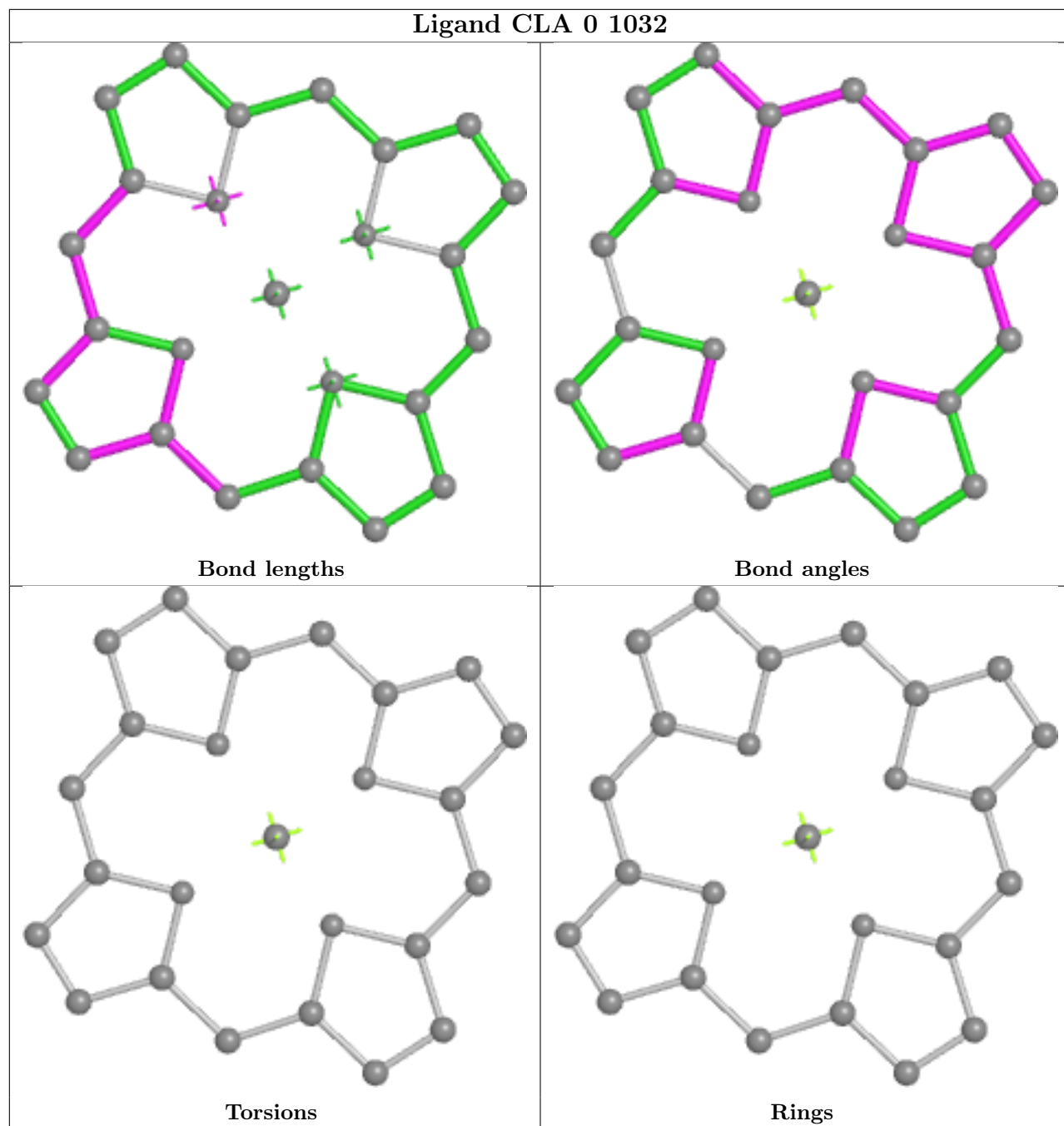


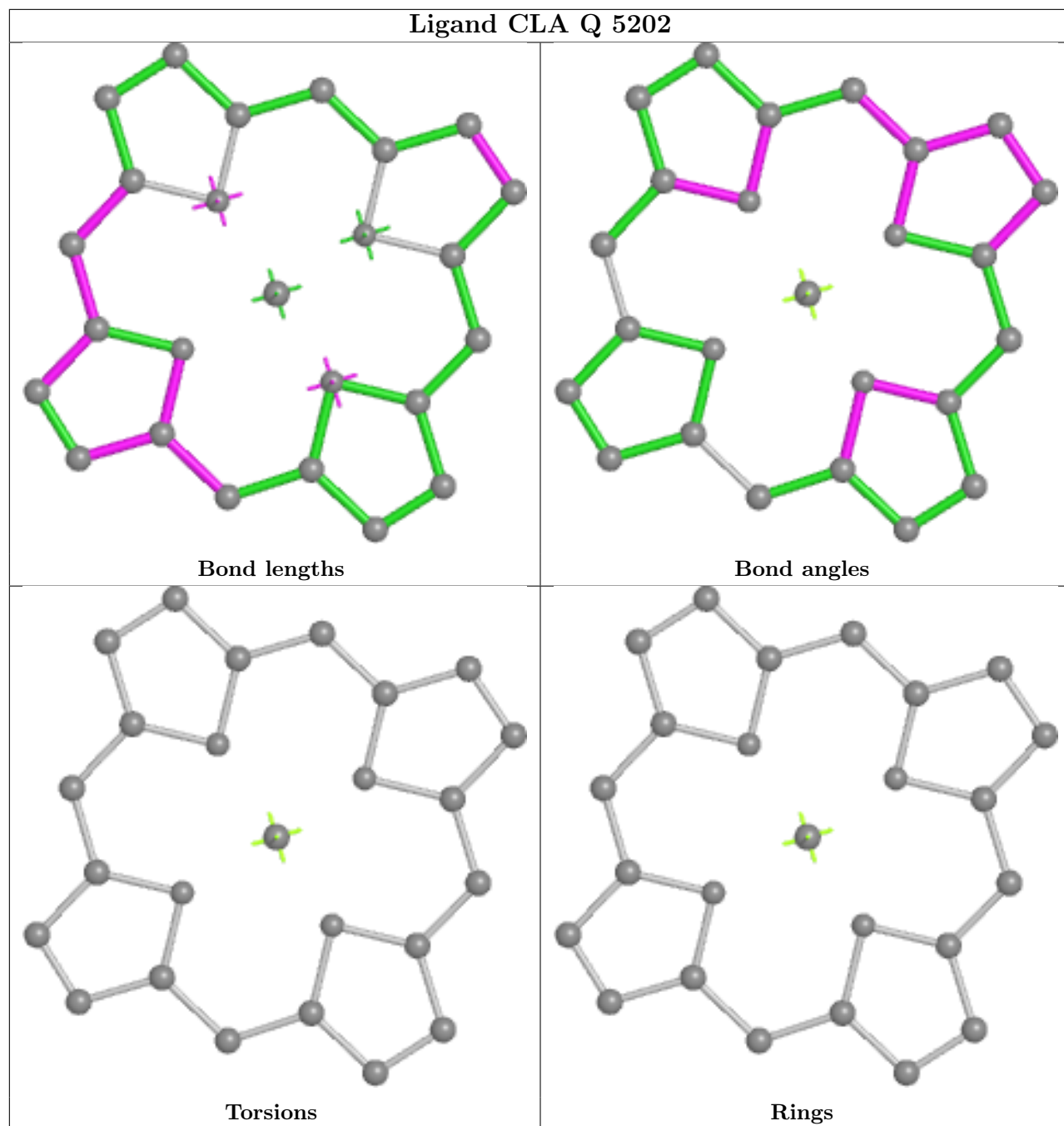


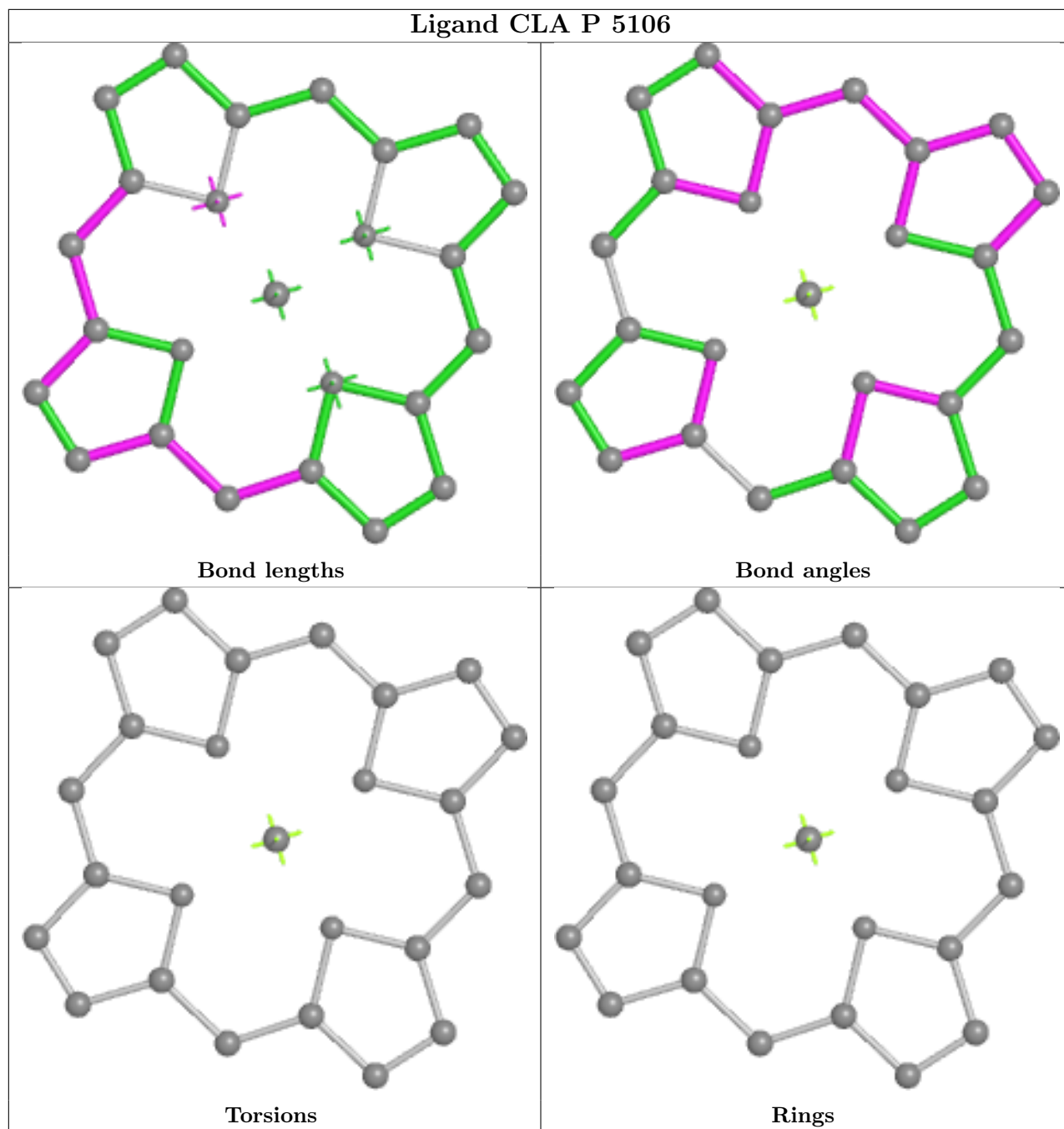


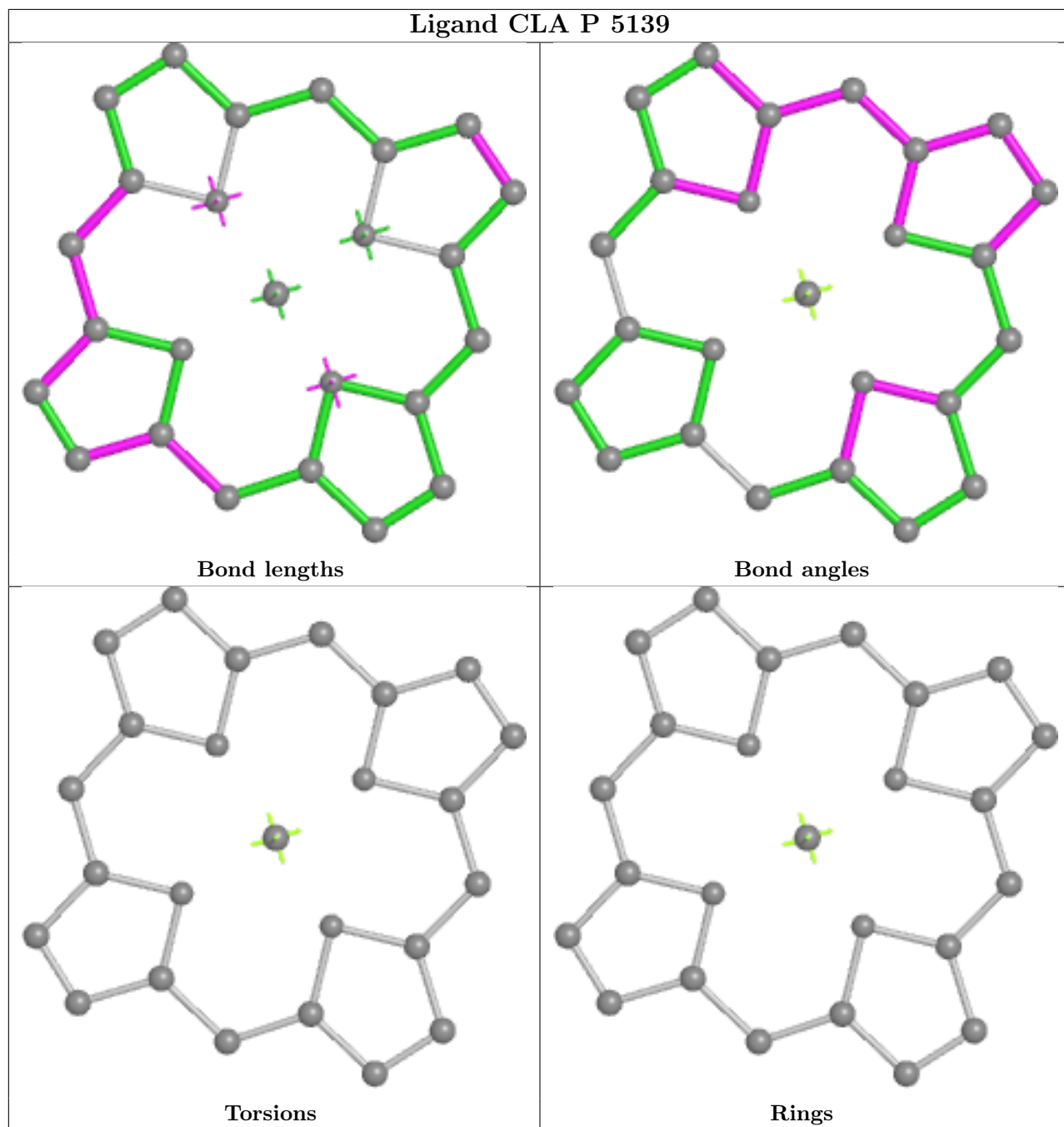


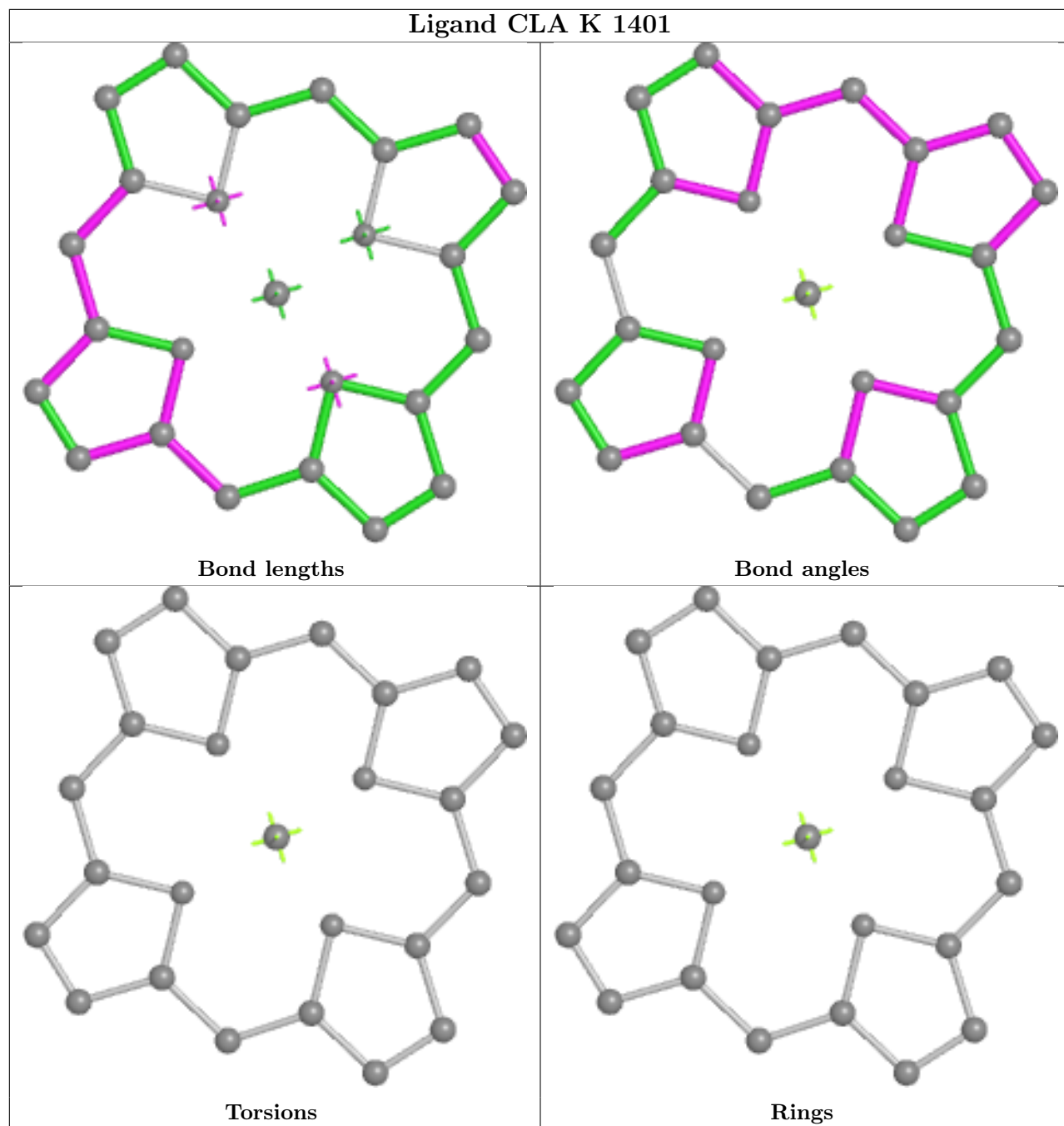


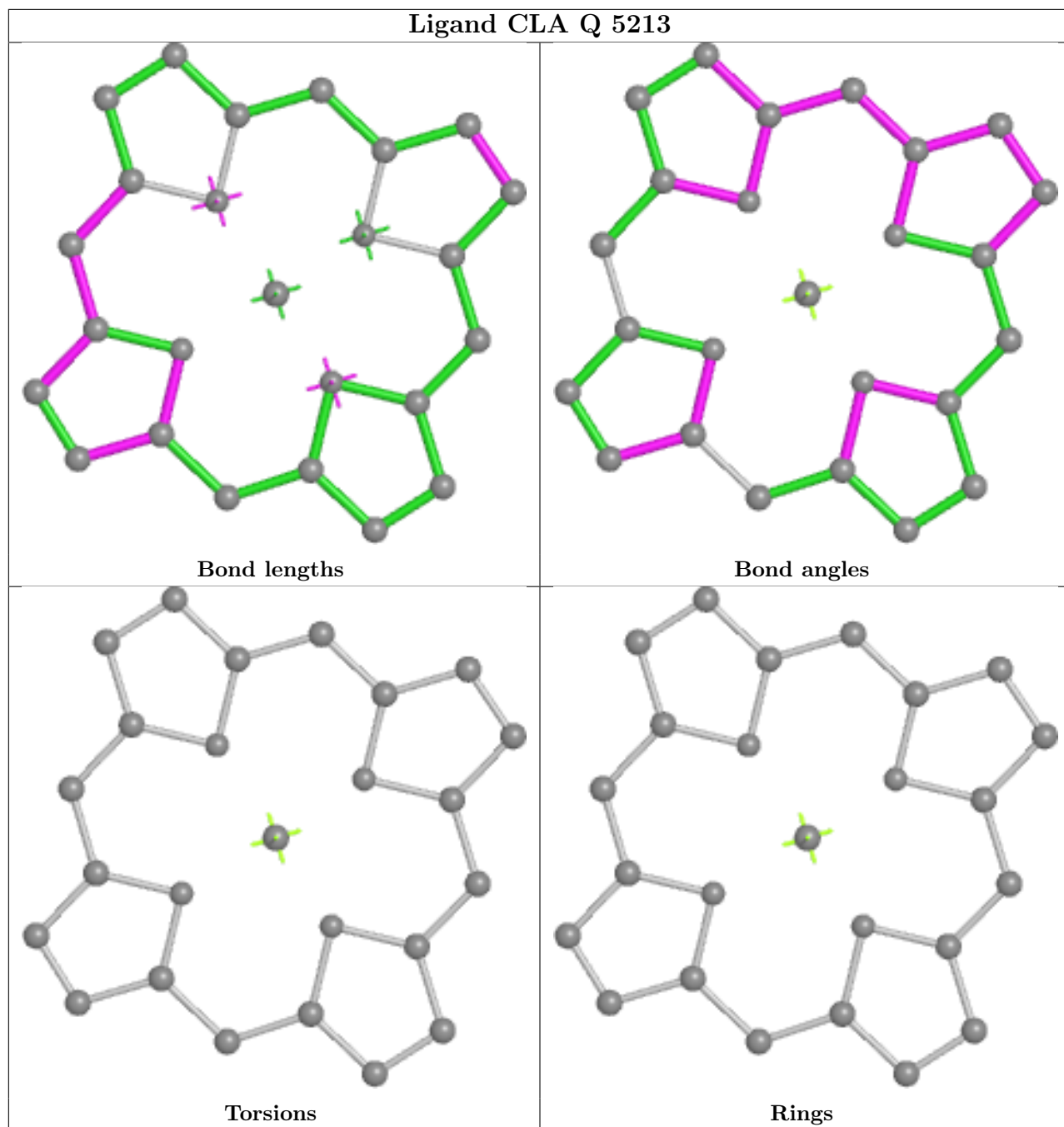


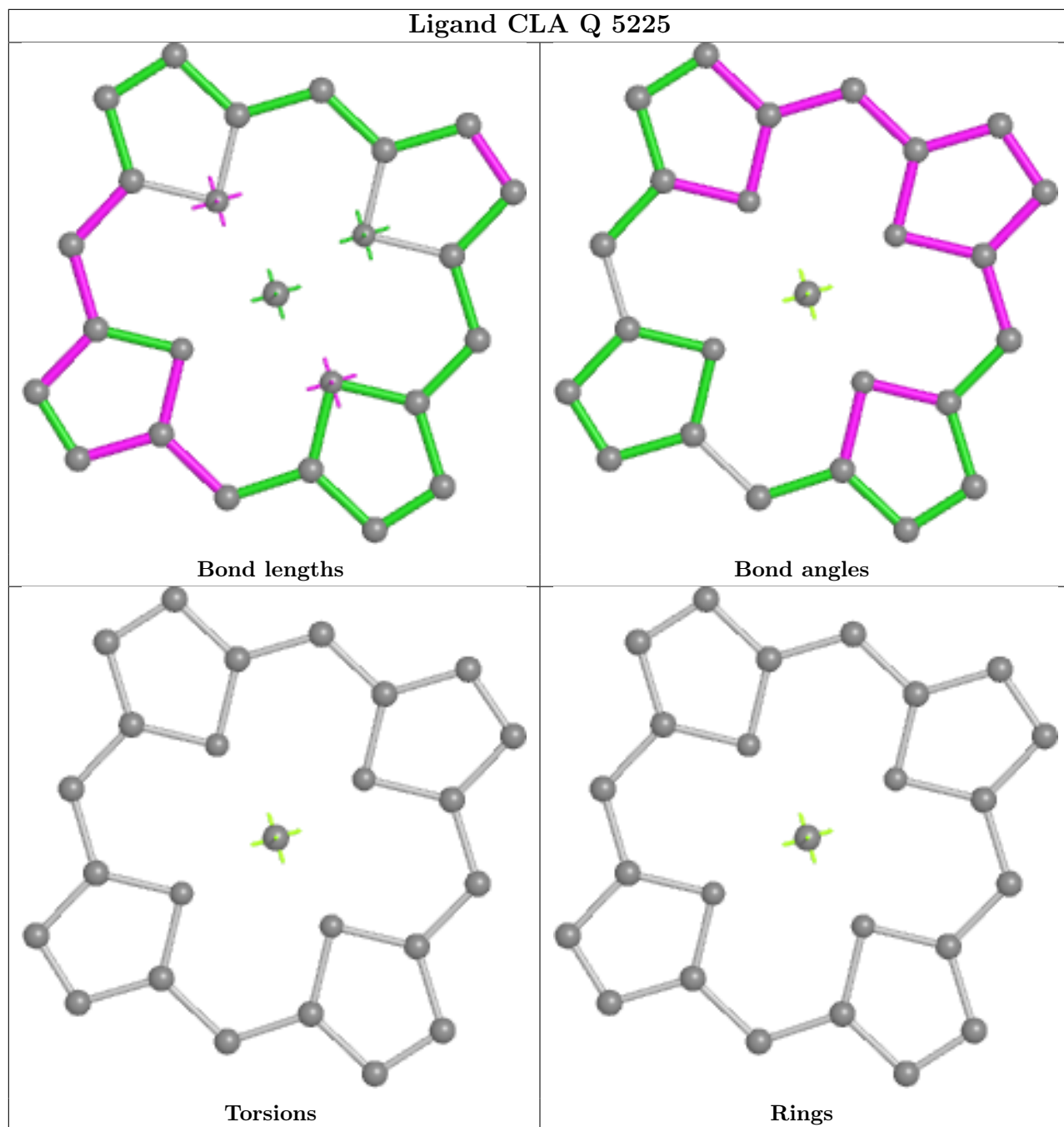


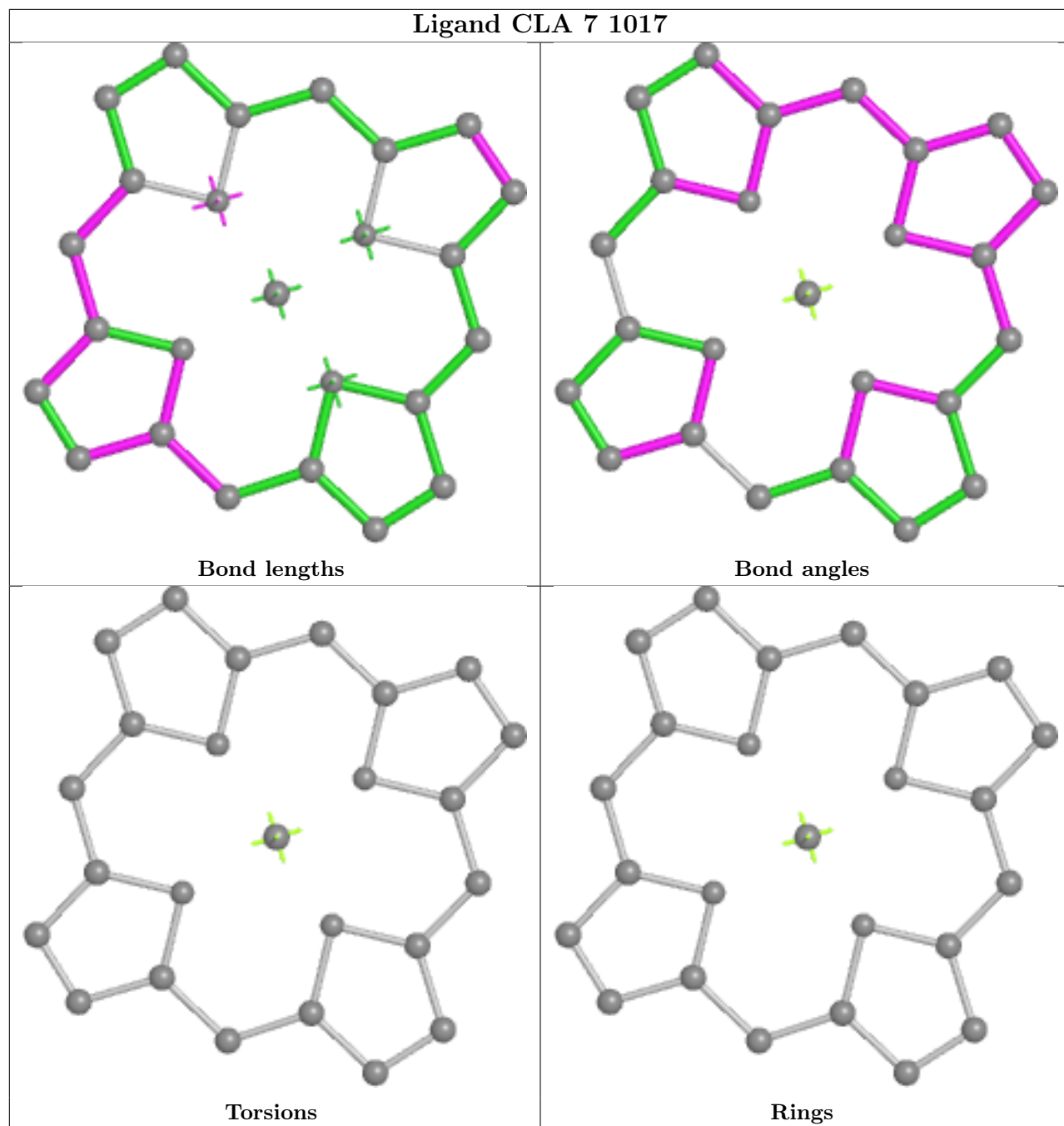


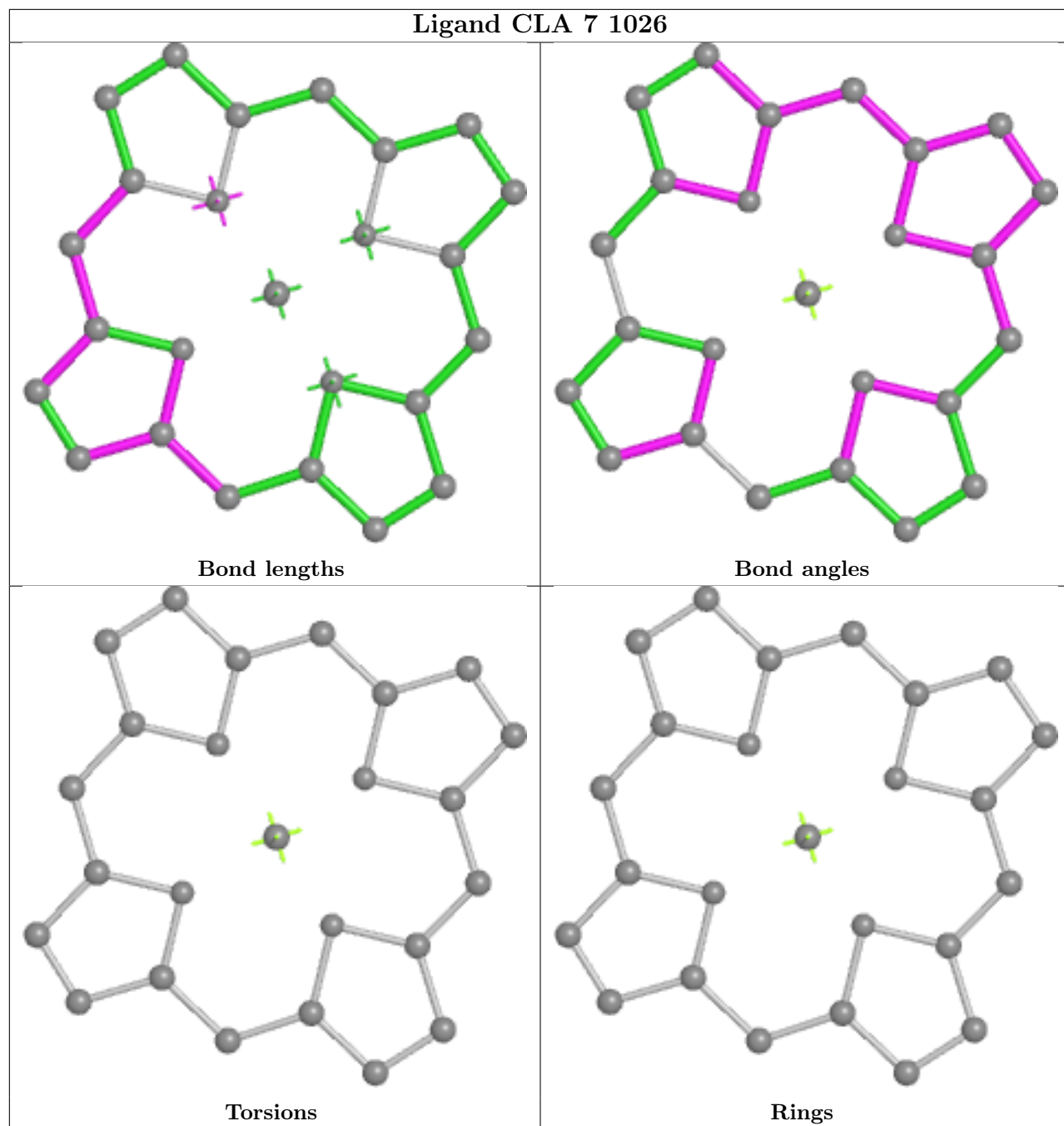


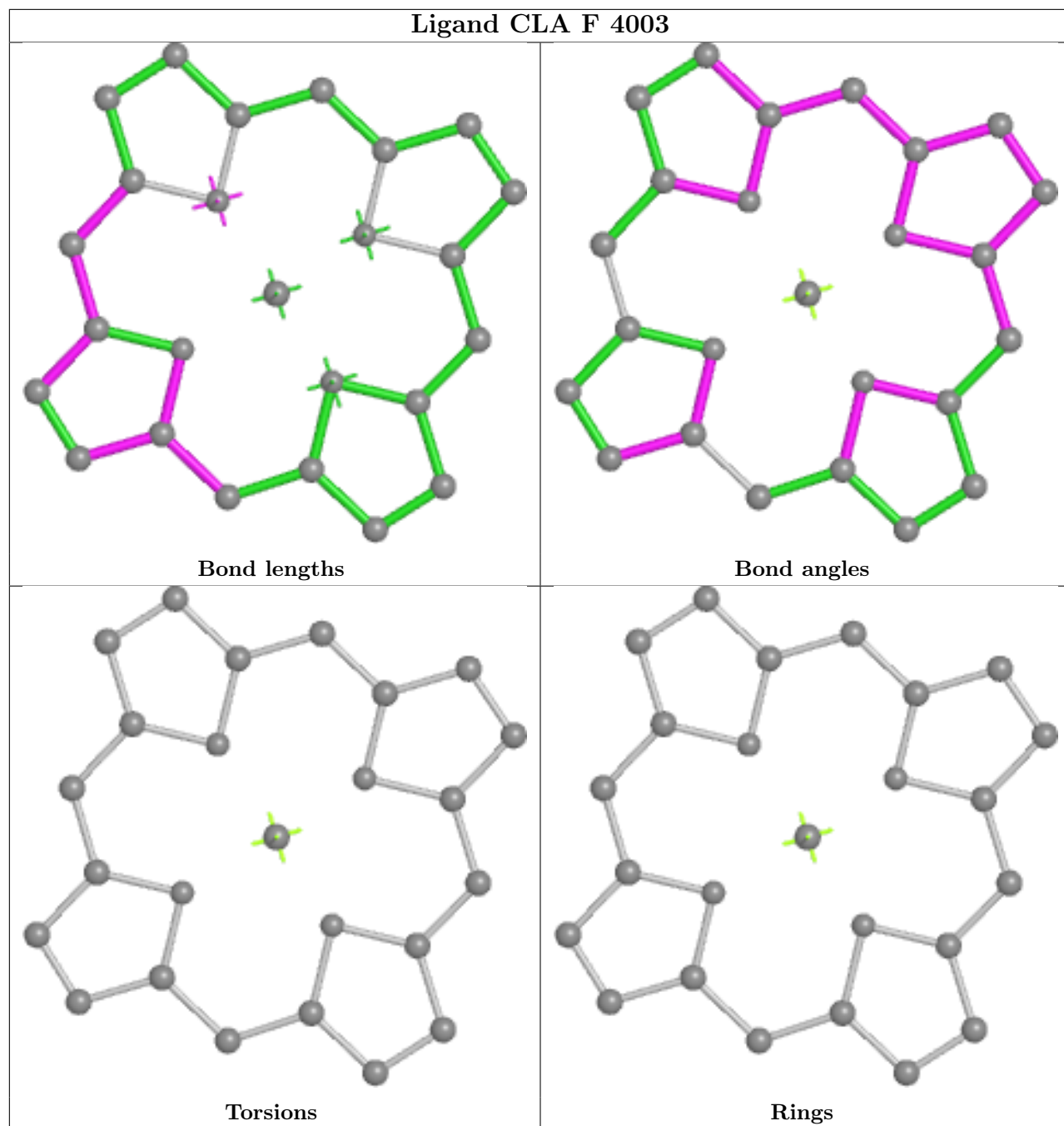


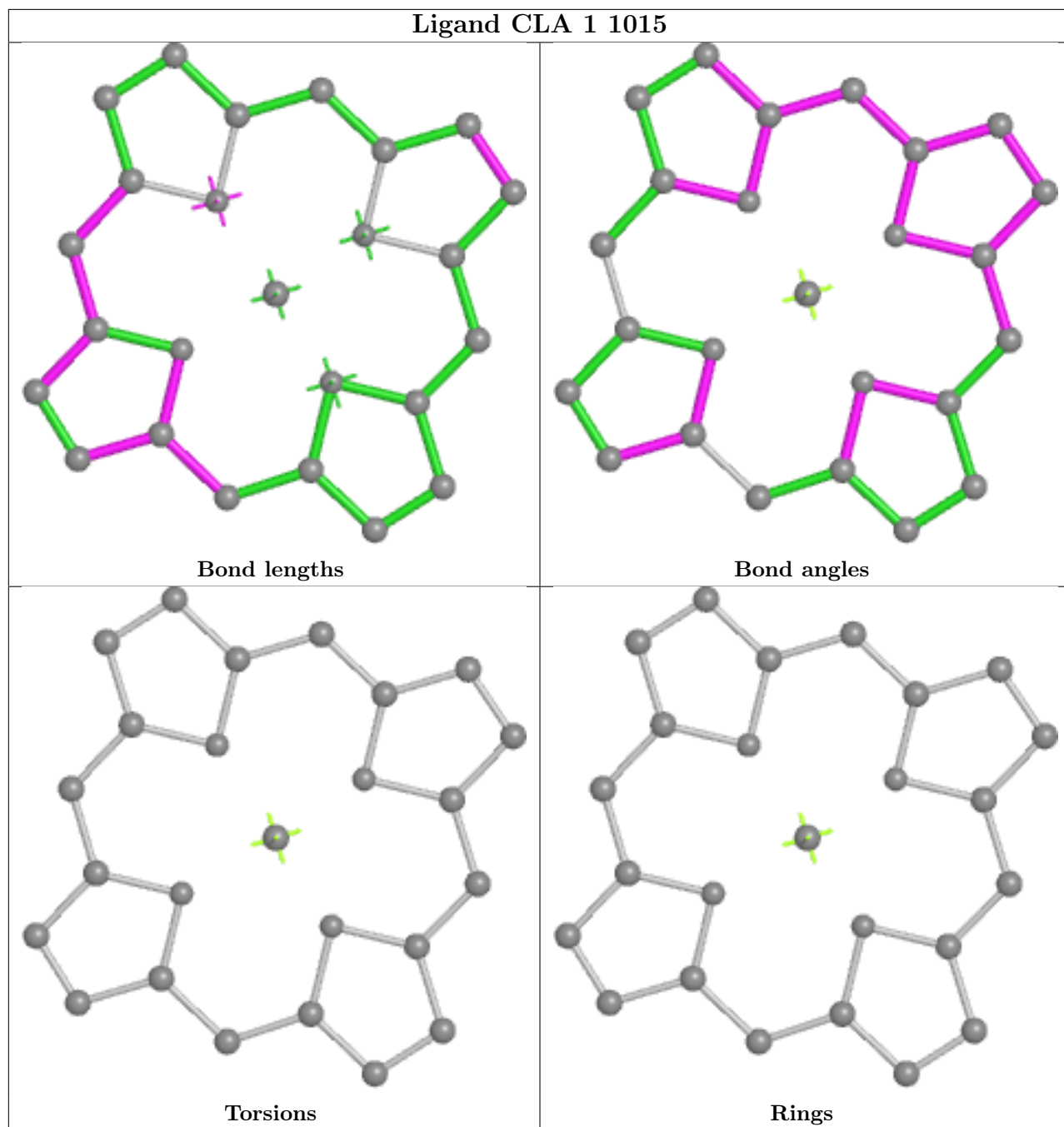


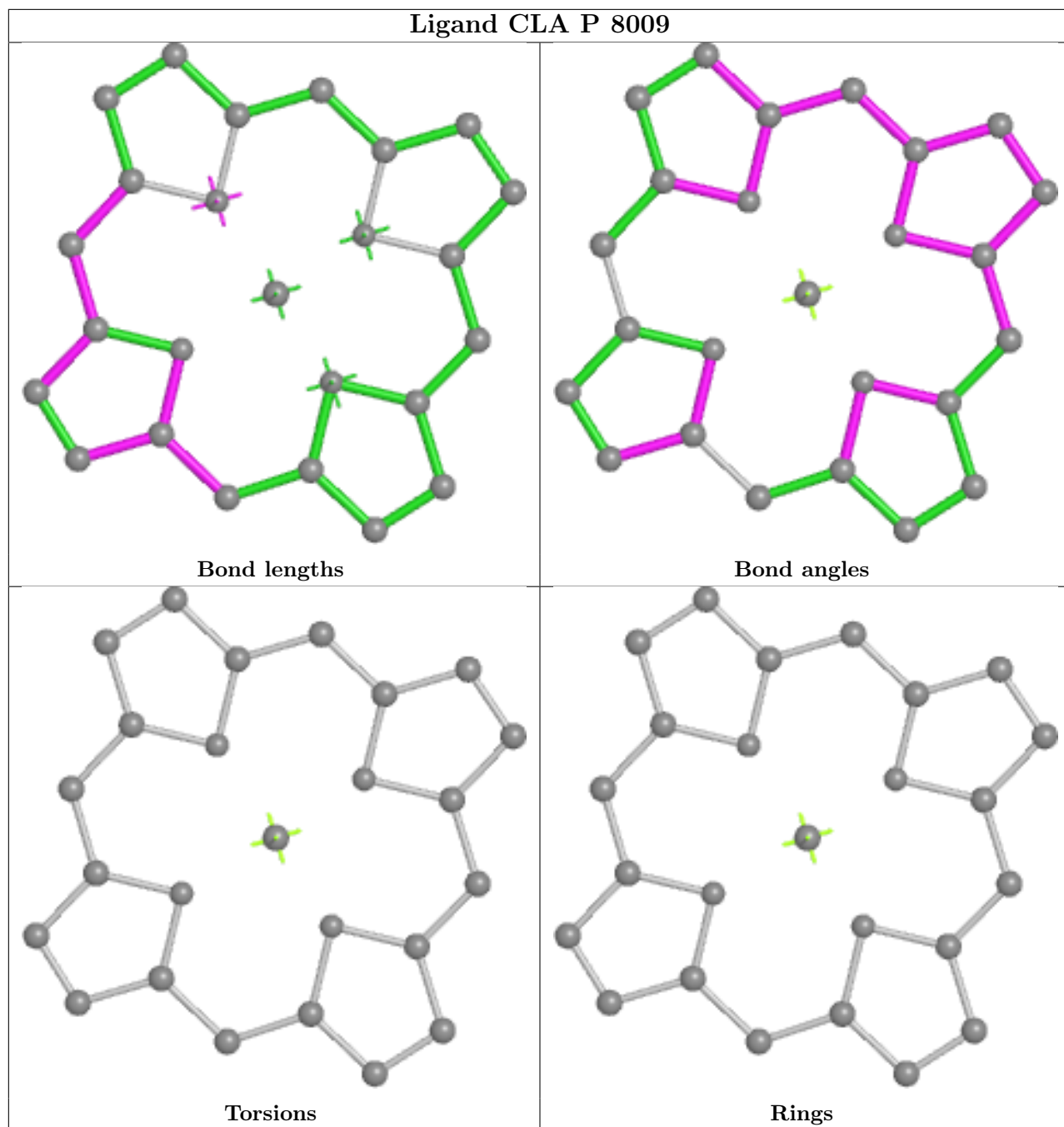


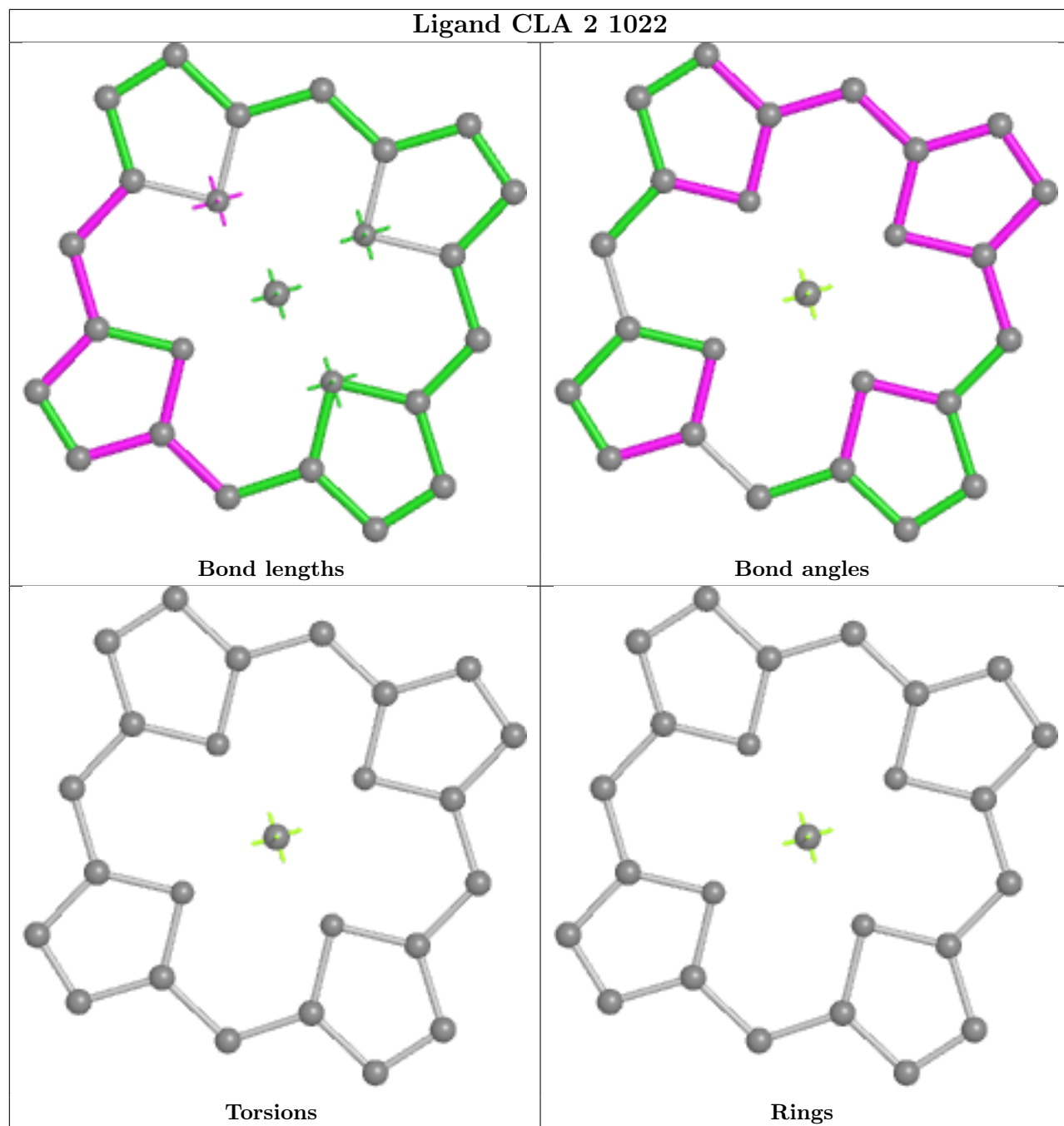


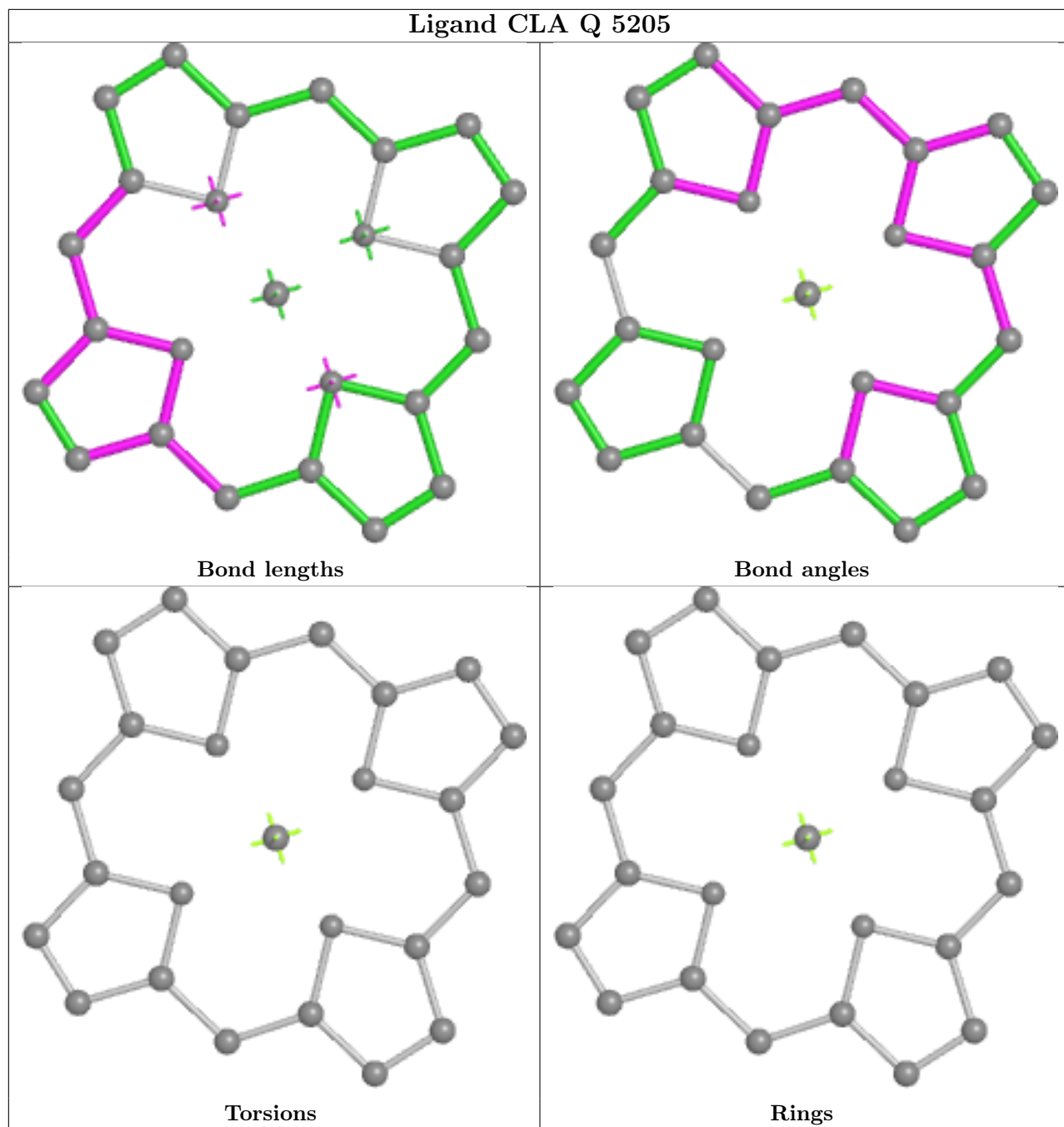


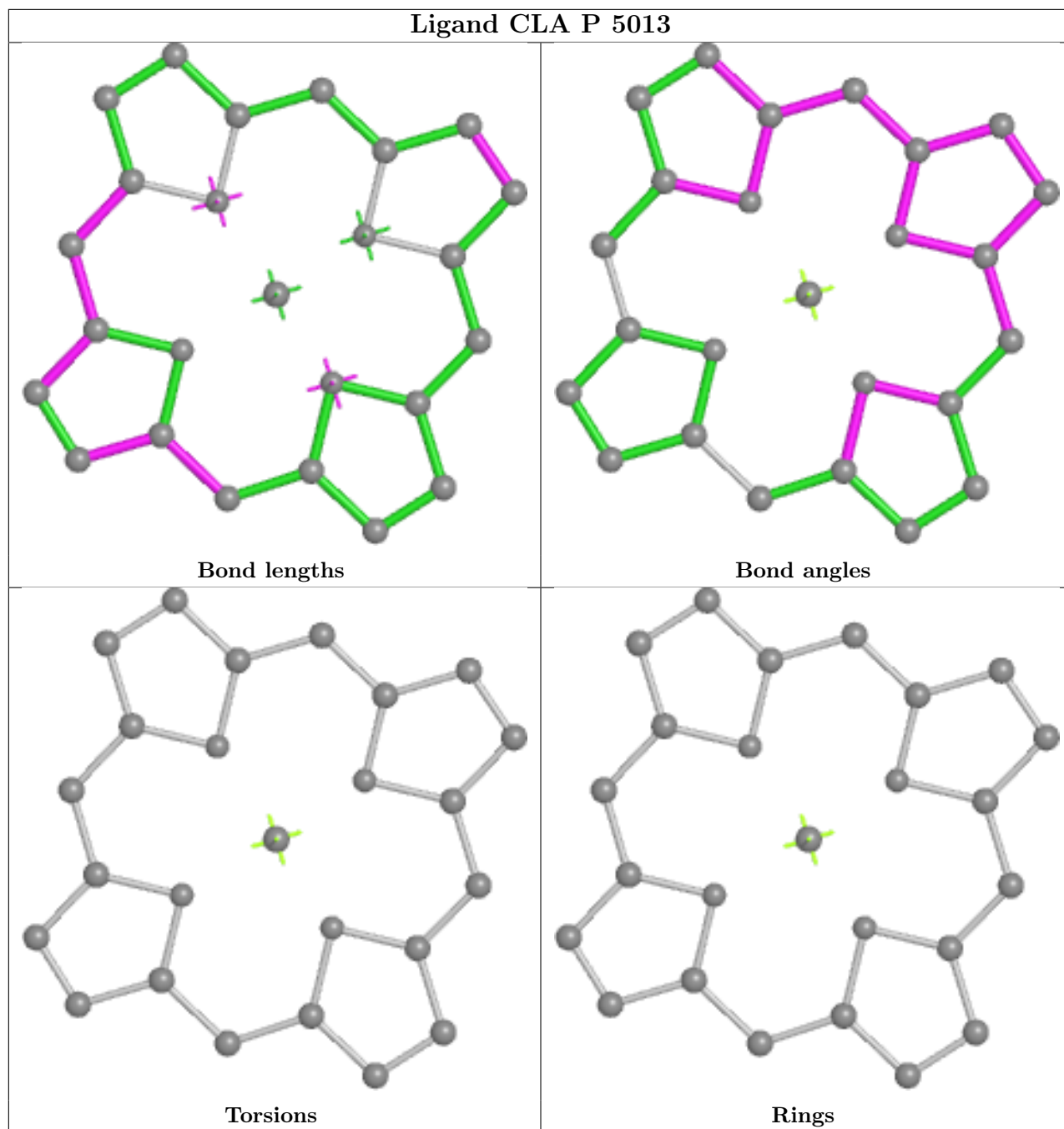


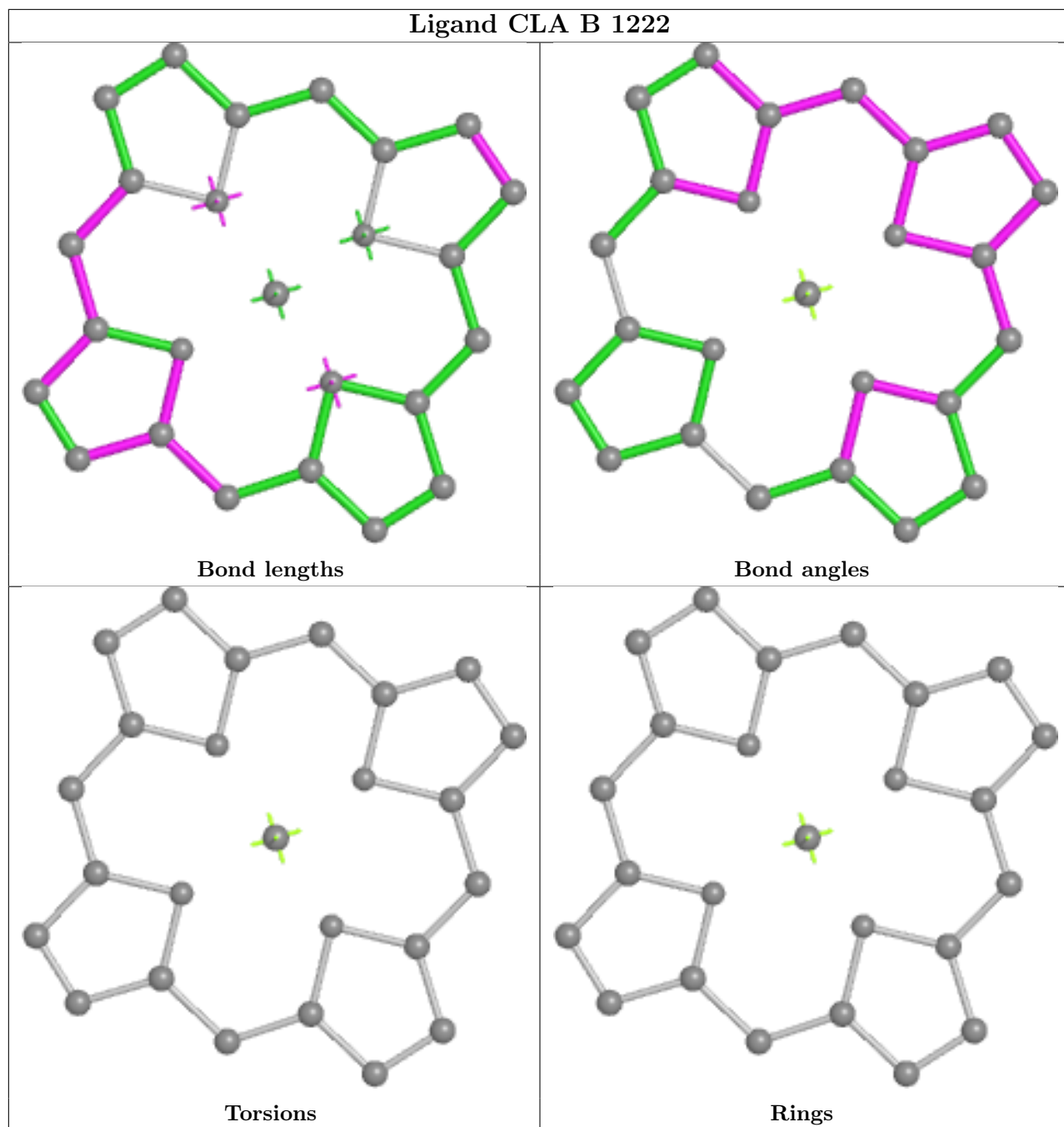


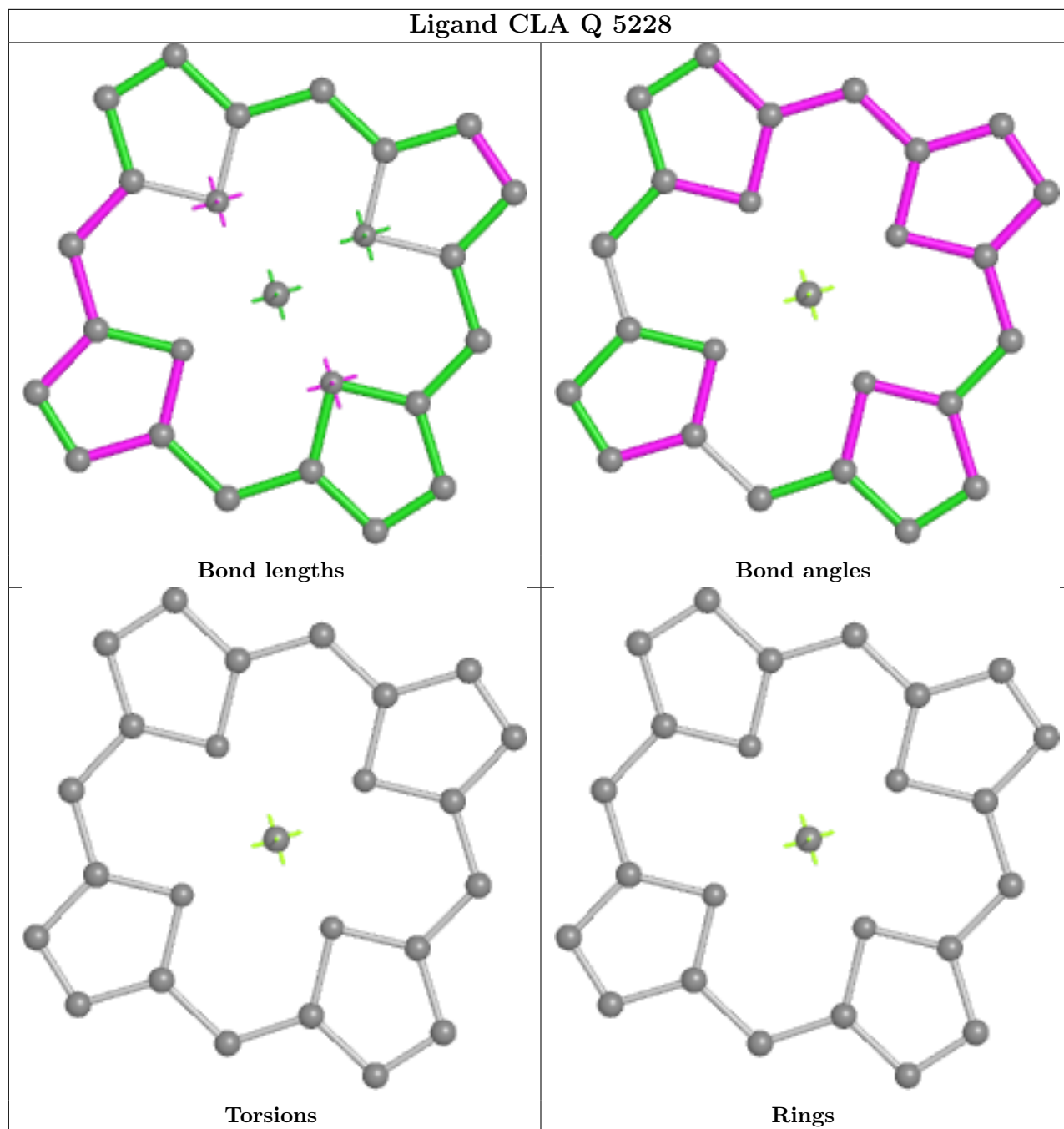


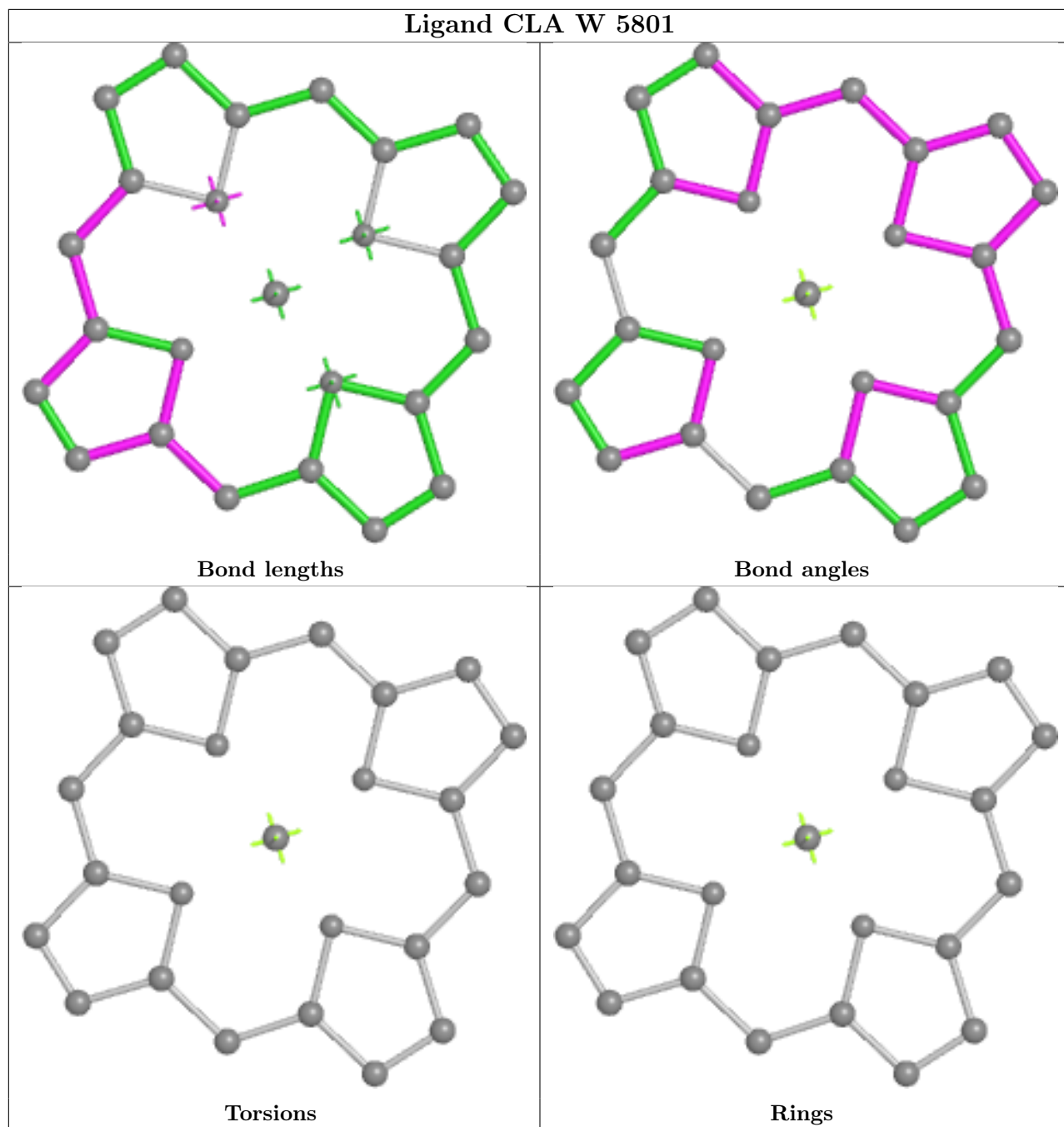


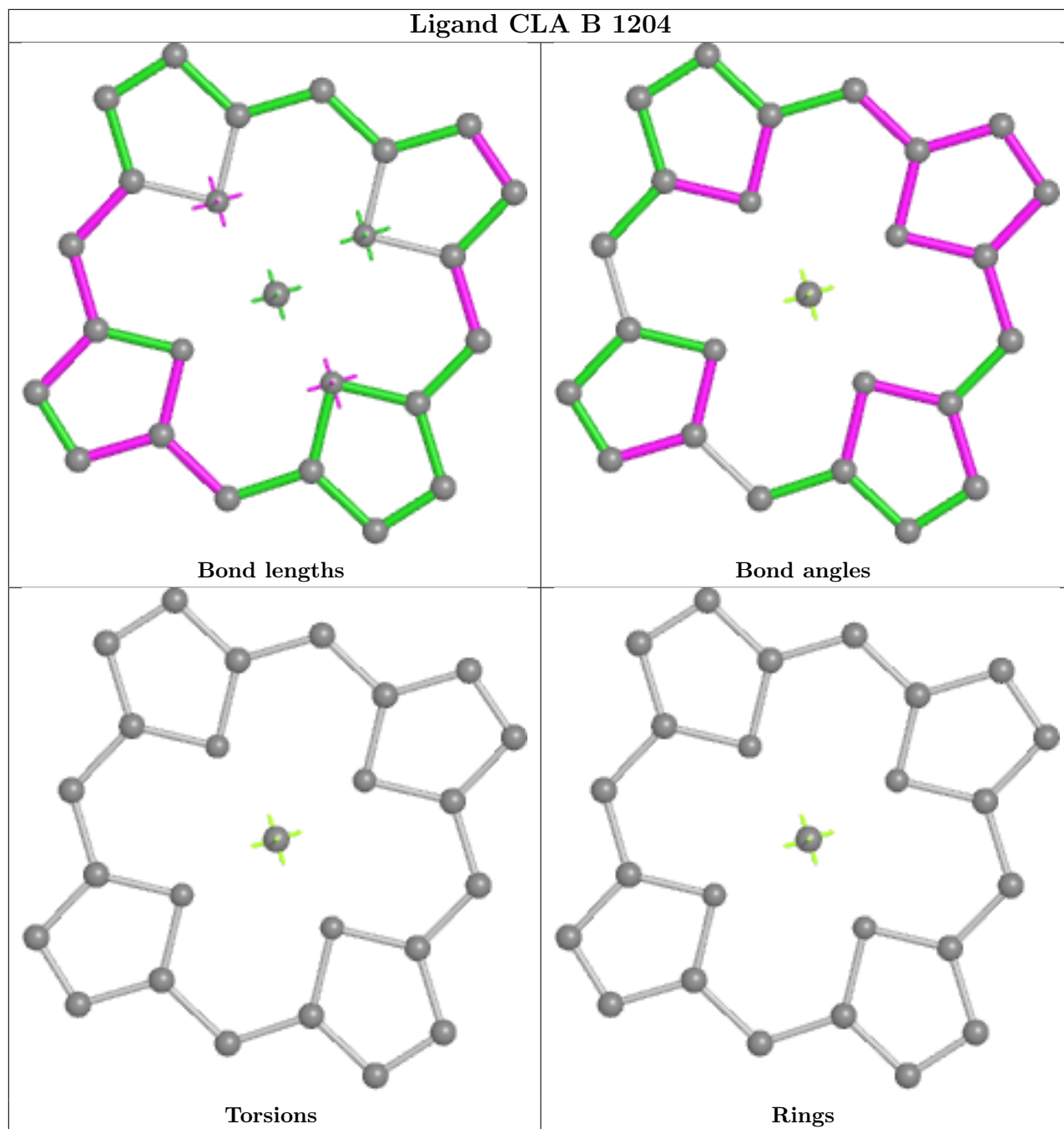


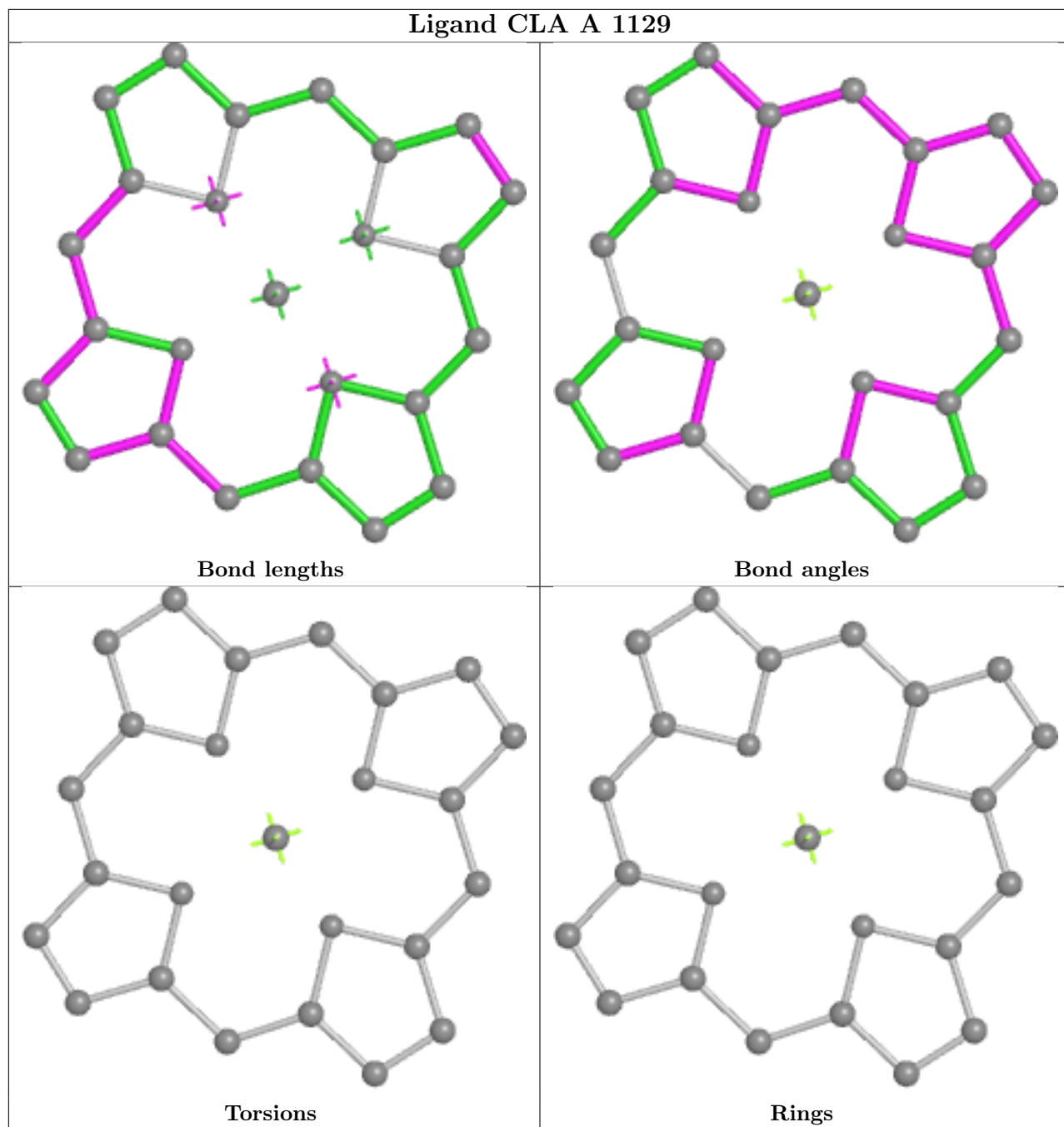


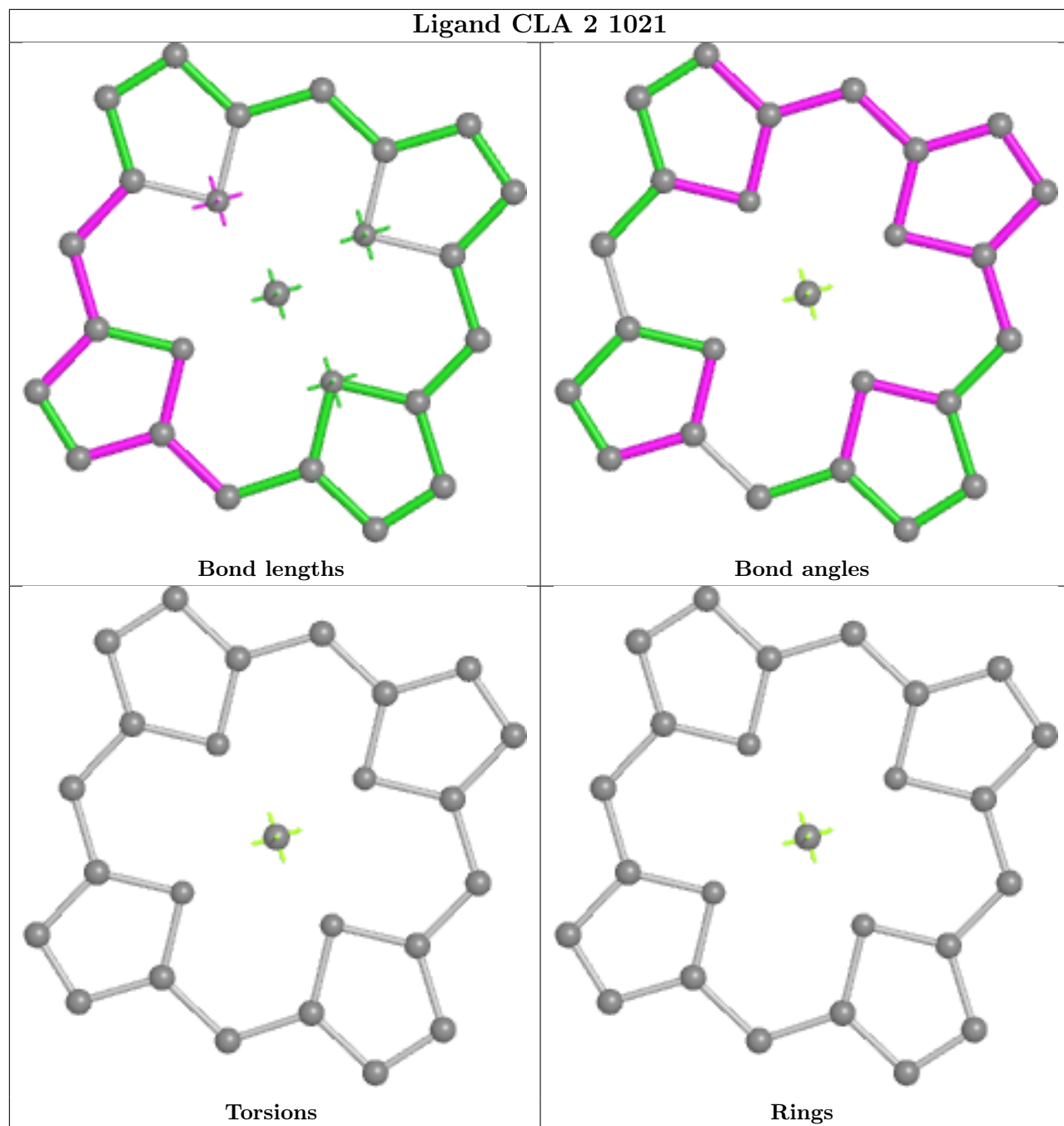


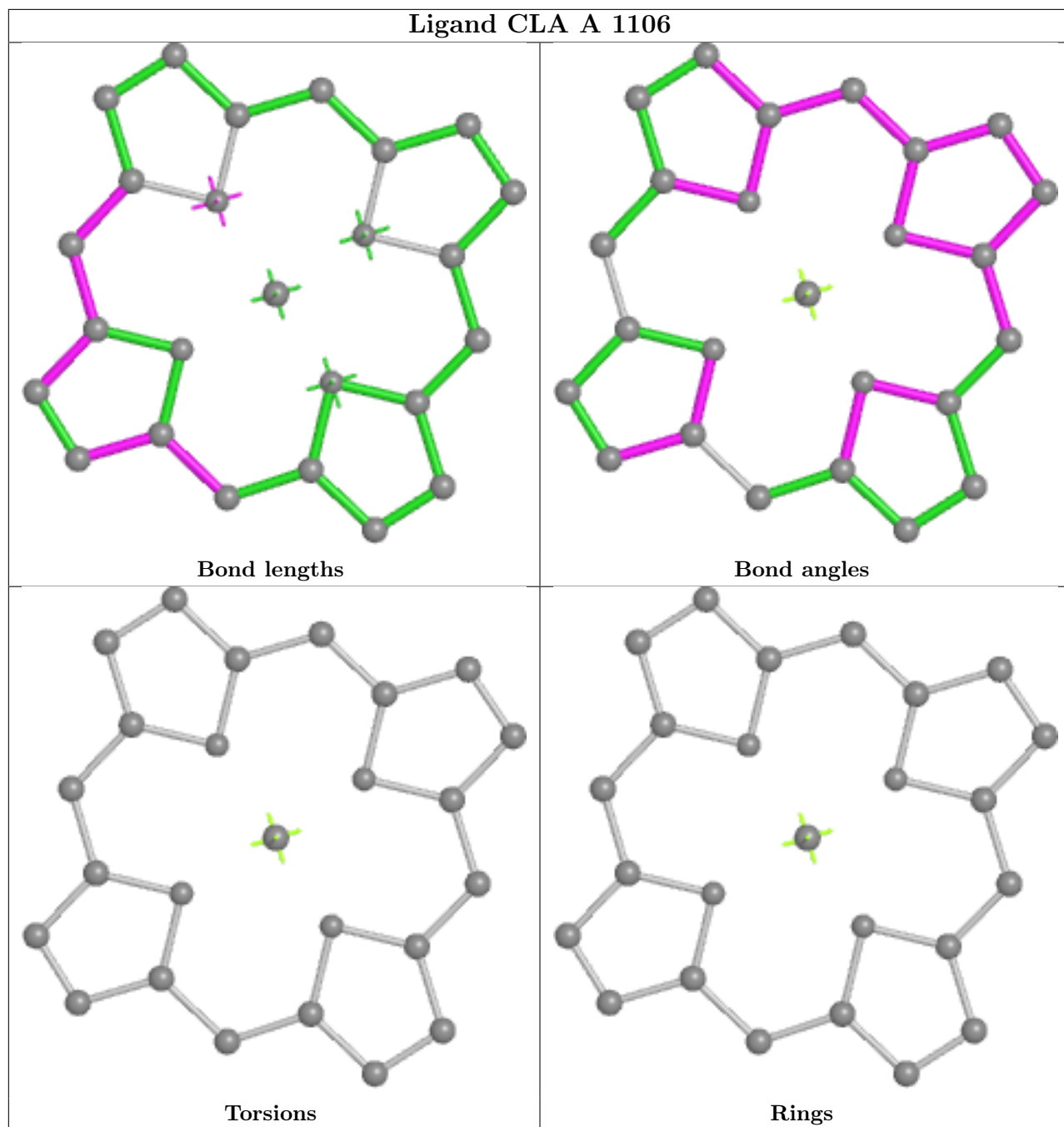


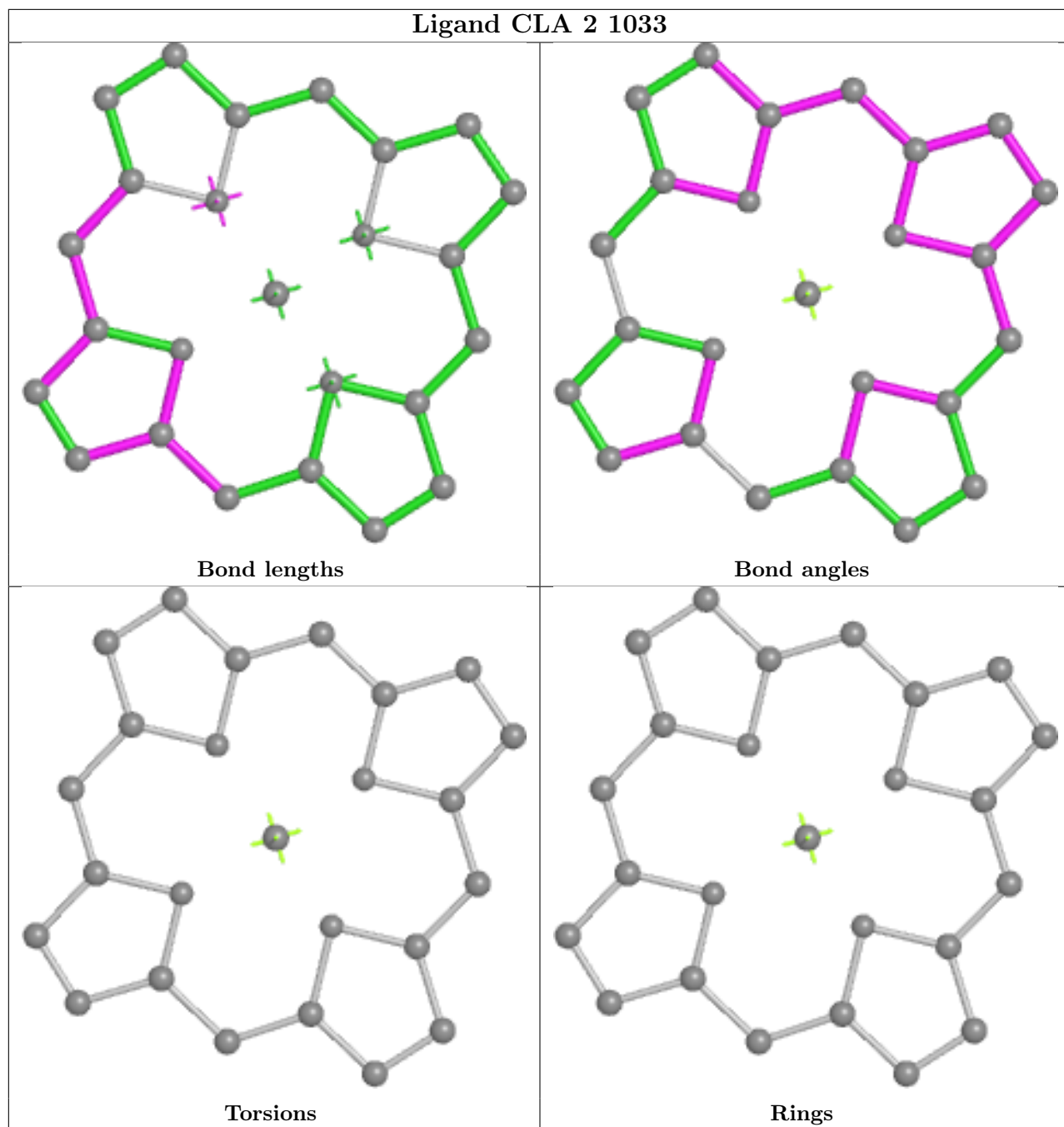


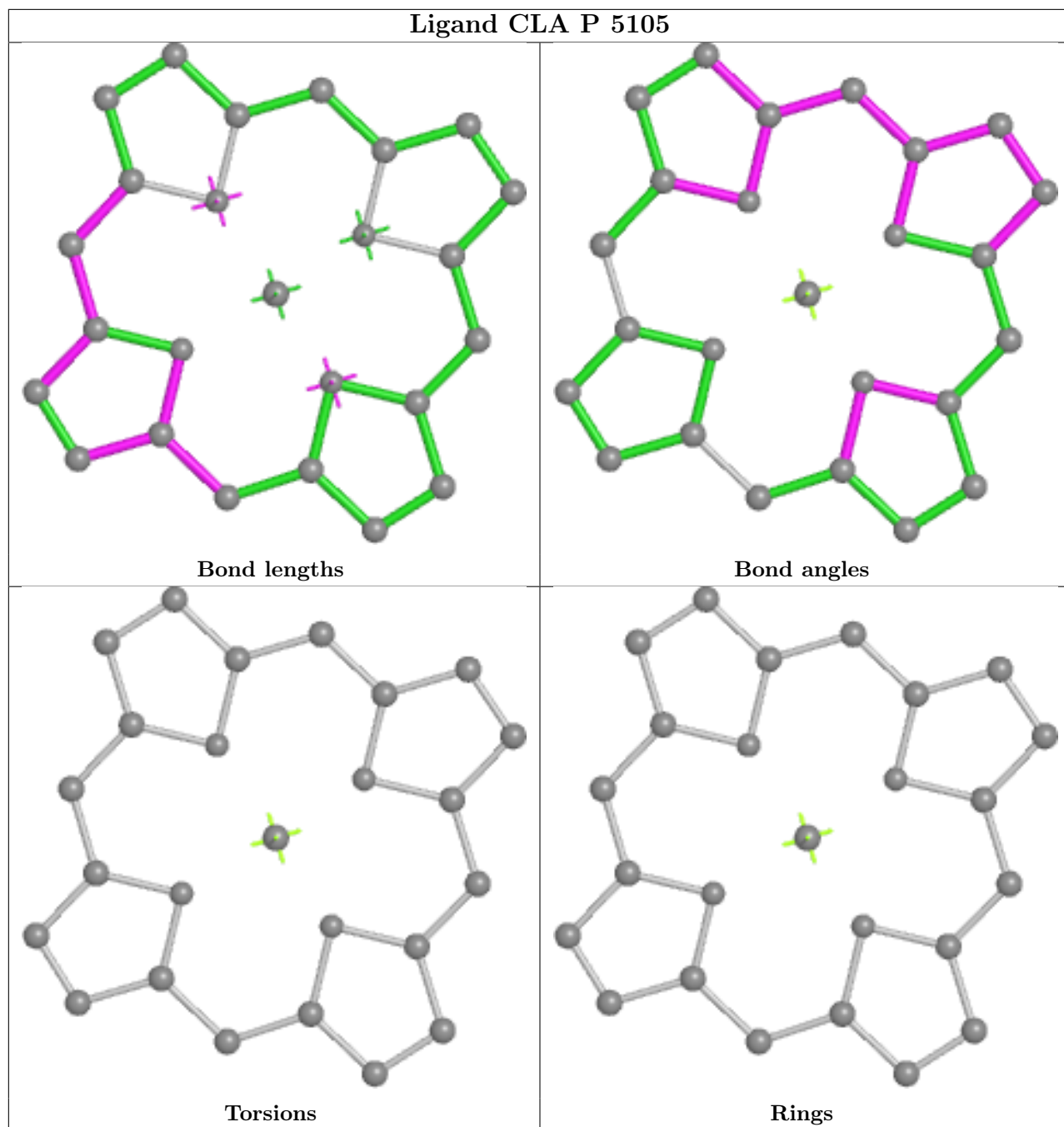


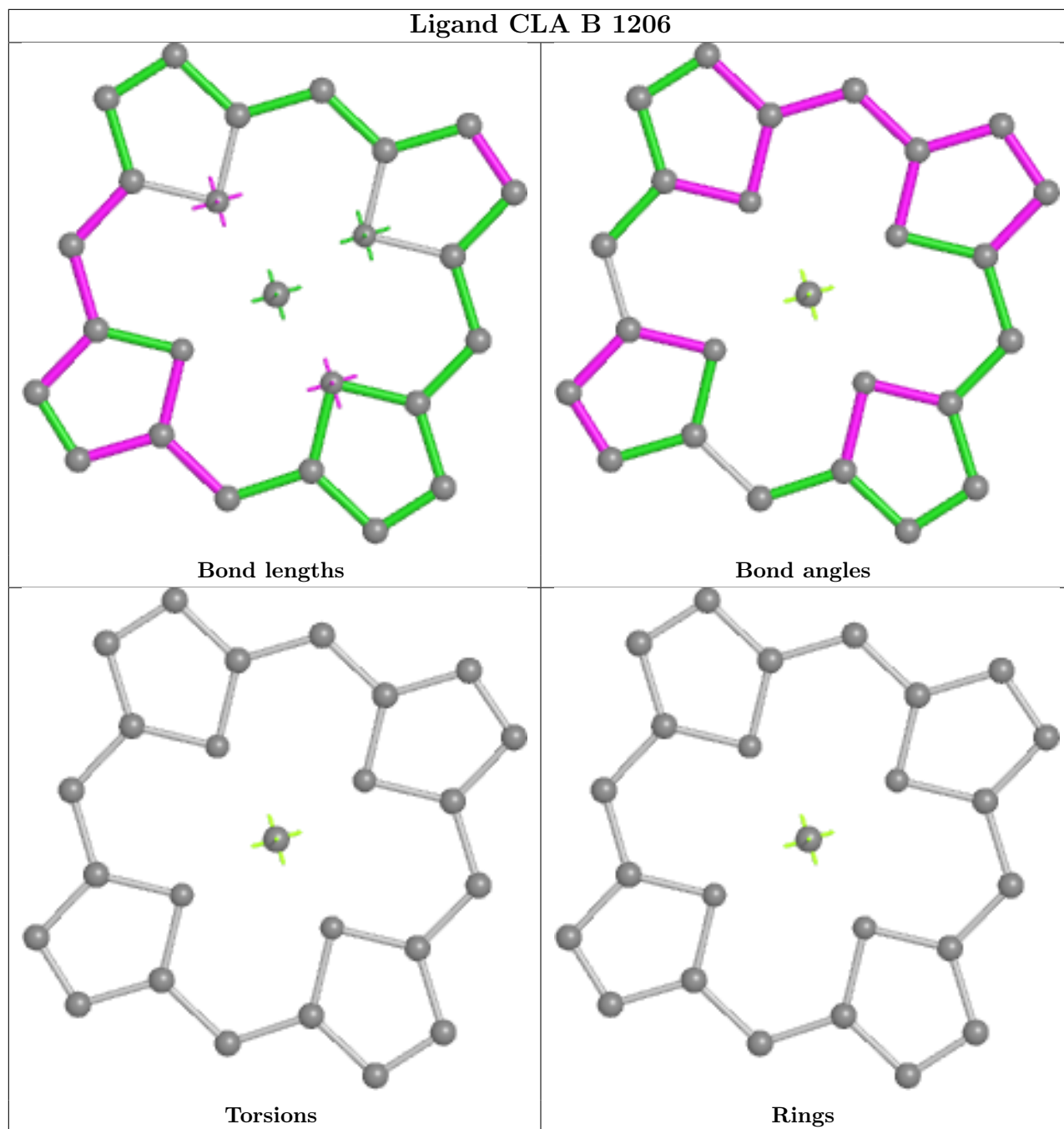


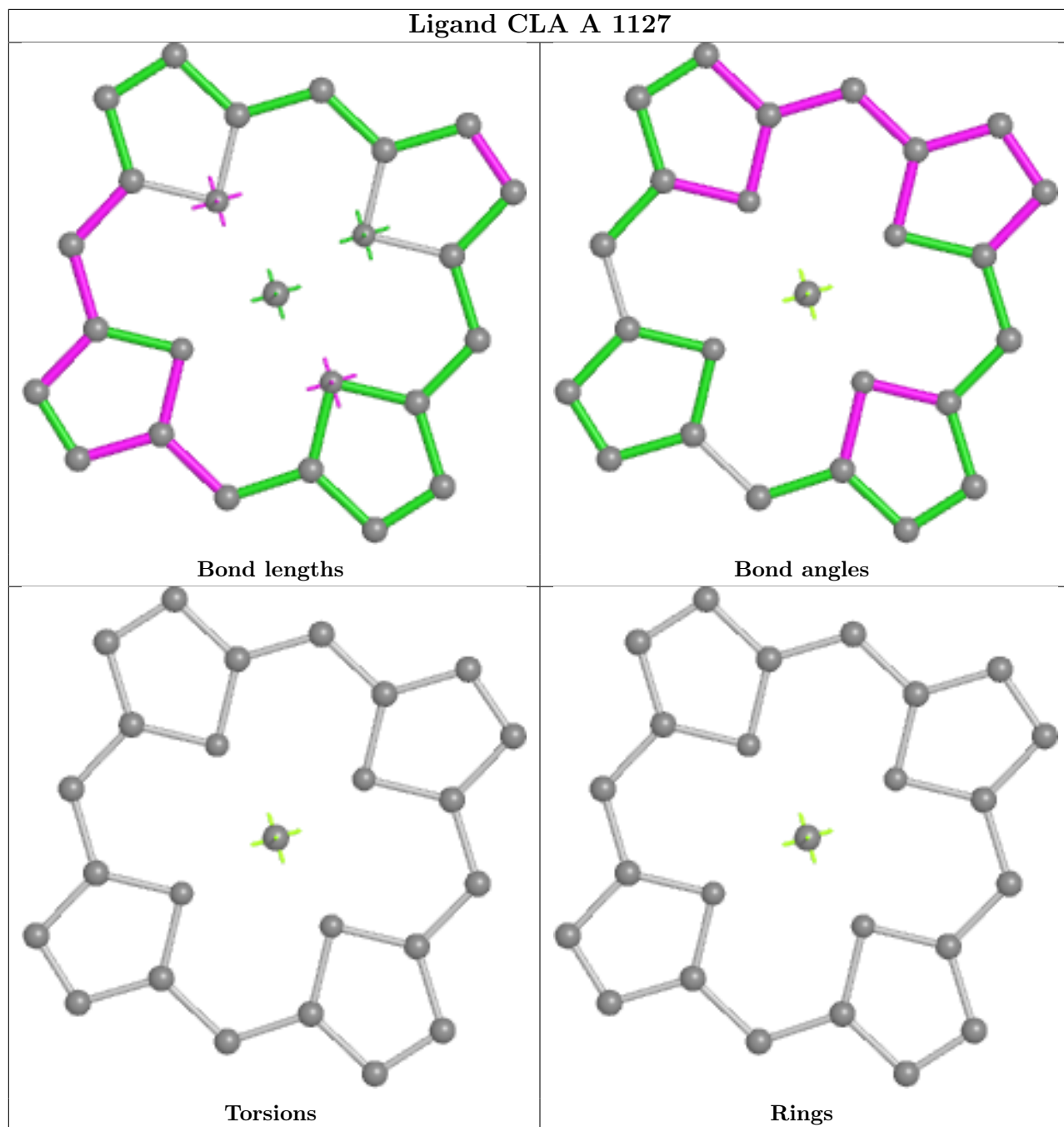


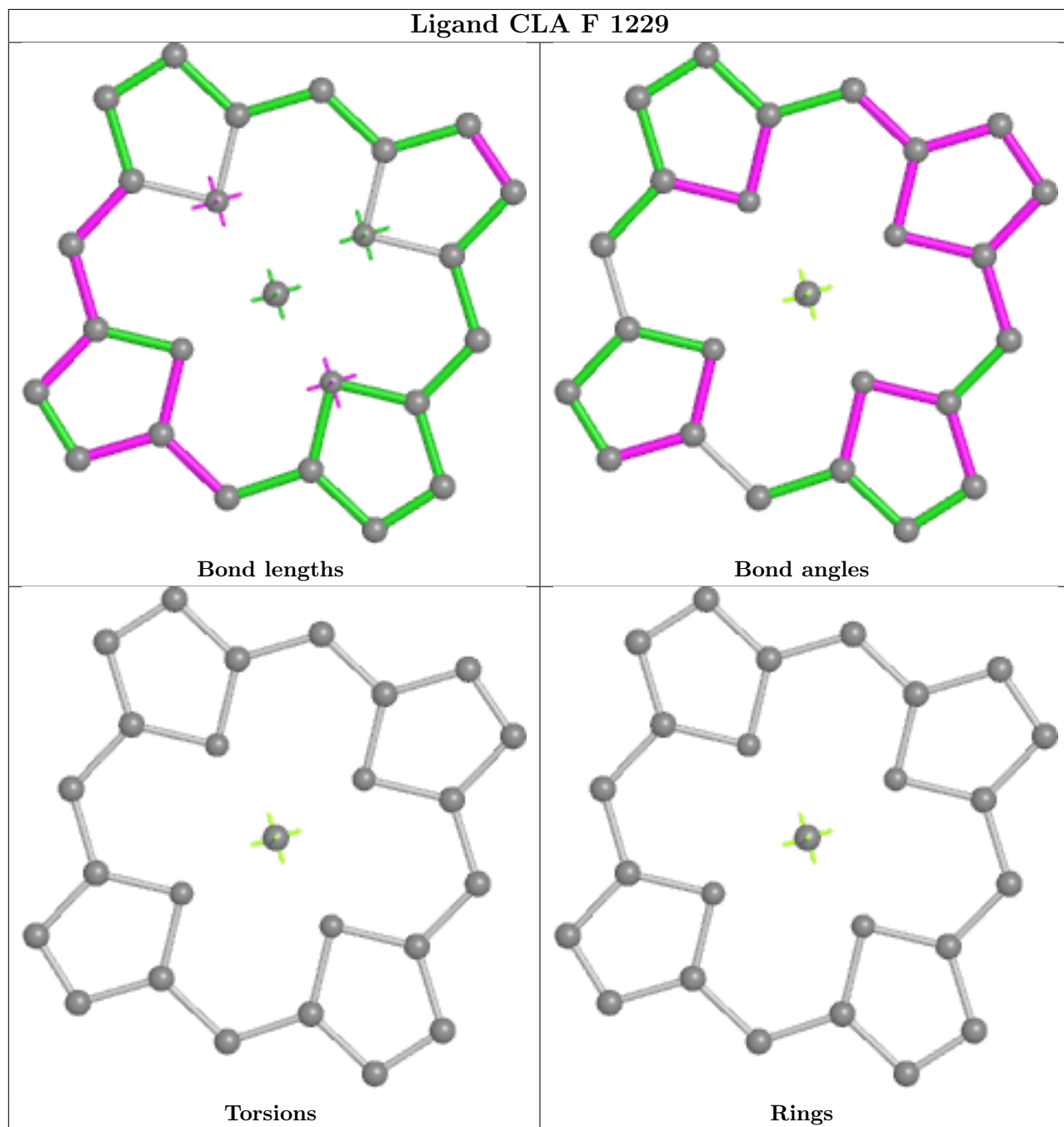


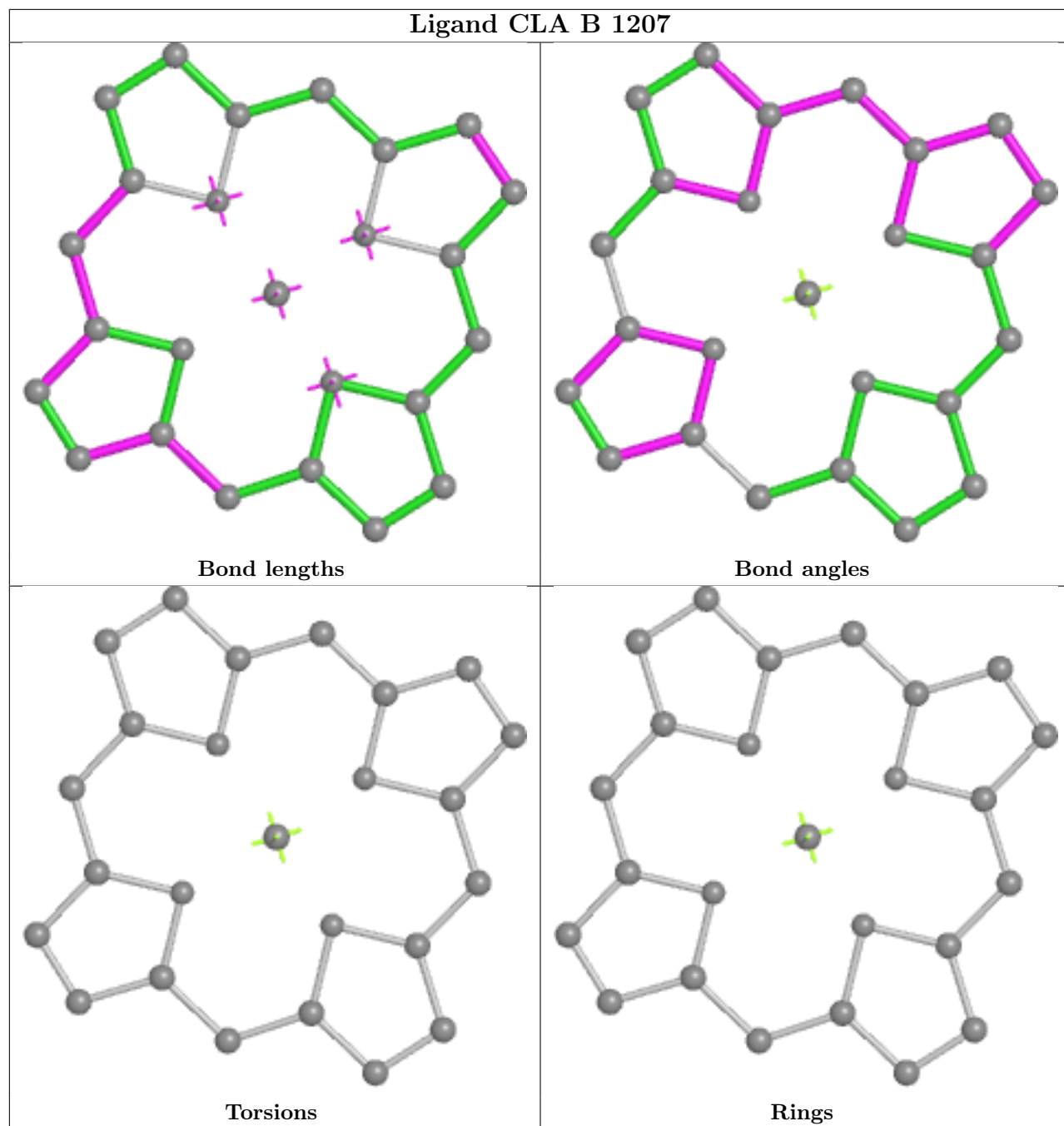


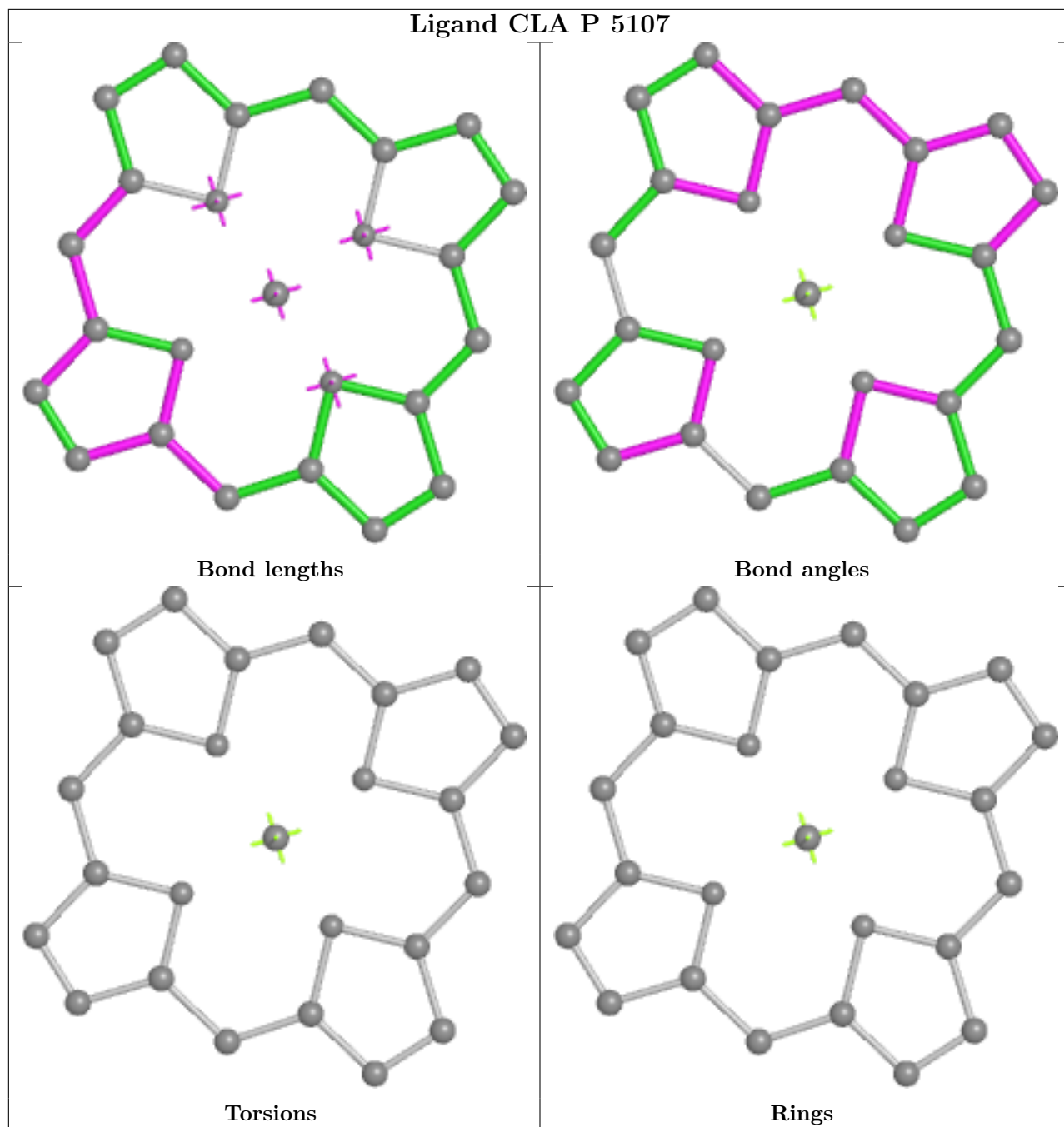


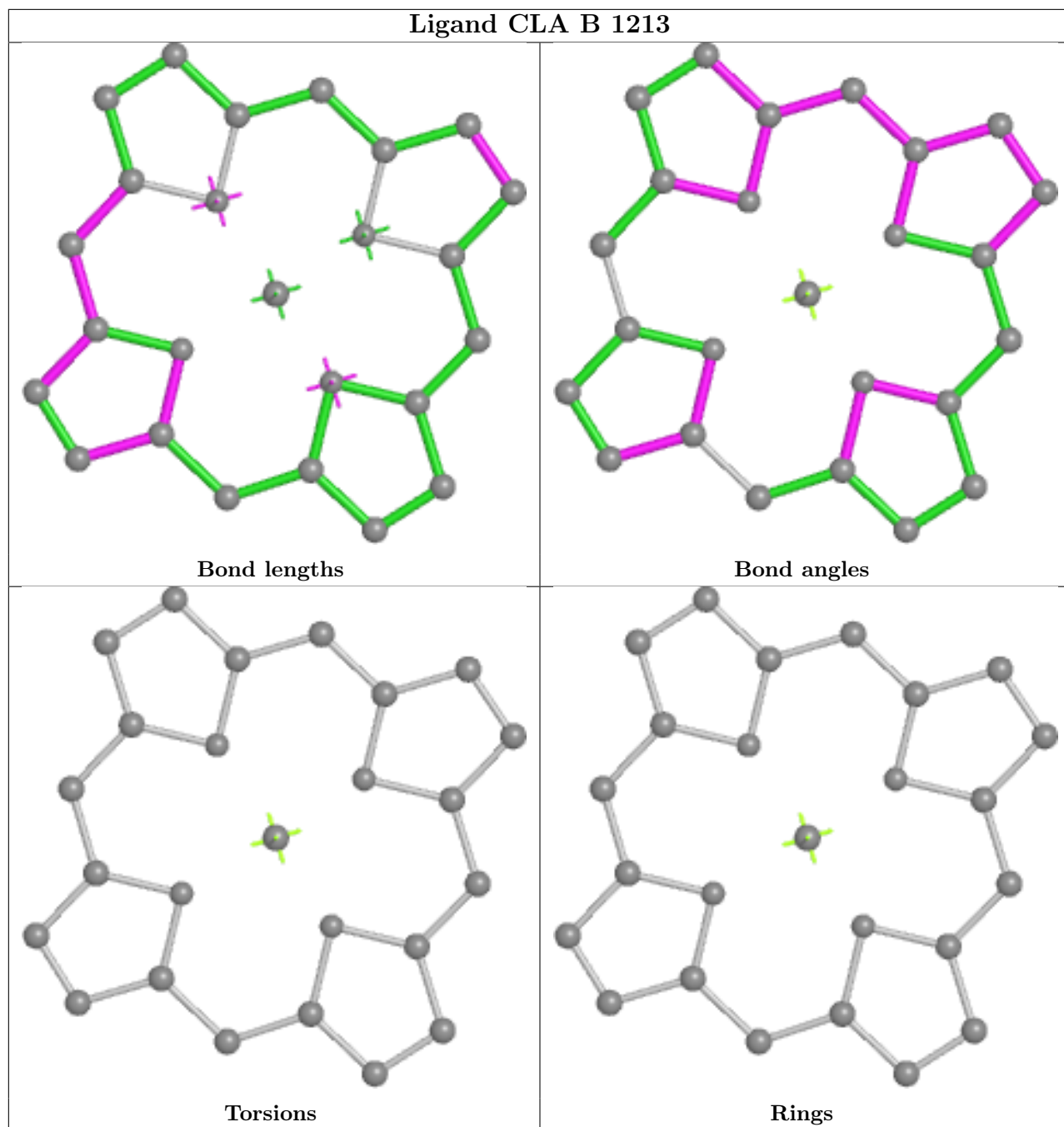


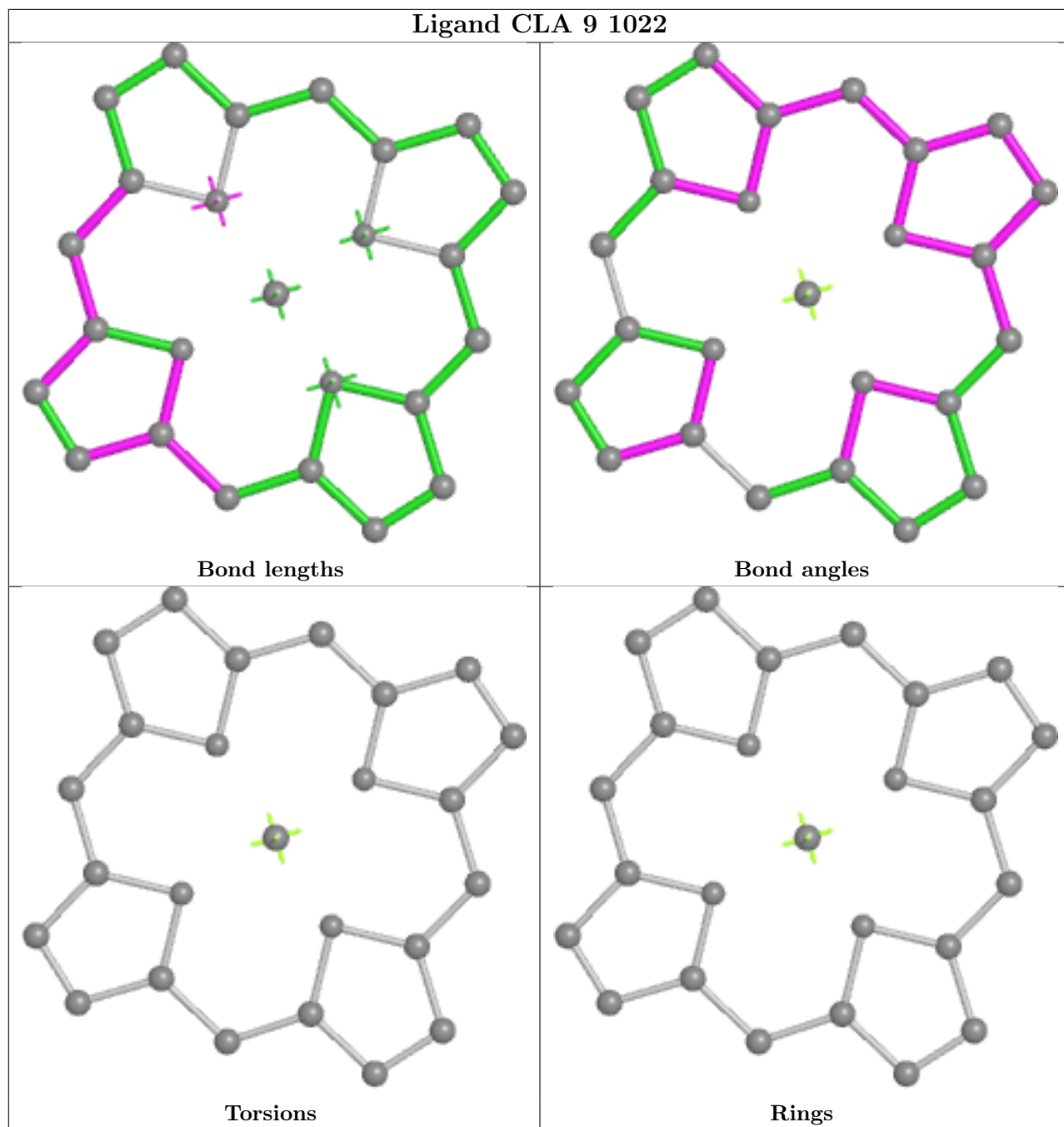


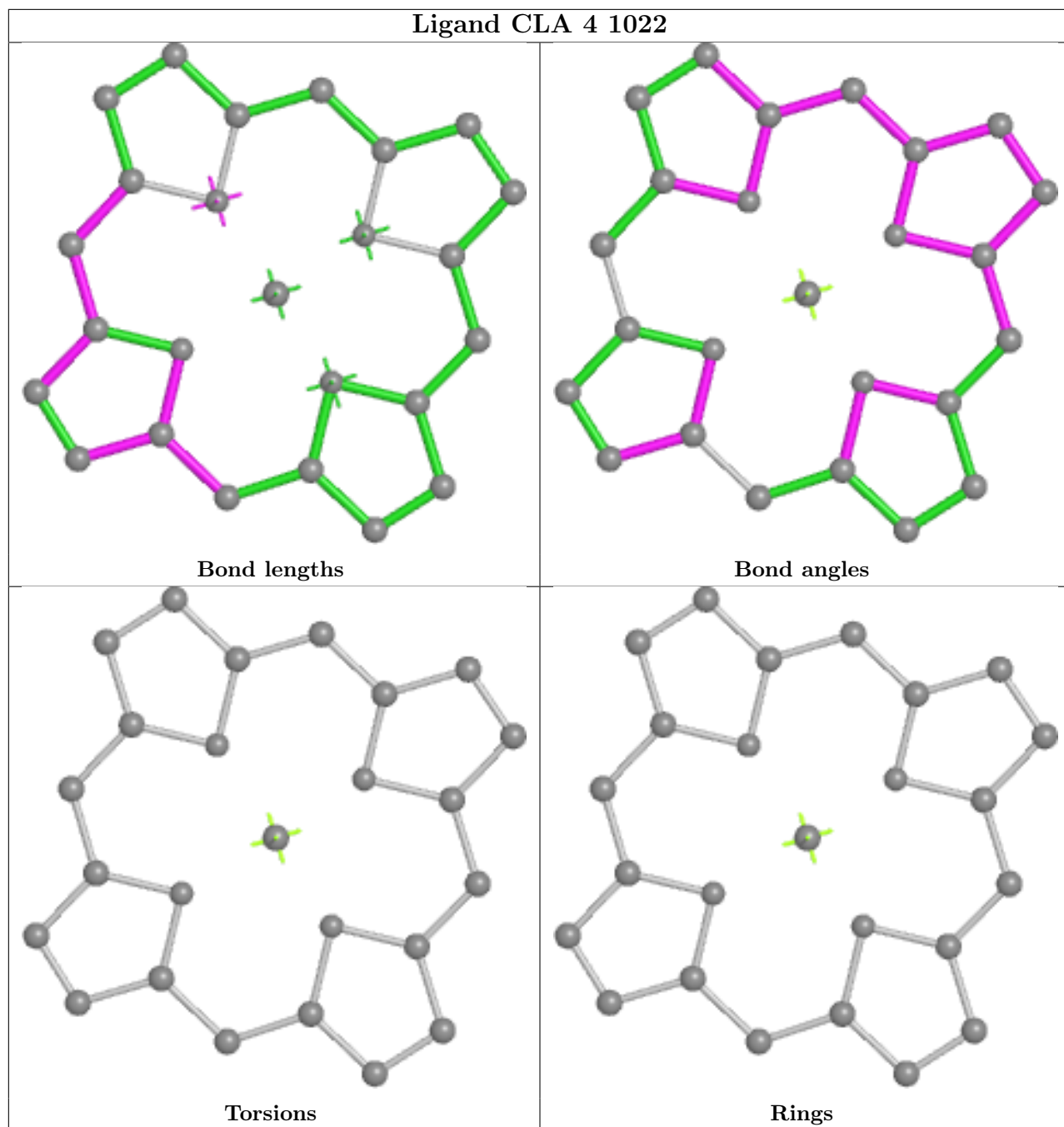


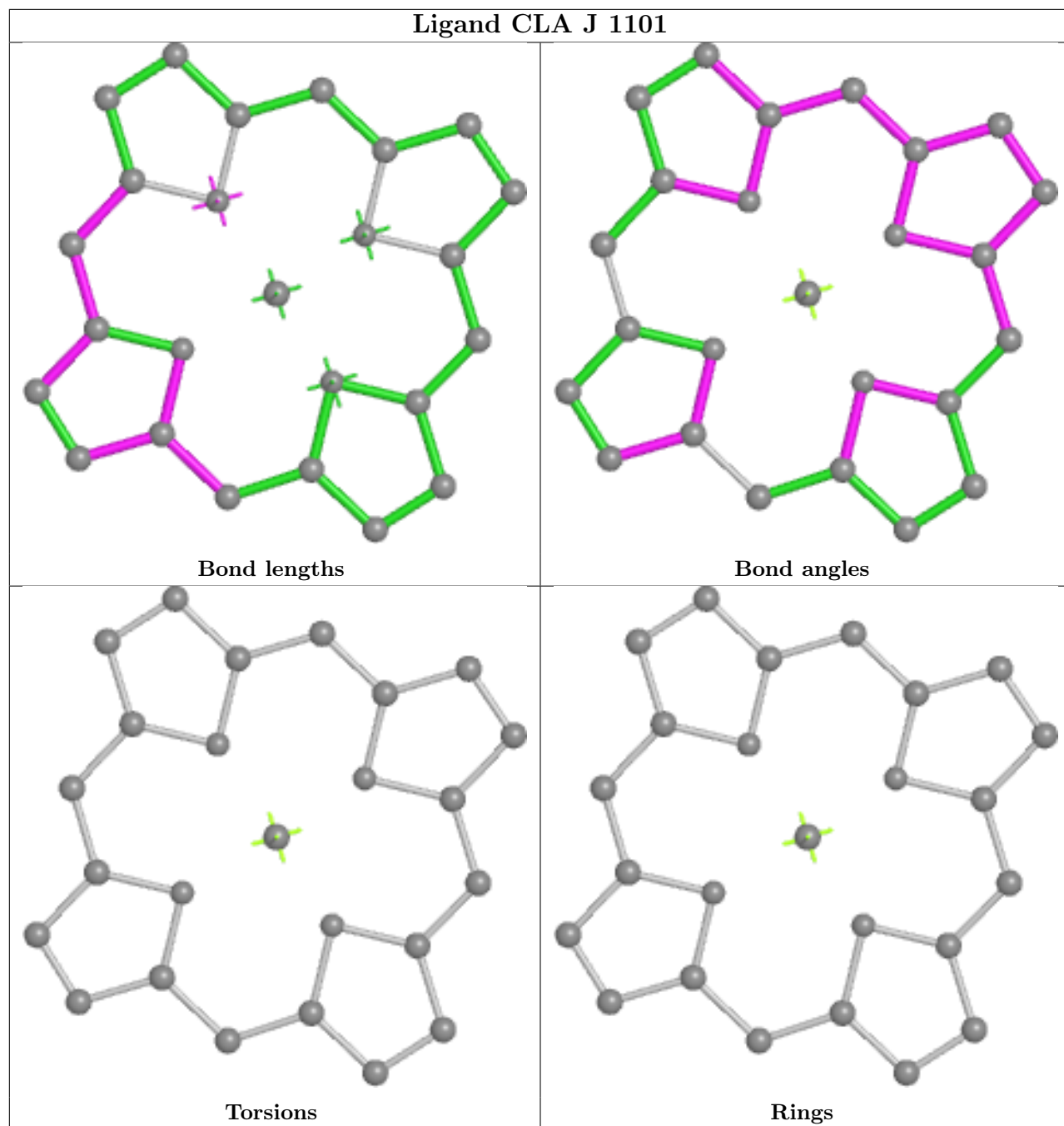


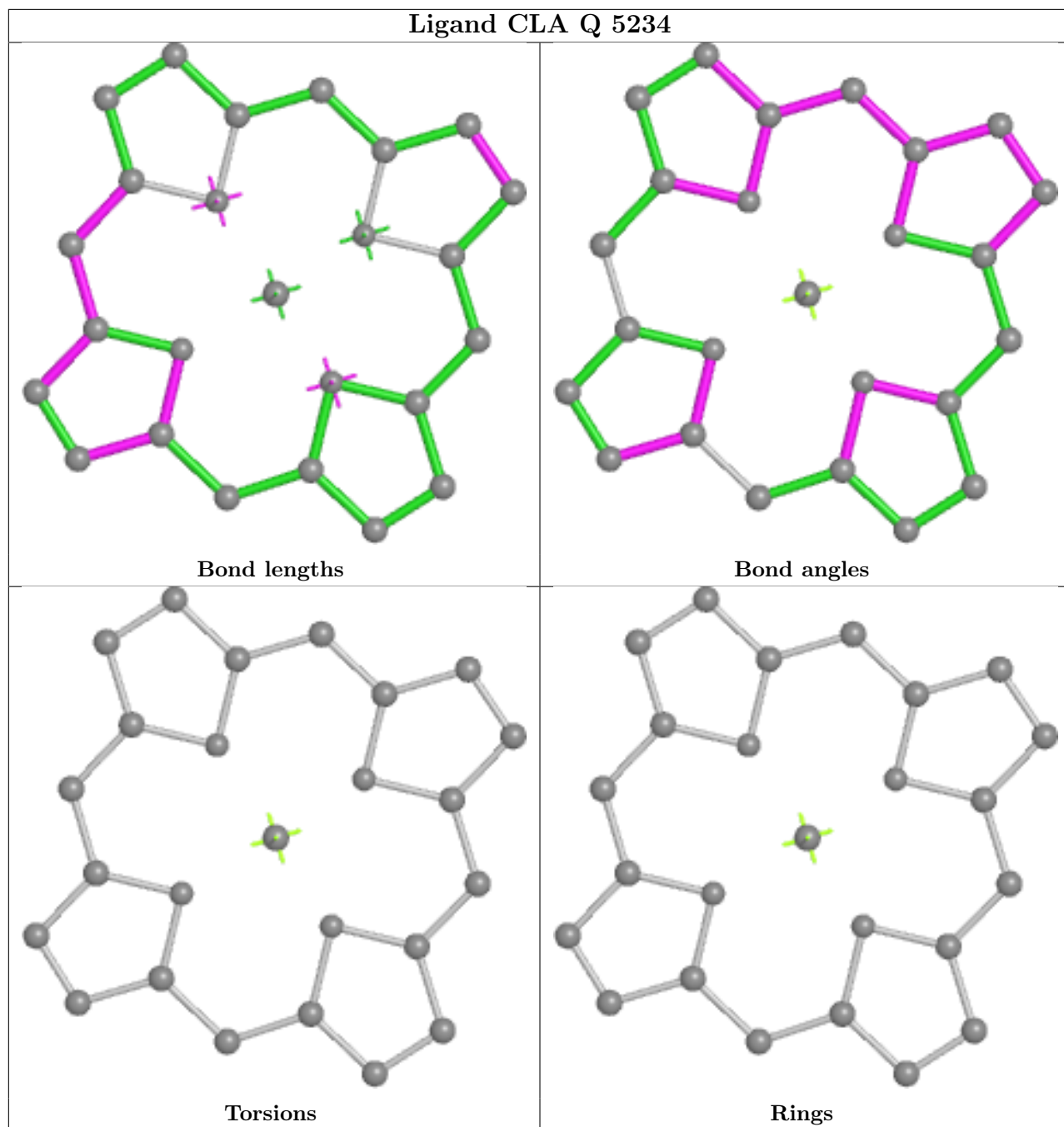


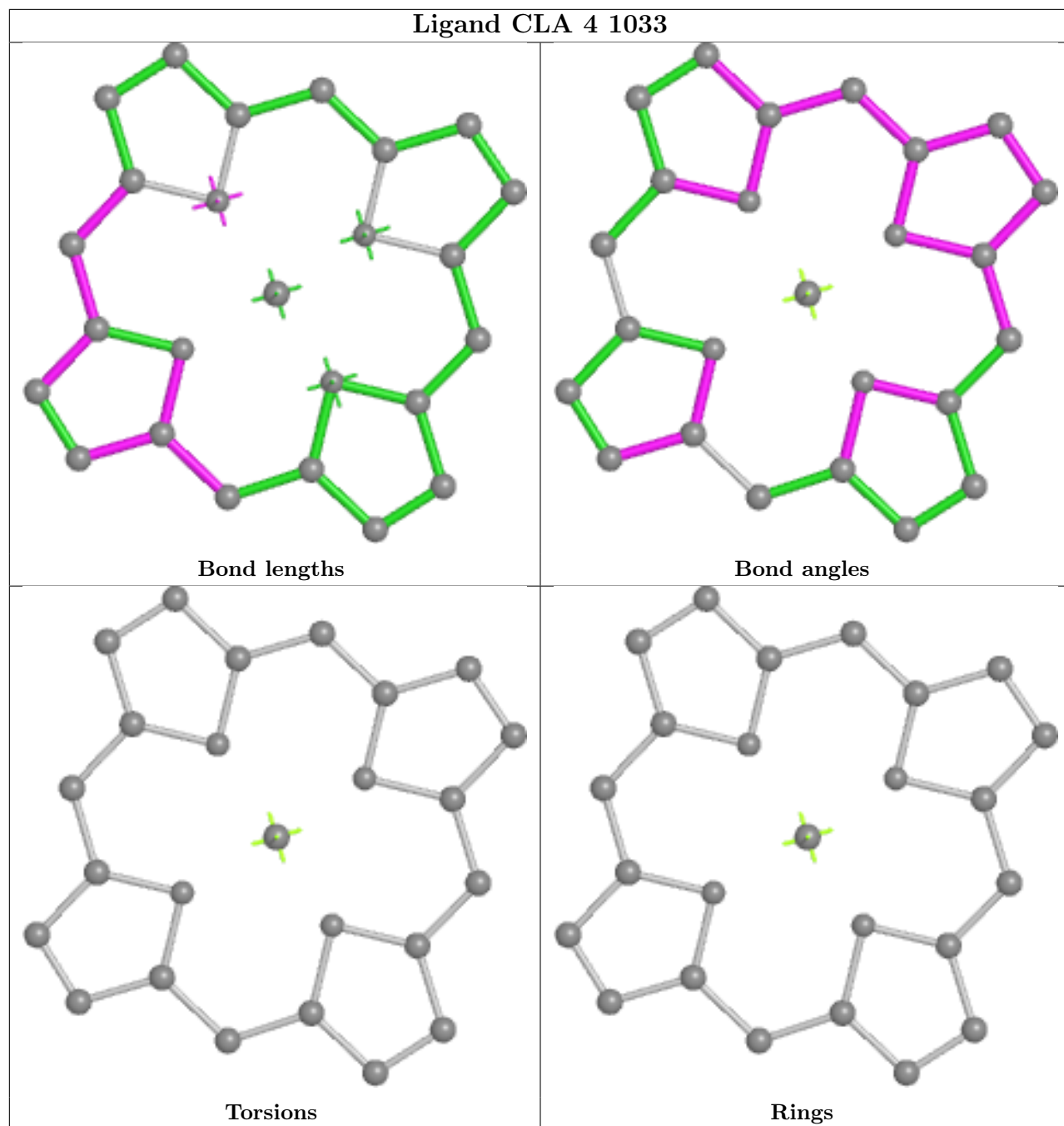


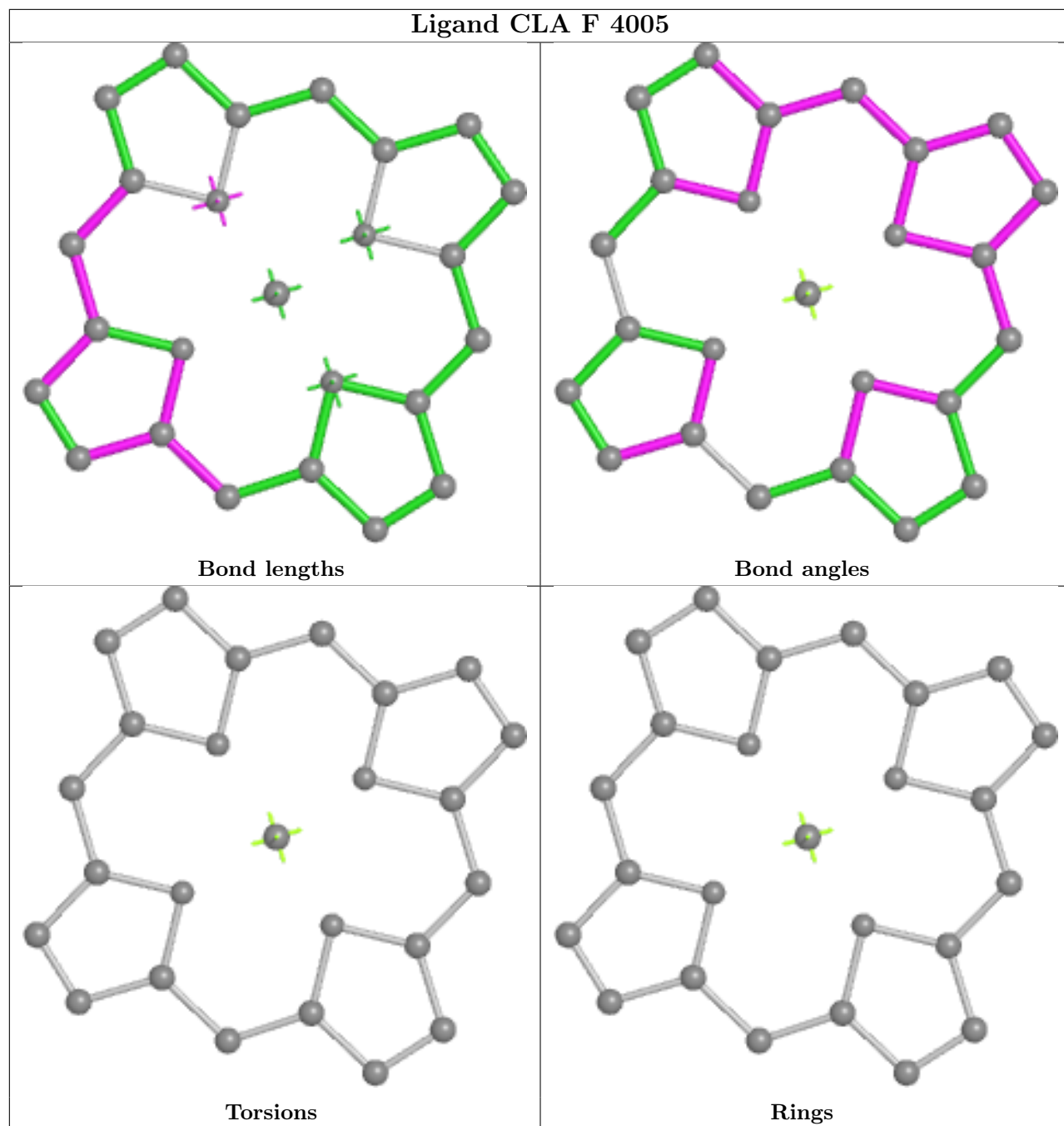


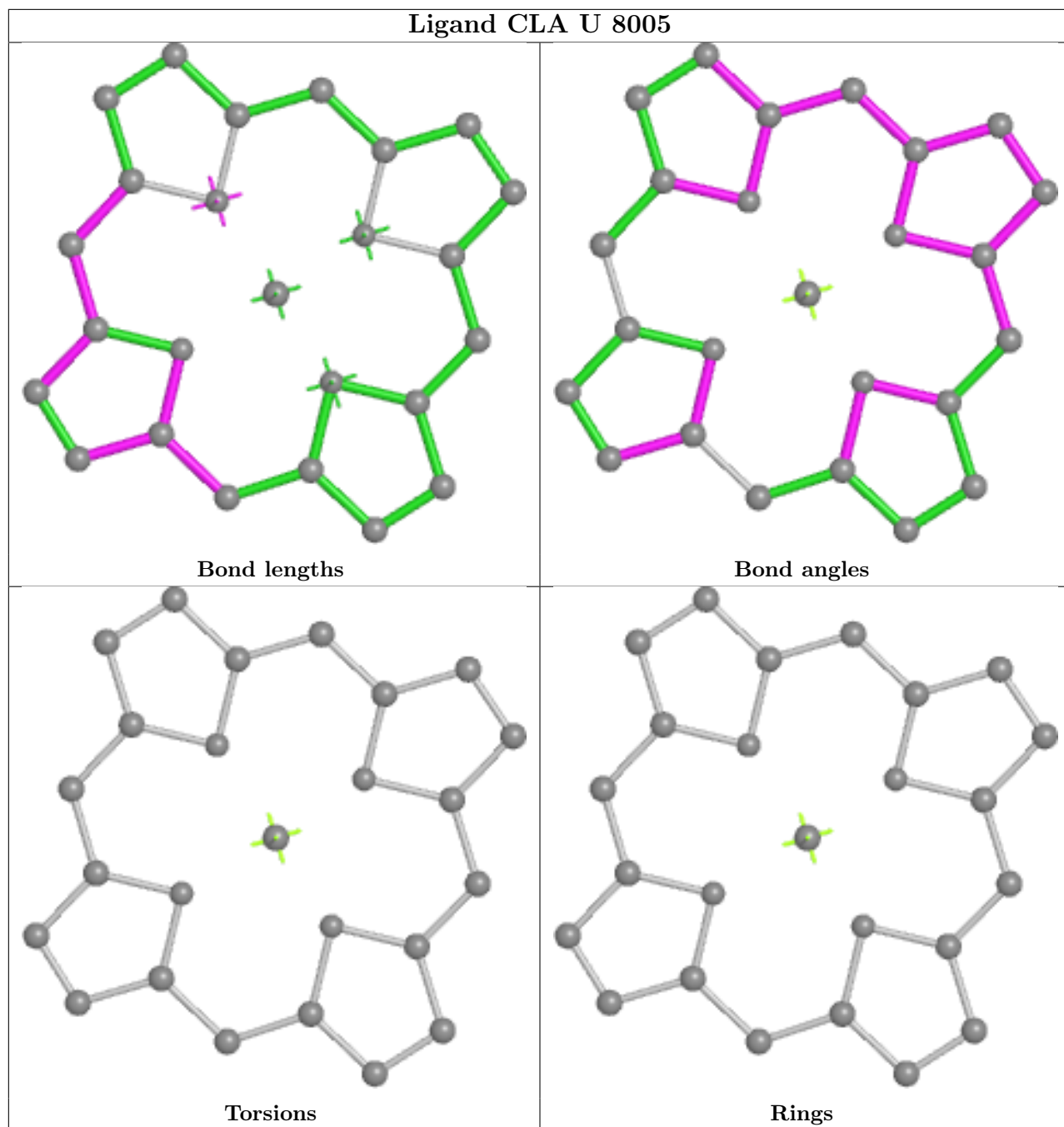


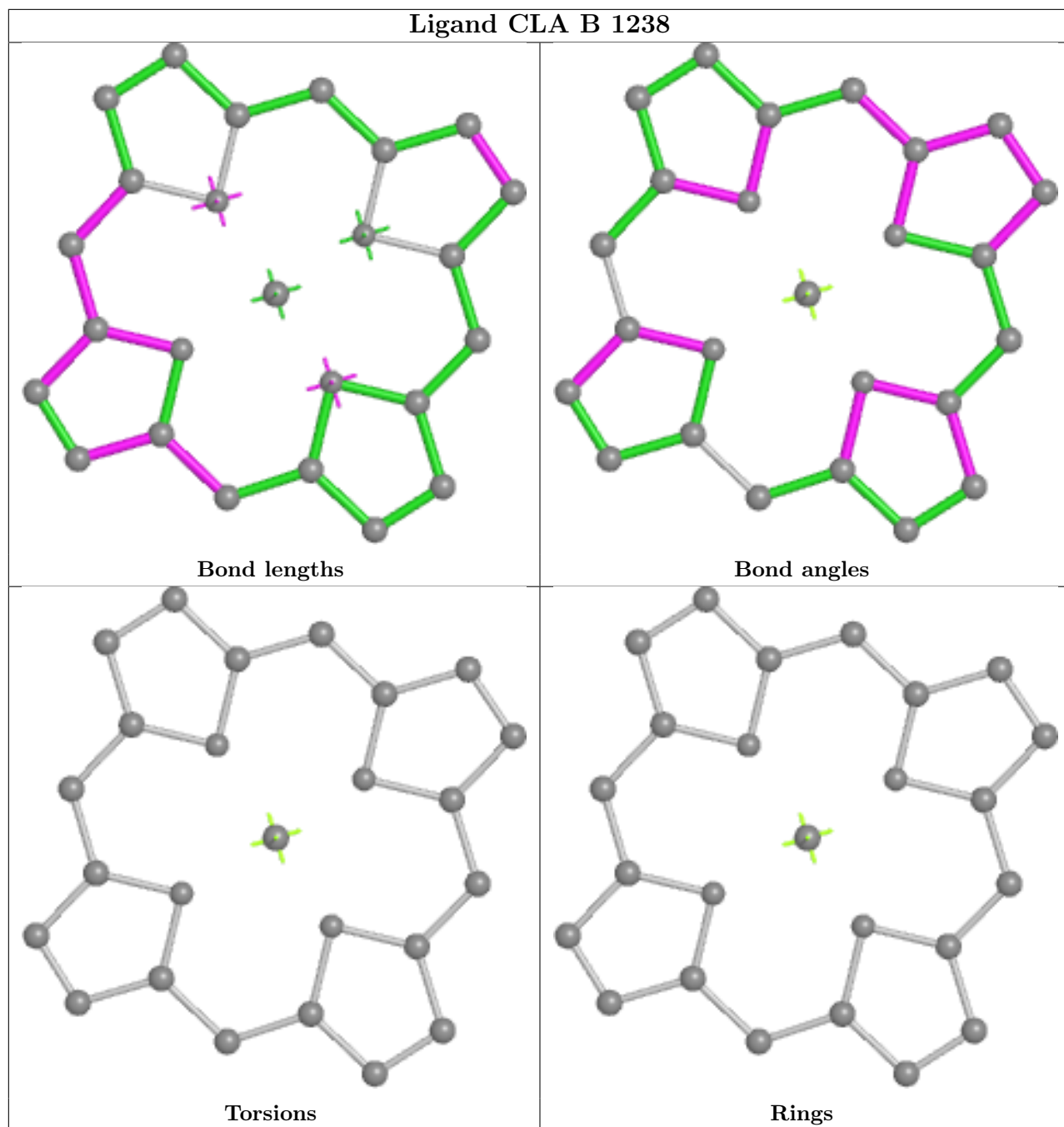


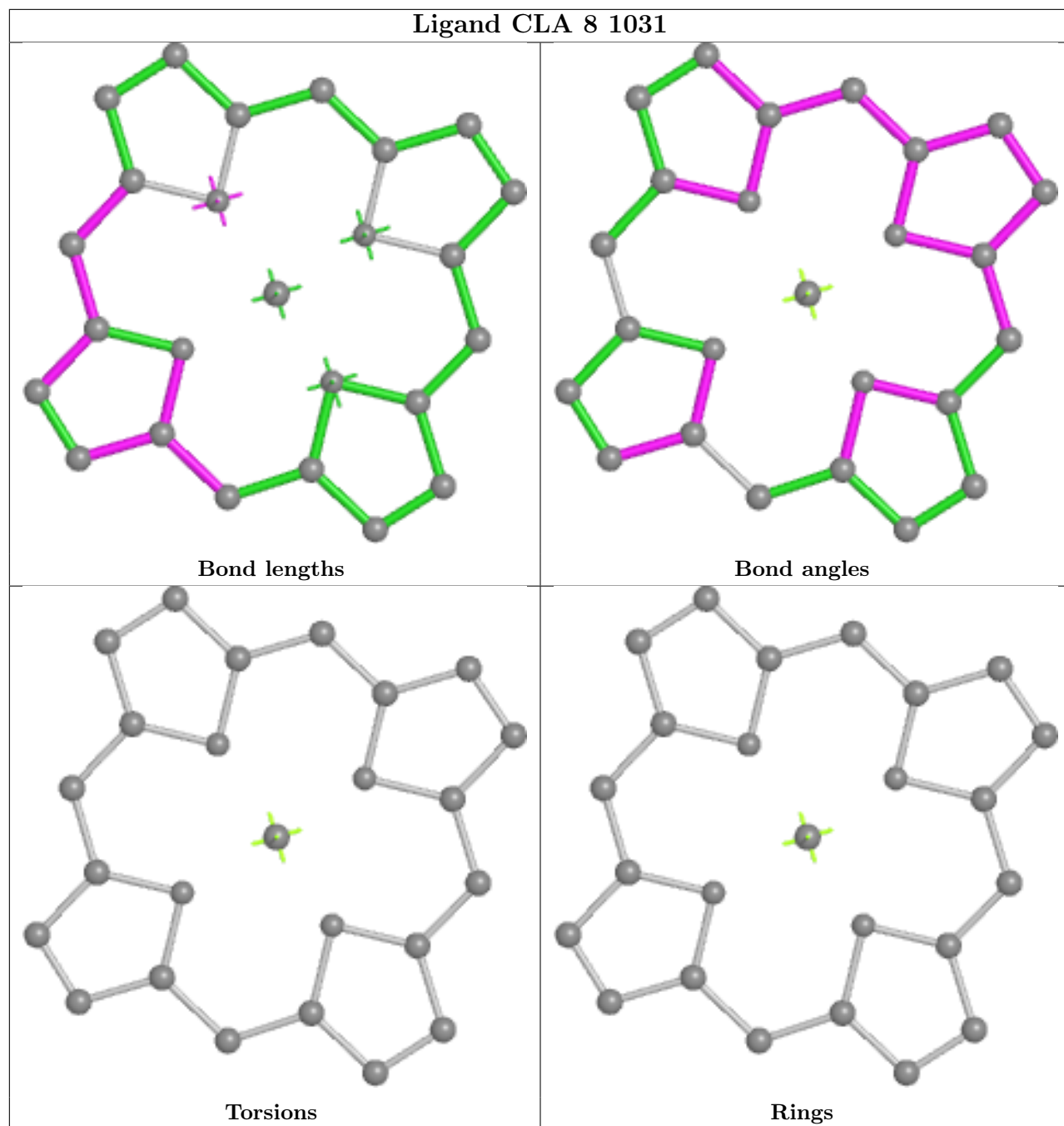


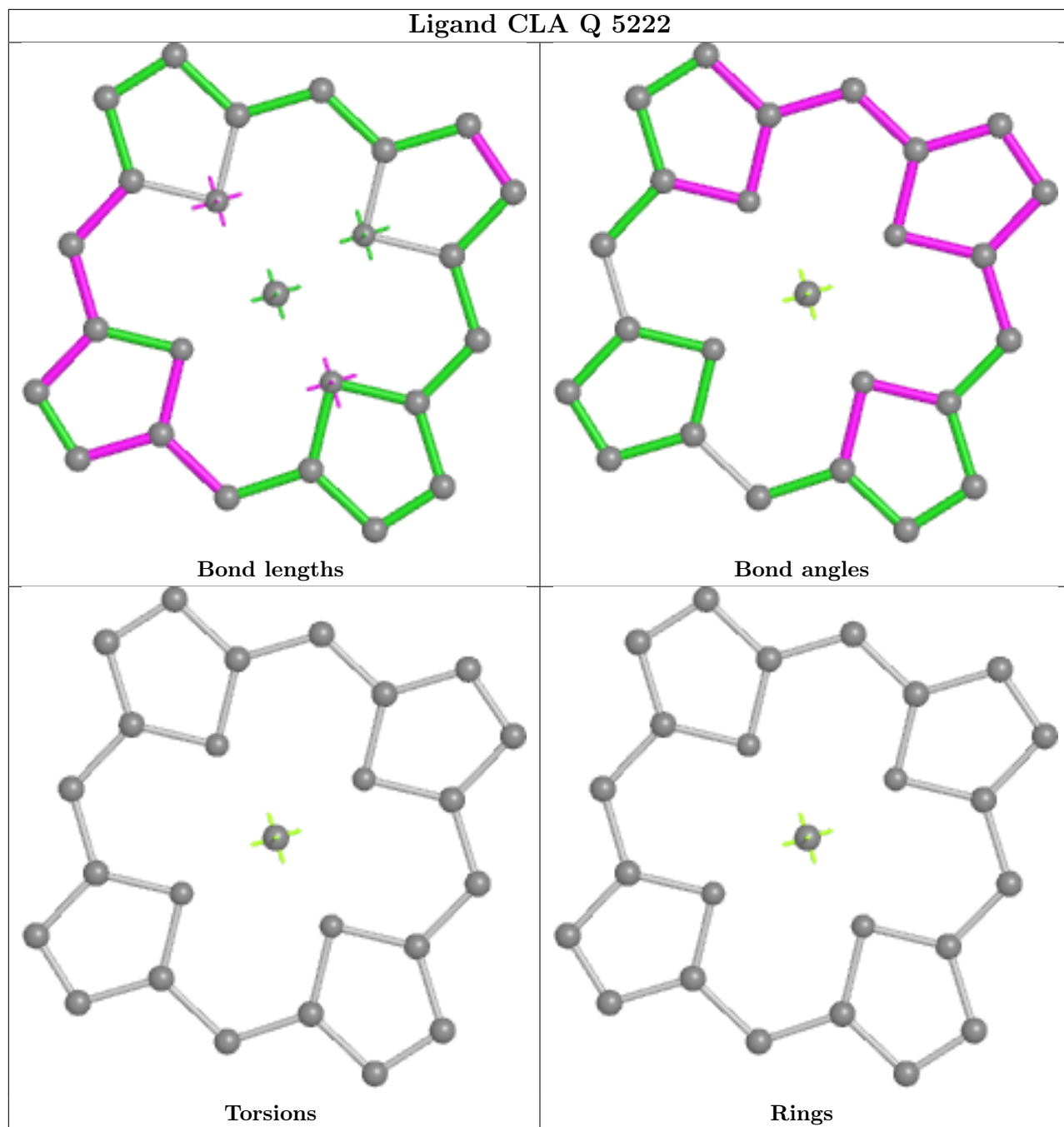


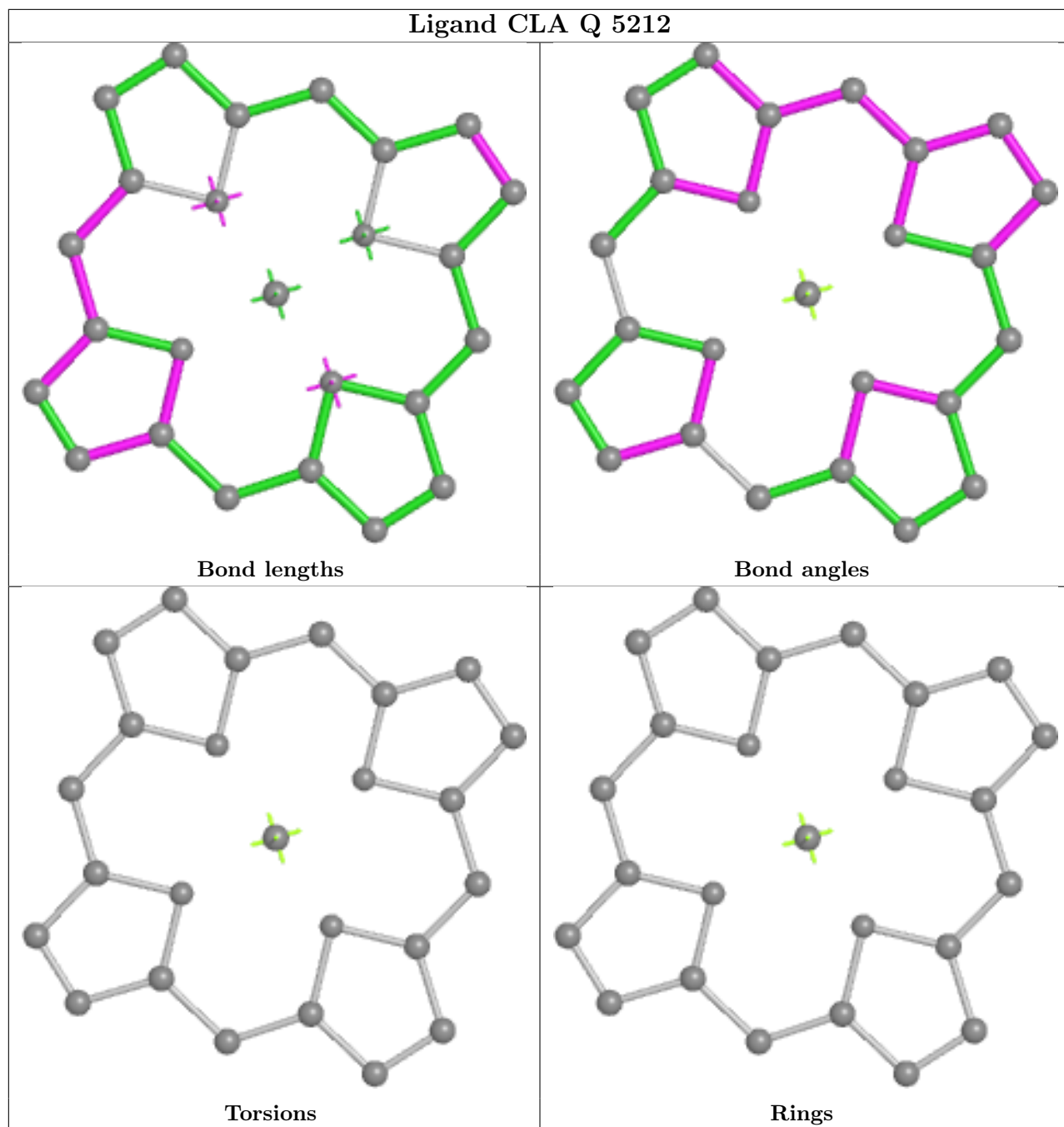


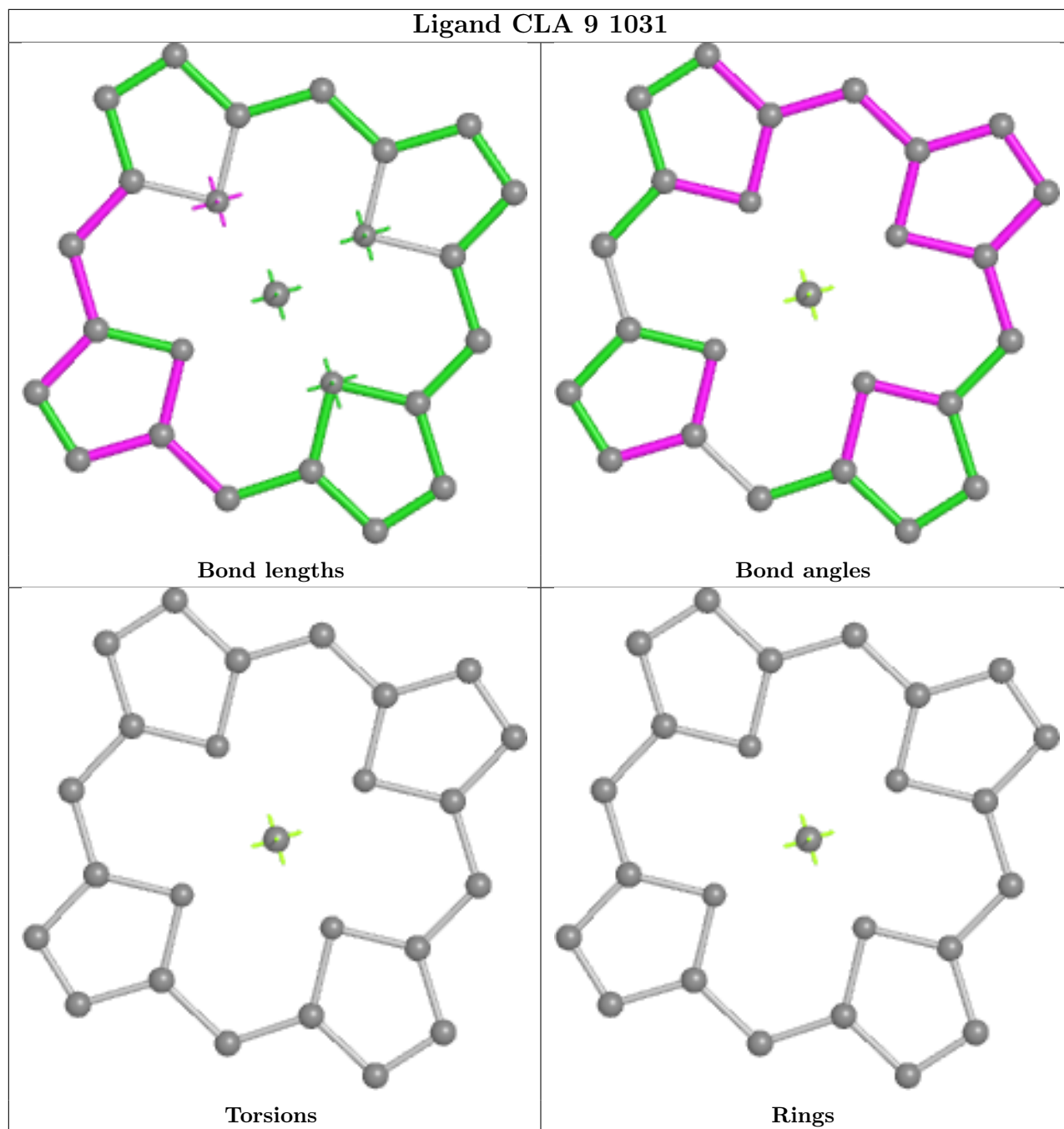


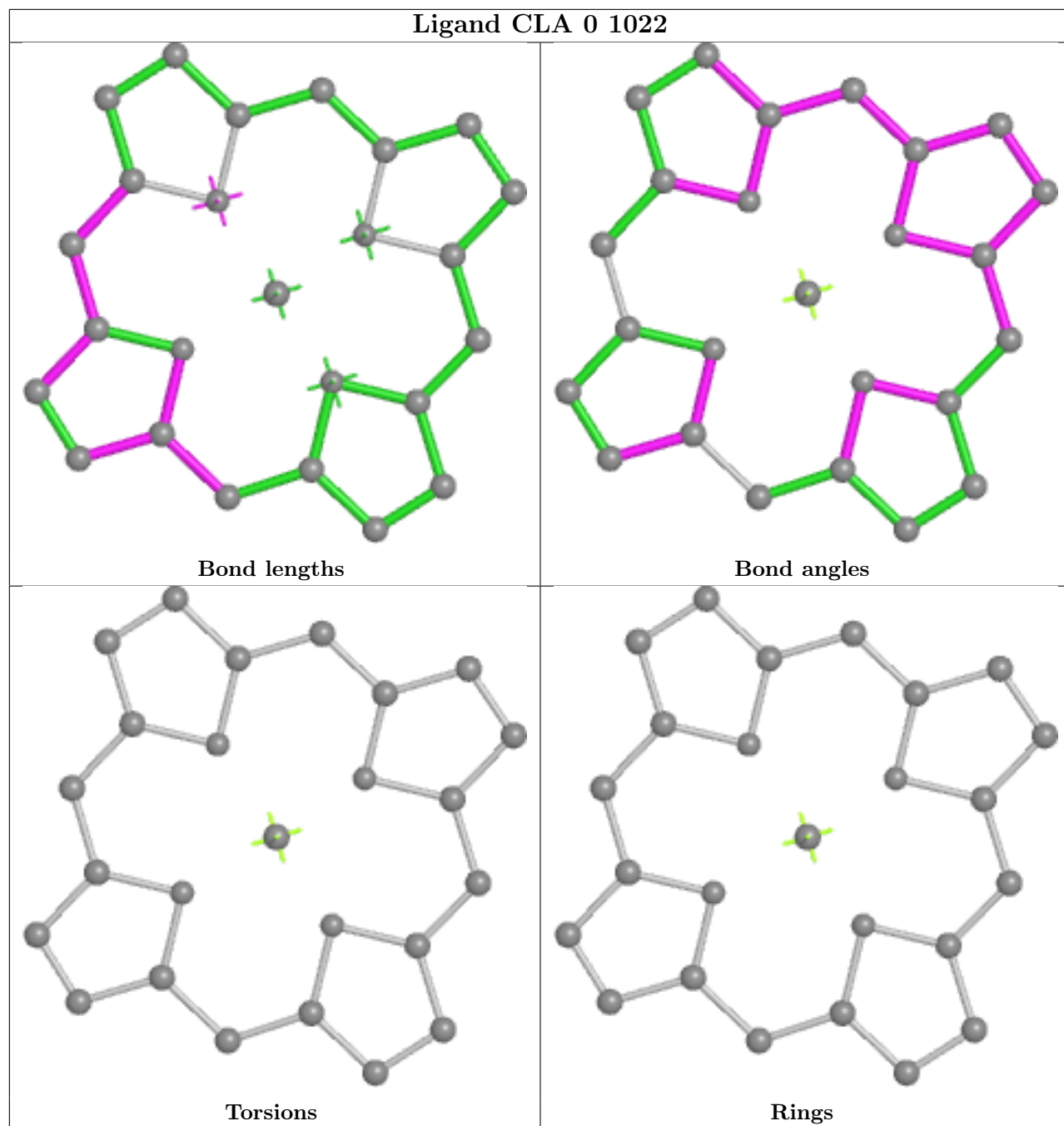


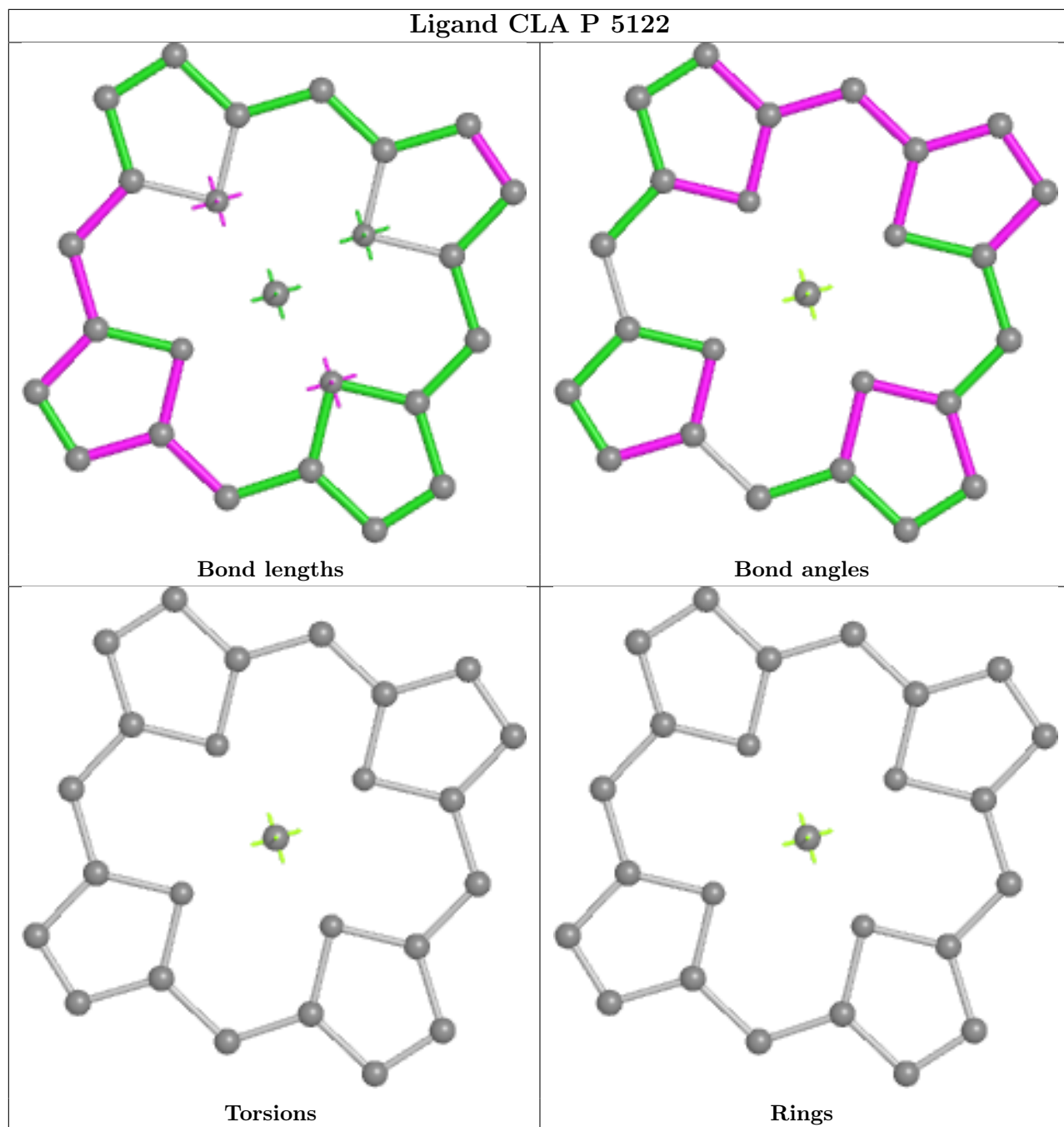


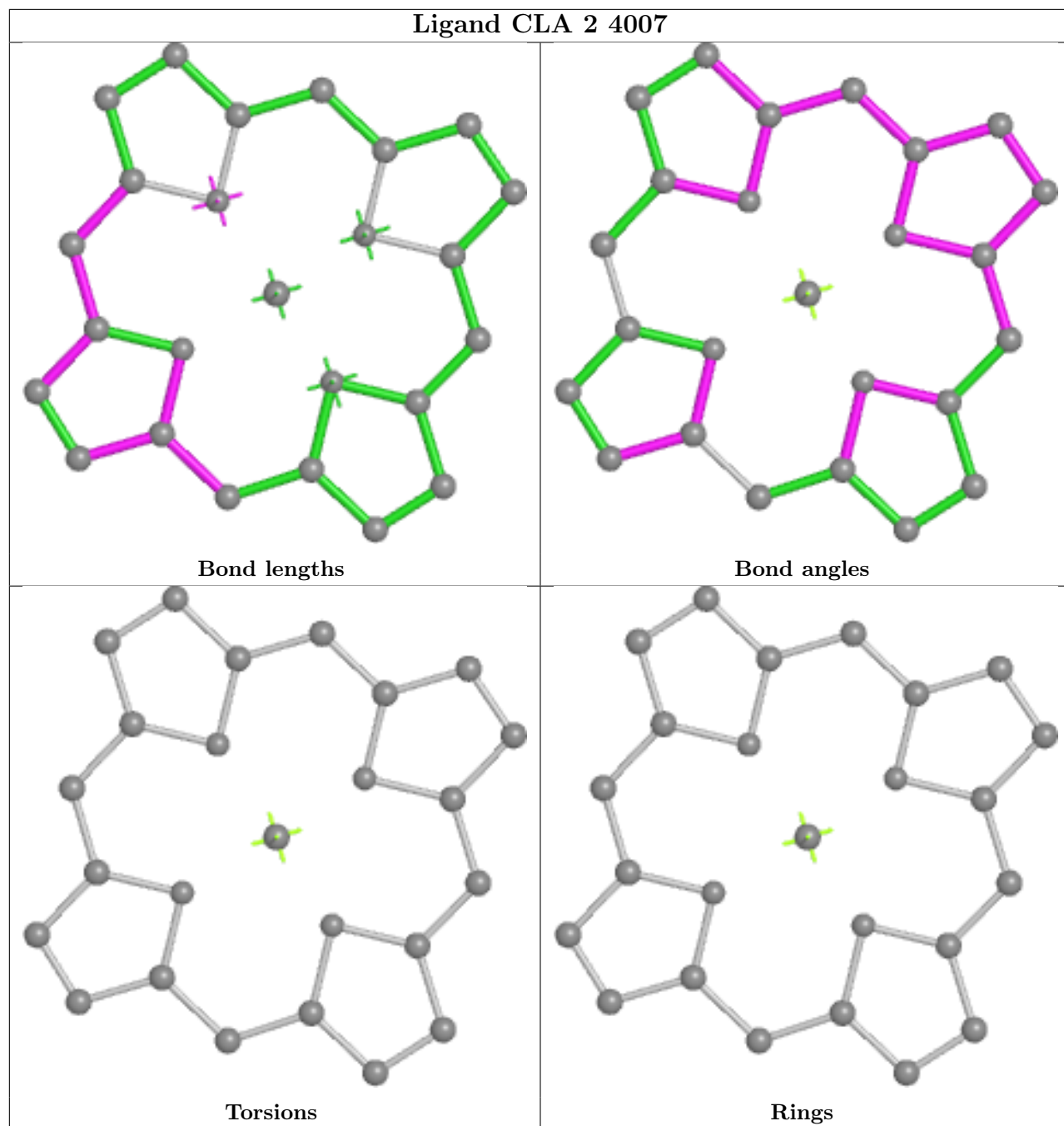


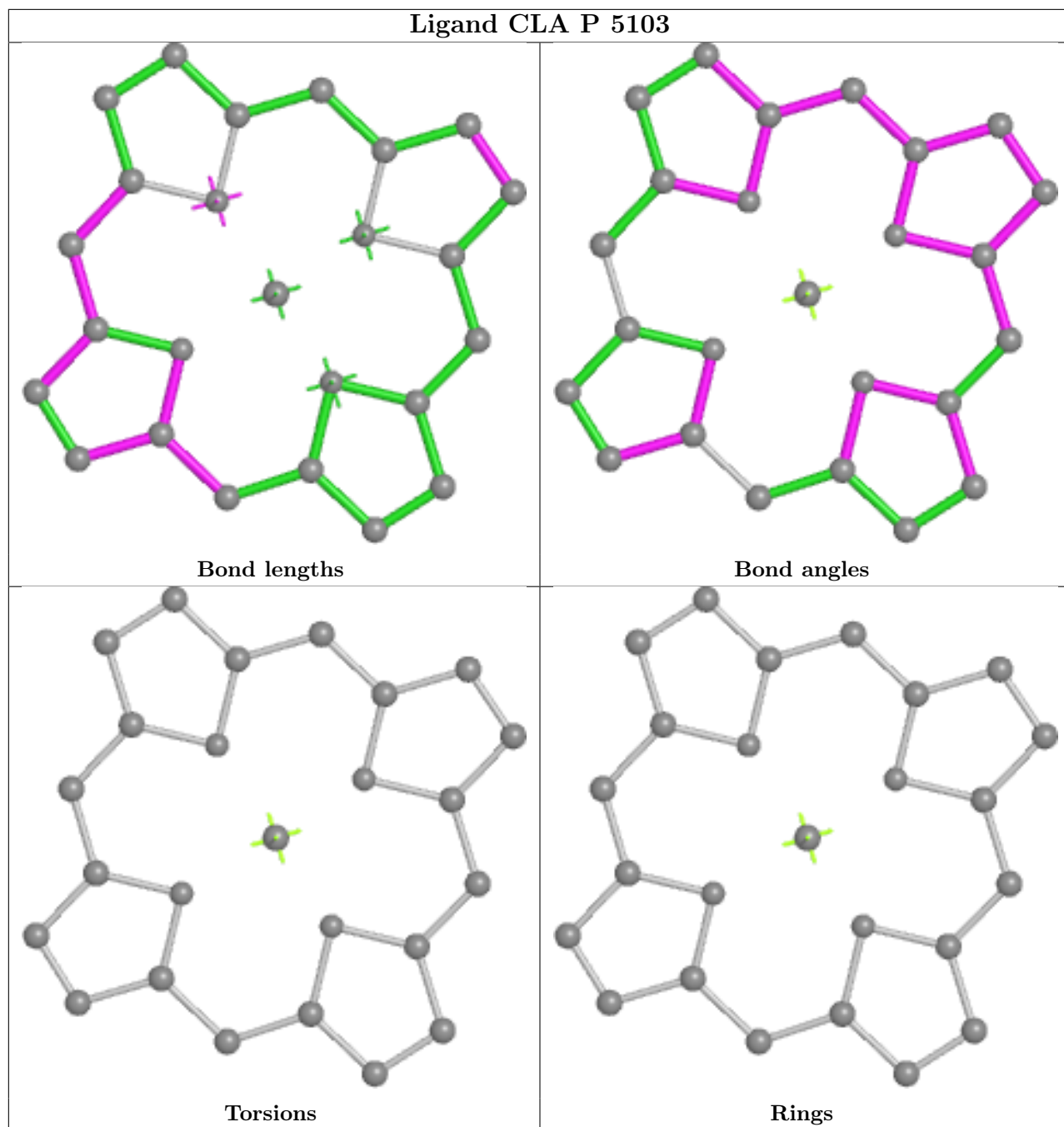


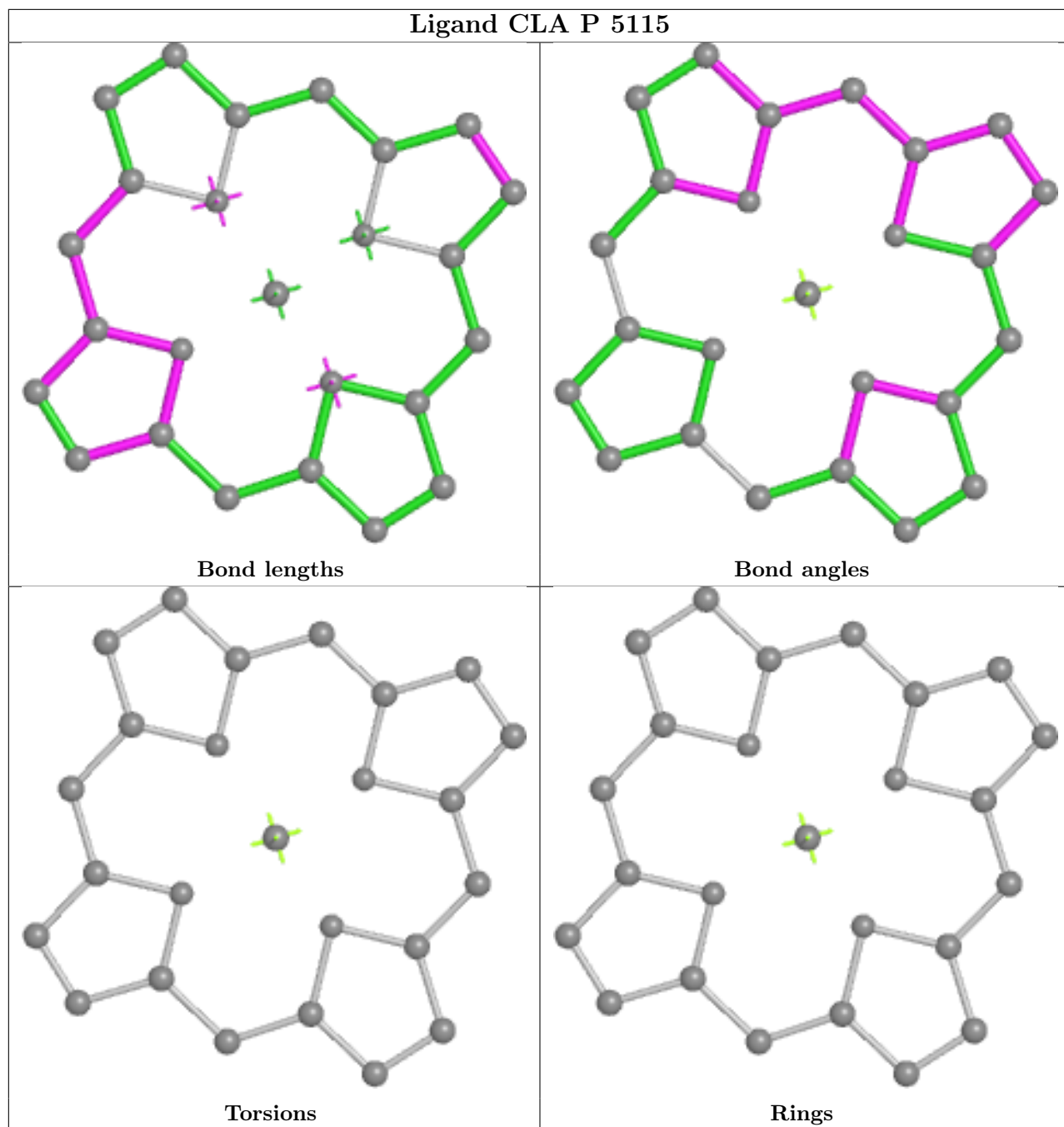


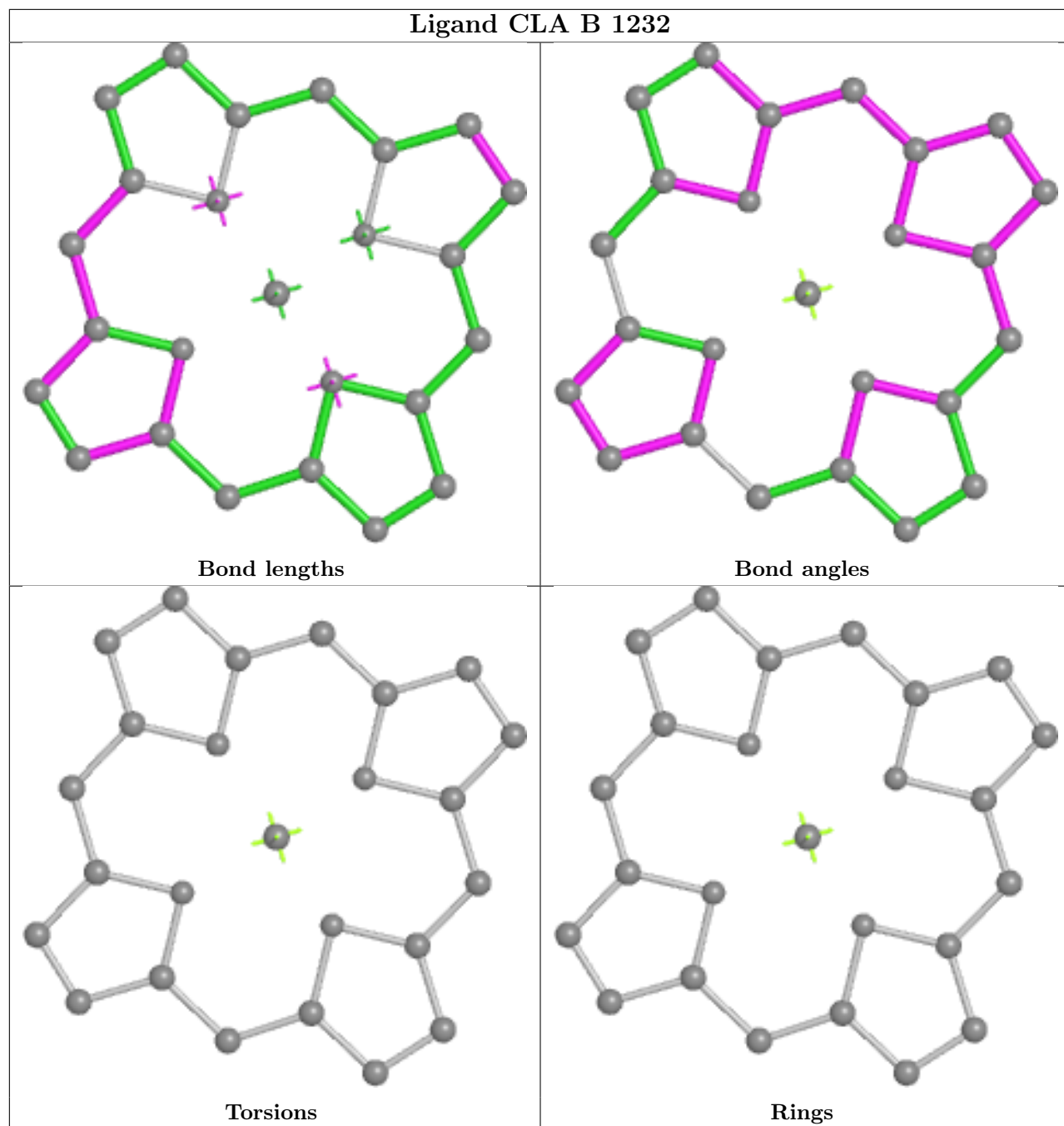


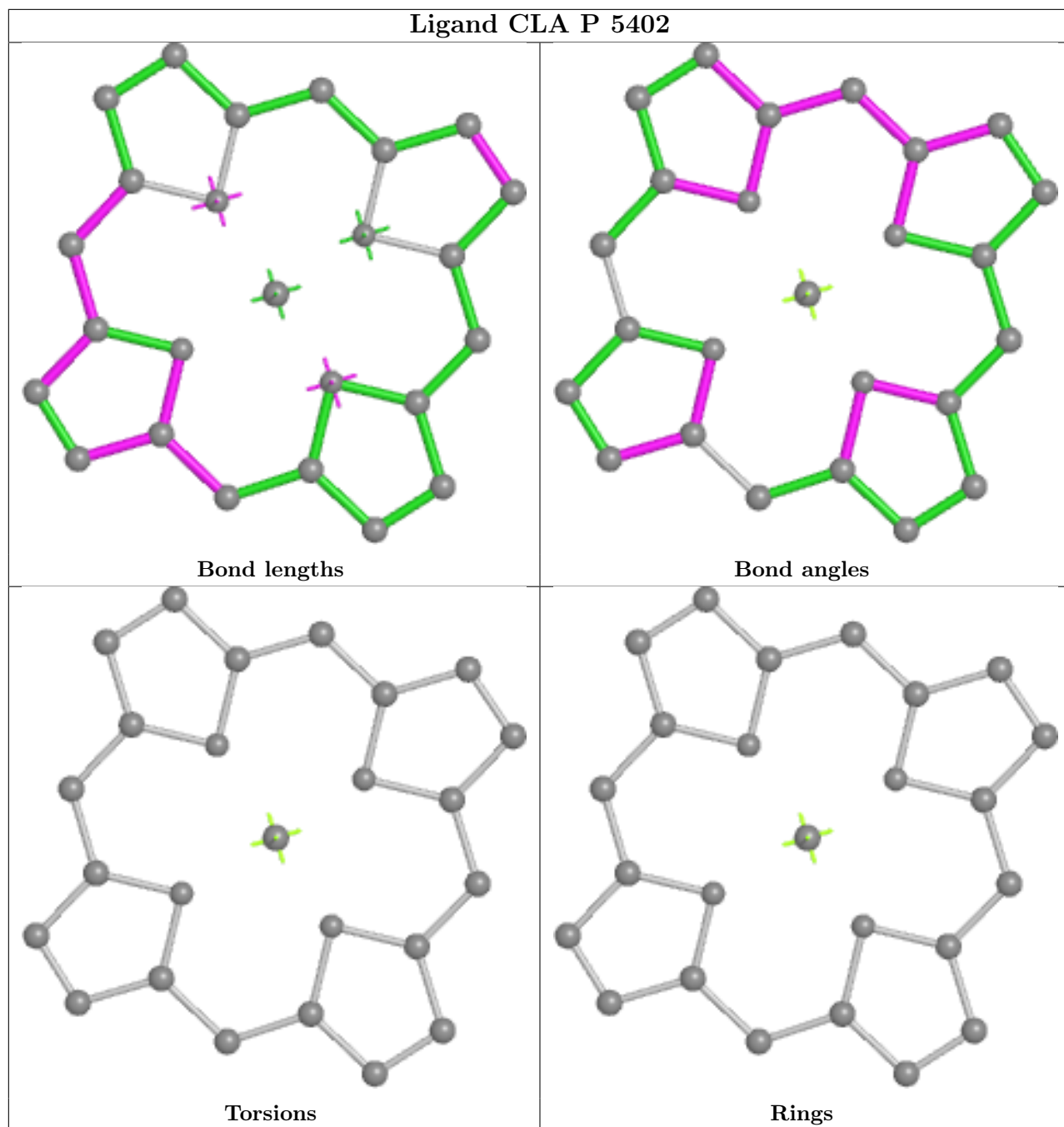


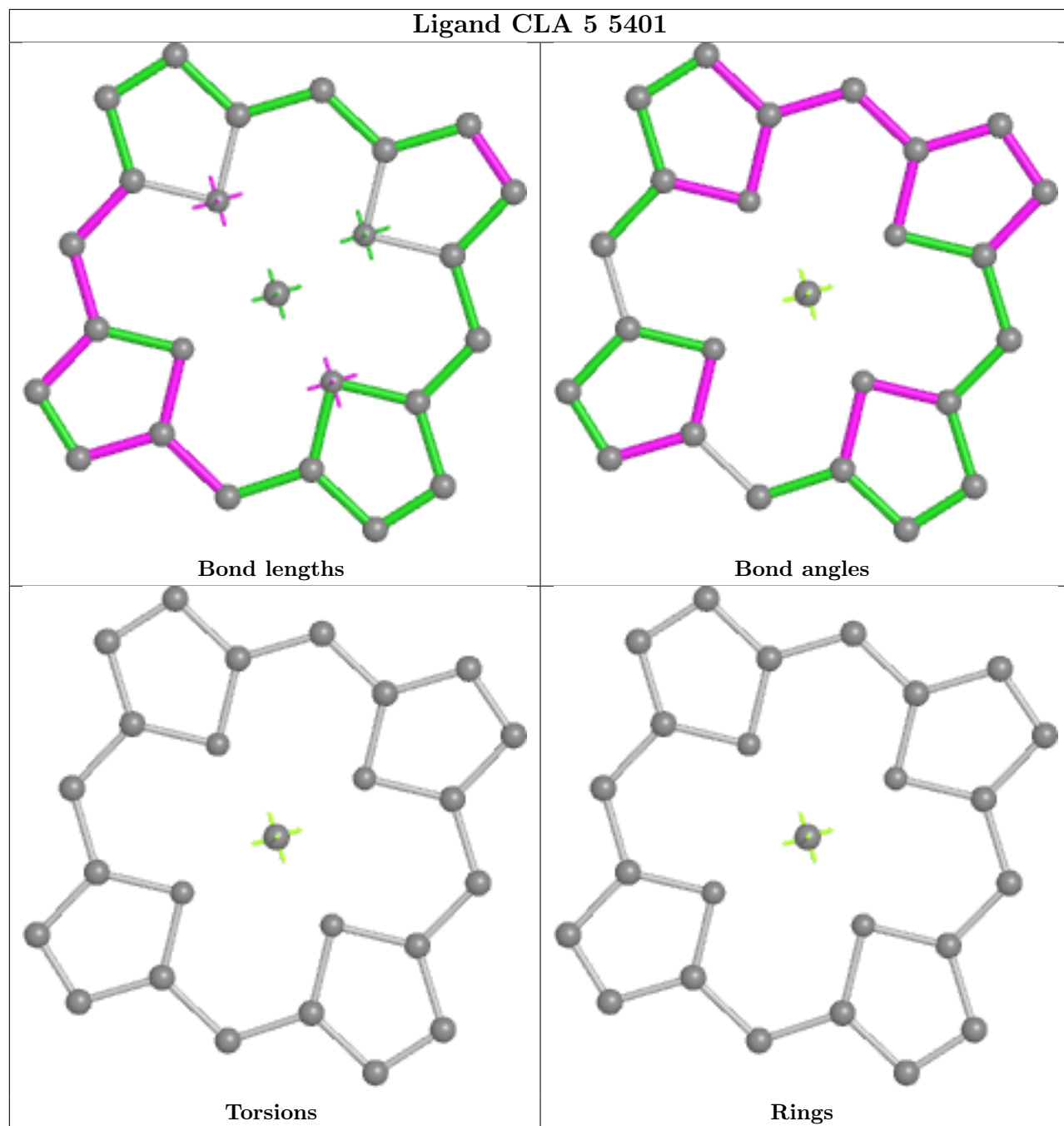


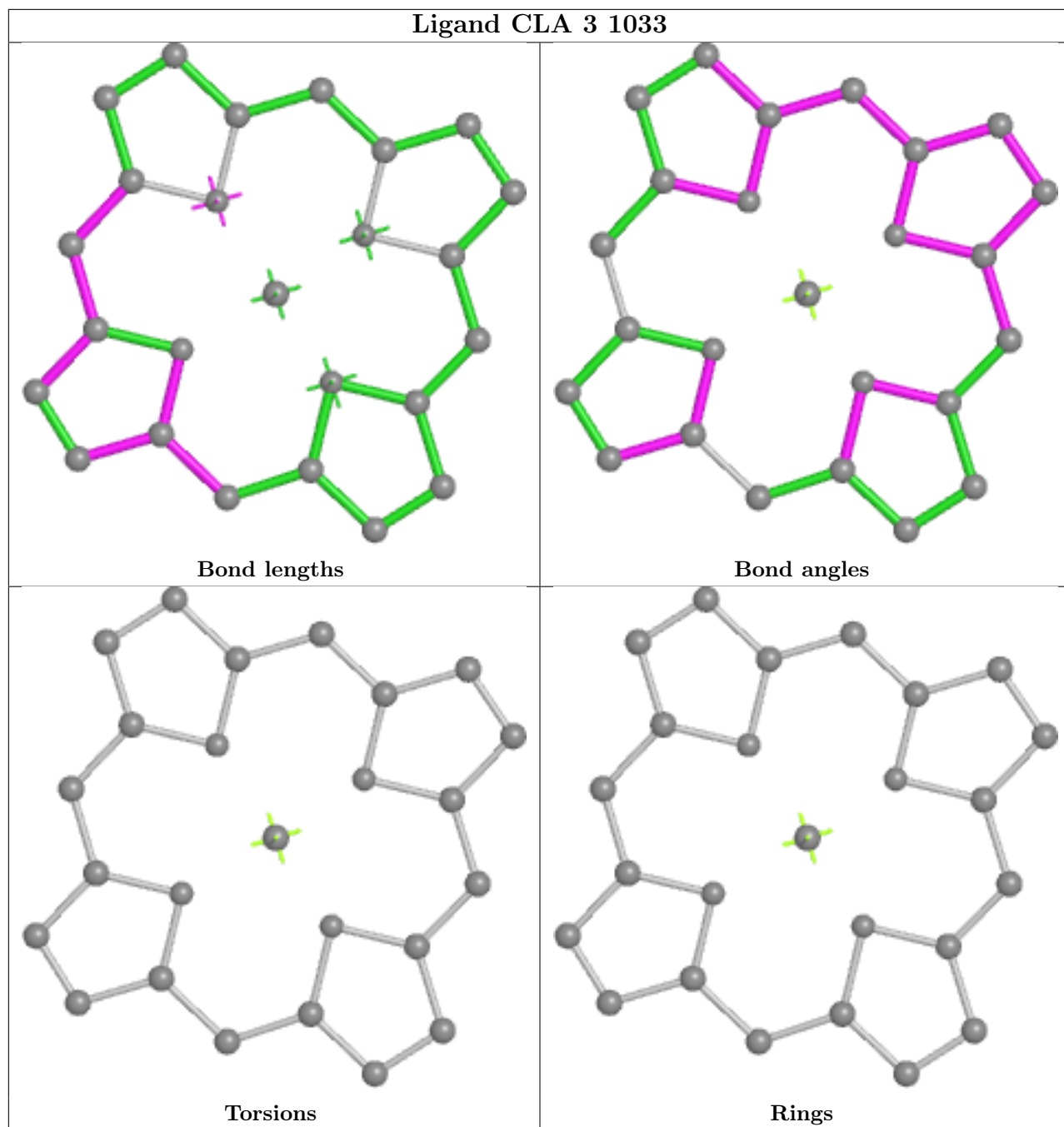


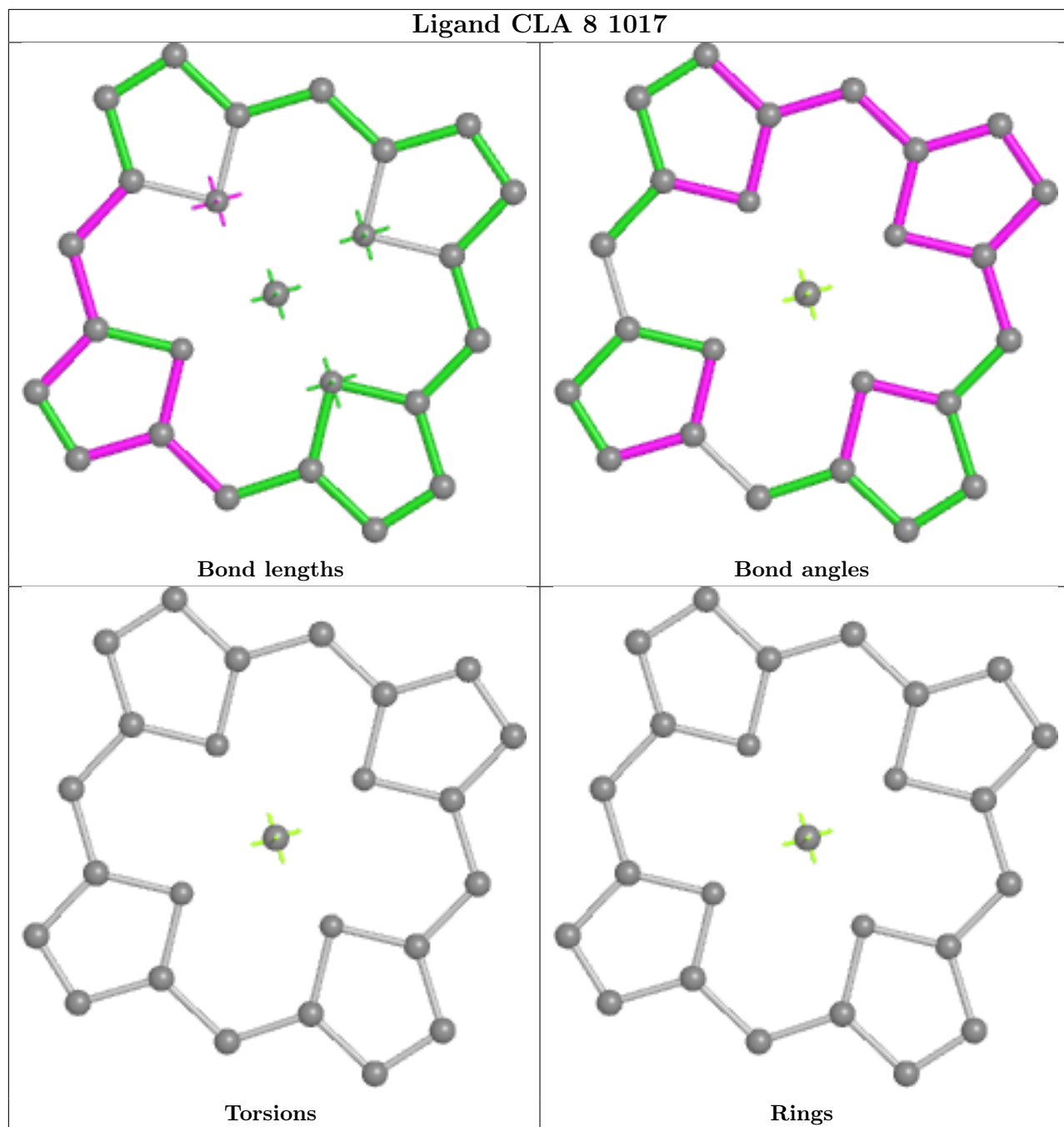


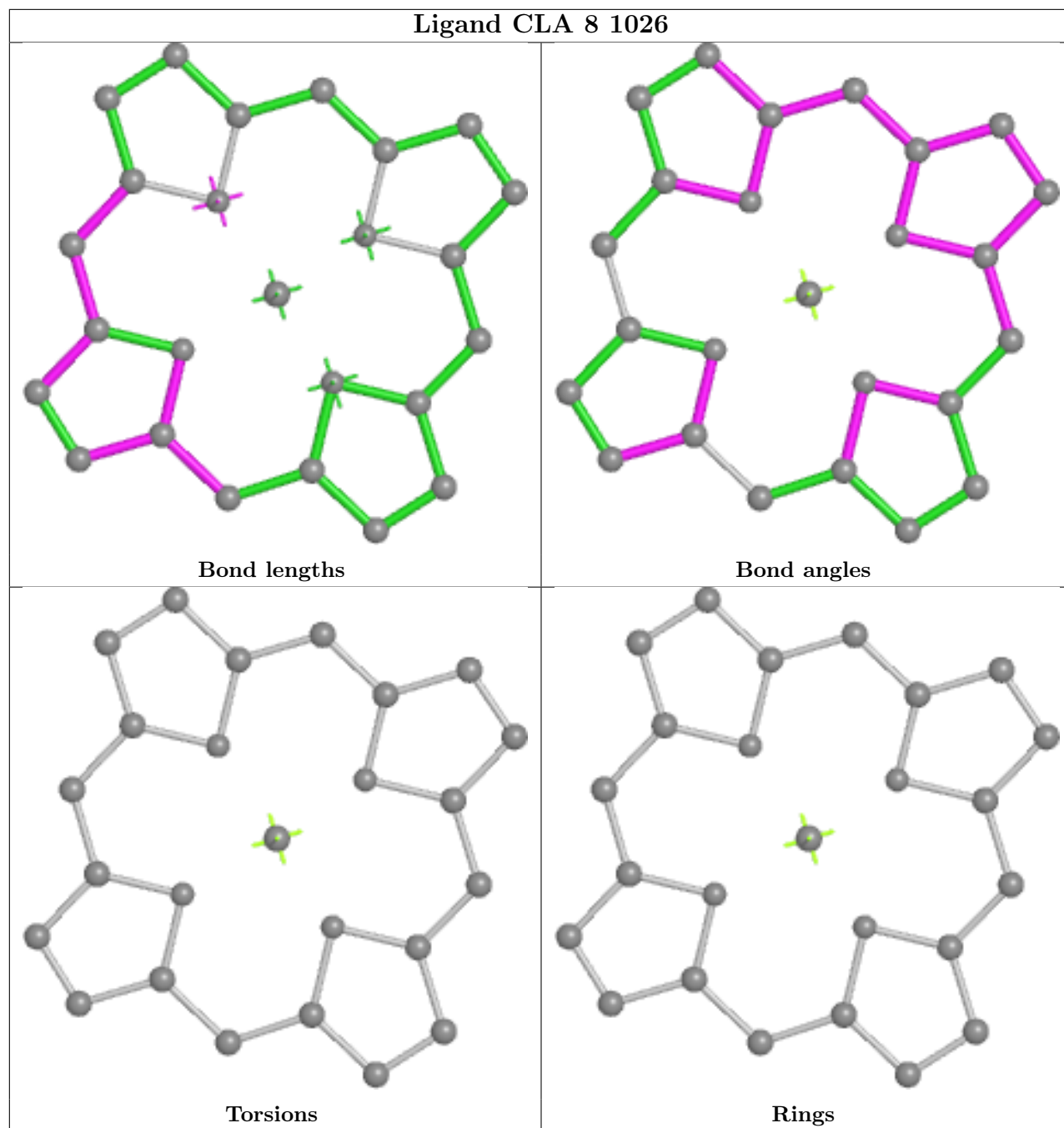


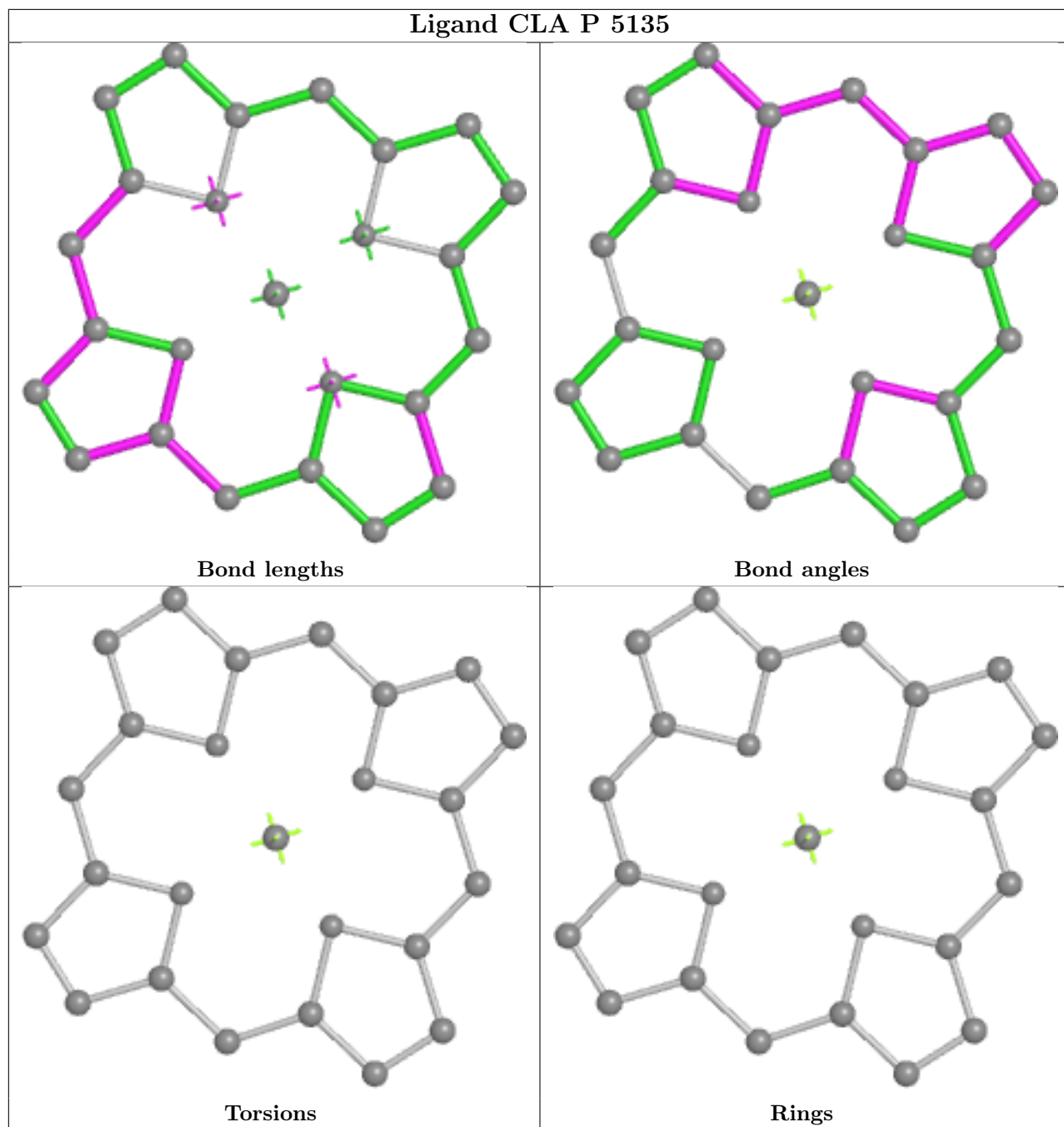


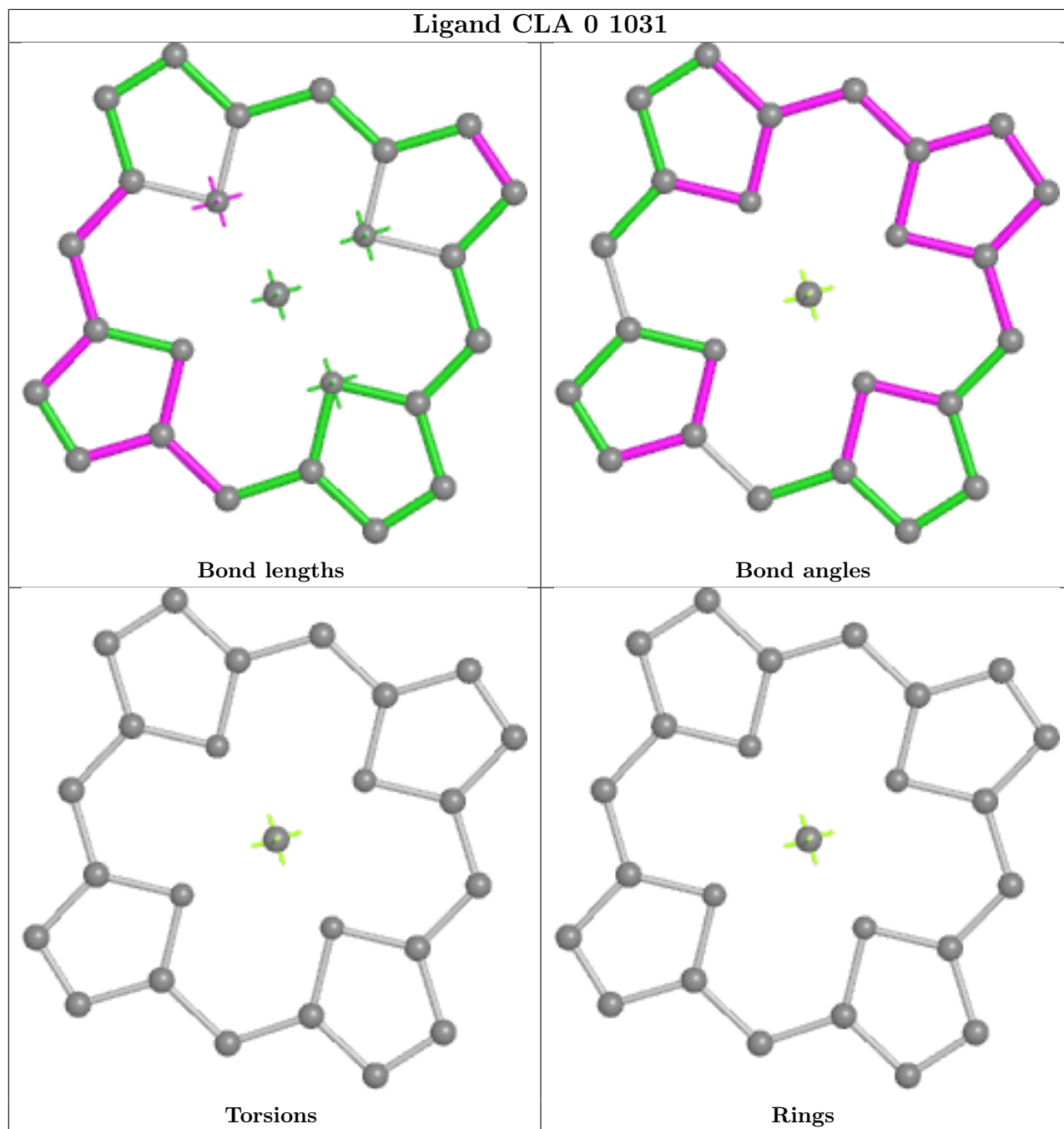


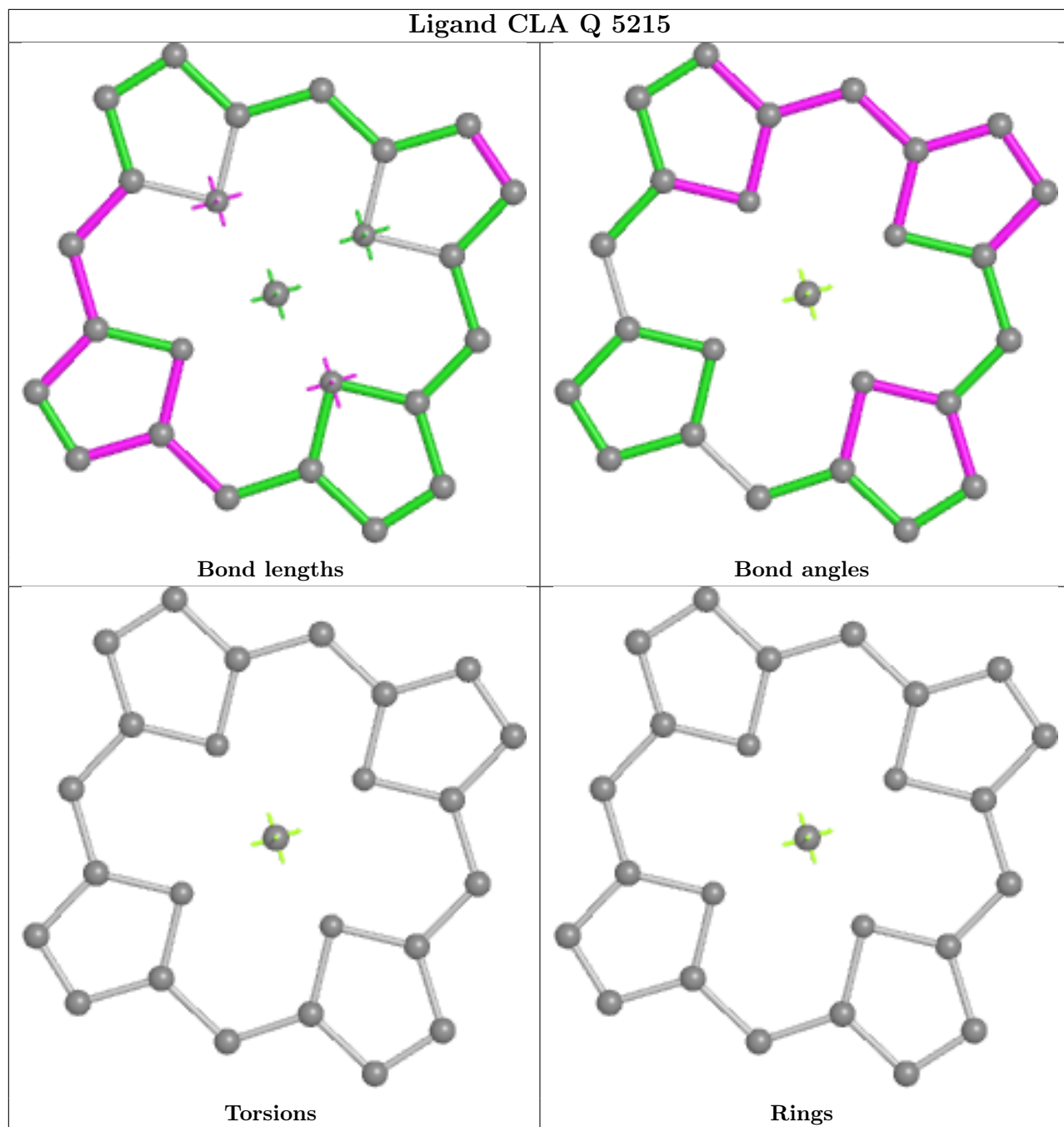


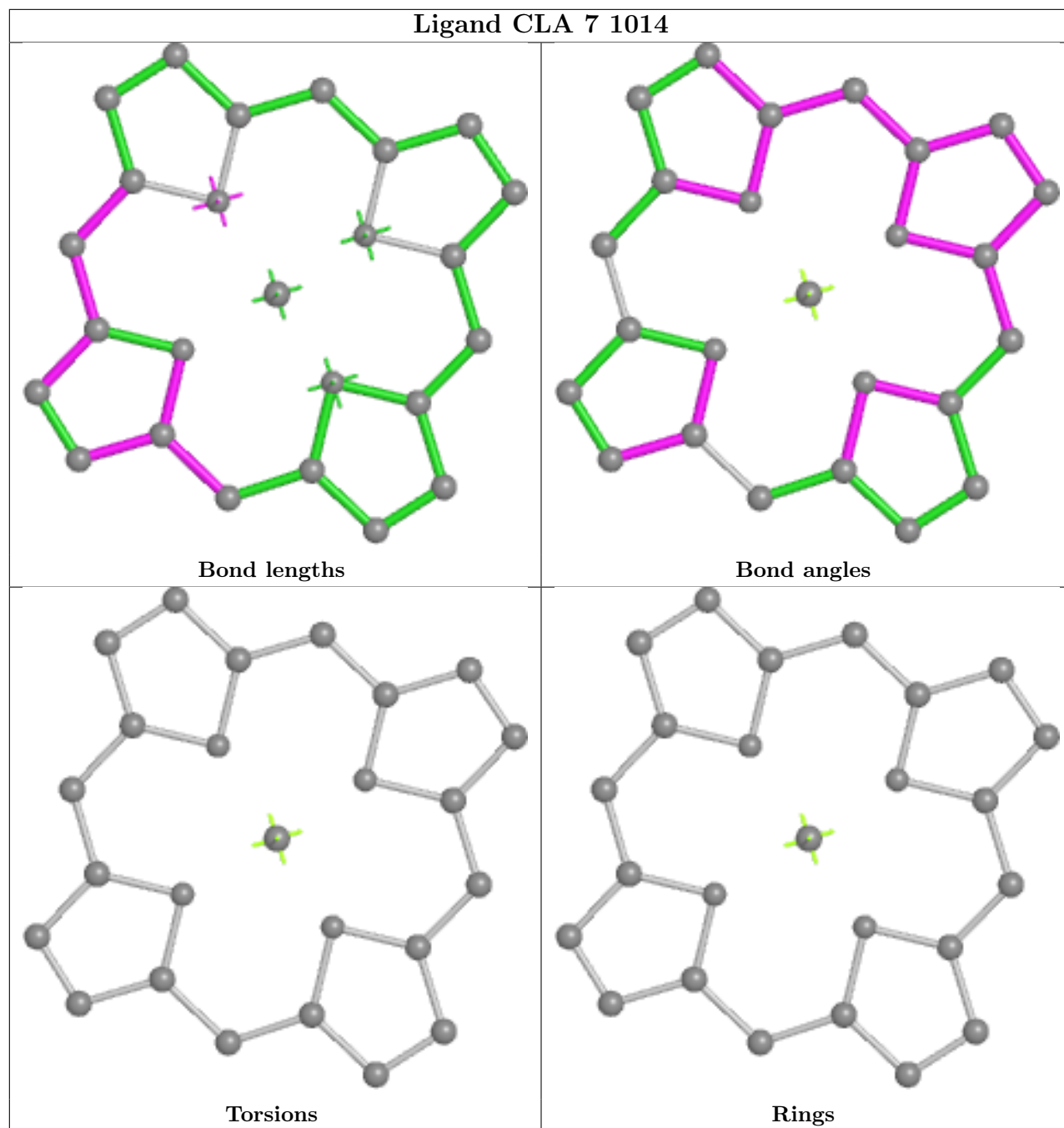


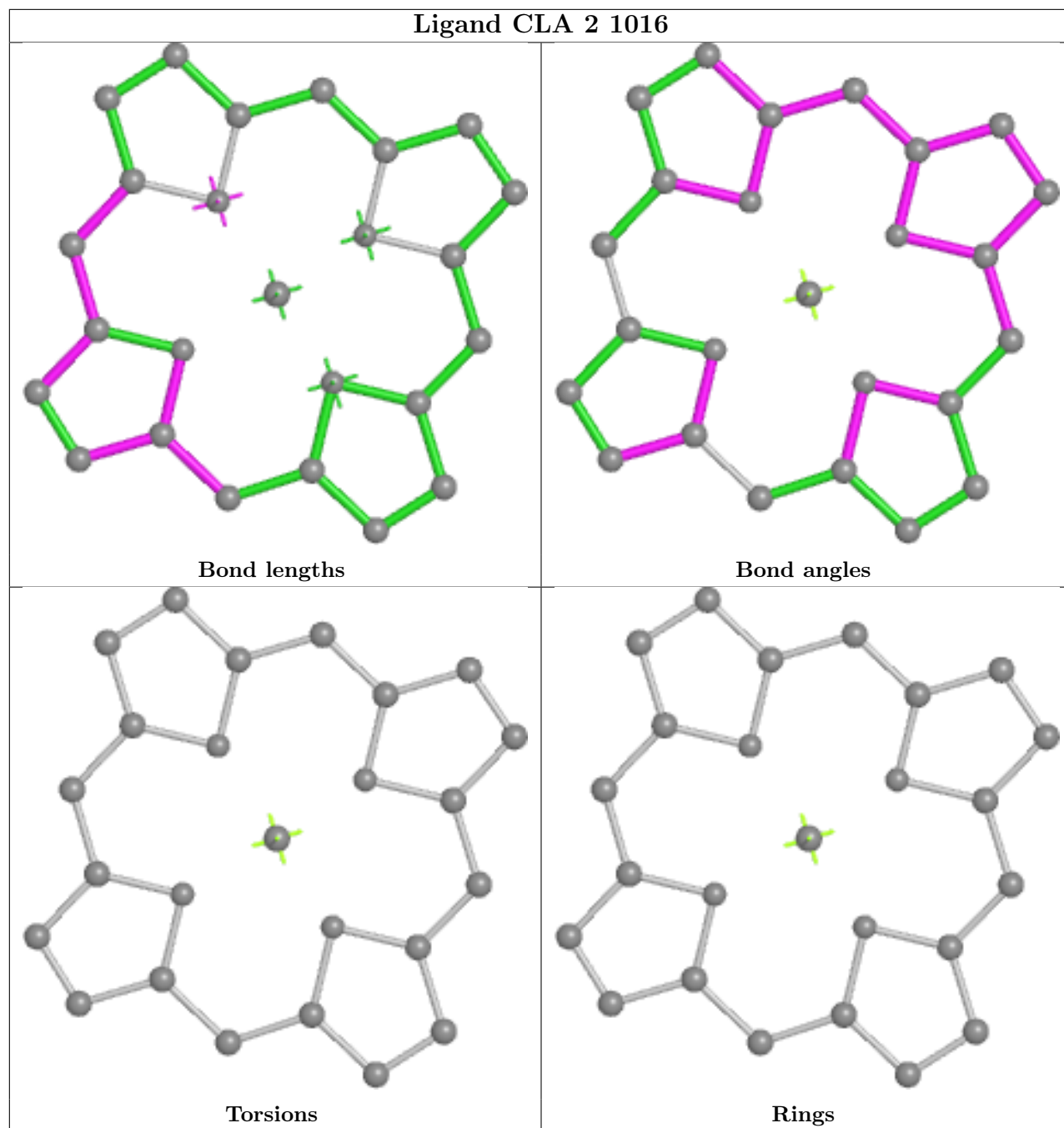


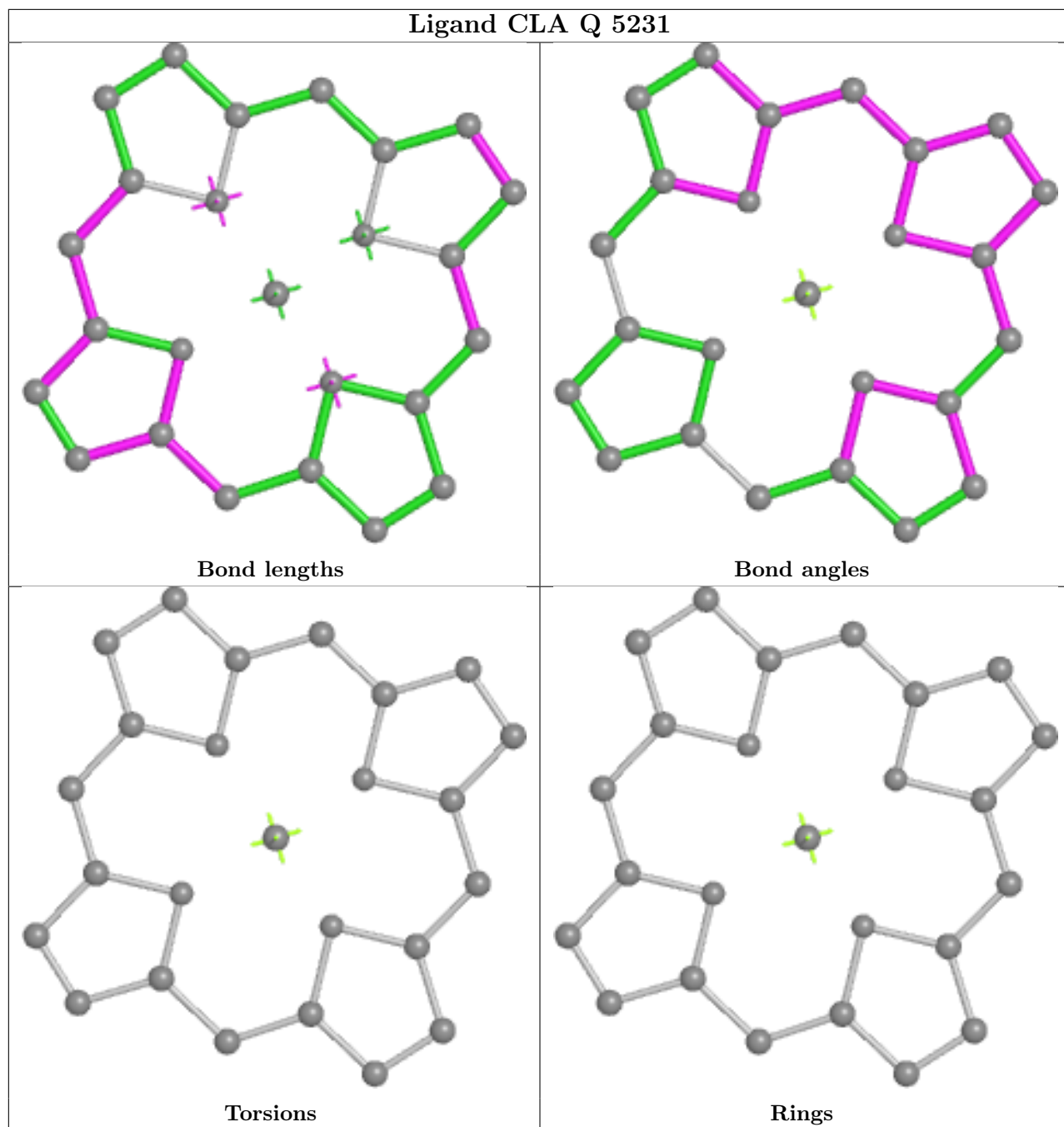


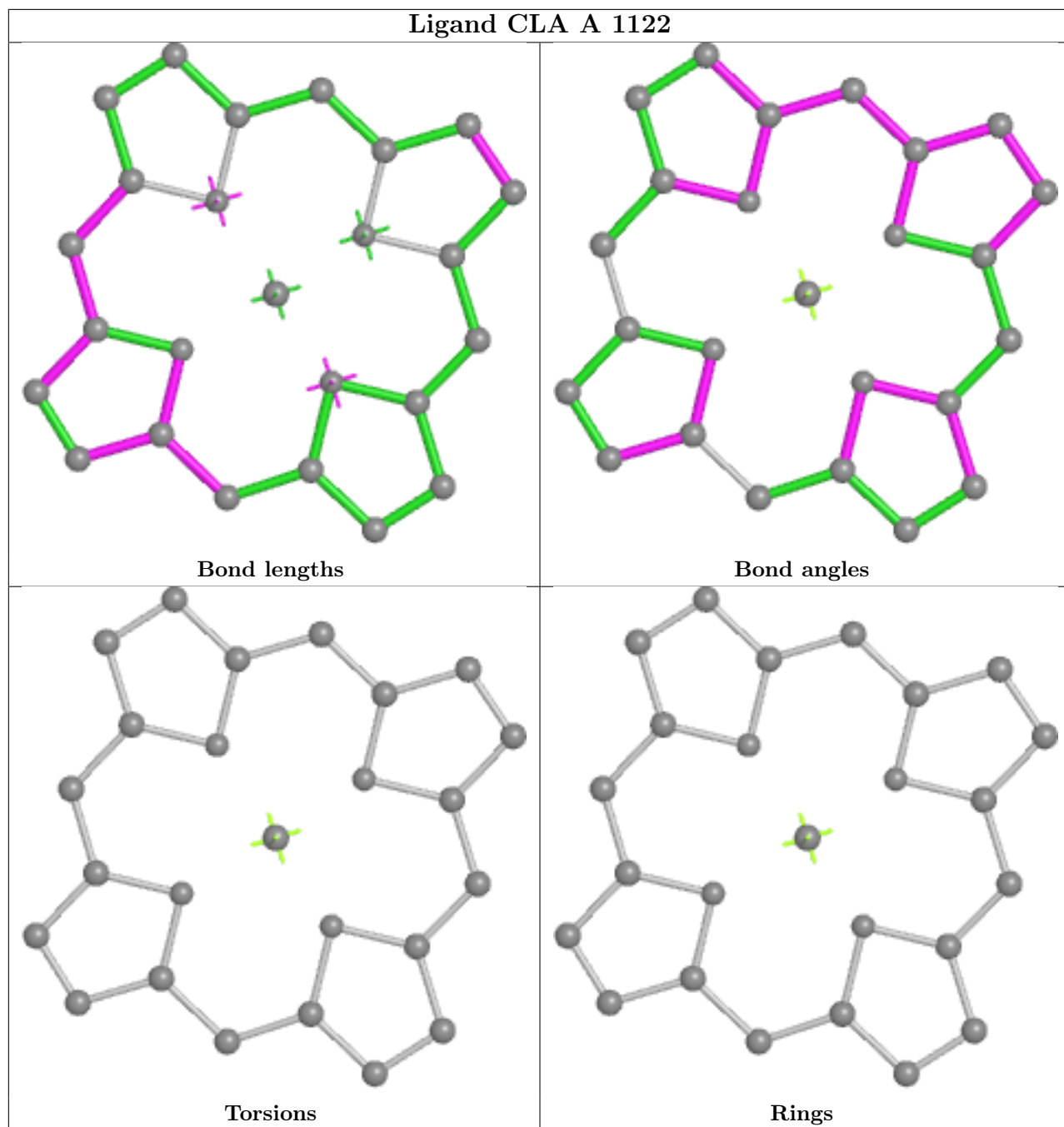


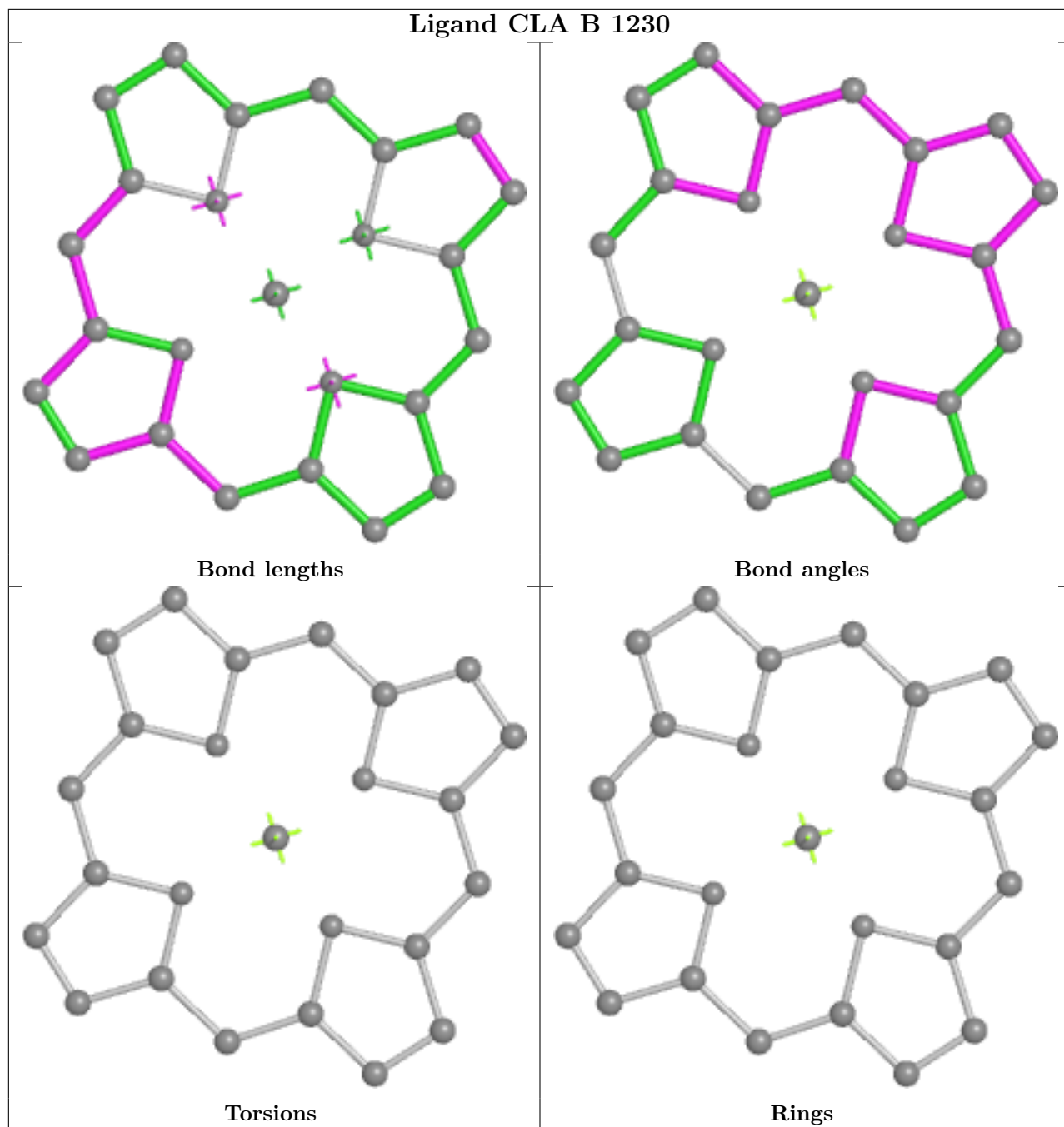


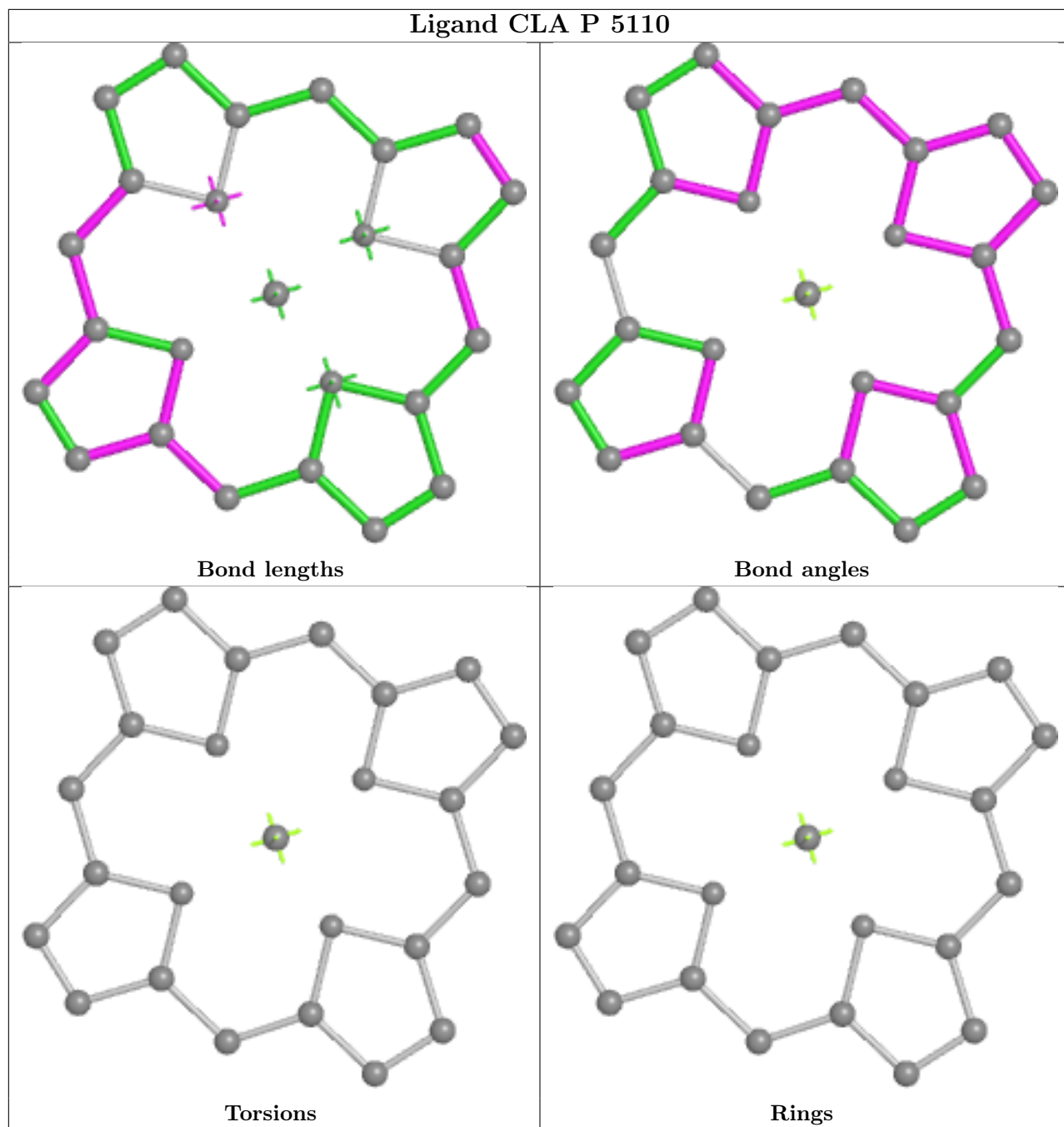


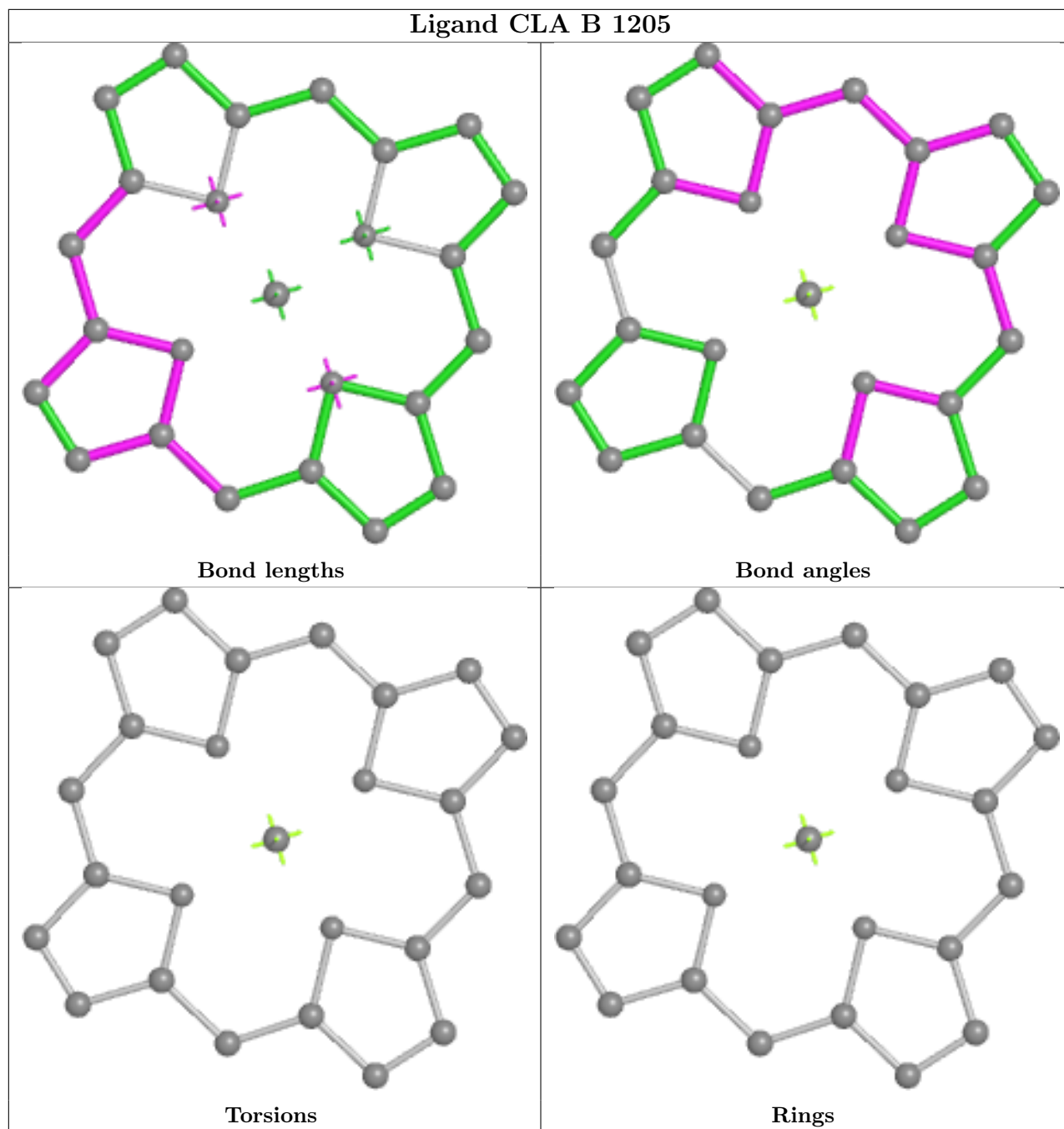


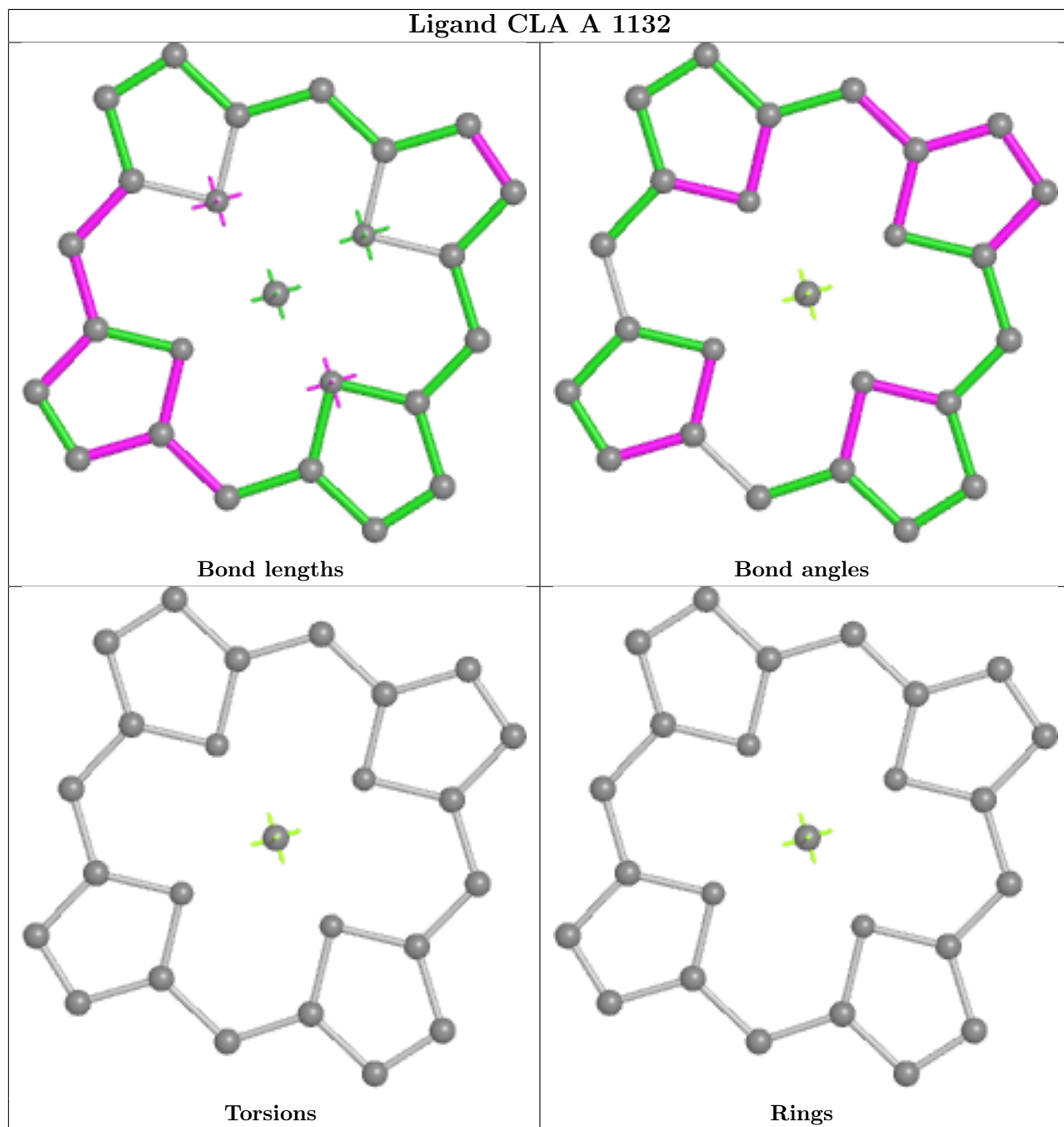


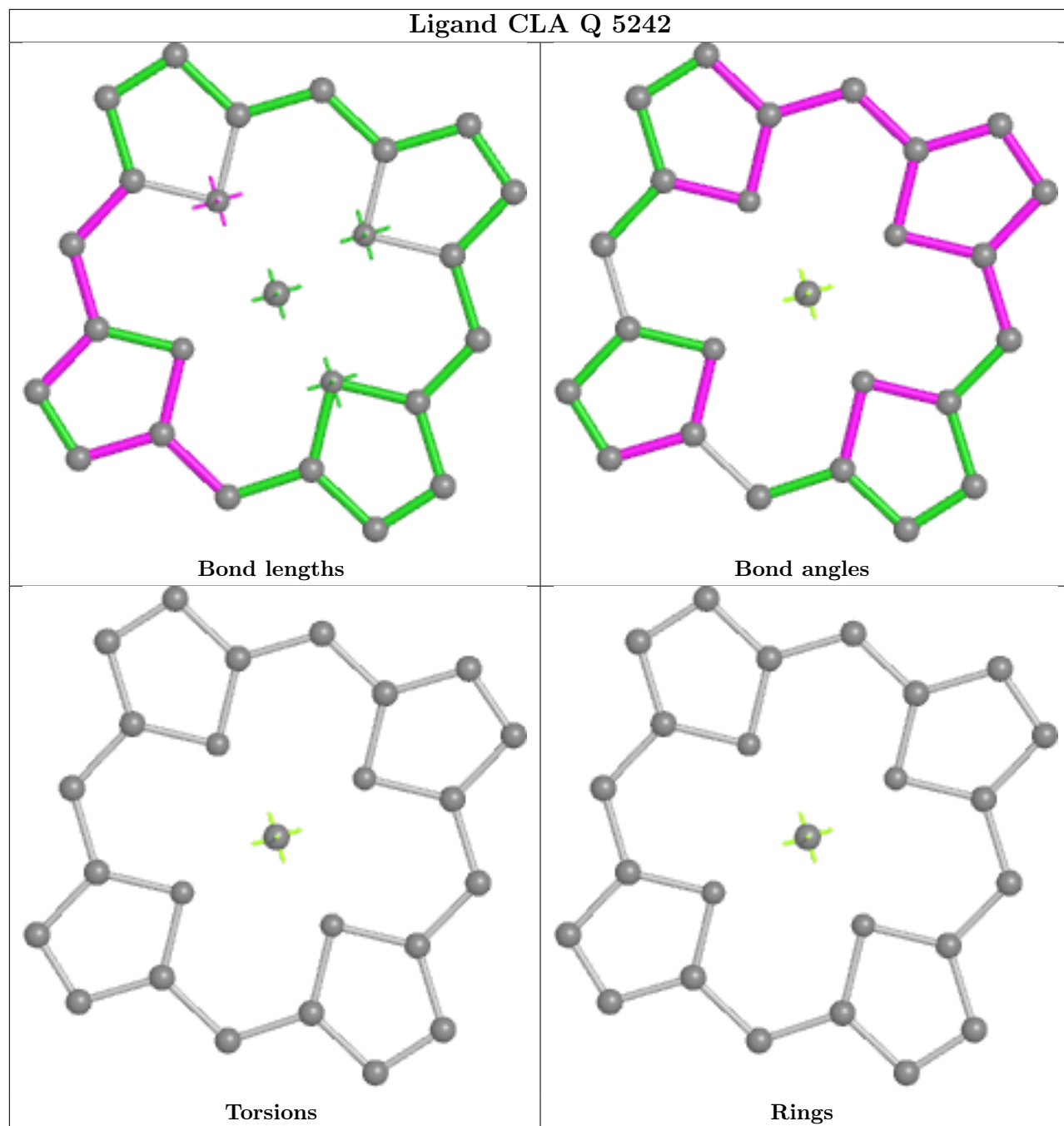


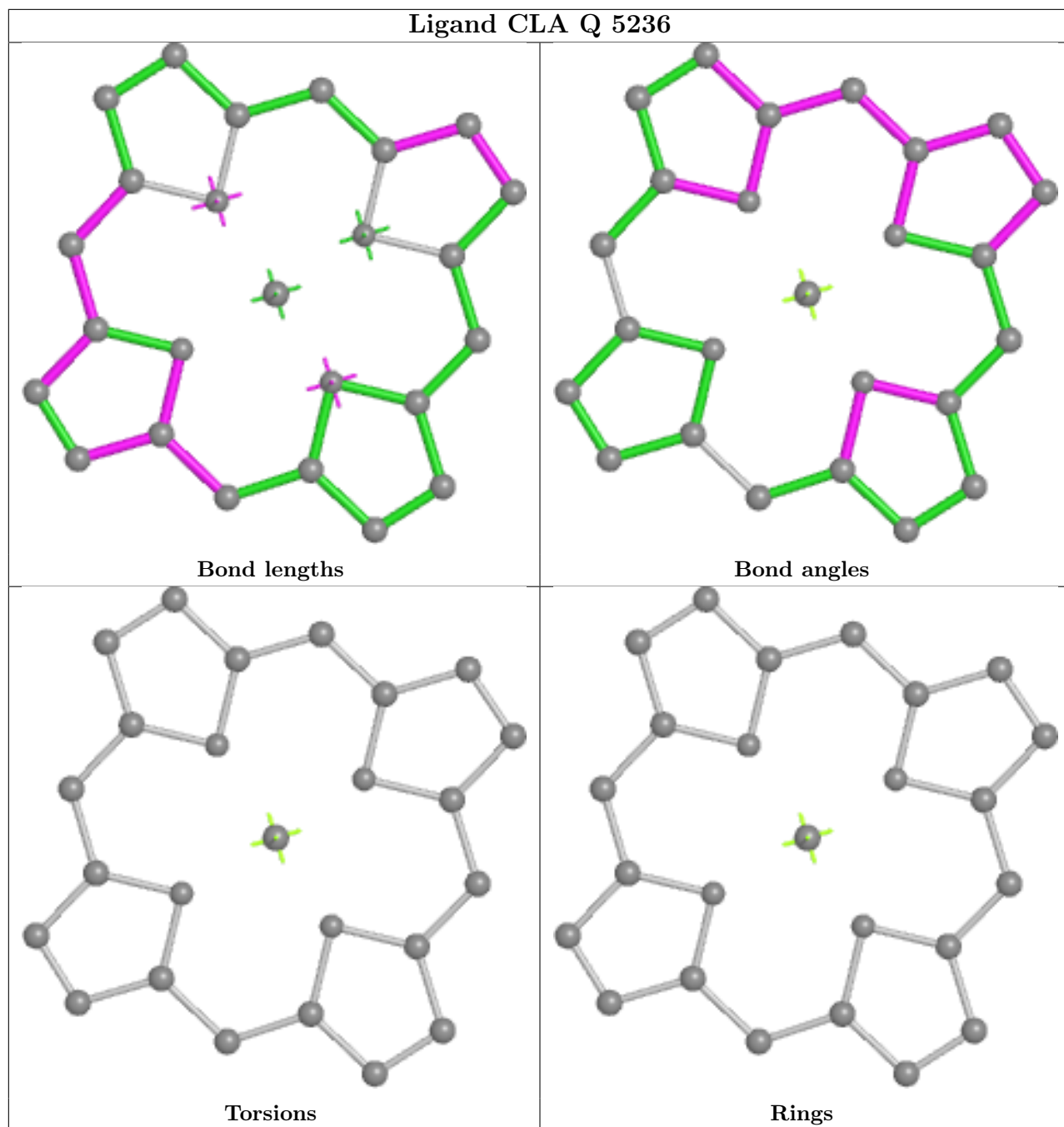


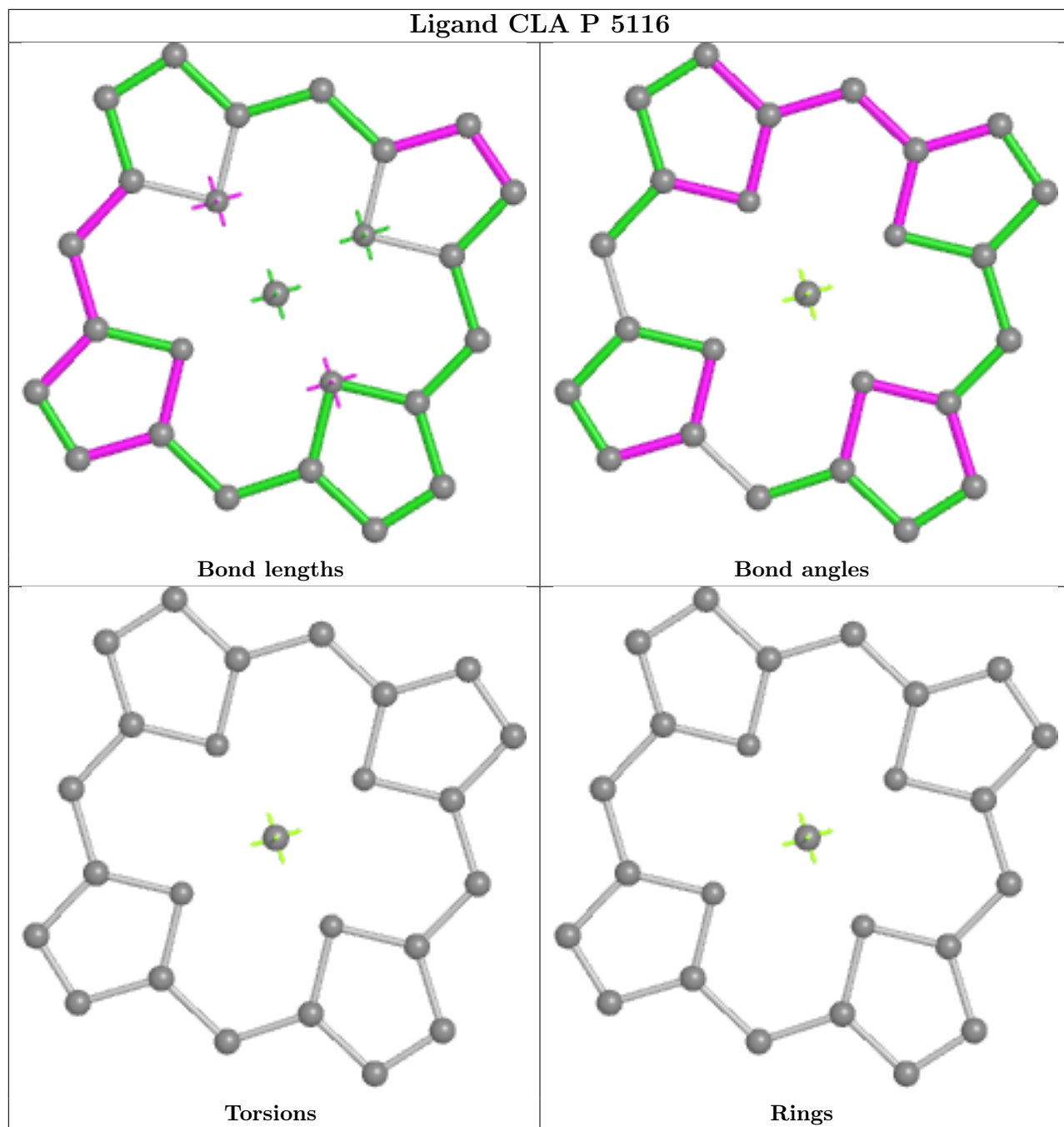


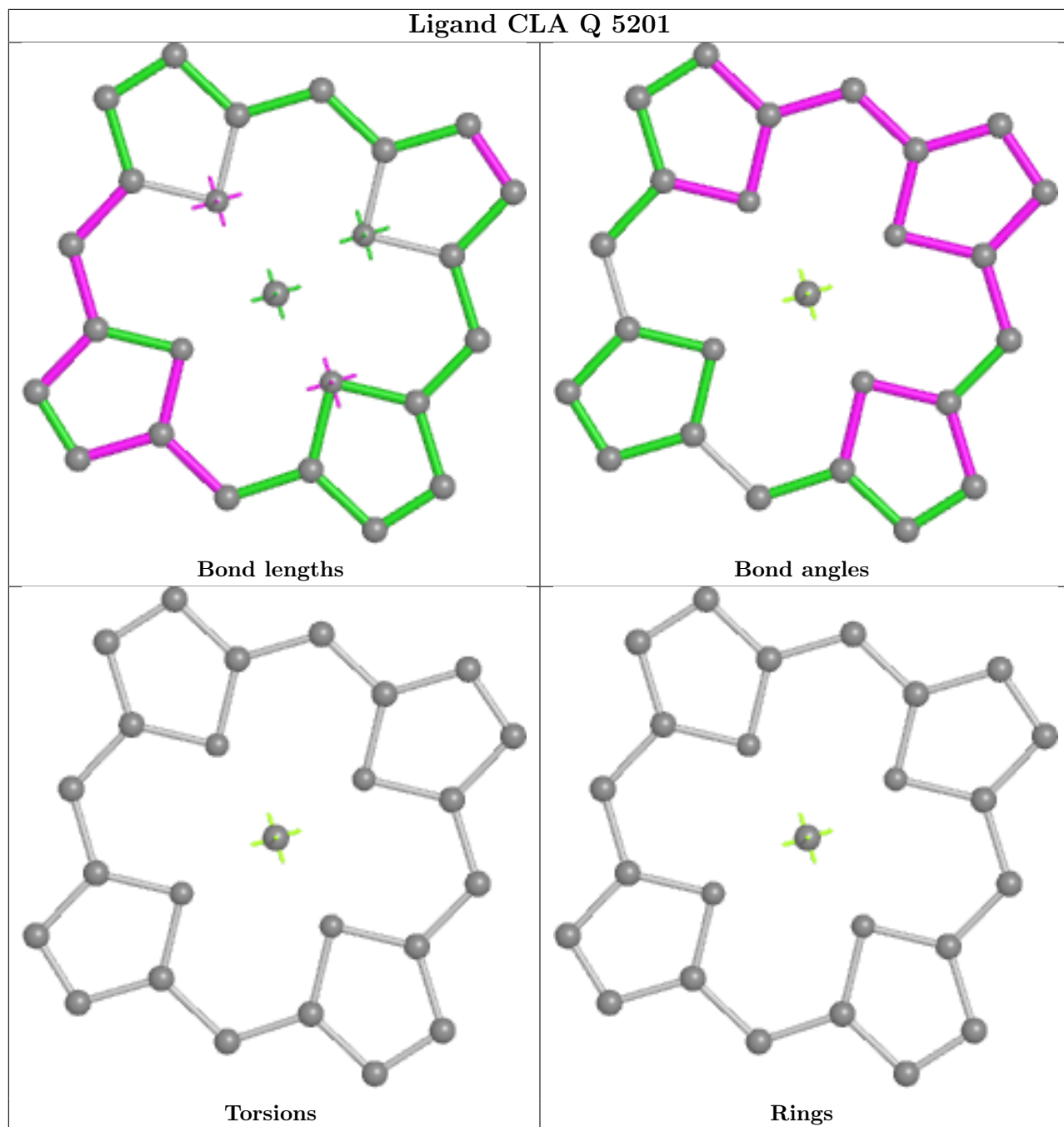


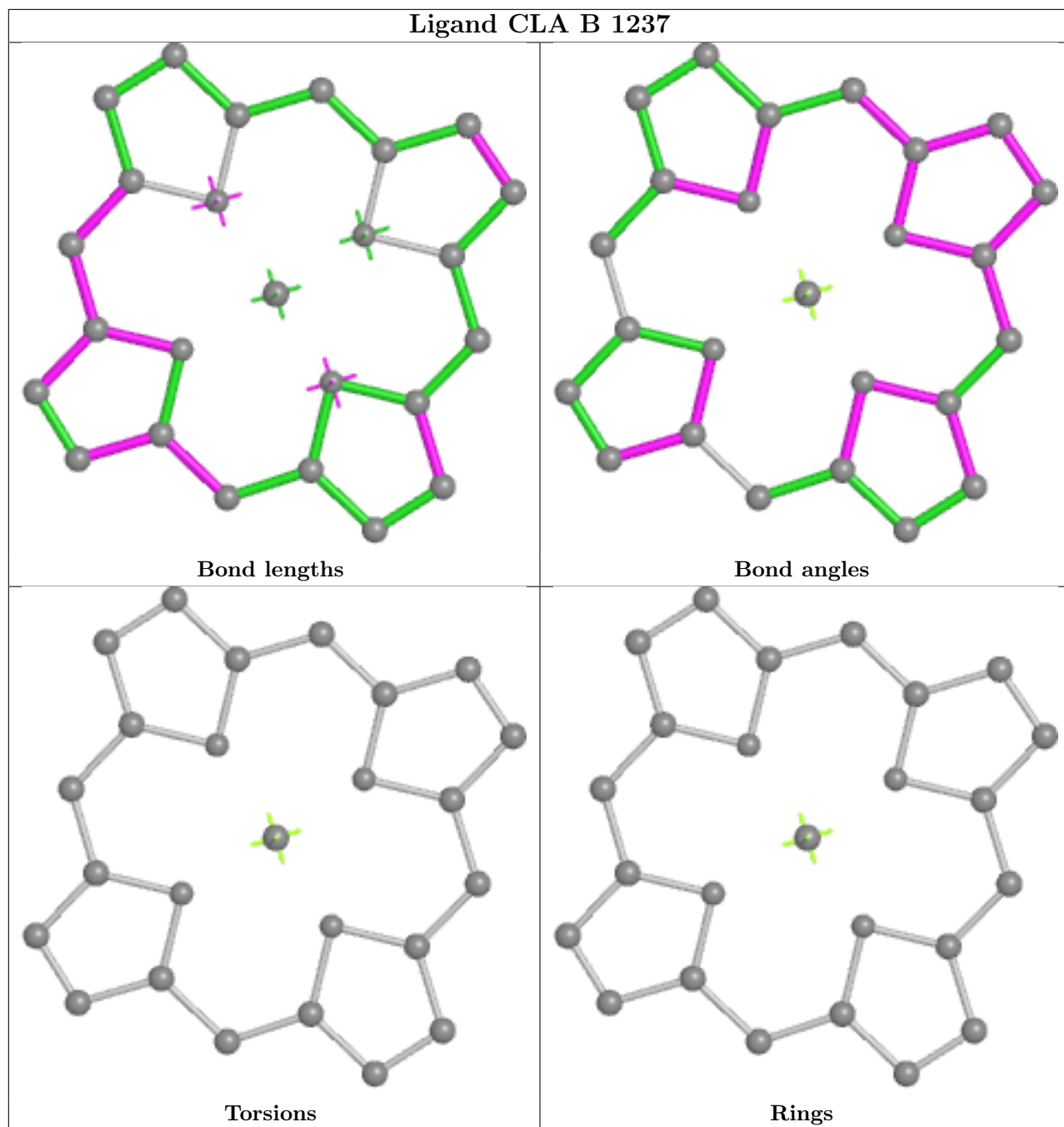


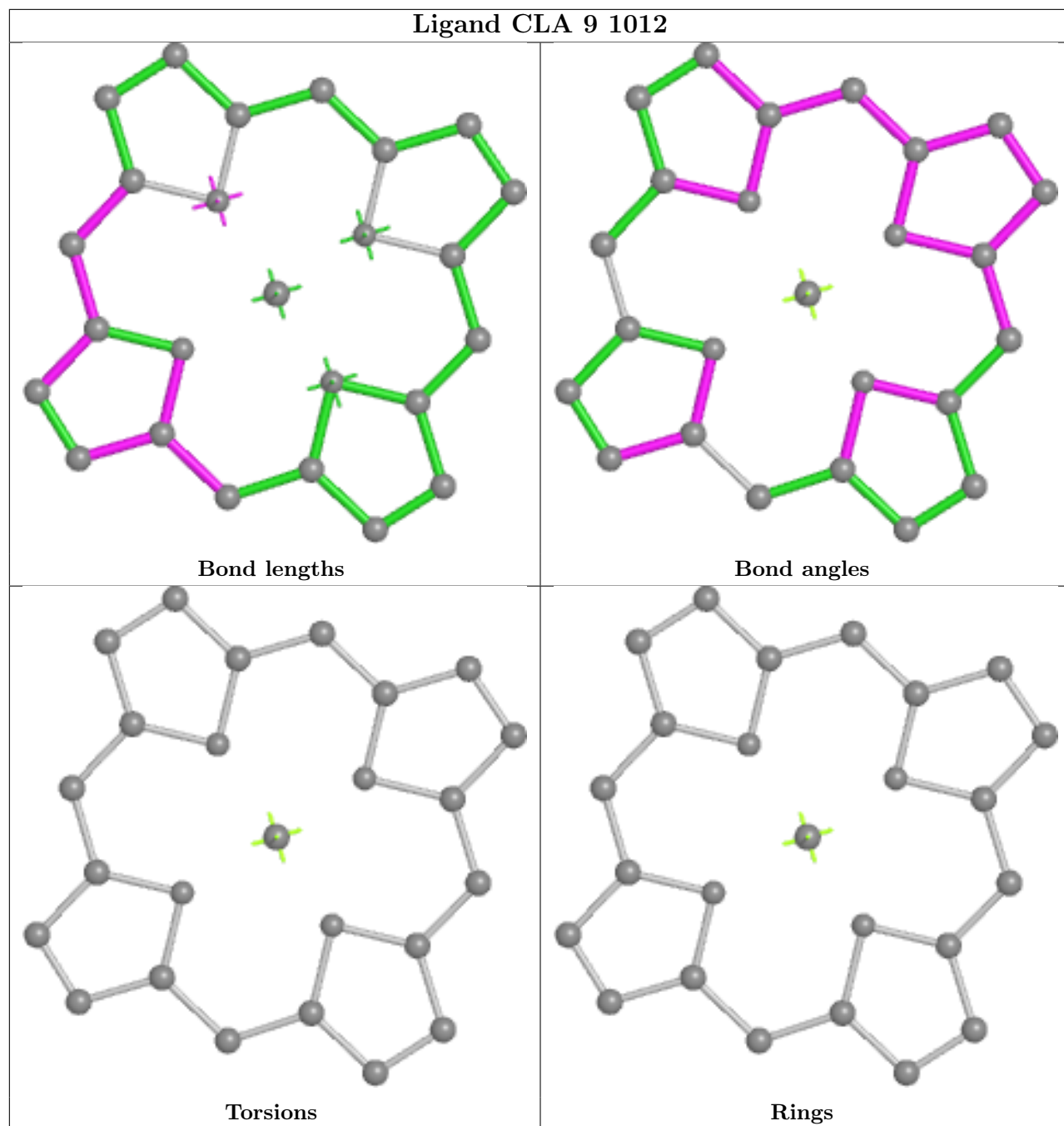


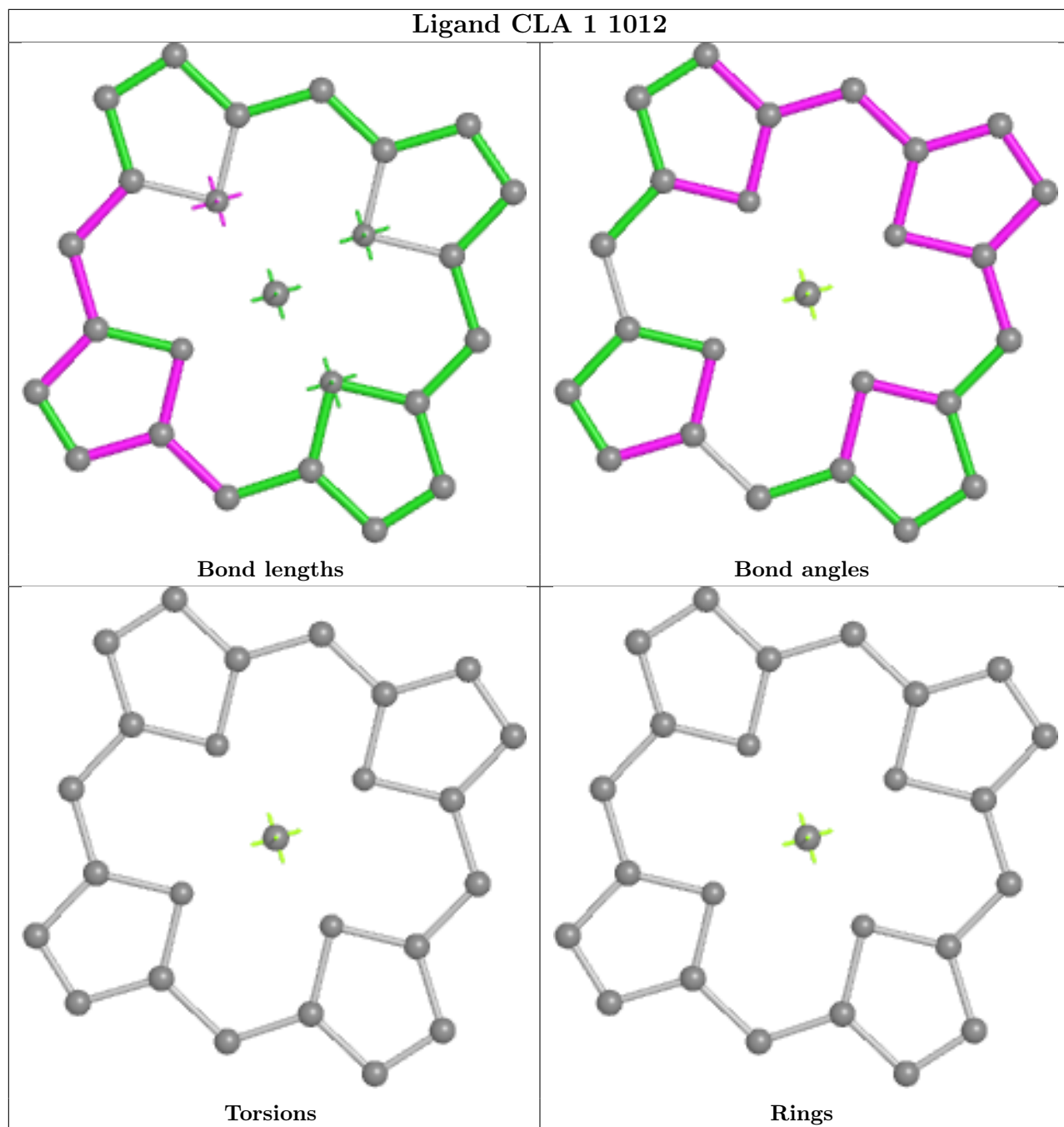


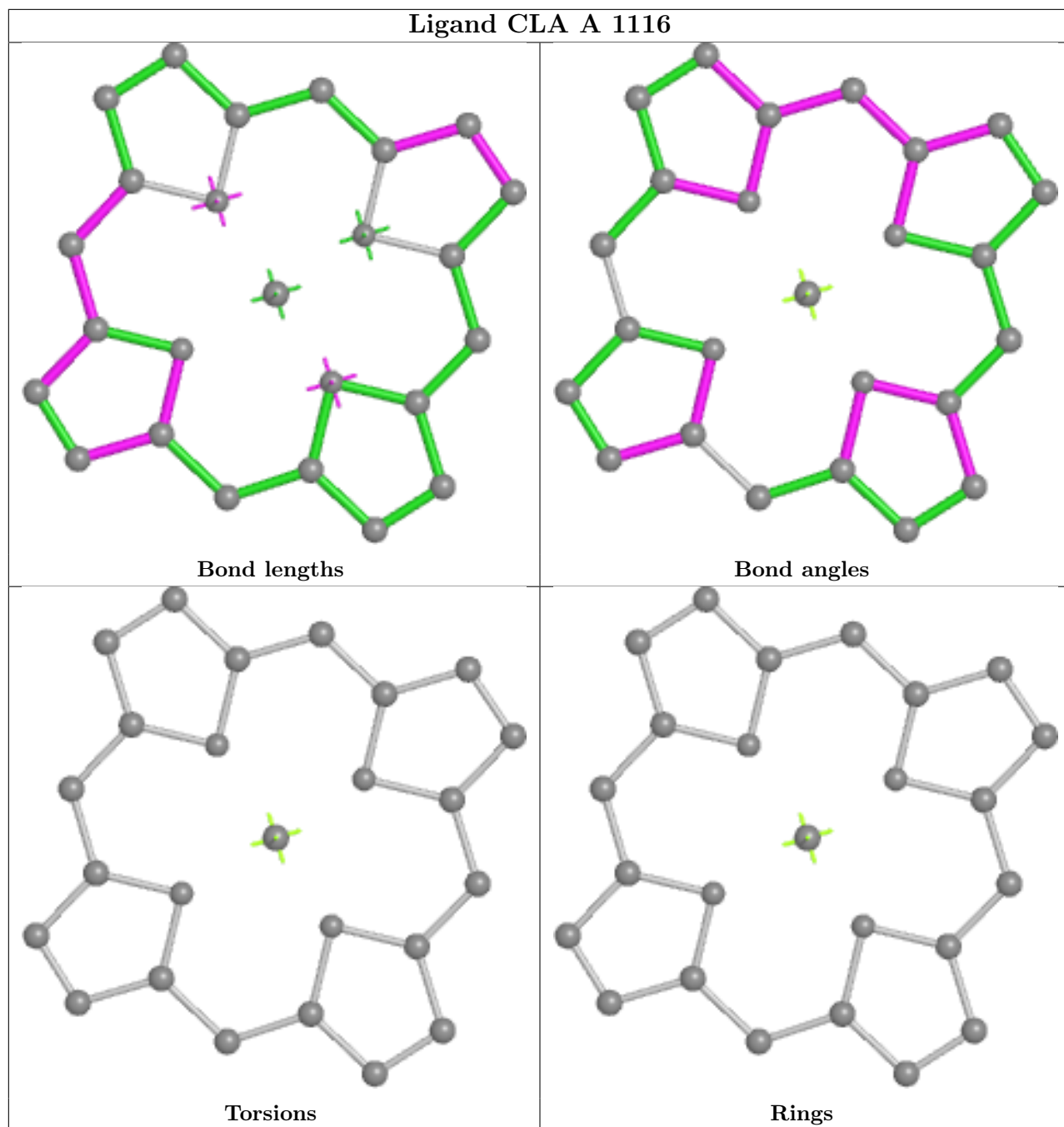


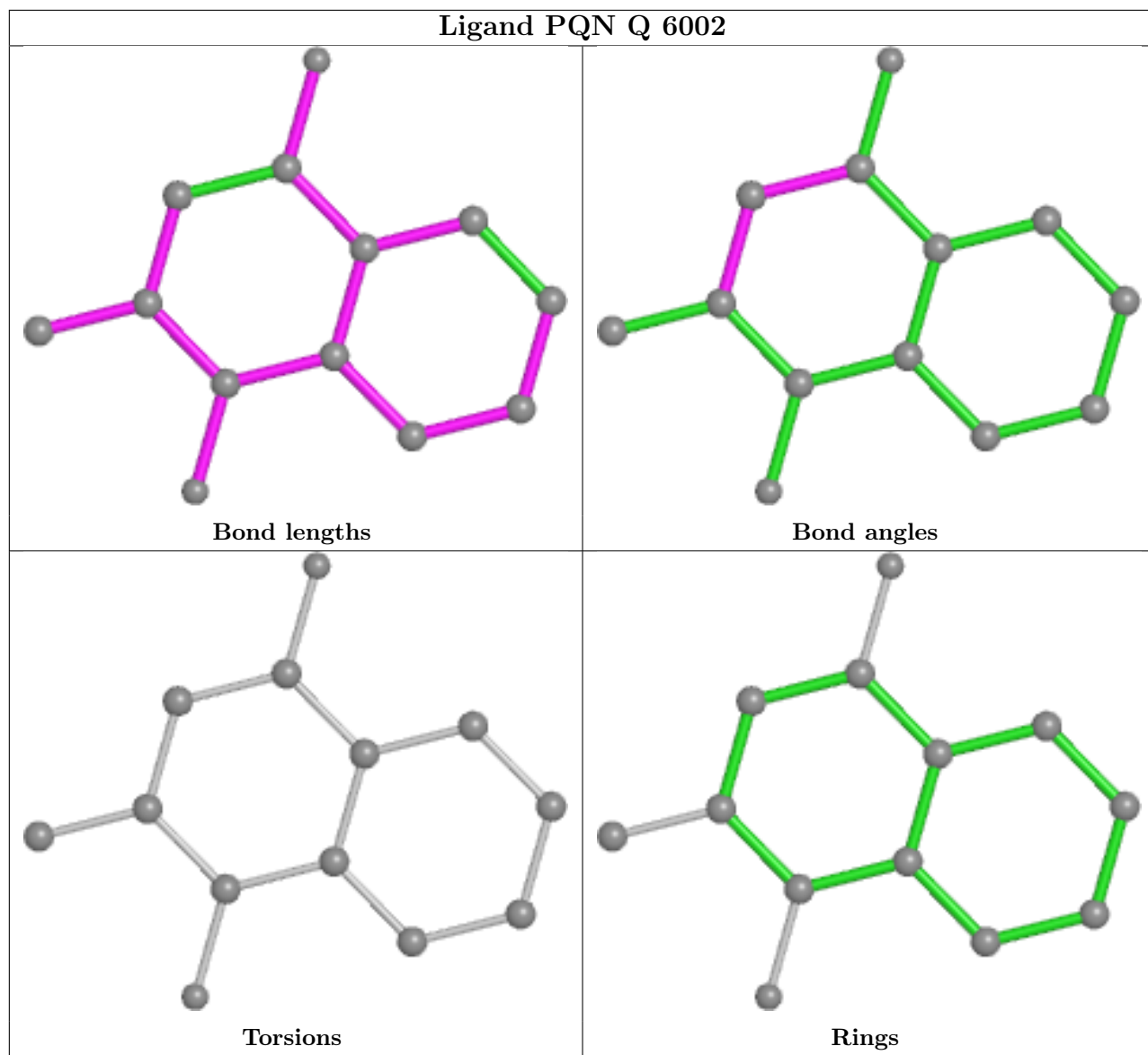


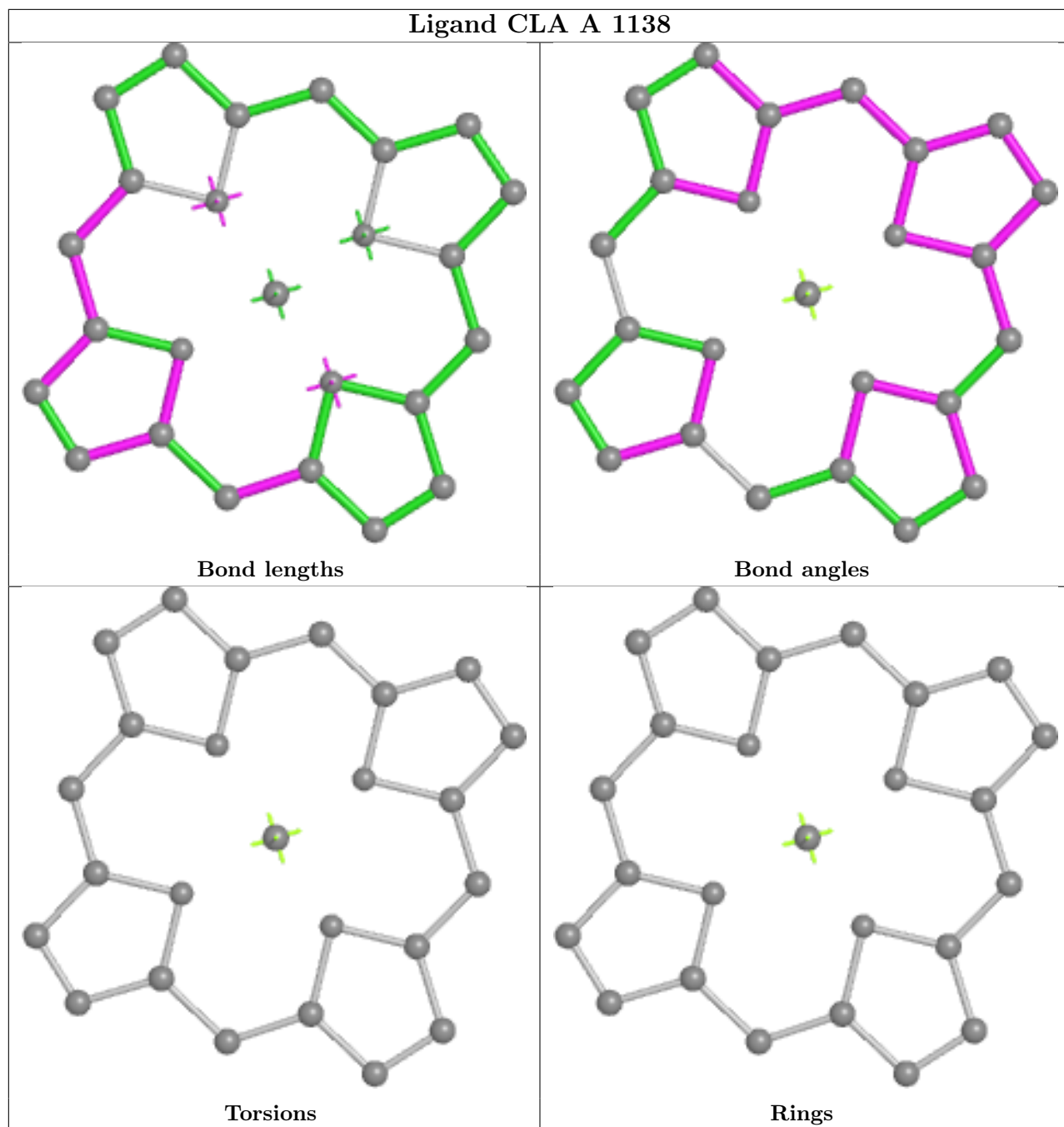


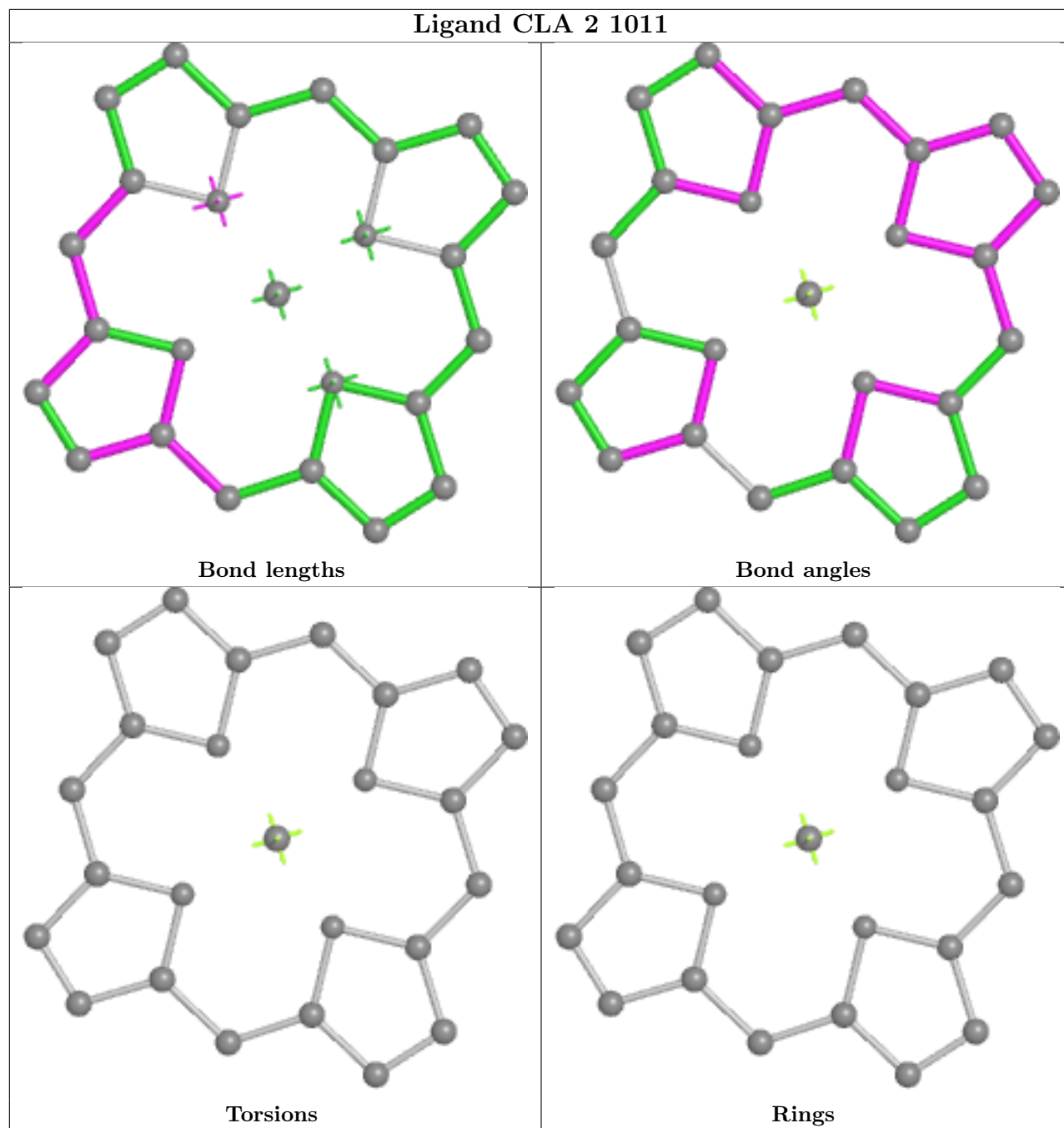


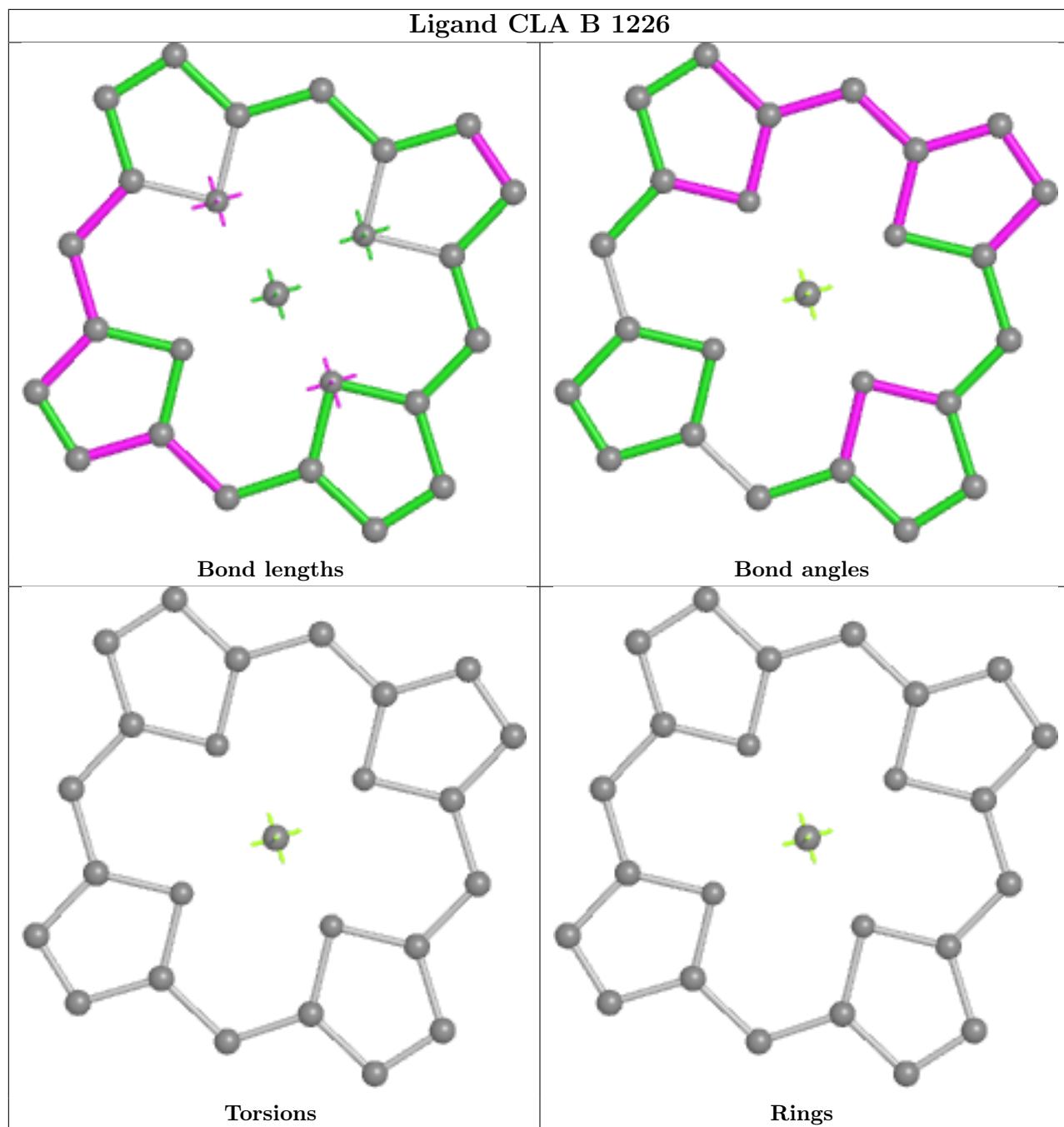


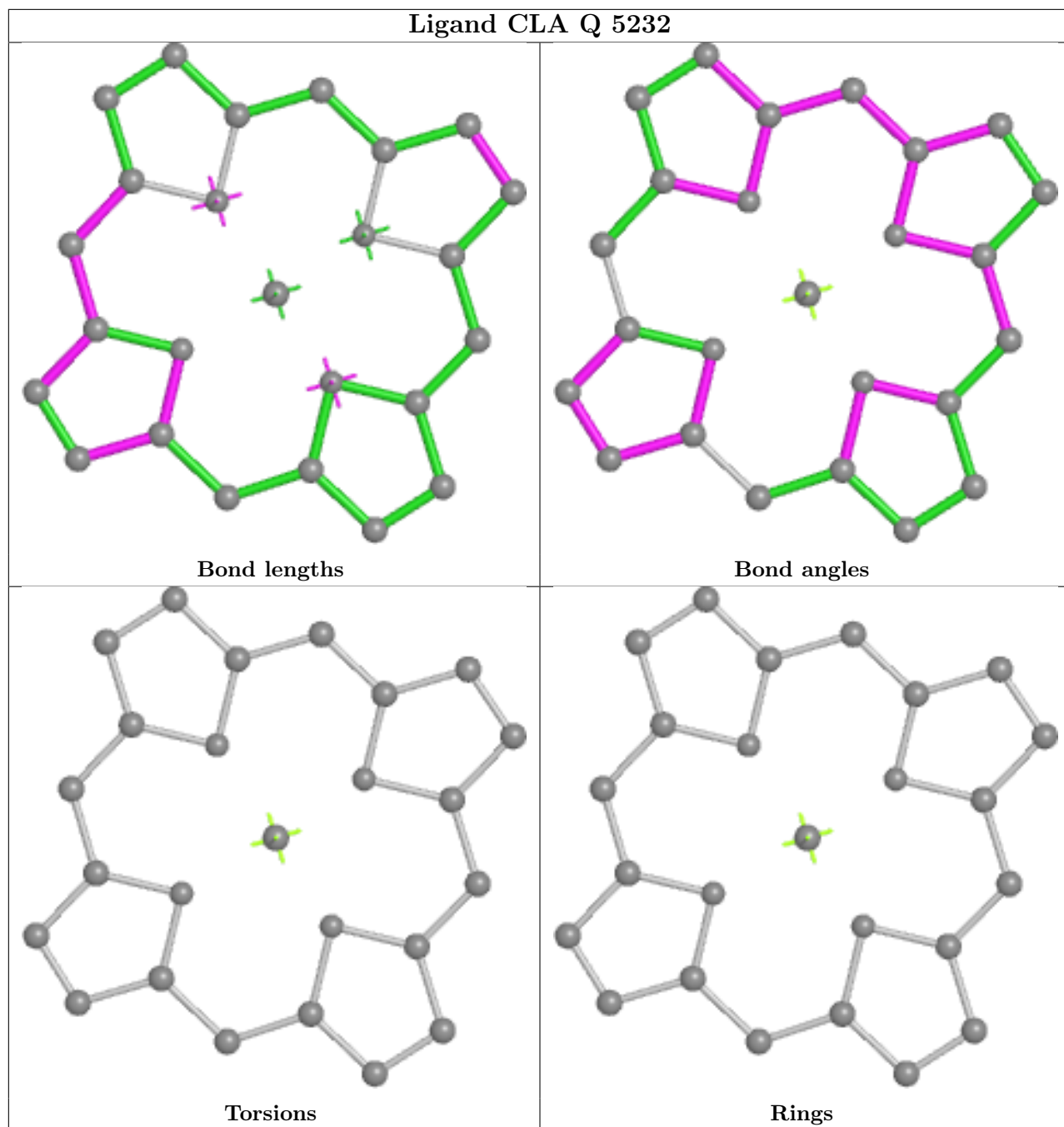


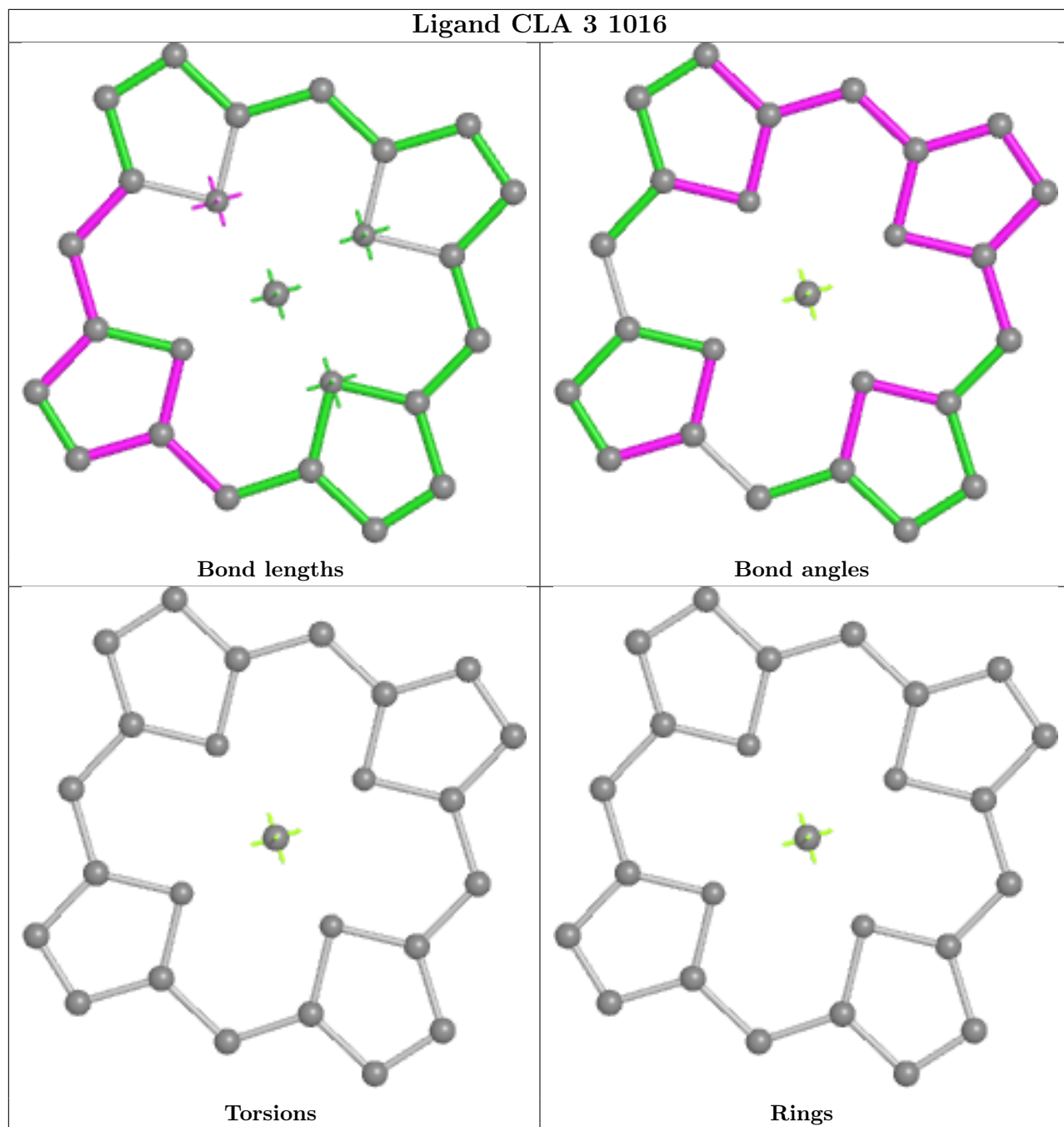


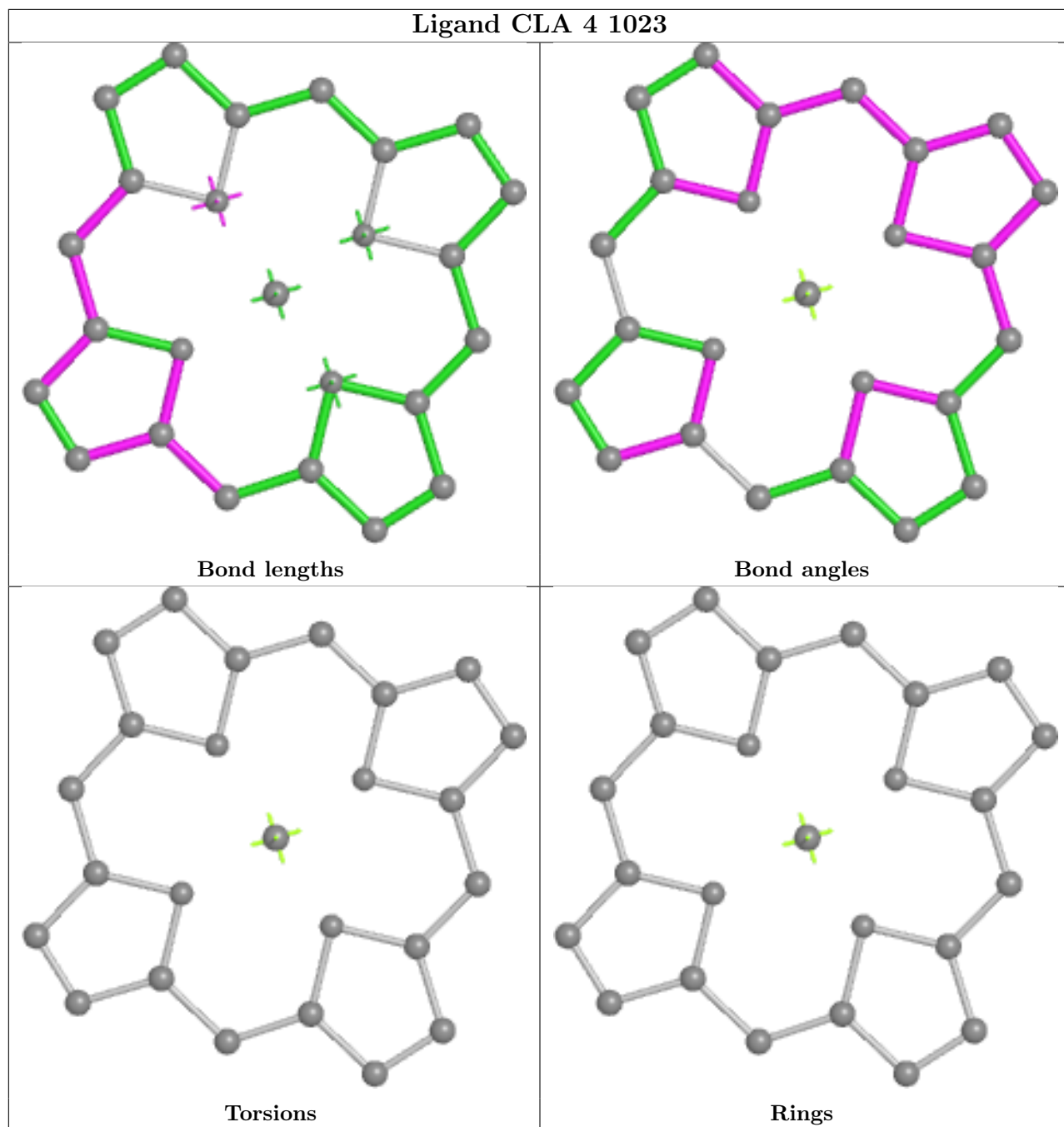


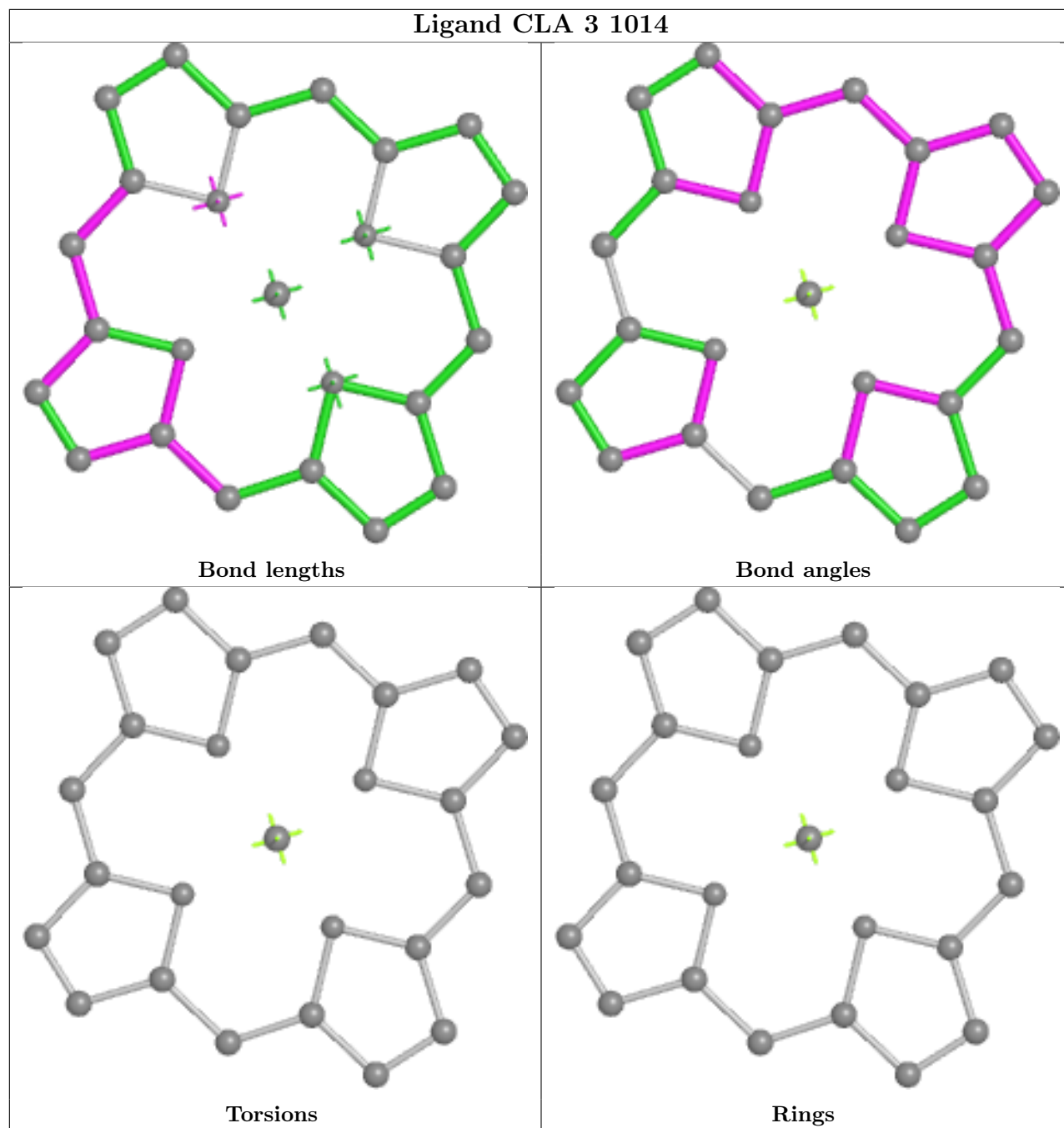


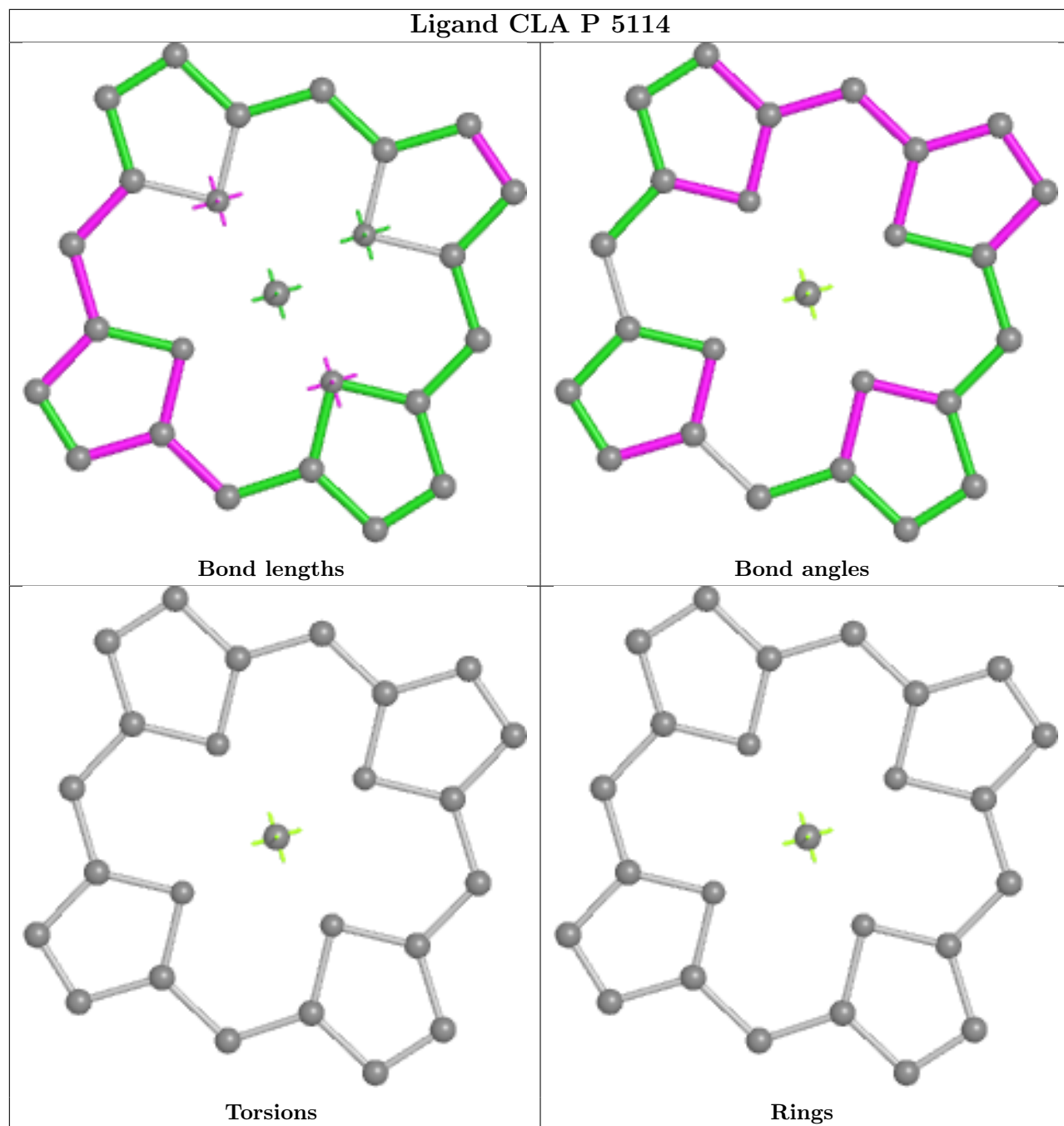


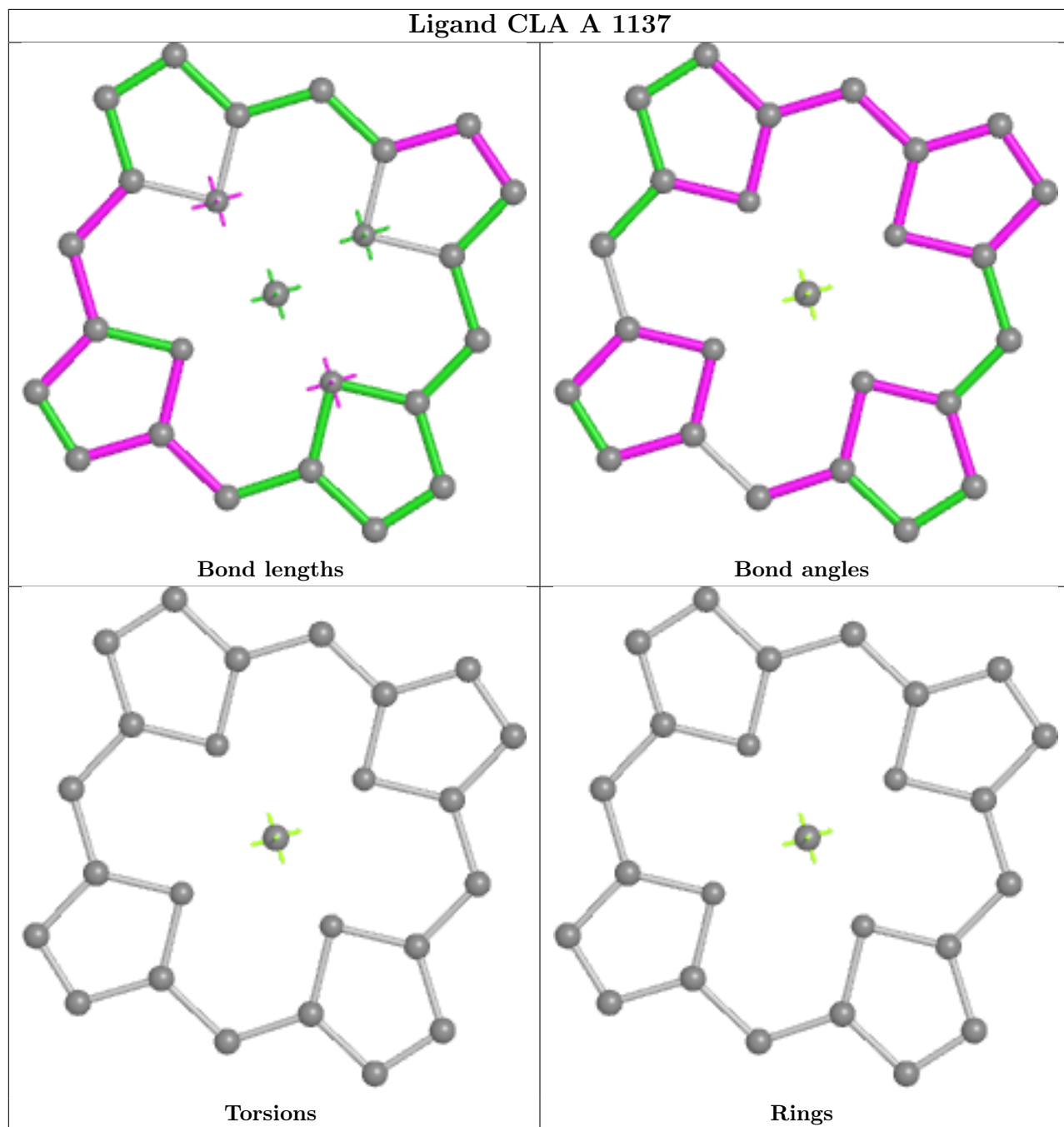


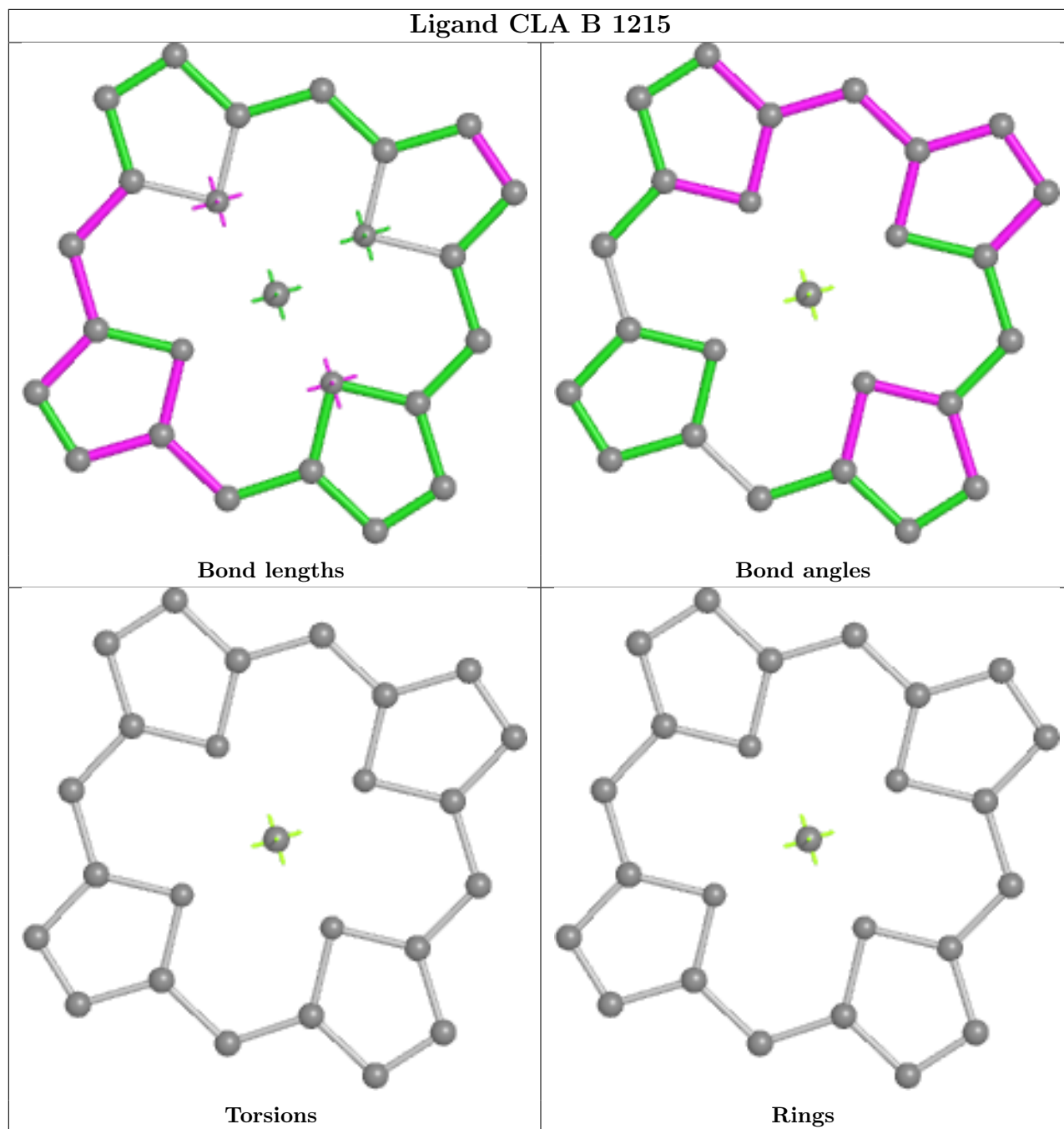


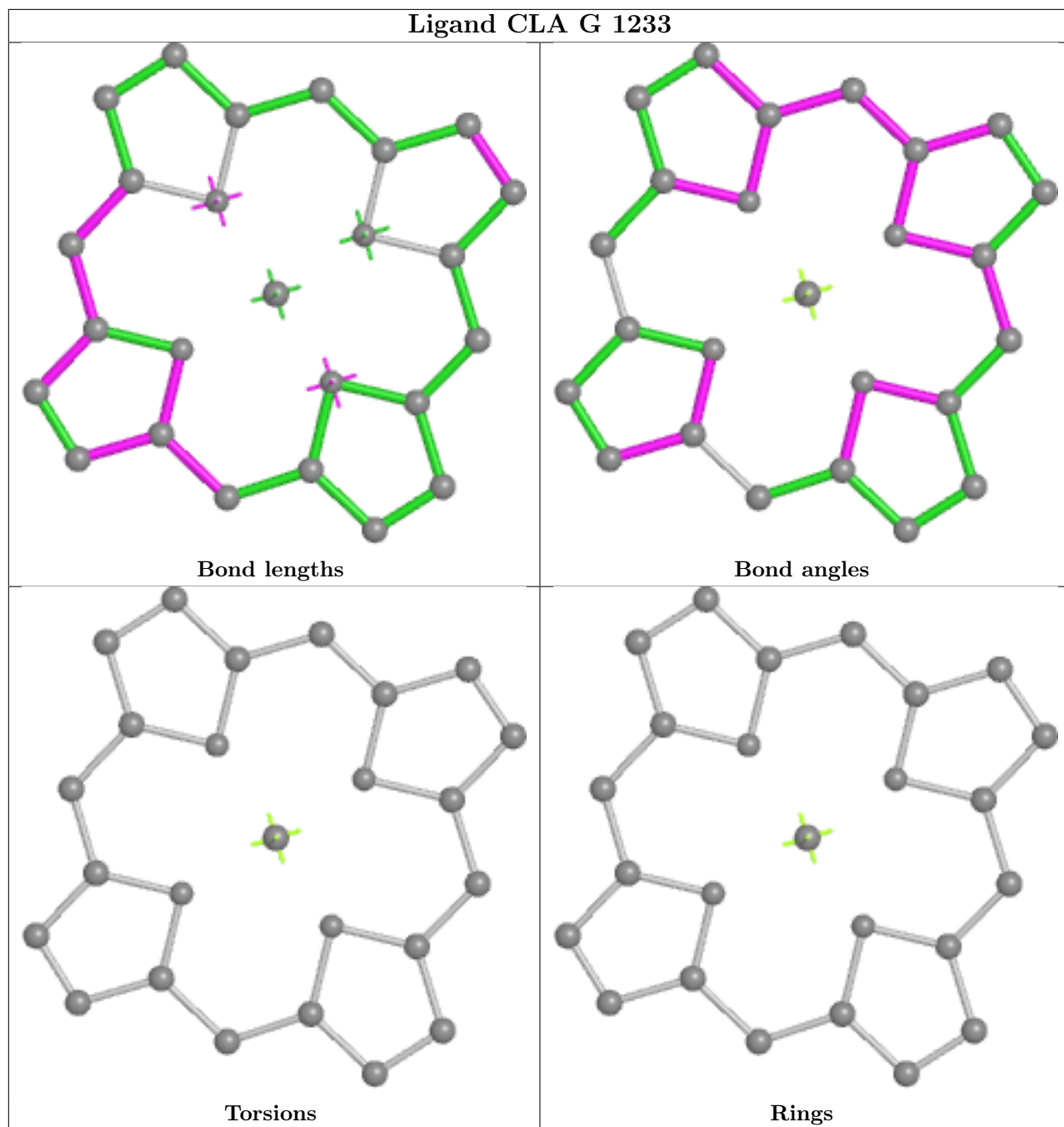


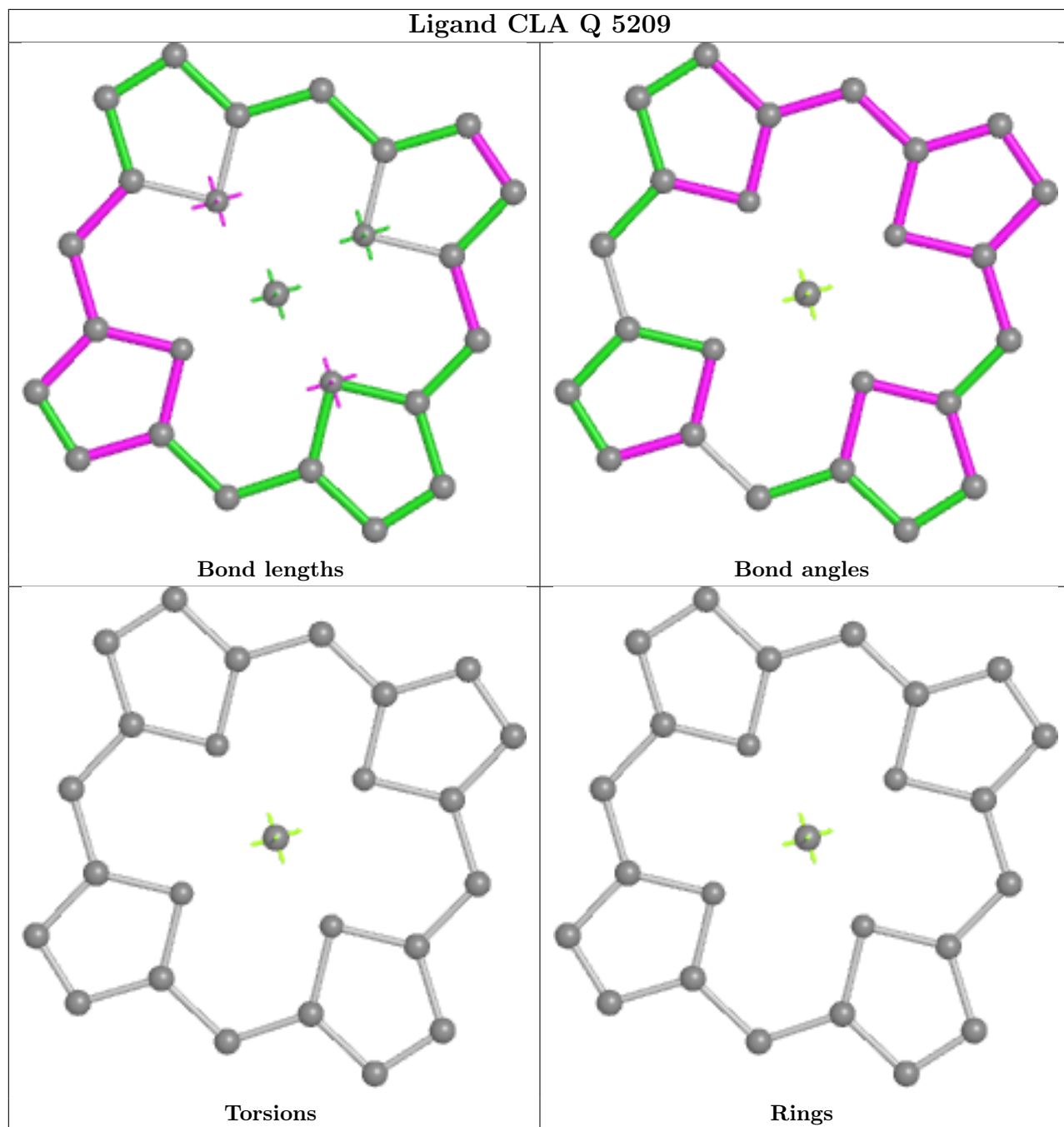


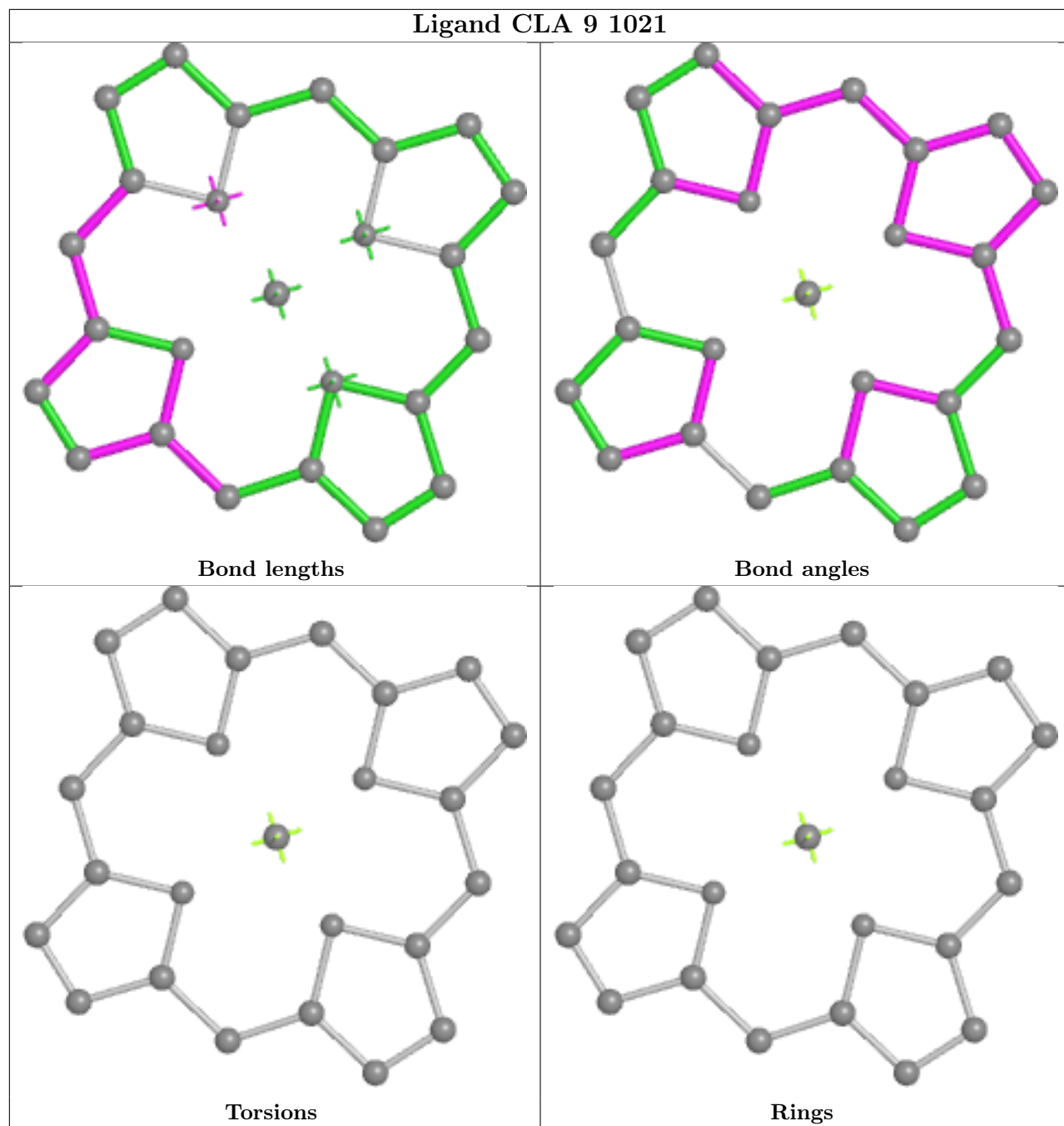


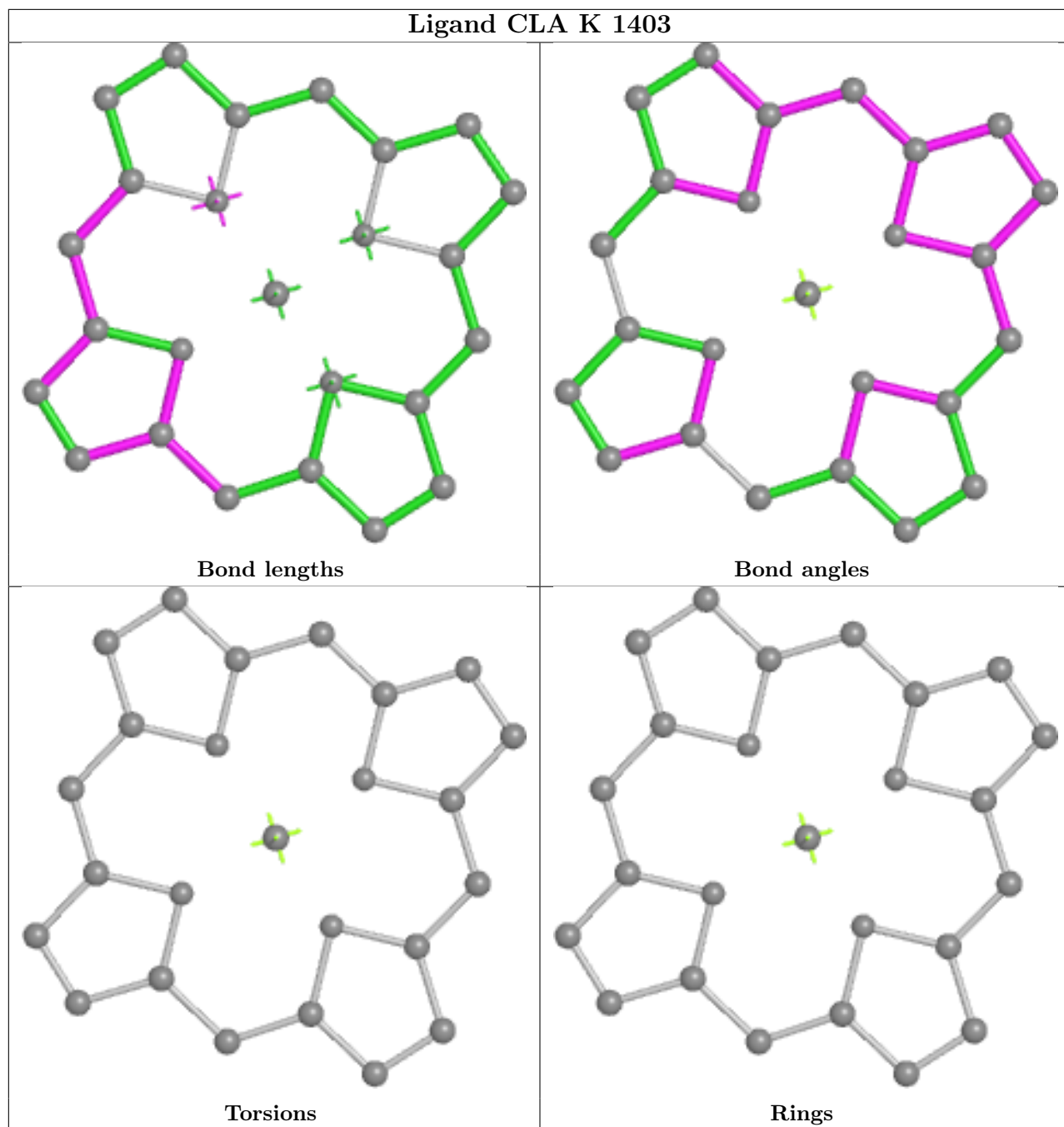


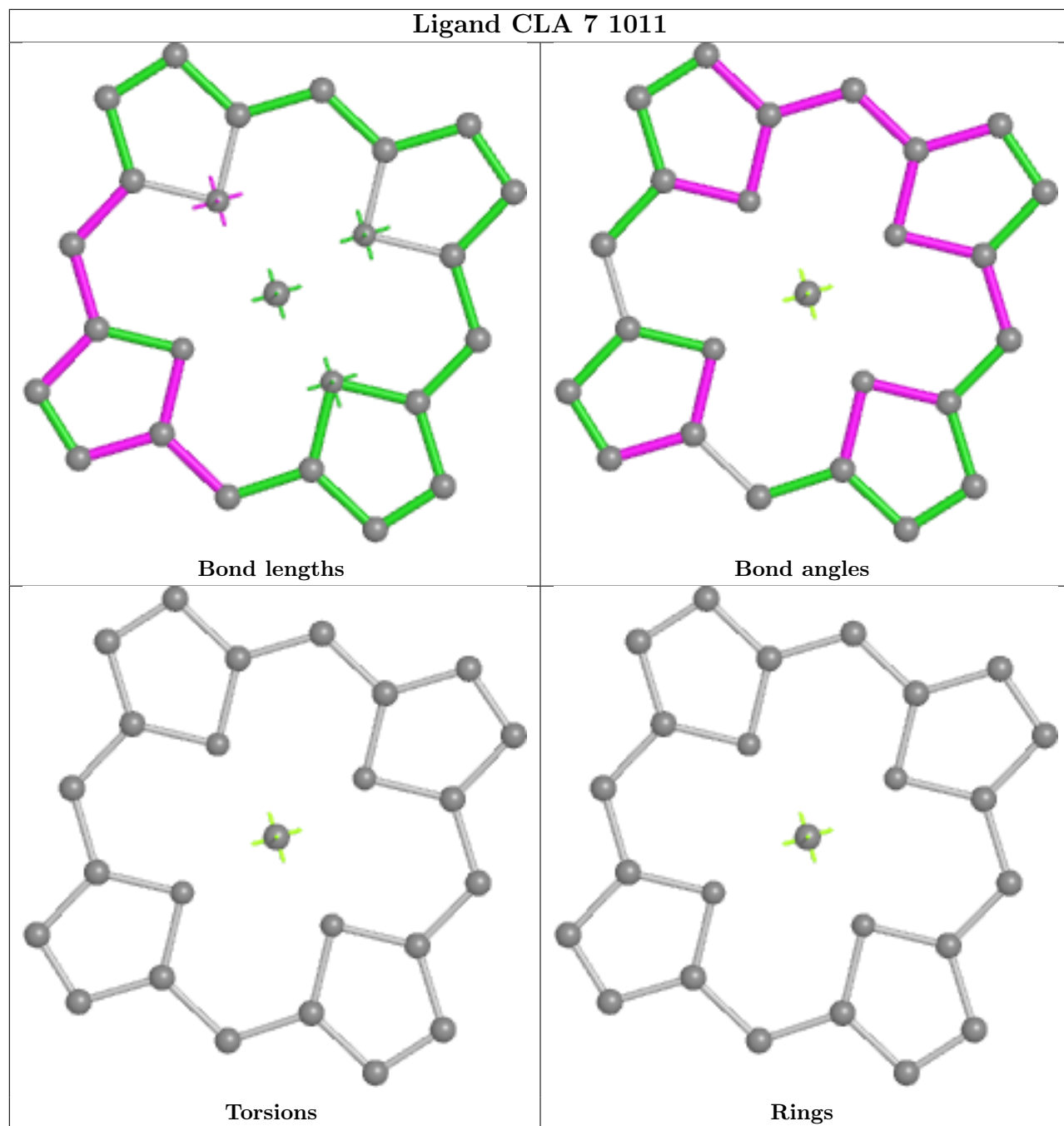


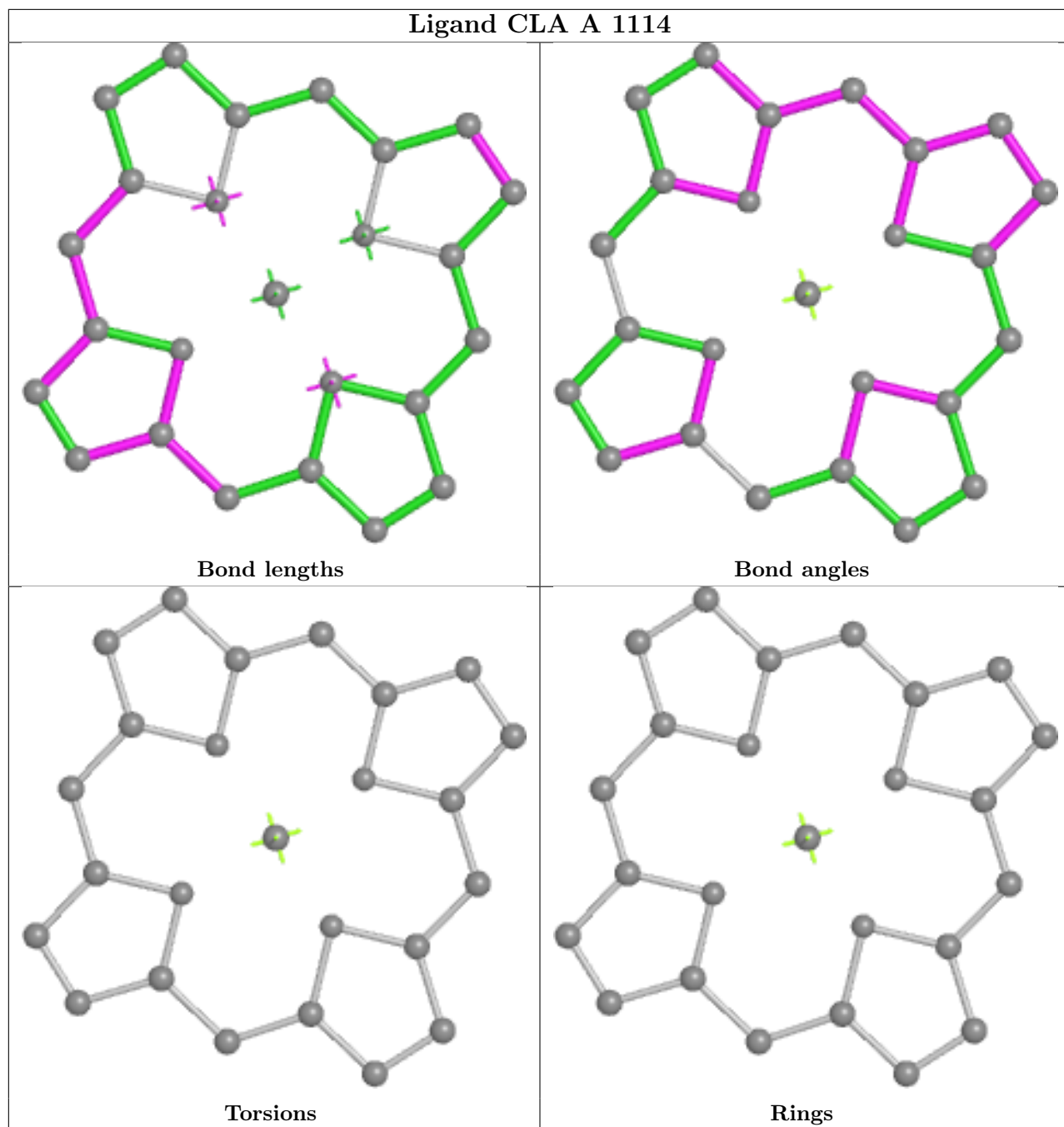


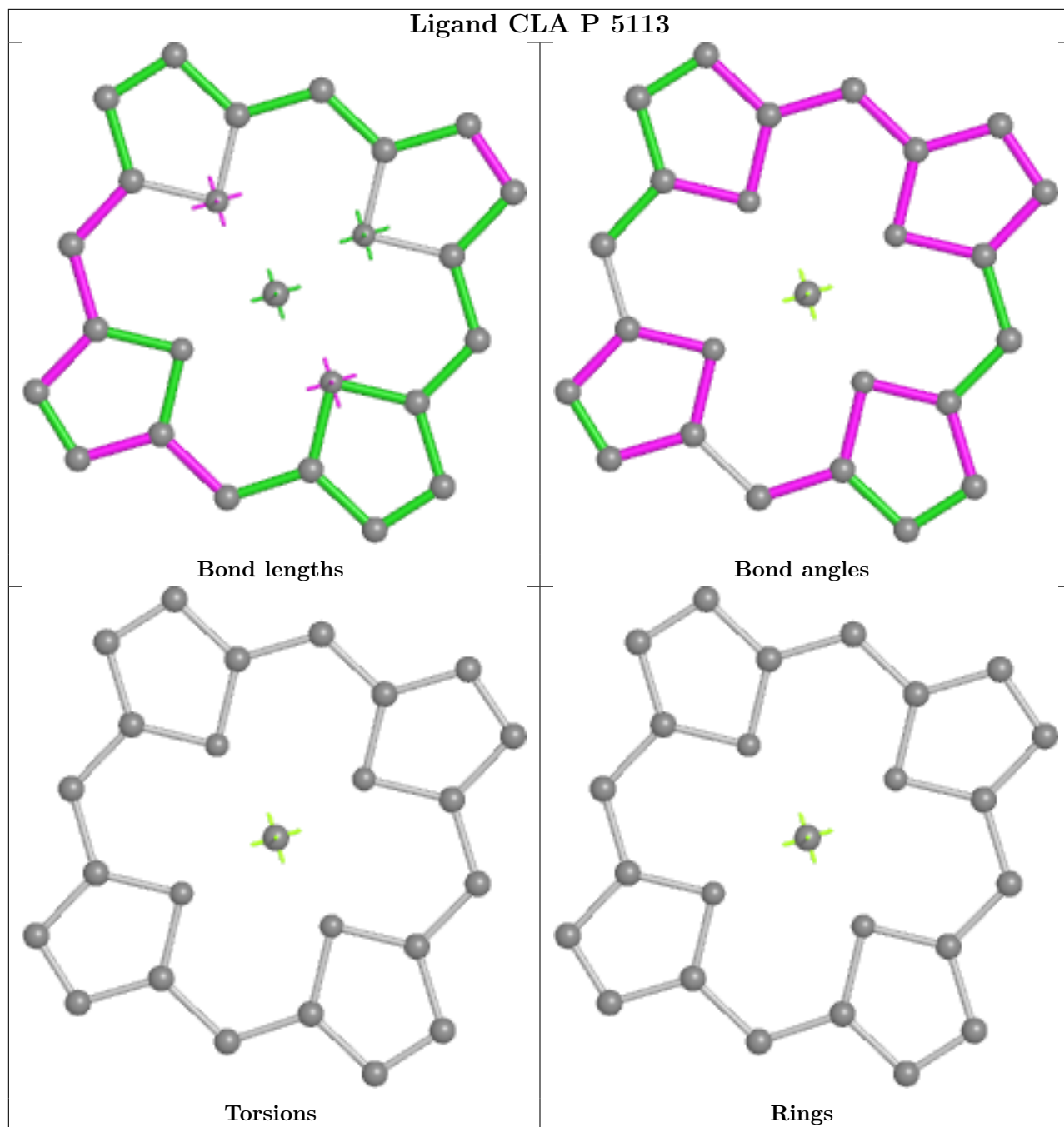


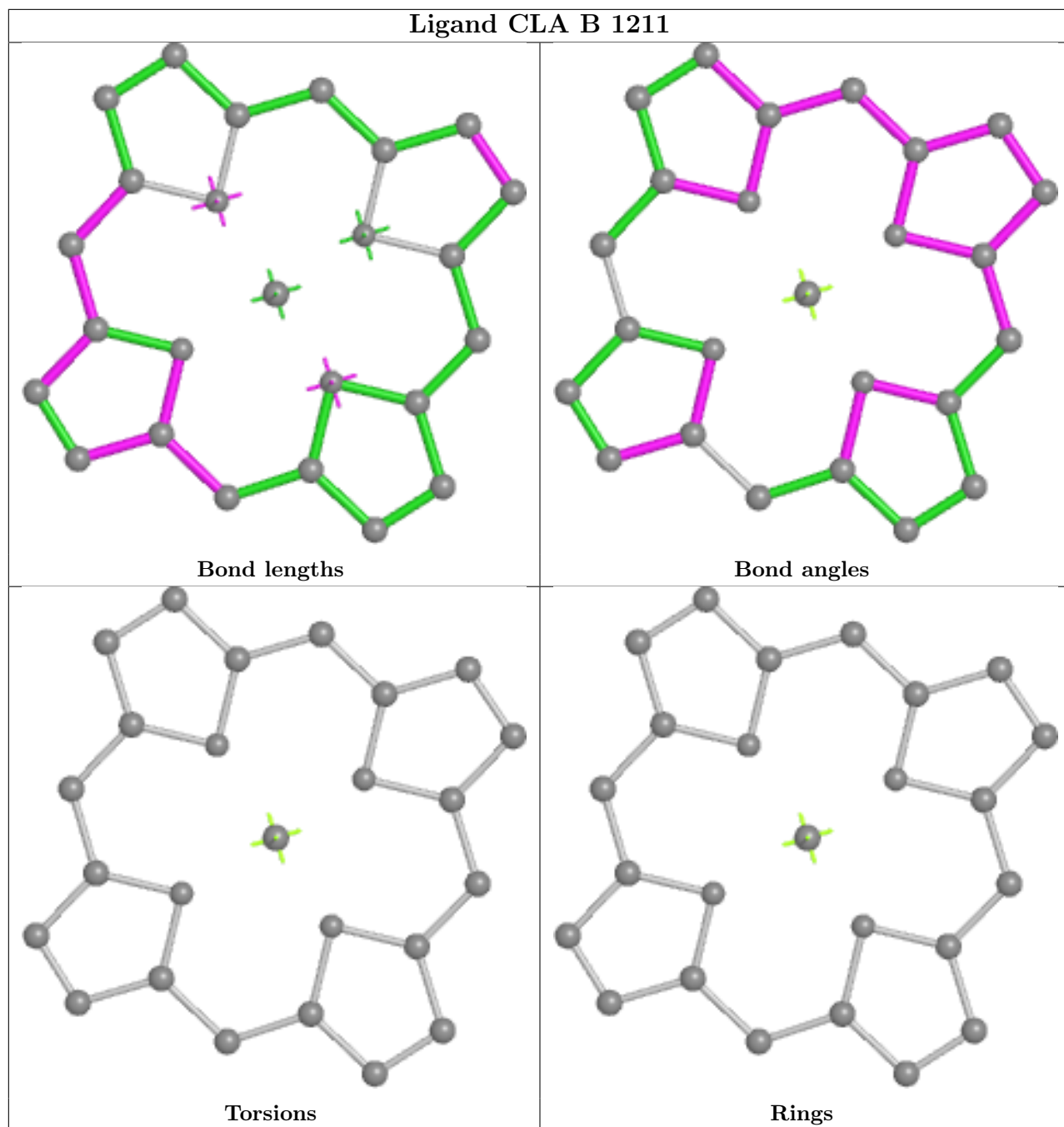


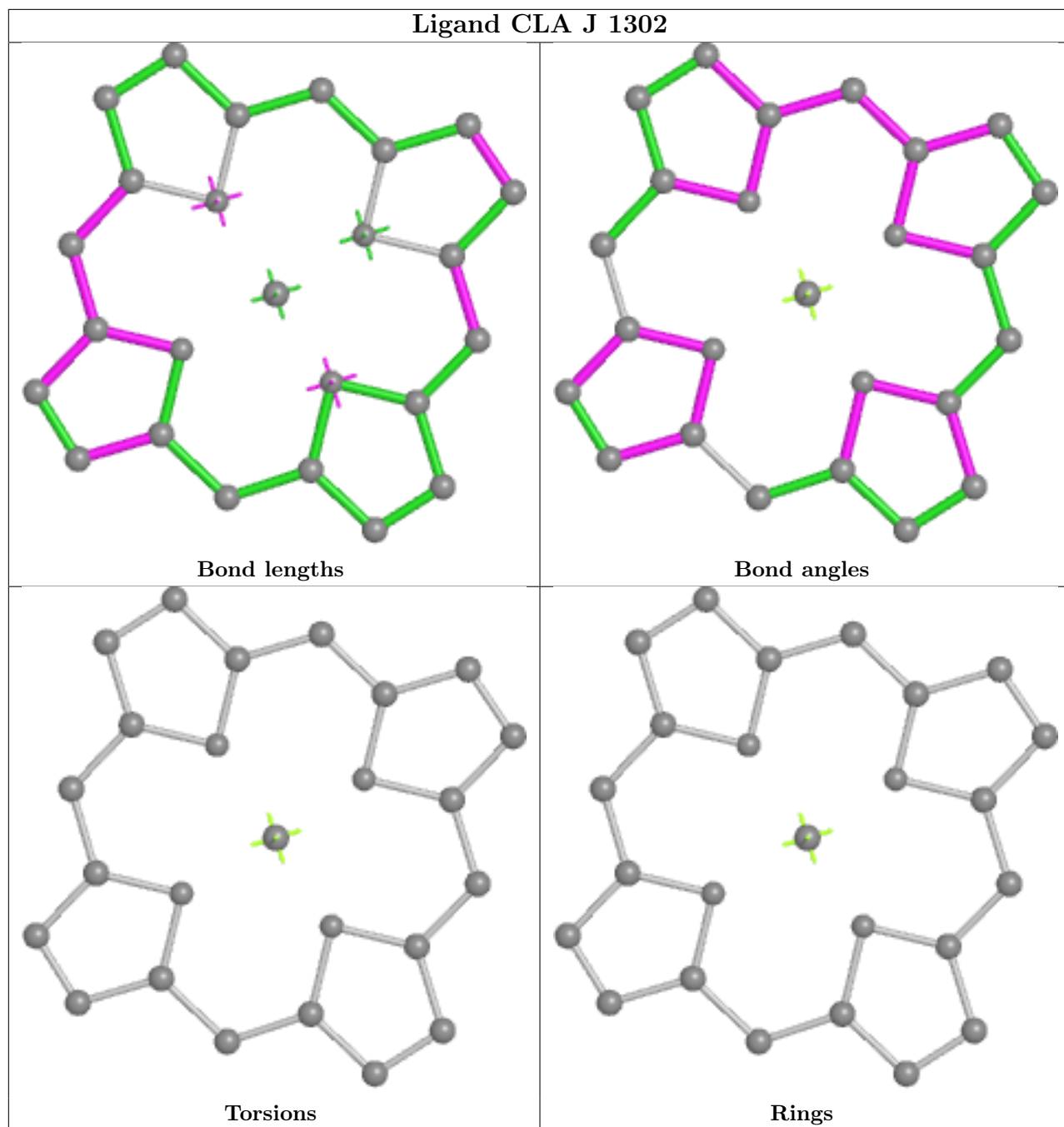


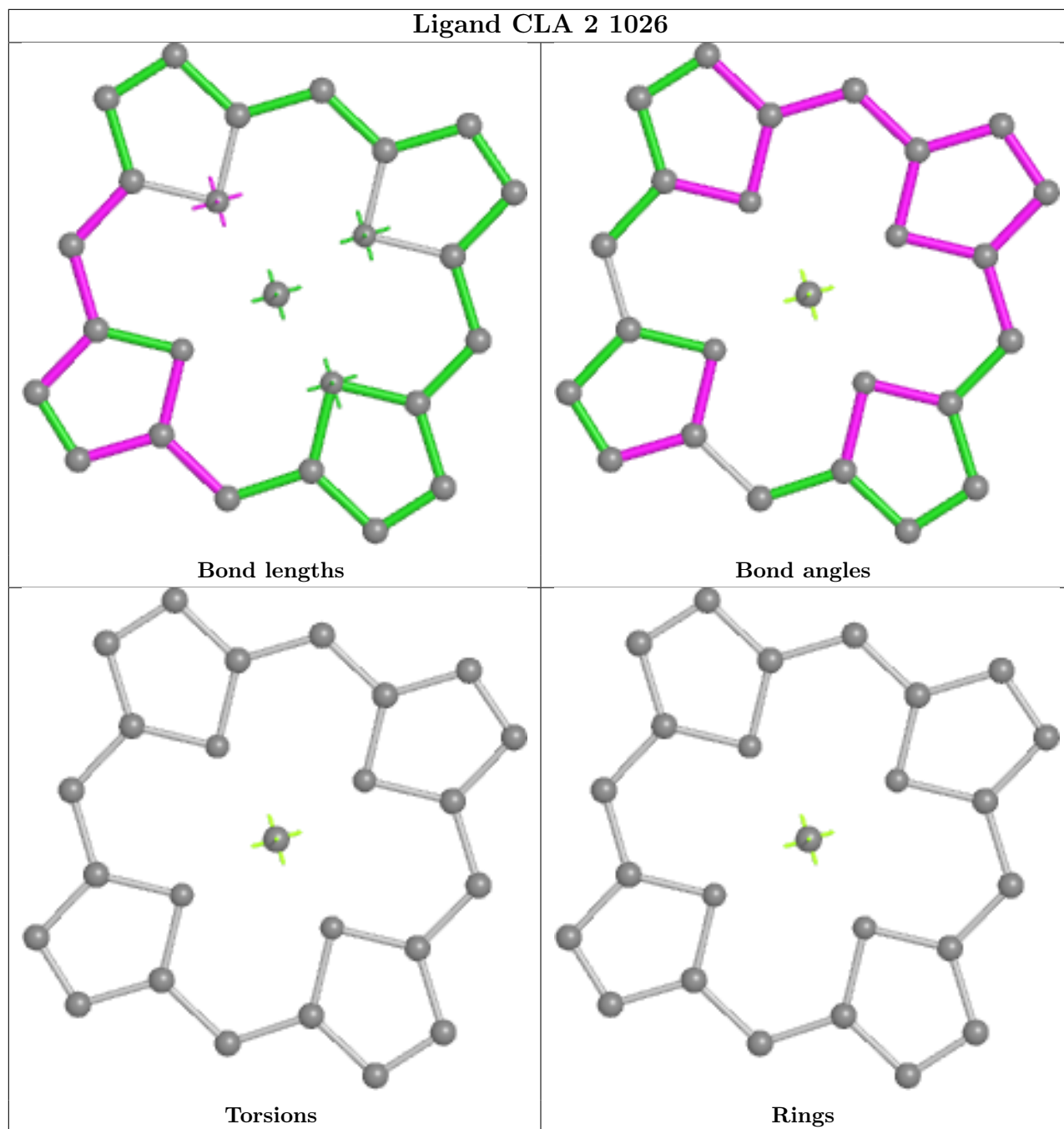


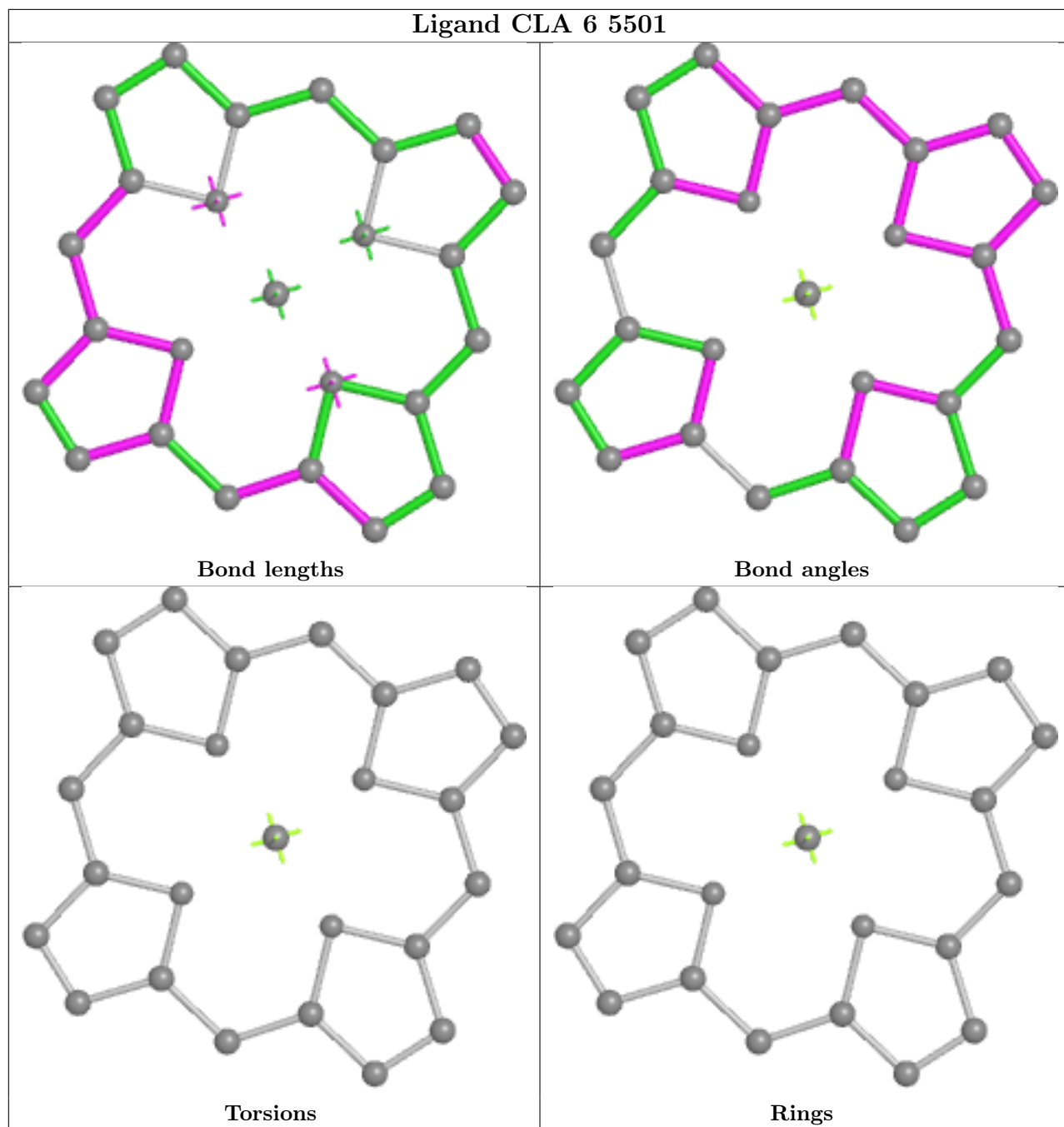


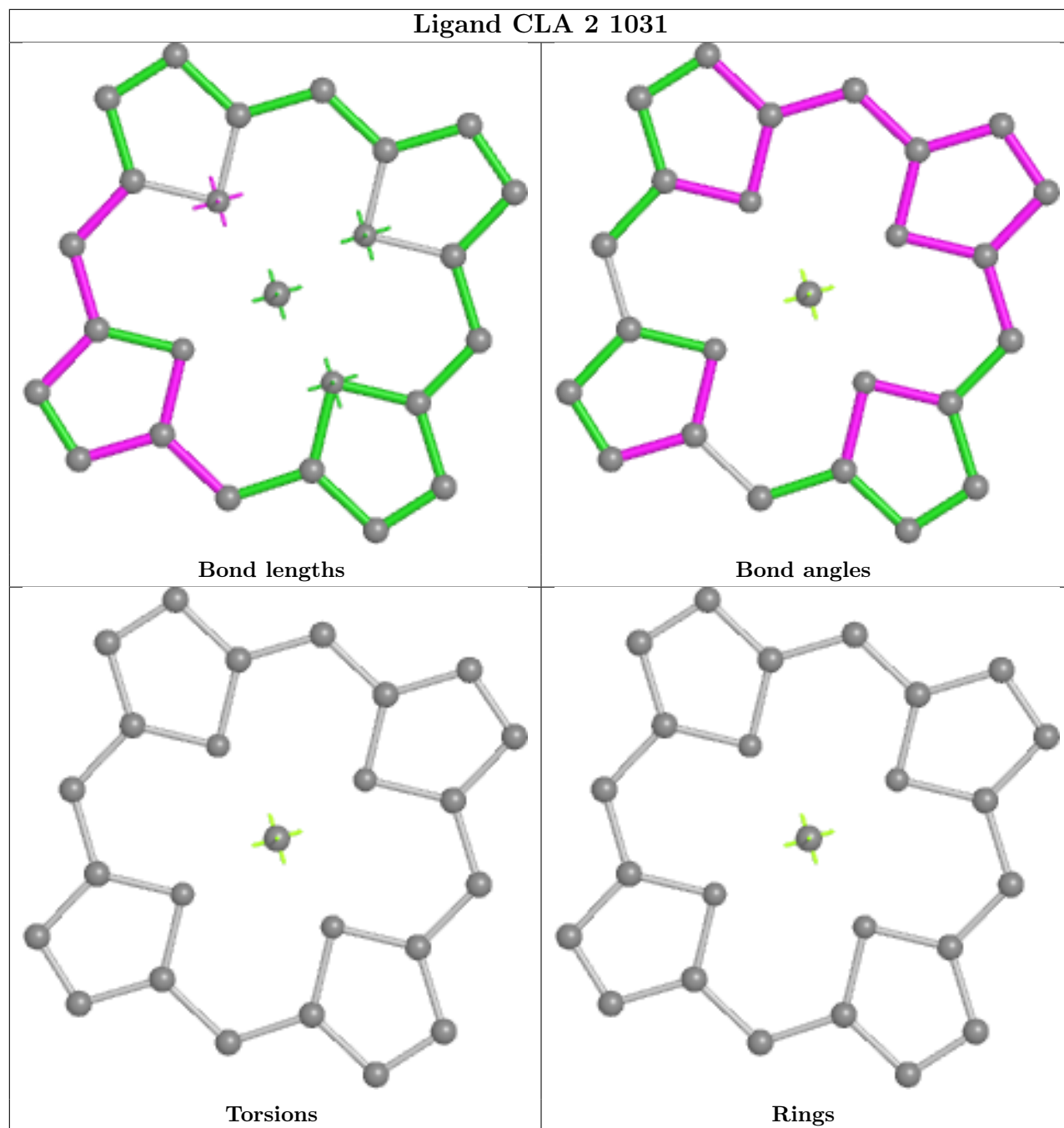


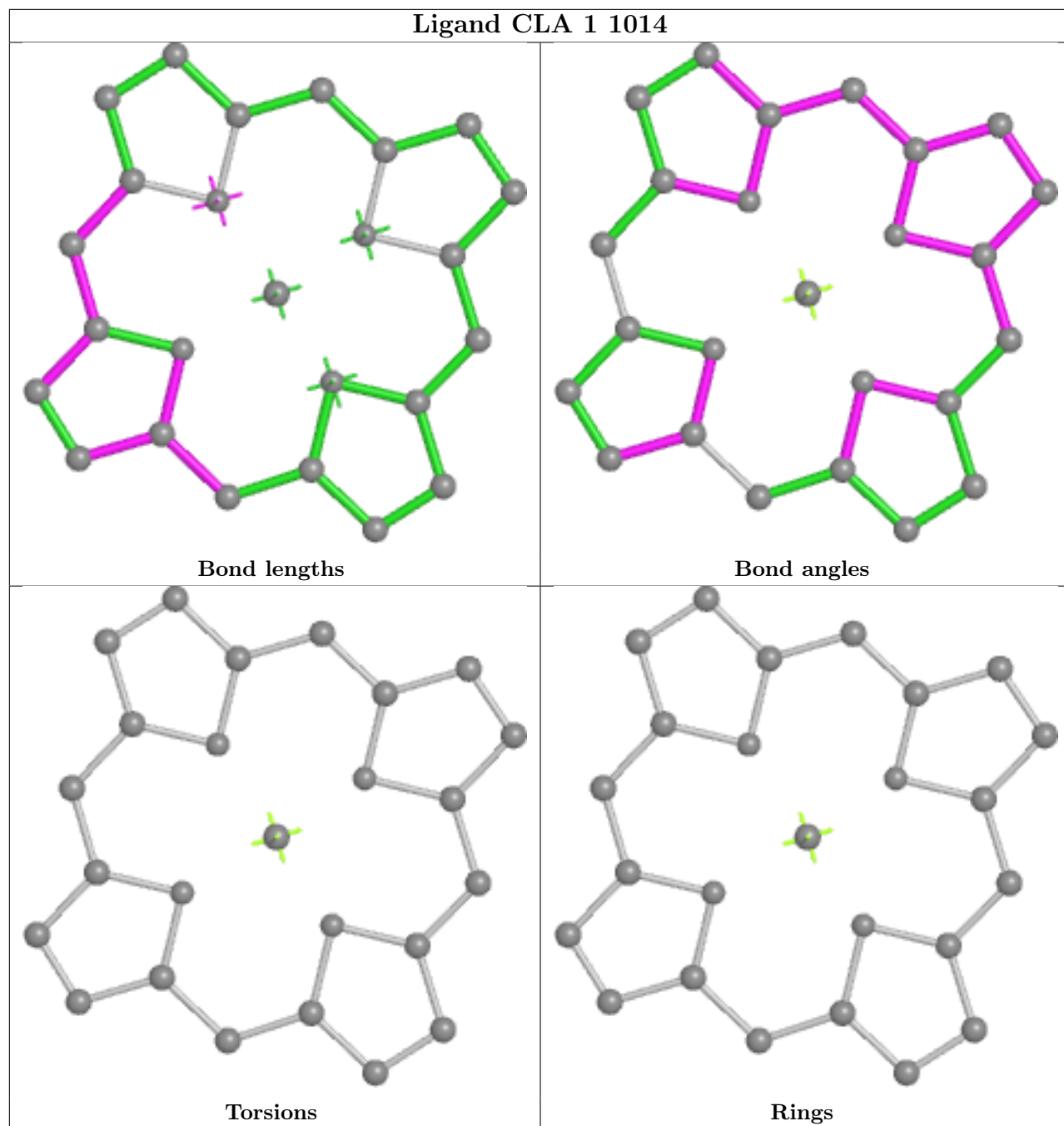


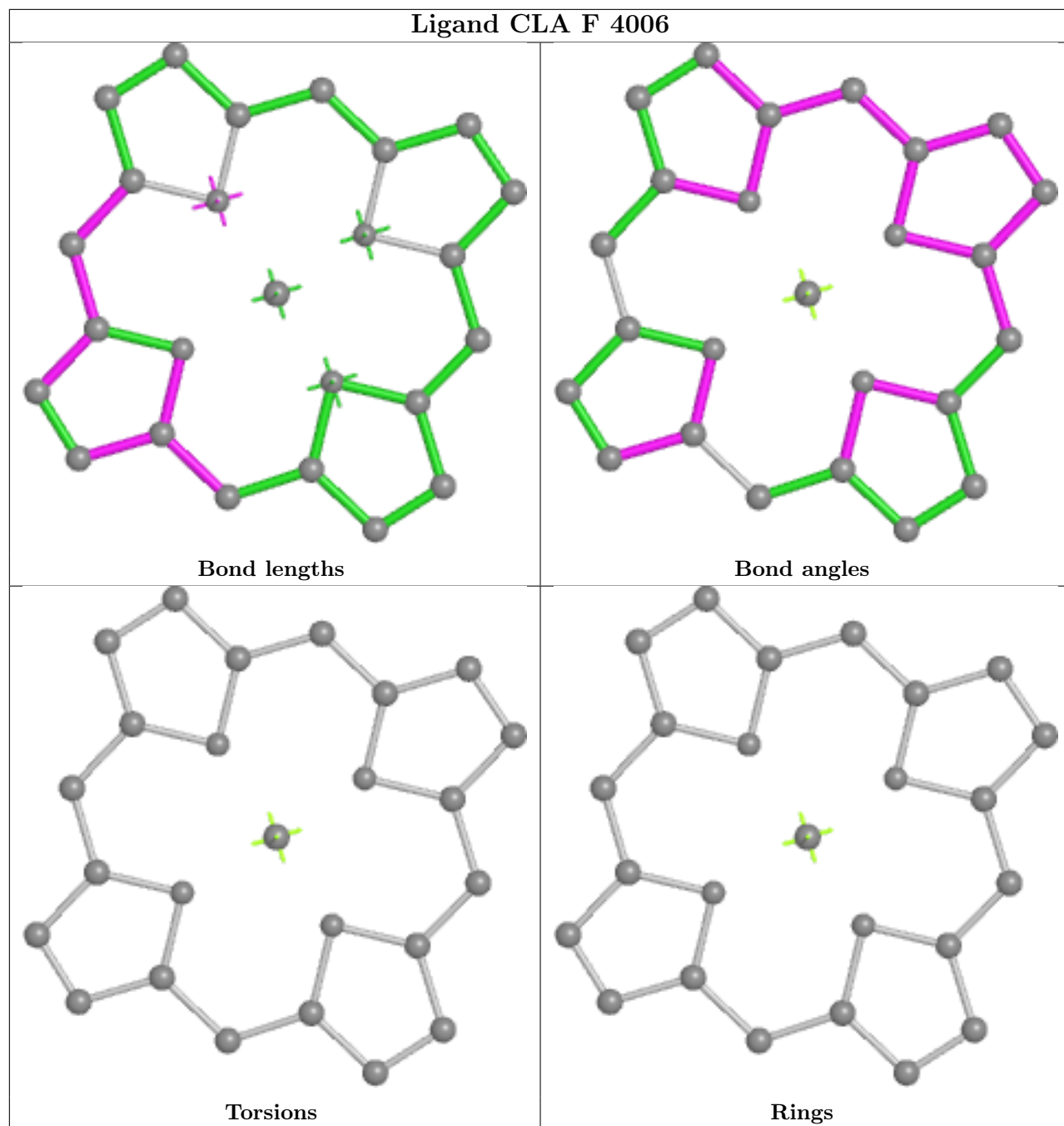


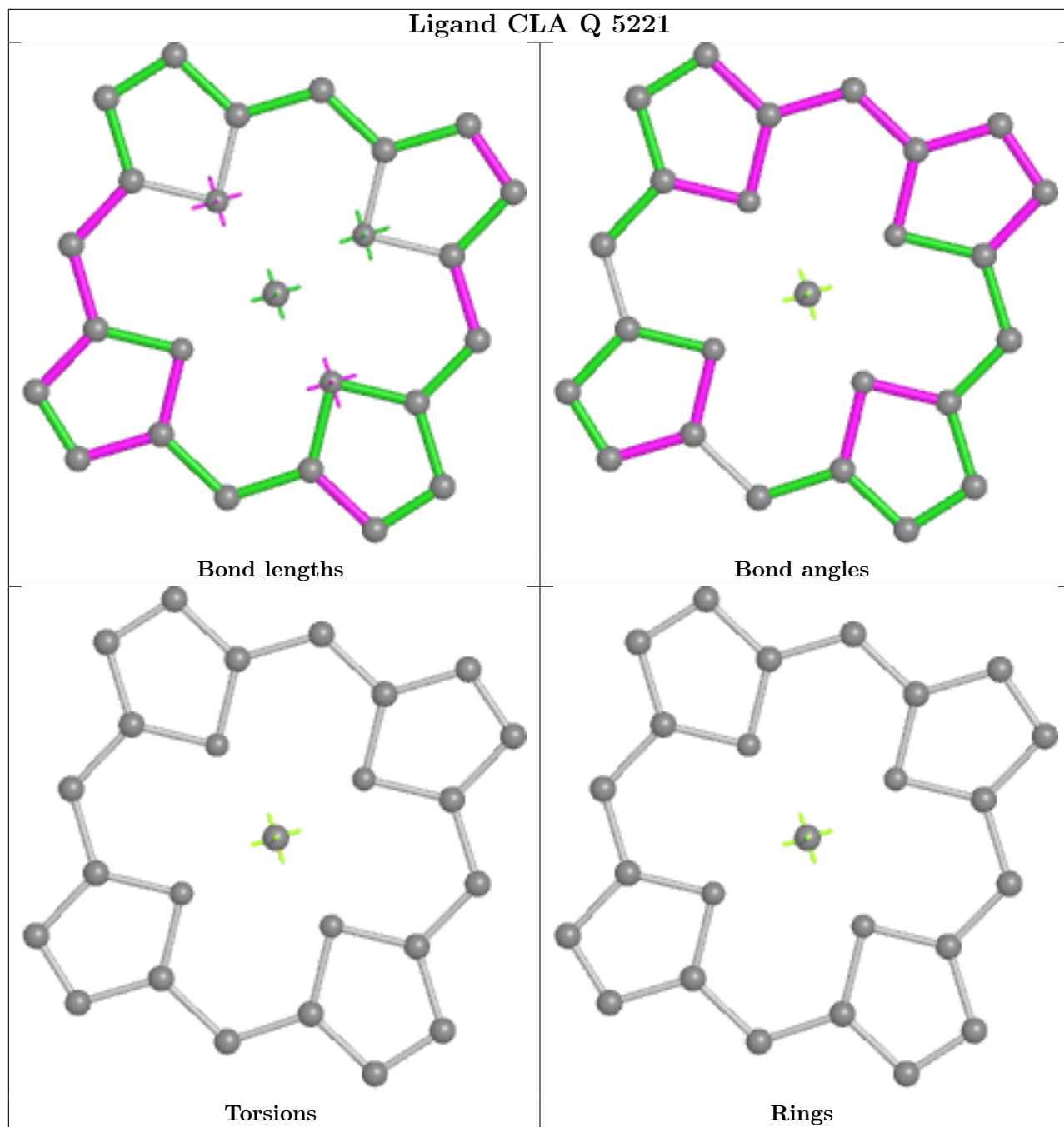


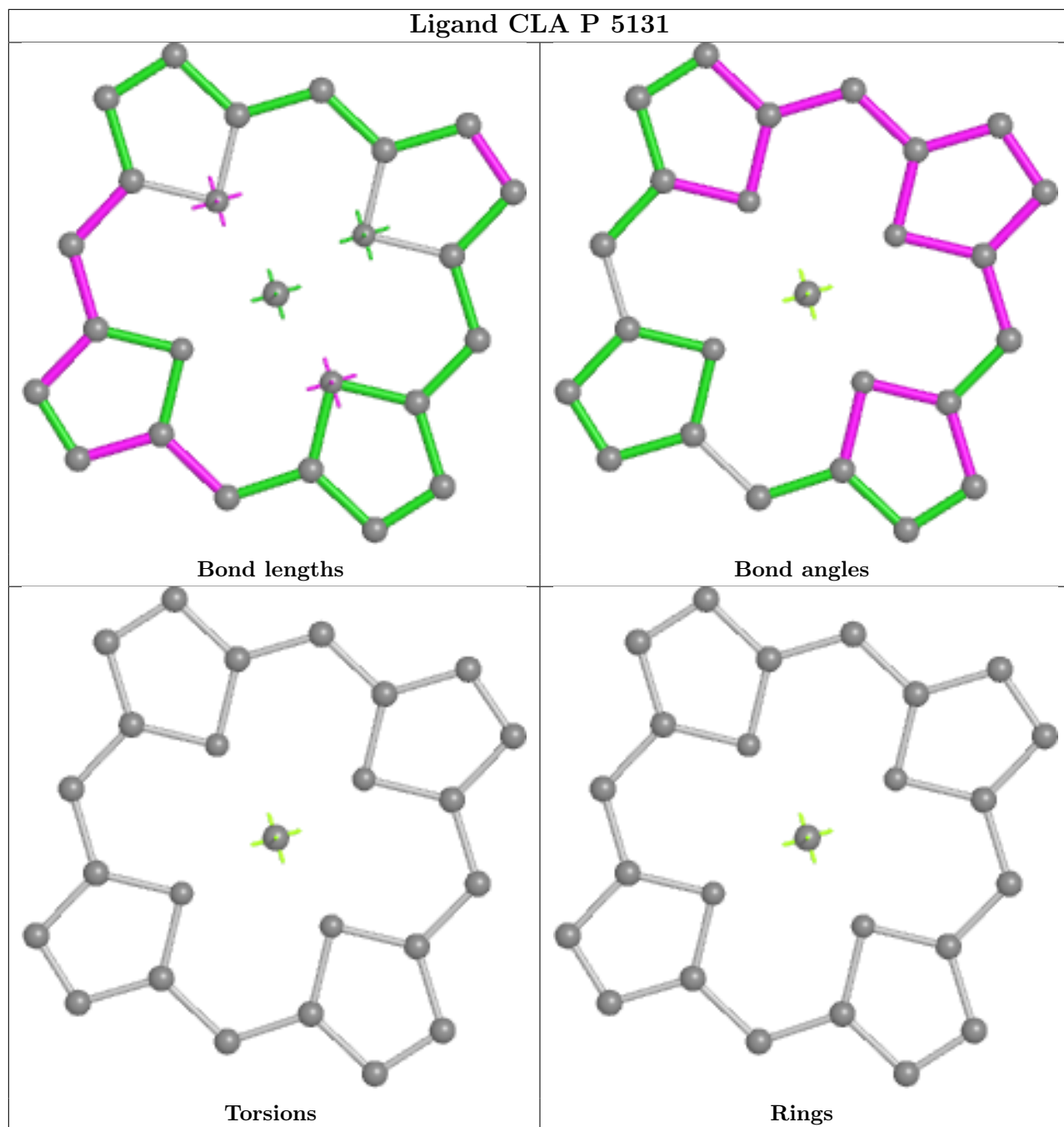


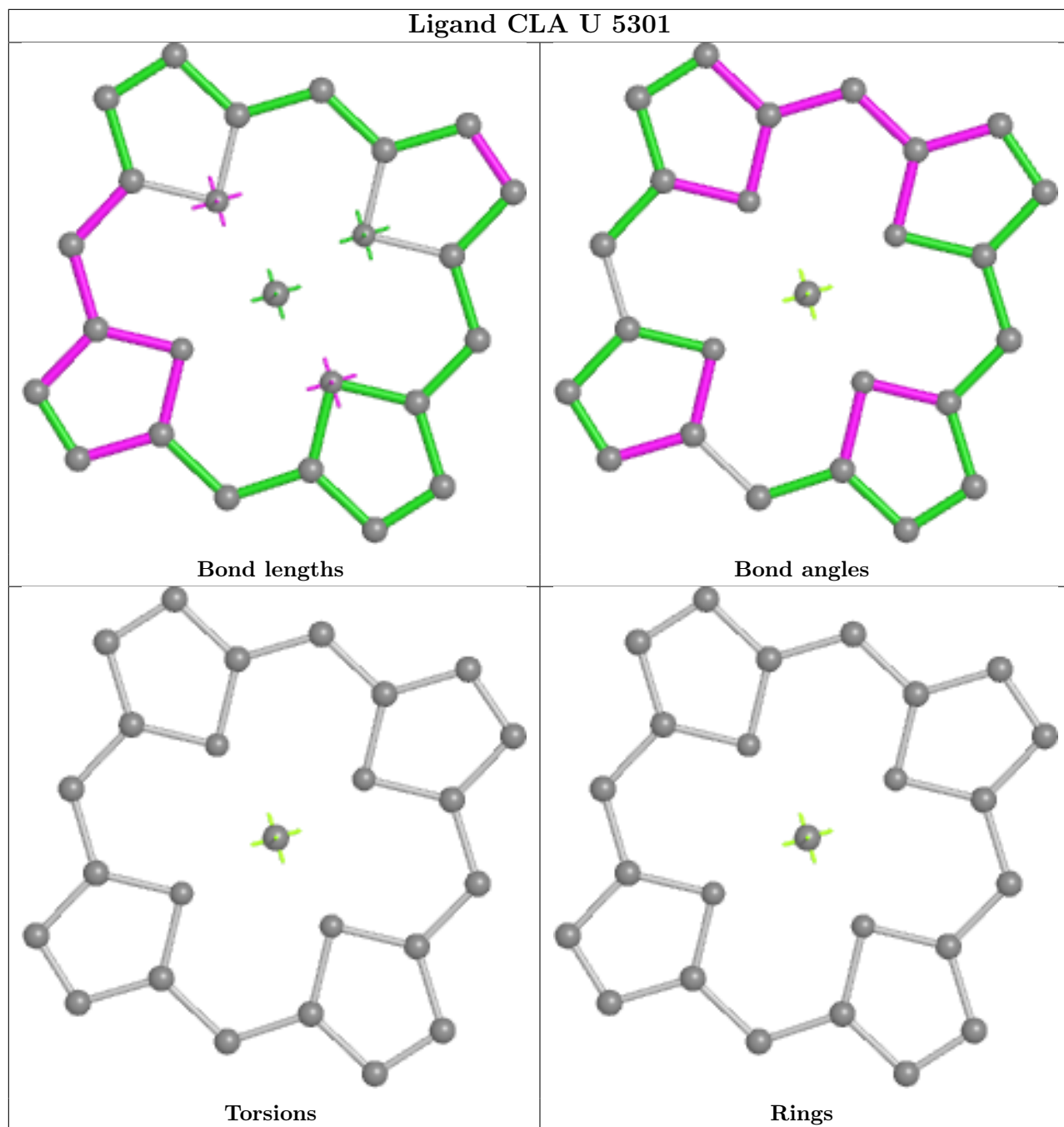


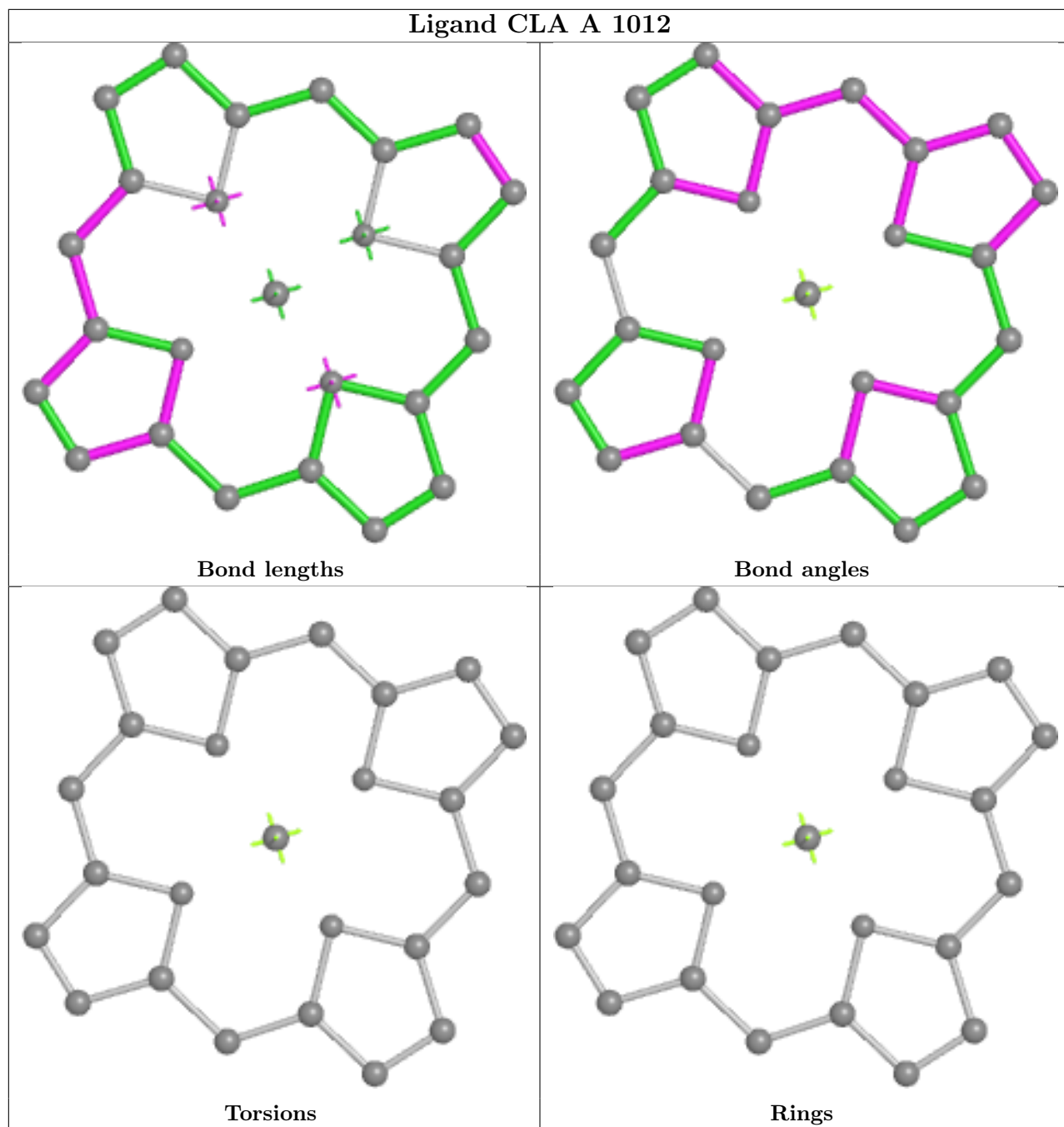


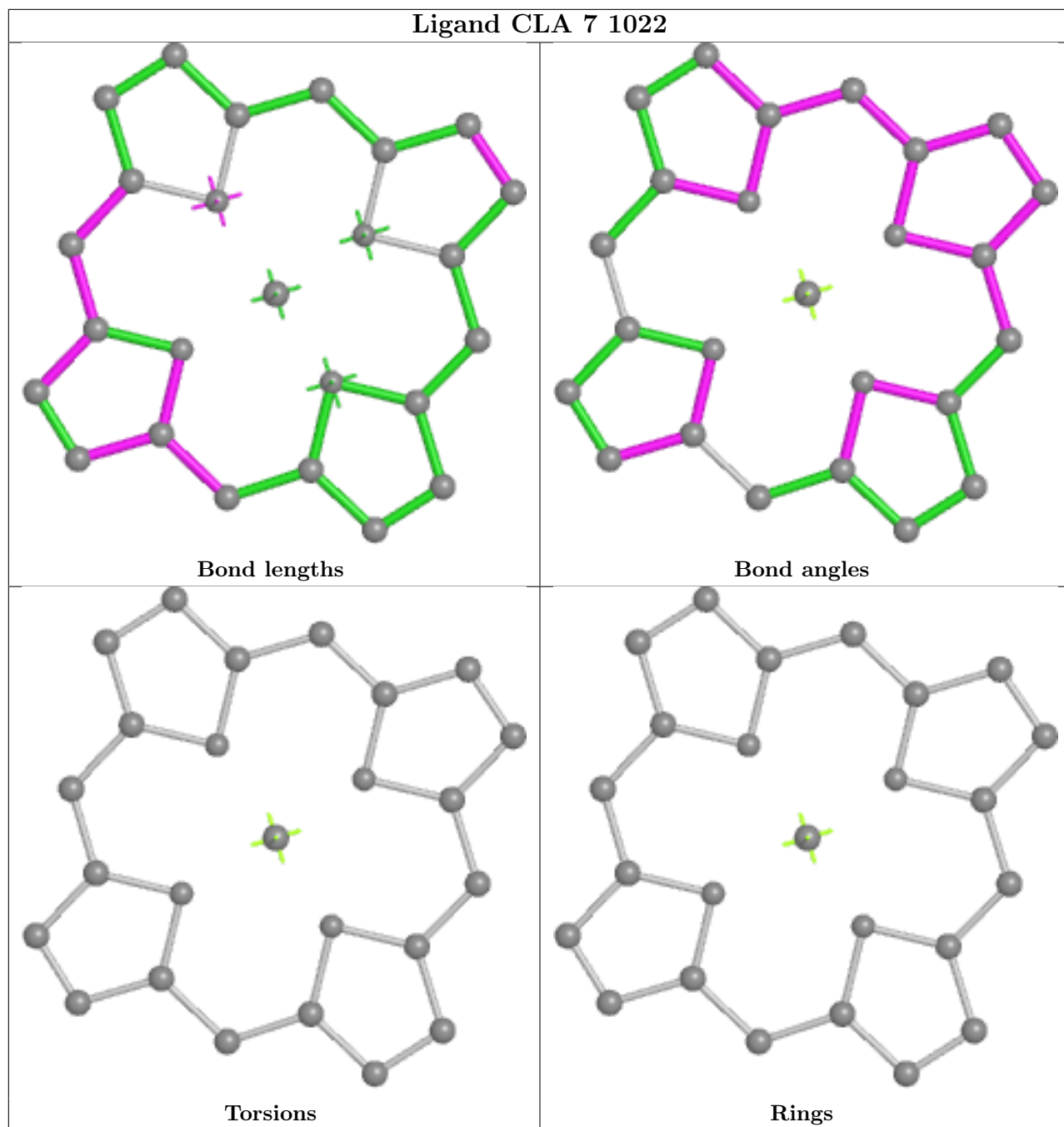


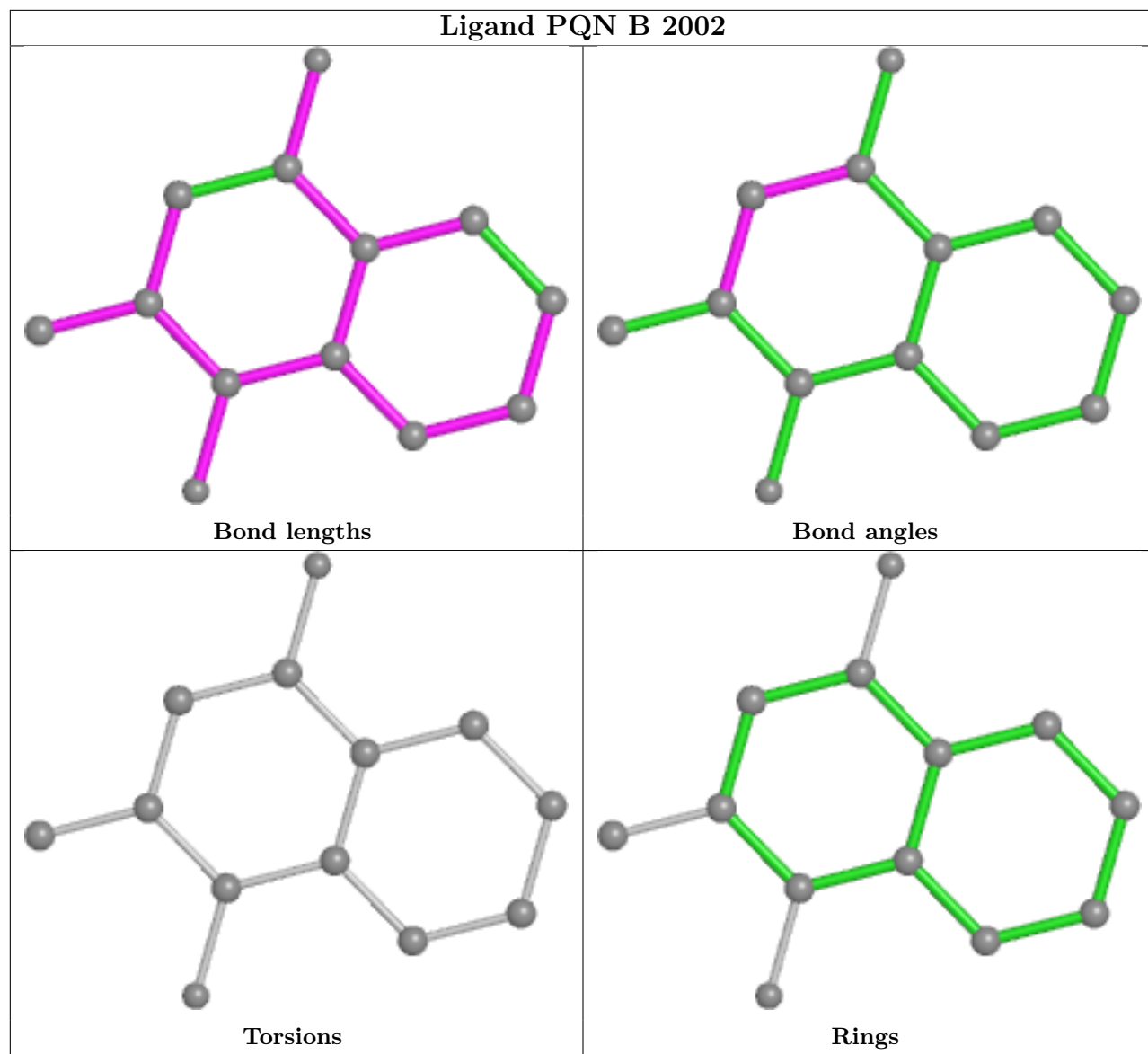


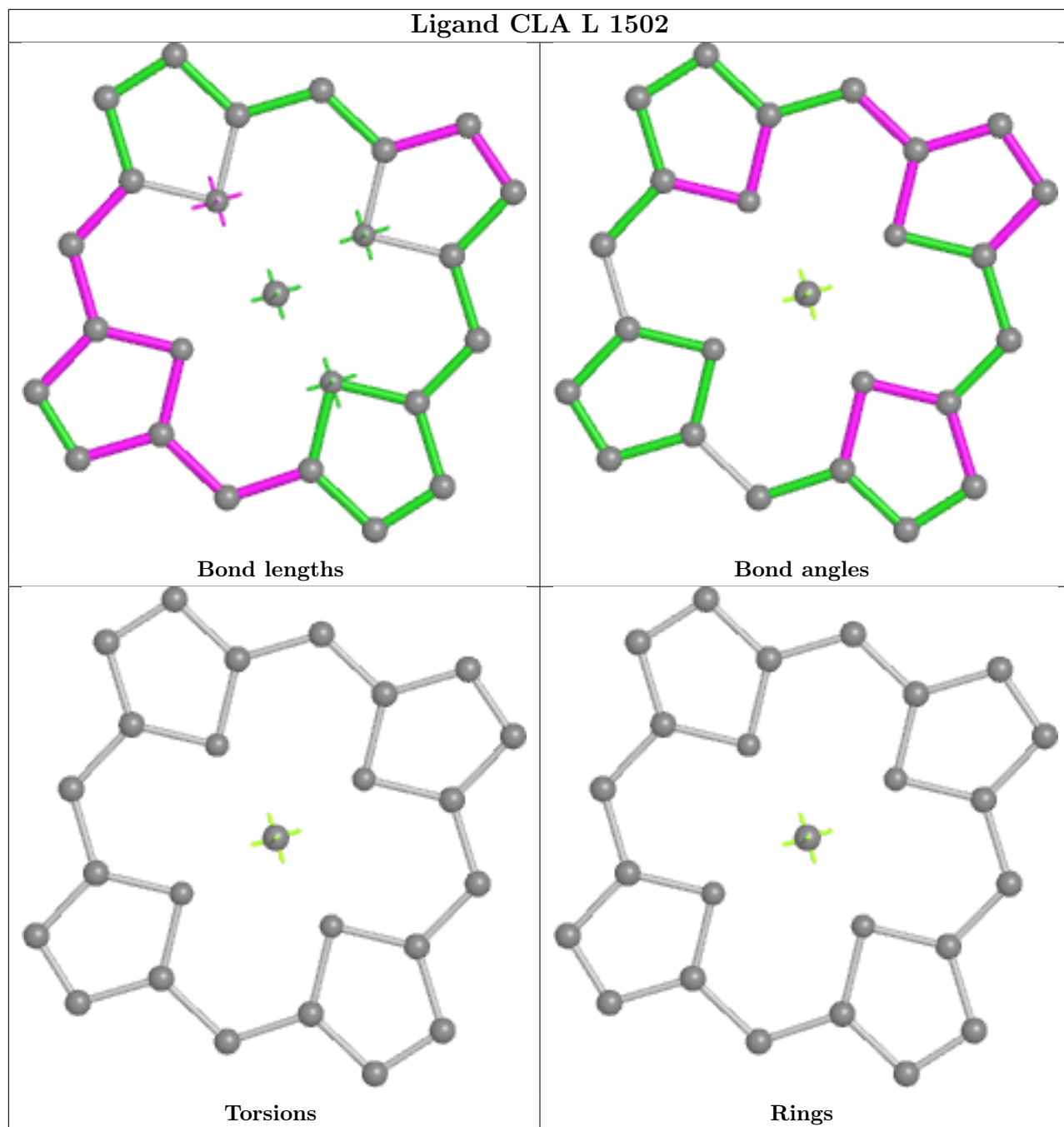


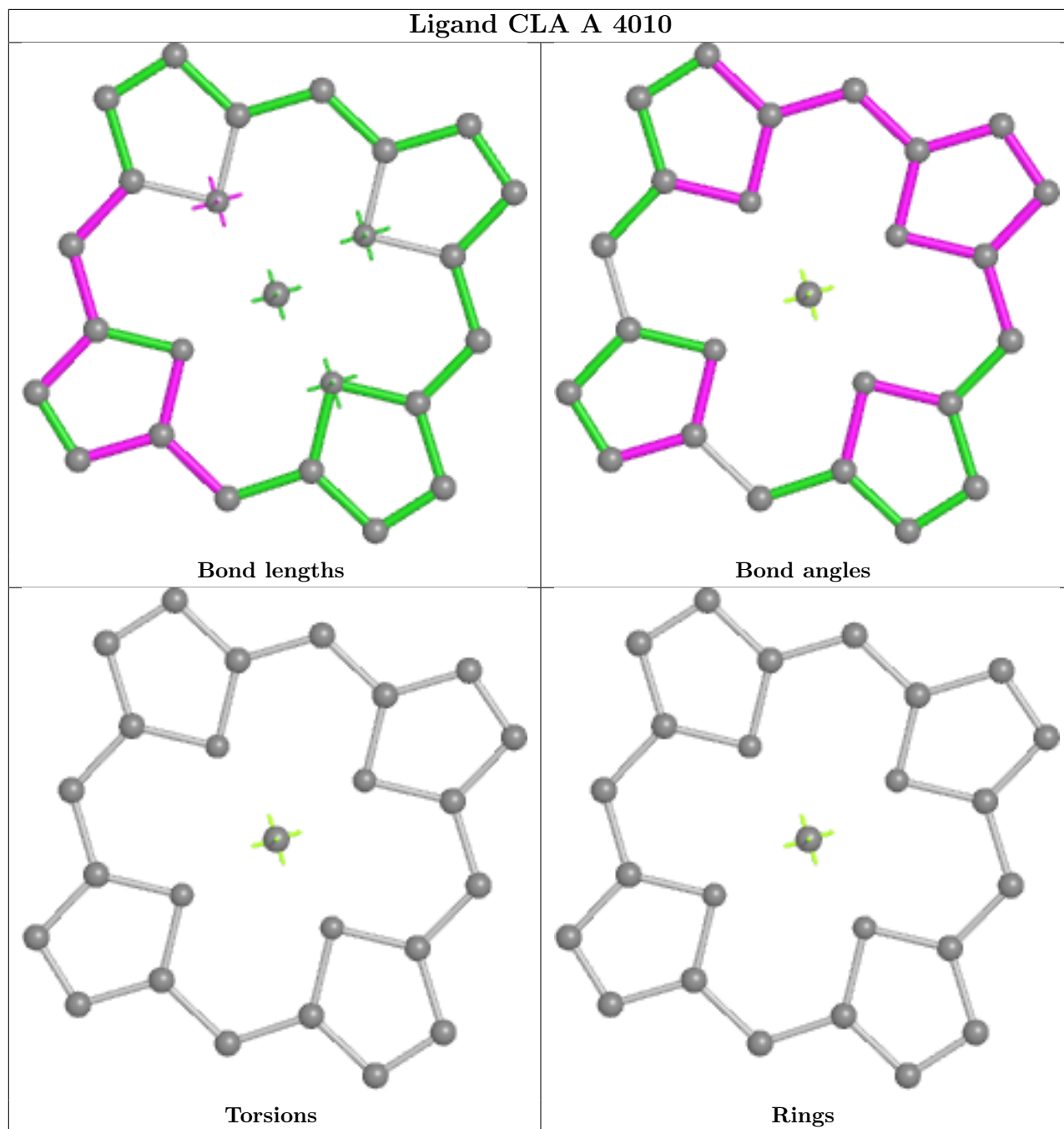


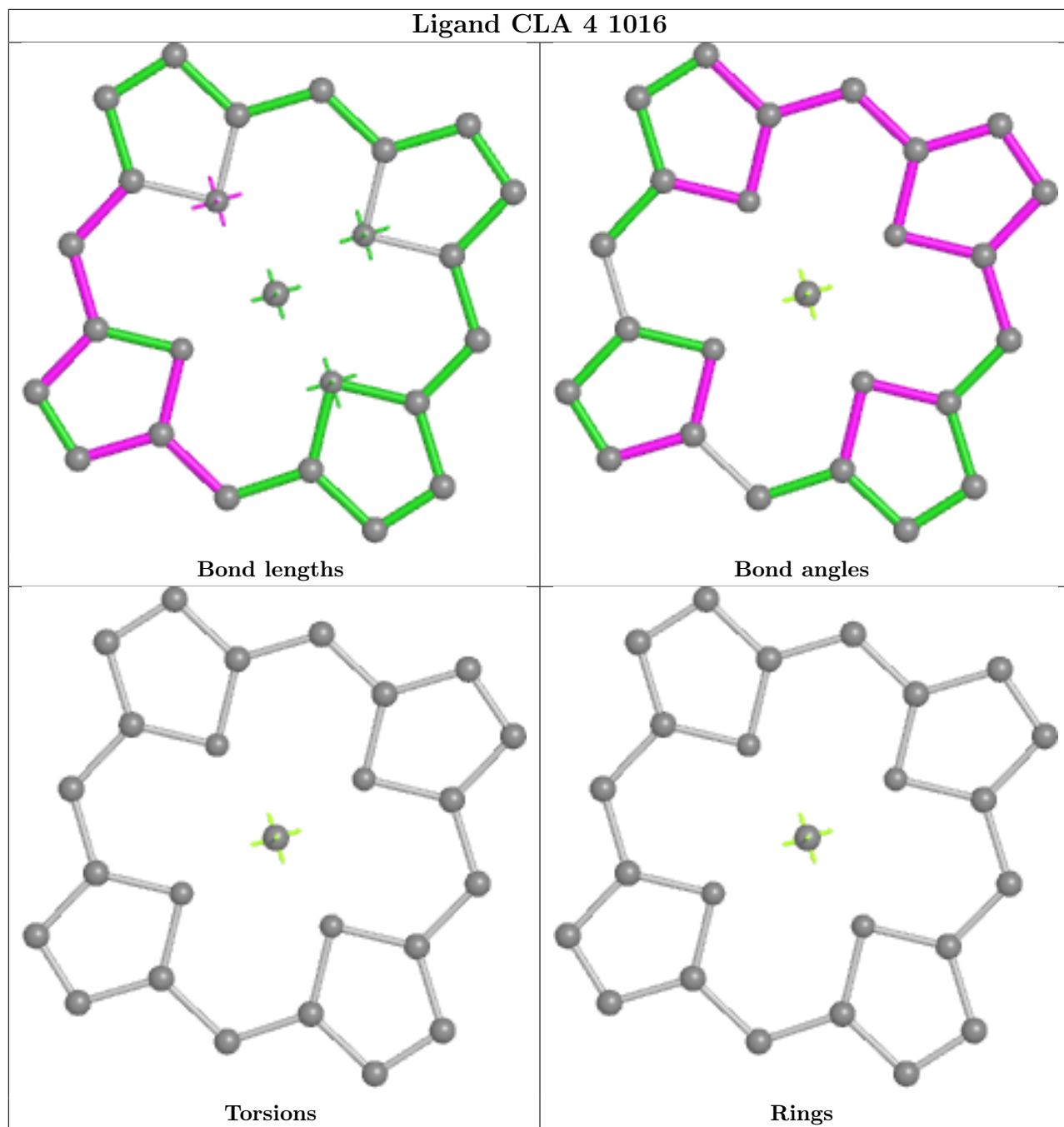


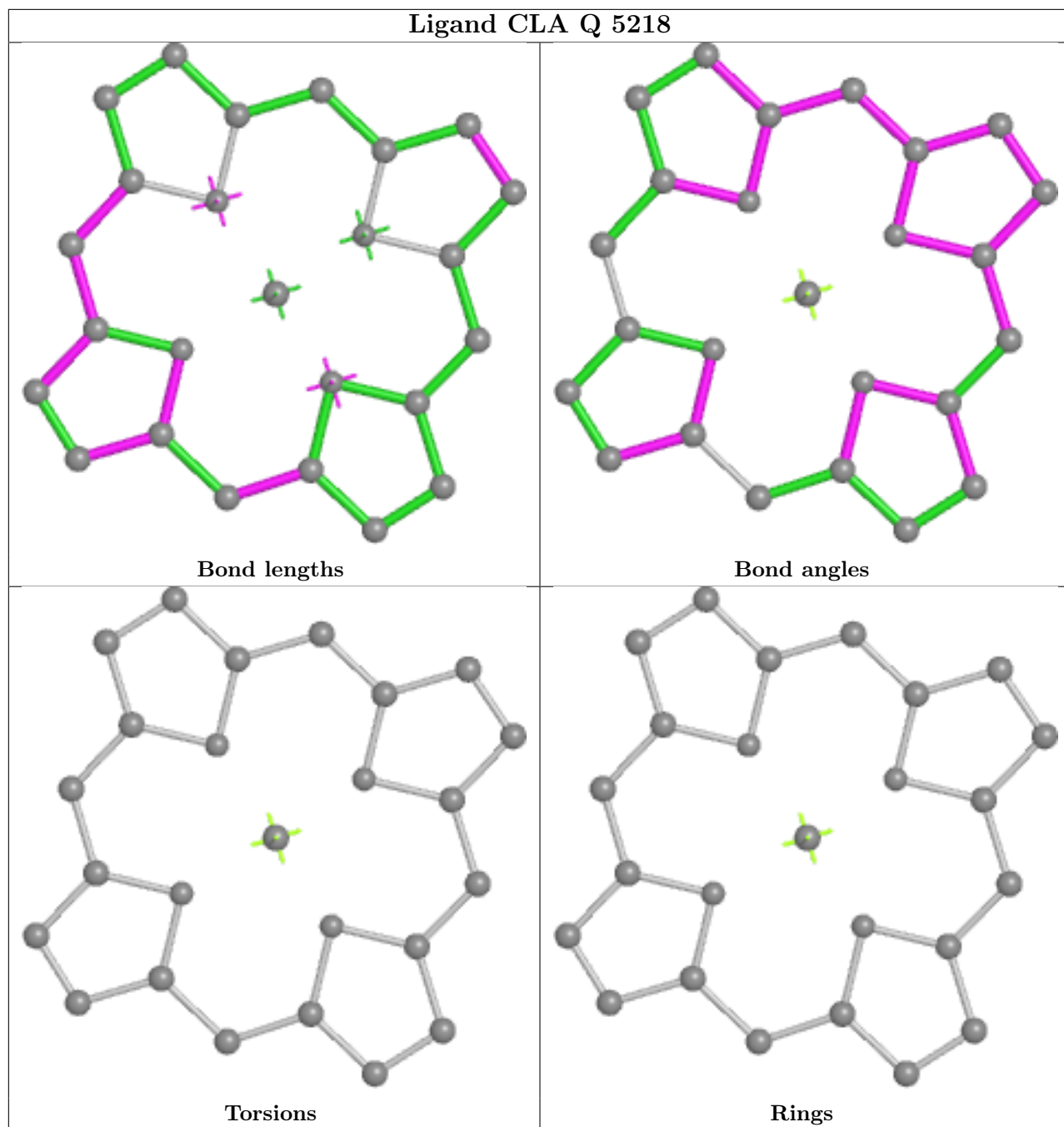


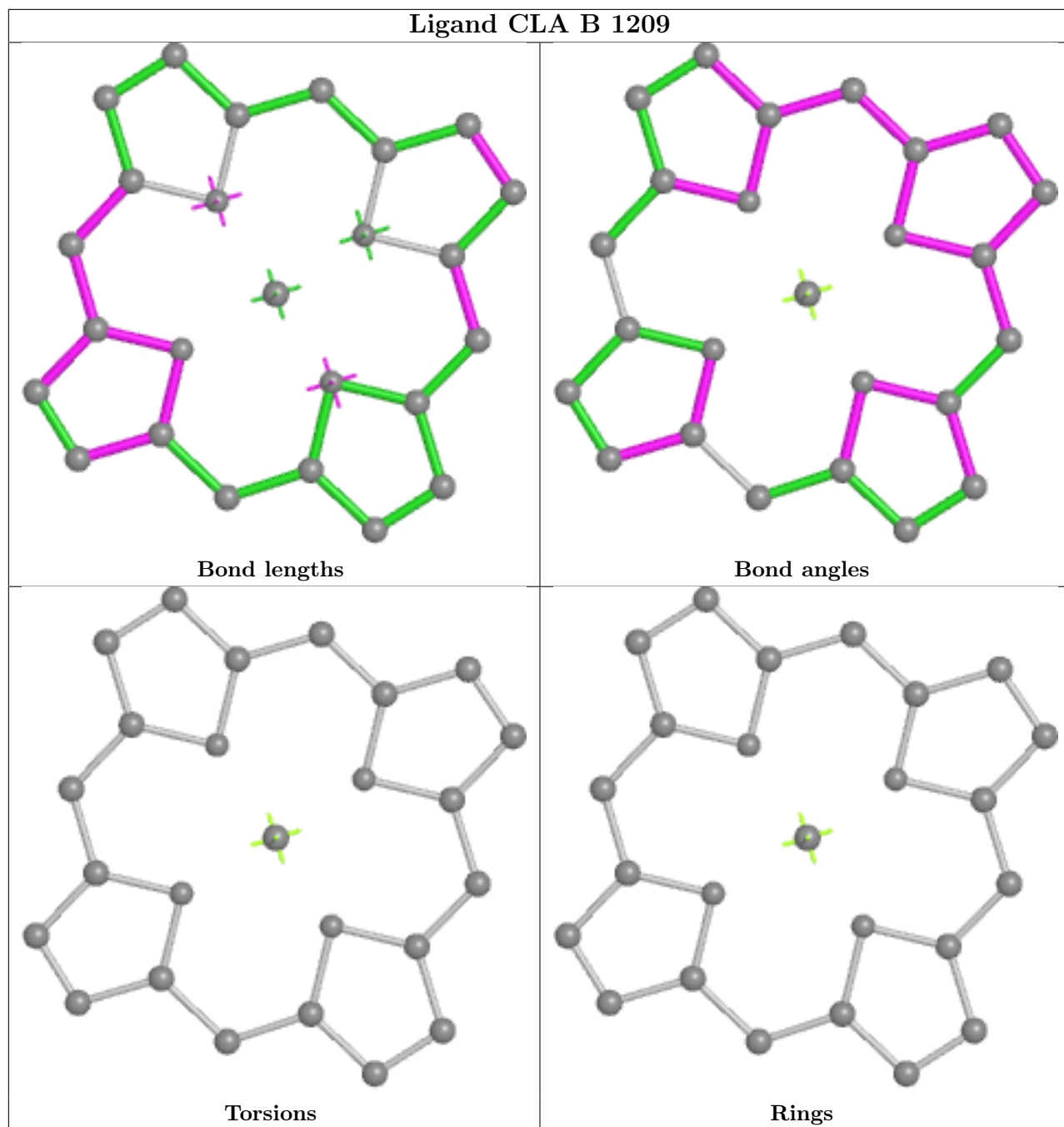


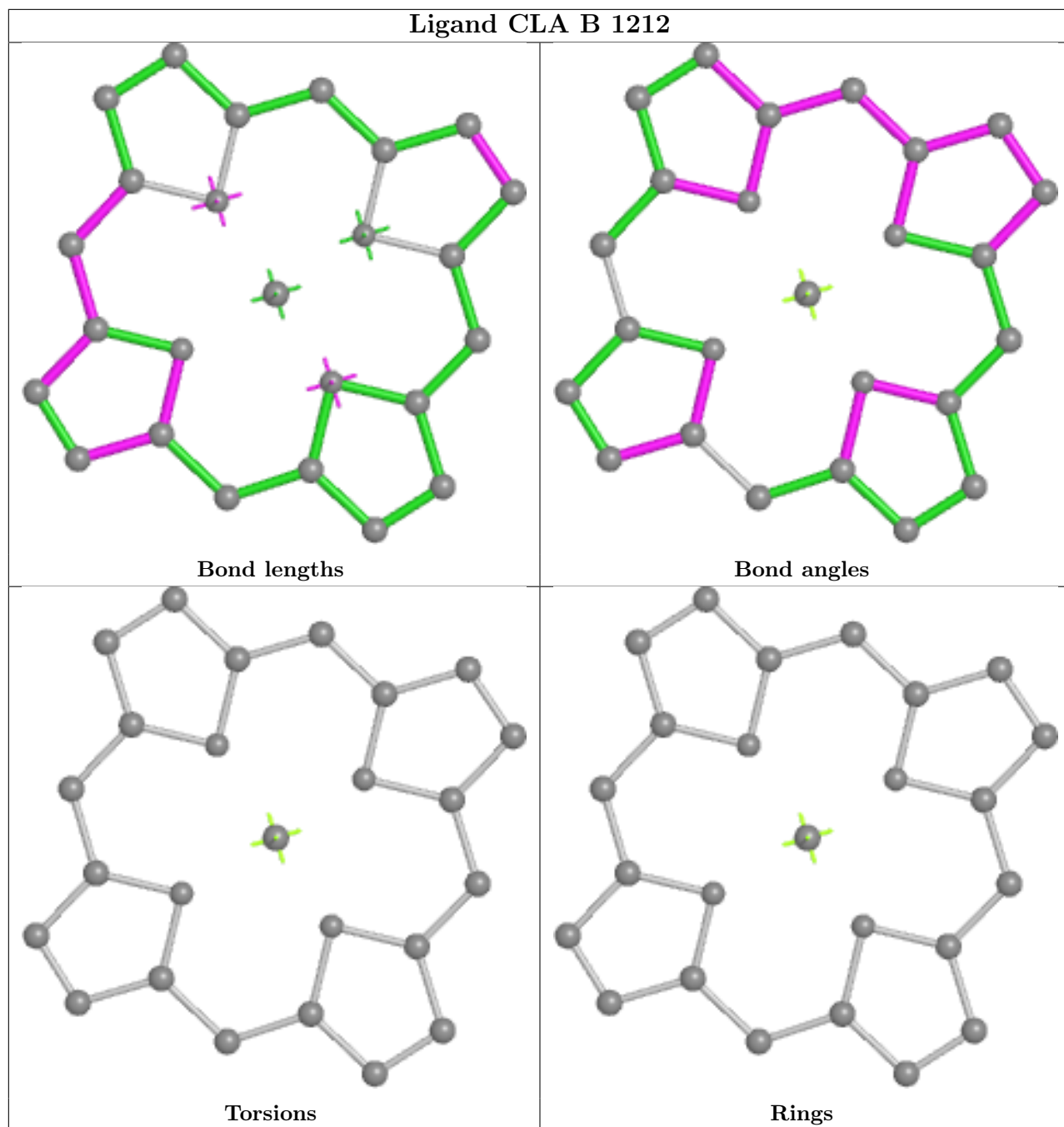


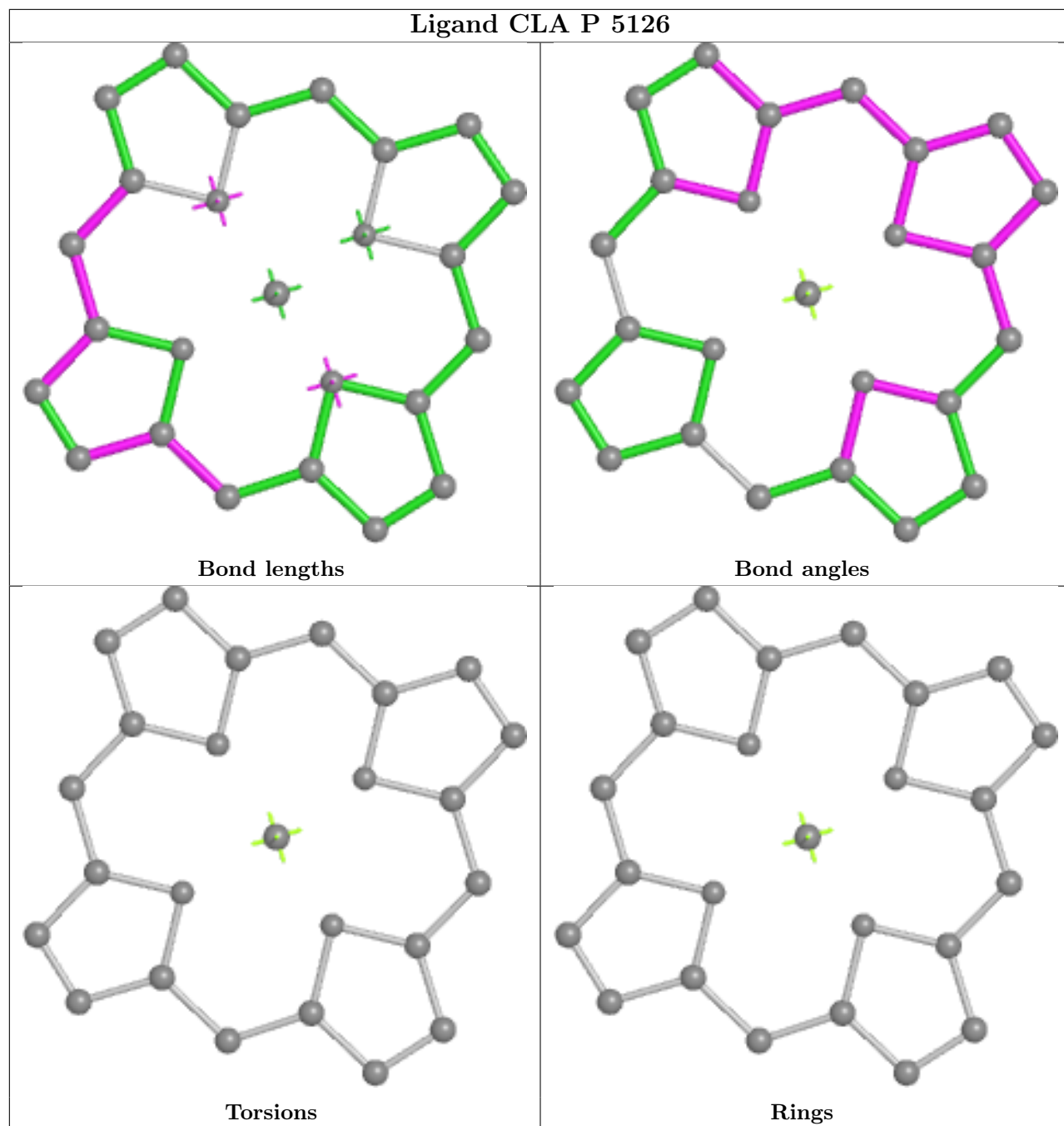


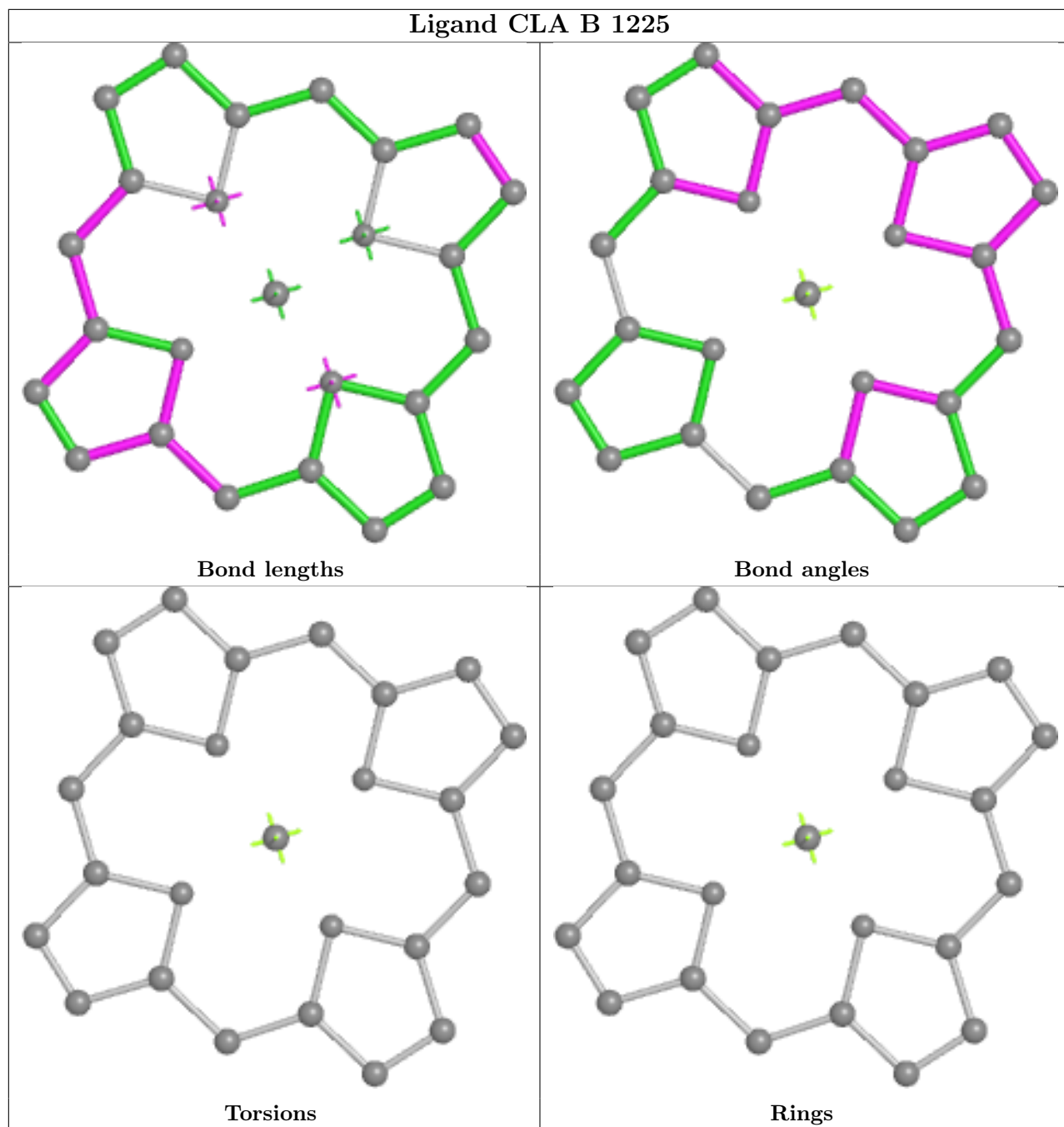


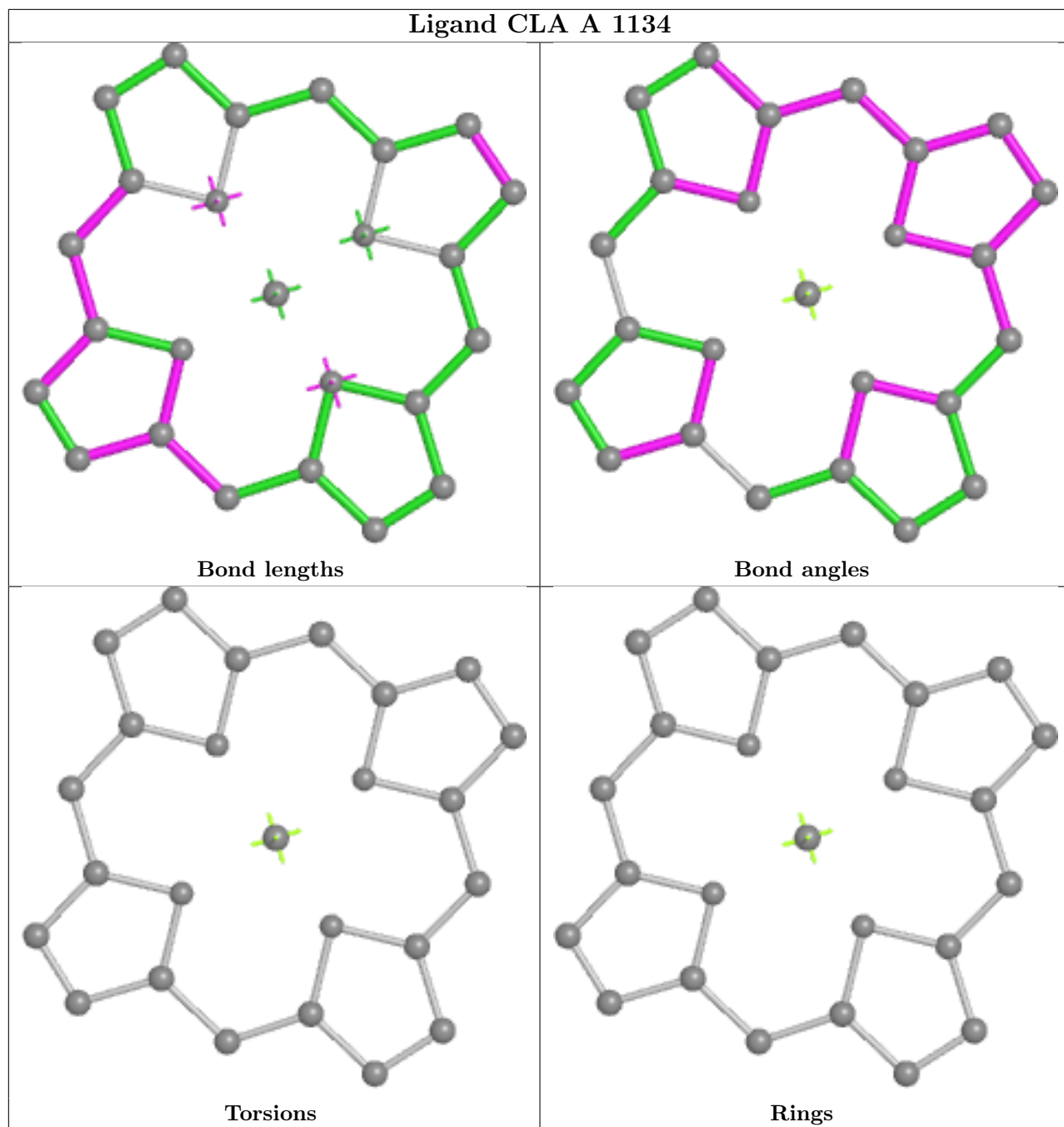


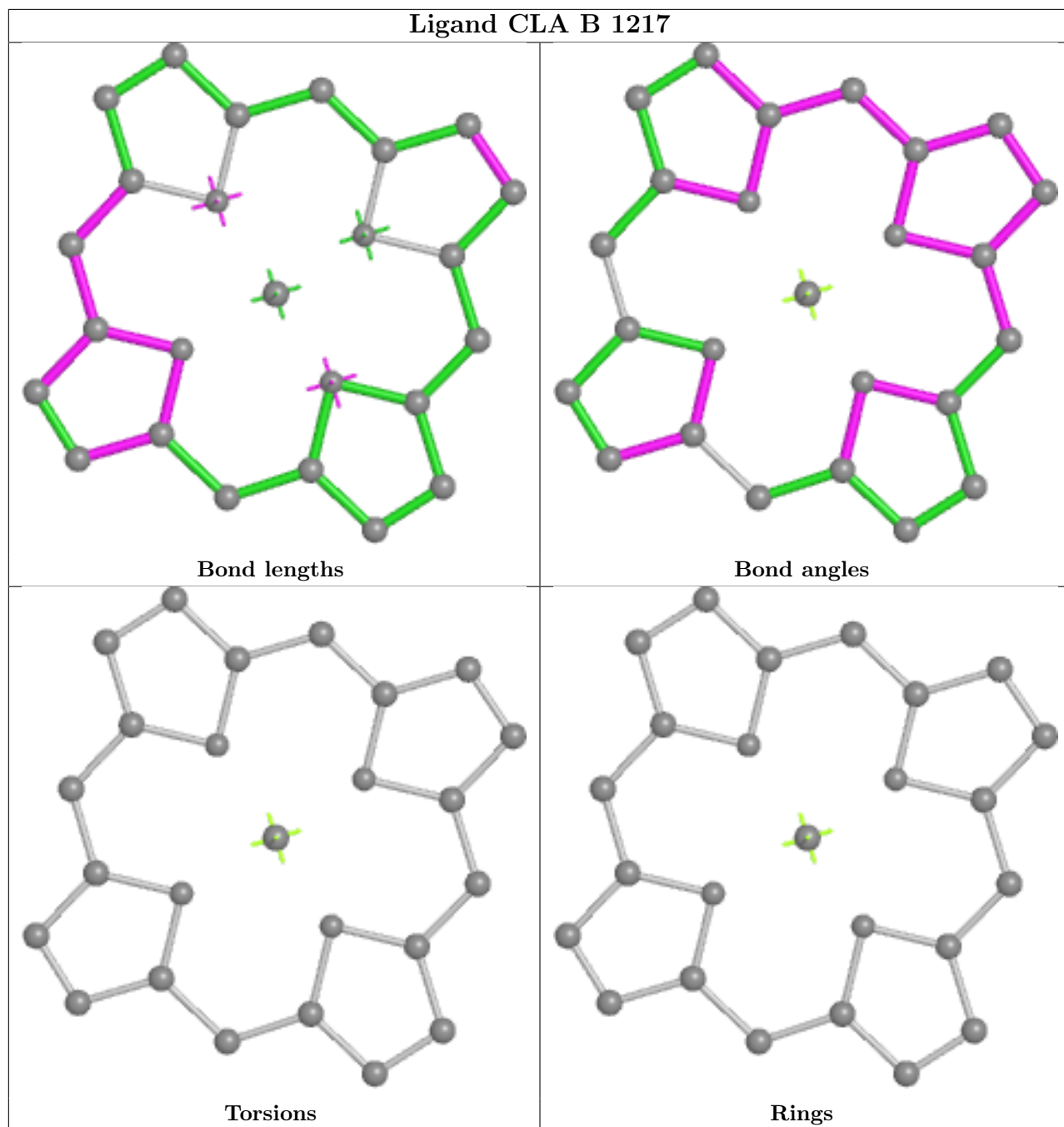


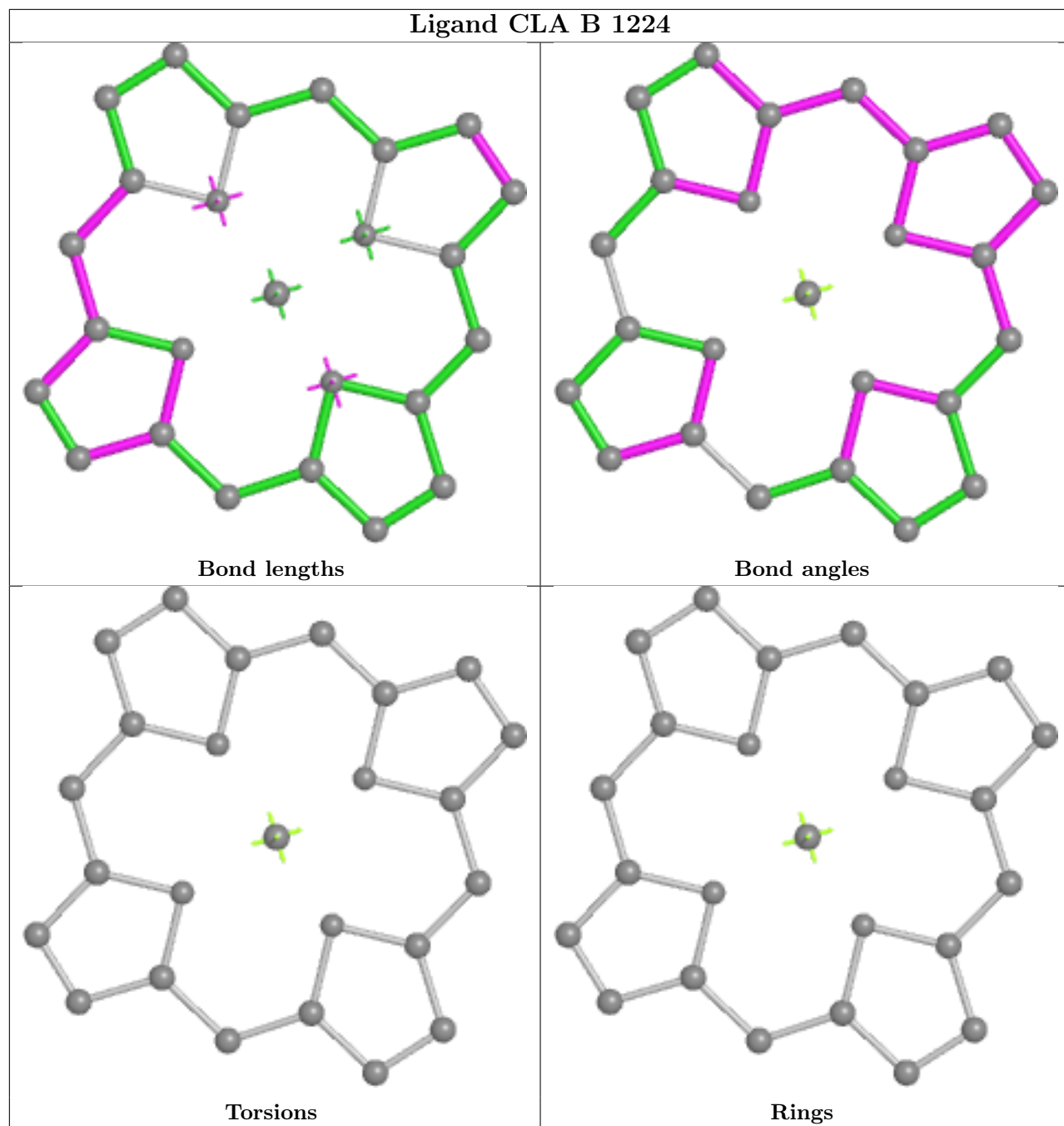


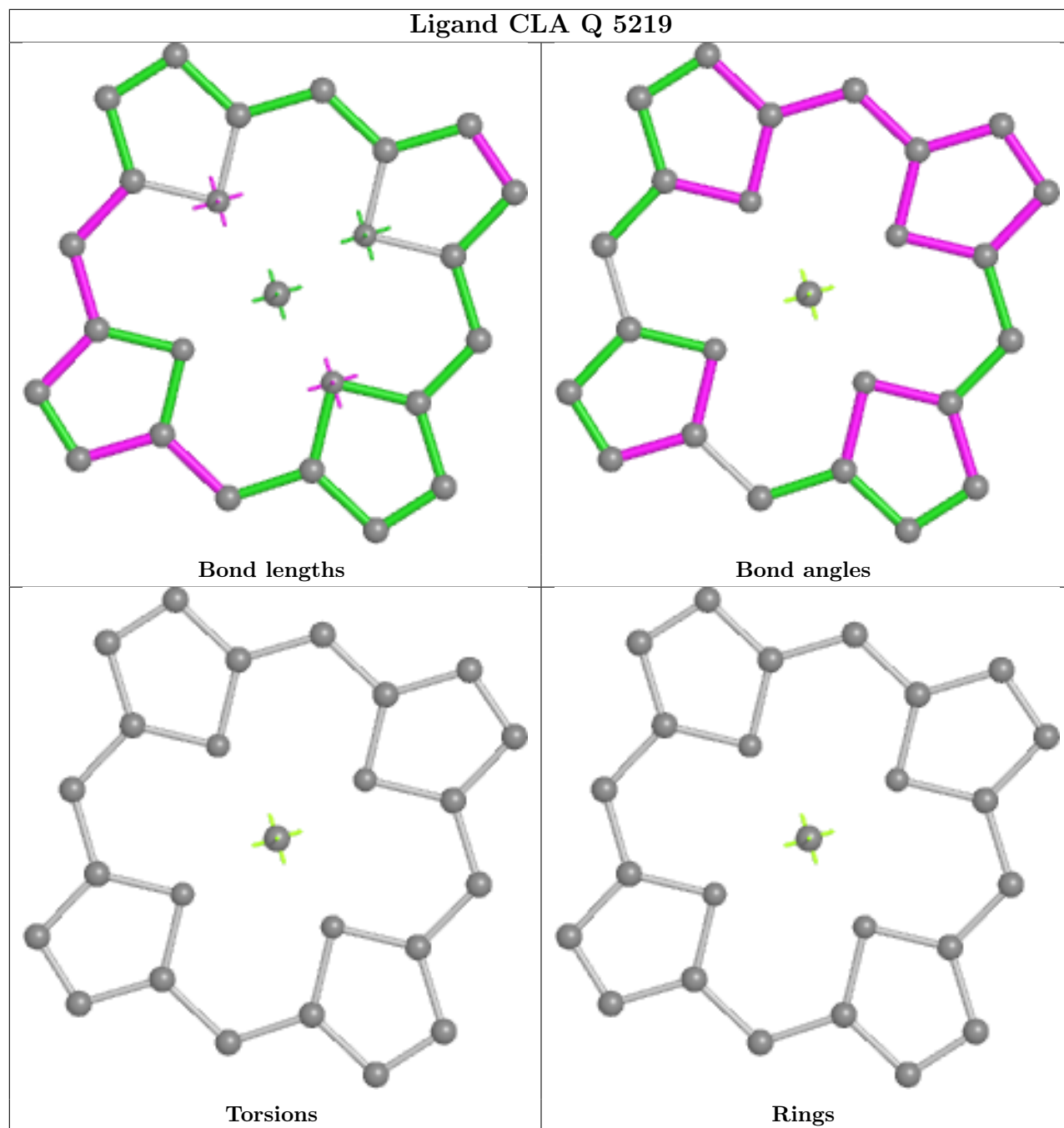


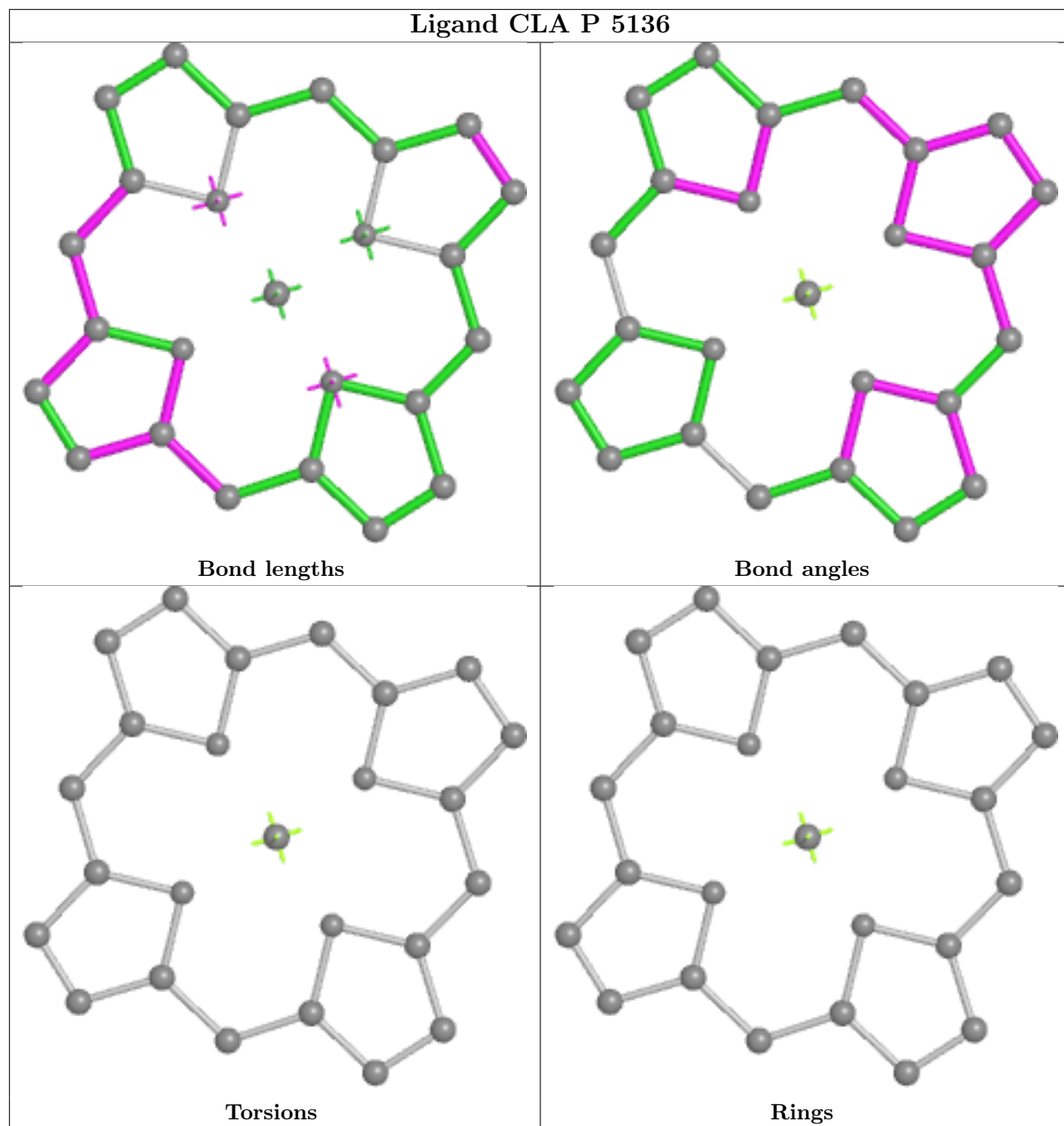


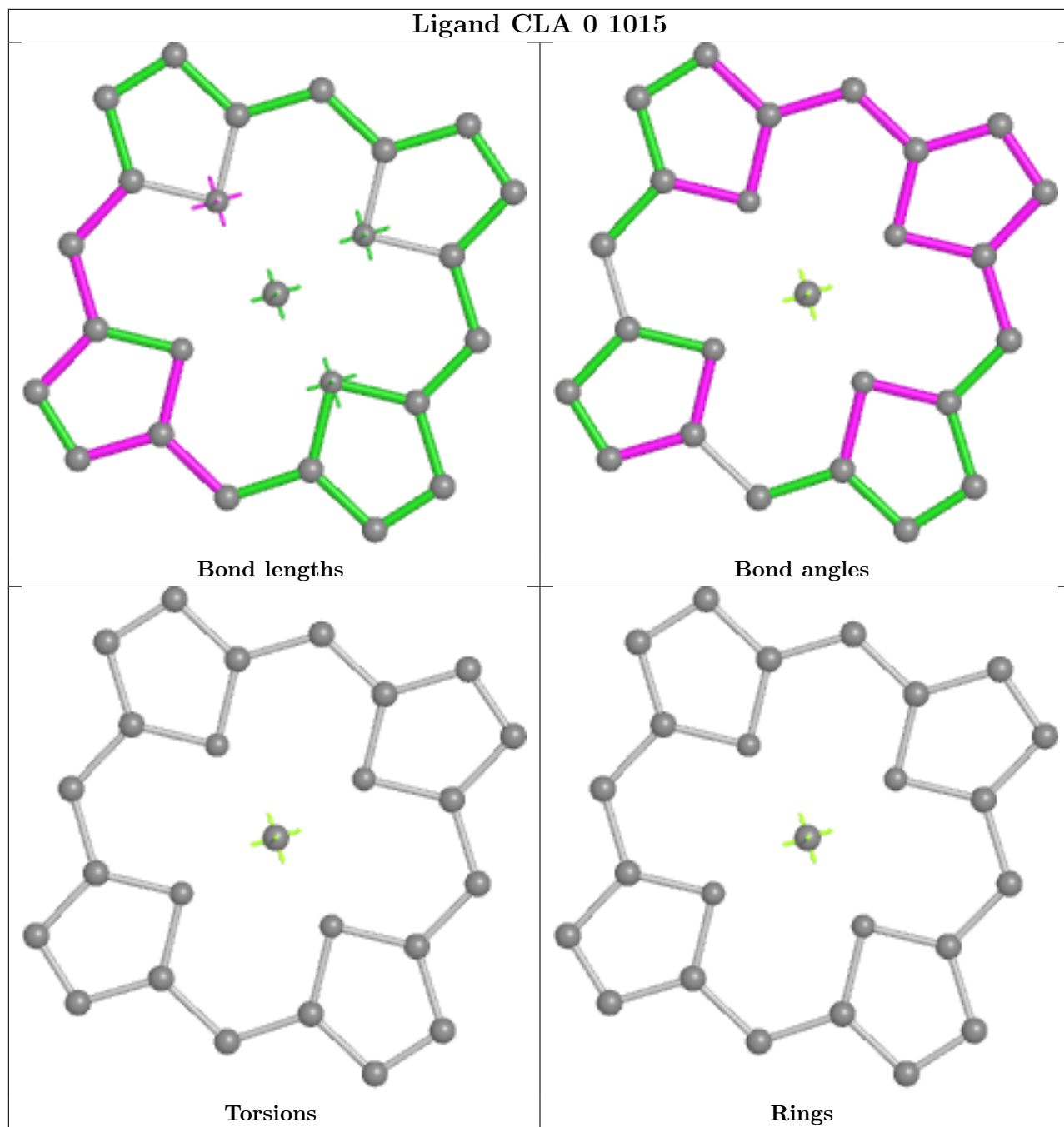


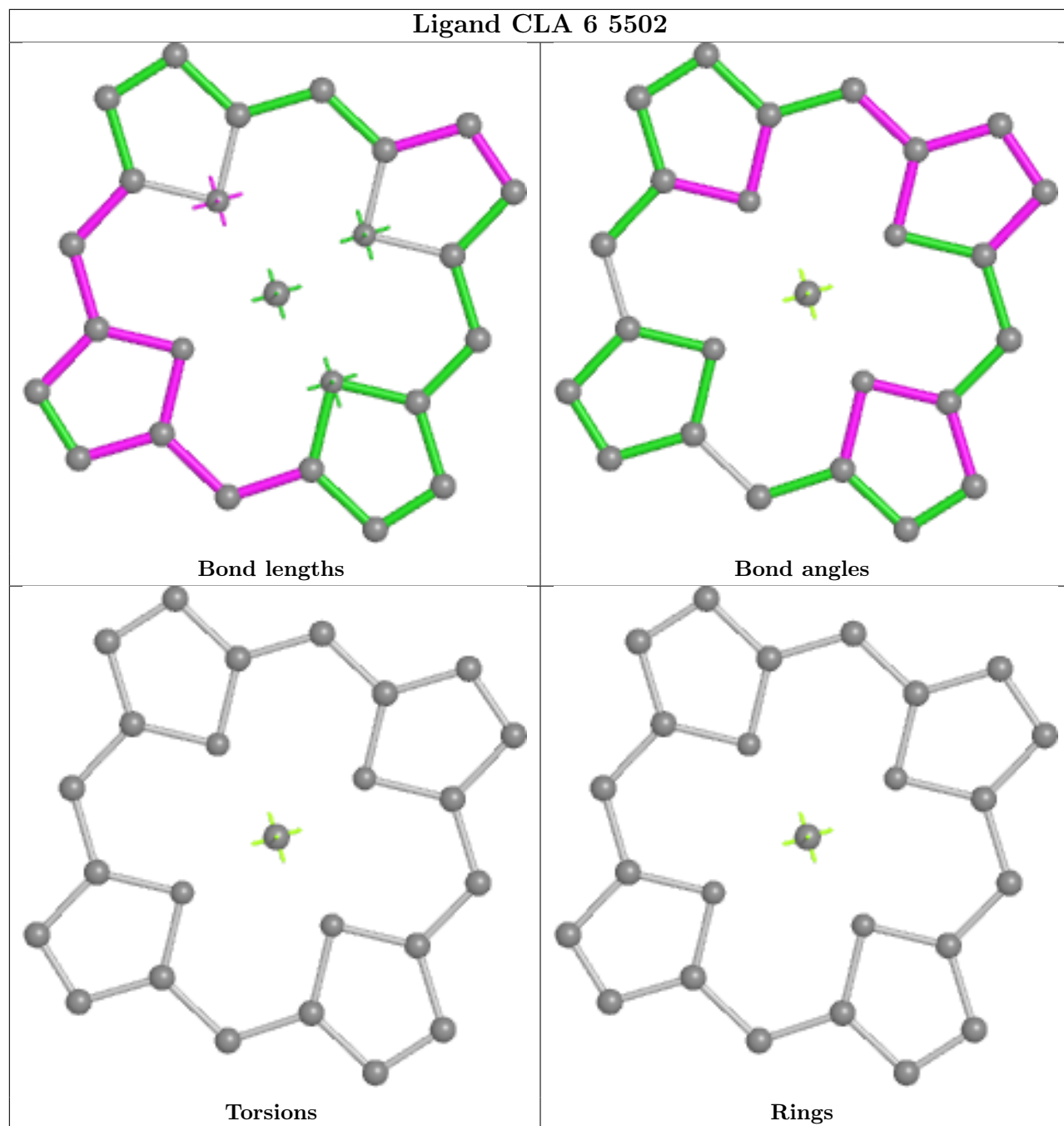


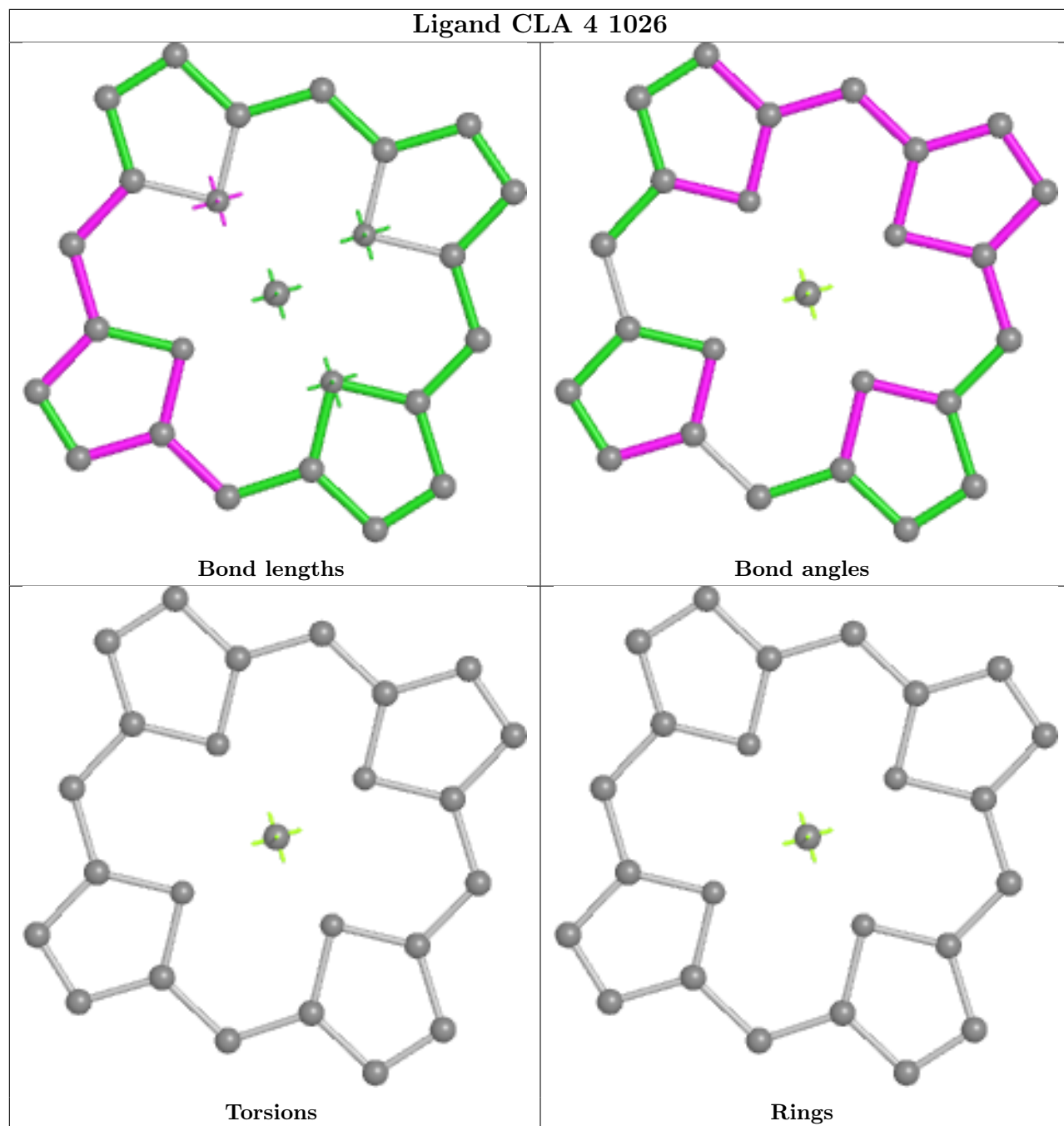


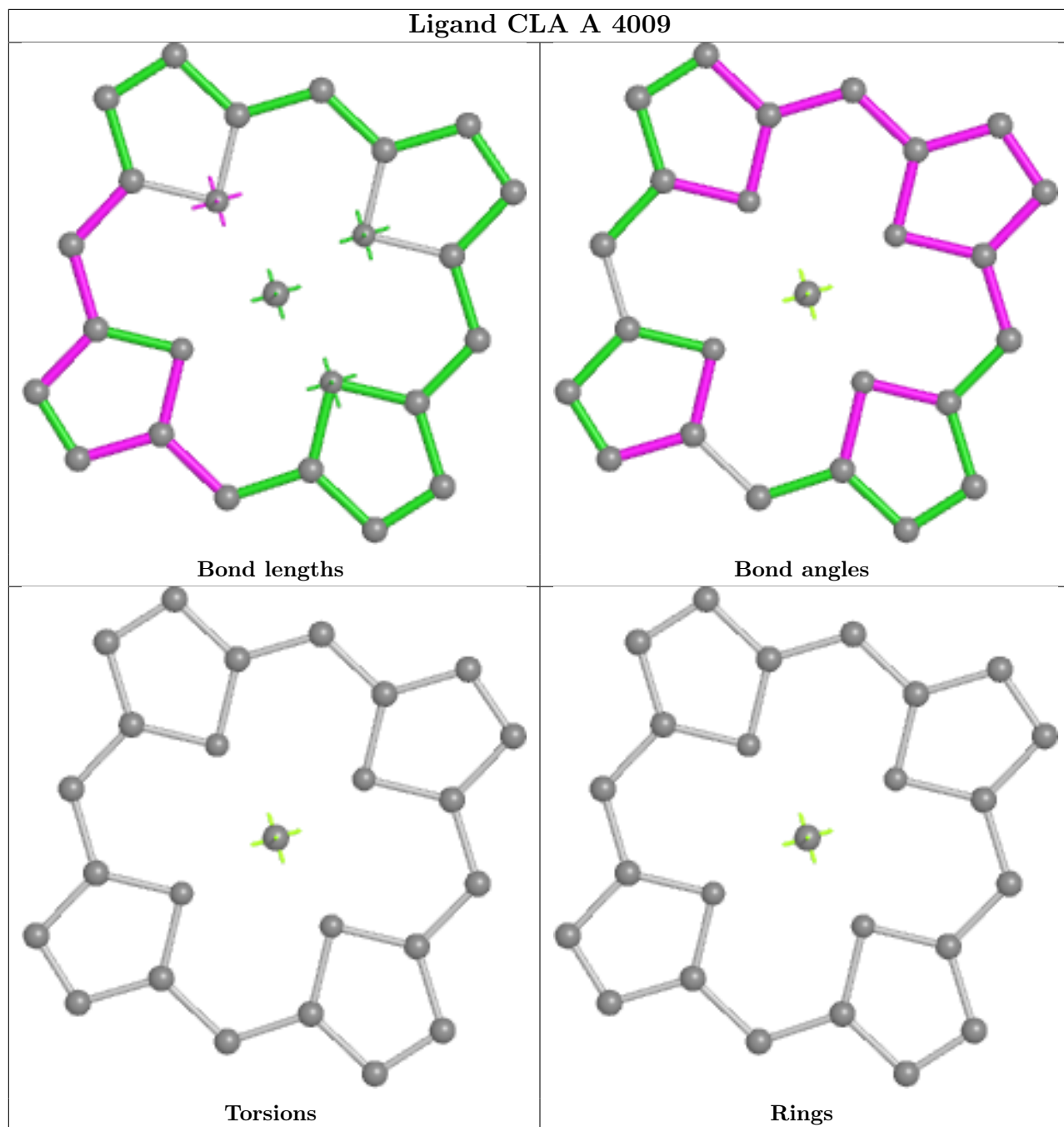


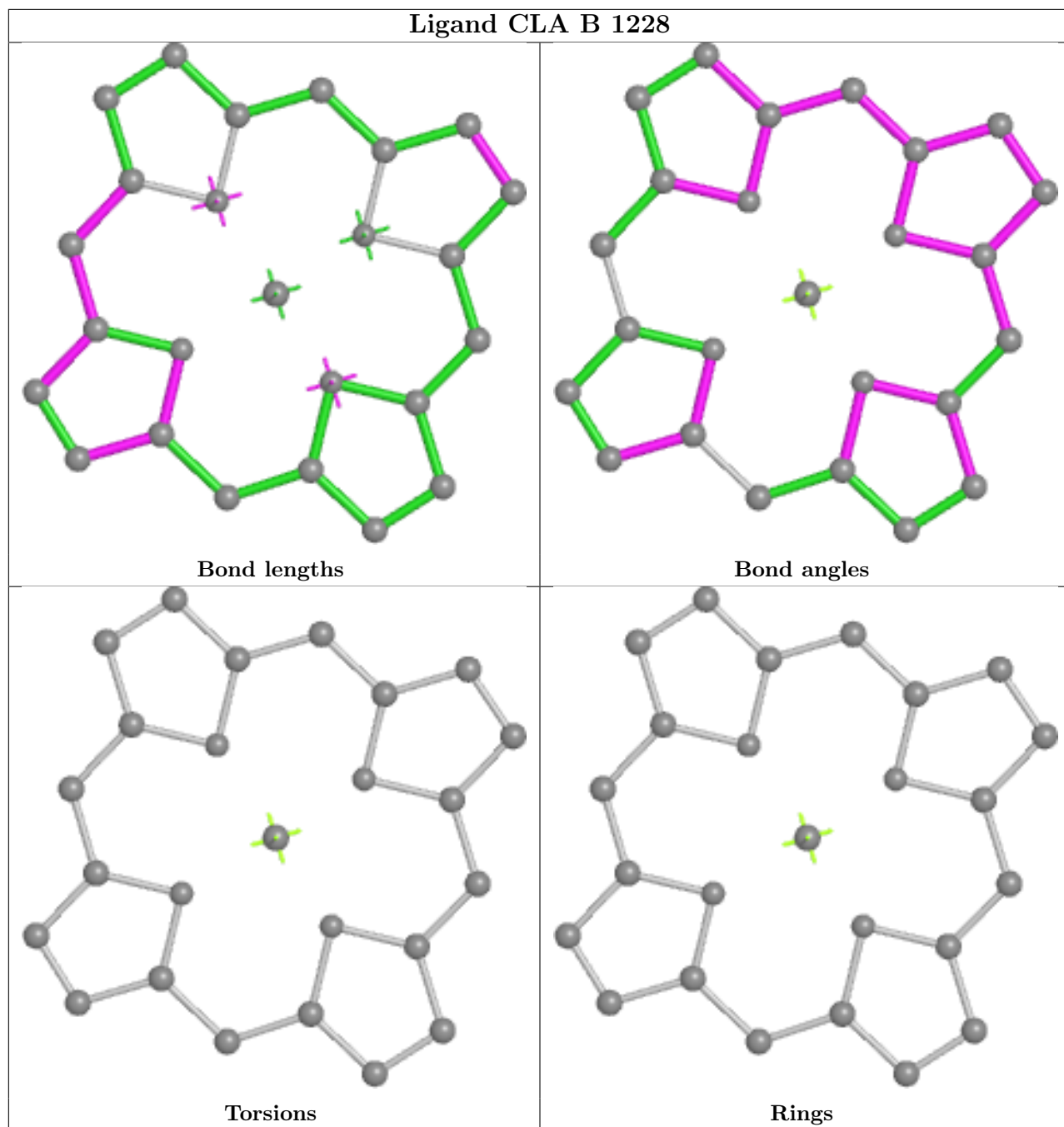


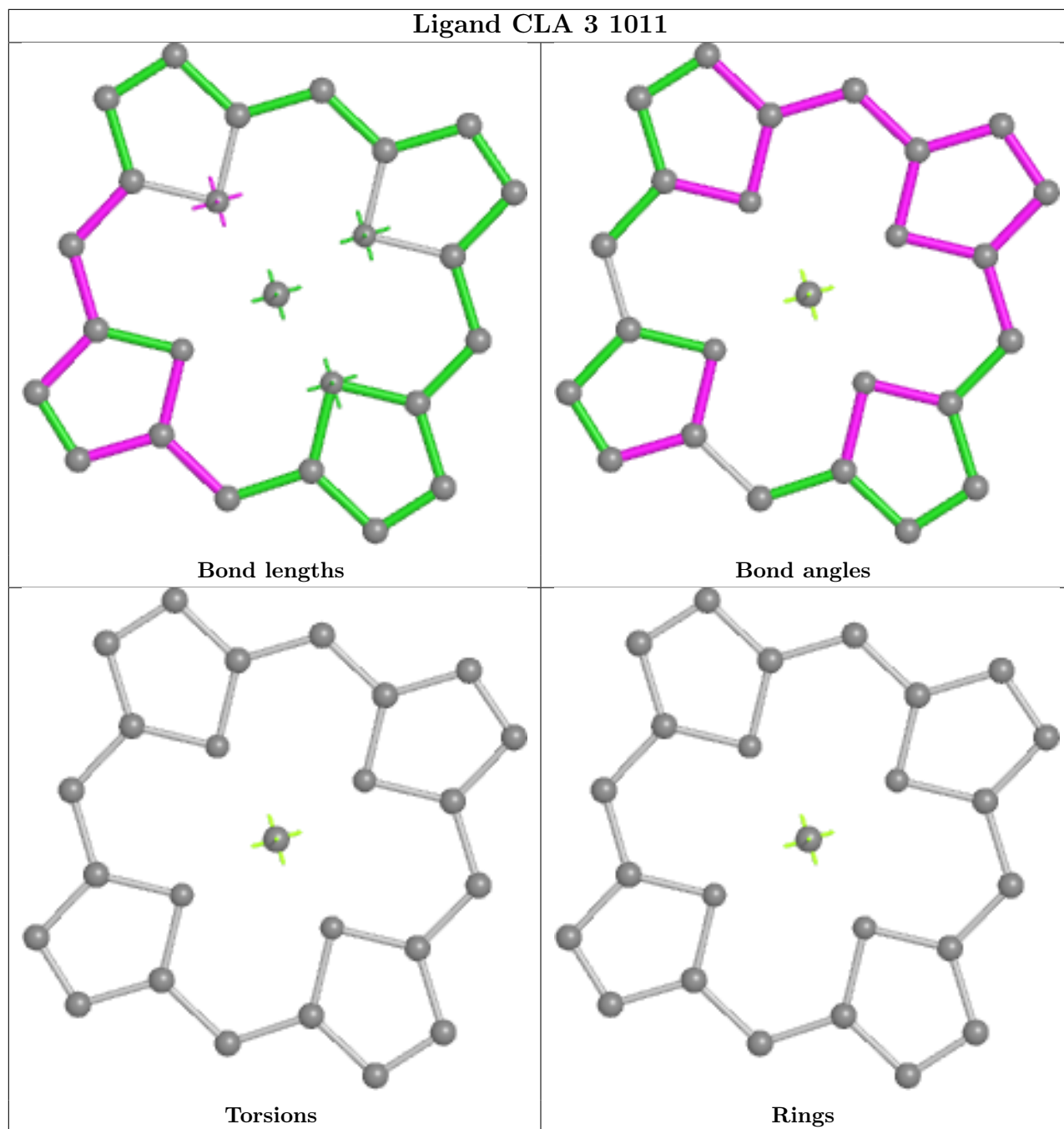


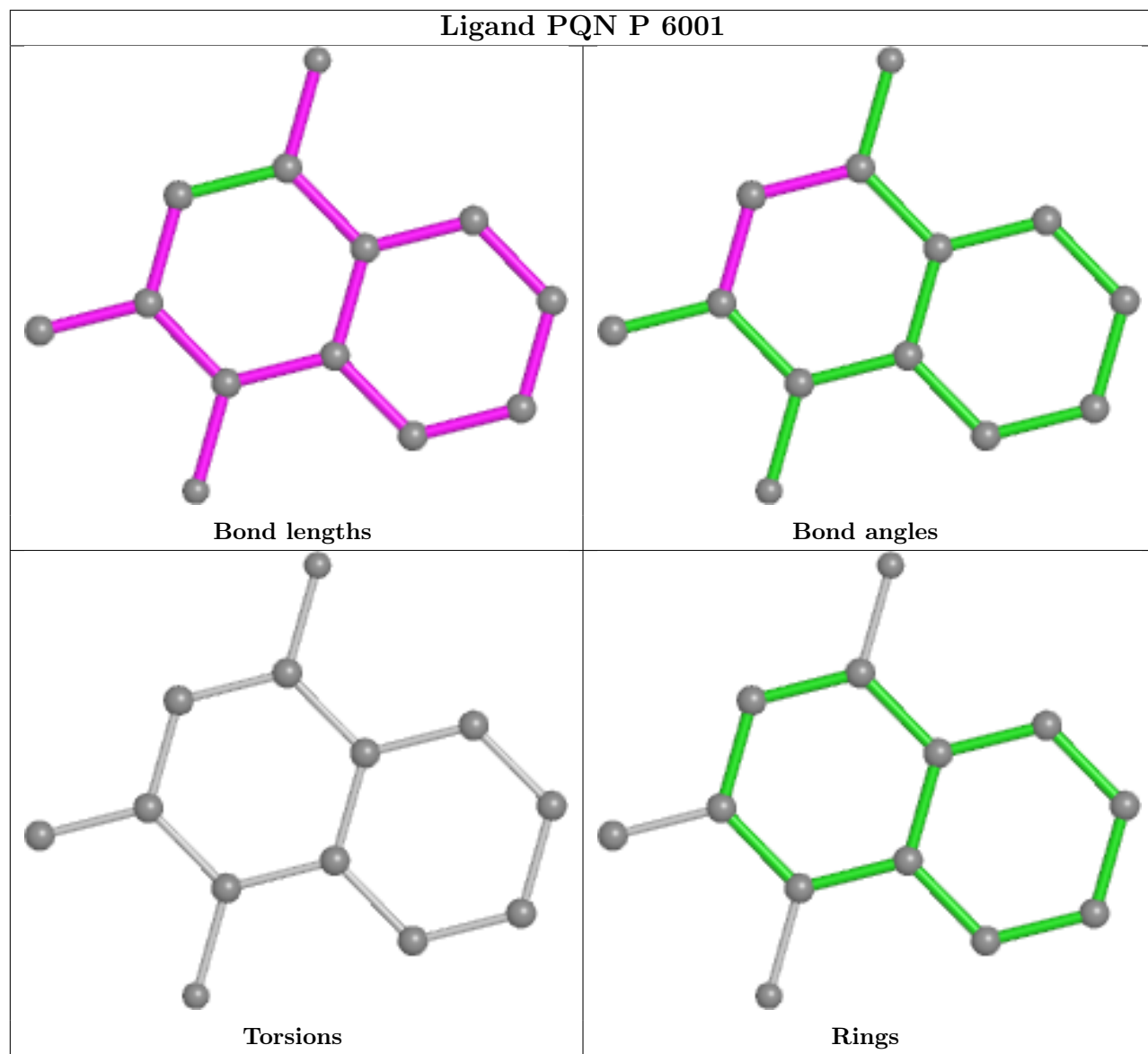


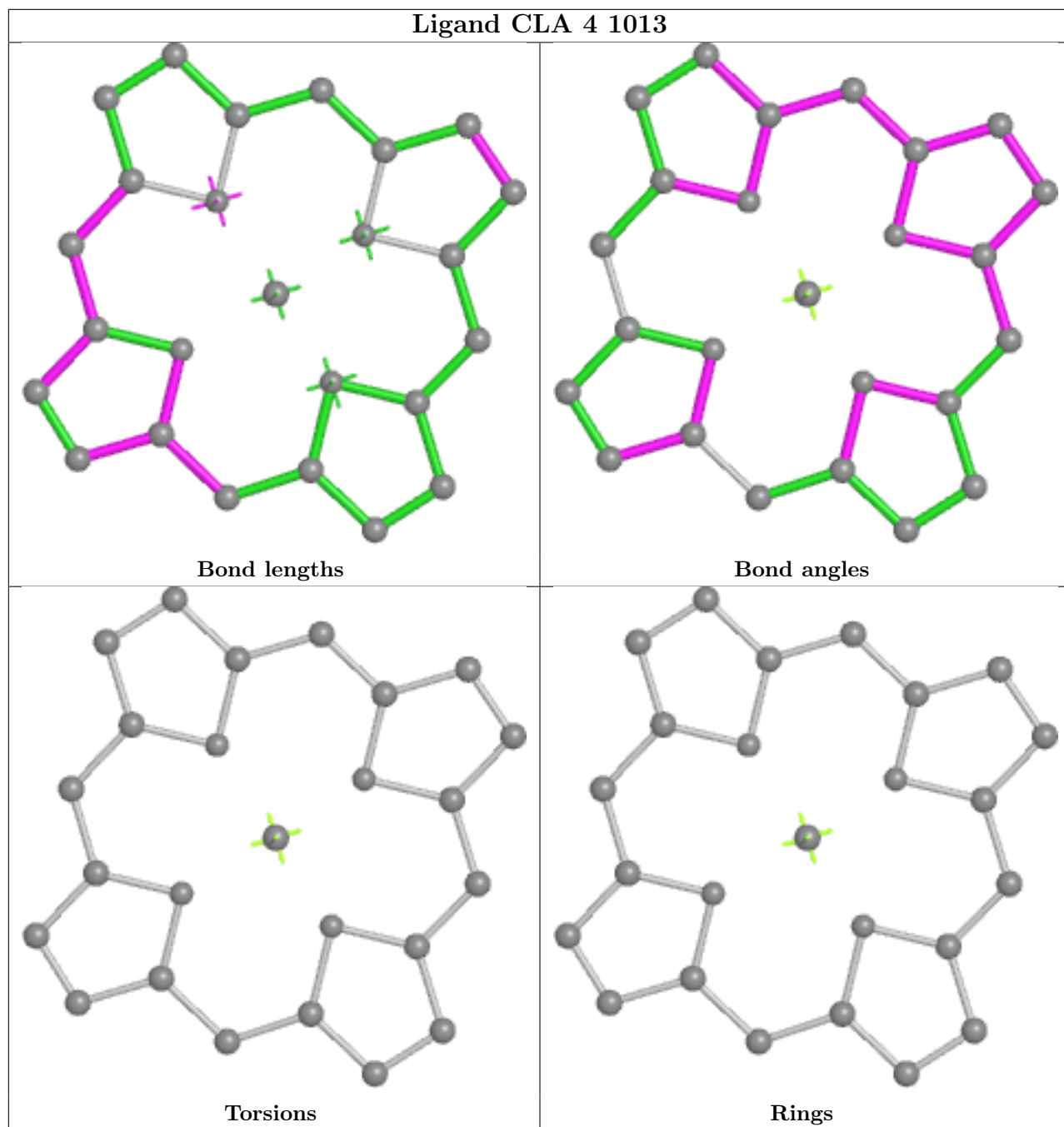


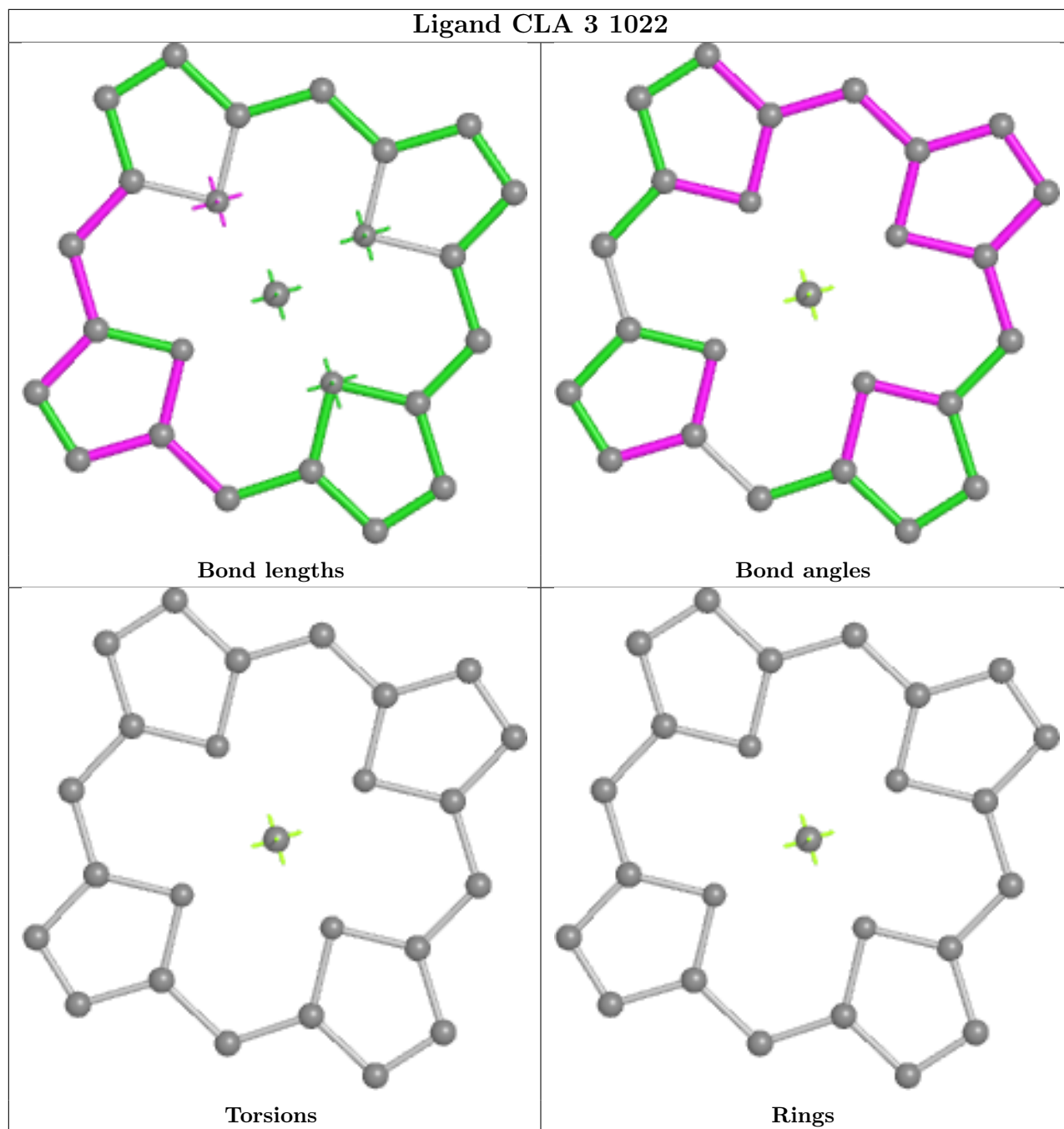


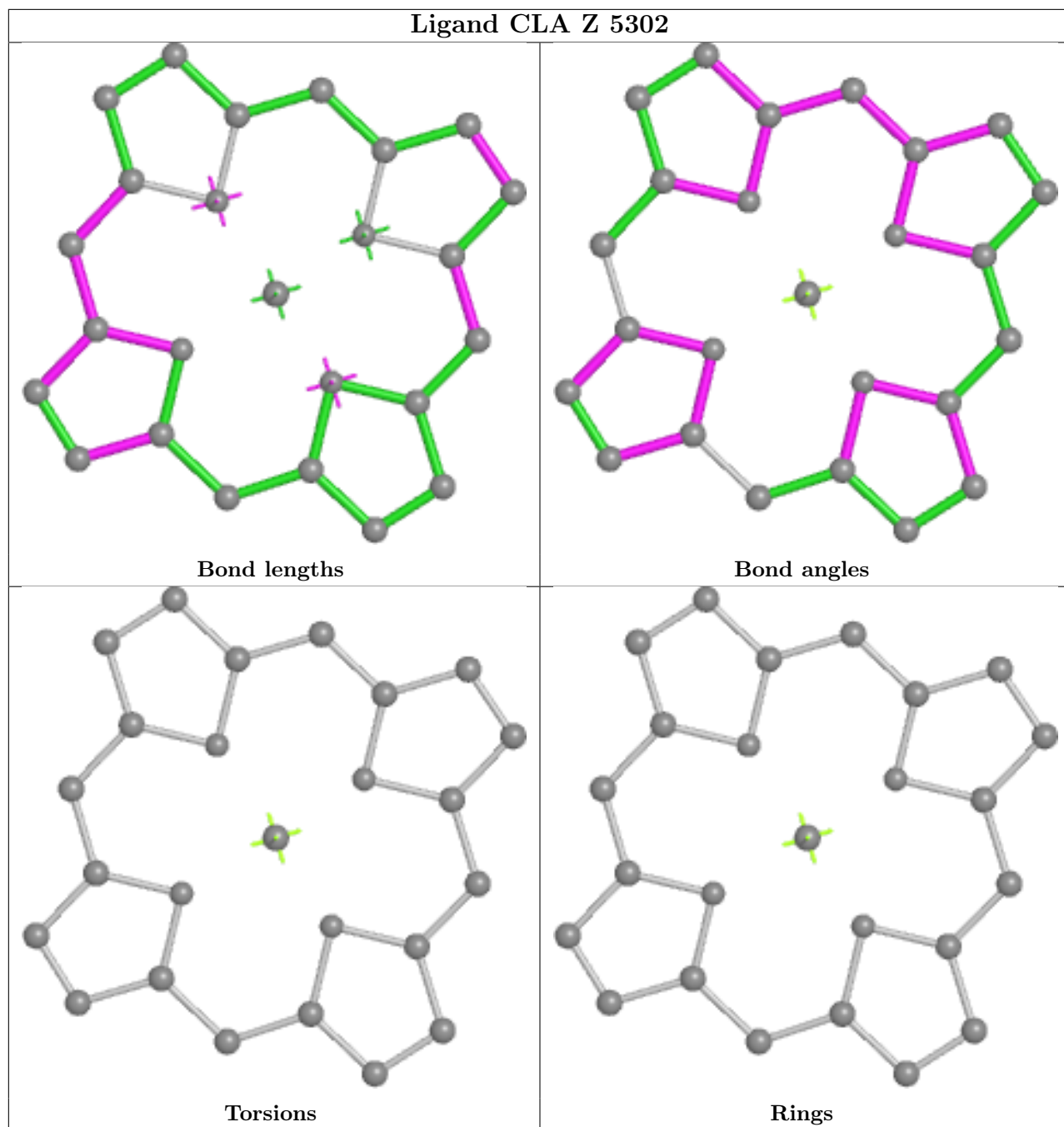


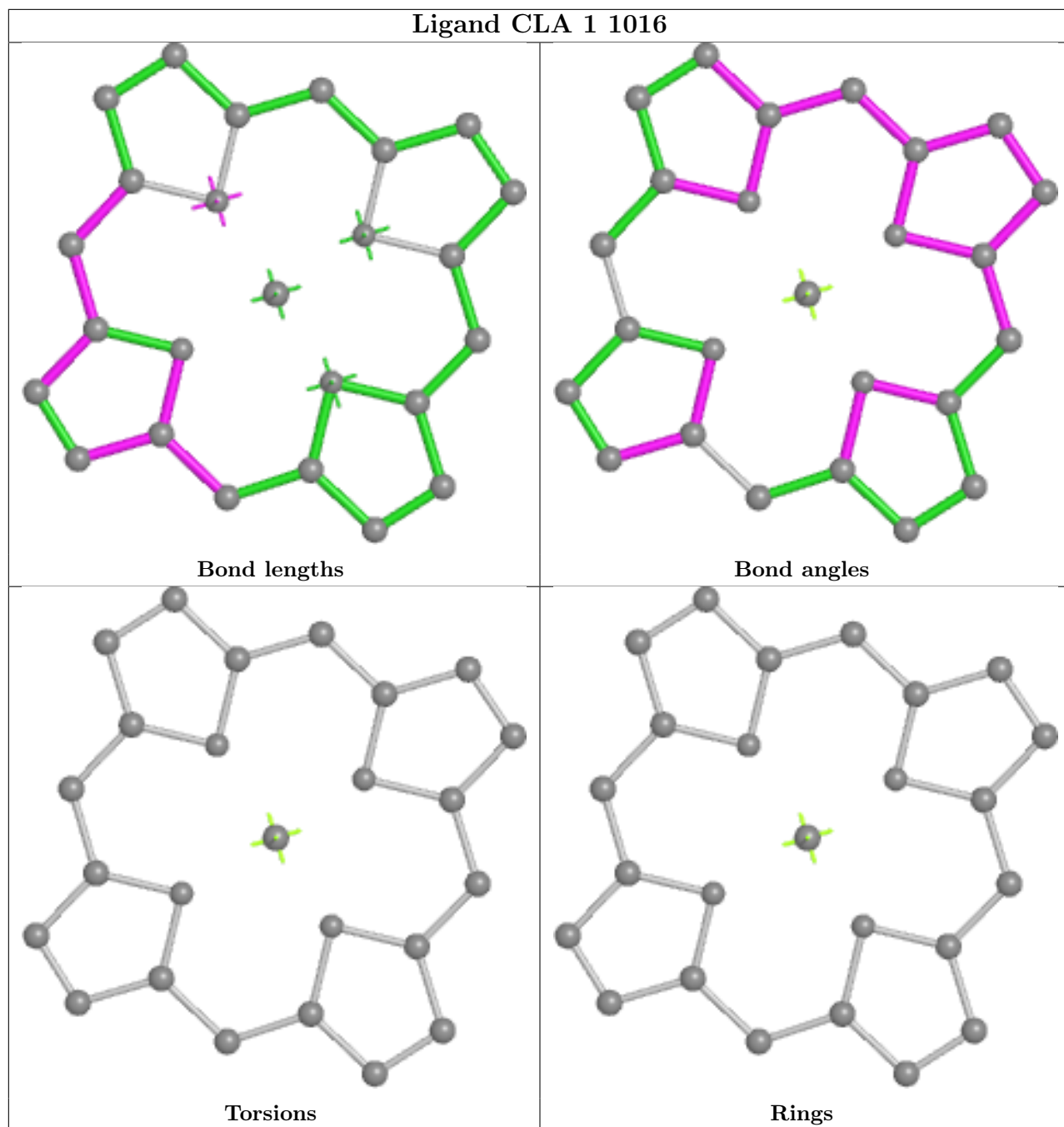


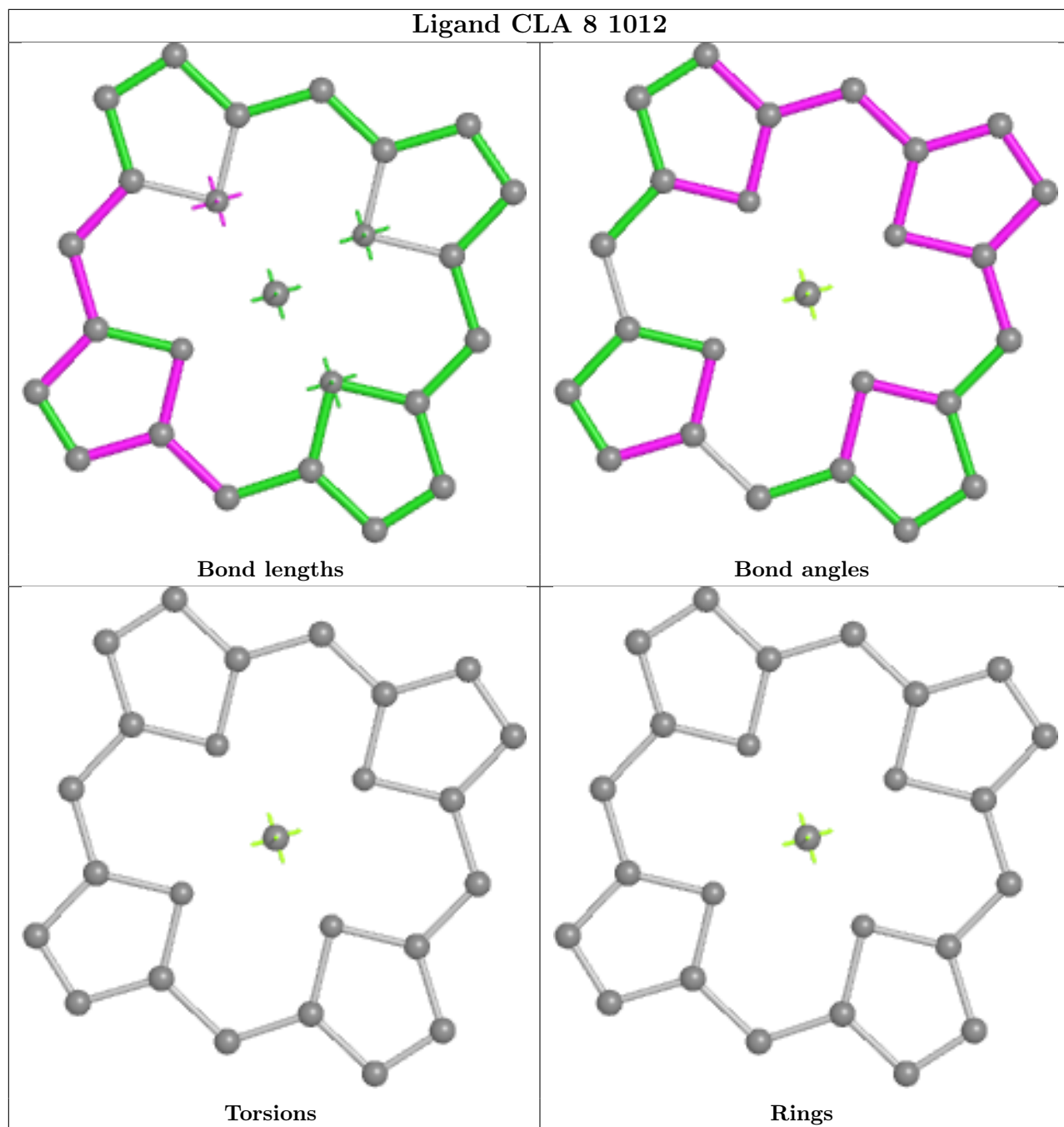


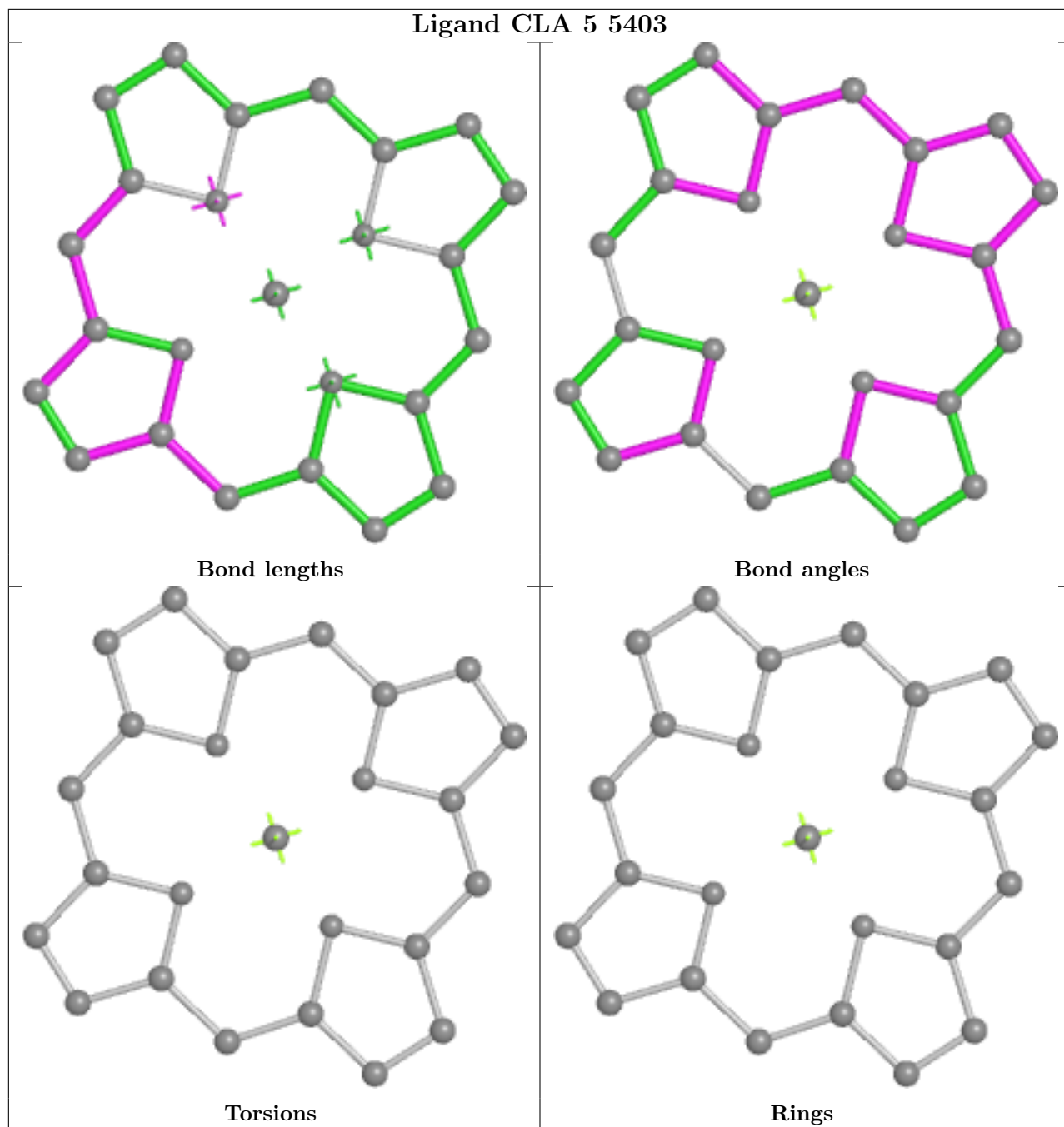


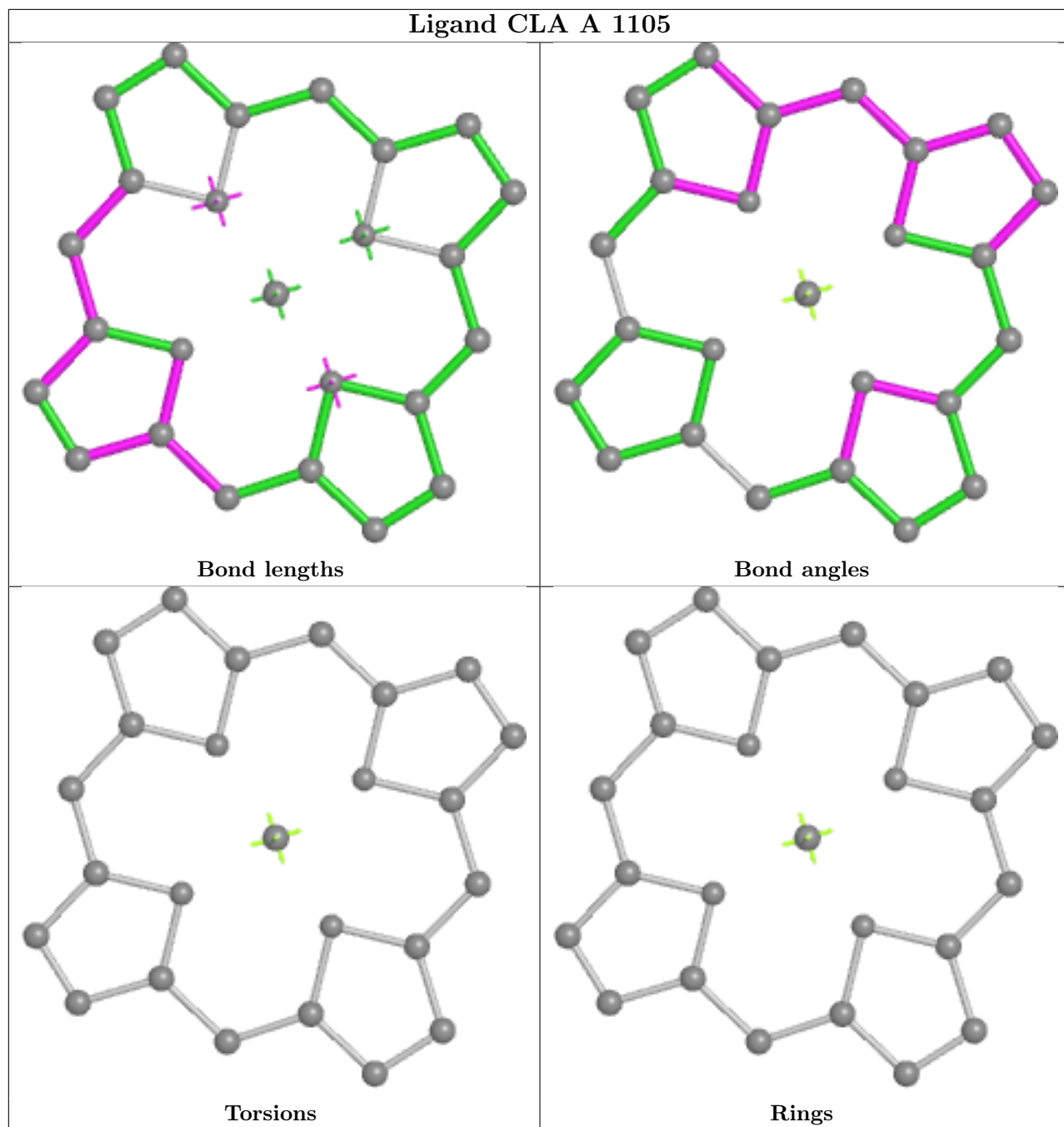


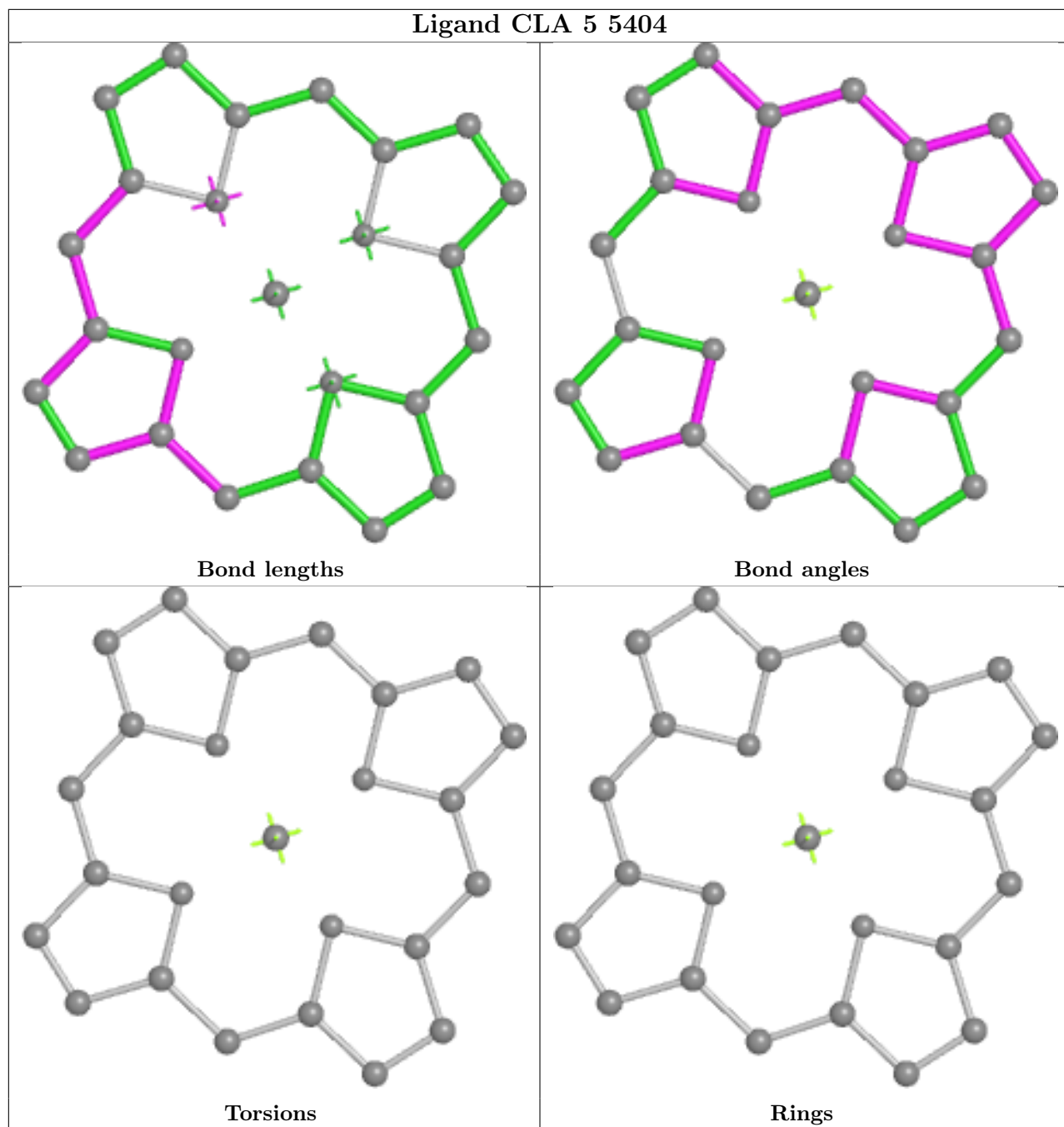


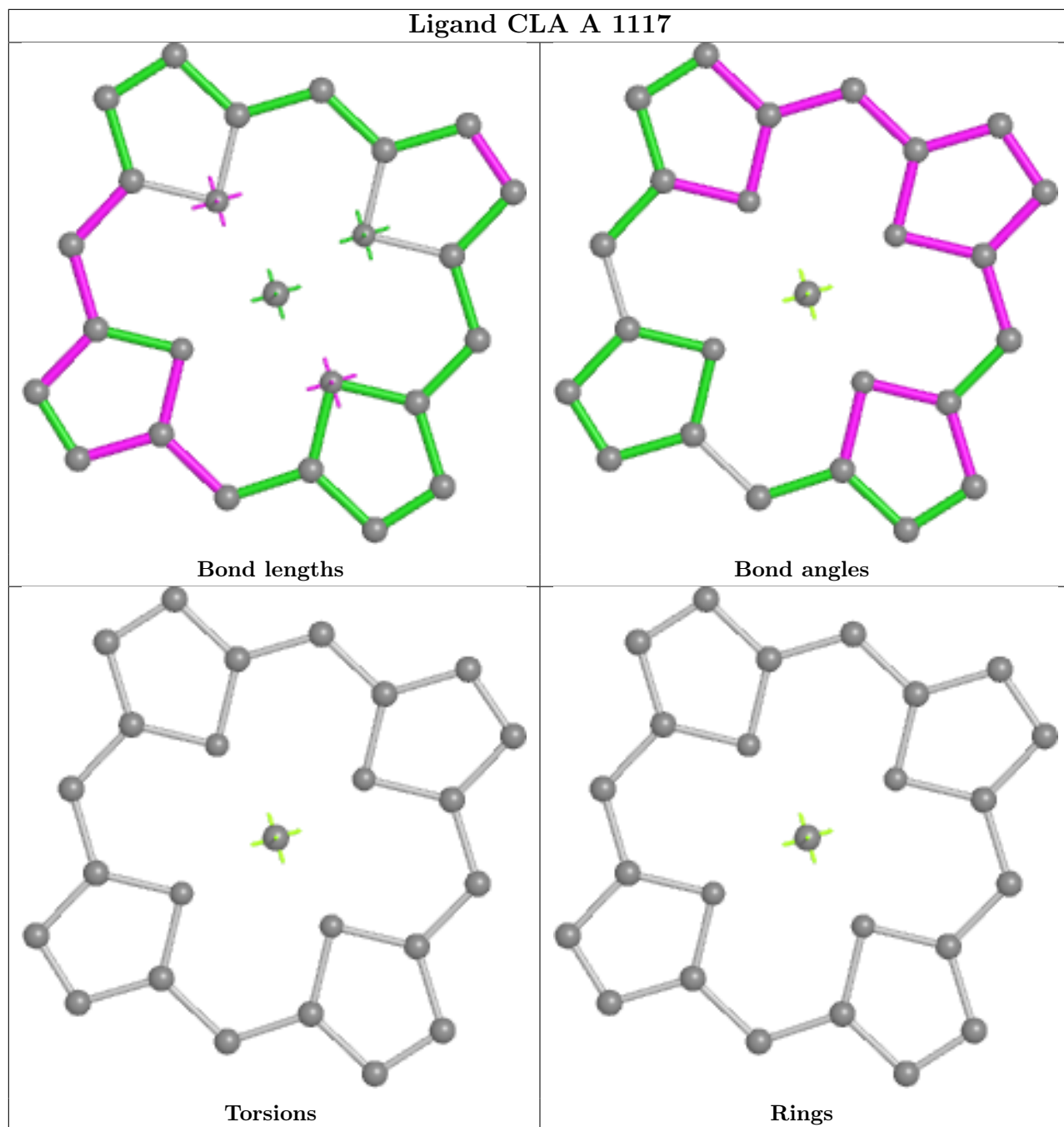


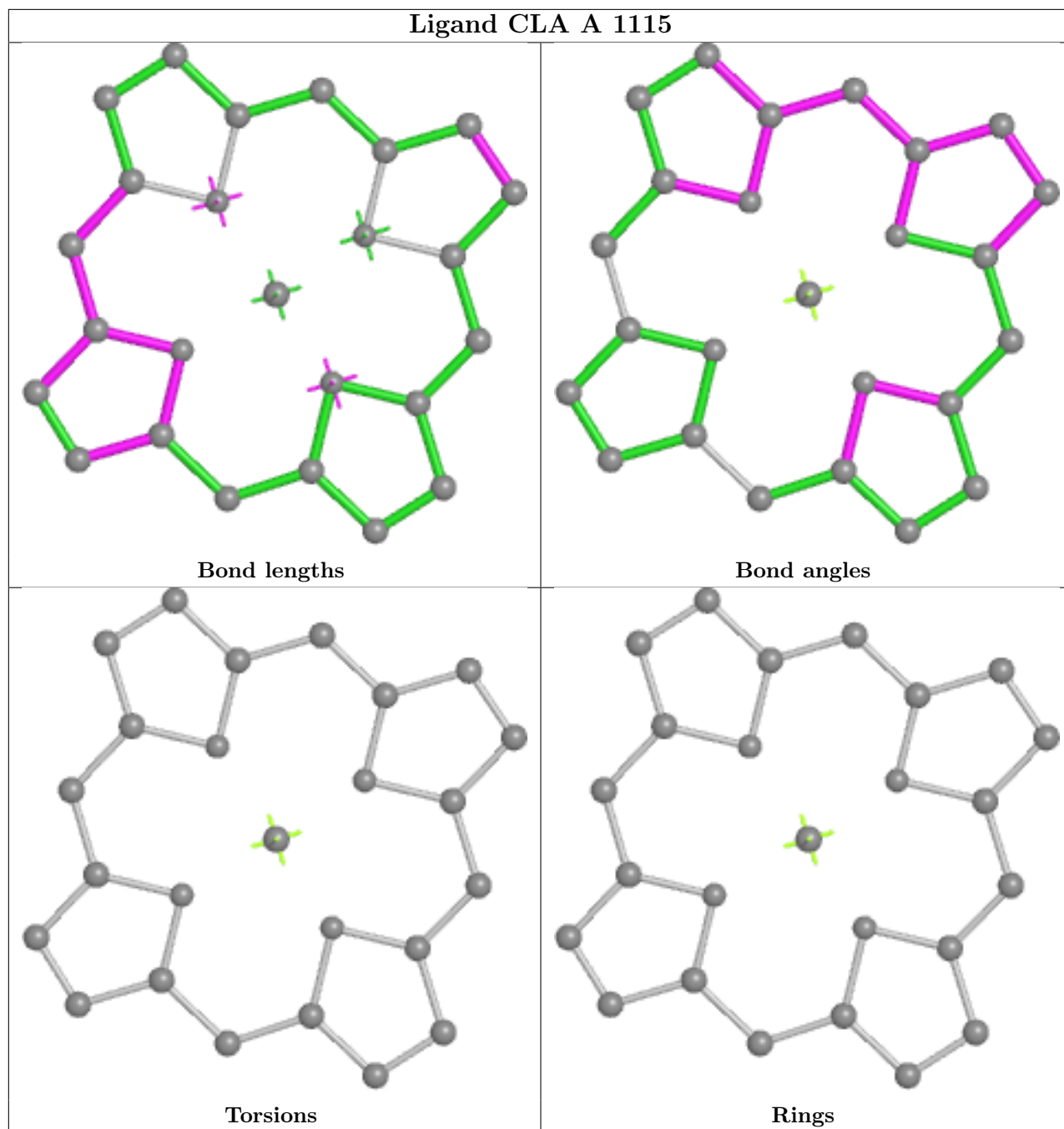


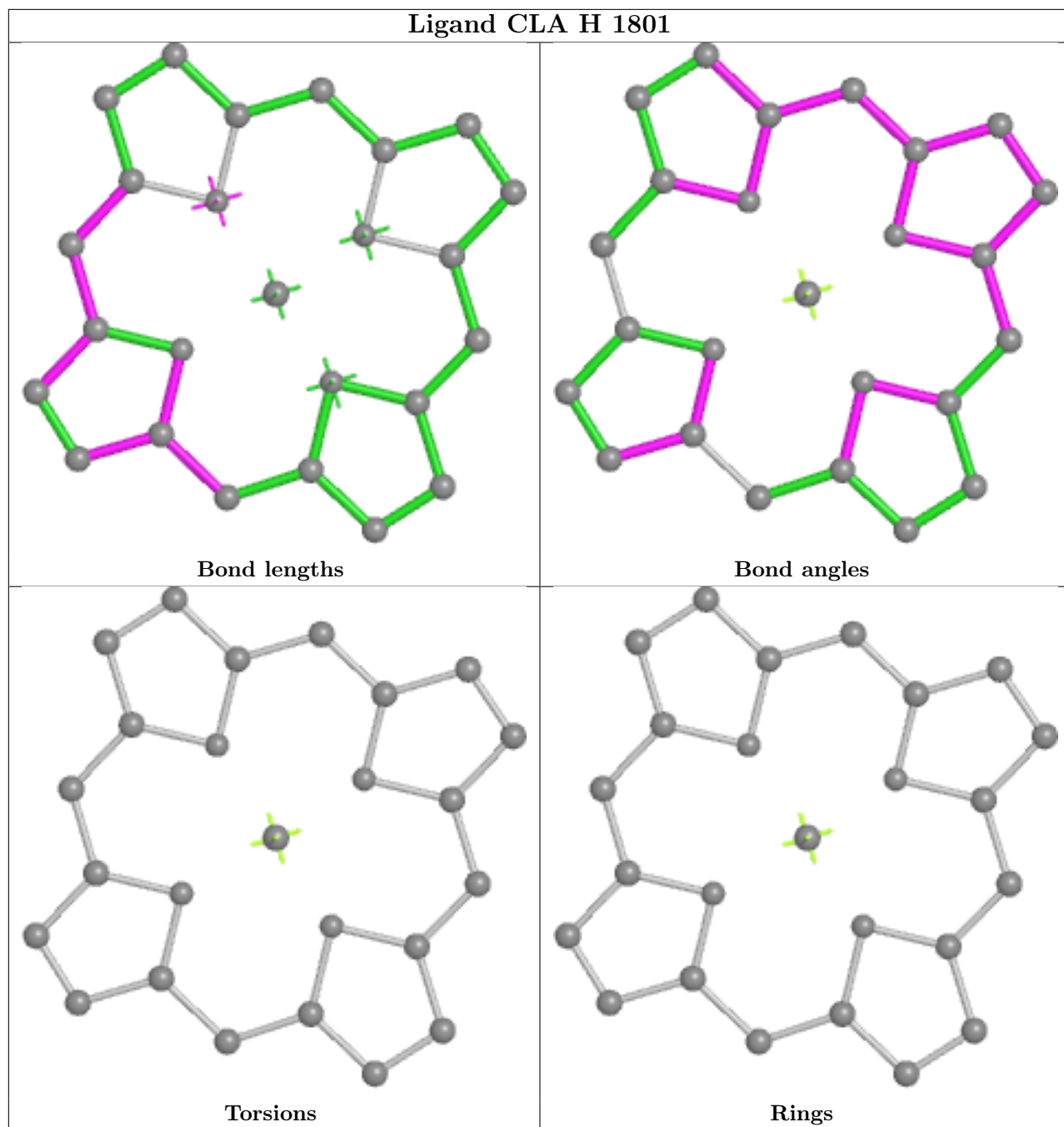


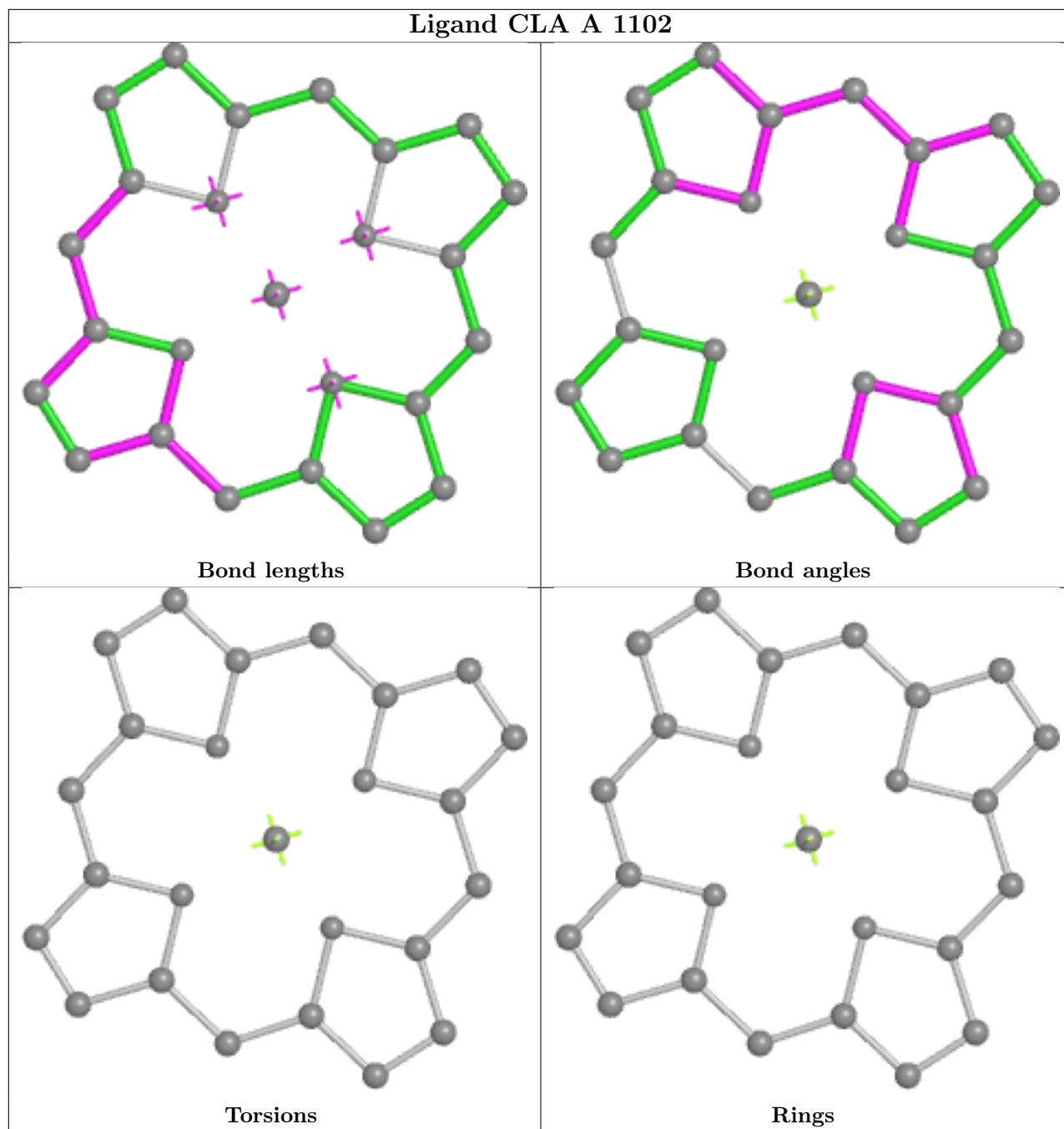


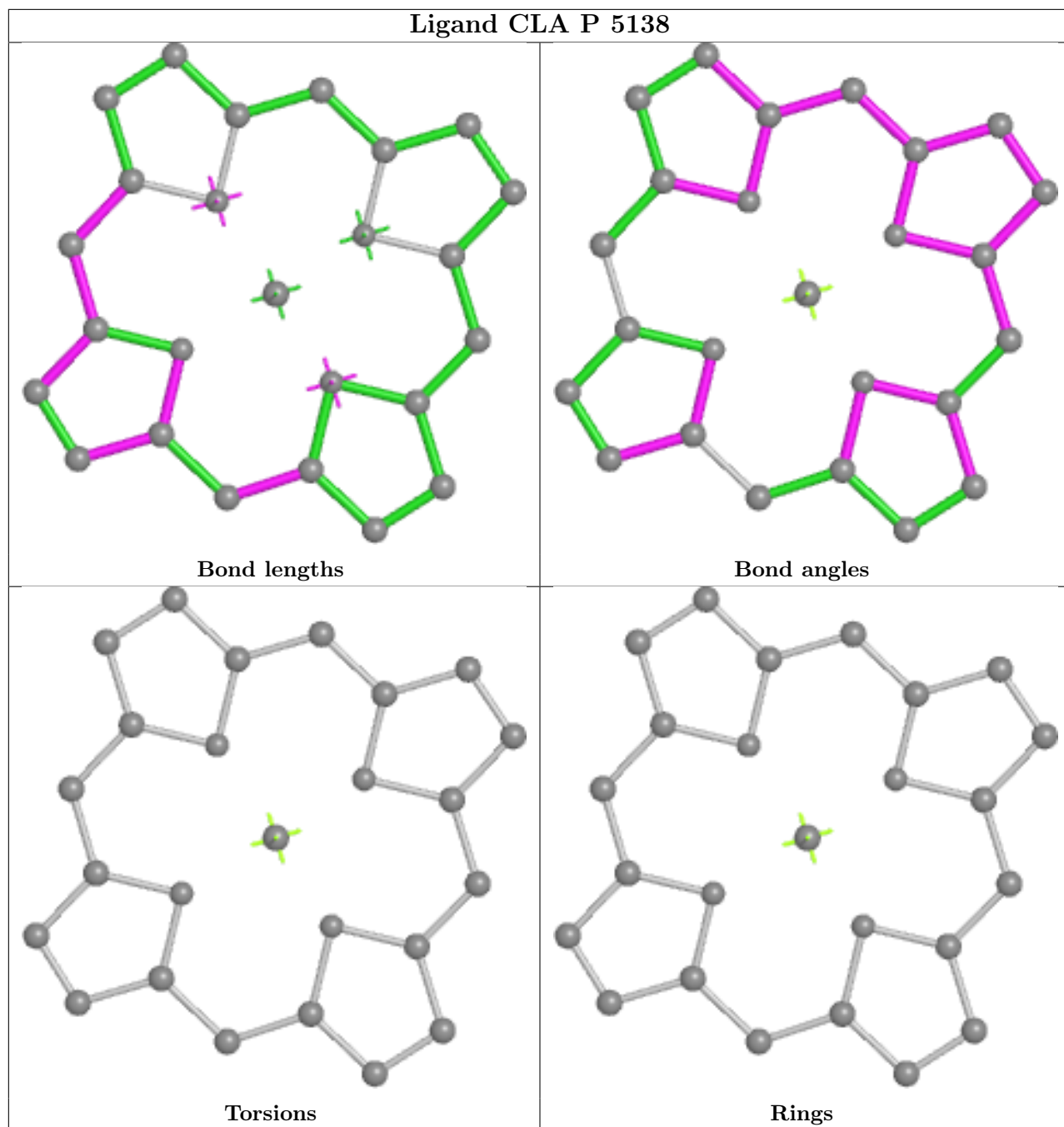


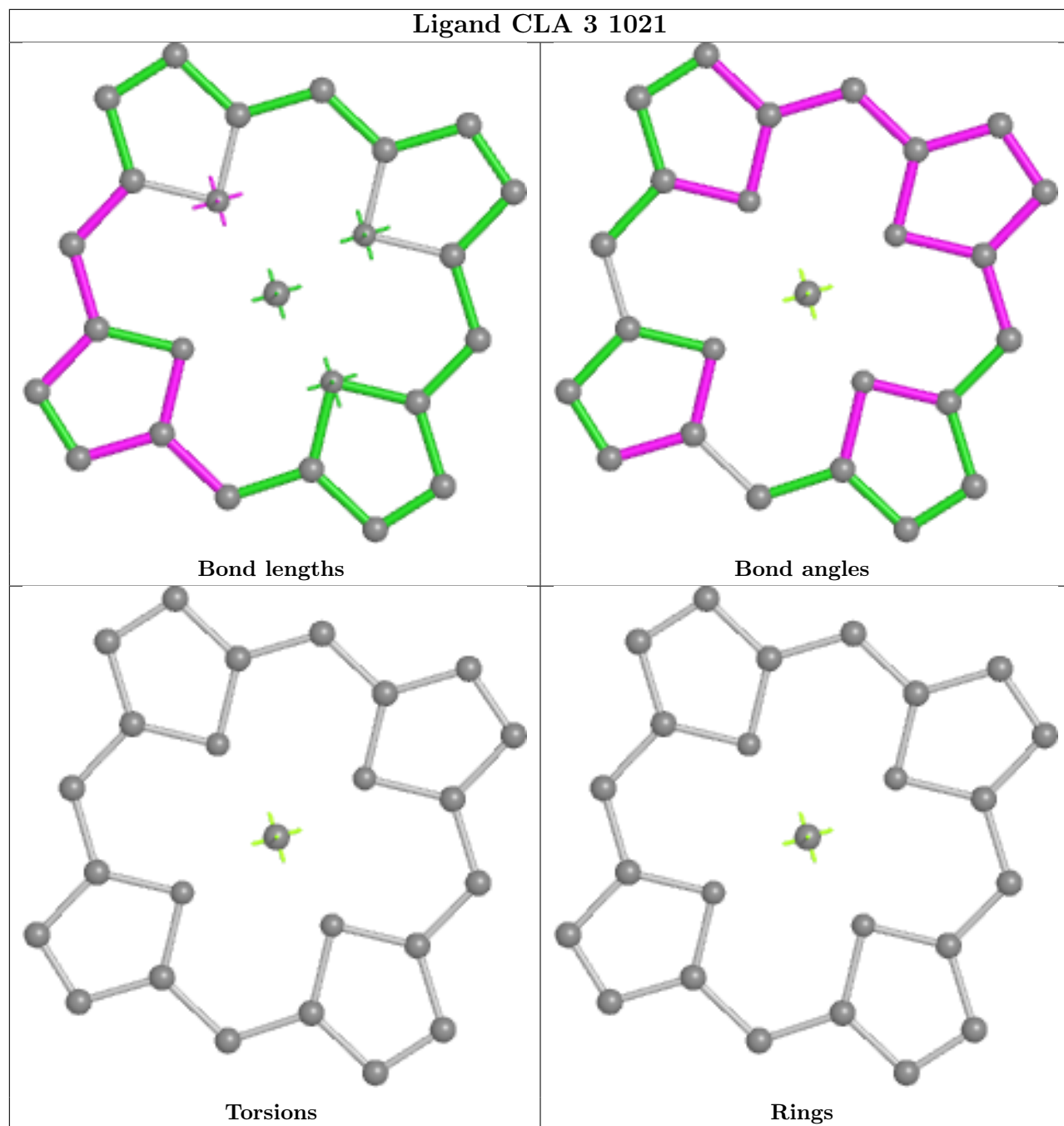


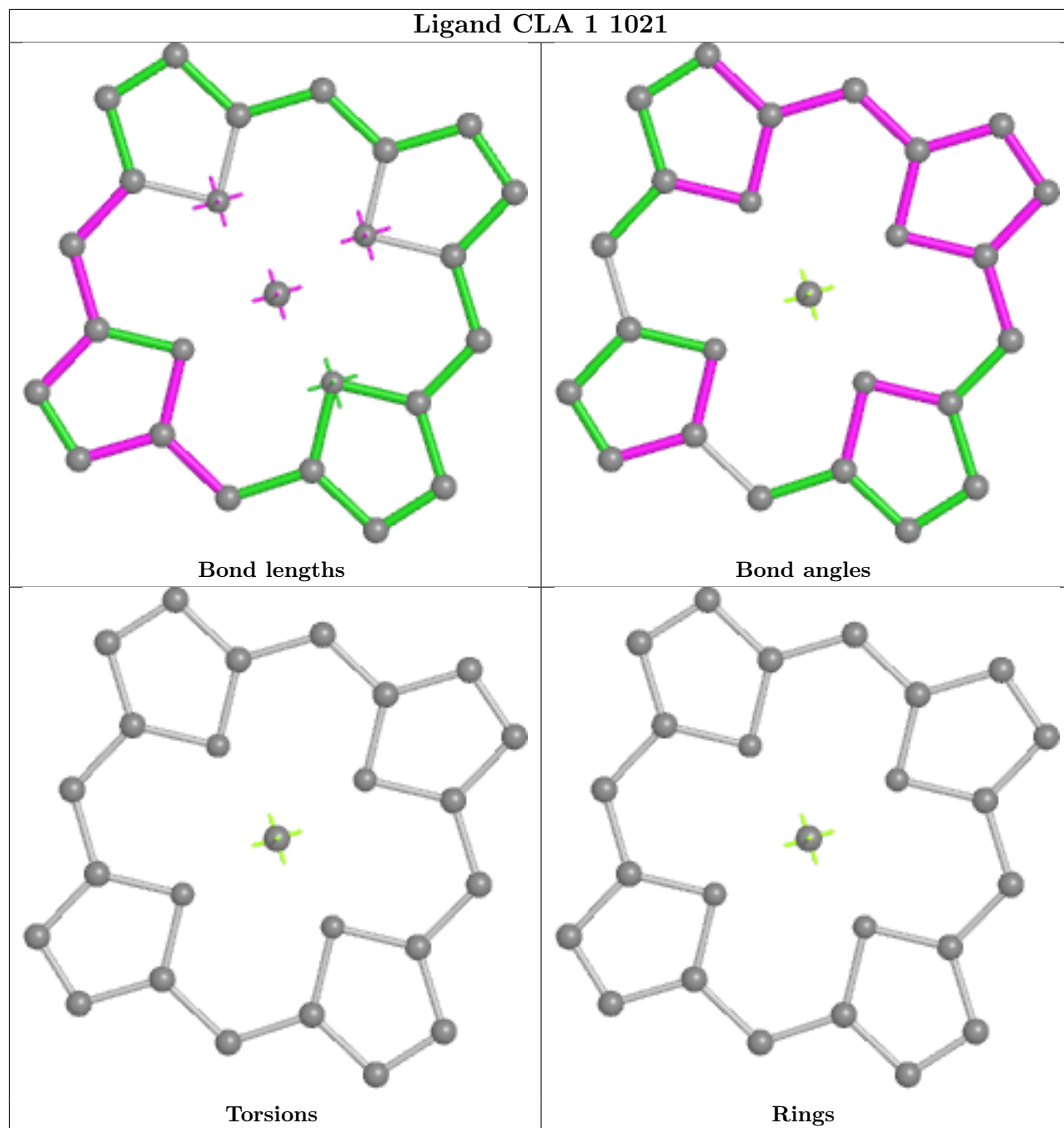


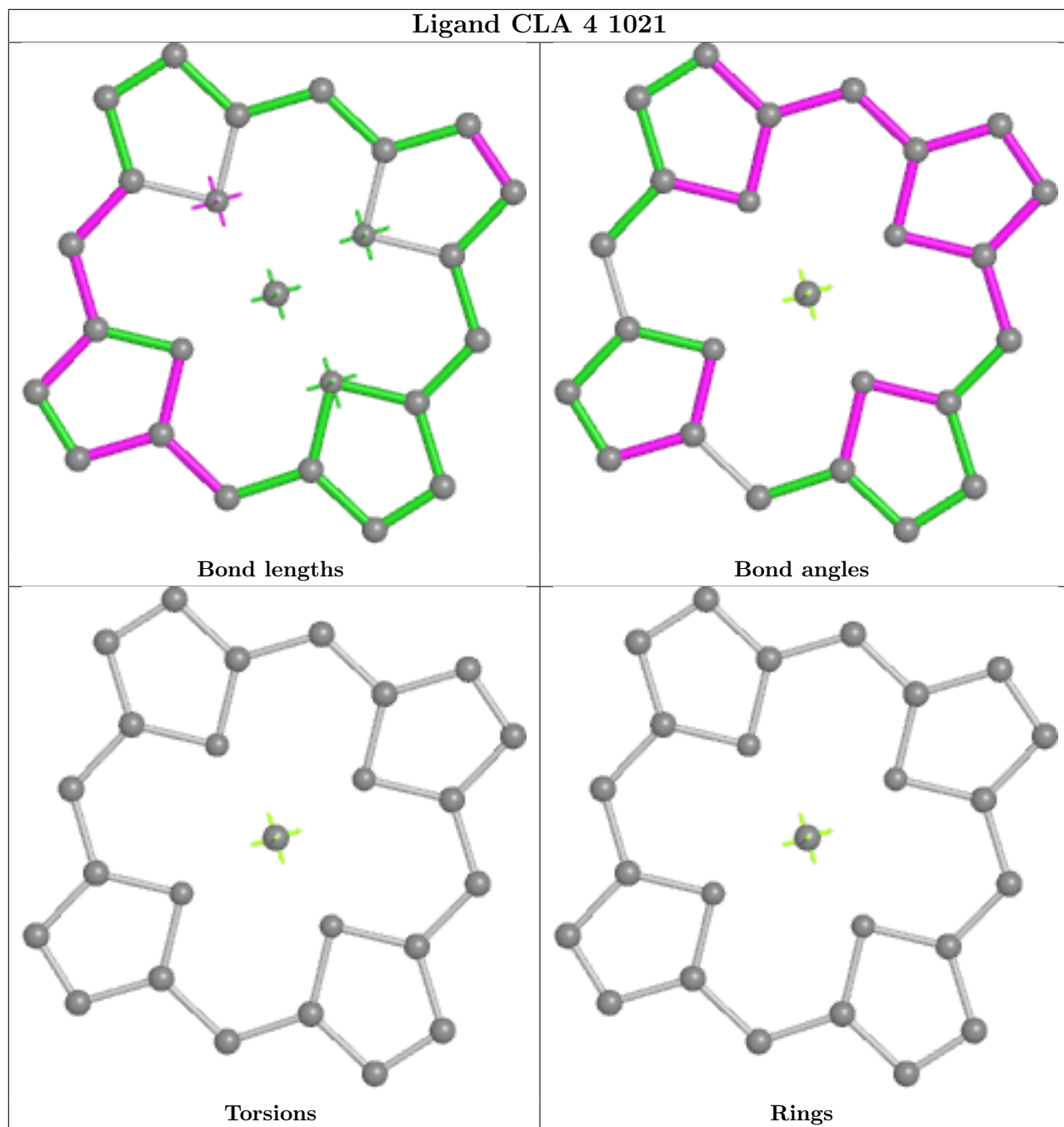


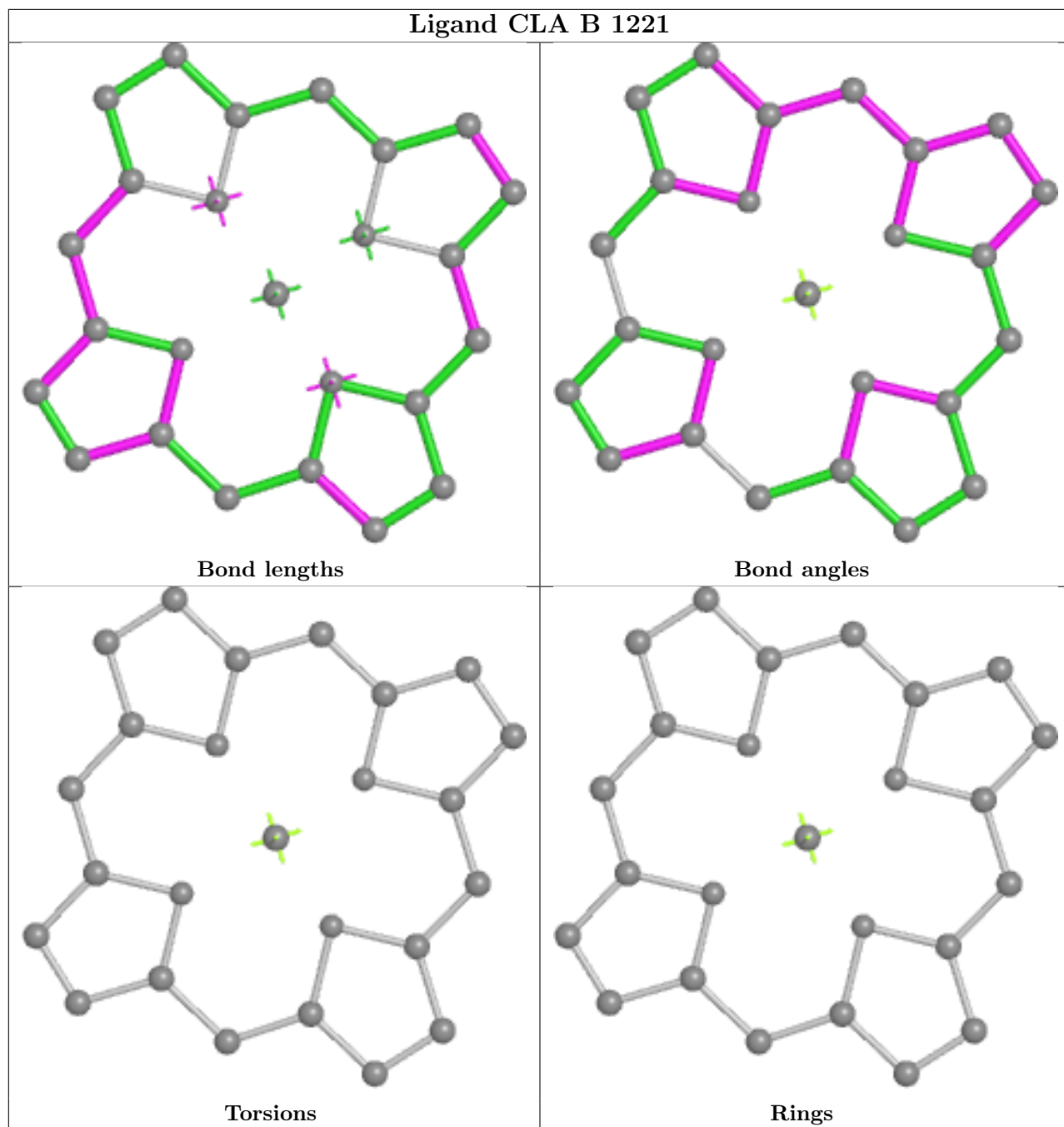


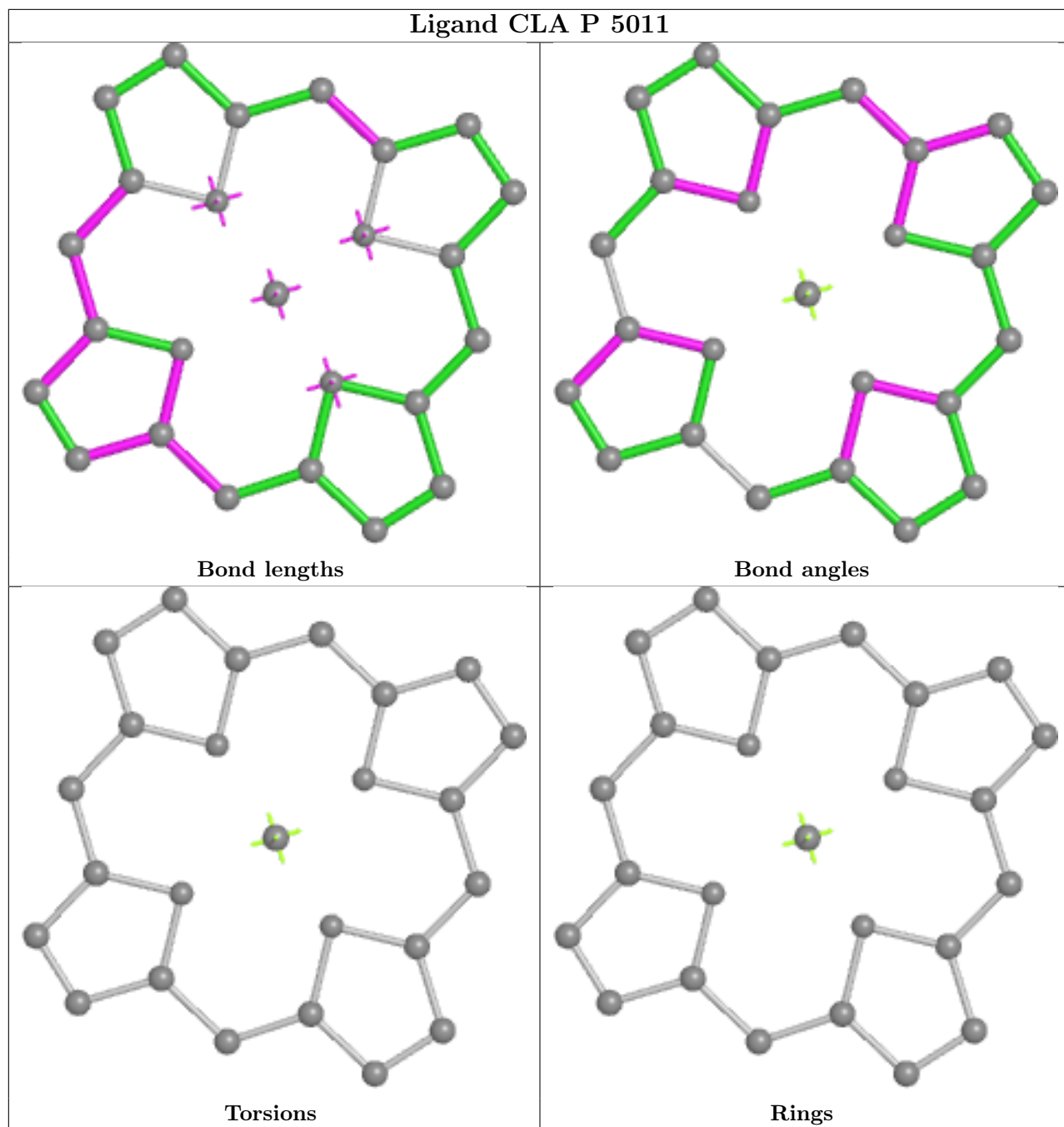


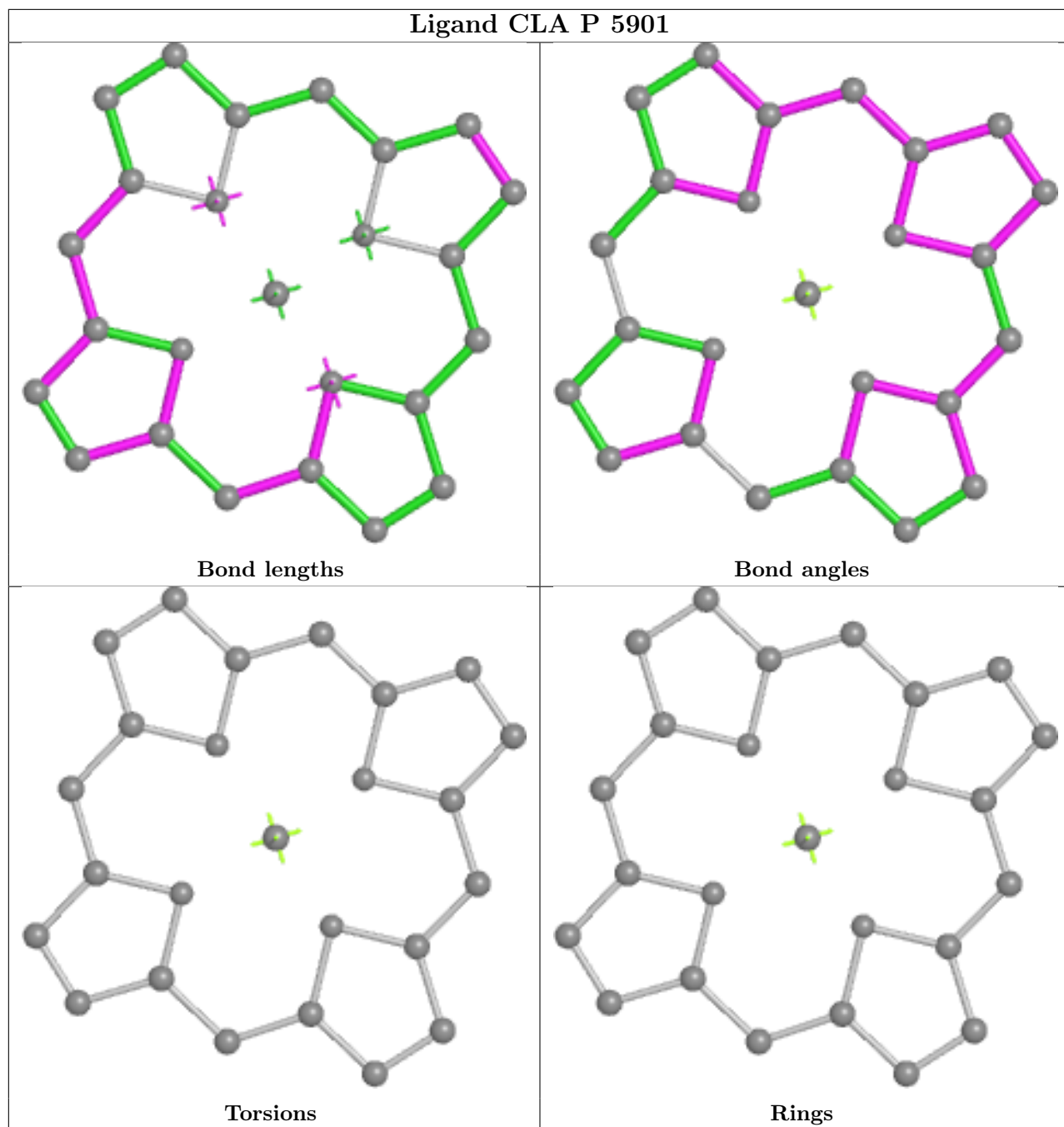


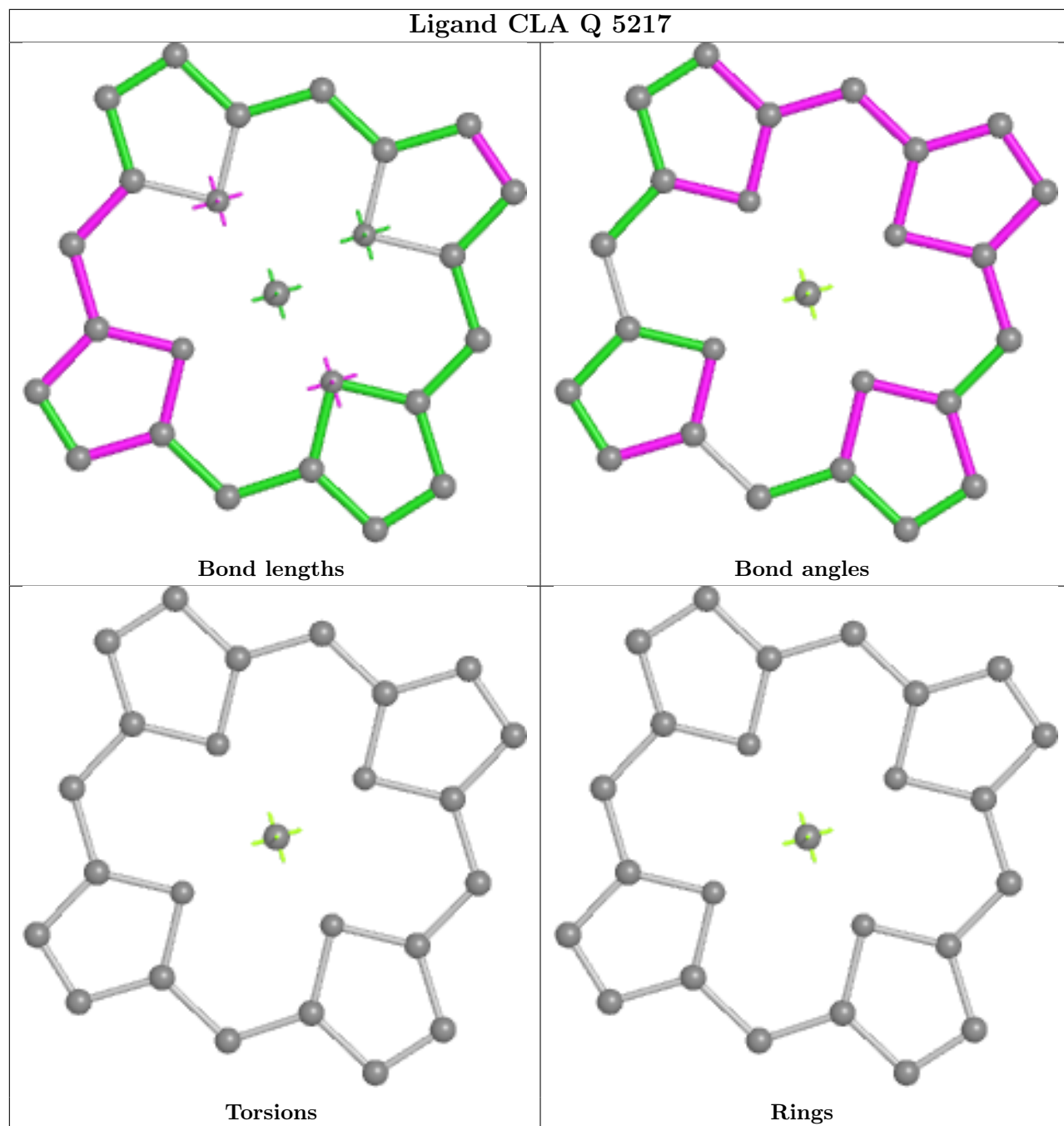


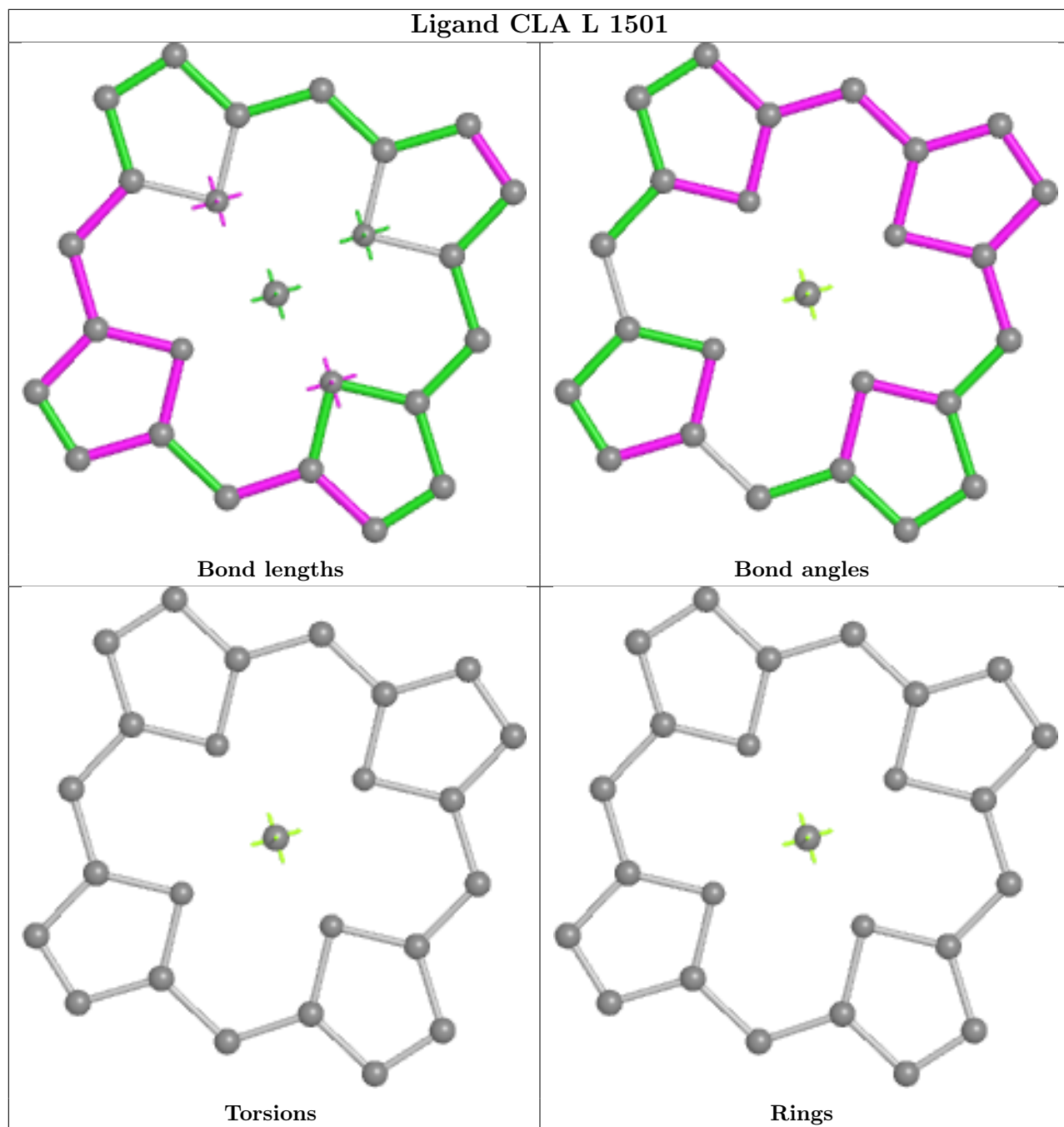


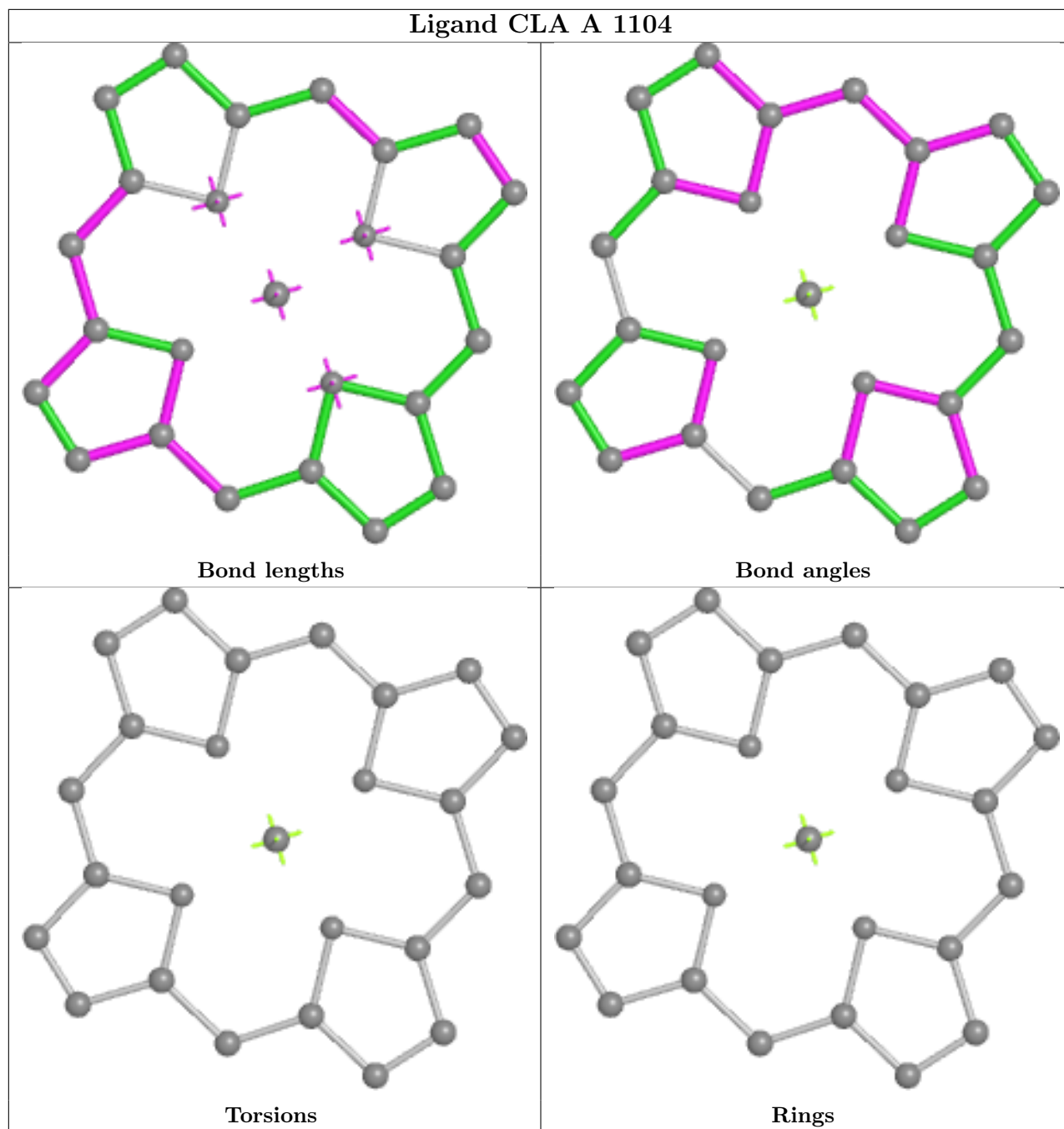


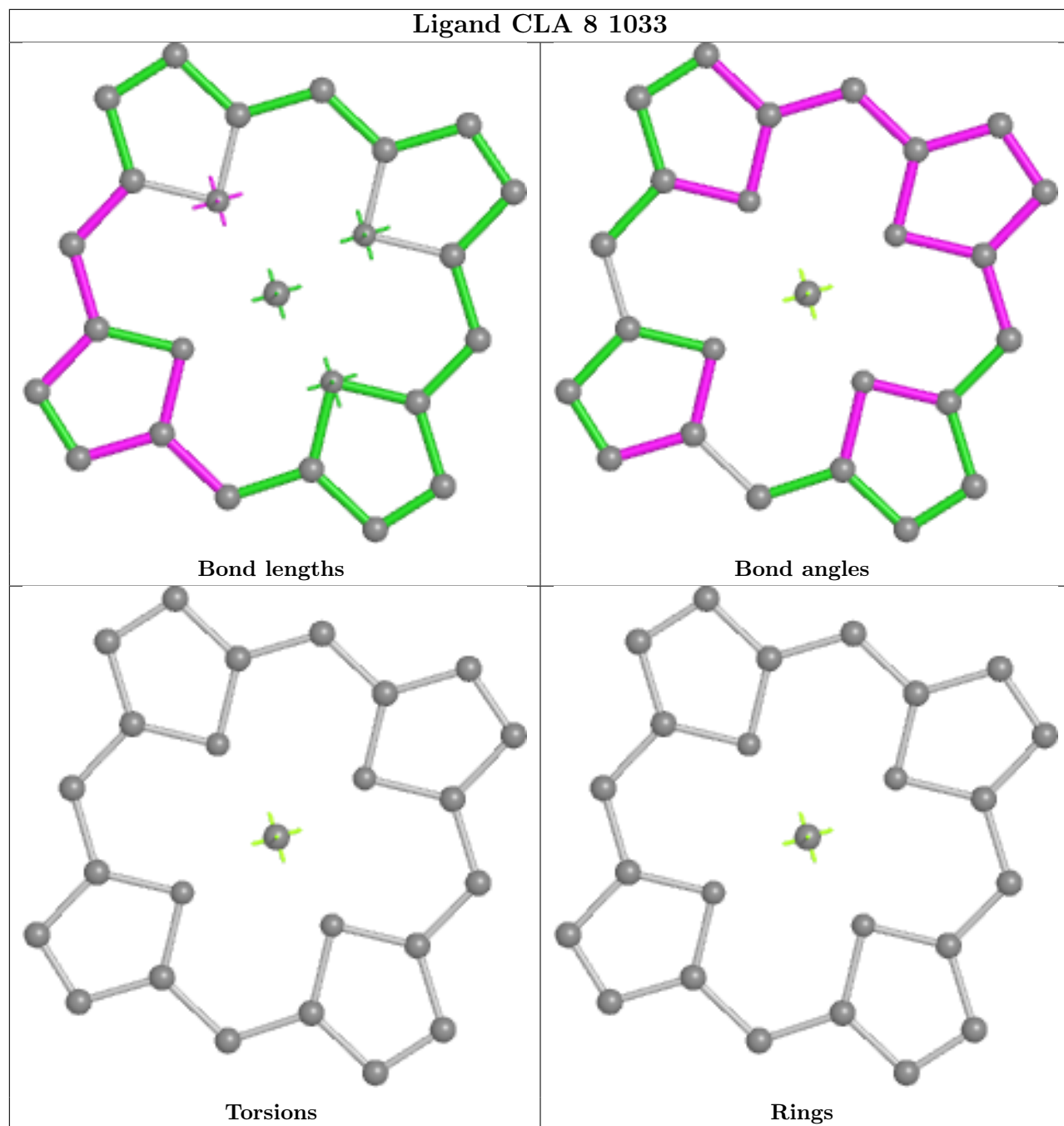


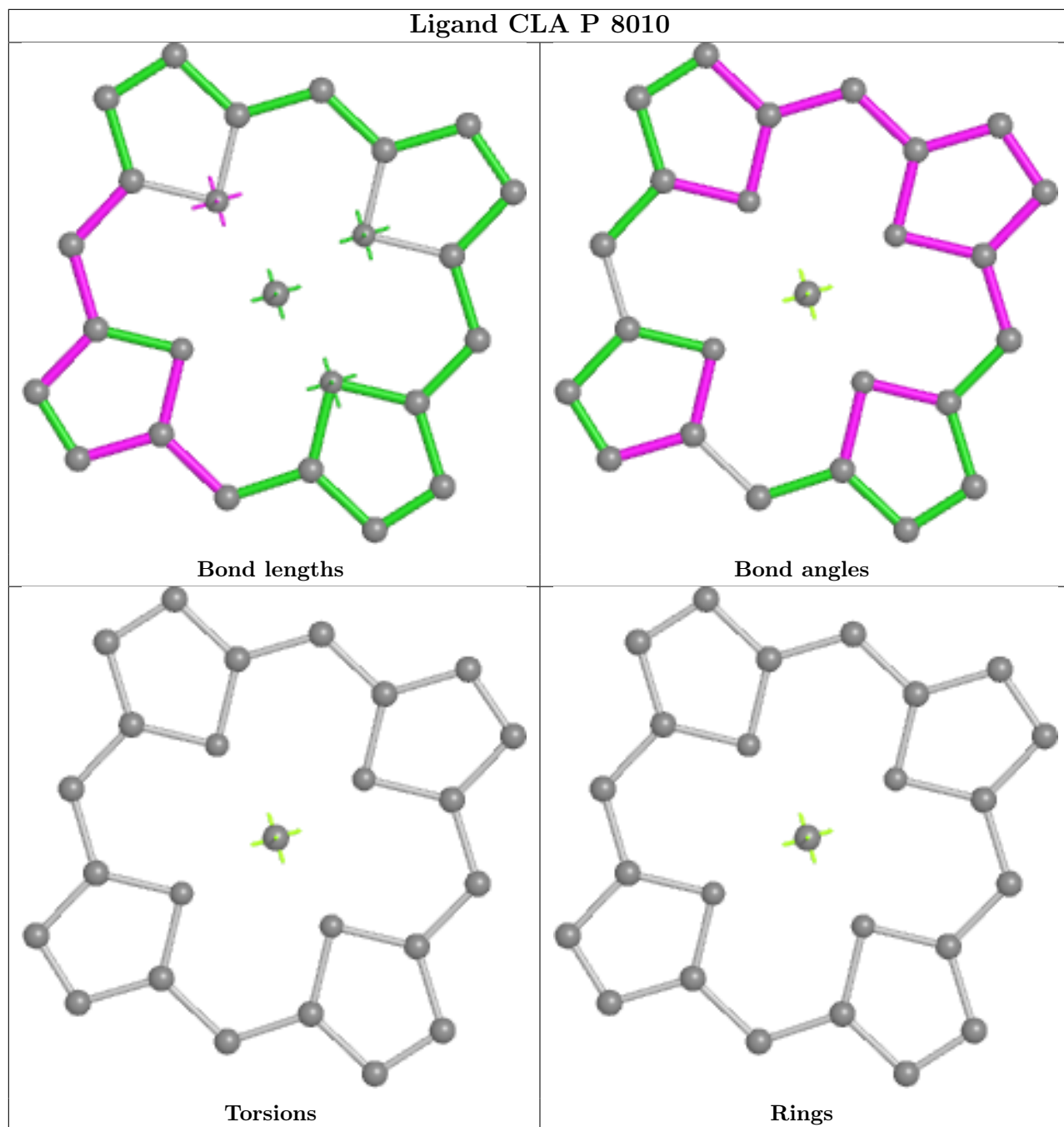


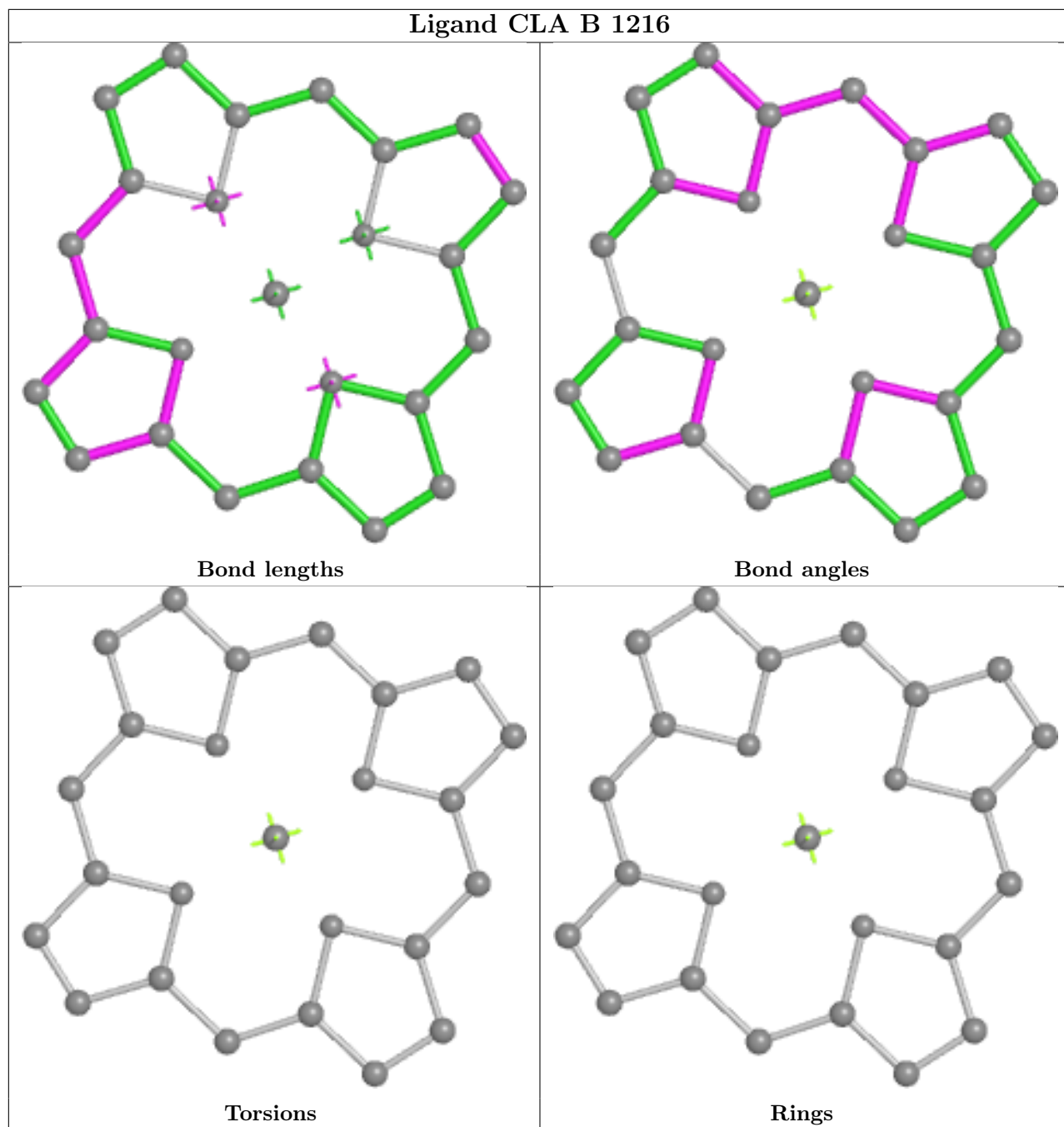


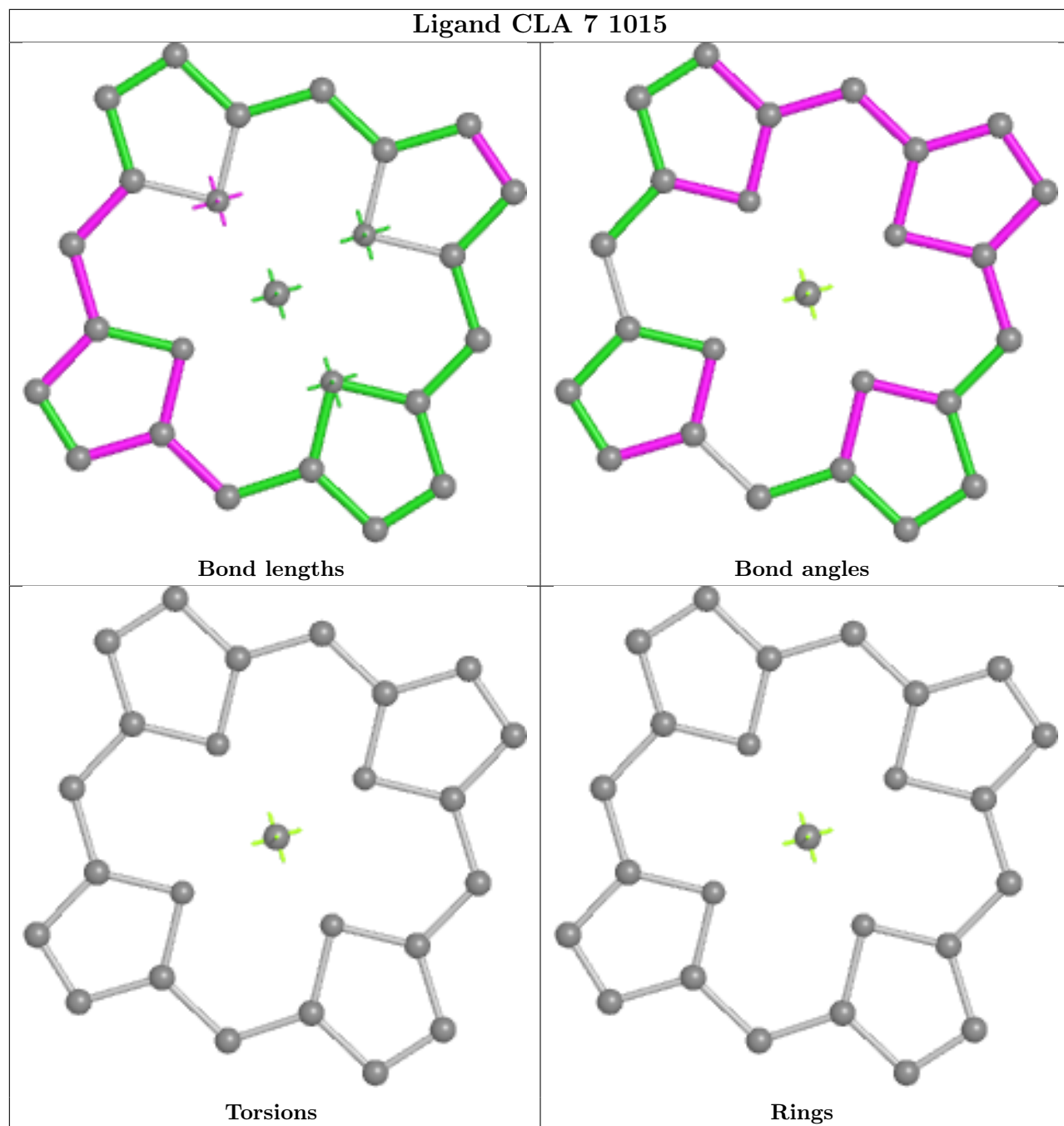


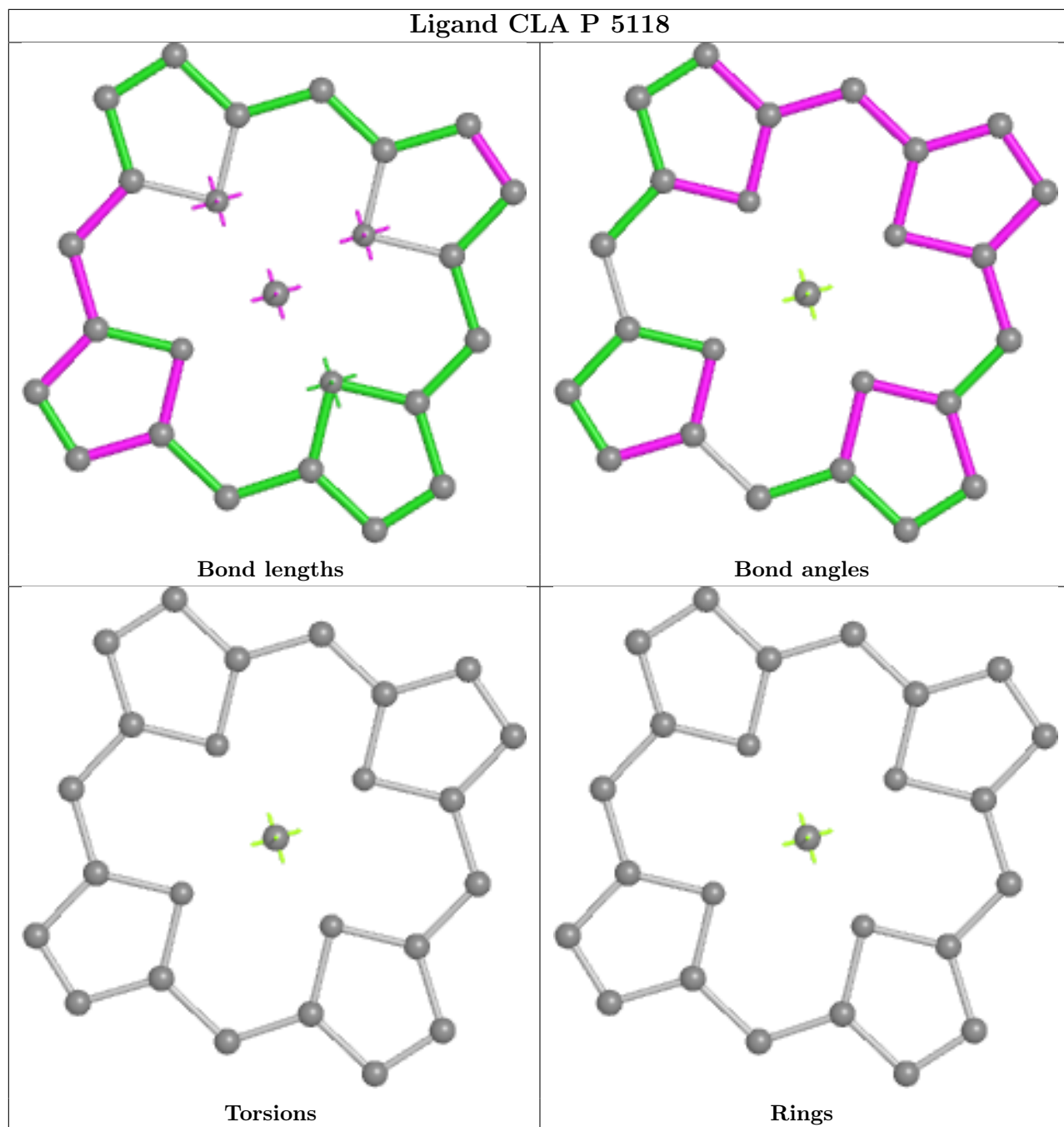


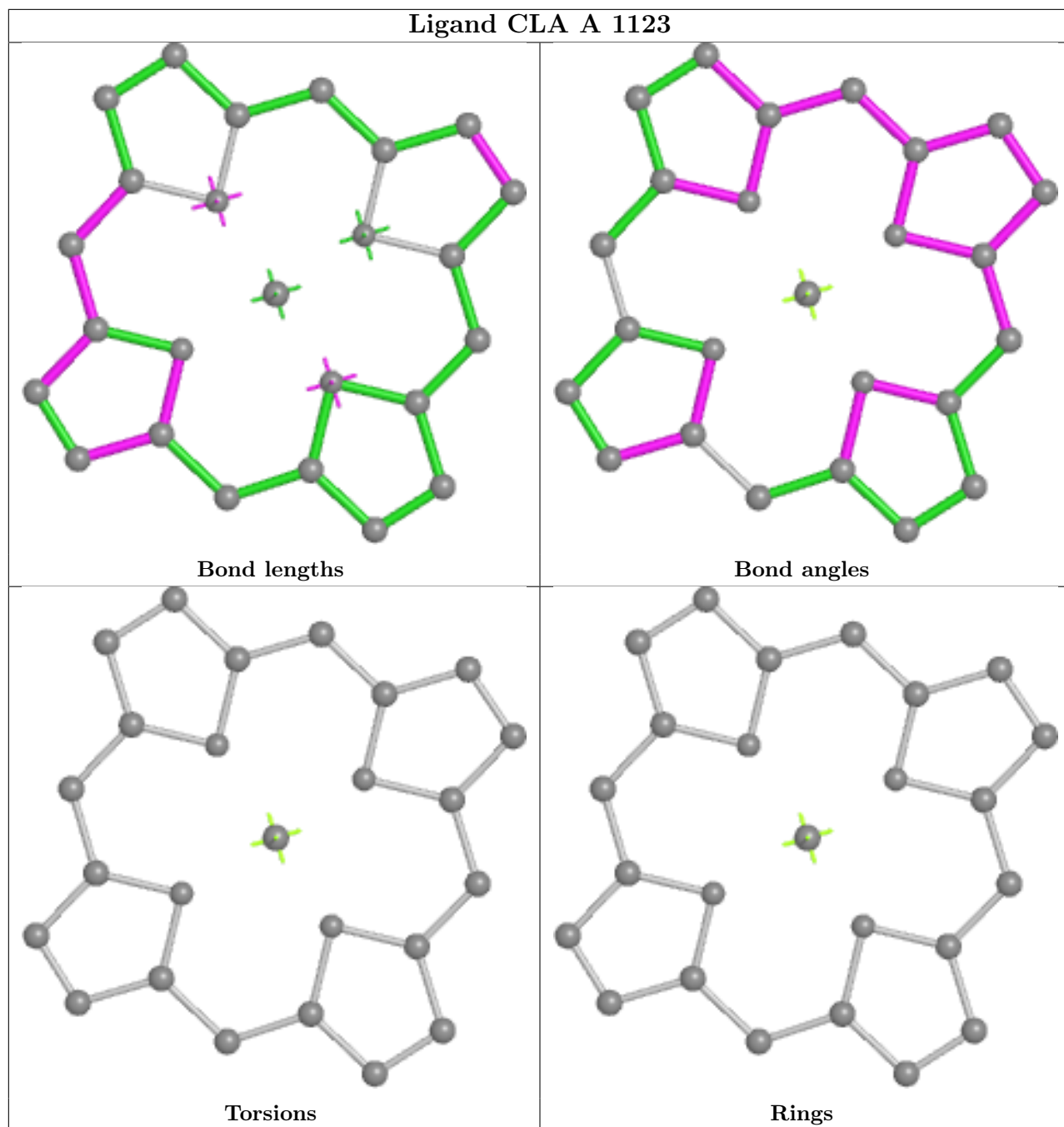


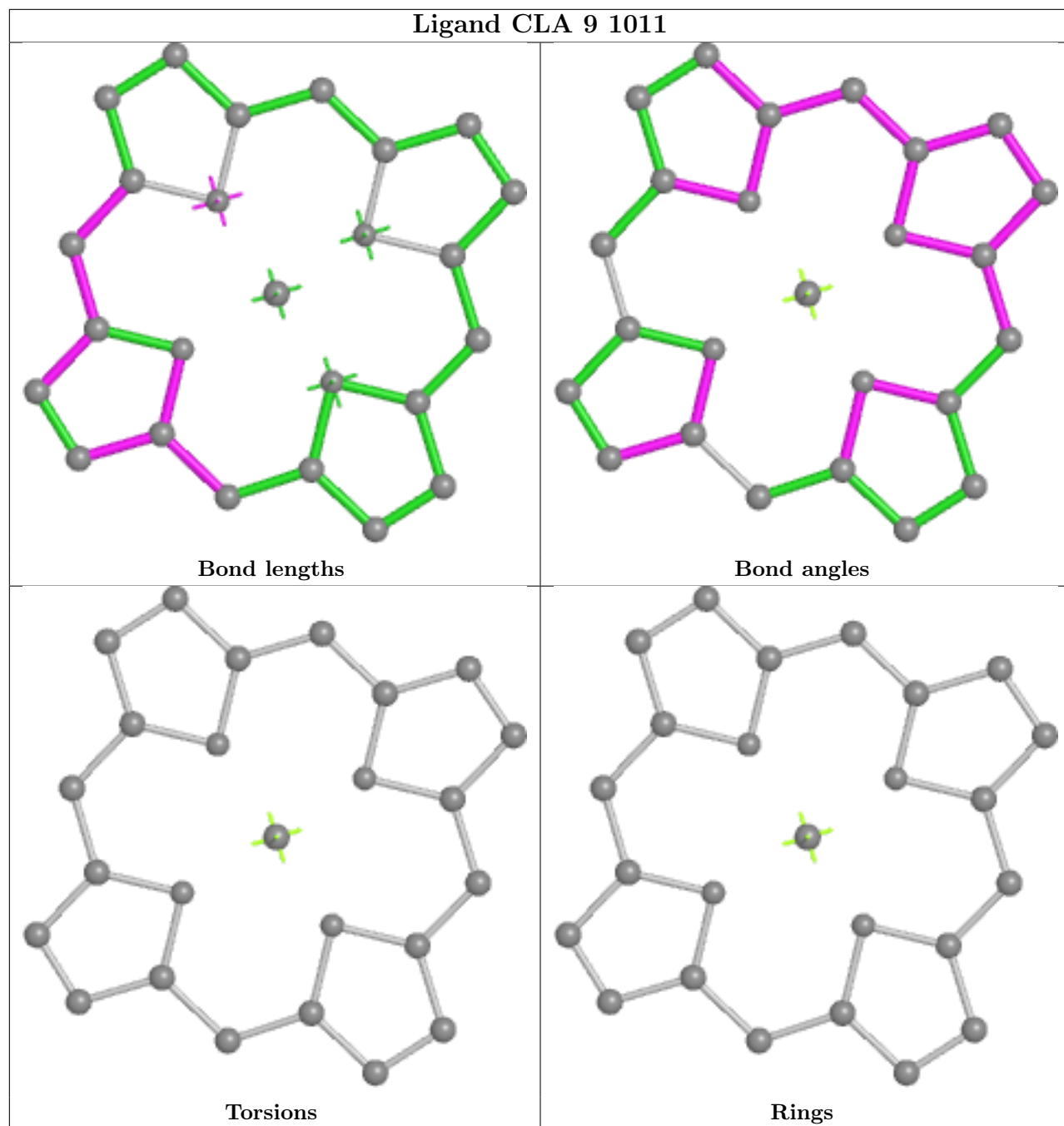


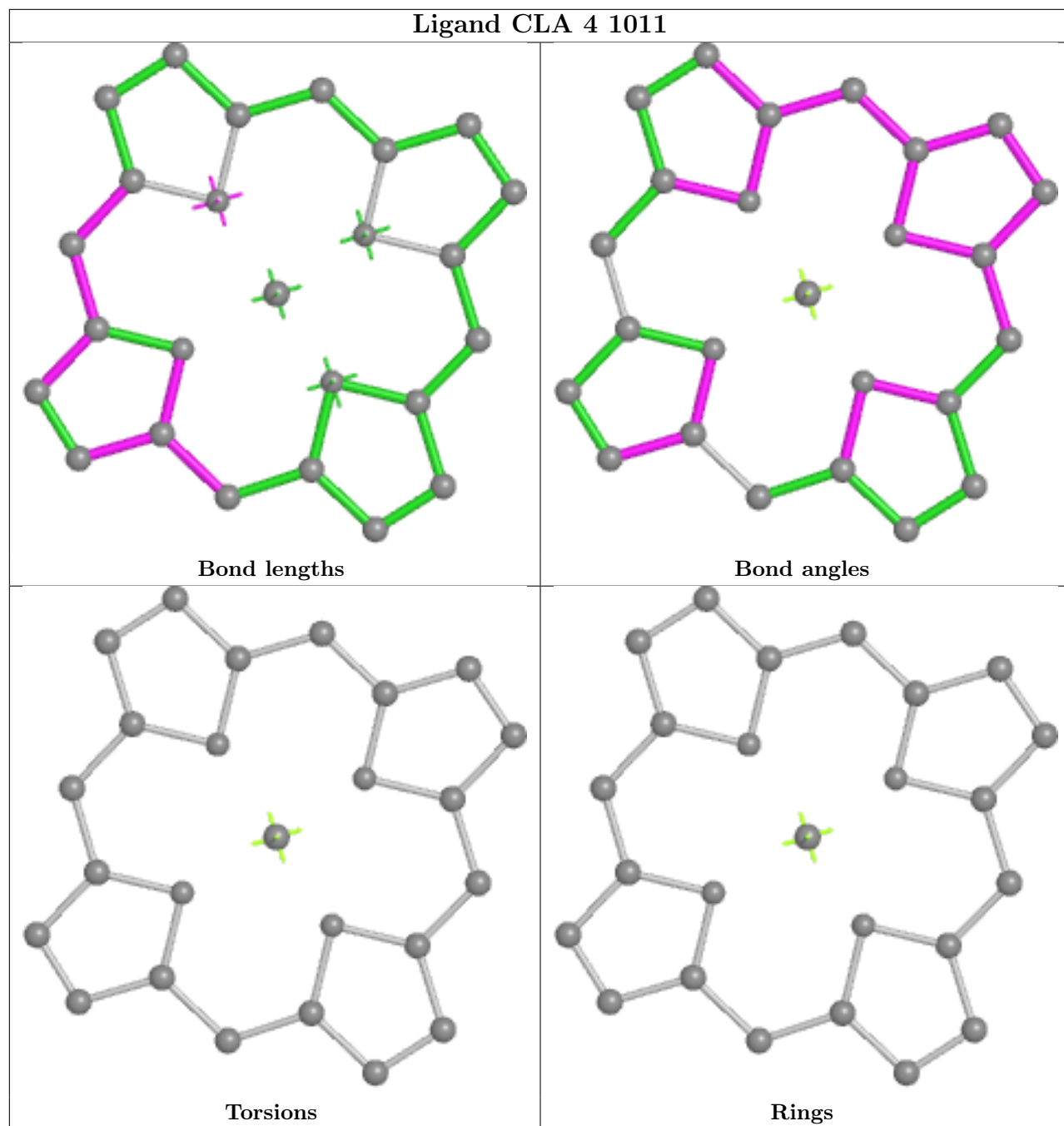


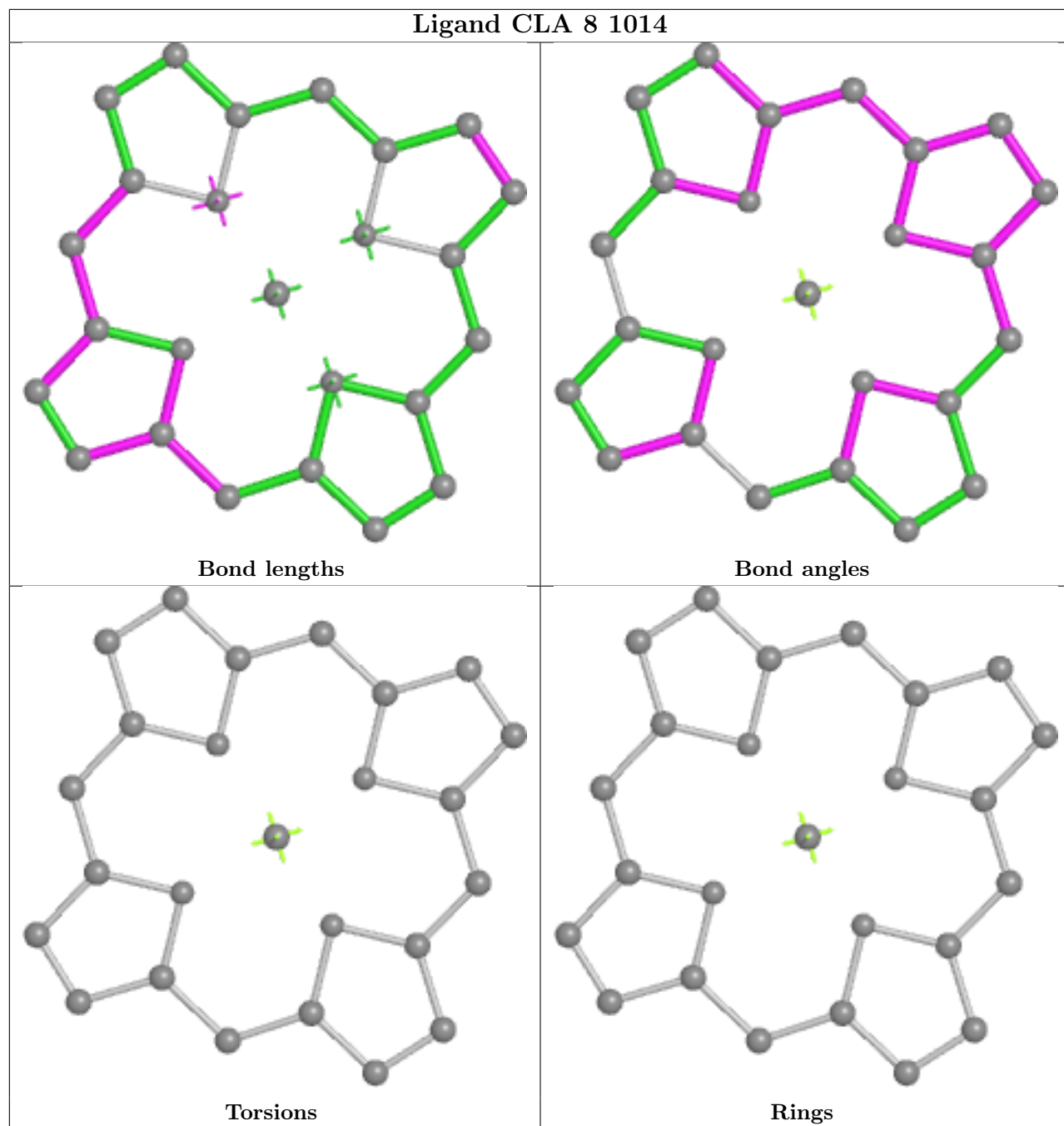


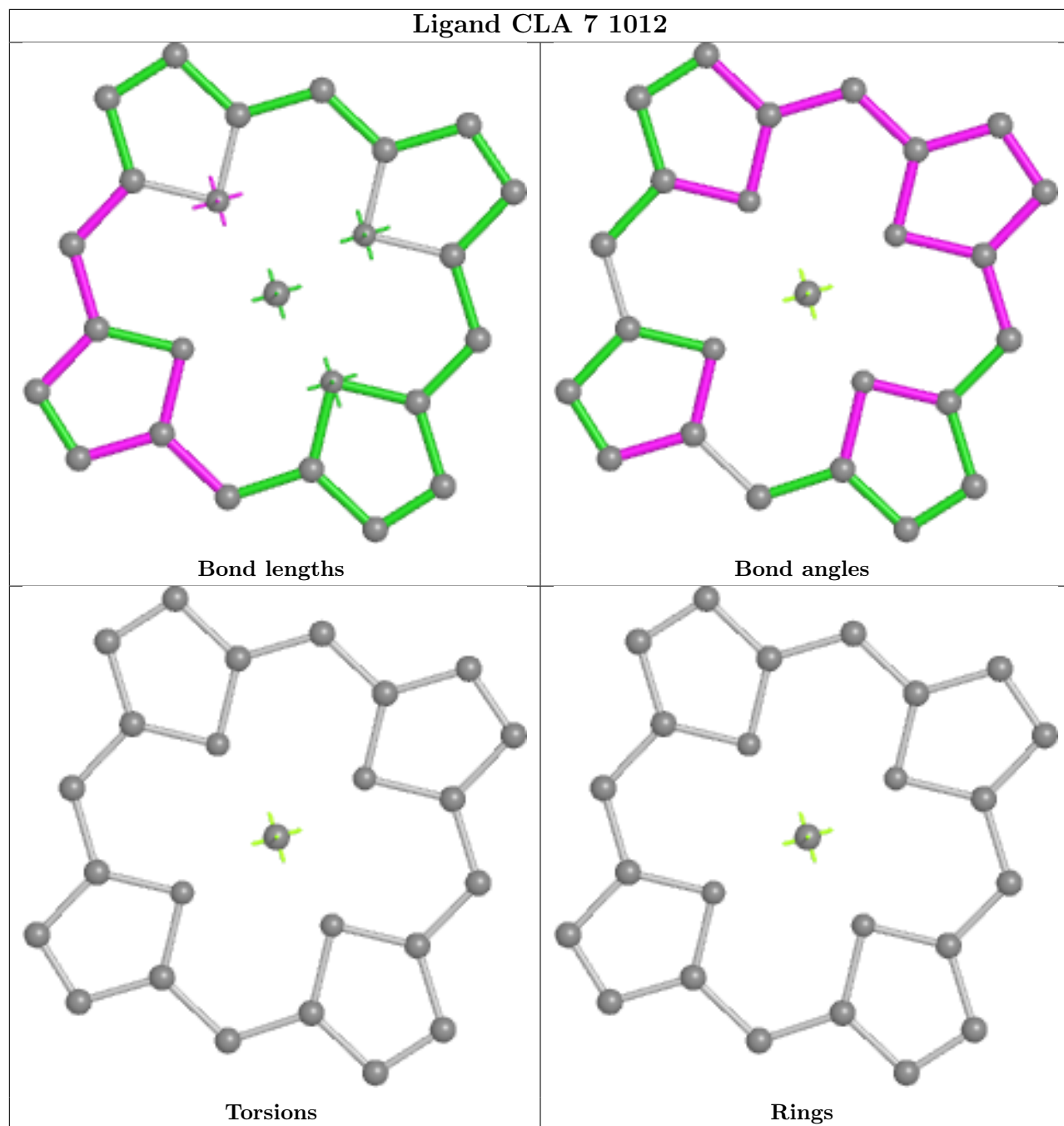


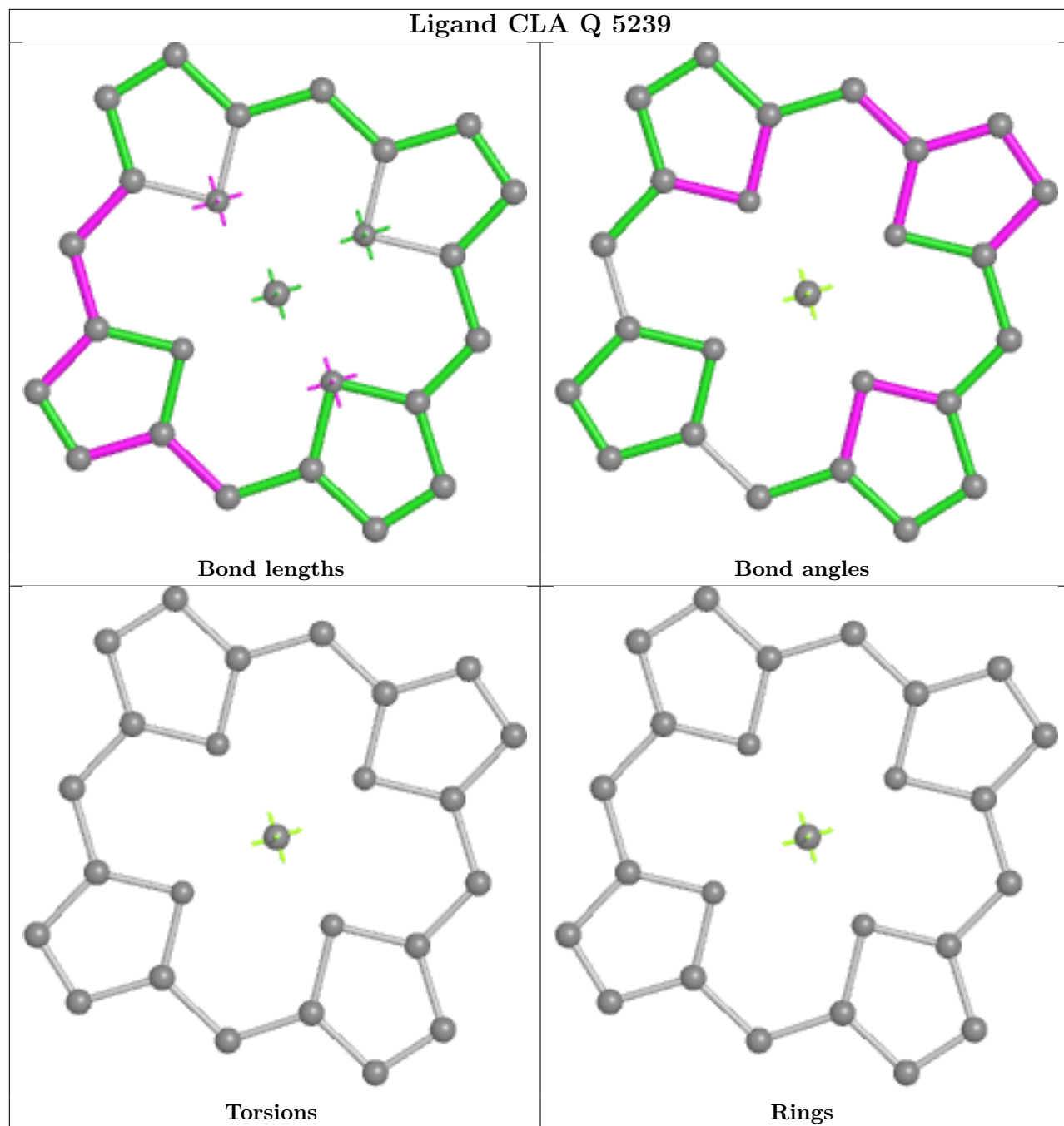


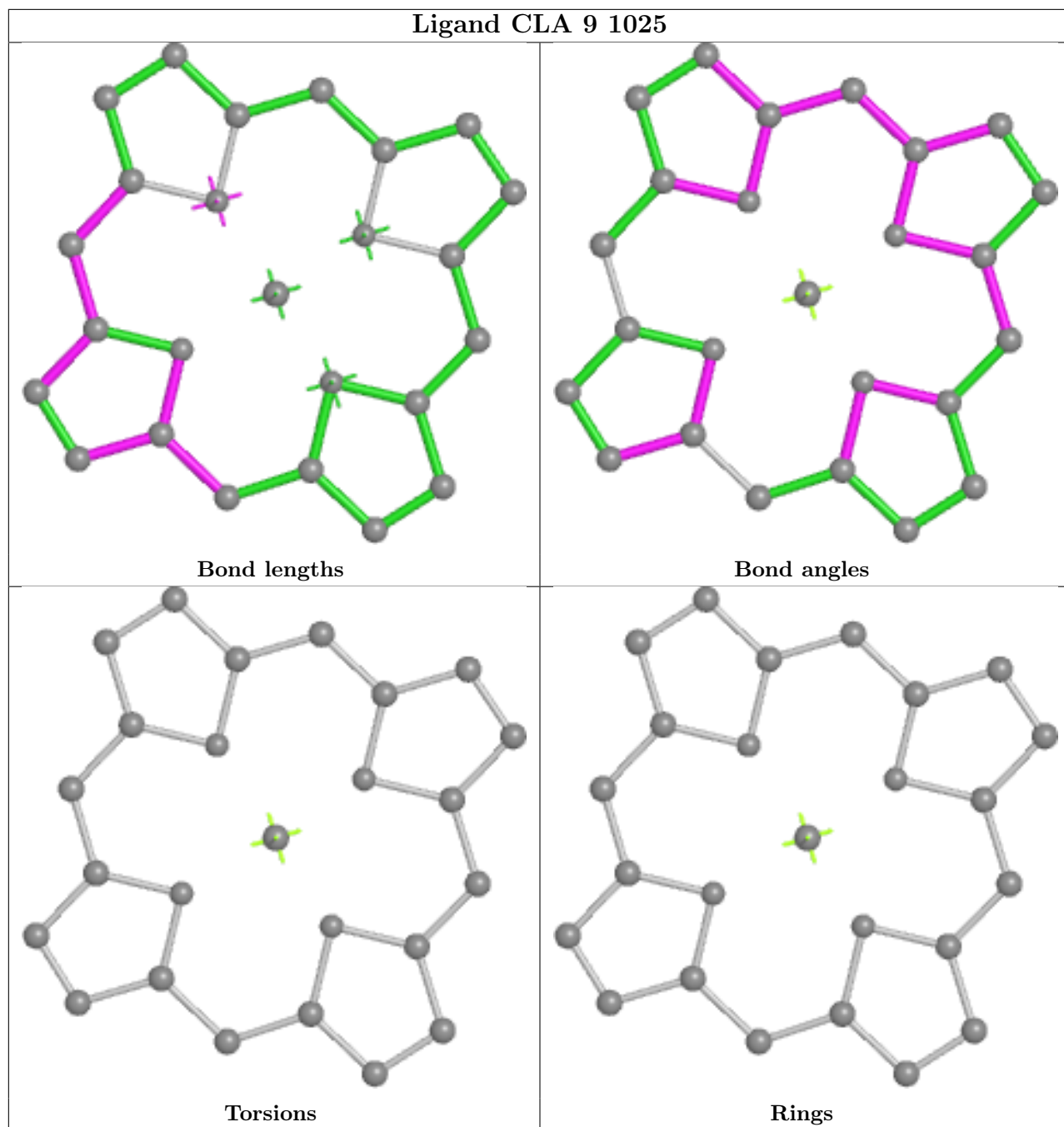


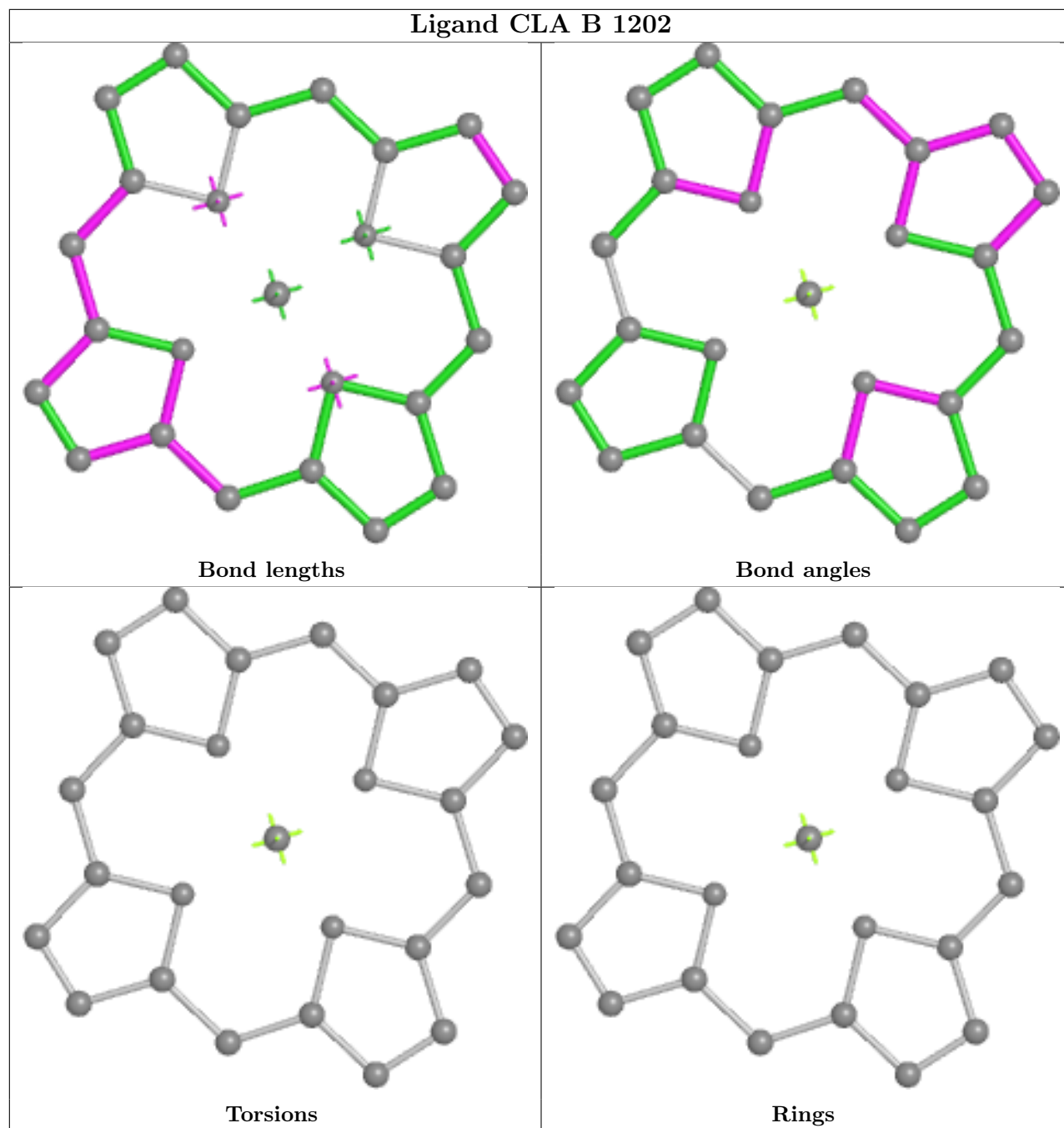


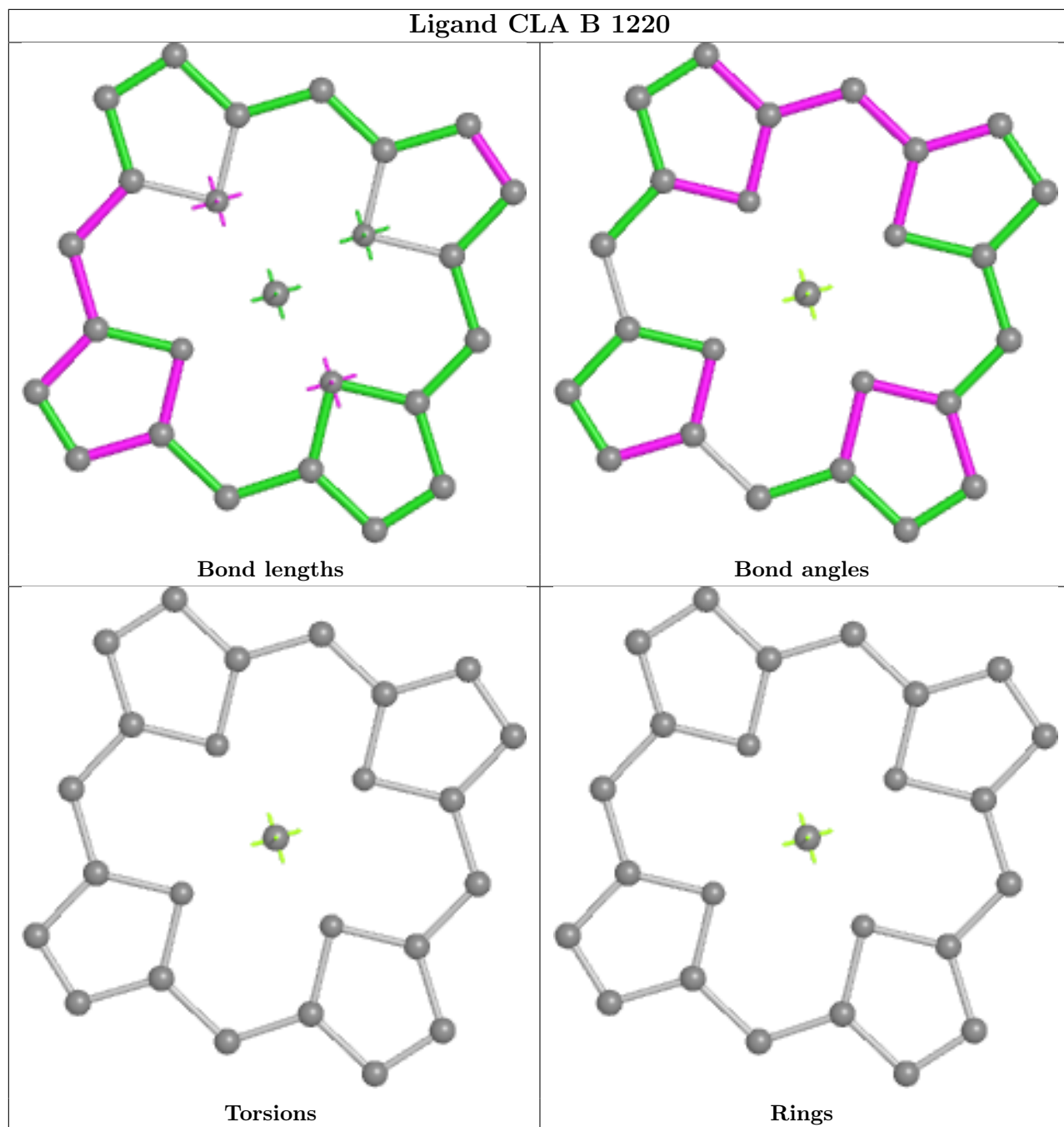


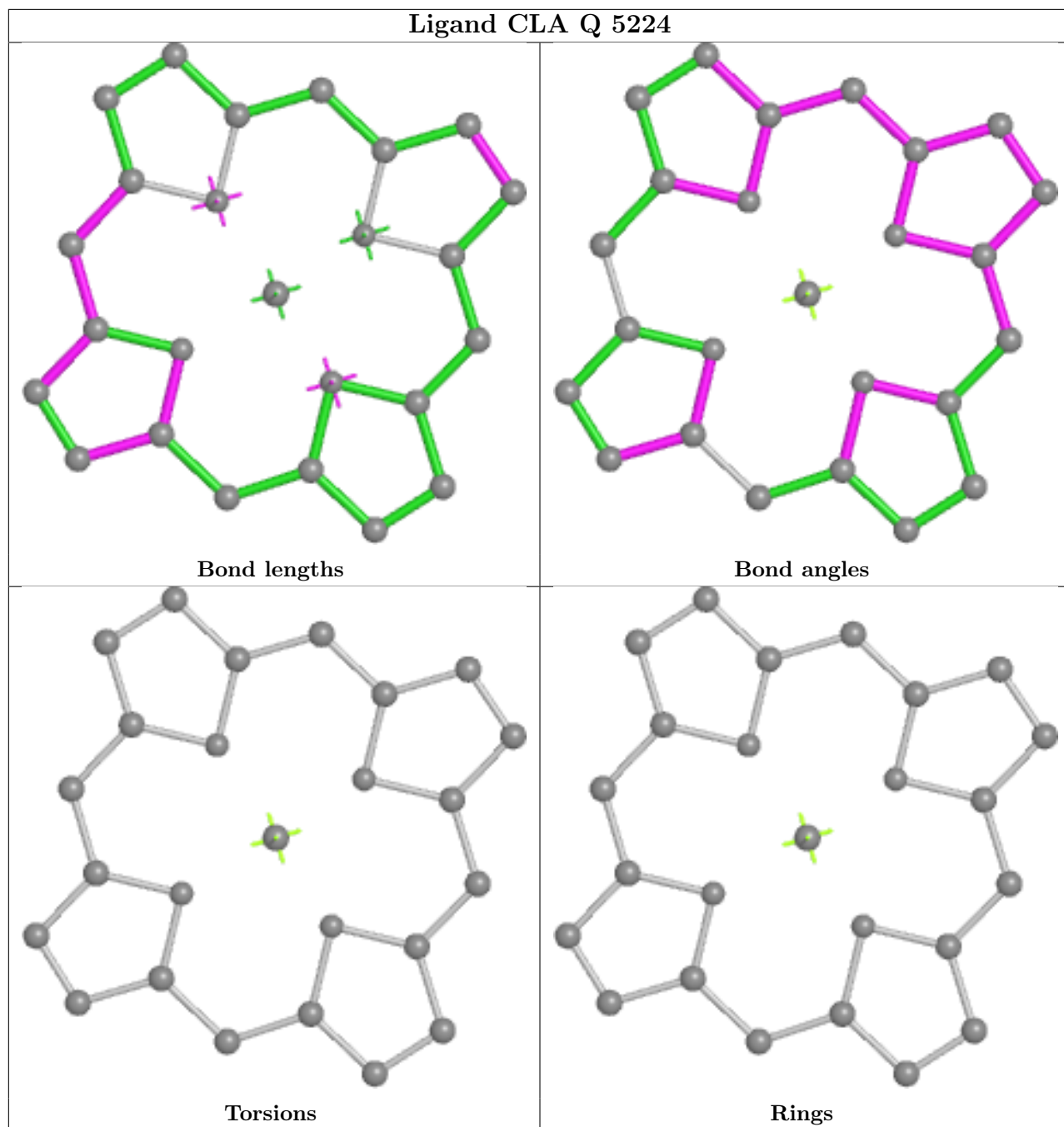


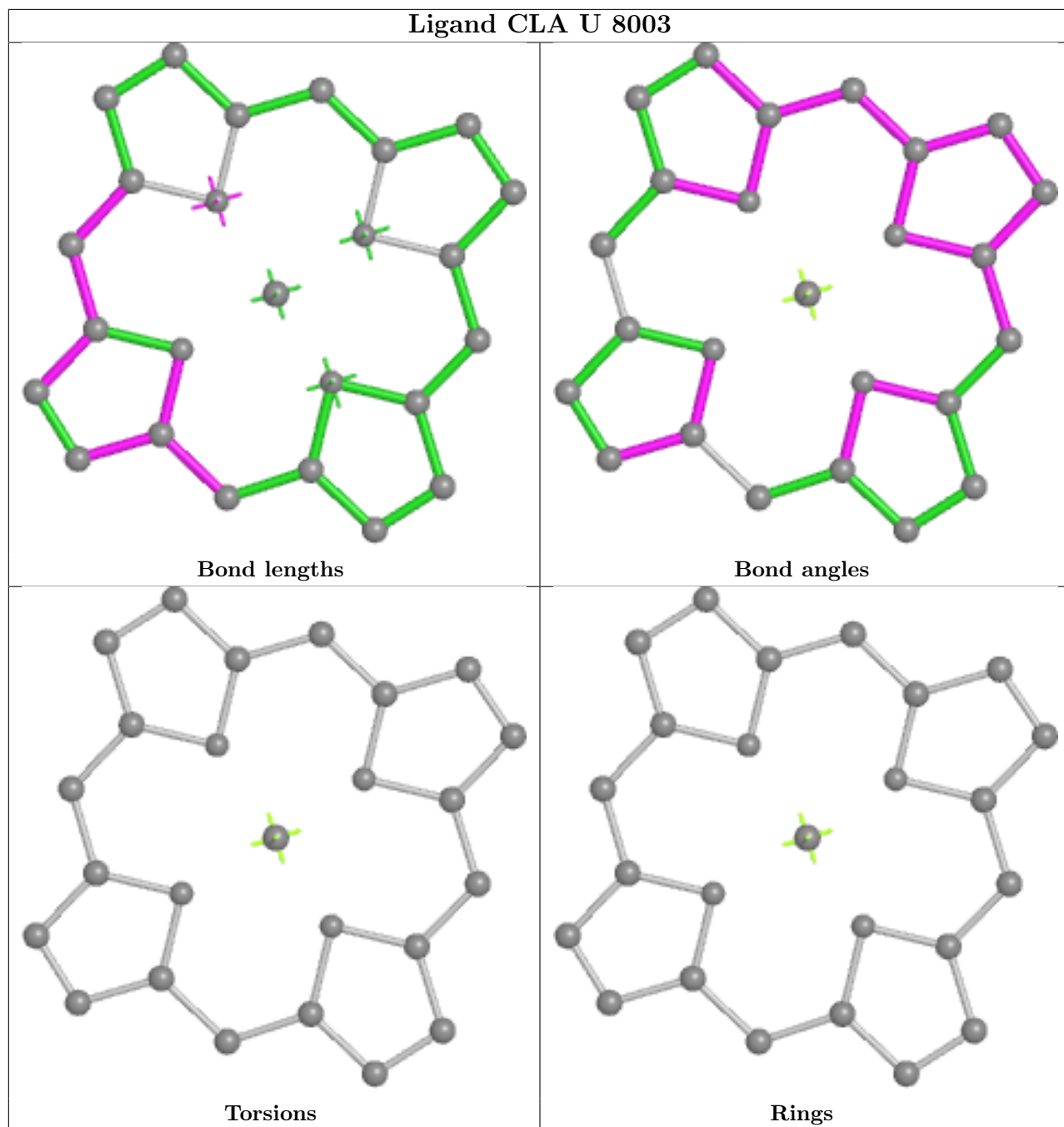


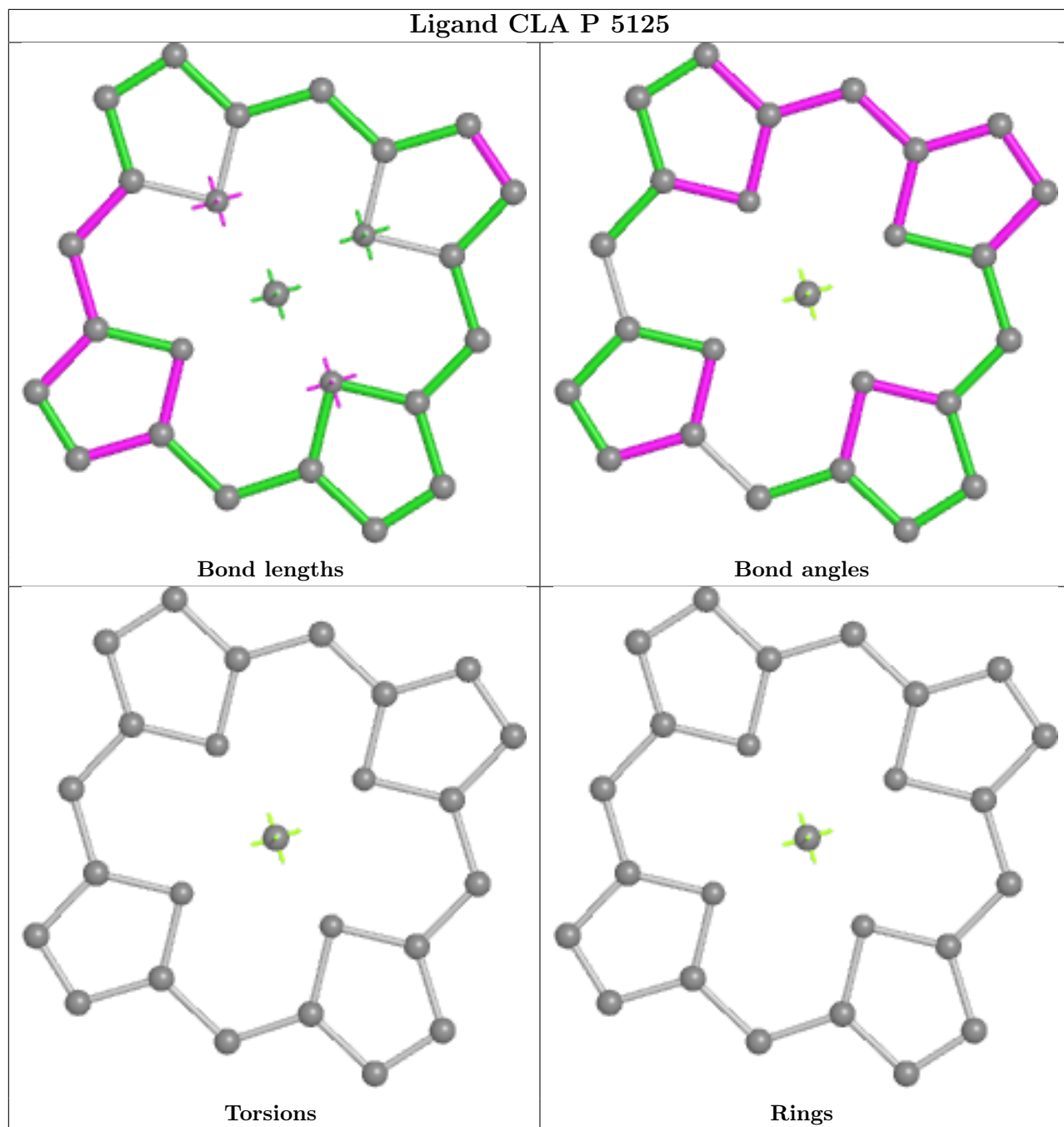


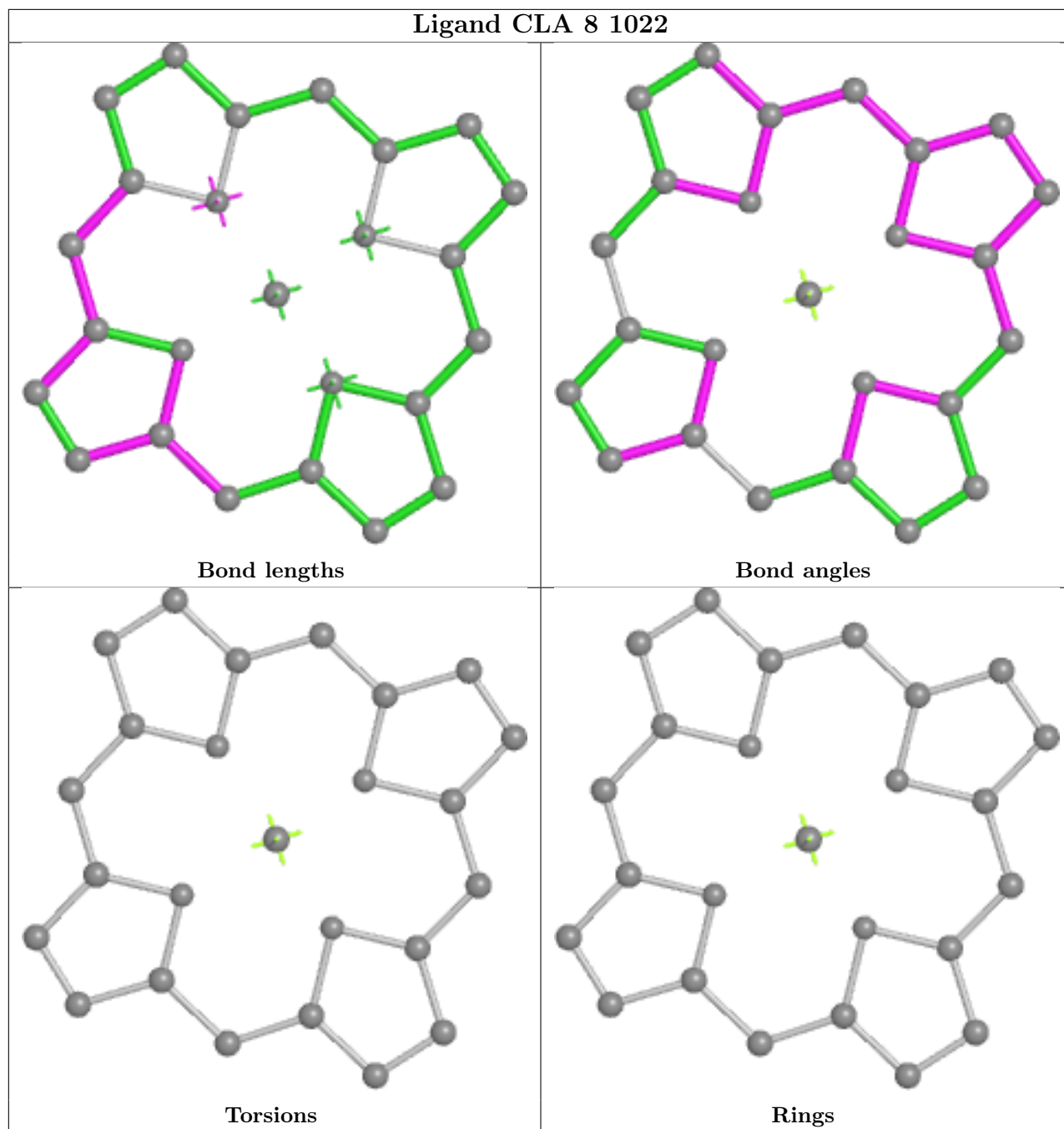


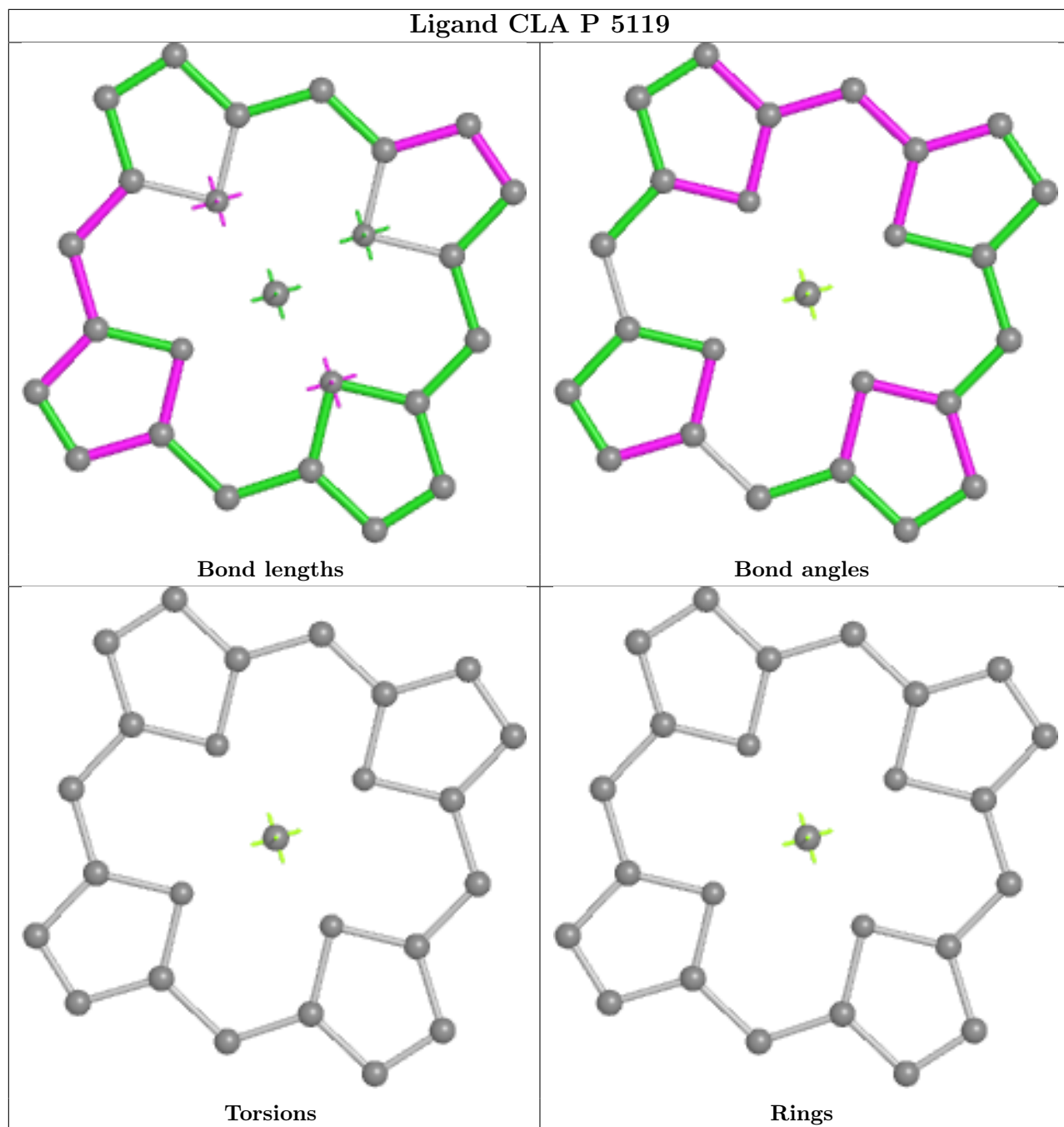


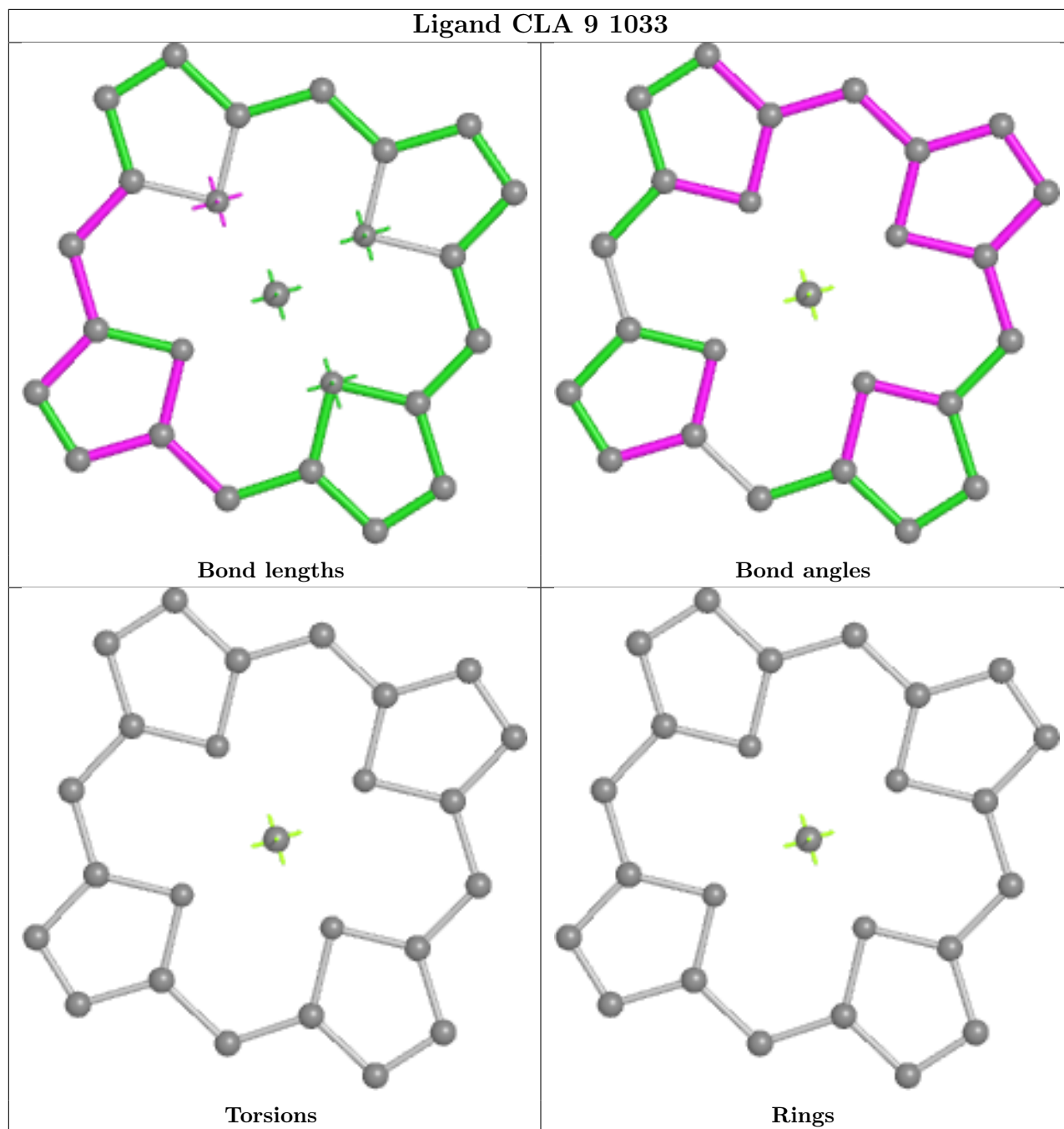


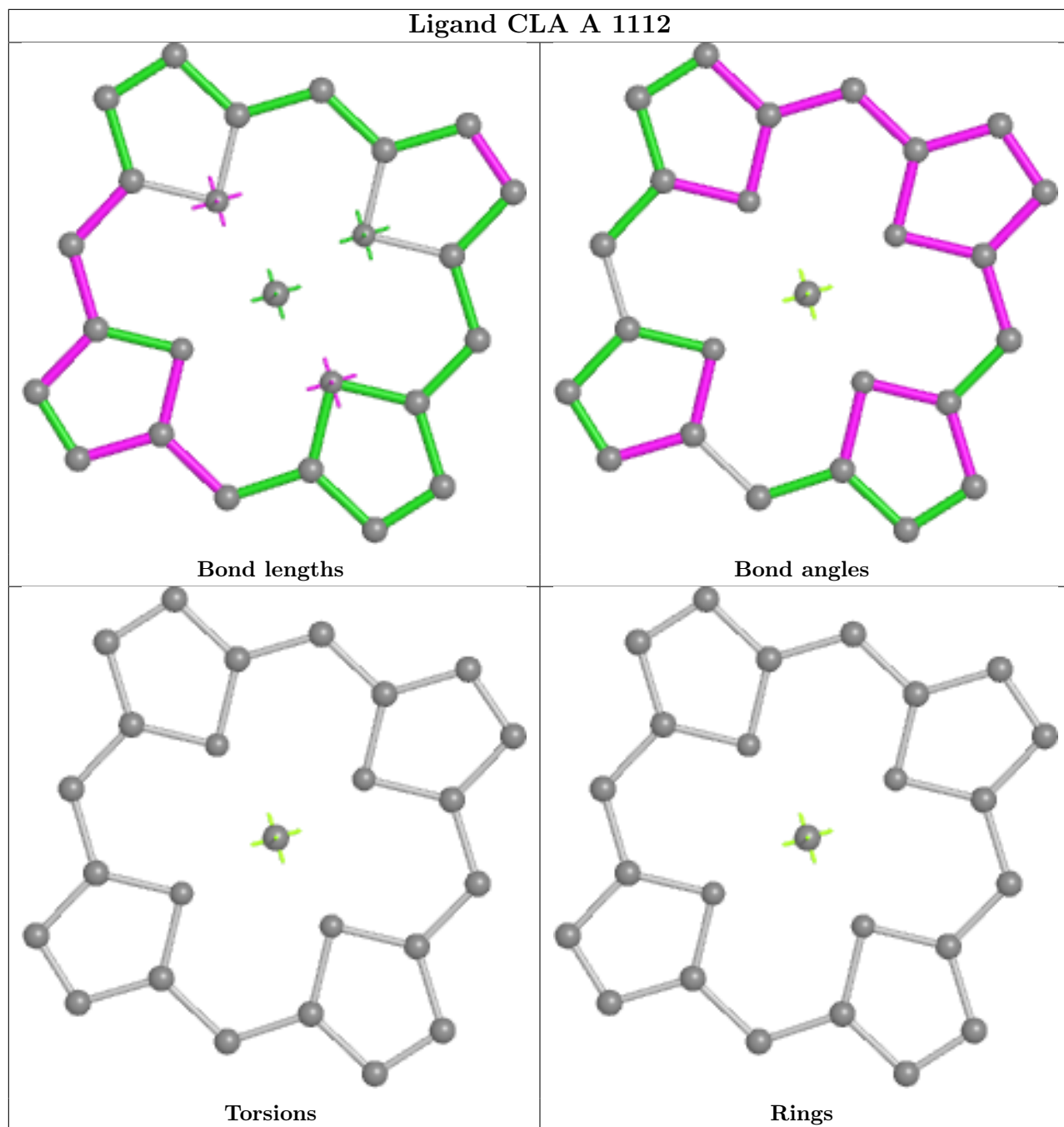


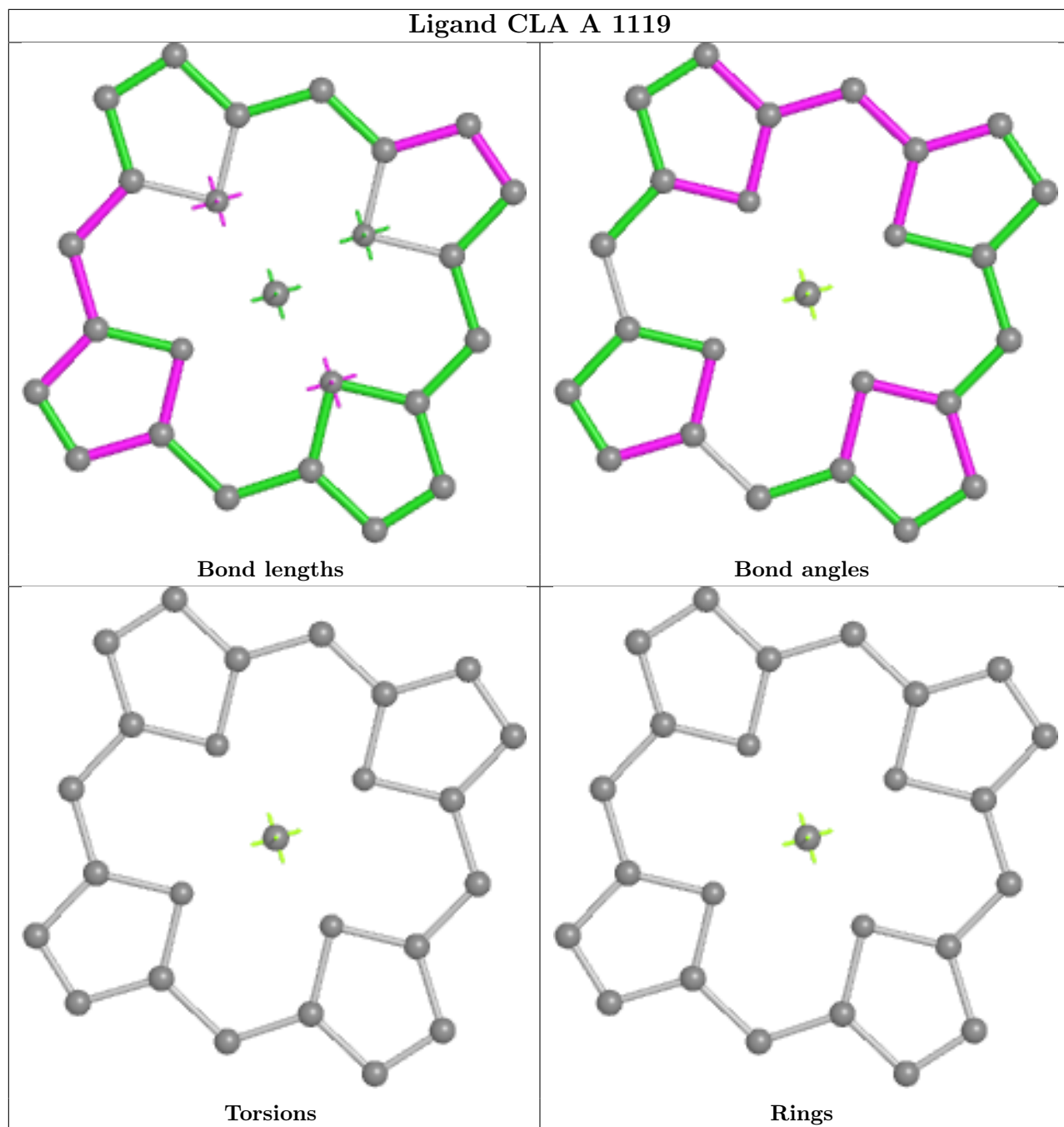


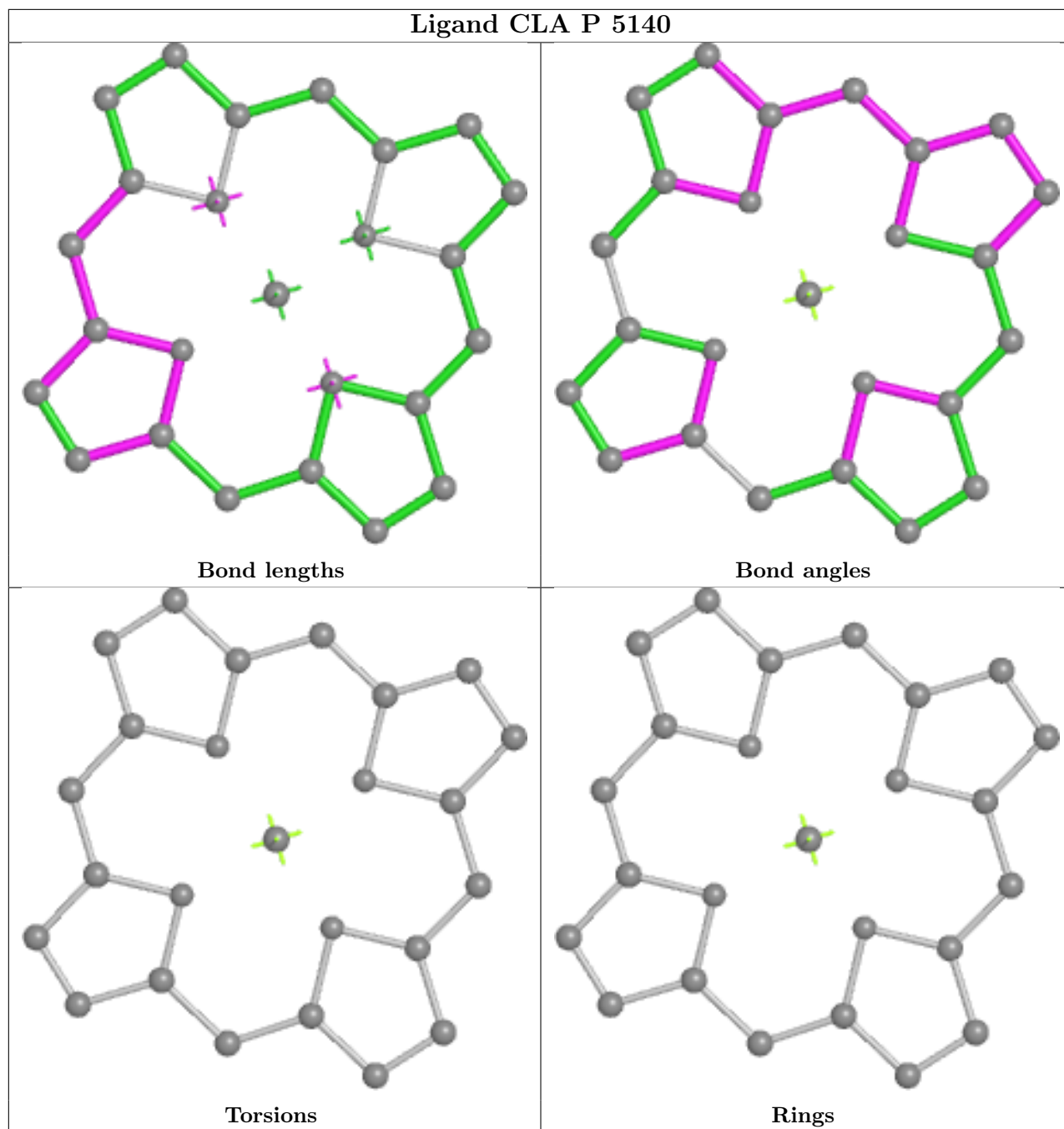


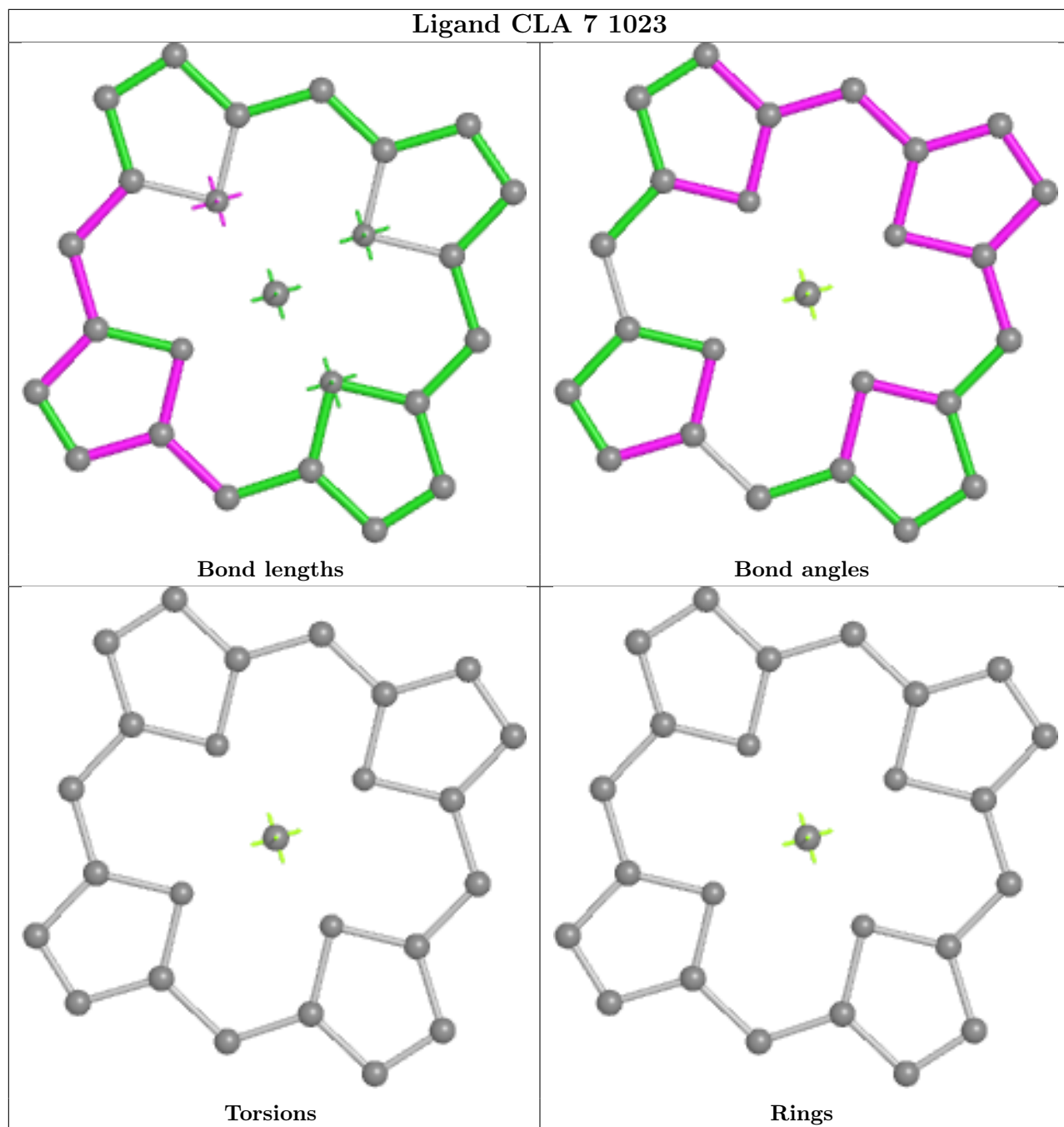


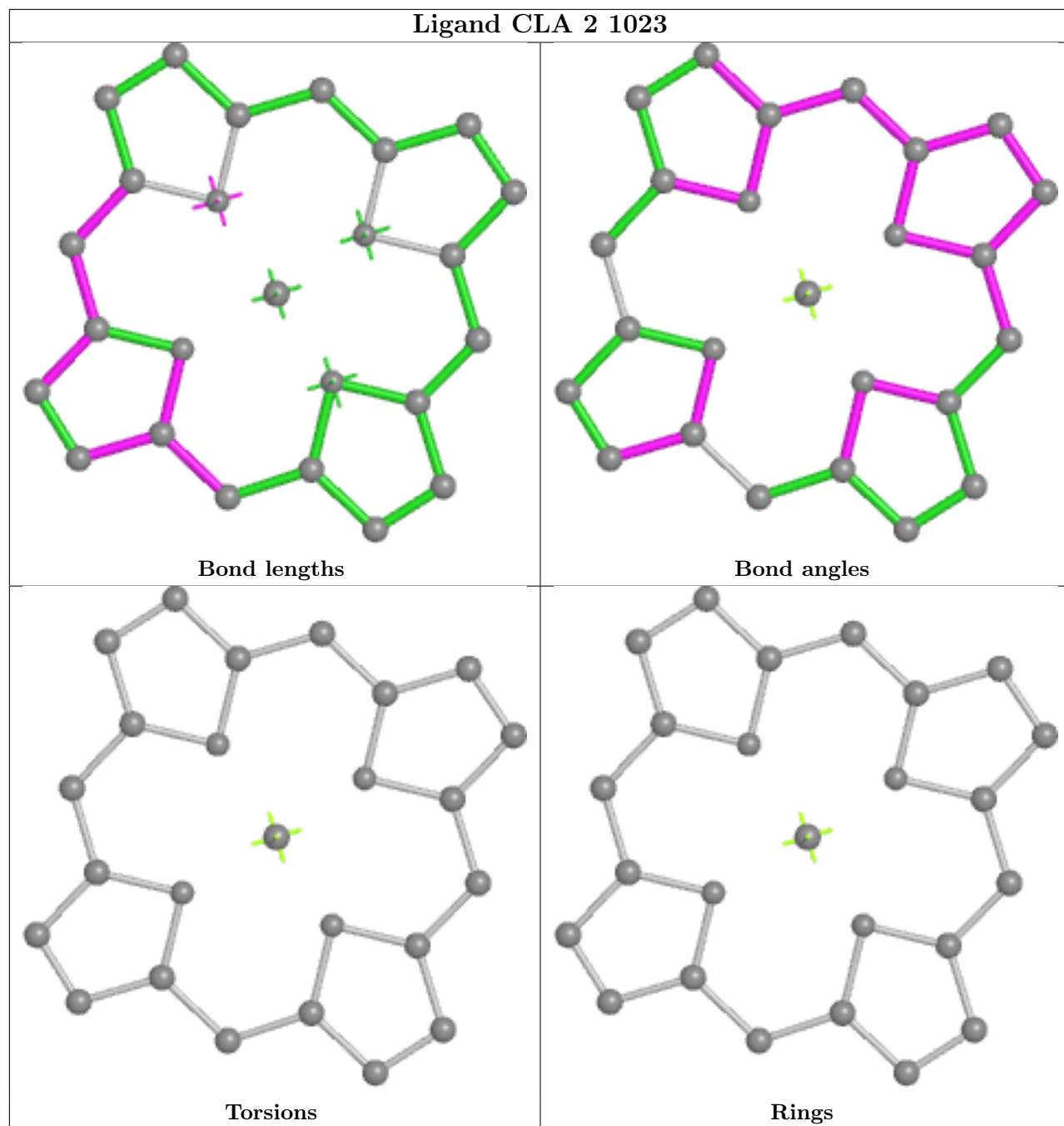


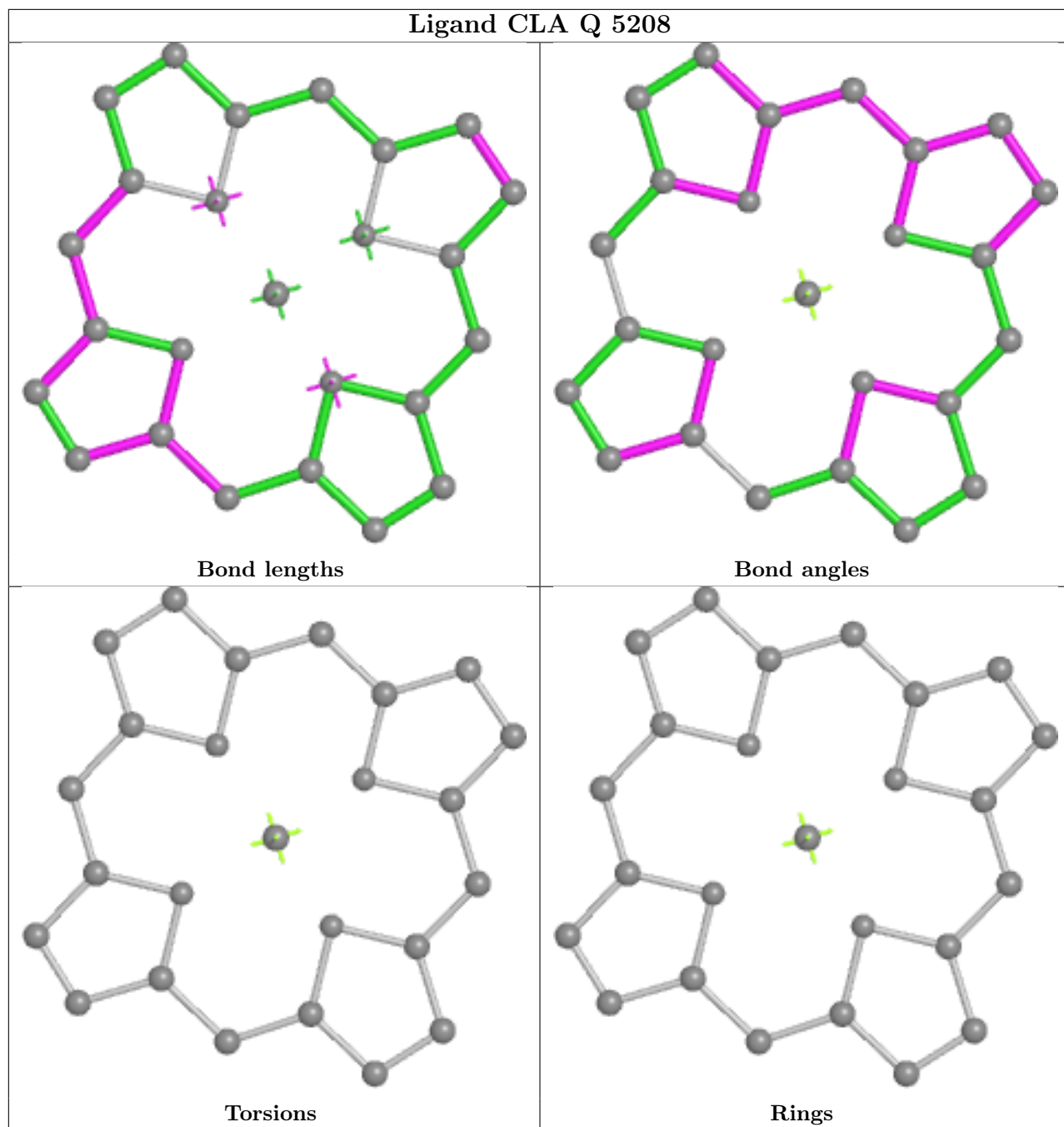


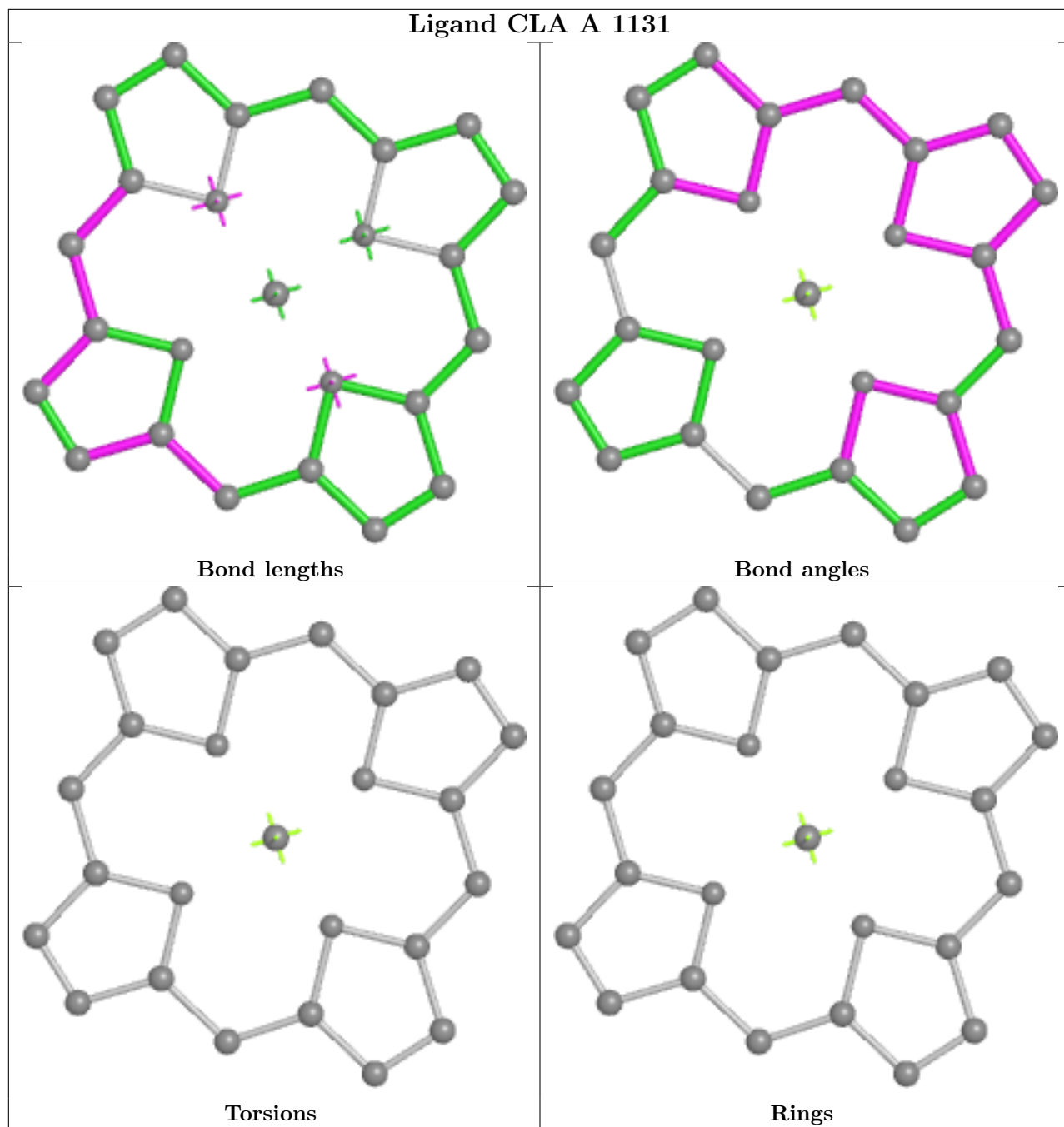


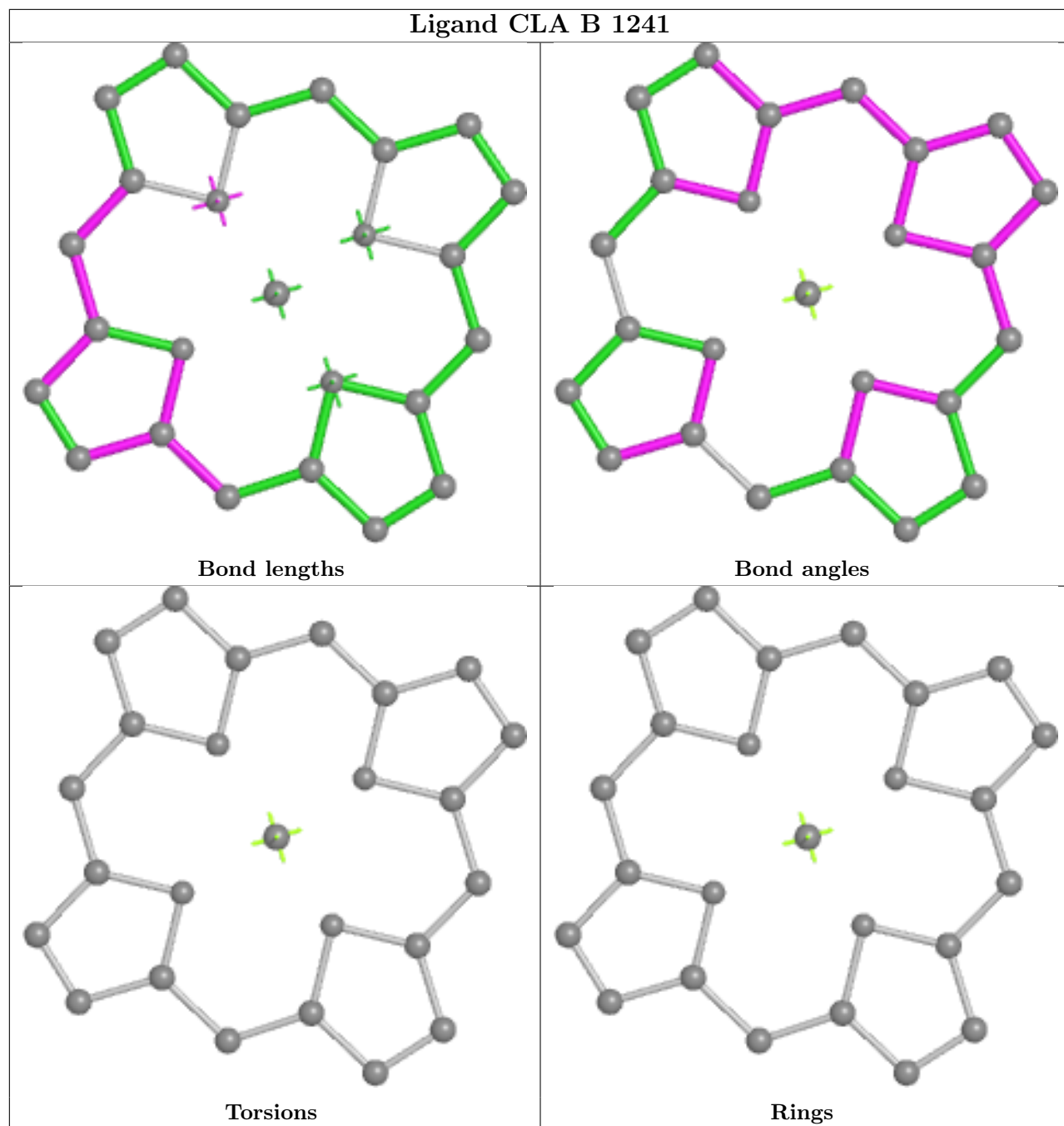


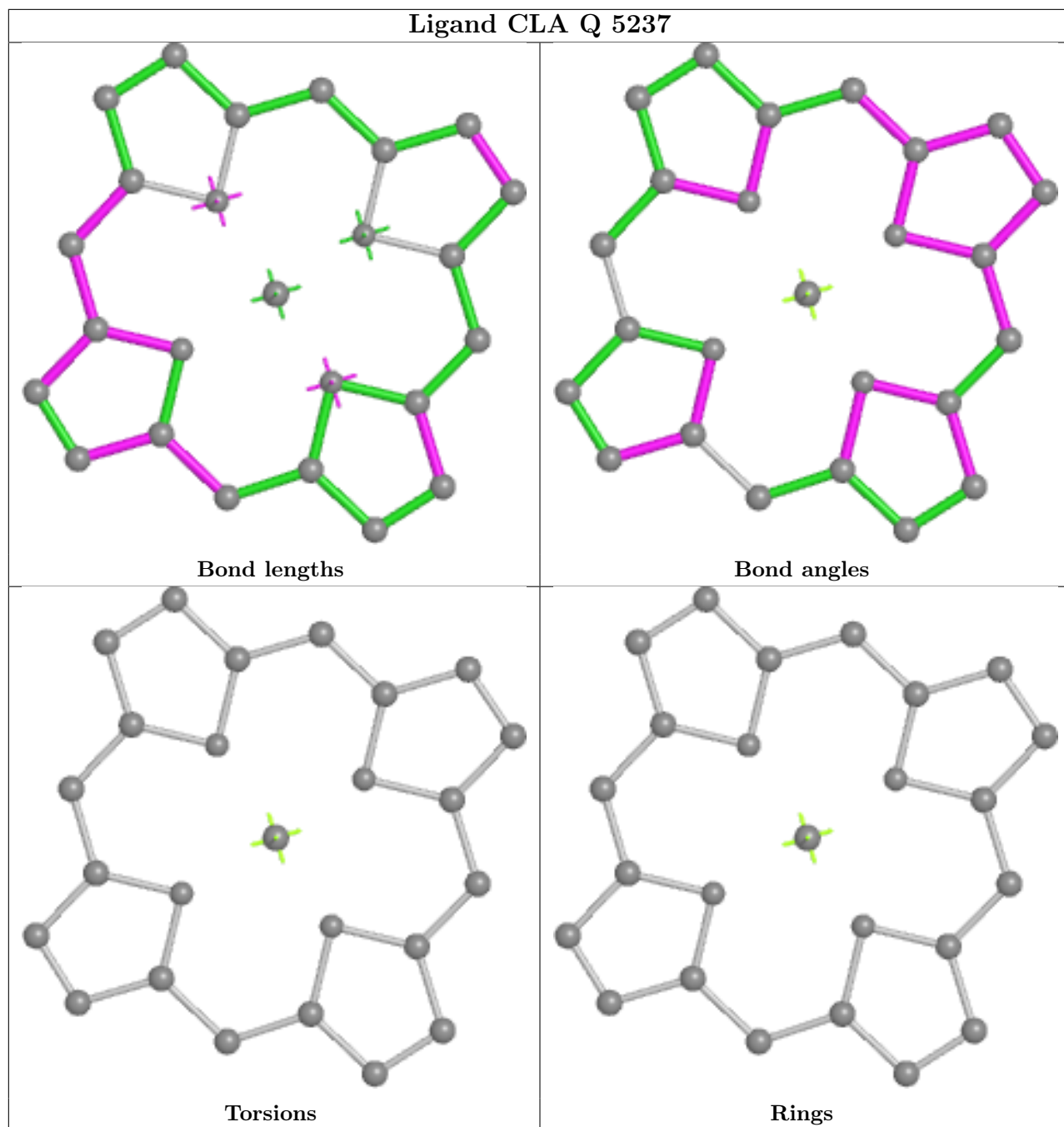


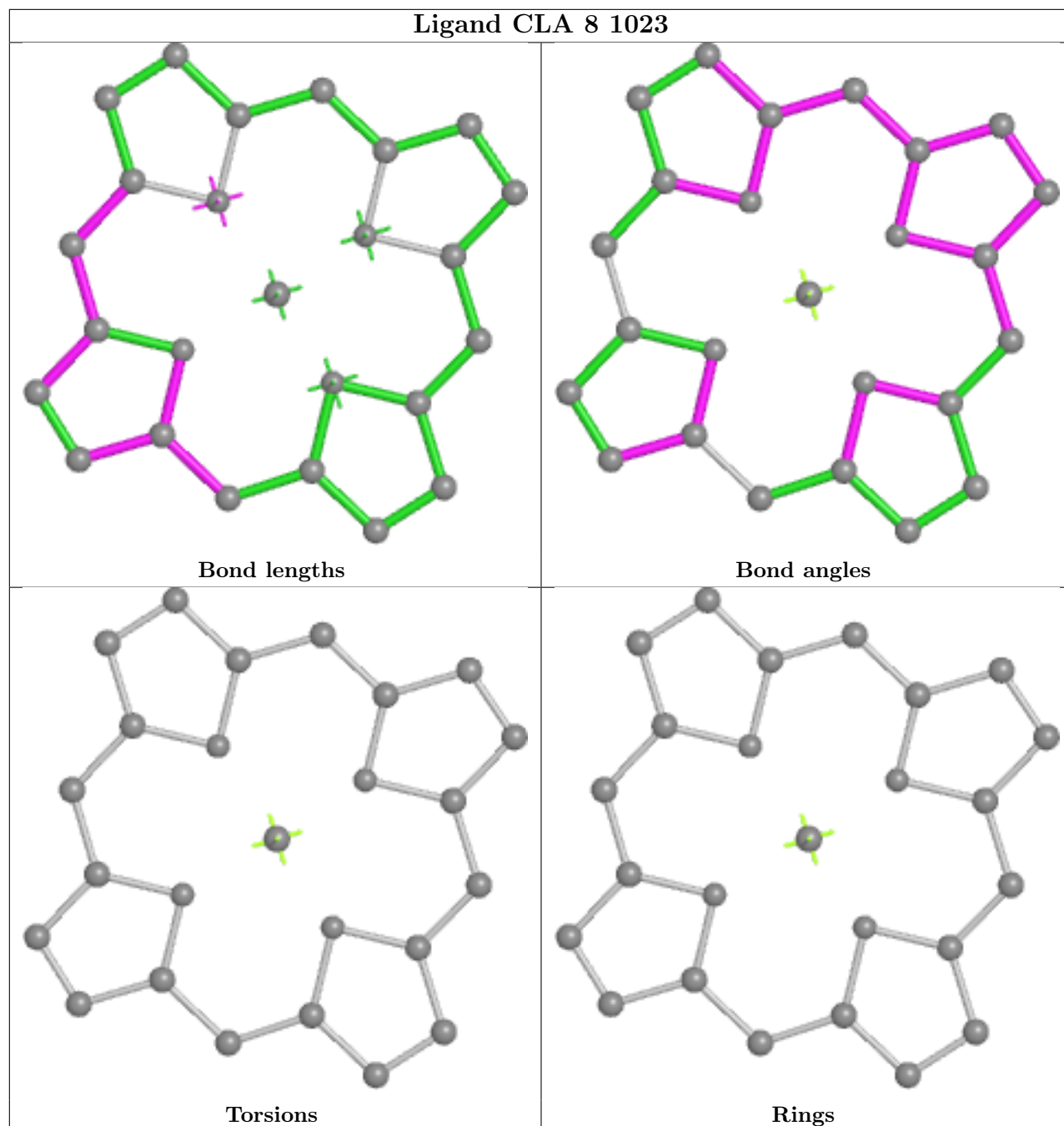


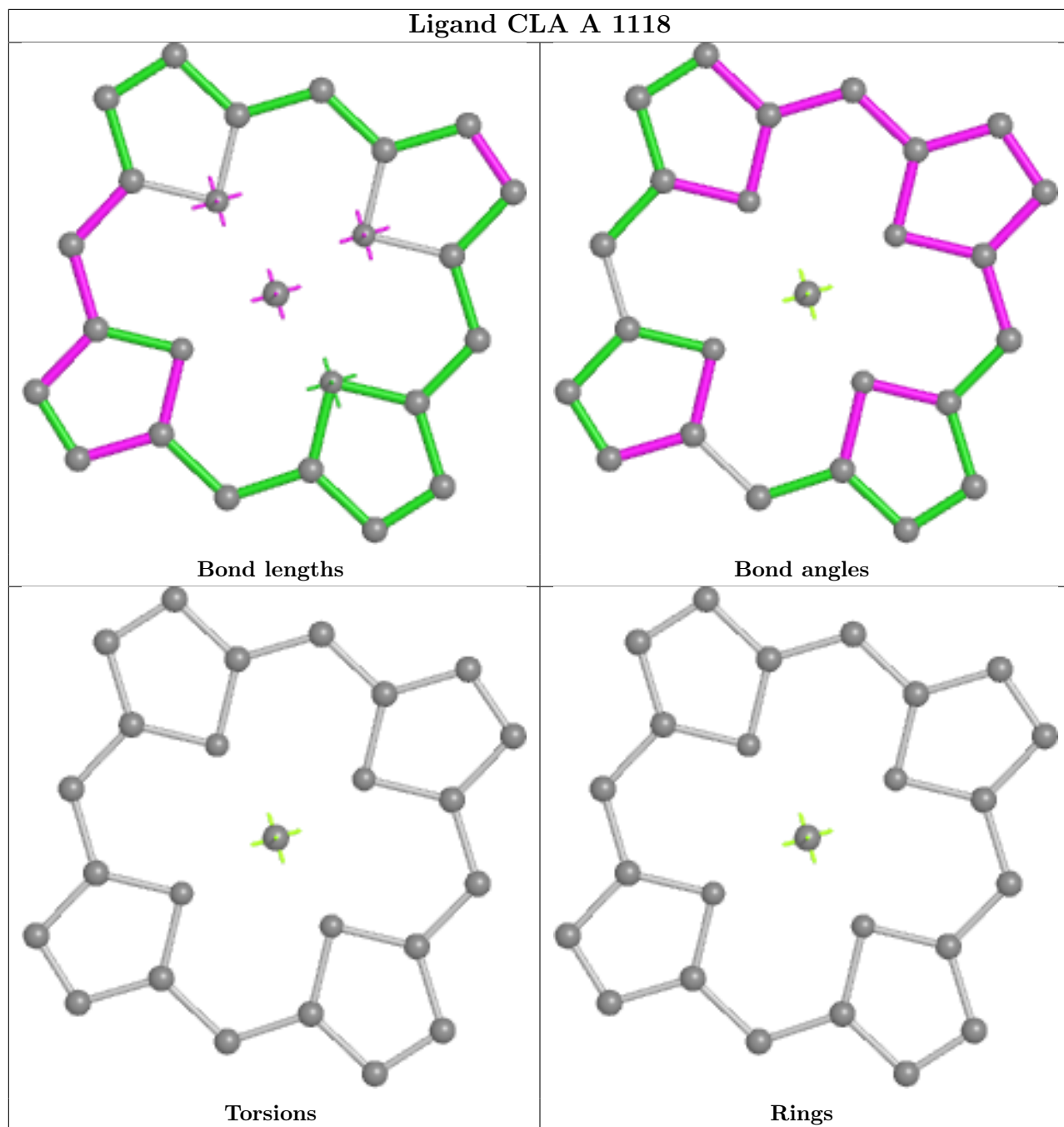


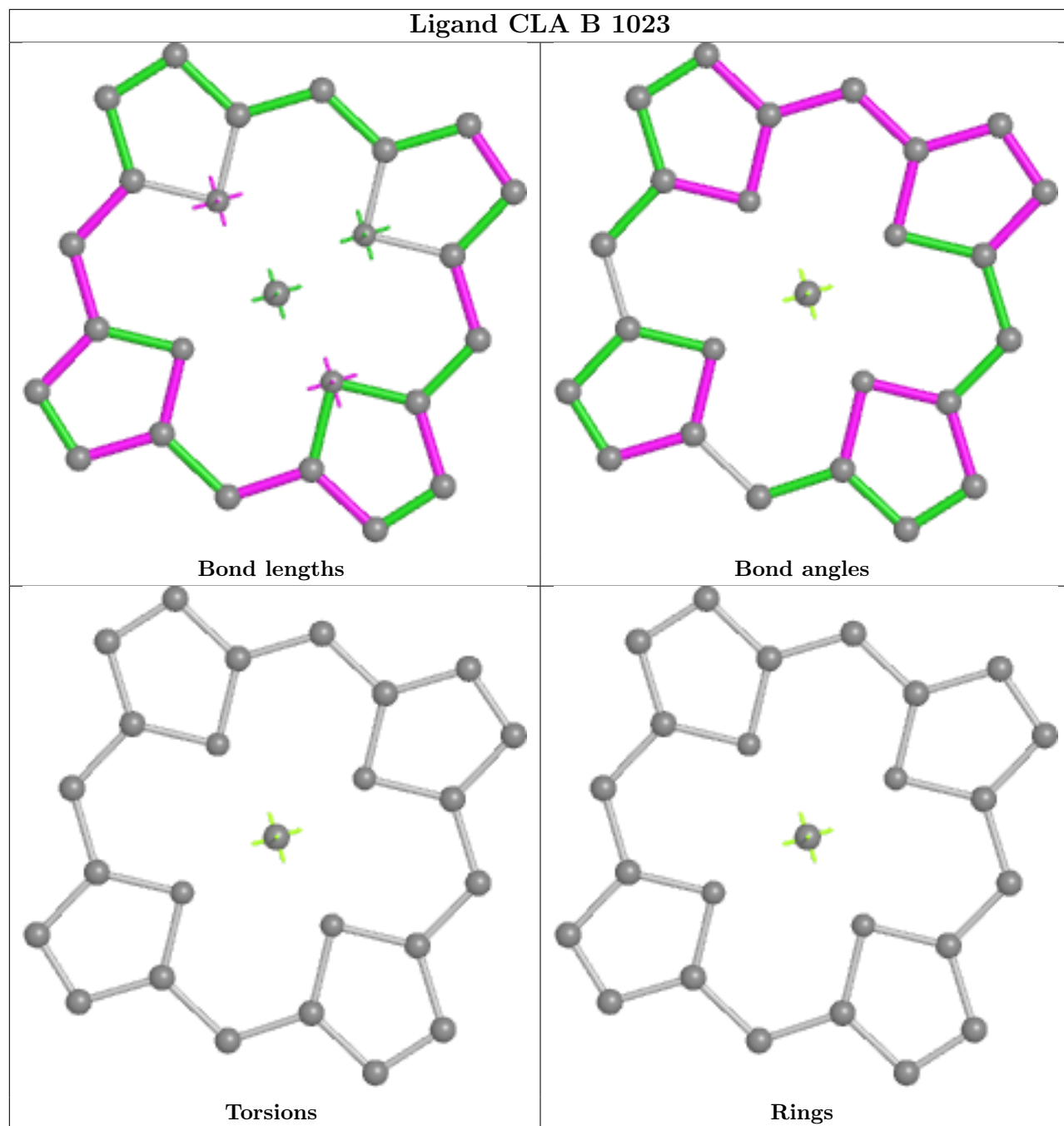


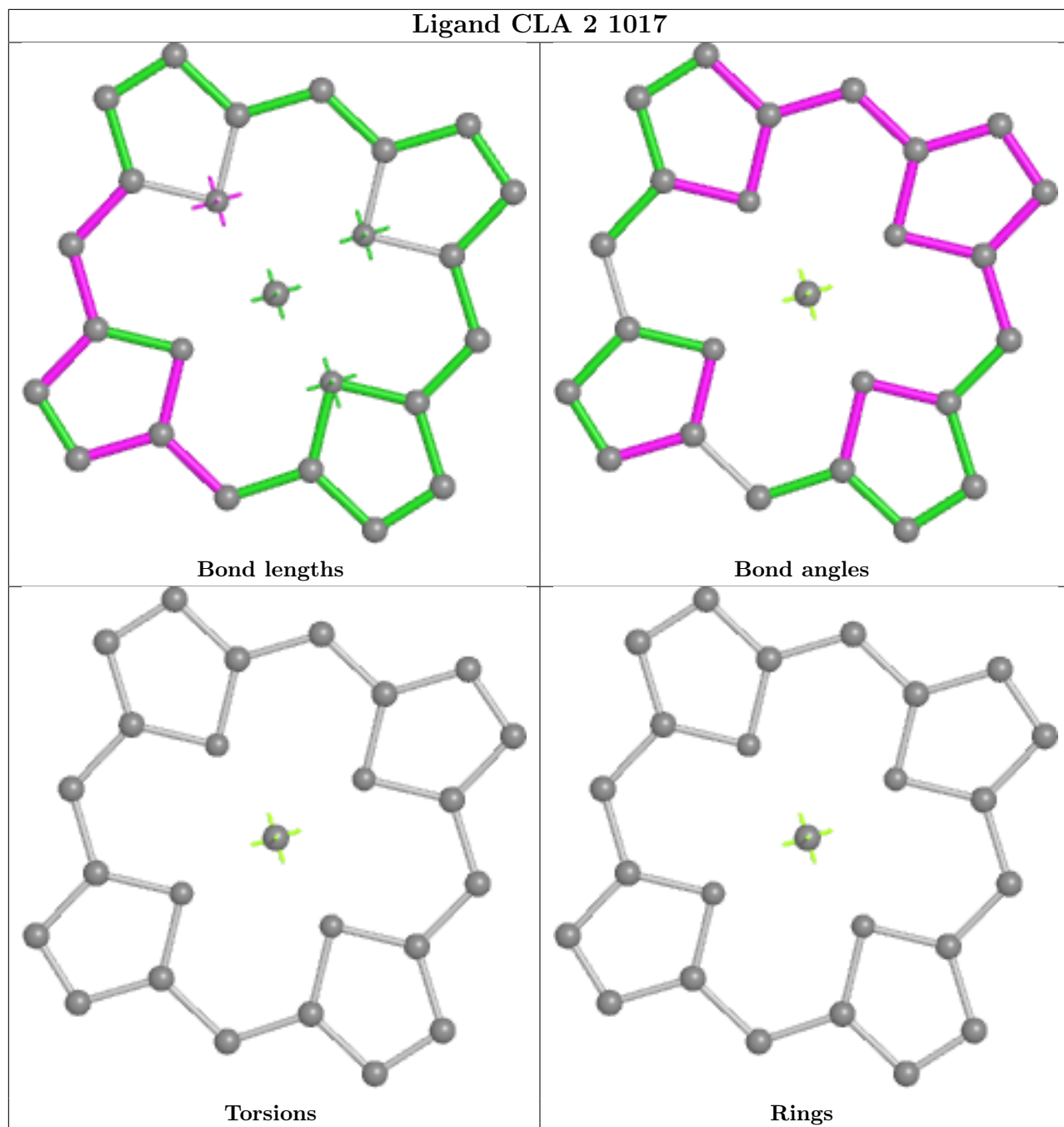


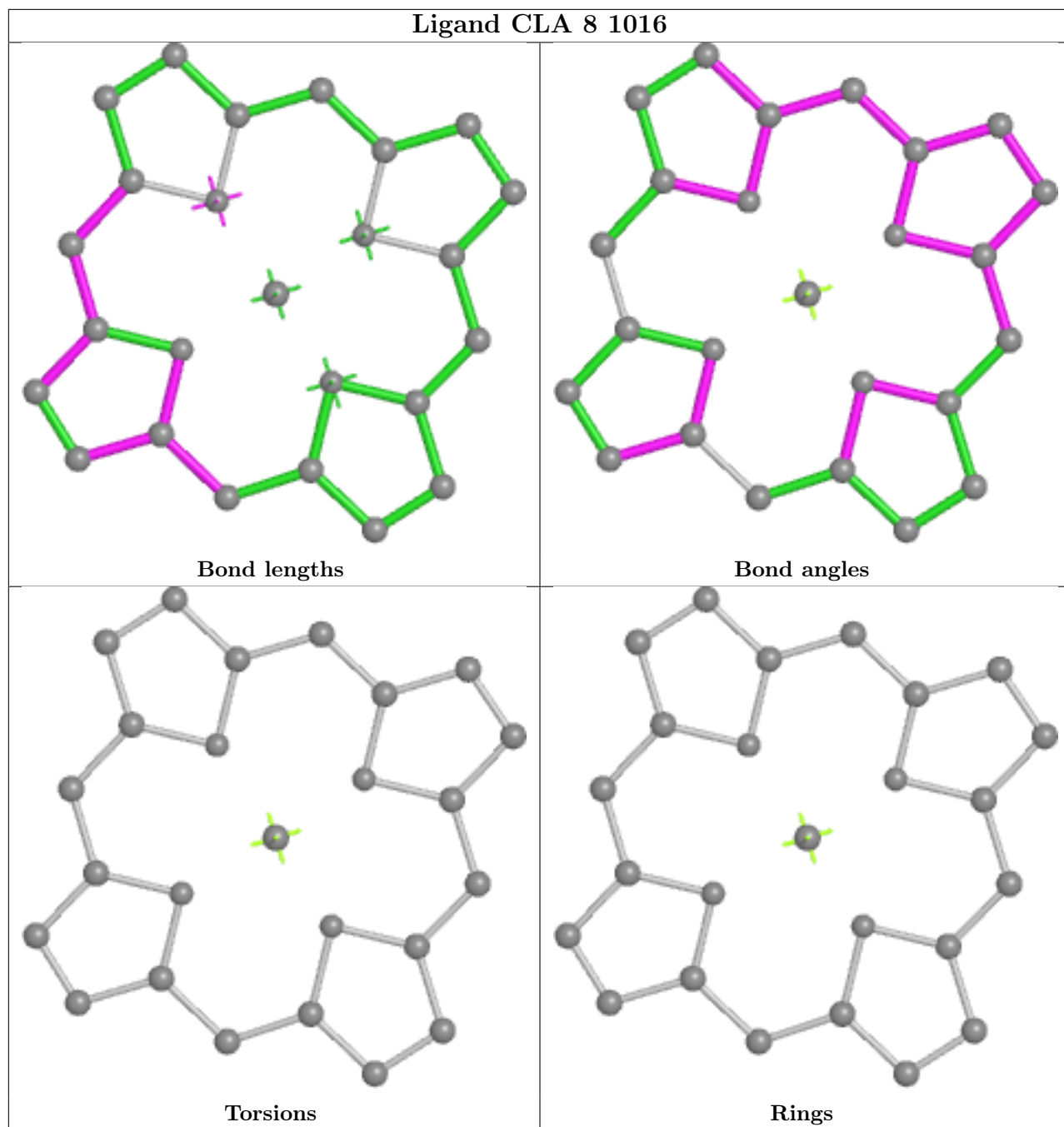


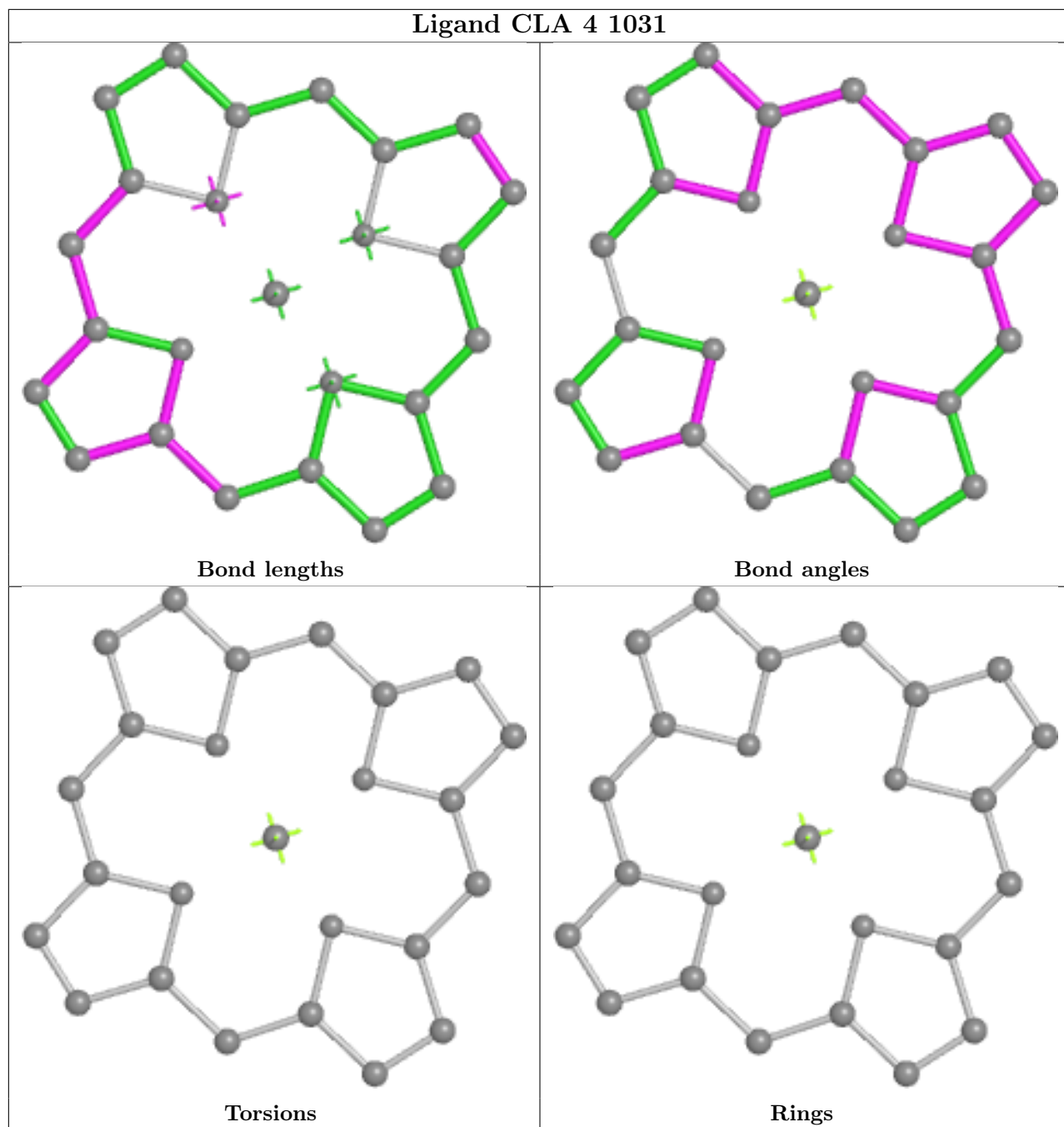


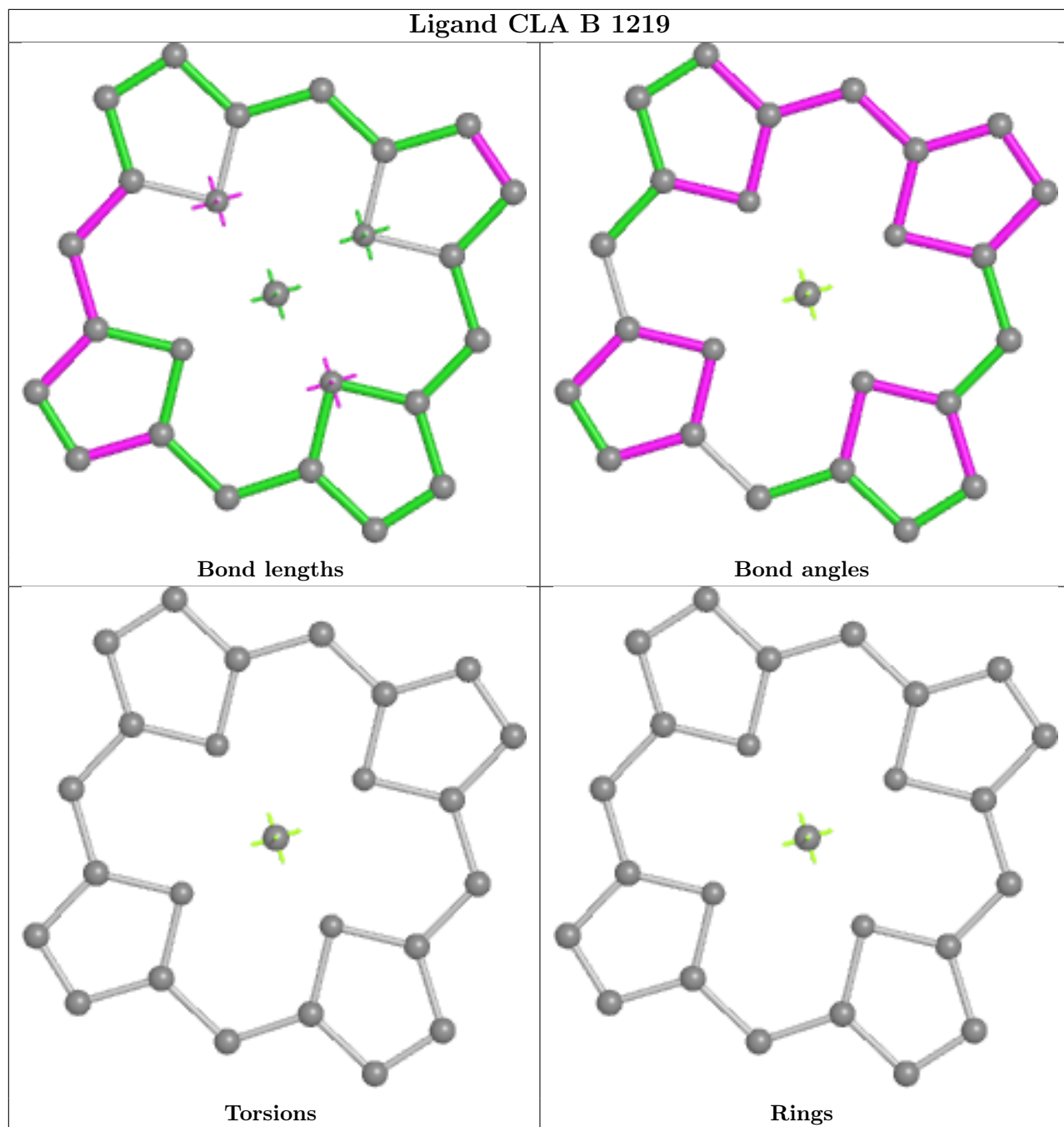


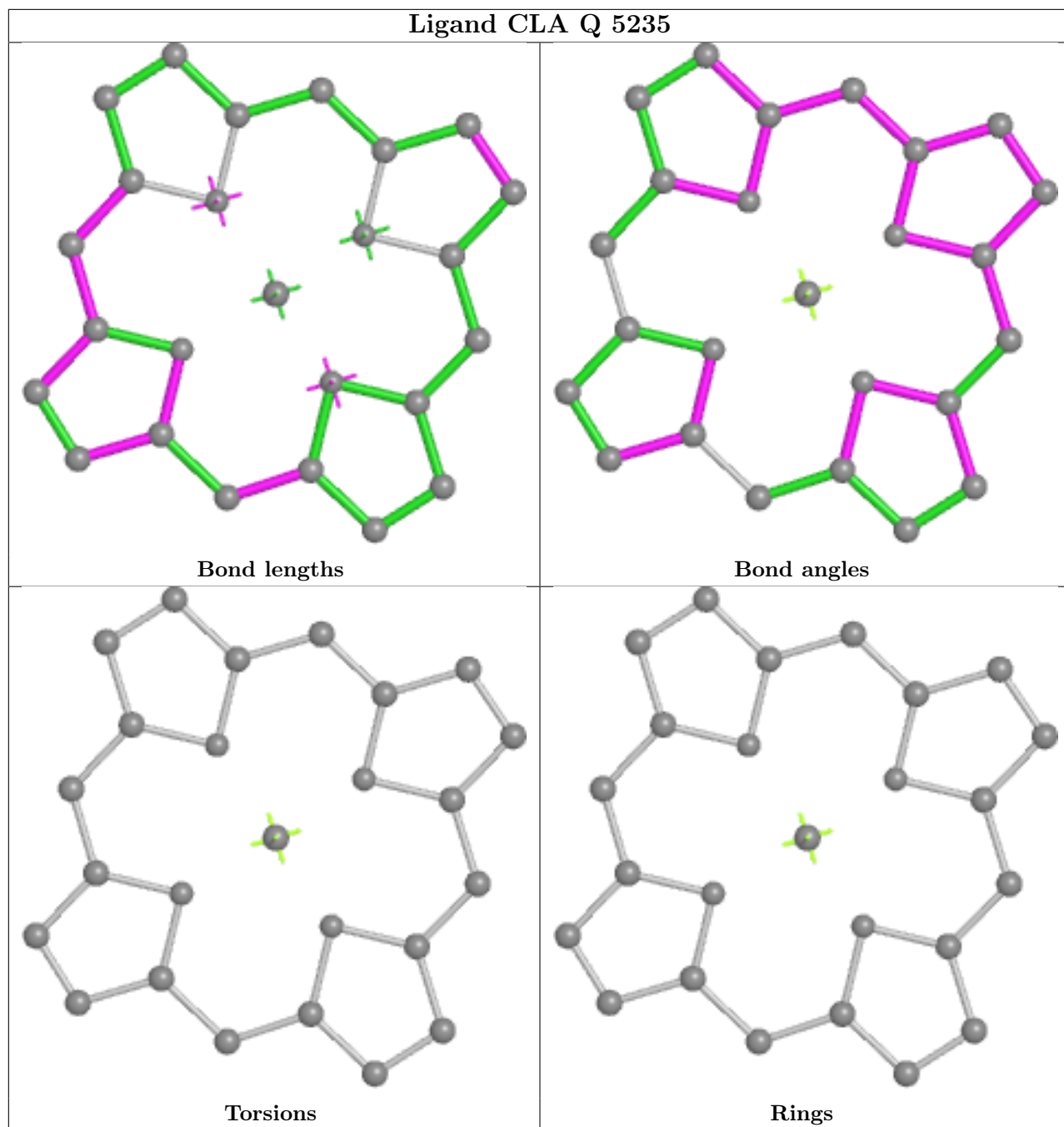


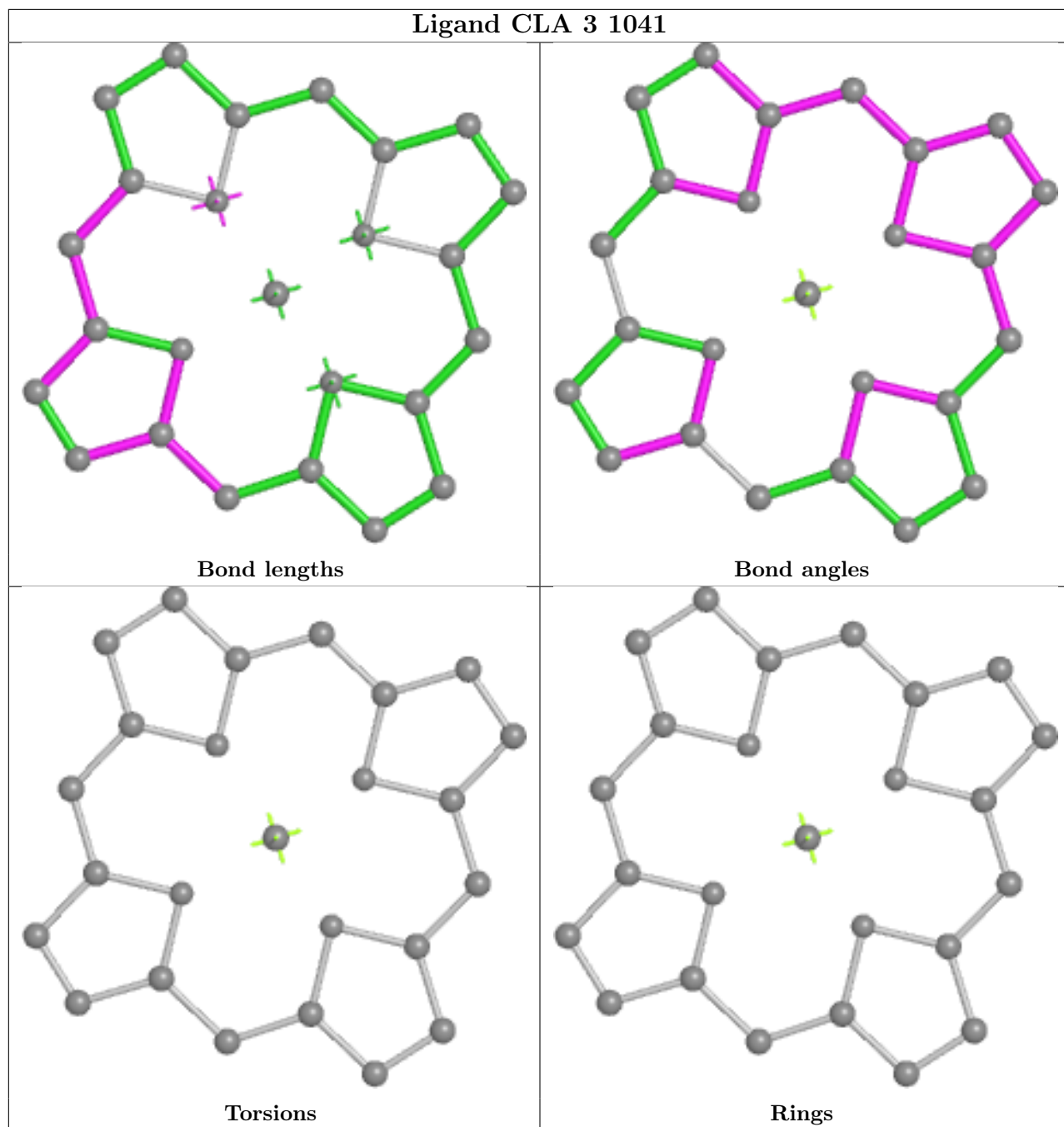


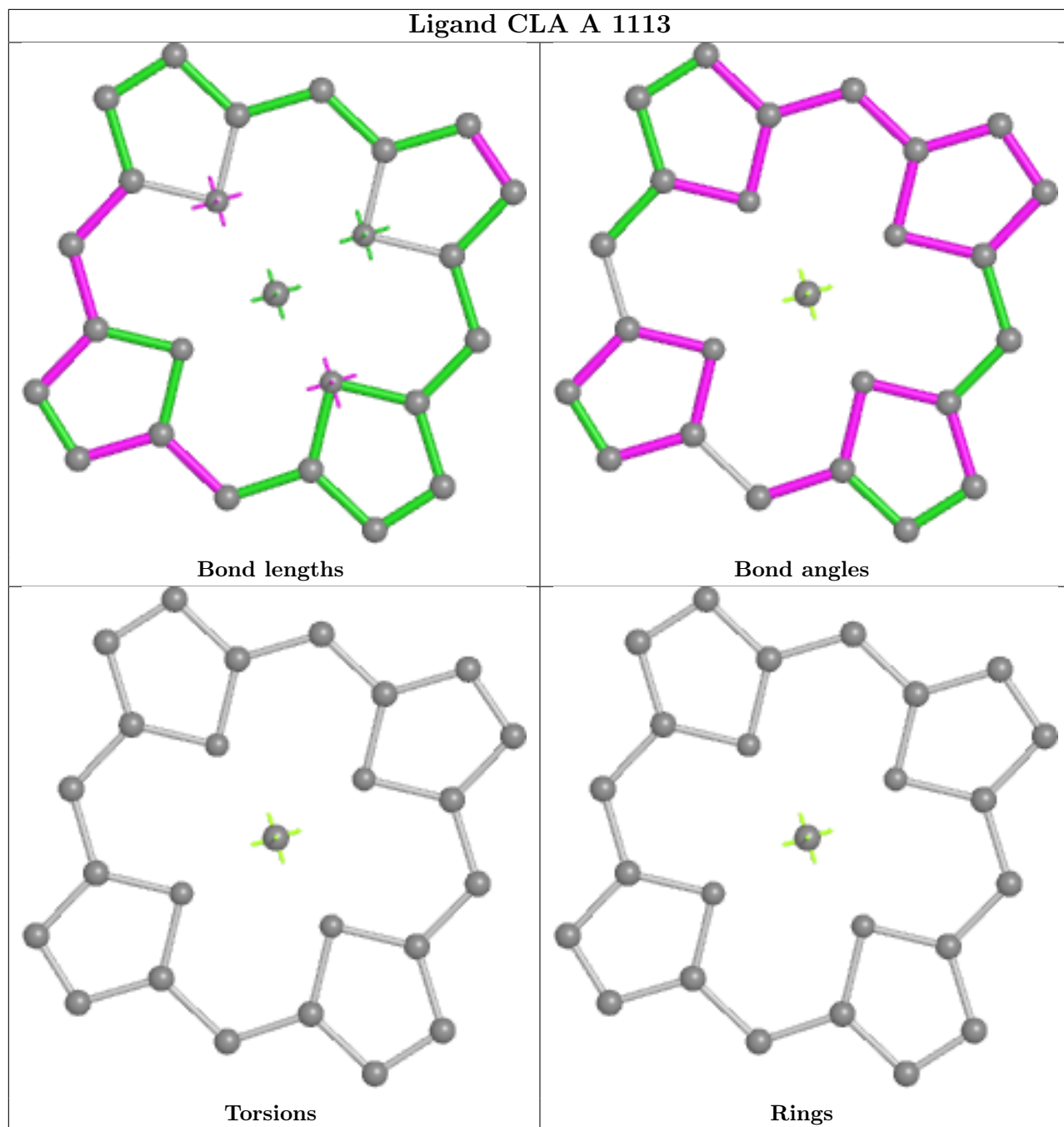


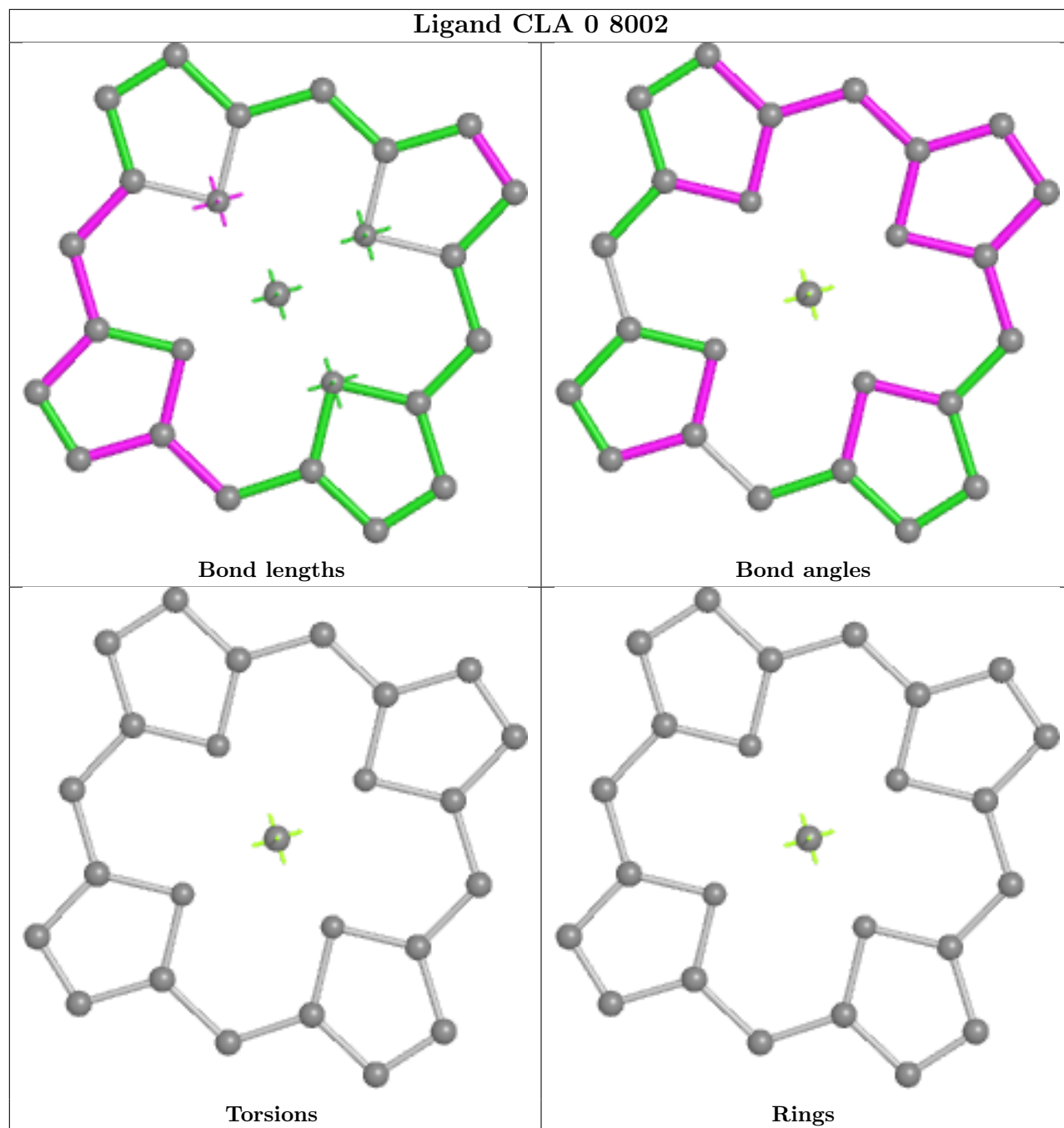


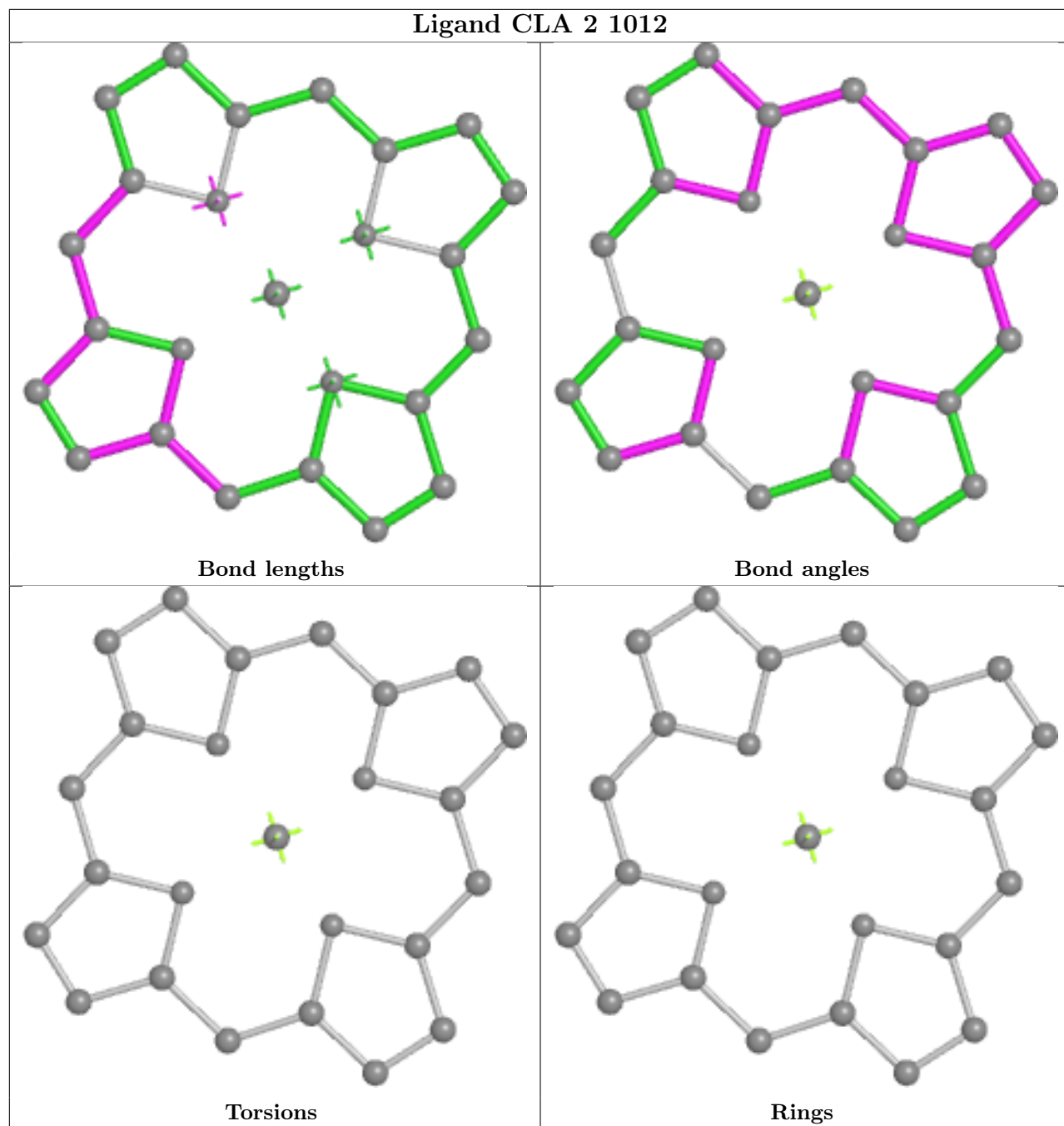


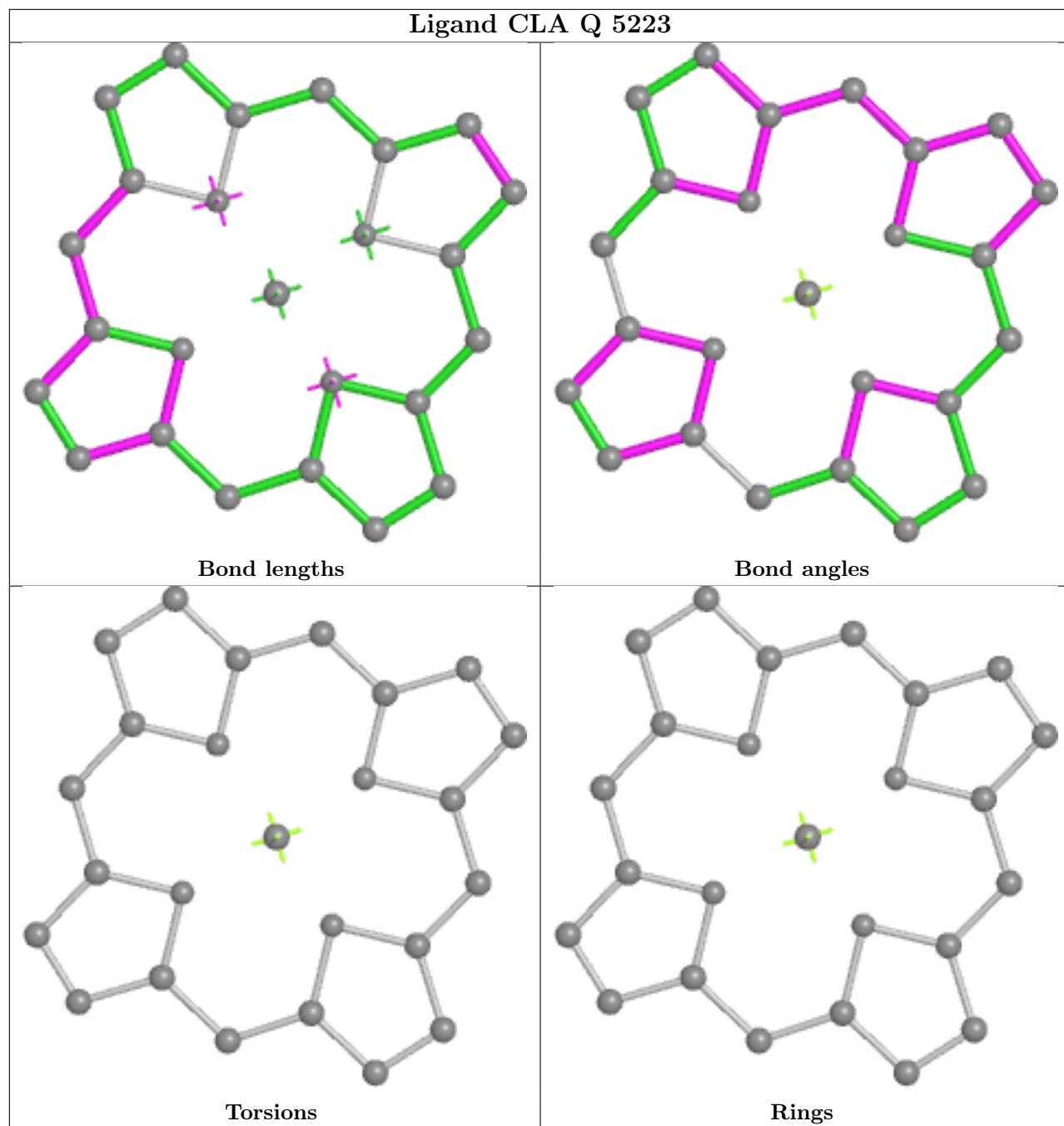


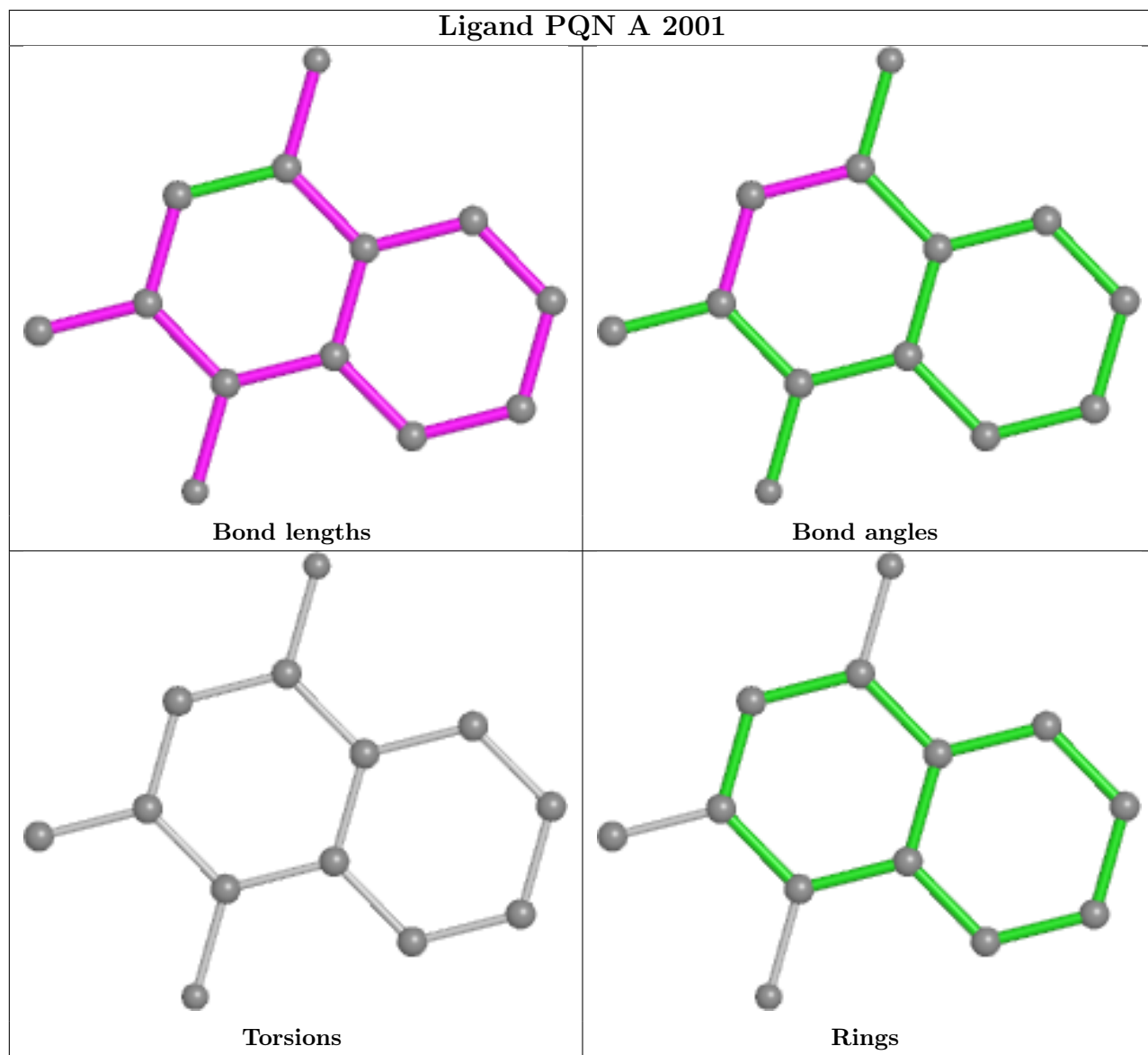


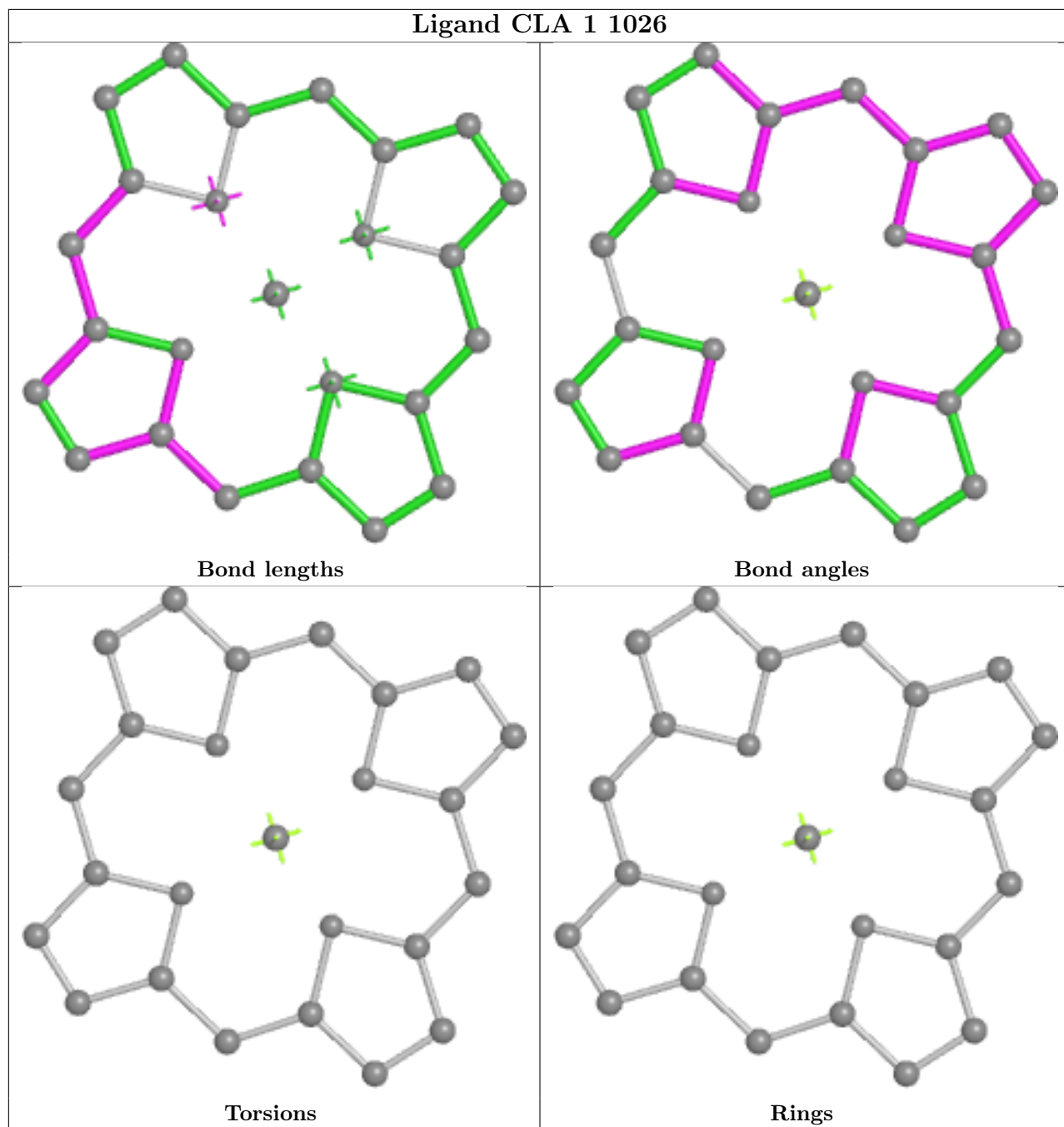


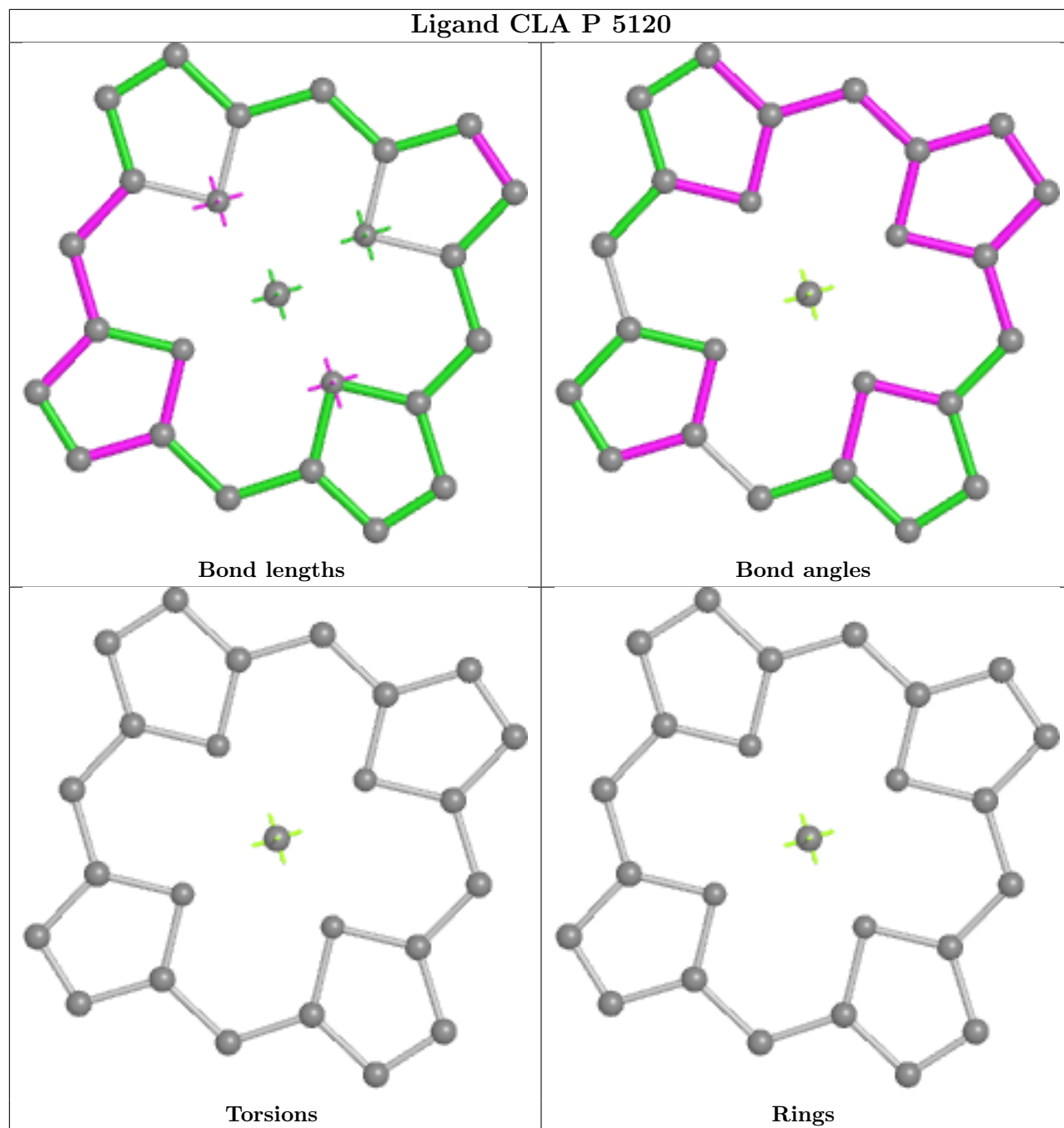


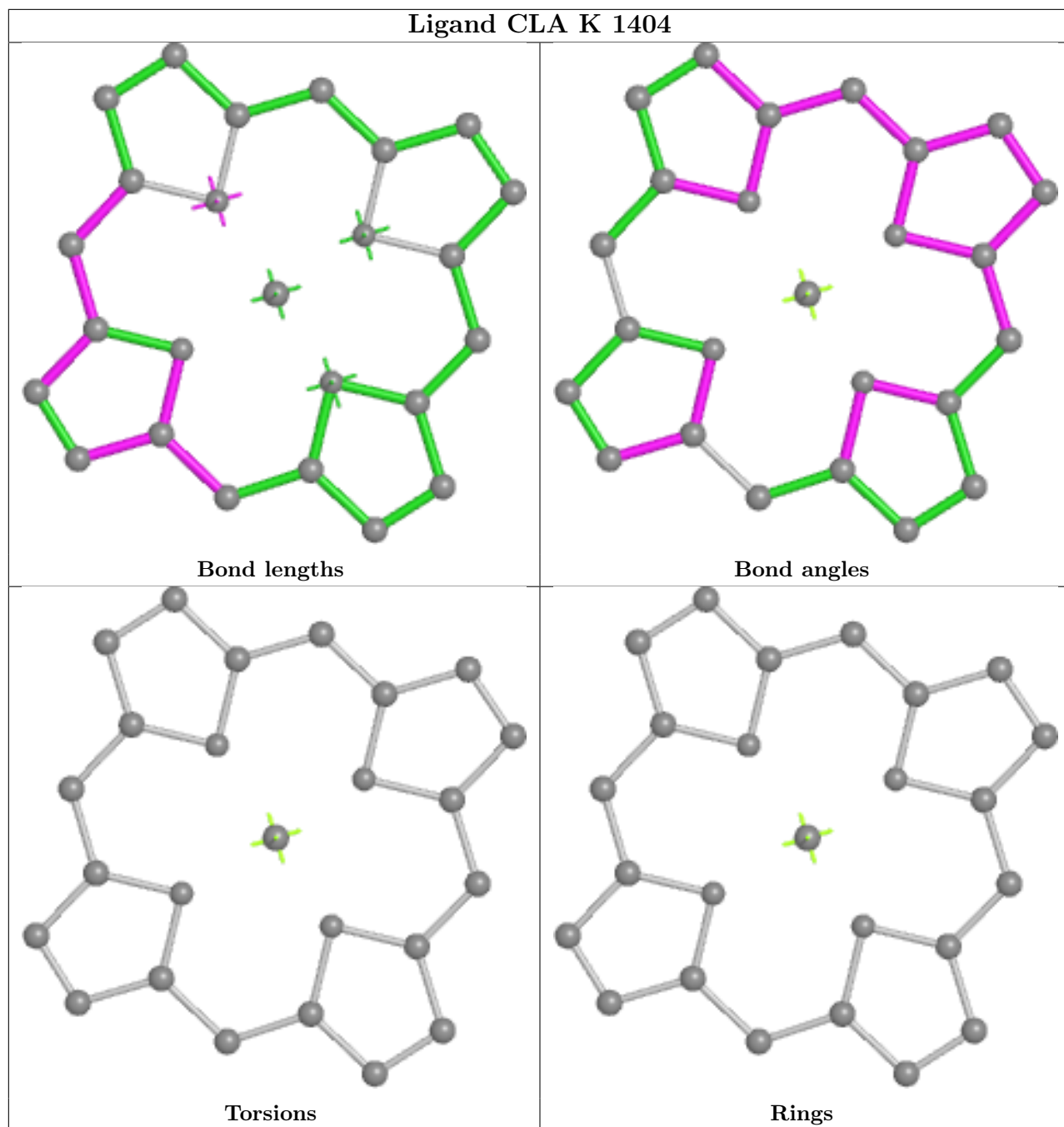


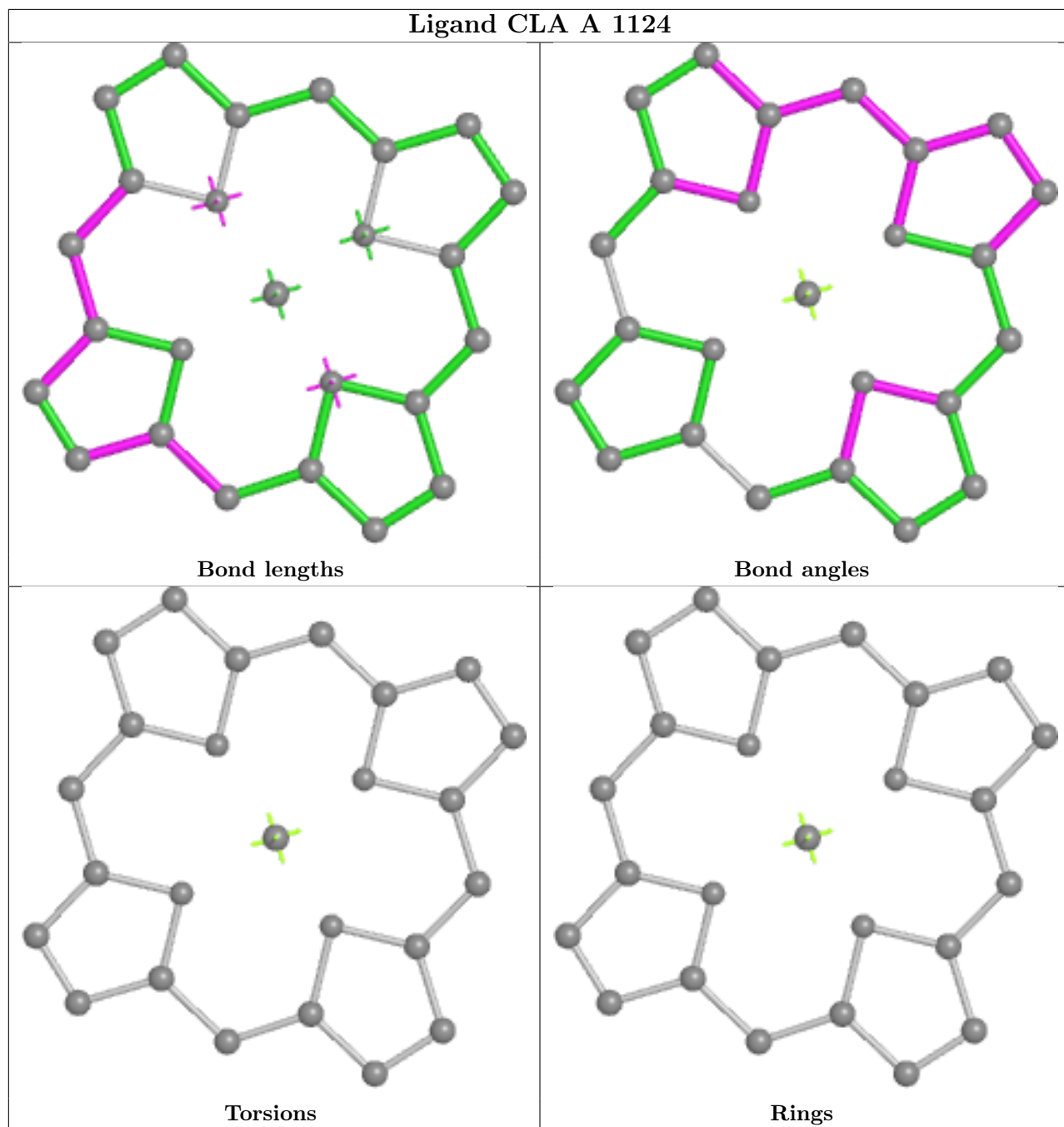


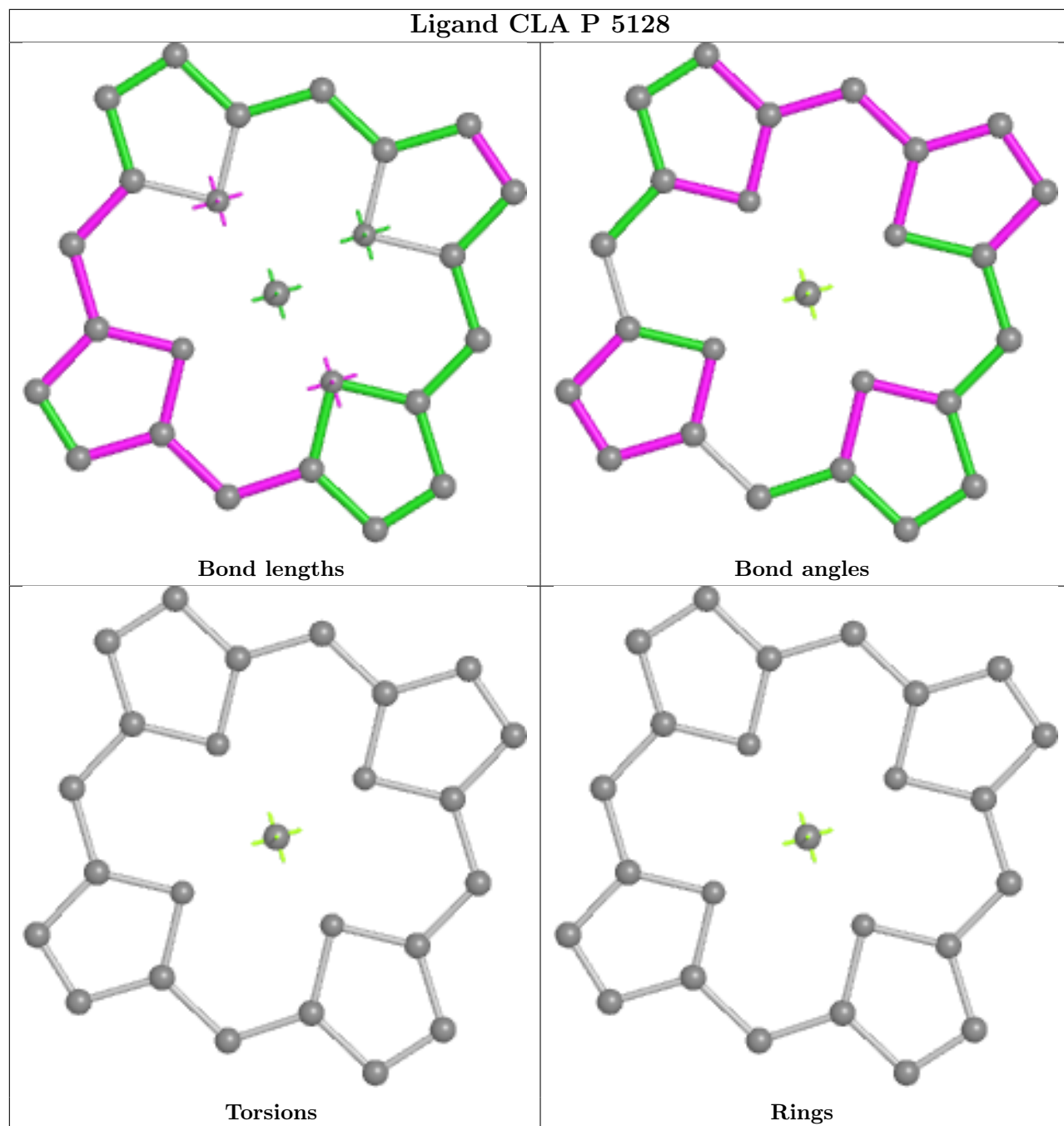


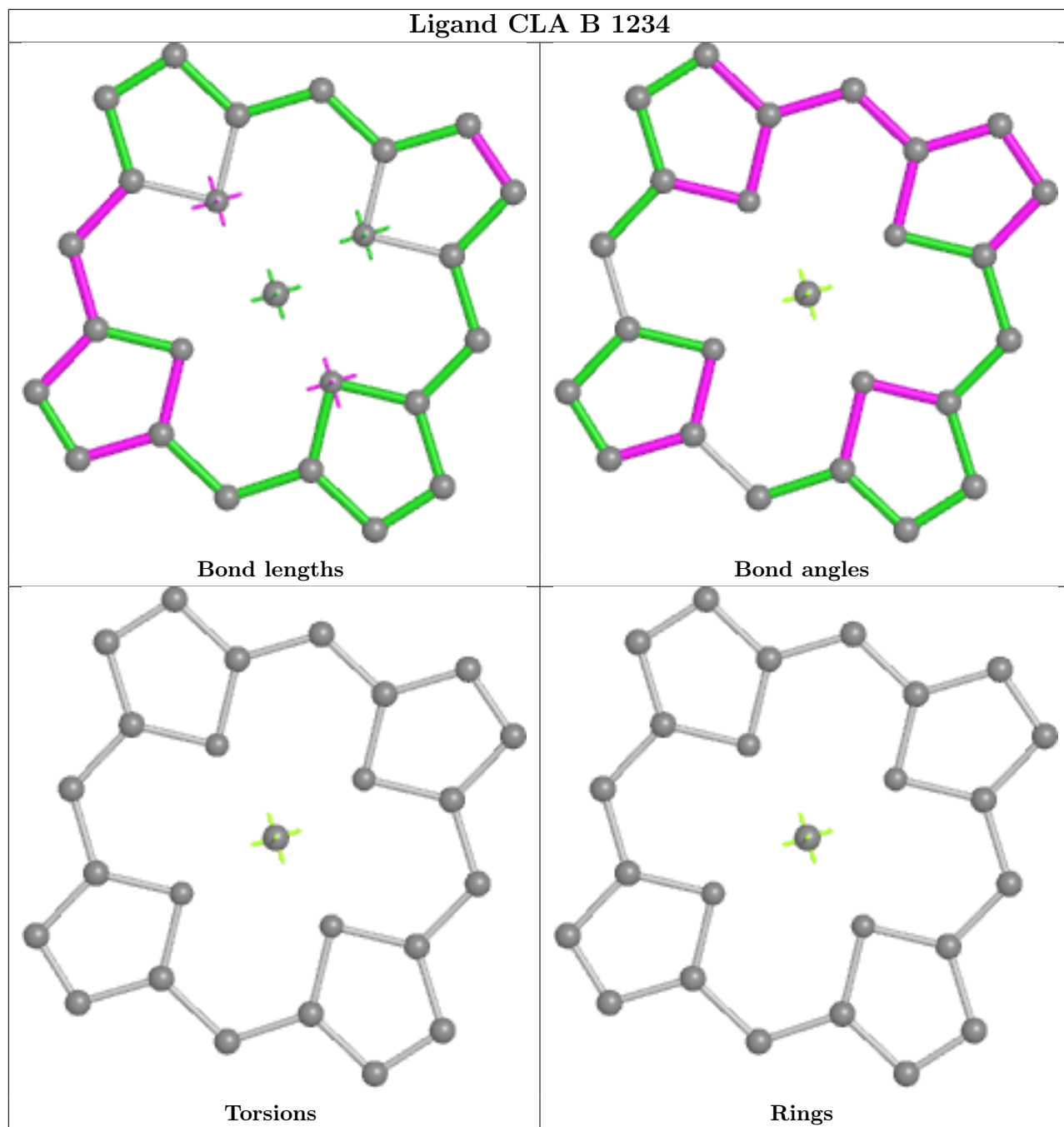


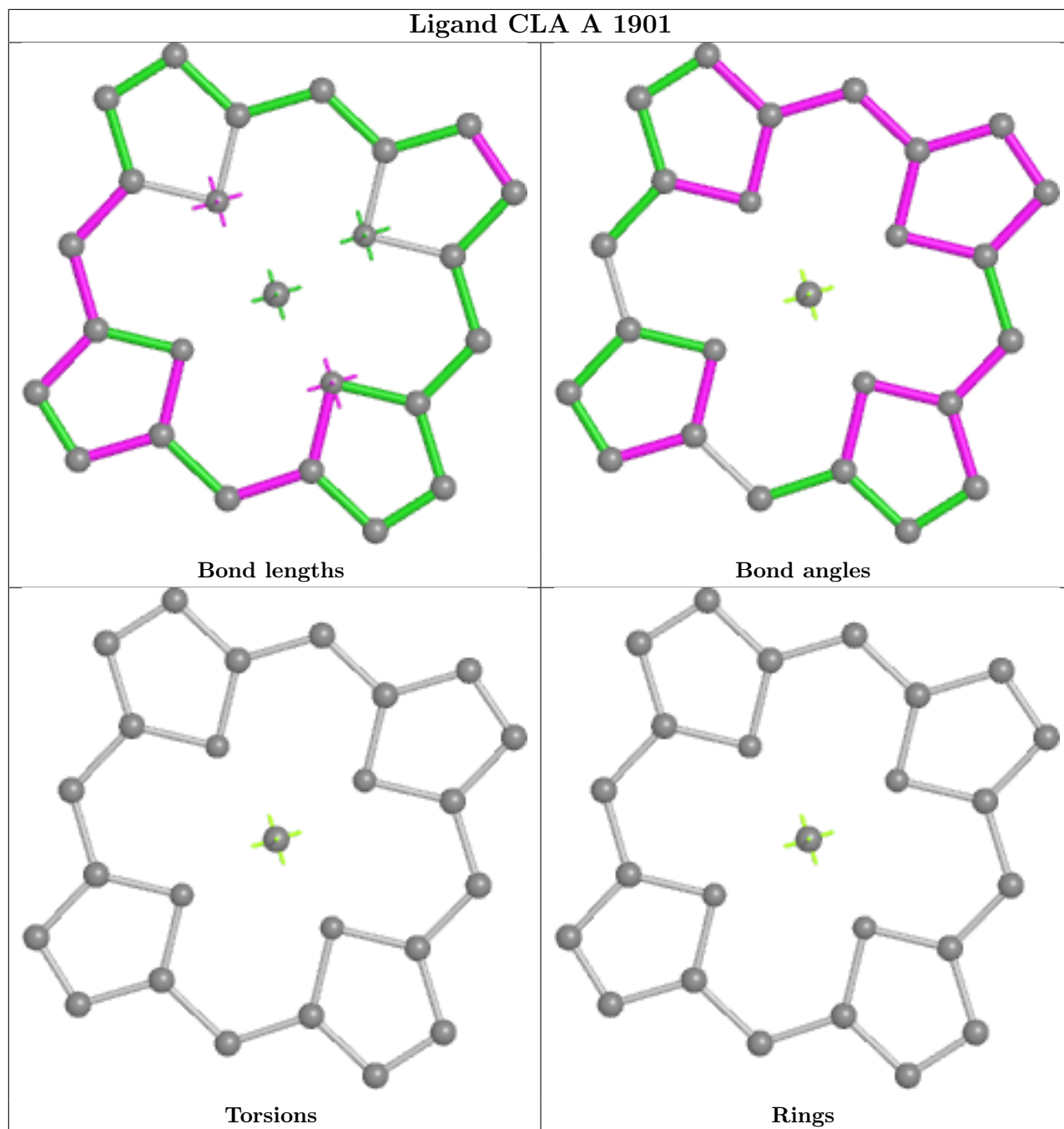


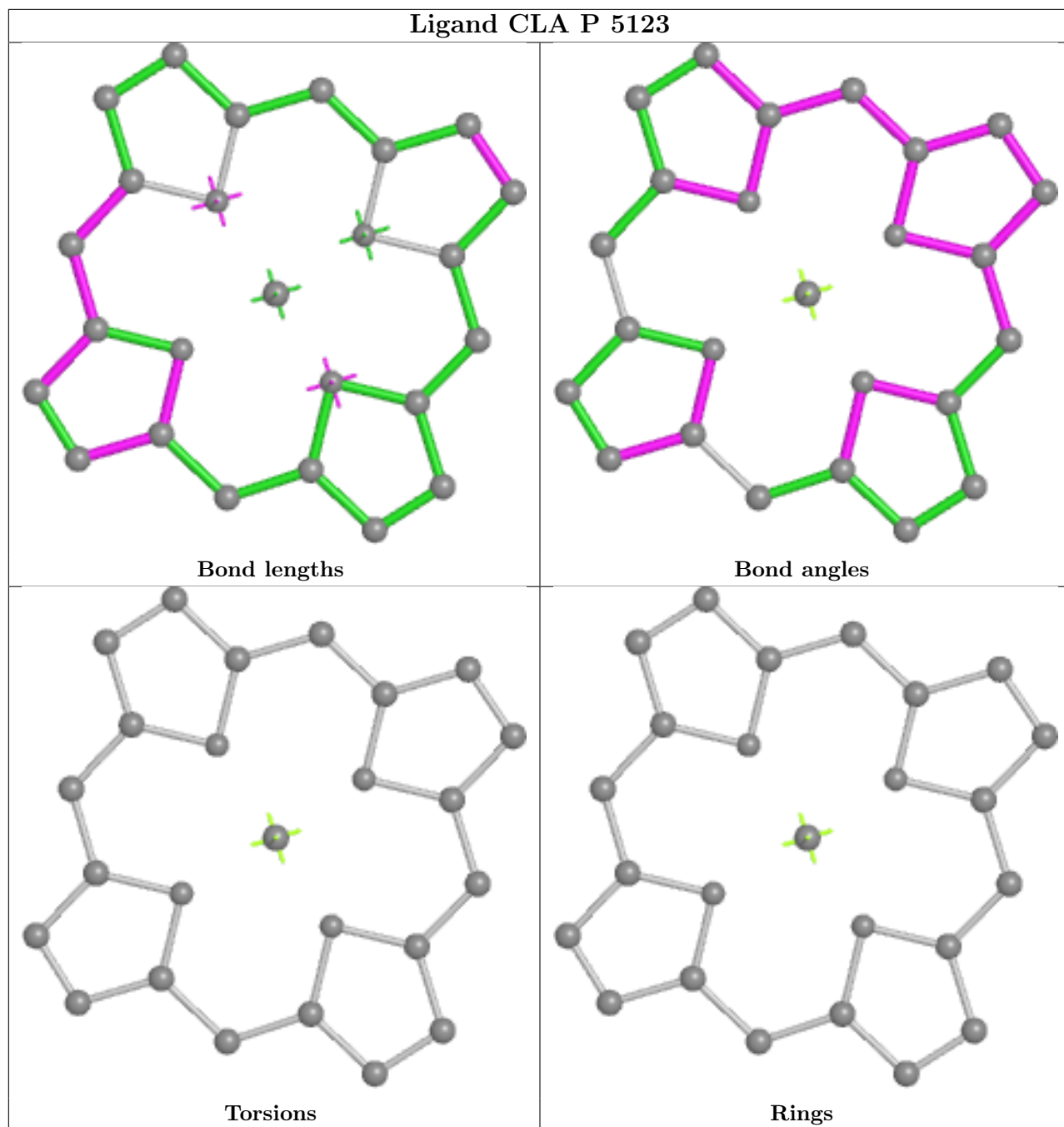


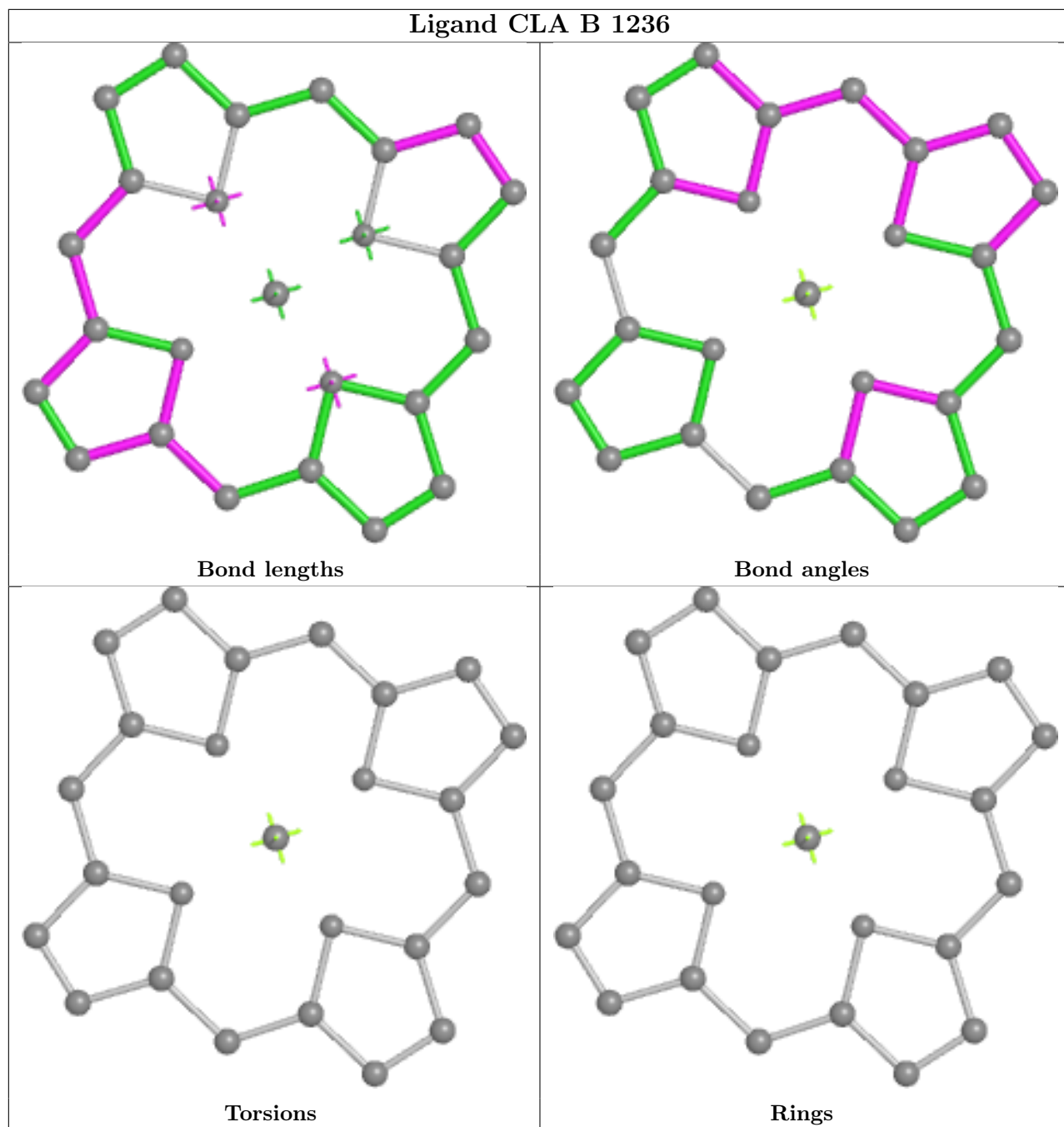


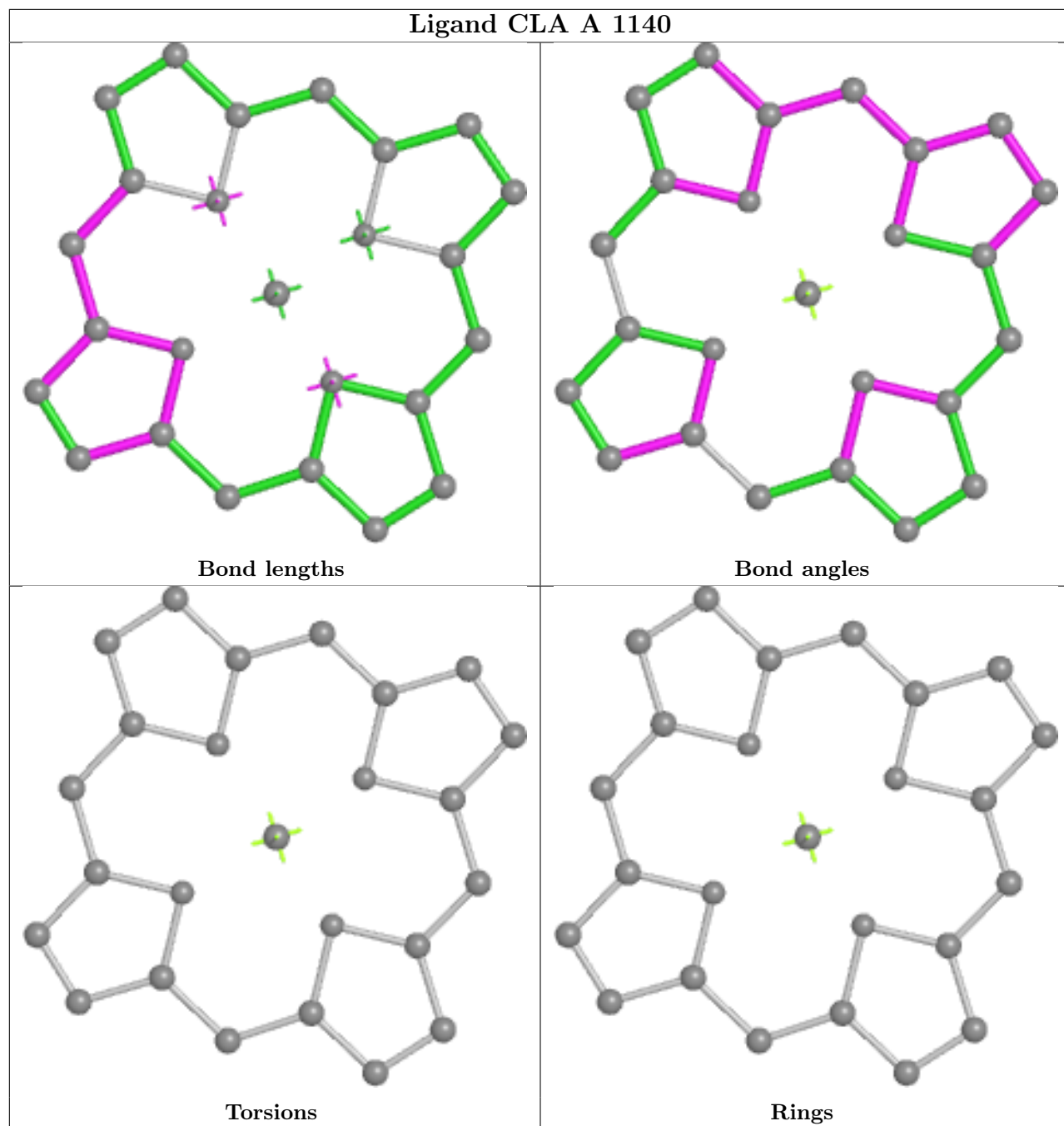


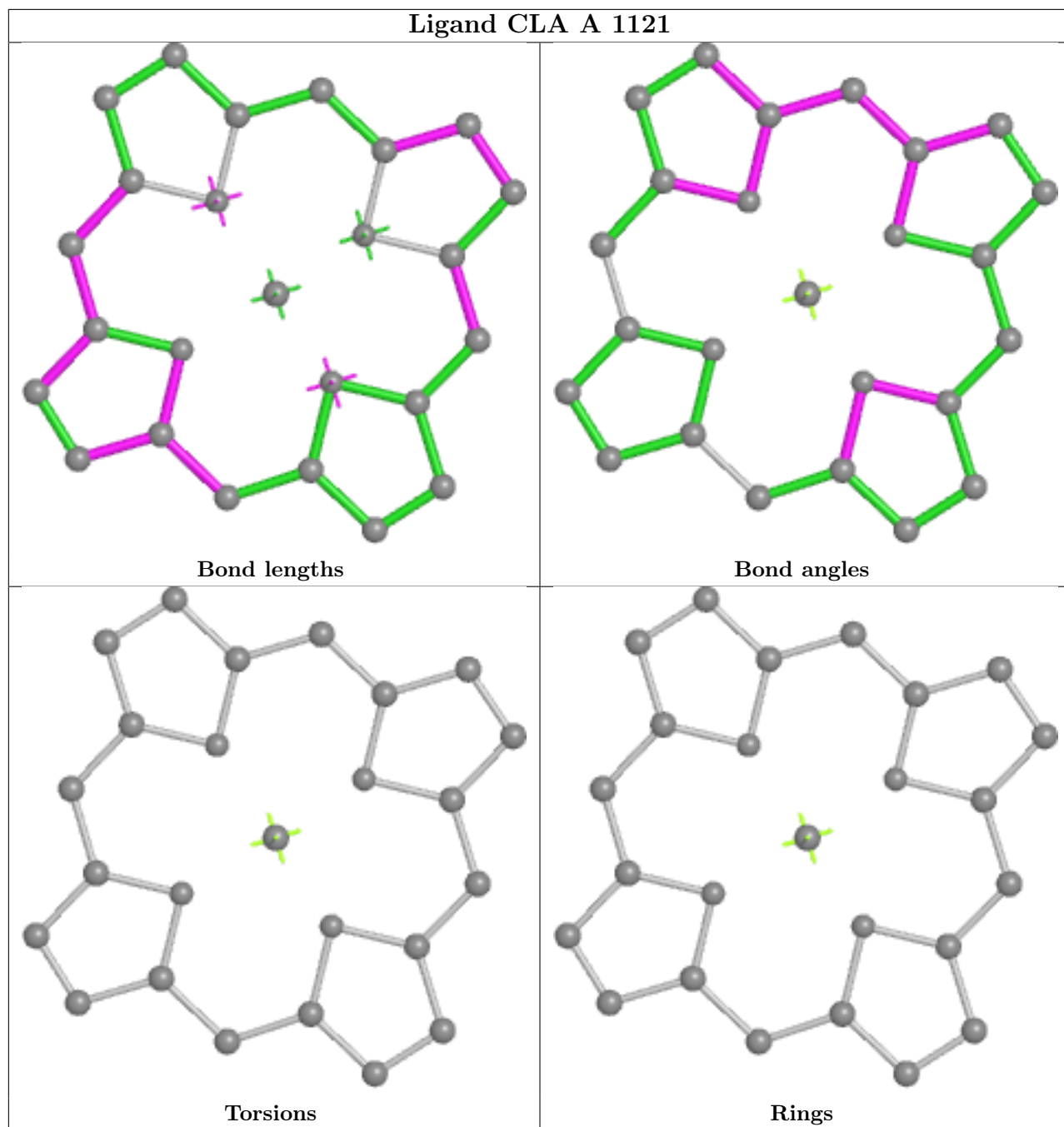


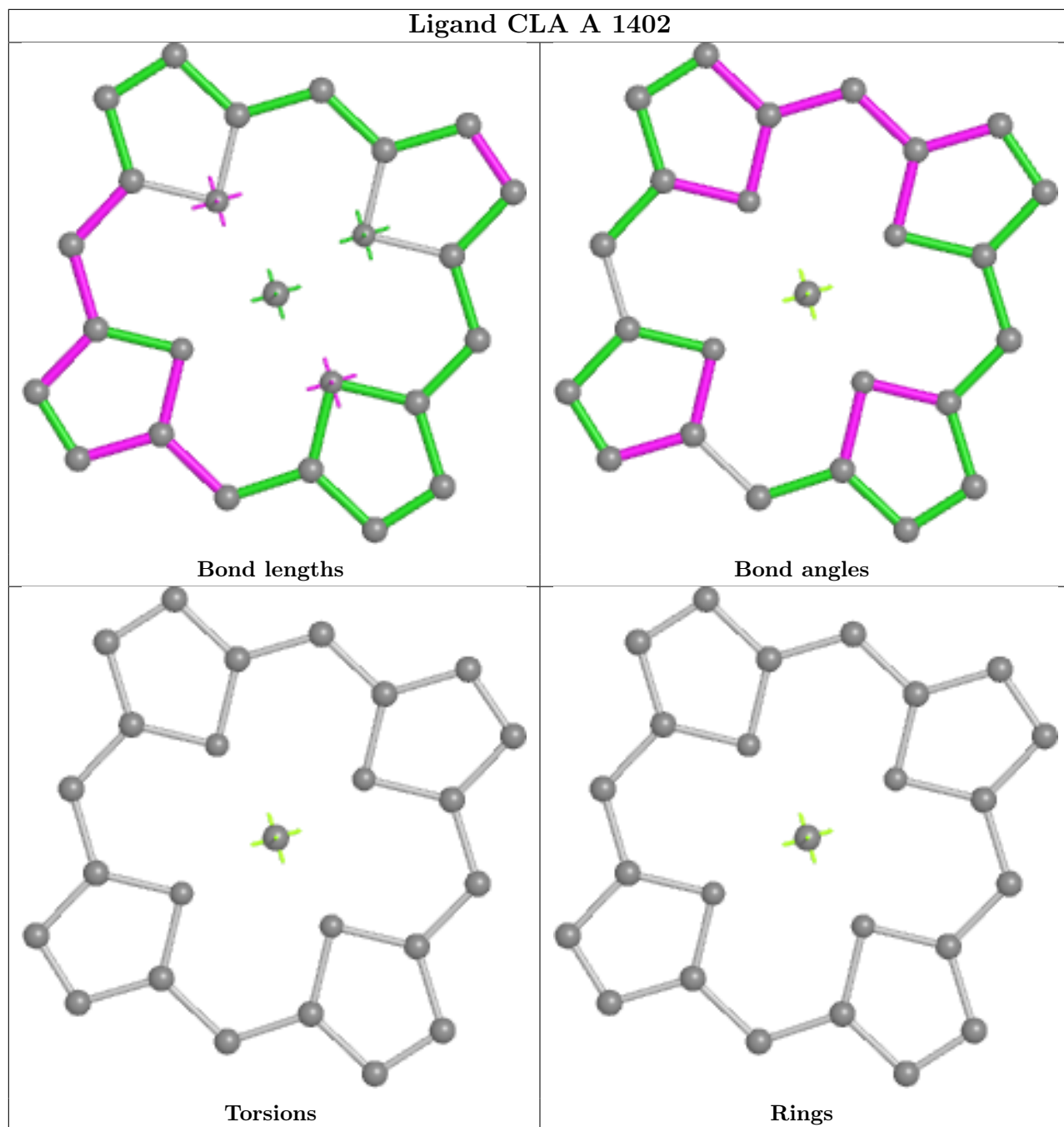


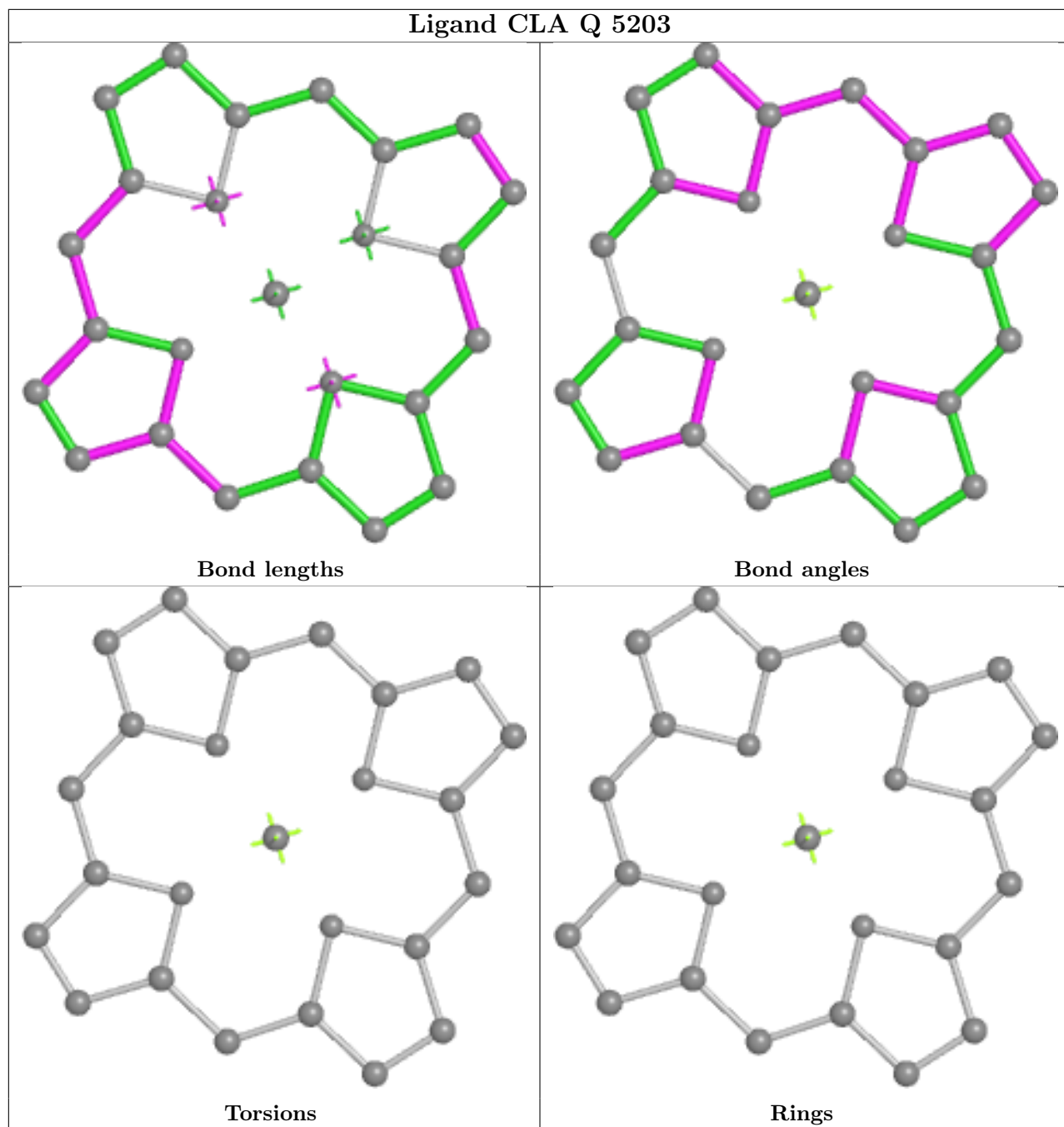


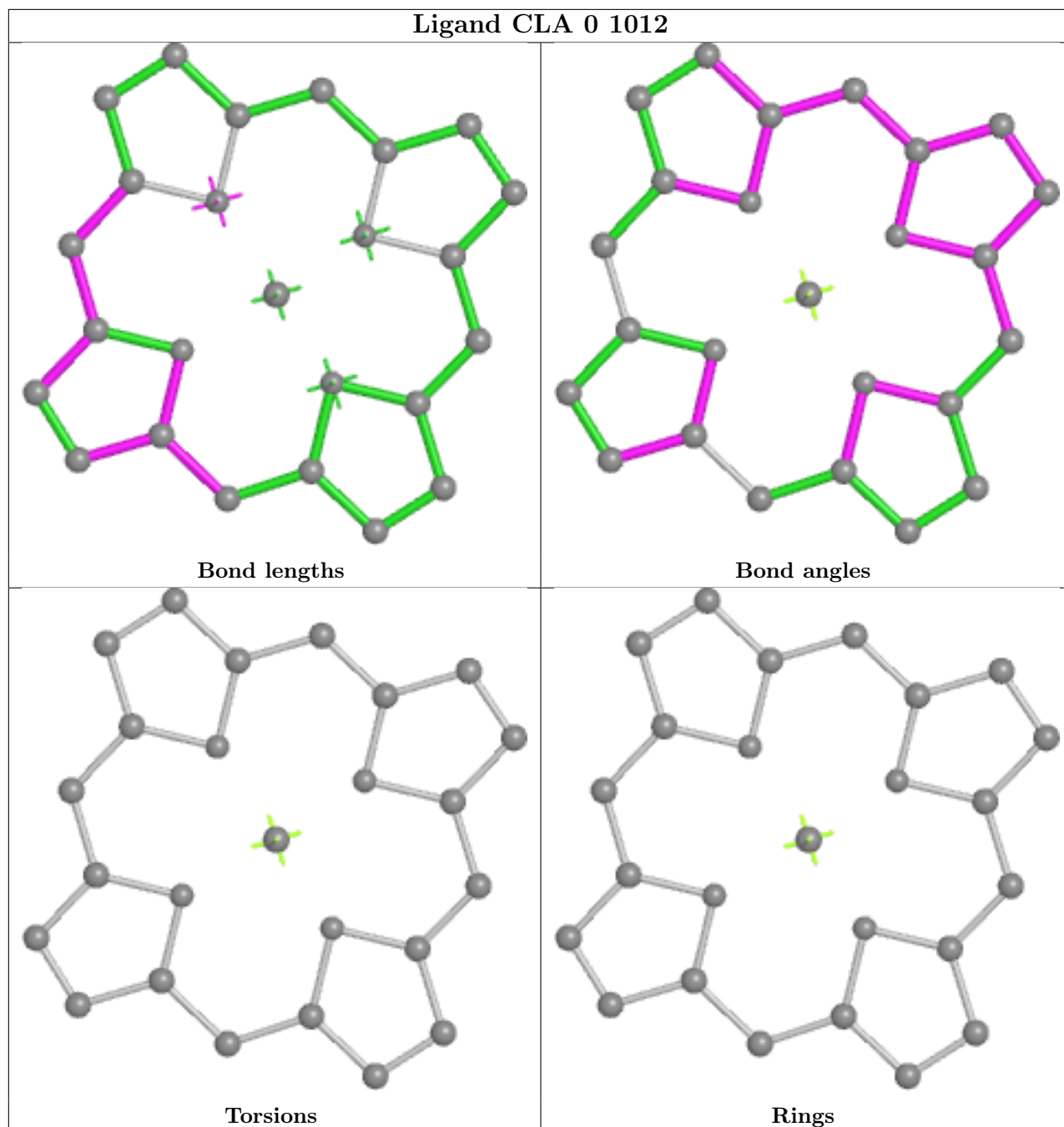


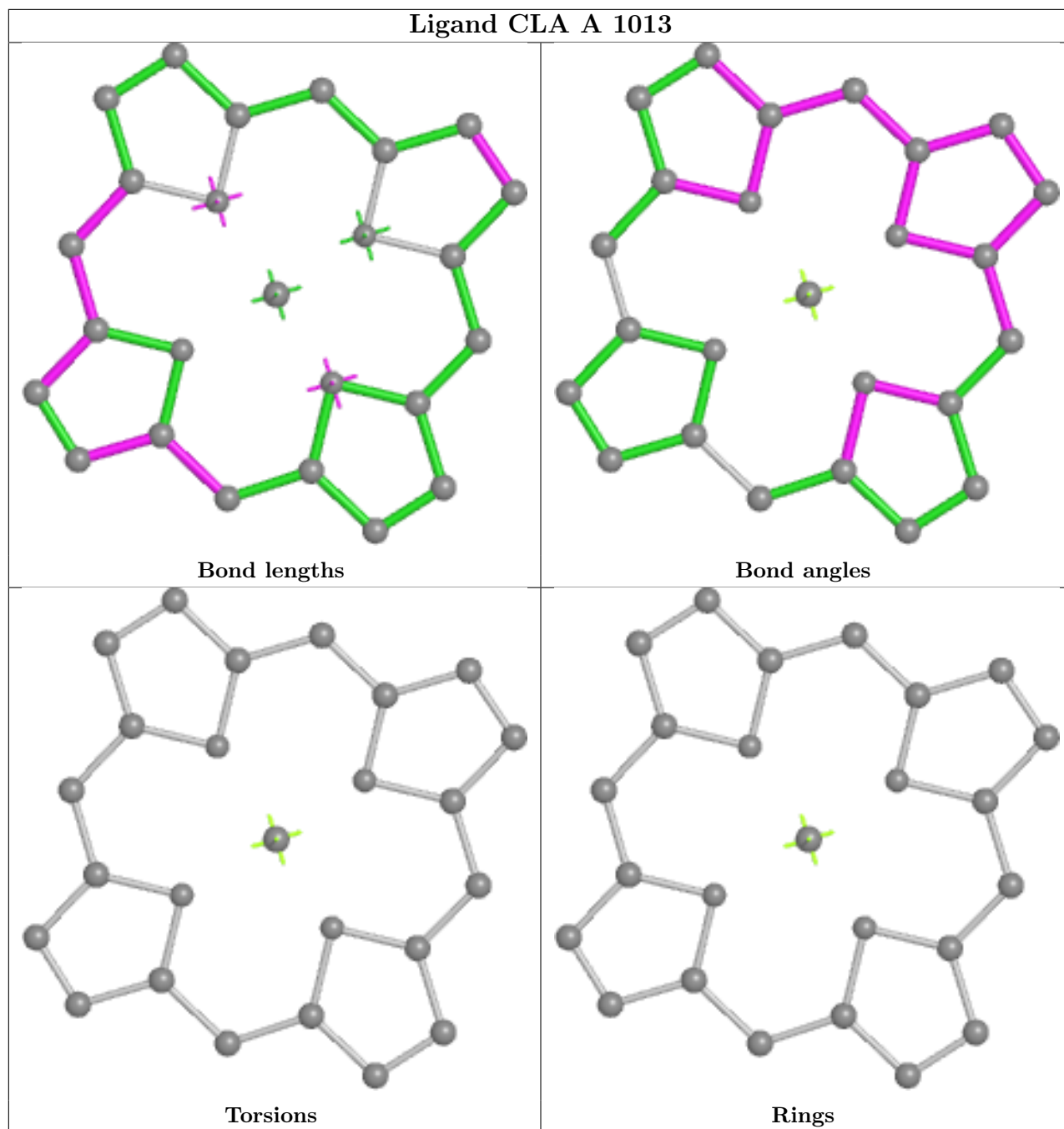


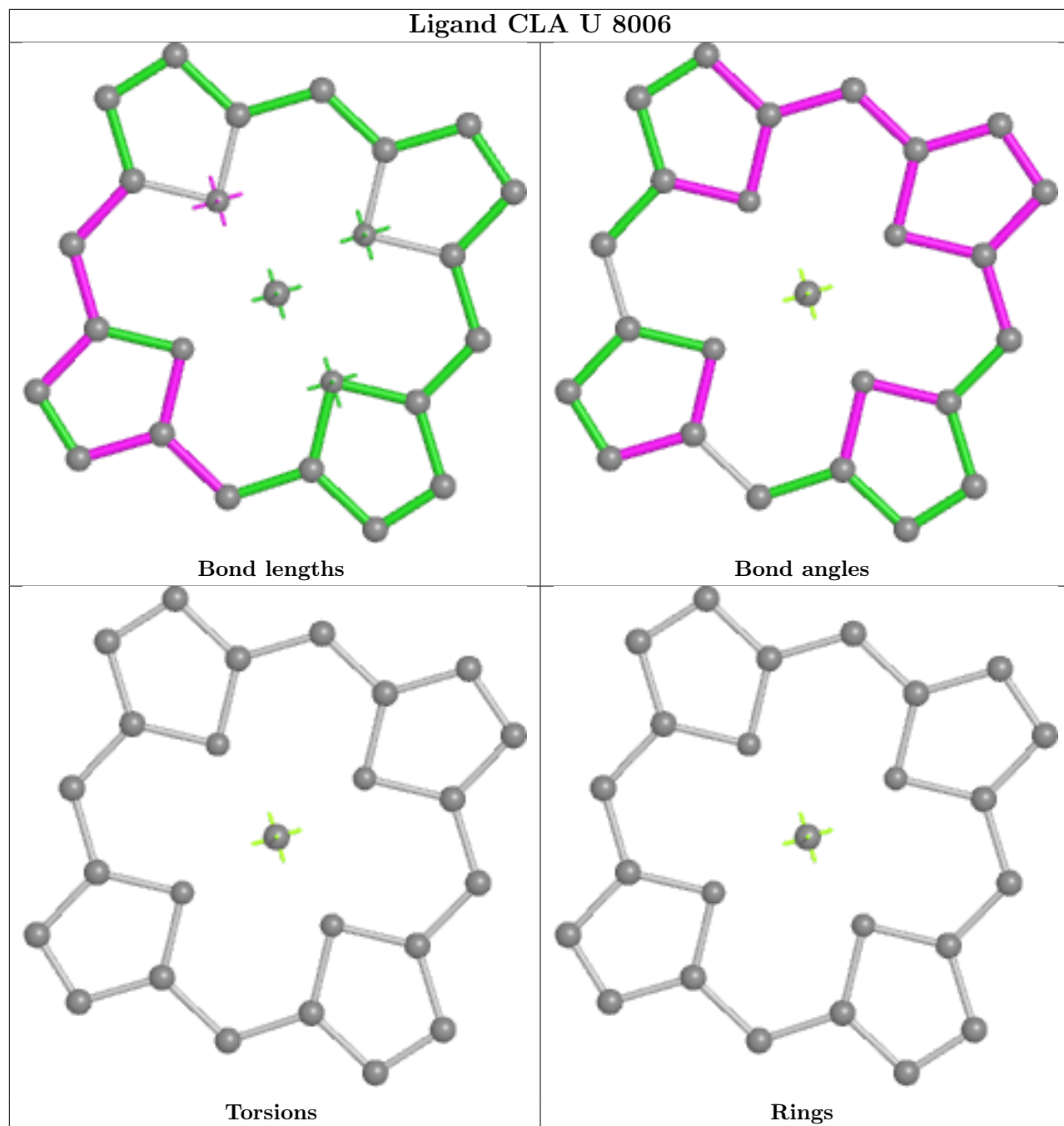


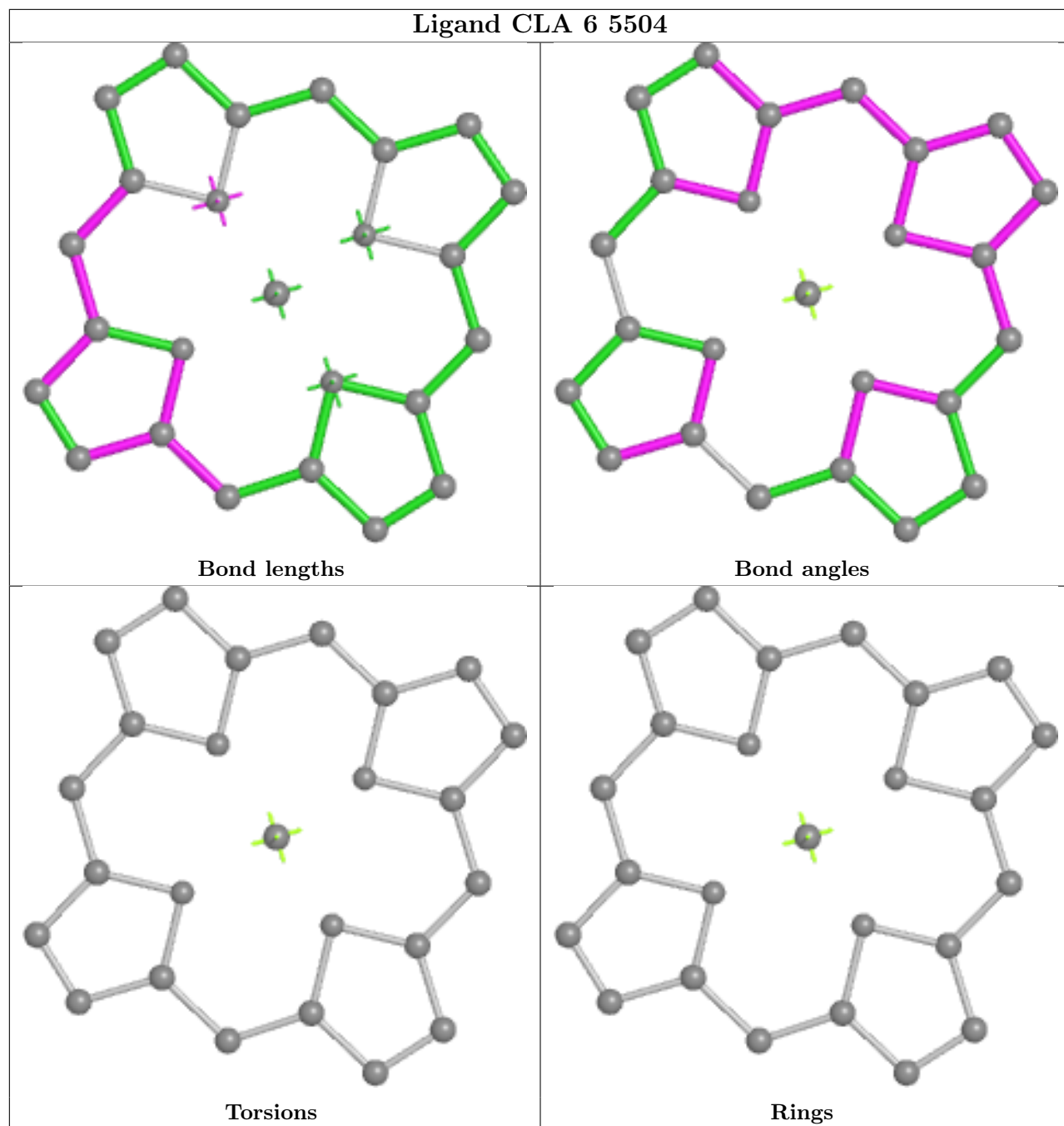


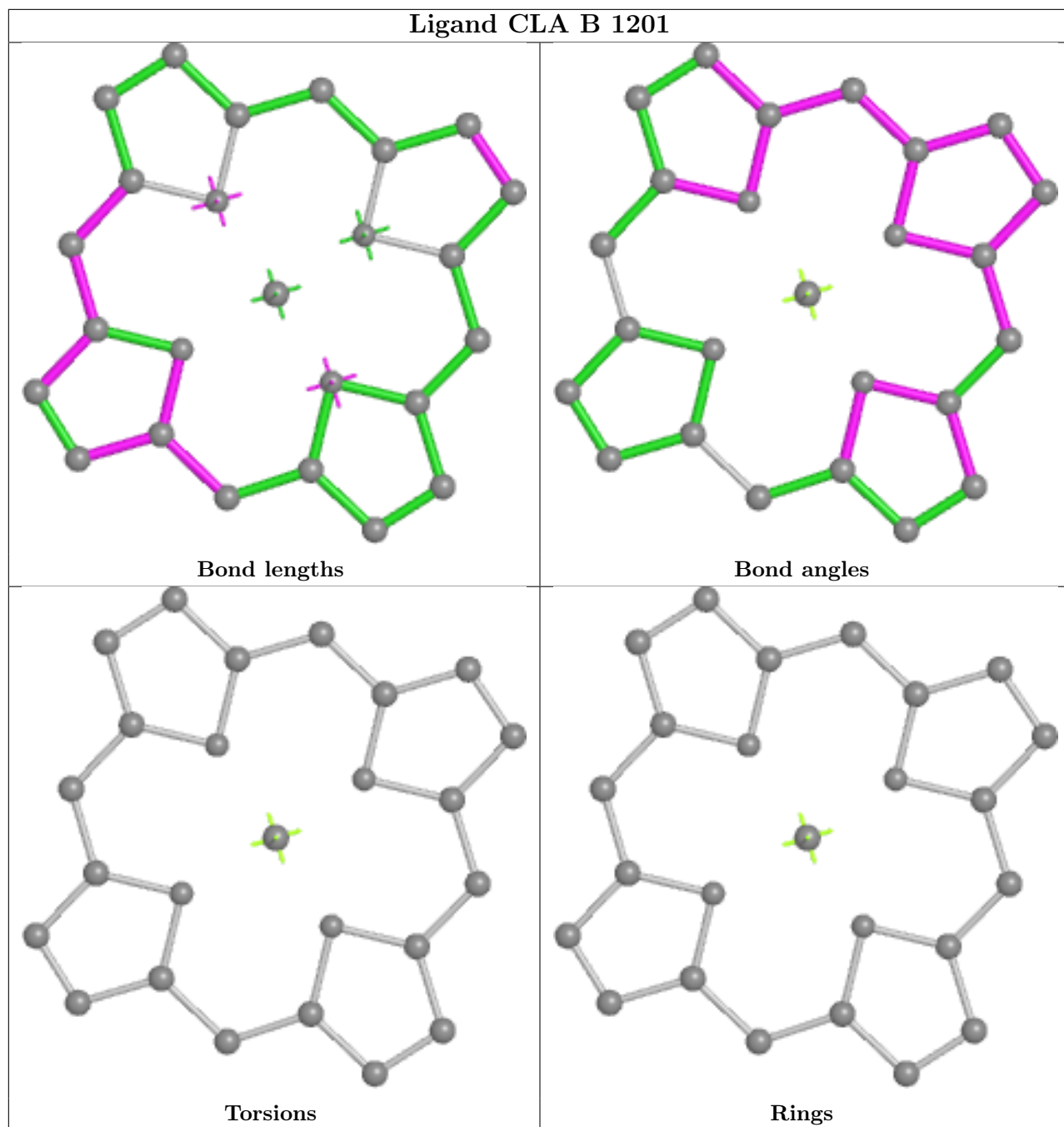


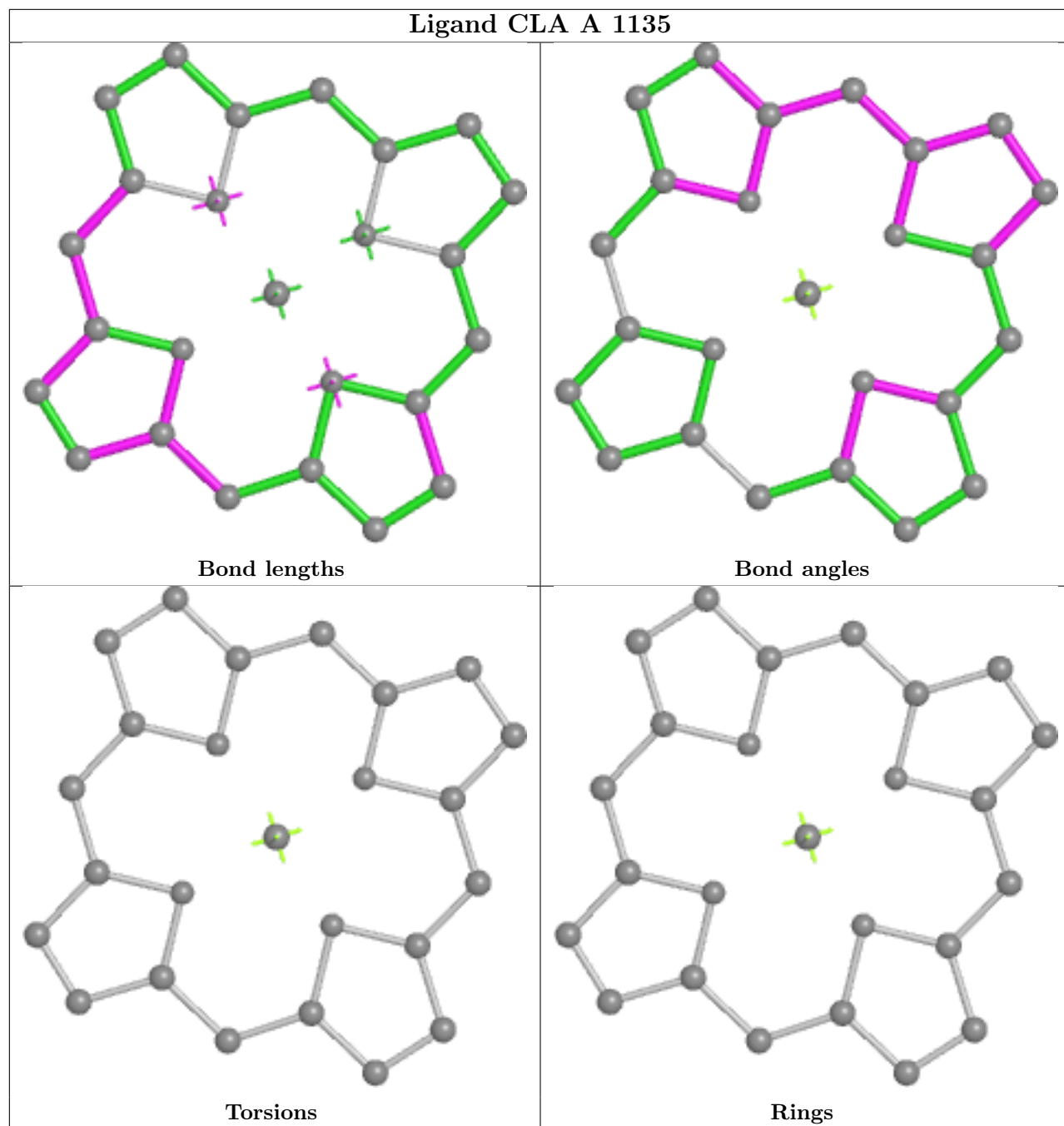


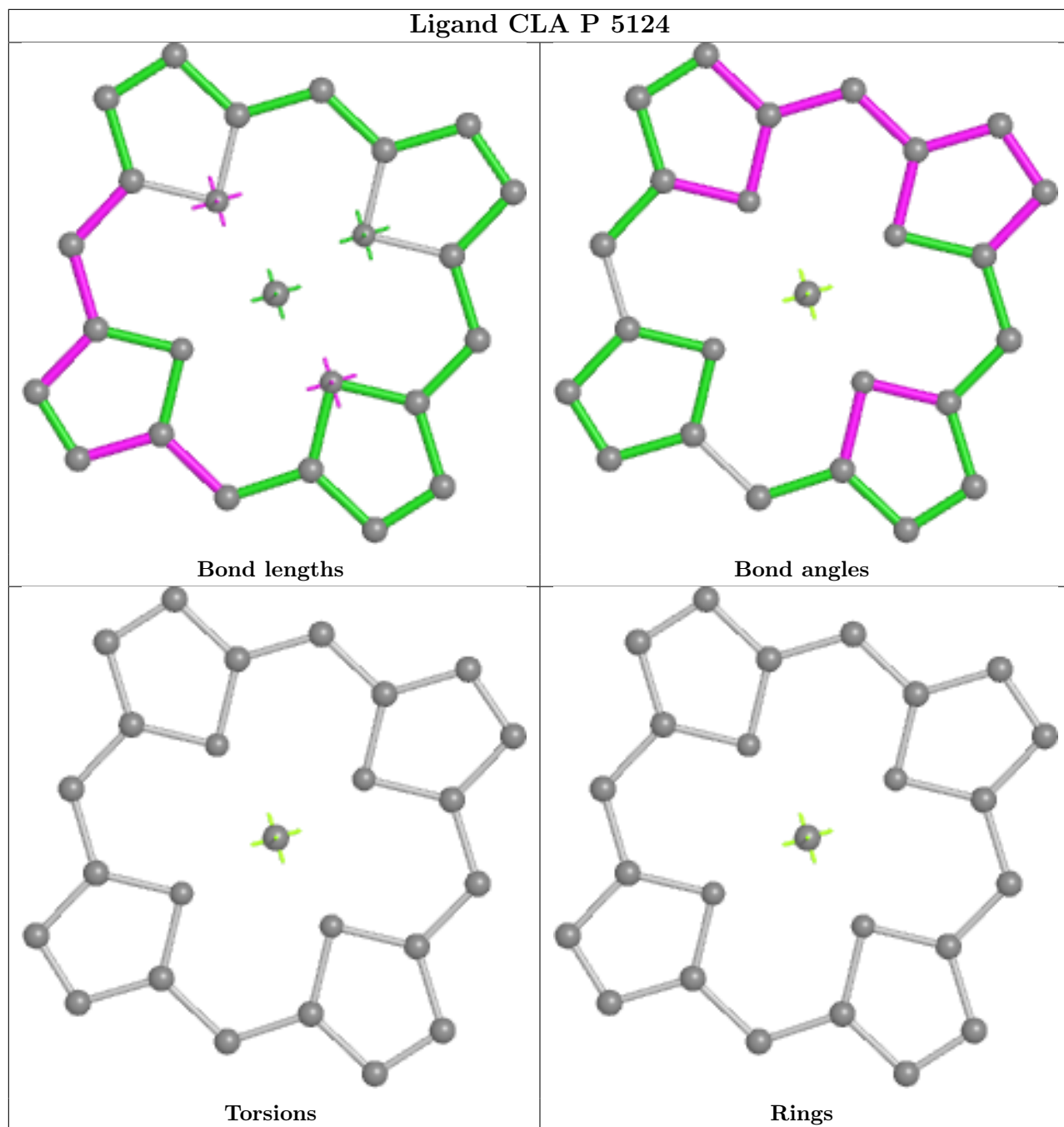


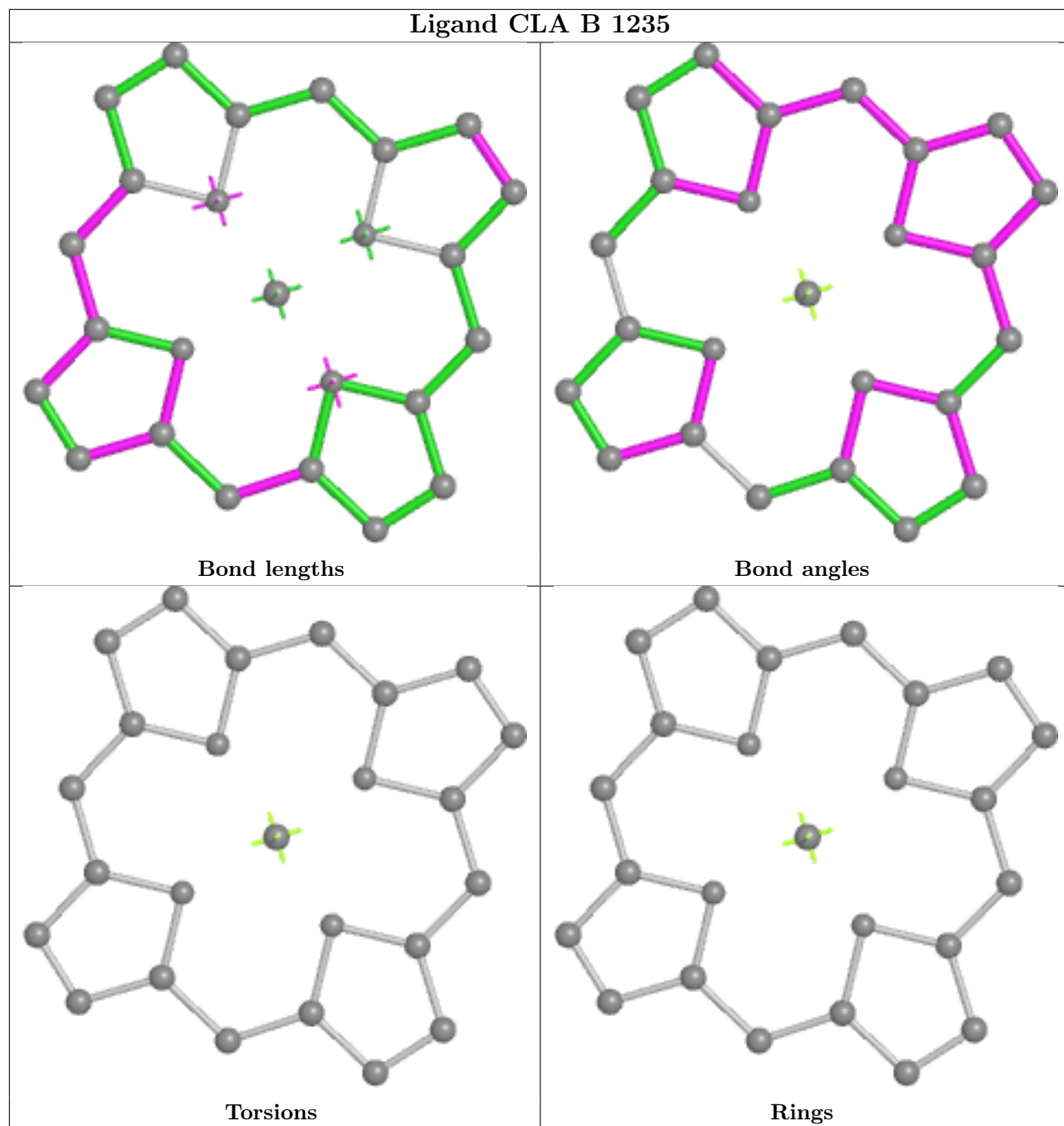


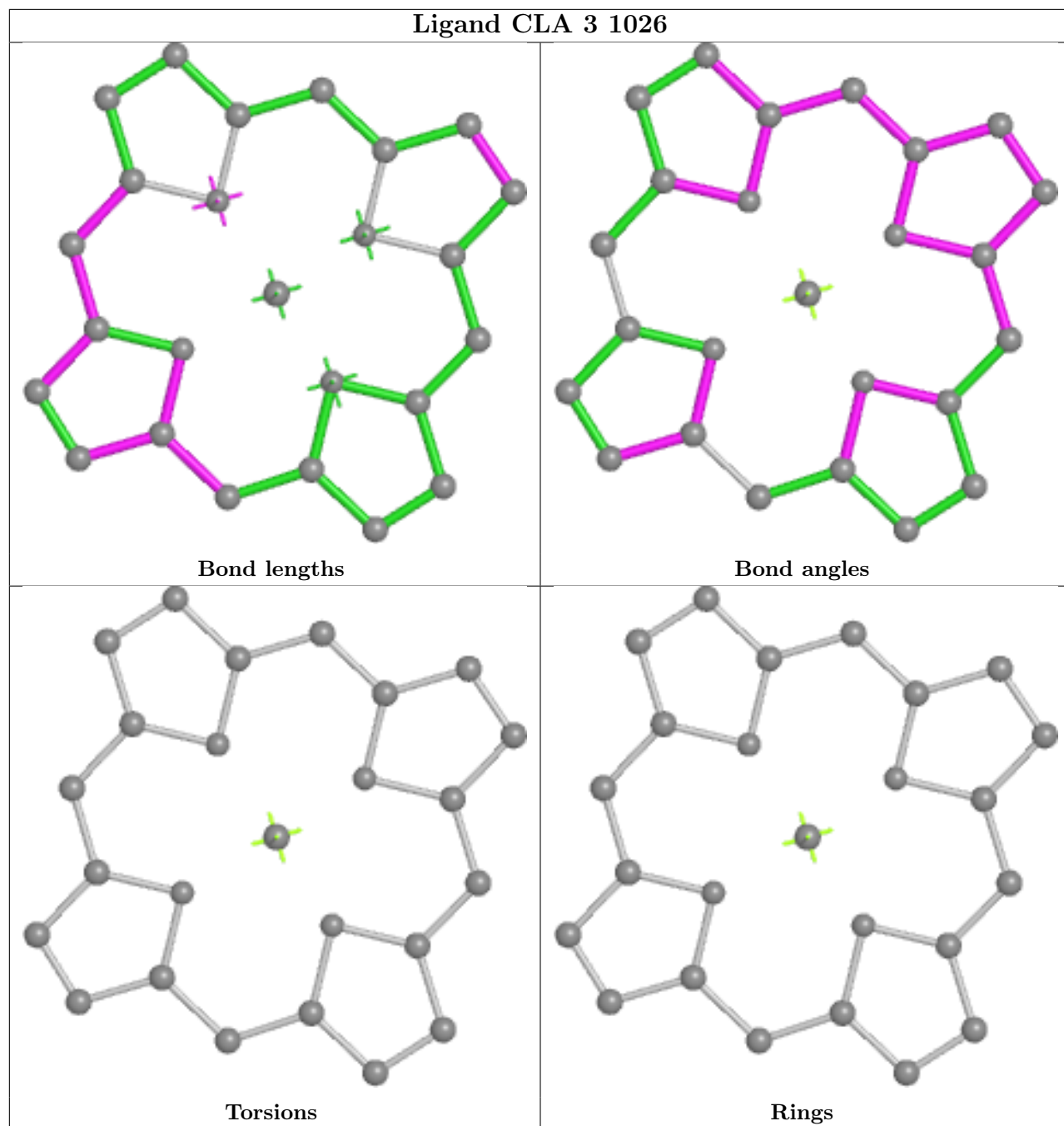


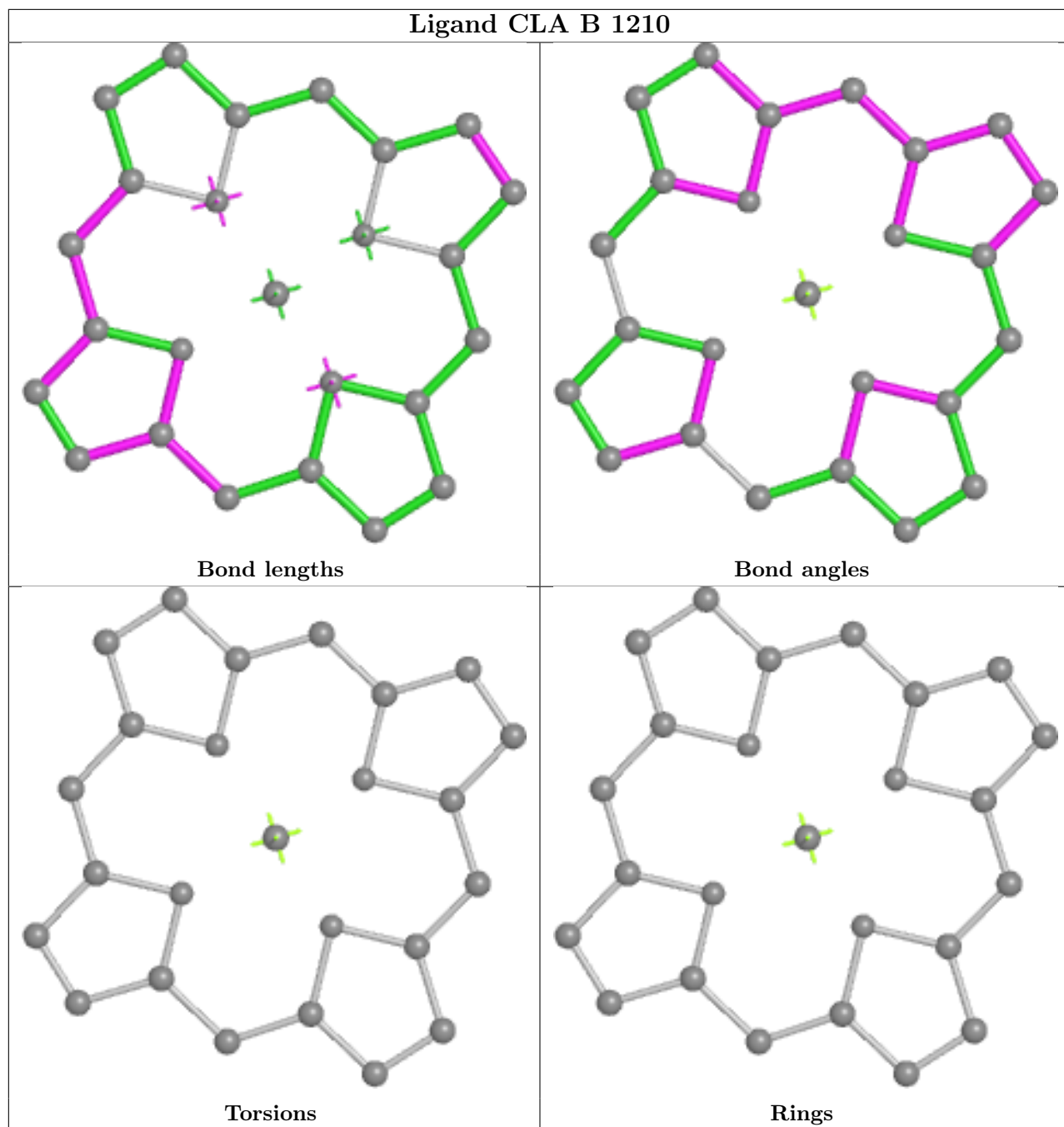


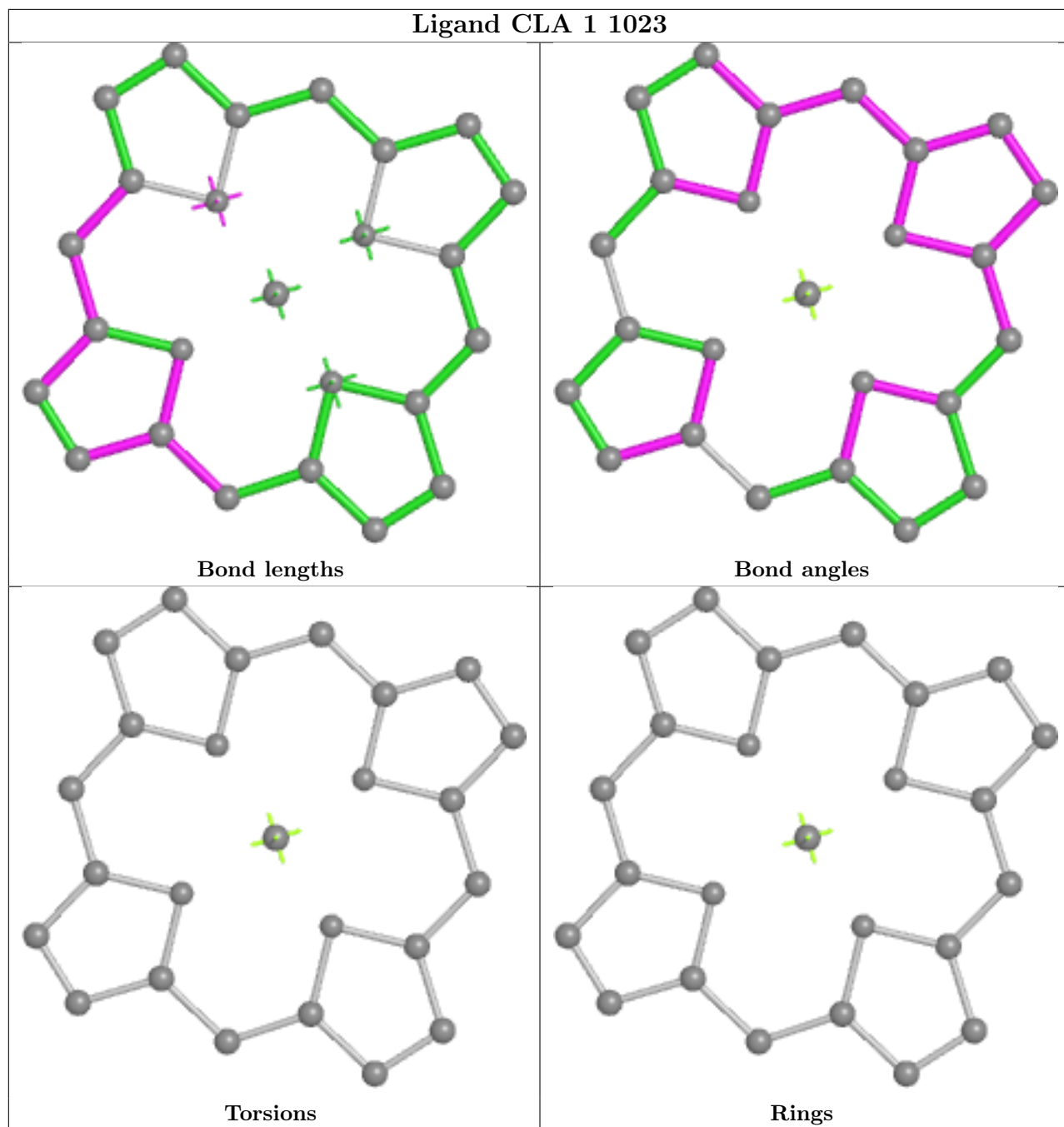


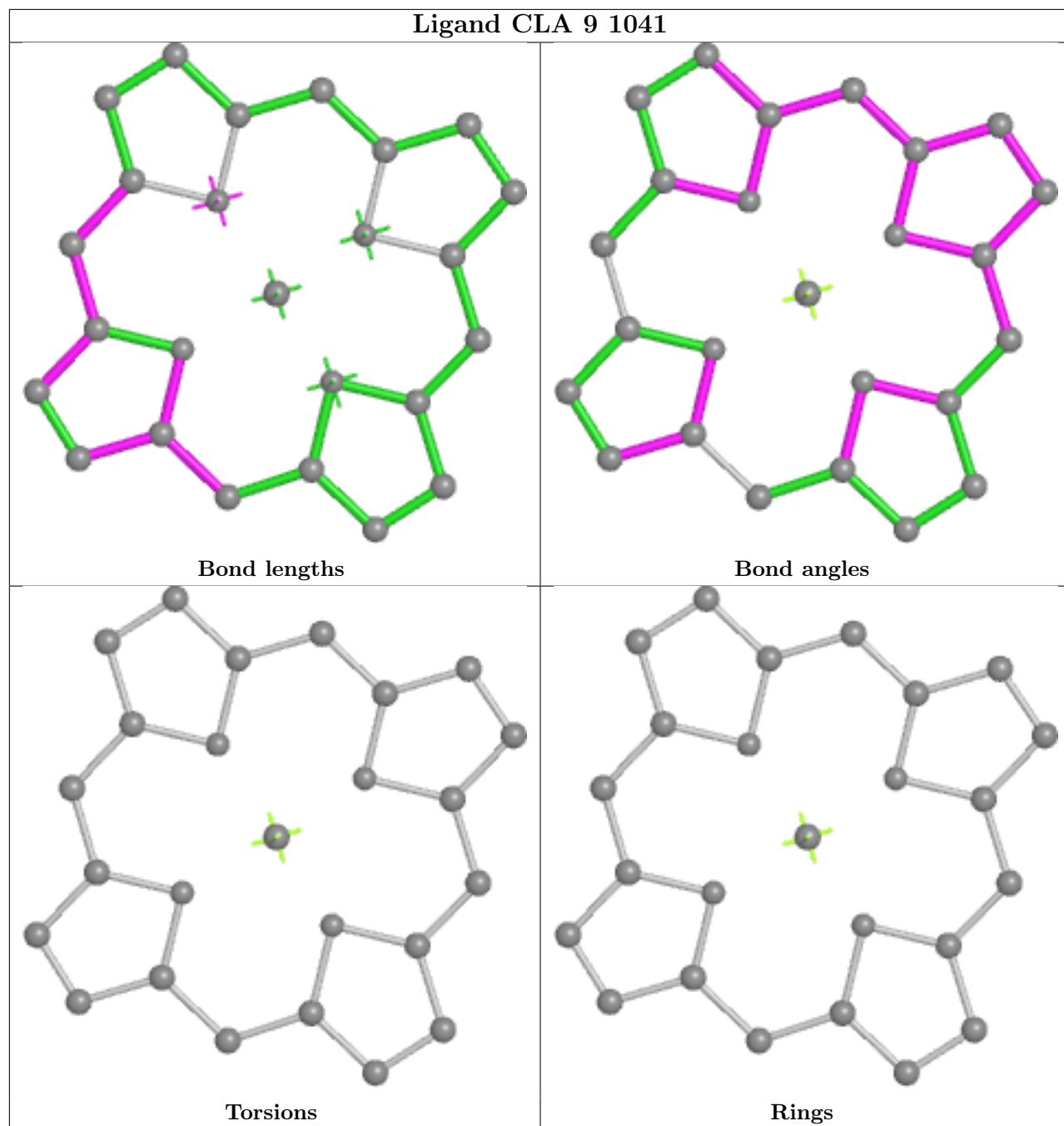


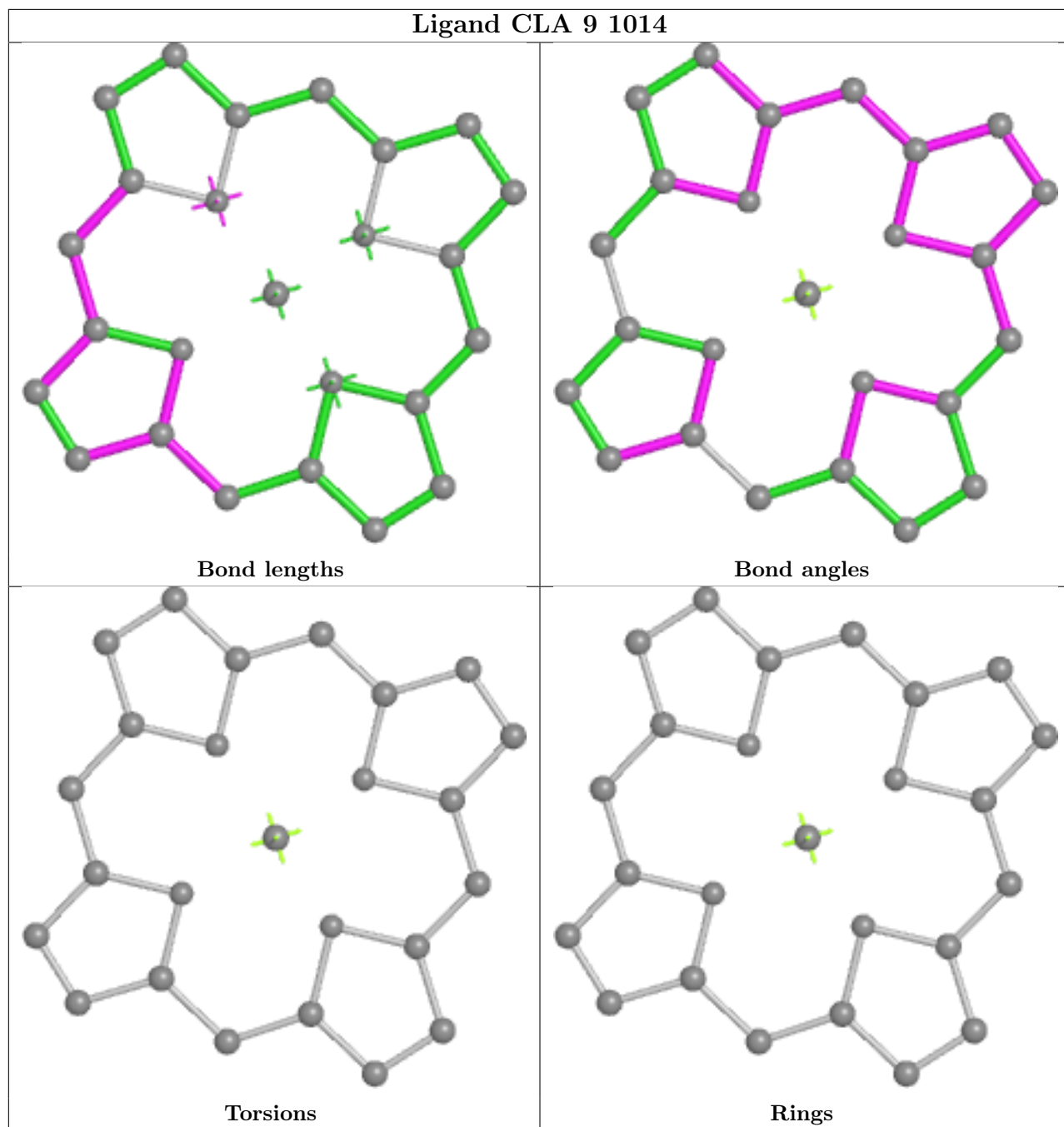


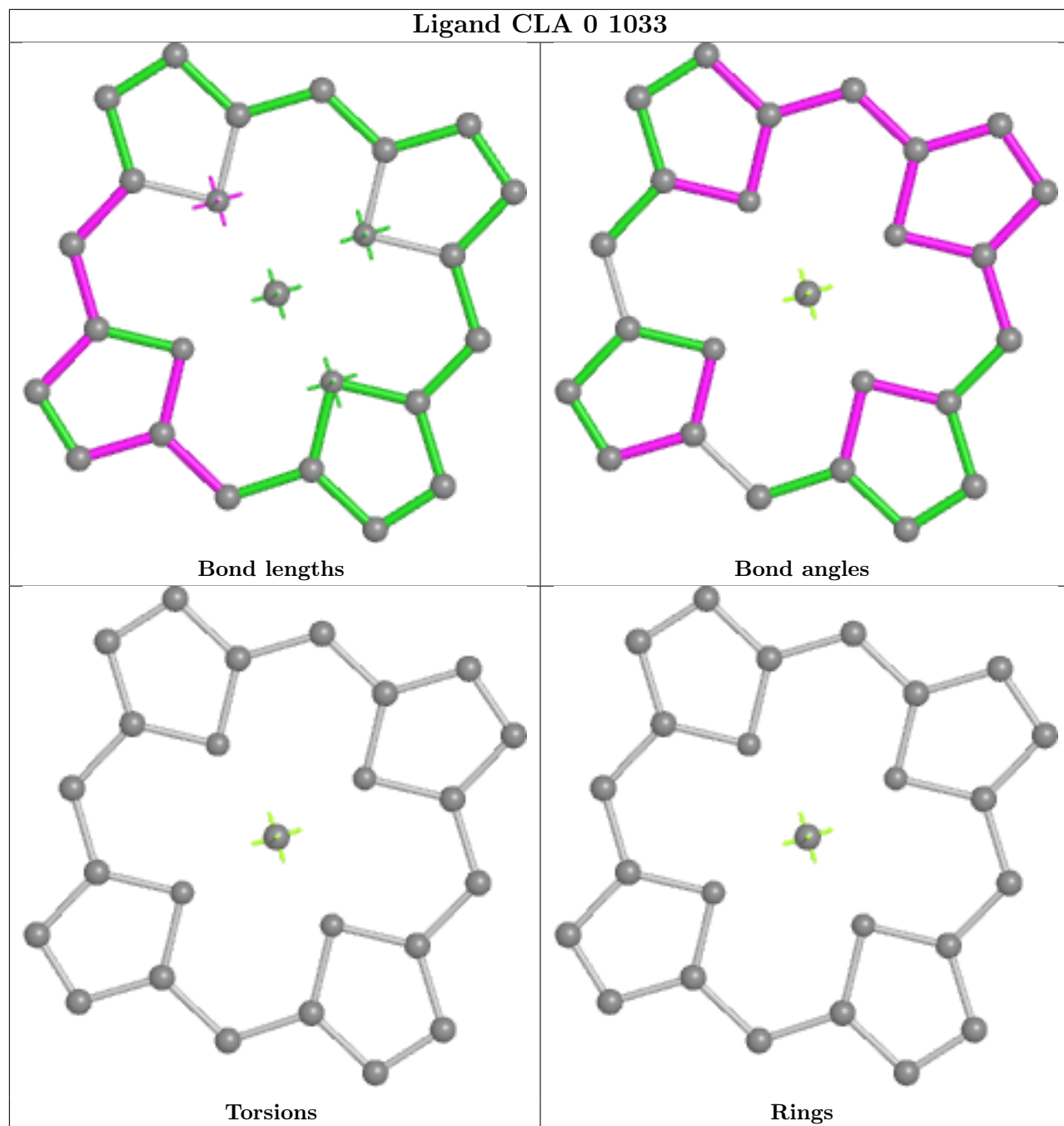


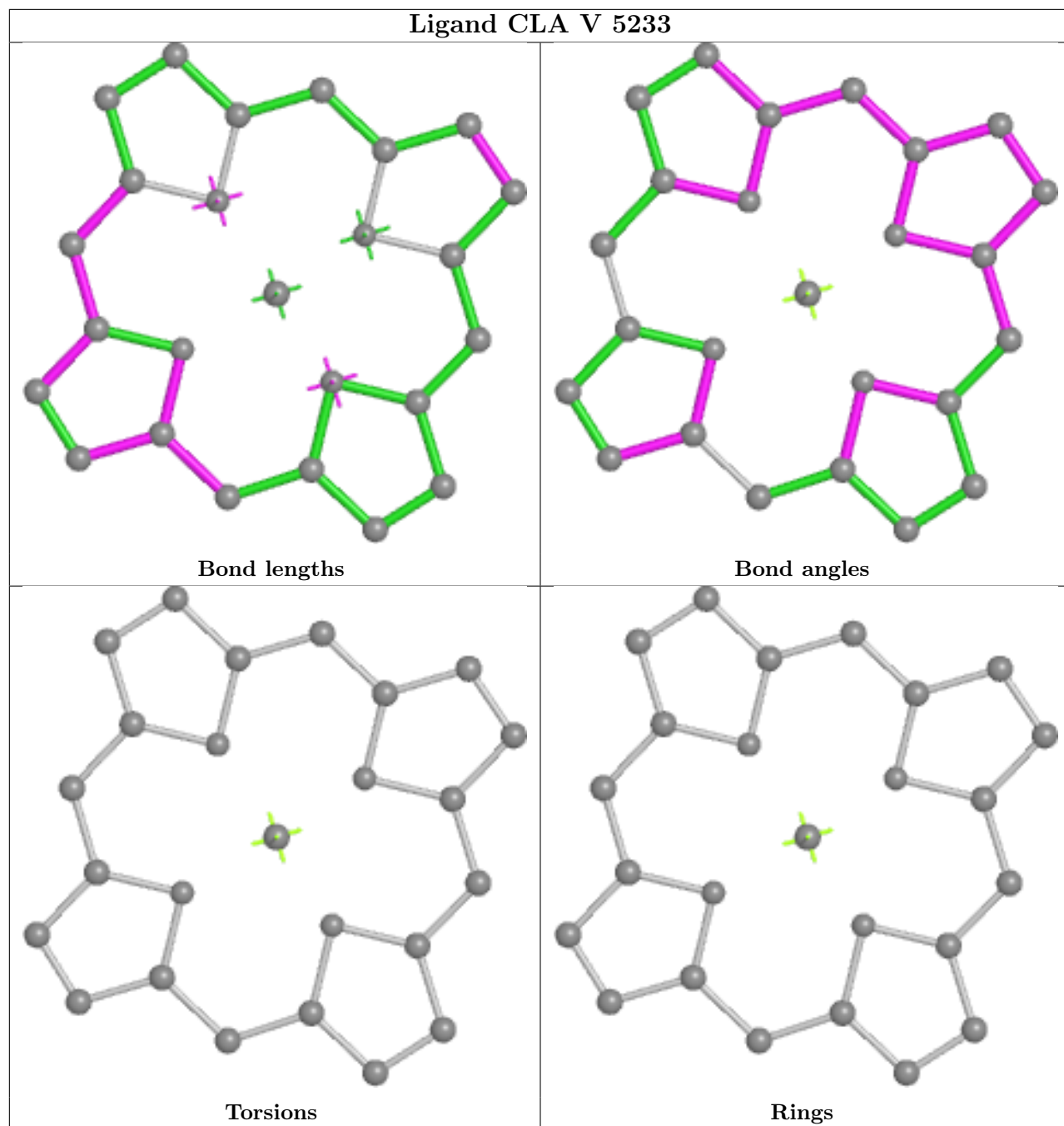


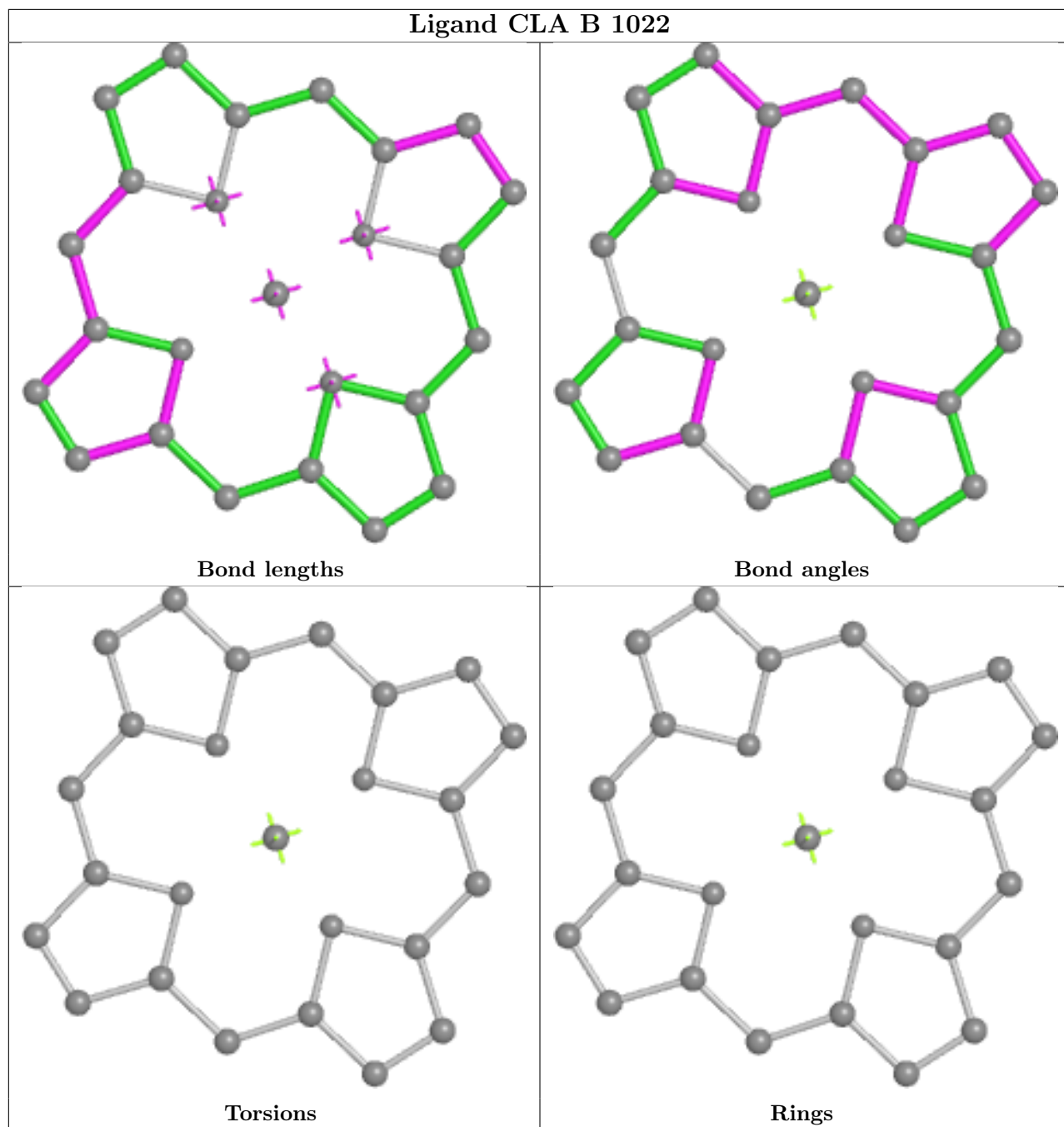


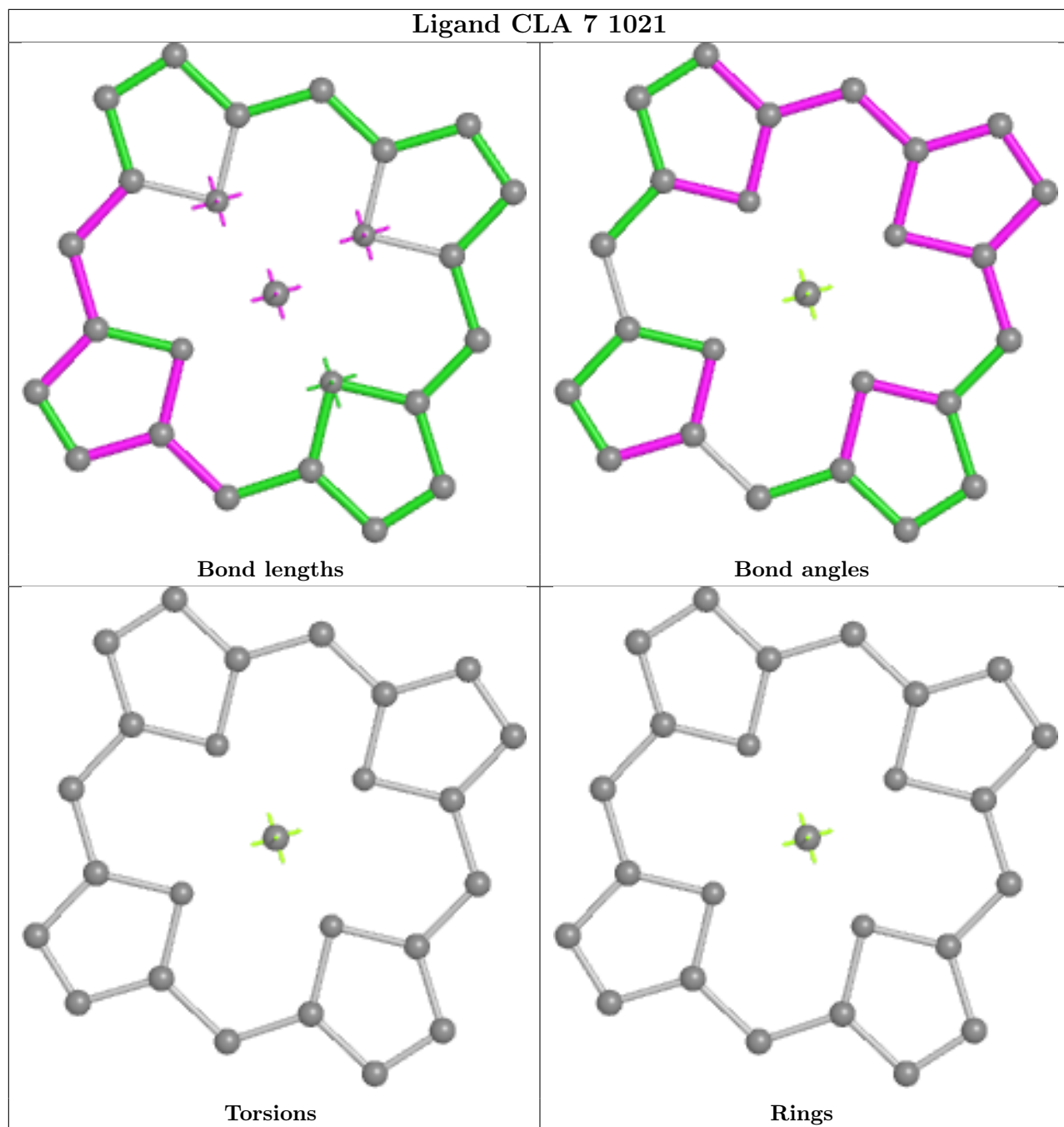


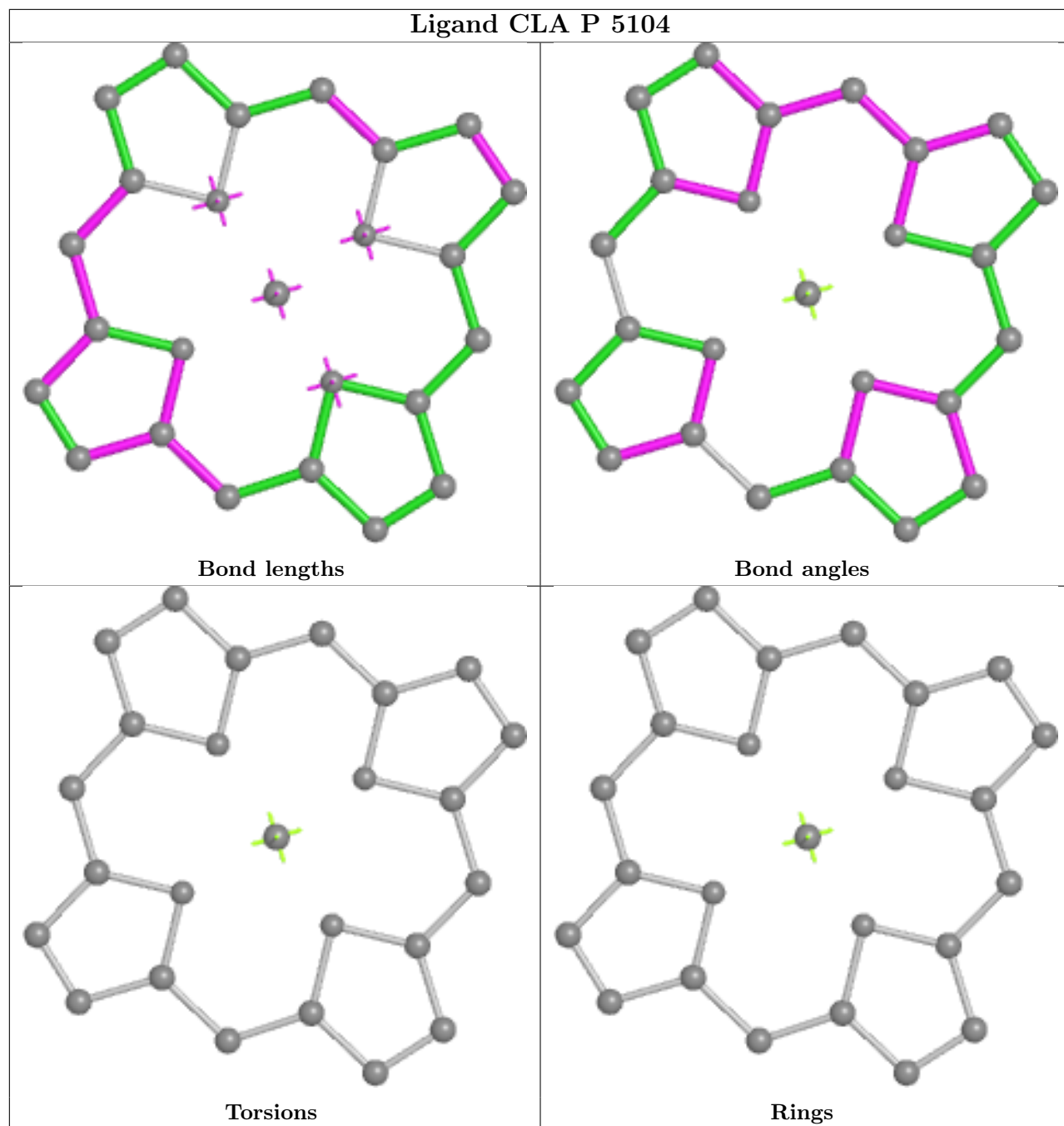


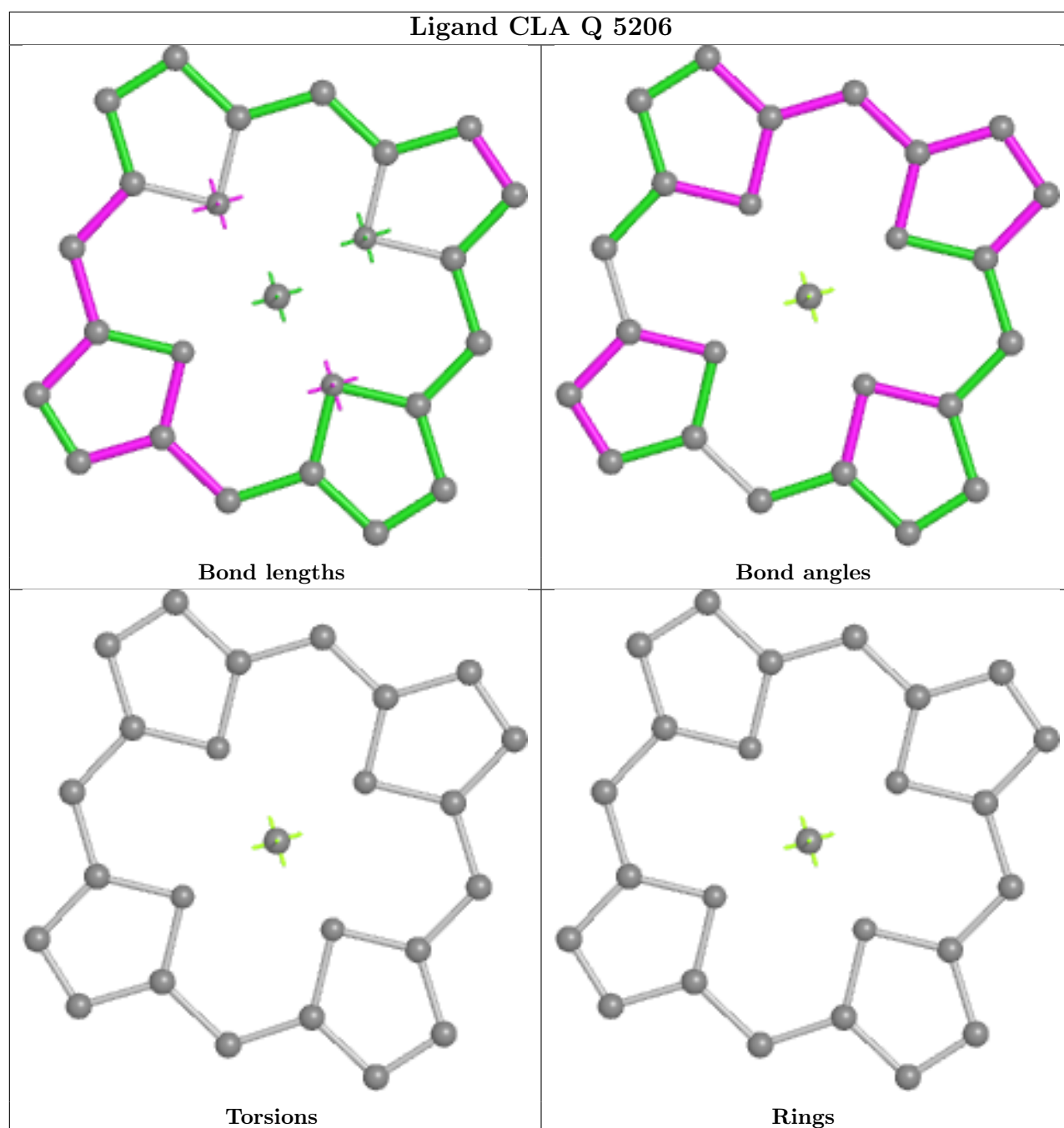












5.7 Other polymers [\(i\)](#)

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.