Supplementary Information

Theoretical Study of the Interaction of 1,2-Dithiolene Ligands with the Mg^{2+} and Ca^{2+} Aquacations: Electronic, Geometric and Energetic Analysis

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Table S1. Base set superposition error (BSSE) correction to the enthalpy and Gibbs free energy values. Calculated through the counterpoise correction

Ligand	Mg^{2+}	Ca^{2+}
Monosubstituted complexes / (kcal mol^{-1})		
tdt	8.08	2.54
bdt	7.11	2.71
Cl_2-bdt	9.51	2.80
edt	5.81	2.54
mdt	6.27	2.64
tfd	6.13	2.83
mnt	3.03	2.40
Disubstituted complexes / (kcal mol^{-1})		
$(tdt)_2$	36.57	21.63
$(bdt)_2$	32.49	9.32
$(Cl_2\text{-}bdt)_2$	30.13	15.64
$(edt)_2$	31.00	28.26
$(mdt)_2$	28.63	25.96
$(tfd)_2$	25.44	16.45
$(mnt)_2$	22.7	13.31

Tdt: toluene-3,4-dithiolate; bdt: benzene-1,2-dithiolate; Cl_2-bdt: 3,6-dichlorobenzene-1,2-dithiolate; edt: ethylene-1,2-dithiolate; mdt: 1,2-dimethyl-1,2-ethylenedithiolate; tfd: bis(trifluoromethyl) ethylenedithiolate; mnt: maleonitrile-2,3-dithiolate.

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Table S2. Natural resonance theory (NRT) analysis of the percentage of the ligand resonance structures that contribute to the final hybridization and NBO delocalization

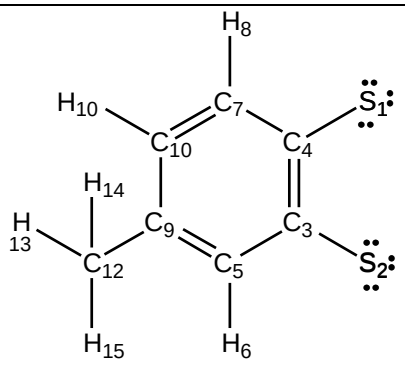
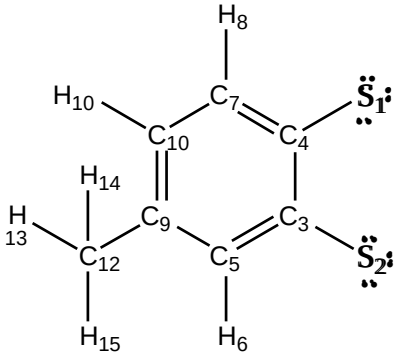
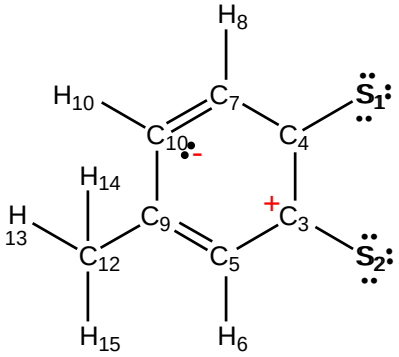
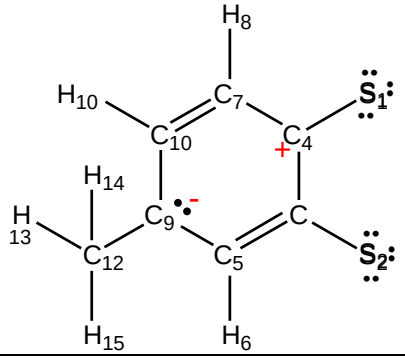
Reference structure	NRT weight / %	Resonance	NBO delocalization
		TDT	
1	18.18		reference
2	11.40		$\pi_{CC} \rightarrow \pi^*_{CC}$
3	8.62		$\pi_{CC} \rightarrow \pi^*_{CC}$
4	7.81		$\pi_{CC} \rightarrow \pi^*_{CC}$

Table S2. Natural resonance theory (NRT) analysis of the percentage of the ligand resonance structures that contribute to the final hybridization and NBO delocalization (cont.)

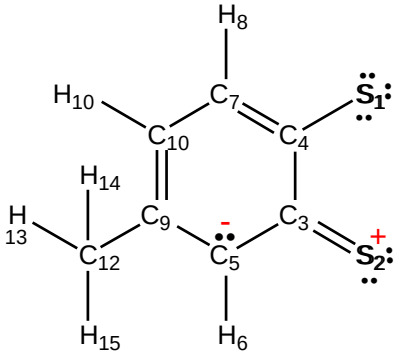
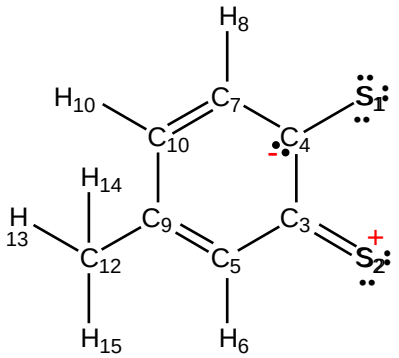
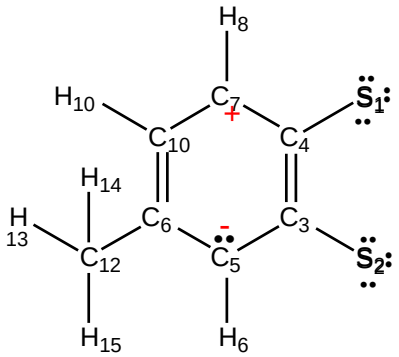
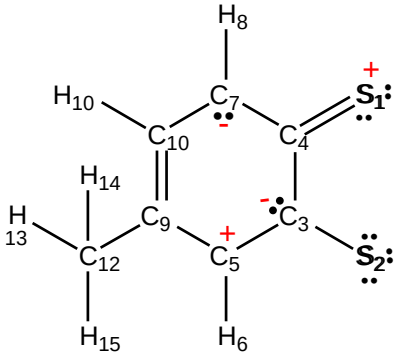
Reference structure	NRT weight / %	Resonance	NBO delocalization
5-6	12.01		$\sigma_S \rightarrow \pi^*_{CC}$
7-8	9.21		$\sigma_S \rightarrow \pi^*_{CC}$
9-10	7.19		$\pi_{CC} \rightarrow \pi^*_{CC}$
11	2.40		$\sigma_S \rightarrow \pi^*_{CC}$ $\pi_{CC} \rightarrow \pi^*_{CC}$

Table S2. Natural resonance theory (NRT) analysis of the percentage of the ligand resonance structures that contribute to the final hybridization and NBO delocalization (cont.)

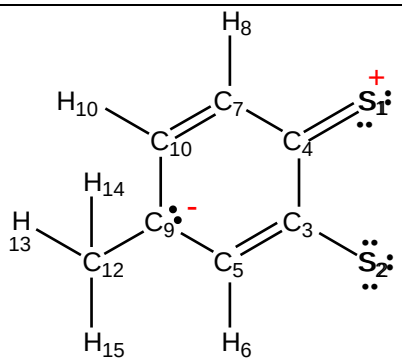
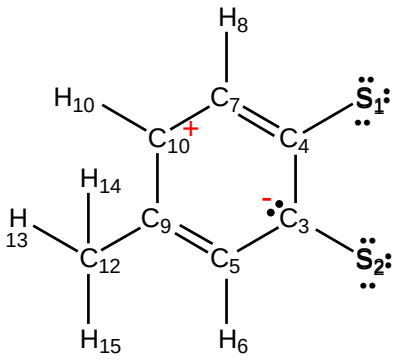
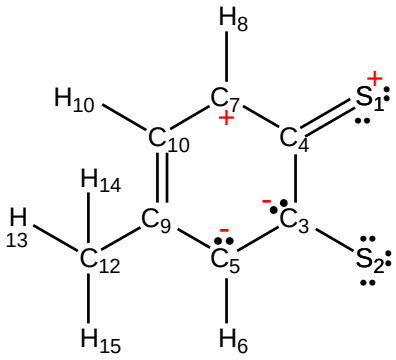
Reference structure	NRT weight / %	Resonance	NBO delocalization
12	1.95		$\sigma_S \rightarrow \pi^*_{CC}$
13	1.44		$\pi_{CC} \rightarrow \pi^*_{CC}$
14	1.31		$\sigma_S \rightarrow \pi^*_{CC}$ $\pi_{CC} \rightarrow \pi^*_{CC}$

Table S2. Natural resonance theory (NRT) analysis of the percentage of the ligand resonance structures that contribute to the final hybridization and NBO delocalization (cont.)

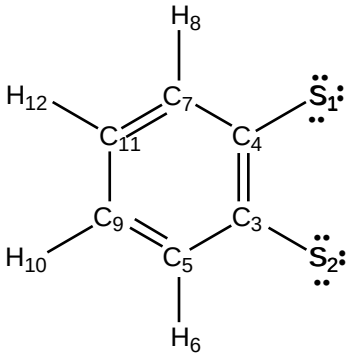
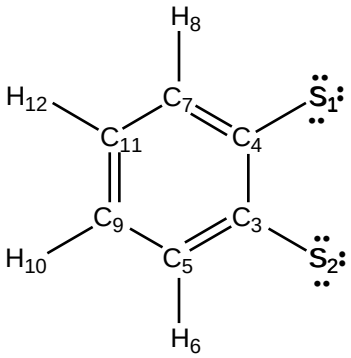
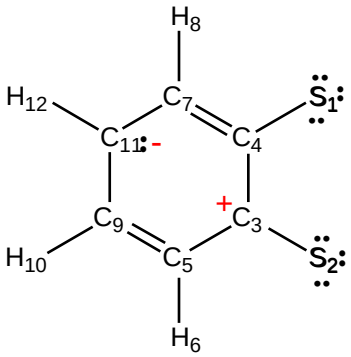
Reference structure	NRT weight / %	Resonance	NBO deloc.
		BDT	
1	23.45		reference
2	12.03		$\pi_{CC} \rightarrow \pi^*_{CC}$
3-4	14.18		$\pi_{CC} \rightarrow \pi^*_{CC}$

Table S2. Natural resonance theory (NRT) analysis of the percentage of the ligand resonance structures that contribute to the final hybridization and NBO delocalization (cont.)

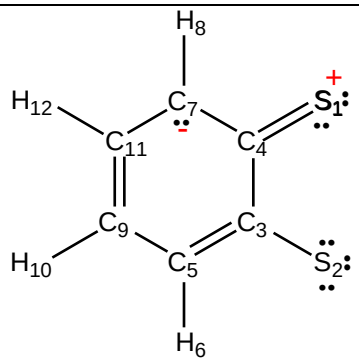
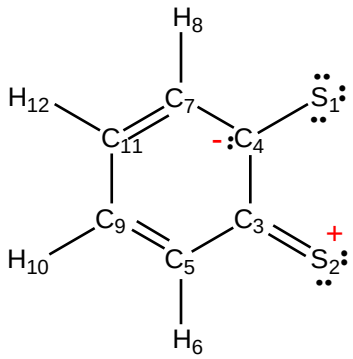
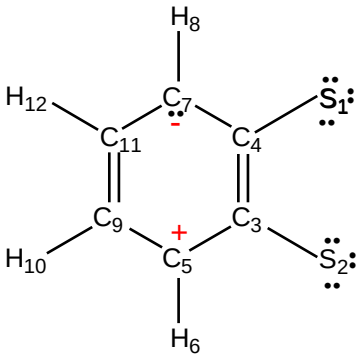
Reference structure	NRT weight / %	Resonance	NBO deloc.
5-6	11.12		$\sigma_S \rightarrow \pi^*_{CC}$
7-8	8.28		$\sigma_S \rightarrow \pi^*_{CC}$
9-10	5.48		$\pi_{CC} \rightarrow \pi^*_{CC}$

Table S2. Natural resonance theory (NRT) analysis of the percentage of the ligand resonance structures that contribute to the final hybridization and NBO delocalization (cont.)

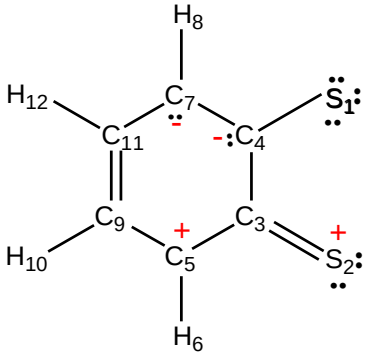
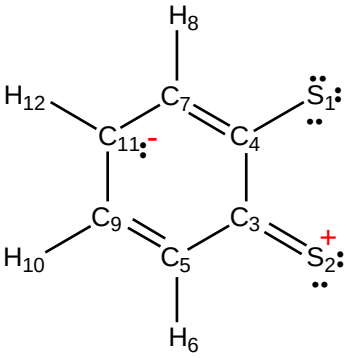
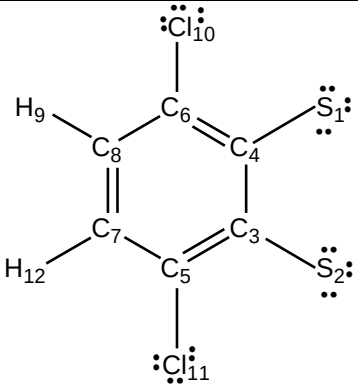
Reference structure	NRT weight / %	Resonance	NBO deloc.
11-12-13-14	7.04		$\sigma_S \rightarrow \pi^*_{CC}$
15-16	2.30		$\sigma_S \rightarrow \pi^*_{CC}$
		Cl_2-BDT	
1	14.03		reference

Table S2. Natural resonance theory (NRT) analysis of the percentage of the ligand resonance structures that contribute to the final hybridization and NBO delocalization (cont.)

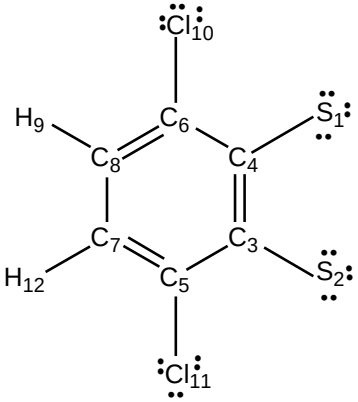
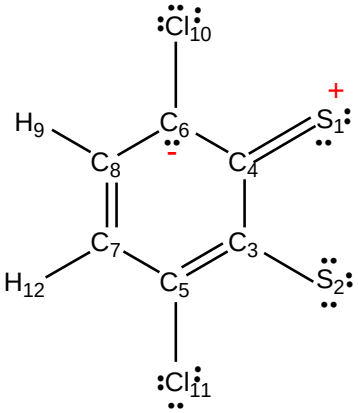
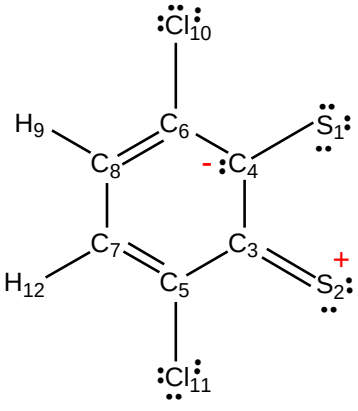
Reference structure	NRT weight / %	Resonance	NBO deloc.
2	13.02		$\pi_{CC} \rightarrow \pi^*_{CC}$
3-4	15.50		$\sigma_S \rightarrow \pi^*_{CC}$
5-6	9.92		$\sigma_S \rightarrow \pi^*_{CC}$

Table S2. Natural resonance theory (NRT) analysis of the percentage of the ligand resonance structures that contribute to the final hybridization and NBO delocalization (cont.)

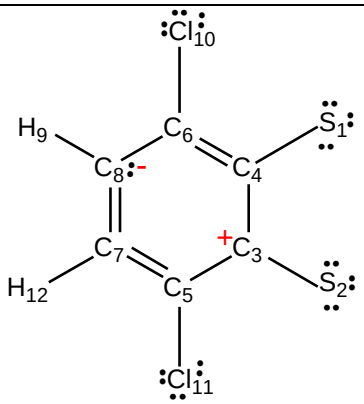
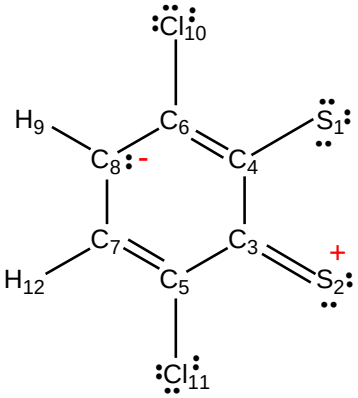
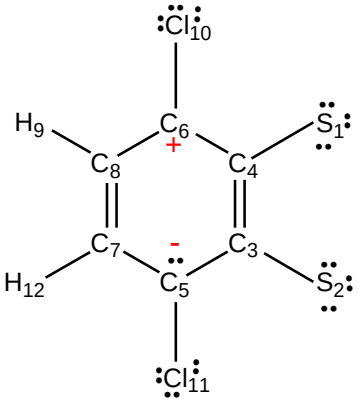
Reference structure	NRT weight / %	Resonance	NBO deloc.
7-8	9.91		$\pi_{CC} \rightarrow \pi^*_{CC}$
9	3.60		$\sigma_S \rightarrow \pi^*_{CC}$
10	3.56		$\pi_{CC} \rightarrow \pi^*_{CC}$

Table S2. Natural resonance theory (NRT) analysis of the percentage of the ligand resonance structures that contribute to the final hybridization and NBO delocalization (cont.)

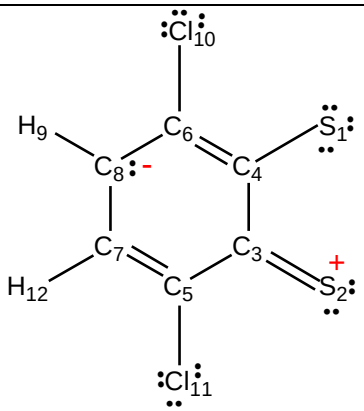
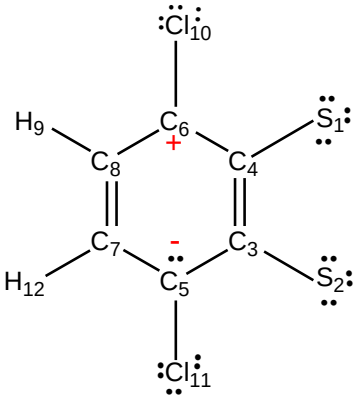
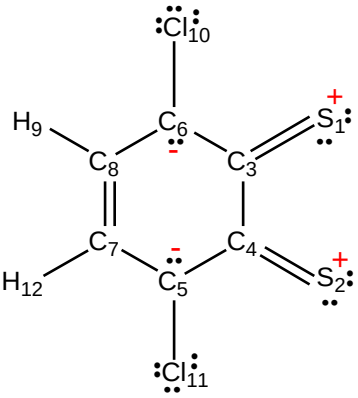
Reference structure	NRT weight / %	Resonance	NBO deloc.
11-9	7.15		$\sigma_S \rightarrow \pi^*_{CC}$
12-10	7.08		$\pi_{CC} \rightarrow \pi^*_{CC}$
13	2.94		$\sigma_S \rightarrow \pi^*_{CC}$

Table S2. Natural resonance theory (NRT) analysis of the percentage of the ligand resonance structures that contribute to the final hybridization and NBO delocalization (cont.)

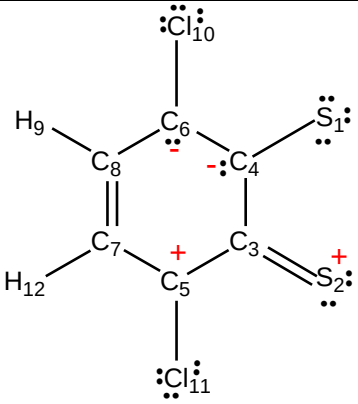
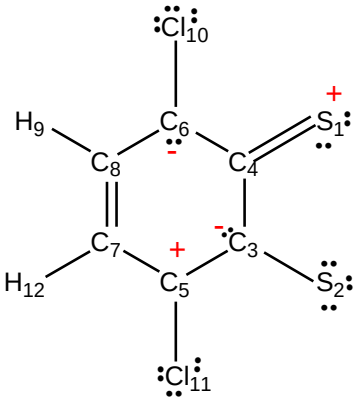
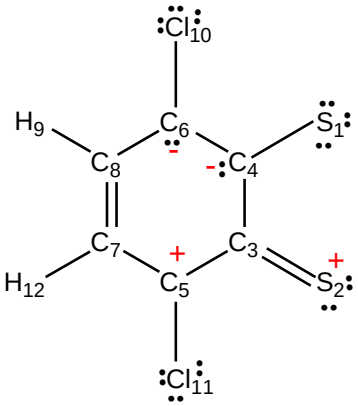
Reference structure	NRT weight / %	Resonance	NBO deloc.
14	1.38		$\sigma_S \rightarrow \pi^*_{CC}$
15-16	2.76		$\sigma_S \rightarrow \pi^*_{CC}$
17-14	2.76		$\sigma_S \rightarrow \pi^*_{CC}$

Table S2. Natural resonance theory (NRT) analysis of the percentage of the ligand resonance structures that contribute to the final hybridization and NBO delocalization (cont.)

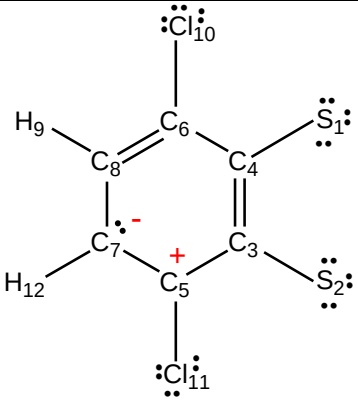
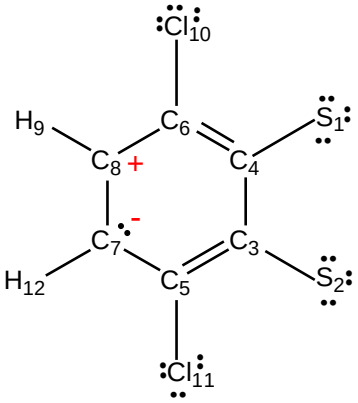
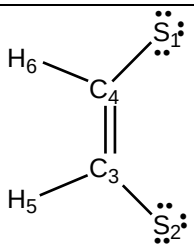
Reference structure	NRT weight / %	Resonance	NBO deloc.
18-19	2.60		$\pi_{CC} \rightarrow \pi^*_{CC}$
20	1.15		$\pi_{CC} \rightarrow \pi^*_{CC}$
		EDT	
1	75.49		reference

Table S2. Natural resonance theory (NRT) analysis of the percentage of the ligand resonance structures that contribute to the final hybridization and NBO delocalization (cont.)

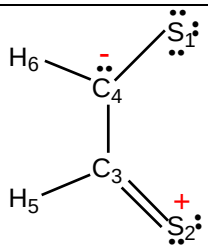
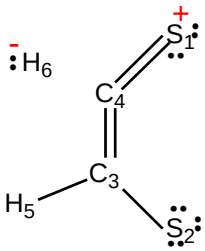
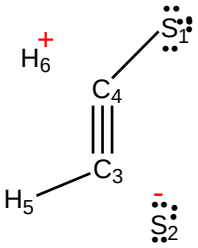
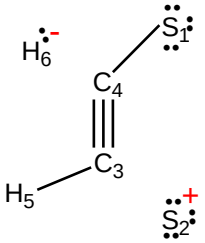
Reference structure	NRT weight / %	Resonance	NBO deloc.
2-3	17.39		$\sigma_S \rightarrow \pi^*_{C\text{-}C}$
4-5	3.58		$\sigma_S \rightarrow \sigma^*_{C\text{-}H}$
6-7	2.90		$\sigma_{C\text{-}H} \rightarrow \eta^*_S$
8-9	0.62		$\sigma_{S\text{-}C} \rightarrow \sigma^*_{C\text{-}H}$

Table S2. Natural resonance theory (NRT) analysis of the percentage of the ligand resonance structures that contribute to the final hybridization and NBO delocalization (cont.)

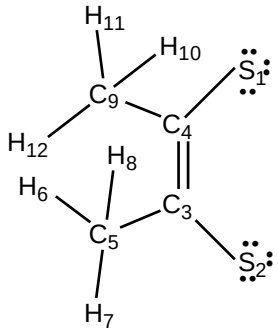
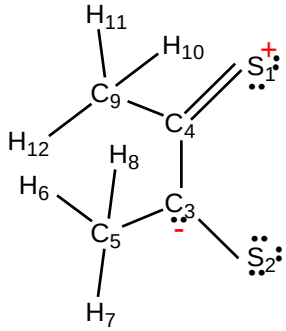
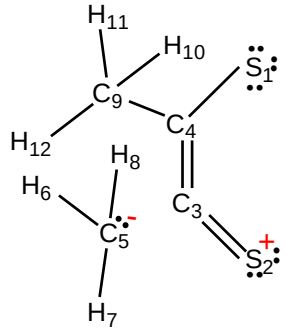
MDT			
Reference structure	NRT weight / %	Resonance	NBO deloc.
1	69.66		reference
2-3	17.84		$\sigma_S \rightarrow \pi^*_{CC}$
4-5	3.96		$\sigma_S \rightarrow \pi^*_{CC}$

Table S2. Natural resonance theory (NRT) analysis of the percentage of the ligand resonance structures that contribute to the final hybridization and NBO delocalization (cont.)

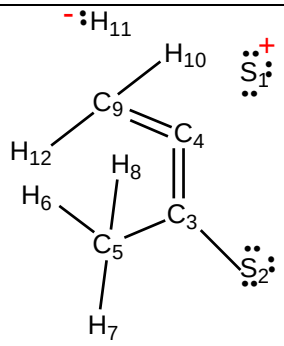
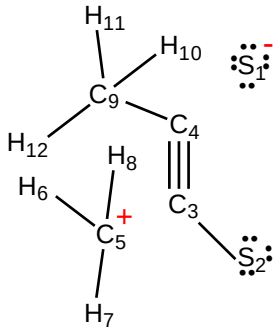
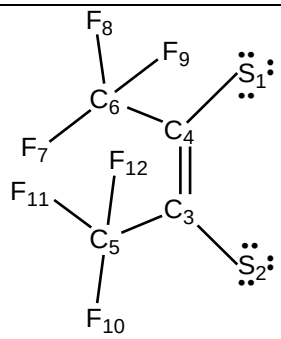
Reference structure	NRT weight / %	Resonance	NBO deloc.
8-9	1.68		$\sigma_{C\text{-}S} \rightarrow \sigma^*_{CH}$
10-11	1.32		$\sigma_{C\text{-}C} \rightarrow \sigma^*_{C\text{-}S}$
69.66/3.71	73.37/23.48		
		TFD	
1	33.26		reference

Table S2. Natural resonance theory (NRT) analysis of the percentage of the ligand resonance structures that contribute to the final hybridization and NBO delocalization (cont.)

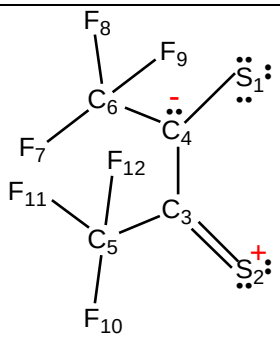
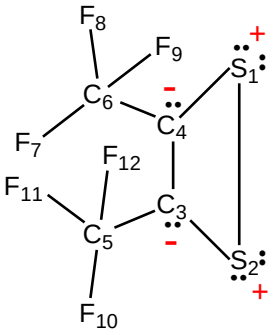
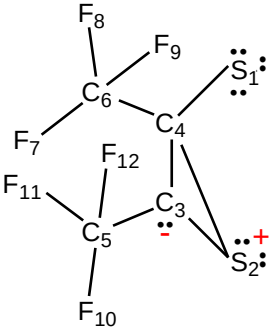
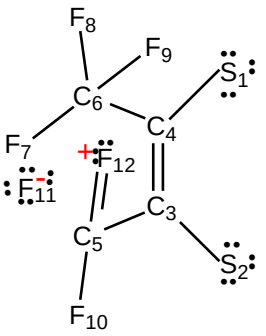
Reference structure	NRT weight / %	Resonance	NBO deloc.
2-3	14.30		$\sigma_S \rightarrow \pi^*_{CC}$
4	2.16		$\sigma_S \rightarrow \pi^*_{CC}$
5-6	4.00		$\sigma_S \rightarrow \pi^{*CC}$
7-8-9-10	5.06		$\sigma_F \rightarrow \sigma^*_{C\text{-}F}$

Table S2. Natural resonance theory (NRT) analysis of the percentage of the ligand resonance structures that contribute to the final hybridization and NBO delocalization (cont.)

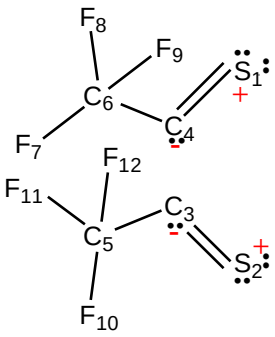
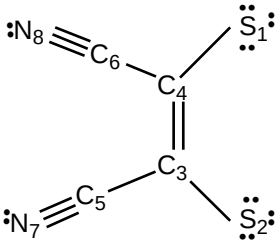
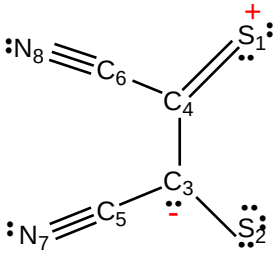
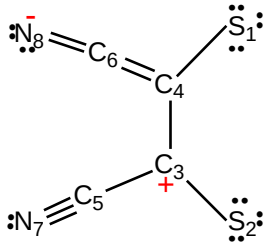
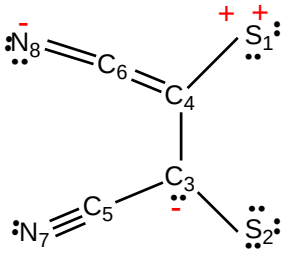
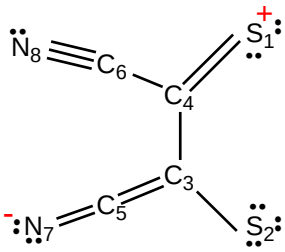
Reference structure	NRT weight / %	Resonance	NBO deloc.
11	1.09		$\sigma_S \rightarrow \sigma^*_{CC}$ $\sigma_S \rightarrow \pi^*_{CC}$
		MNT	
1	44.10		reference
2-3	26.94		$\sigma_S \rightarrow \pi^*_{CC}$

Table S2. Natural resonance theory (NRT) analysis of the percentage of the ligand resonance structures that contribute to the final hybridization and NBO delocalization (cont.)

Reference structure	NRT weight / %	Resonance	NBO deloc.
4-5	5.50		$\pi_{CC} \rightarrow \pi^*_{\eta\text{-}C}$
6-7	3.52		$\sigma_S \rightarrow \pi^*_{\eta\text{-}C}$
8	2.90		$\sigma_S \rightarrow \pi^*_{\eta\text{-}C}$

NBO: natural bond order; tdt: toluene-3,4-dithiolate; bdt: benzene-1,2-dithiolate; Cl_2-bdt: 3,6-dichlorobenzene-1,2-dithiolate; edt: ethylene-1,2-dithiolate; mdt: 1,2-dimethyl-1,2-ethylenedithiolate; tfd: bis(trifluoromethyl) ethylenedithiolate; mnt: maleonitrile-2,3-dithiolate.

Table S3. Cartesian coordinates of the structures, E_{HF}, E_{HOMO} and E_{LUMO}

Structure	$Mg(H_2O)_4$_tdt
E_{HF} / Hartree	-1572.3419000
E_{HOMO} / Hartree	-0.131
E_{LUMO} / Hartree	-0.074

Cartesian Coordinates

MgC7H14S2O4

MAGNESIUM	12.0	1.9852400000	0.0115640000	0.0100970000
OXYGEN	8.0	2.0861060000	-0.5974710000	-2.1168940000
OXYGEN	8.0	3.6201750000	-1.4278540000	0.0735820000
OXYGEN	8.0	3.6180060000	1.3958690000	-0.0483340000
OXYGEN	8.0	1.9416500000	-0.2760530000	2.1968770000

HYDROGEN 1.0 1.8638120000 0.1151100000 -2.7295490000
HYDROGEN 1.0 1.2473340000 -1.0902490000 -1.9533660000
HYDROGEN 1.0 3.6653430000 -1.8993380000 -0.7683160000
HYDROGEN 1.0 3.5967710000 -2.0886070000 0.7754310000
HYDROGEN 1.0 3.4150860000 2.3329230000 0.0557630000
HYDROGEN 1.0 4.5053920000 1.2335830000 0.2879850000
HYDROGEN 1.0 1.5552970000 0.5348250000 2.5572760000
HYDROGEN 1.0 1.1752350000 -0.8778590000 2.0643180000
SULFUR 16.0 0.4155480000 1.8396930000 -0.0845420000
SULFUR 16.0 0.1084090000 -1.6376900000 0.0360270000
CARBON 6.0 -1.2642400000 -0.4729980000 0.0041050000
CARBON 6.0 -1.1314000000 0.9356020000 -0.0450690000
CARBON 6.0 -2.5527240000 -1.0355130000 0.0310450000
HYDROGEN 1.0 -2.6311320000 -2.1168590000 0.0700740000
CARBON 6.0 -2.3109110000 1.7026340000 -0.0652470000
HYDROGEN 1.0 -2.2166990000 2.7820110000 -0.1015470000
CARBON 6.0 -3.7134640000 -0.2684040000 0.0094460000
CARBON 6.0 -3.5708160000 1.1239720000 -0.0387260000
HYDROGEN 1.0 -4.4507060000 1.7605140000 -0.0549930000
CARBON 6.0 -5.0792720000 -0.9134240000 0.0254670000
HYDROGEN 1.0 -5.7113840000 -0.4916390000 0.8133980000
HYDROGEN 1.0 -5.6037840000 -0.7622430000 -0.9245740000
HYDROGEN 1.0 -5.0072910000 -1.9901270000 0.1951980000
$END

Structure	$Mg(H_2O)_4$_bdt
E_{HF} / Hartree	-1533.6528213
E_{HOMO} / Hartree	-0.133
E_{LUMO} / Hartree	-0.075

Cartesian Coordinates

MgC6H12S2O4

C1

MAGNESIUM 12.0 1.6483770000 0.1028010000 0.0003840000
OXYGEN 8.0 1.7344840000 -0.3883910000 -2.1542980000
OXYGEN 8.0 3.4211230000 -1.1528650000 0.0033970000
OXYGEN 8.0 3.1019500000 1.6676900000 0.0002630000
OXYGEN 8.0 1.7259800000 -0.3842030000 2.1562910000
HYDROGEN 1.0 1.3822170000 0.3336620000 -2.6908490000
HYDROGEN 1.0 0.9731890000 -0.9934300000 -1.9921590000
HYDROGEN 1.0 3.5047380000 -1.7124560000 -0.7781910000

HYDROGEN 1.0 3.5013700000 -1.7183620000 0.7810230000
HYDROGEN 1.0 2.8167520000 2.5883520000 0.0087550000
HYDROGEN 1.0 4.0632390000 1.6332040000 0.0156270000
HYDROGEN 1.0 1.3675640000 0.3381710000 2.6883810000
HYDROGEN 1.0 0.9673960000 -0.9919050000 1.9908960000
SULFUR 16.0 -0.0952970000 1.7682810000 -0.0034940000
SULFUR 16.0 -0.0754050000 -1.7165240000 -0.0011210000
CARBON 6.0 -1.5523490000 -0.6878610000 -0.0006080000
CARBON 6.0 -1.5535450000 0.7309150000 -0.0013630000
CARBON 6.0 -2.7820060000 -1.3672350000 0.0006320000
HYDROGEN 1.0 -2.7672530000 -2.4511070000 0.0011420000
CARBON 6.0 -2.7951690000 1.3935550000 -0.0007340000
HYDROGEN 1.0 -2.7936290000 2.4774930000 -0.0012890000
CARBON 6.0 -3.9954790000 -0.6911730000 0.0011720000
HYDROGEN 1.0 -4.9257060000 -1.2487210000 0.0021060000
CARBON 6.0 -4.0001020000 0.7038780000 0.0005080000
HYDROGEN 1.0 -4.9355720000 1.2530370000 0.0009200000
$END

Structure	$Mg(H_2O)_4\_Cl_2\_bdt$
E_{HF} / Hartree	-2452.8929014
E_{HOMO} / Hartree	-0.150
E_{LUMO} / Hartree	-0.080

Cartesian Coordinates
MgC6H10S2O4Cl2
C1
MAGNESIUM 12.0 2.2562730000 0.1035840000 -0.0006290000
OXYGEN 8.0 2.3699820000 -0.3759300000 -2.1576710000
OXYGEN 8.0 4.0337770000 -1.1272930000 0.0040910000
OXYGEN 8.0 3.6606740000 1.7129100000 -0.0044130000
OXYGEN 8.0 2.3664880000 -0.3726360000 2.1585280000
HYDROGEN 1.0 1.5963920000 -0.9702140000 -2.0364030000
HYDROGEN 1.0 2.0606720000 0.3431240000 -2.7234110000
HYDROGEN 1.0 4.1495150000 -1.6846770000 -0.7748610000
HYDROGEN 1.0 4.1456880000 -1.6809870000 0.7862560000
HYDROGEN 1.0 3.3471010000 2.6246620000 -0.0007980000
HYDROGEN 1.0 4.6227650000 1.7109860000 0.0037890000
HYDROGEN 1.0 2.0524920000 0.3474140000 2.7204670000
HYDROGEN 1.0 1.5941410000 -0.9681820000 2.0344760000
SULFUR 16.0 0.4896370000 1.7393320000 0.0002860000

SULFUR 16.0 0.5330380000 -1.6903160000 0.0000770000
CARBON 6.0 -0.9598520000 -0.7062940000 -0.0000590000
CARBON 6.0 -0.9710360000 0.7280820000 0.0000290000
CARBON 6.0 -2.1963220000 -1.3783000000 -0.0002580000
CARBON 6.0 -2.2274120000 1.3681780000 -0.0000350000
CARBON 6.0 -3.4153110000 -0.7126410000 -0.0003400000
CARBON 6.0 -3.4289970000 0.6733480000 -0.0002150000
HYDROGEN 1.0 -4.3650320000 1.2160700000 -0.0002580000
CHLORINE 17.0 -2.3468030000 3.1285940000 0.0001050000
CHLORINE 17.0 -2.2741750000 -3.1415540000 -0.0004580000
HYDROGEN 1.0 -4.3389710000 -1.2757770000 -0.0005180000
$END

Structure	$Mg(H_2O)_4$_edt
E_{HF} / Hartree	-1379.9645622
E_{HOMO} / Hartree	-0.123
E_{LUMO} / Hartree	-0.071

Cartesian Coordinates
MgC2H10S2O4
C1
MAGNESIUM 12.0 0.6969020000 0.0908990000 0.0169030000
OXYGEN 8.0 0.8709570000 -0.6263260000 -2.0689360000
OXYGEN 8.0 2.4465660000 -1.2167650000 0.1731190000
OXYGEN 8.0 2.2432860000 1.5722860000 -0.0993830000
OXYGEN 8.0 0.5597460000 0.0735980000 2.2056380000
HYDROGEN 1.0 0.5623760000 0.0280670000 -2.7092500000
HYDROGEN 1.0 0.0986940000 -1.2099480000 -1.8773200000
HYDROGEN 1.0 2.5460020000 -1.6470670000 -0.6867880000
HYDROGEN 1.0 2.4063690000 -1.9167390000 0.8352430000
HYDROGEN 1.0 1.9612070000 2.4923240000 -0.0339310000
HYDROGEN 1.0 3.0961260000 1.4835770000 0.3394460000
HYDROGEN 1.0 0.0272190000 0.8699550000 2.3598250000
HYDROGEN 1.0 -0.0964000000 -0.6538840000 2.1620700000
SULFUR 16.0 -1.0172160000 1.8008730000 -0.2364210000
SULFUR 16.0 -1.0061730000 -1.7538630000 0.1376880000
CARBON 6.0 -2.4043750000 -0.6486560000 0.0198130000
CARBON 6.0 -2.4002610000 0.6905710000 -0.1186690000
HYDROGEN 1.0 -3.3638480000 -1.1543770000 0.0704010000
HYDROGEN 1.0 -3.3629680000 1.1913150000 -0.1731770000
$END

Structure	$Mg(H_2O)_4$_mdt
E_{HF} / Hartree	-1458.6127519
E_{HOMO} / Hartree	-0.111
E_{LUMO} / Hartree	-0.069

Cartesian Coordinates

MgC4H14S2O4

C1

MAGNESIUM 12.0 1.2649480000 0.0670270000 0.0217890000

OXYGEN 8.0 1.4525210000 -0.7278180000 -2.0453360000

OXYGEN 8.0 3.0037230000 -1.2337090000 0.2100880000

OXYGEN 8.0 2.7742380000 1.5774860000 -0.2248980000

OXYGEN 8.0 1.1377070000 0.2912490000 2.2088660000

HYDROGEN 1.0 1.1871930000 -0.1182280000 -2.7451940000

HYDROGEN 1.0 0.6552540000 -1.2705250000 -1.8257910000

HYDROGEN 1.0 3.0995950000 -1.6526410000 -0.6564180000

HYDROGEN 1.0 2.9585910000 -1.9431680000 0.8615340000

HYDROGEN 1.0 2.4221280000 2.4760580000 -0.2409080000

HYDROGEN 1.0 3.5837790000 1.5843680000 0.2975530000

HYDROGEN 1.0 0.5278530000 1.0495420000 2.1155210000

HYDROGEN 1.0 0.5357710000 -0.4680240000 2.3163410000

SULFUR 16.0 -0.4773390000 1.7387410000 -0.1862780000

SULFUR 16.0 -0.4467570000 -1.7074380000 0.1783290000

CARBON 6.0 -1.9240590000 -0.6725960000 0.0366460000

CARBON 6.0 -1.9316670000 0.6751990000 -0.1021630000

CARBON 6.0 -3.1708430000 -1.5303510000 0.0988260000

HYDROGEN 1.0 -3.2051970000 -2.0831740000 1.0436410000

HYDROGEN 1.0 -4.0951730000 -0.9614270000 0.0075010000

HYDROGEN 1.0 -3.1551970000 -2.2794530000 -0.6997490000

CARBON 6.0 -3.1936870000 1.5064020000 -0.2118310000

HYDROGEN 1.0 -3.2068190000 2.0494530000 -1.1625690000

HYDROGEN 1.0 -4.1091130000 0.9202060000 -0.1441750000

HYDROGEN 1.0 -3.2164830000 2.2622520000 0.5798040000

$END

Structure	$Mg(H_2O)_4$_tfd
E_{HF} / Hartree	-2054.2496503
E_{HOMO} / Hartree	-0.155
E_{LUMO} / Hartree	-0.084

Cartesian Coordinates

MgC4H8S2O4F6

C1

MAGNESIUM 12.0 2.3488970000 0.0924960000 0.0054960000

OXYGEN 8.0 2.6064050000 -0.4695970000 -2.1136310000

OXYGEN 8.0 4.1129020000 -1.1421150000 0.1641320000

OXYGEN 8.0 3.7539940000 1.6982920000 0.0460280000

OXYGEN 8.0 2.3114630000 -0.2671720000 2.1799260000

HYDROGEN 1.0 2.3809020000 0.2274980000 -2.7431080000

HYDROGEN 1.0 1.8136950000 -1.0449870000 -2.0598390000

HYDROGEN 1.0 4.2883100000 -1.7064930000 -0.5986690000

HYDROGEN 1.0 4.1972110000 -1.6807120000 0.9599610000

HYDROGEN 1.0 3.4486400000 2.6106720000 0.1107640000

HYDROGEN 1.0 4.7060460000 1.6771110000 0.1857600000

HYDROGEN 1.0 1.9786180000 0.4637680000 2.7164950000

HYDROGEN 1.0 1.5568620000 -0.8845900000 2.0684930000

SULFUR 16.0 0.5785190000 1.7247660000 -0.2127680000

SULFUR 16.0 0.6099250000 -1.6886800000 -0.0272100000

CARBON 6.0 -0.8539720000 -0.6692870000 -0.0515980000

CARBON 6.0 -0.8548410000 0.6964870000 -0.0605930000

CARBON 6.0 -2.1205570000 -1.5183940000 -0.0079040000

CARBON 6.0 -2.1391550000 1.5262130000 0.0187530000

FLUORINE 9.0 -1.9103540000 2.7833920000 0.4552670000

FLUORINE 9.0 -2.7422010000 1.6541460000 -1.1892110000

FLUORINE 9.0 -3.0513300000 1.0119320000 0.8753980000

FLUORINE 9.0 -3.1541210000 -0.9902730000 -0.6982080000

FLUORINE 9.0 -2.5523750000 -1.7254570000 1.2653110000

FLUORINE 9.0 -1.9272970000 -2.7465140000 -0.5385280000

$END

Structure	$Mg(H_2O)_4$_mnt
E_{HF} / Hartree	-1564.502594
E_{HOMO} / Hartree	-0.174
E_{LUMO} / Hartree	-0.093

Cartesian Coordinates

MgC4N2H8S2O4

C1

MAGNESIUM 12.0 0.1068060000 -0.0678750000 0.0104440000

OXYGEN 8.0 2.1817110000 0.3759790000 -0.5573350000

OXYGEN 8.0 0.1672990000 -1.1142650000 -1.8835010000

OXYGEN 8.0 0.4718420000 -2.0262980000 0.7770120000

OXYGEN 8.0 -2.0495860000 -0.3333010000 -0.3241790000
HYDROGEN 1.0 2.8278970000 0.3998620000 0.1601990000
HYDROGEN 1.0 1.9662240000 1.3094940000 -0.7598040000
HYDROGEN 1.0 0.8772000000 -0.8713620000 -2.4900010000
HYDROGEN 1.0 -0.6580180000 -1.1310290000 -2.3831580000
HYDROGEN 1.0 0.5681070000 -2.2117670000 1.7179170000
HYDROGEN 1.0 0.5976500000 -2.8432590000 0.2836010000
HYDROGEN 1.0 -2.5887590000 -0.5192550000 0.4552940000
HYDROGEN 1.0 -2.1732530000 0.6181790000 -0.5194430000
SULFUR 16.0 0.0926740000 0.7914440000 2.2935900000
SULFUR 16.0 -0.3294390000 2.2487220000 -0.8563770000
CARBON 6.0 -0.3521930000 3.0817390000 0.7142470000
CARBON 6.0 -0.1841660000 2.5000950000 1.9484880000
CARBON 6.0 -0.5688750000 4.4873570000 0.6156240000
CARBON 6.0 -0.2288840000 3.3208100000 3.1174730000
NITROGEN 7.0 -0.7469560000 5.6244750000 0.4893960000
NITROGEN 7.0 -0.2569770000 3.9491590000 4.0888630000
$END

Structure	$Ca(H_2O)_4$_tdt
E_{HF} / Hartree	-2050.5150628
E_{HOMO} / Hartree	-0.136
E_{LUMO} / Hartree	-0.068

Cartesian Coordinates
CaC7H14S2O4
C1
CALCIUM 20.0 -2.0709370000 0.2089260000 -0.6032240000
OXYGEN 8.0 -1.6911120000 2.1899710000 -1.8838860000
OXYGEN 8.0 -3.6771740000 0.1853600000 1.0926370000
OXYGEN 8.0 -2.0979010000 -1.4600630000 -2.3090810000
OXYGEN 8.0 -1.8035870000 -0.2448630000 2.8549430000
HYDROGEN 1.0 -1.6467170000 2.7120540000 -2.6903300000
HYDROGEN 1.0 -0.9334470000 2.4321150000 -1.2931400000
HYDROGEN 1.0 -4.5958210000 0.2505650000 1.3634410000
HYDROGEN 1.0 -3.1049460000 0.0203250000 1.9079330000
HYDROGEN 1.0 -1.4241430000 -1.9849780000 -1.8052550000
HYDROGEN 1.0 -2.1488850000 -1.7870000000 -3.2120500000
HYDROGEN 1.0 -1.3632470000 -1.0064920000 2.4275860000
HYDROGEN 1.0 -1.1978560000 0.4857060000 2.6216520000
SULFUR 16.0 -0.4759970000 -1.8337000000 0.2628110000

SULFUR 16.0 -0.0941710000 1.5994550000 0.6696820000
CARBON 6.0 1.2441500000 0.4517350000 0.3003770000
CARBON 6.0 1.0864050000 -0.9455350000 0.1345710000
CARBON 6.0 2.5348330000 1.0019860000 0.1998950000
CARBON 6.0 2.2343640000 -1.7135610000 -0.1253460000
CARBON 6.0 3.6672560000 0.2346080000 -0.0569580000
CARBON 6.0 3.4960310000 -1.1451410000 -0.2226520000
CARBON 6.0 5.0379010000 0.8645630000 -0.1335970000
HYDROGEN 1.0 2.6377400000 2.0732820000 0.3356210000
HYDROGEN 1.0 2.1158160000 -2.7840540000 -0.2477260000
HYDROGEN 1.0 4.3538610000 -1.7797650000 -0.4242570000
HYDROGEN 1.0 5.6418960000 0.6089690000 0.7440570000
HYDROGEN 1.0 5.5872100000 0.5197230000 -1.0149950000

$END

Structure	$Ca(H_2O)_4$_bdt
E_{HF} / Hartree	-2011.1880226
E_{HOMO} / Hartree	-0.139
E_{LUMO} / Hartree	-0.069

Cartesian Coordinates
CaC6H12S2O4
C1
CALCIUM 20.0 -1.7842040000 0.0032480000 -0.5923230000
OXYGEN 8.0 -1.6369700000 1.8535570000 -2.0948940000
OXYGEN 8.0 -3.3516730000 0.0018130000 1.1387260000
OXYGEN 8.0 -1.6496590000 -1.8483800000 -2.0939200000
OXYGEN 8.0 -1.4175420000 -0.0046820000 2.8871150000
HYDROGEN 1.0 -1.6527180000 2.2750910000 -2.9591900000
HYDROGEN 1.0 -0.9028380000 2.2408670000 -1.5535700000
HYDROGEN 1.0 -4.2677460000 0.0020360000 1.4256030000
HYDROGEN 1.0 -2.7521670000 -0.0007580000 1.9513430000
HYDROGEN 1.0 -0.9147880000 -2.2391320000 -1.5563720000
HYDROGEN 1.0 -1.6827200000 -2.2809340000 -2.9522220000
HYDROGEN 1.0 -0.8996040000 -0.7596270000 2.5441450000
HYDROGEN 1.0 -0.8998590000 0.7537380000 2.5521100000
SULFUR 16.0 0.0441580000 -1.7359600000 0.4599710000
SULFUR 16.0 0.0476360000 1.7362600000 0.4651600000
CARBON 6.0 1.5001780000 0.7083820000 0.1892100000
CARBON 6.0 1.4988210000 -0.7103230000 0.1869620000

CARBON 6.0 2.7197370000 1.3788710000 -0.0089070000
HYDROGEN 1.0 2.7133900000 2.4626120000 0.0027250000
CARBON 6.0 2.7169570000 -1.3827150000 -0.0133130000
HYDROGEN 1.0 2.7083840000 -2.4664700000 -0.0050960000
CARBON 6.0 3.9118430000 0.6945340000 -0.2081600000
HYDROGEN 1.0 4.8337020000 1.2467770000 -0.3547830000
CARBON 6.0 3.9104490000 -0.7001830000 -0.2104100000
HYDROGEN 1.0 4.8311880000 -1.2538060000 -0.3588320000
$END

Structure	$Ca(H_2O)_4\_Cl_2\_bdt$
E_{HF} / Hartree	-2930.4255062
E_{HOMO} / Hartree	-0.155
E_{LUMO} / Hartree	-0.075

Cartesian Coordinates
CaC6H10S2O4Cl2
C1
CALCIUM 20.0 2.3936400000 0.0019740000 0.3283660000
OXYGEN 8.0 2.3803020000 1.8212030000 1.883948000
0XYGEN 8.0 4.4922010000 -0.0085450000 -0.8352600000
OXYGEN 8.0 2.3729370000 -1.8076710000 1.8949430000
OXYGEN 8.0 2.3180350000 -0.0038550000 -2.3572850000
HYDROGEN 1.0 2.5945890000 2.2634680000 2.7105190000
HYDROGEN 1.0 1.5457260000 2.1995530000 1.5174730000
HYDROGEN 1.0 5.4522630000 -0.0184450000 -0.8642590000
HYDROGEN 1.0 4.1368000000 -0.0095900000 -1.7441650000
HYDROGEN 1.0 1.5410730000 -2.1890810000 1.5255070000
HYDROGEN 1.0 2.5814060000 -2.2436110000 2.7263480000
HYDROGEN 1.0 1.7016340000 -0.7599590000 -2.2868260000
HYDROGEN 1.0 1.7079410000 0.7577030000 -2.2987370000
SULFUR 16.0 0.3834210000 -1.7102040000 -0.4119940000
SULFUR 16.0 0.3820520000 1.7104160000 -0.4136980000
CARBON 6.0 -1.0827510000 0.7164470000 -0.1807620000
CARBON 6.0 -1.0822180000 -0.7169320000 -0.1800990000
CARBON 6.0 -2.3164680000 1.3733560000 -0.0084740000
CARBON 6.0 -2.3153300000 -1.3747320000 -0.0071160000
CARBON 6.0 -3.5147210000 0.6916960000 0.1606250000
CARBON 6.0 -3.5141650000 -0.6939150000 0.1613340000
HYDROGEN 1.0 -4.4350890000 -1.2467450000 0.2908800000
CHLORINE 17.0 -2.4123650000 -3.1357890000 0.0137010000

CHLORINE 17.0 -2.4149560000 3.1343400000 0.0106270000

HYDROGEN 1.0 -4.4361090000 1.2438880000 0.2896380000

$END

Structure	$Ca(H_2O)_4$_edt
E_{HF} / Hartree	-1857.5010196
E_{HOMO} / Hartree	-0.185
E_{LUMO} / Hartree	-0.045

Cartesian Coordinates

CaC2H10S2O4

C1

CALCIUM 20.0 0.7223720000 0.0042000000 0.6123480000

OXYGEN 8.0 2.1544950000 -1.9163150000 0.4241730000

OXYGEN 8.0 -0.5698820000 -0.0019890000 2.5641300000

OXYGEN 8.0 2.1367350000 1.9370800000 0.4223920000

OXYGEN 8.0 - 2.7606990000 -0.0139560000 1.1116090000

HYDROGEN 1.0 2.9976390000 -2.3514330000 0.2668650000

HYDROGEN 1.0 1.4478430000 -2.3848450000 -0.0849850000

HYDROGEN 1.0 -0.6116580000 0.0045730000 3.5229800000

HYDROGEN 1.0 -1.5046030000 -0.0073180000 2.1957210000

HYDROGEN 1.0 1.4268870000 2.4002830000 -0.0868050000

HYDROGEN 1.0 2.9776360000 2.3749790000 0.2607320000

HYDROGEN 1.0 -2.5549740000 0.7415220000 0.5287360000

HYDROGEN 1.0 -2.5513910000 -0.7698580000 0.5308010000

SULFUR 16.0 -0.7192220000 1.8337160000 -0.7954560000

SULFUR 16.0 -0.6995190000 -1.8414040000 -0.7951610000

CARBON 6.0 -0.1320830000 -0.6796060000 -2.0242100000

CARBON 6.0 -0.1393200000 0.6779100000 -2.0243320000

HYDROGEN 1.0 0.2903220000 -1.1499390000 -2.9090570000

HYDROGEN 1.0 0.2779360000 1.1526560000 -2.9092670000

$END

Structure	$Ca(H_2O)_4$_mdt
E_{HF} / Hartree	-1936.1483312
E_{HOMO} / Hartree	-0.115
E_{LUMO} / Hartree	-0.064

Cartesian Coordinates

CaC4H14S2O4

C1

CALCIUM 20.0 1.4328000000 -0.0004970000 -0.5506020000

OXYGEN 8.0 1.3551720000 -1.8614220000 -2.0475980000
OXYGEN 8.0 2.9390980000 -0.0046040000 1.2378100000
OXYGEN 8.0 1.3614020000 1.8671150000 -2.0390070000
OXYGEN 8.0 0.9387860000 -0.0049980000 2.9137900000
HYDROGEN 1.0 1.4059470000 -2.3081380000 -2.8977060000
HYDROGEN 1.0 0.6128060000 -2.2482340000 -1.5136160000
HYDROGEN 1.0 3.8429710000 -0.0087230000 1.5607850000
HYDROGEN 1.0 2.3083970000 -0.0049300000 2.0264090000
HYDROGEN 1.0 0.6187960000 2.2537170000 -1.5052890000
HYDROGEN 1.0 1.4279880000 2.3292290000 -2.8797140000
HYDROGEN 1.0 0.4391340000 0.7522550000 2.5480340000
HYDROGEN 1.0 0.4377110000 -0.7598150000 2.5448510000
SULFUR 16.0 -0.4173450000 1.7283280000 0.4490820000
SULFUR 16.0 -0.4196290000 -1.7293190000 0.4448750000
CARBON 6.0 -1.8417040000 -0.6768690000 0.0585810000
CARBON 6.0 -1.8408640000 0.6788050000 0.0602940000
CARBON 6.0 -3.0661930000 -1.5221800000 -0.2241560000
HYDROGEN 1.0 -3.2766410000 -2.1690580000 0.6335200000
HYDROGEN 1.0 -3.9617570000 -0.9396950000 -0.4374640000
HYDROGEN 1.0 -2.8825900000 -2.1862000000 -1.0753890000
CARBON 6.0 -3.0643070000 1.5264430000 -0.2199280000
HYDROGEN 1.0 -2.8806710000 2.1913510000 -1.0704710000
HYDROGEN 1.0 -3.9610810000 0.9456820000 -0.4328530000
HYDROGEN 1.0 -3.2726770000 2.1724240000 0.6389160000
$END

Structure	$Ca(H_2O)_4$_tfd
E_{HF} / Hartree	-2531.7819309
E_{HOMO} / Hartree	-0.198
E_{LUMO} / Hartree	-0.060

Cartesian Coordinates
CaC4H8S2O4F6
C1
CALCIUM 20.0 -2.3570440000 0.1489170000 0.3300310000
OXYGEN 8.0 -1.9917340000 -1.5827080000 1.9564880000
OXYGEN 8.0 -4.6272530000 -0.3670450000 -0.2905660000
OXYGEN 8.0 -2.2180080000 2.0049800000 1.8364500000
OXYGEN 8.0 -2.8229230000 0.0581660000 -2.2201400000
HYDROGEN 1.0 -1.7691090000 -1.7612120000 2.8757010000
HYDROGEN 1.0 -1.3488970000 -2.0593210000 1.3822730000

HYDROGEN 1.0 -5.4421150000 -0.8001770000 -0.0212490000
HYDROGEN 1.0 -4.5531370000 -0.4051770000 -1.2583920000
HYDROGEN 1.0 -1.4065560000 2.3700030000 1.4120840000
HYDROGEN 1.0 -2.3827650000 2.4732860000 2.6606280000
HYDROGEN 1.0 -2.5619320000 0.8619180000 -2.6872740000
HYDROGEN 1.0 -2.0044730000 -0.4931220000 -2.2136220000
SULFUR 16.0 -0.3730500000 1.7932350000 -0.6020740000
SULFUR 16.0 -0.5517140000 -1.6186150000 -0.7835380000
CARBON 6.0 0.8933960000 -0.6809040000 -0.3064400000
CARBON 6.0 0.9820730000 0.6820150000 -0.3114120000
CARBON 6.0 2.0537410000 -1.5970190000 0.0801070000
CARBON 6.0 2.2894870000 1.4363630000 -0.0595900000
FLUORINE 9.0 2.2930100000 2.6543120000 -0.6377550000
FLUORINE 9.0 2.5021090000 1.6504040000 1.2681810000
FLUORINE 9.0 3.3806730000 0.8061160000 -0.5448700000
FLUORINE 9.0 2.8398250000 -1.0845960000 1.0559280000
FLUORINE 9.0 2.8532410000 -1.9007400000 -0.9678100000
FLUORINE 9.0 1.6170570000 -2.7819780000 0.5757900000
$END

Structure	$Ca(H_2O)_4$_mnt
E_{HF} / Hartree	-2042.0350616
E_{HOMO} / Hartree	-0.179
E_{LUMO} / Hartree	-0.088

Cartesian Coordinates
CaC4N2H8S2O4
C1
CALCIUM 20.0 -1.6615870000 0.1406740000 0.2536870000
OXYGEN 8.0 -1.3476950000 -1.1440100000 2.2526030000
OXYGEN 8.0 -3.8685820000 -0.5692380000 -0.4026260000
OXYGEN 8.0 -1.8023050000 2.2523930000 1.3851440000
OXYGEN 8.0 -1.8945380000 -0.4543240000 -2.2242290000
HYDROGEN 1.0 -1.2396690000 -1.1039560000 3.2081780000
HYDROGEN 1.0 -0.6329480000 -1.7058070000 1.8797340000
HYDROGEN 1.0 -4.7088540000 -0.9297860000 -0.1050400000
HYDROGEN 1.0 -3.7477680000 -0.7885210000 -1.3402300000
HYDROGEN 1.0 -0.9421360000 2.5977120000 1.0618200000
HYDROGEN 1.0 -2.1705780000 2.8727350000 2.0218270000
HYDROGEN 1.0 -1.5819970000 0.2412510000 -2.8173060000
HYDROGEN 1.0 -1.1025650000 -1.0201140000 -2.0711230000

SULFUR 16.0 0.3836340000 1.7035070000 -0.7132830000

SULFUR 16.0 0.2728070000 -1.7931630000 -0.3150720000

CARBON 6.0 1.6910550000 -0.7314960000 -0.1432300000

CARBON 6.0 1.7296780000 0.6345020000 -0.2871140000

CARBON 6.0 2.8877050000 -1.4369590000 0.1854500000

CARBON 6.0 2.9715650000 1.3185240000 -0.1063110000

NITROGEN 7.0 3.8308270000 -2.0476290000 0.4649110000

NITROGEN 7.0 3.9520500000 1.9149870000 0.0439700000

$END

Structure	$Mg(H_2O)_2\_tdt\_2$
E_{HF} / Hartree	-2487.0176879
E_{HOMO} / Hartree	0.067
E_{LUMO} / Hartree	0.131

Cartesian Coordinates

MgC14H16S4O2

C1

MAGNESIUM 12.0 -0.1288540000 0.4626980000 0.1131220000

OXYGEN 8.0 2.2751070000 3.2617410000 -1.5935380000

OXYGEN 8.0 0.1650300000 -3.3461320000 -1.3664590000

HYDROGEN 1.0 2.1132320000 2.3683830000 -1.9375580000

HYDROGEN 1.0 2.1131820000 3.1242330000 -0.6448480000

HYDROGEN 1.0 0.7511000000 -2.5855990000 -1.5191320000

HYDROGEN 1.0 -0.4901190000 -2.9750510000 -0.7503590000

SULFUR 16.0 1.6696420000 -0.1999590000 -1.4943530000

SULFUR 16.0 1.6641510000 1.5906650000 1.4067520000

CARBON 6.0 3.0576190000 -0.1224480000 -0.3761460000

CARBON 6.0 3.0519580000 0.6290720000 0.8344010000

CARBON 6.0 4.2227030000 -0.8308950000 -0.7204290000

CARBON 6.0 4.2193650000 0.6149000000 1.6173710000

CARBON 6.0 5.3780100000 -0.8294670000 0.0607460000

CARBON 6.0 5.3607600000 -0.0913250000 1.2488290000

HYDROGEN 1.0 4.2051920000 -1.4048590000 -1.6423800000

HYDROGEN 1.0 4.2126980000 1.1771360000 2.5455560000

HYDROGEN 1.0 6.2372520000 -0.0721270000 1.8934360000

CARBON 6.0 6.6148700000 -1.5793060000 -0.3817930000

HYDROGEN 1.0 6.3540850000 -2.4618370000 -0.9744450000

HYDROGEN 1.0 7.2057190000 -1.9163560000 0.4772200000

HYDROGEN 1.0 7.2726510000 -0.9554270000 -1.0025240000

SULFUR 16.0 -1.5296370000 -1.3858160000 0.9569890000

SULFUR 16.0 -2.1667440000 1.6660240000 -0.5173270000
CARBON 6.0 -3.1516370000 -0.7865300000 0.5311080000
CARBON 6.0 -3.4121360000 0.4795100000 -0.0729820000
CARBON 6.0 -4.2506070000 -1.6170260000 0.8151340000
CARBON 6.0 -4.7537830000 0.8211890000 -0.3412010000
HYDROGEN 1.0 -4.0484940000 -2.5831300000 1.2666620000
HYDROGEN 1.0 -4.9376980000 1.7866080000 -0.8045490000
CARBON 6.0 -5.8344910000 -0.0090710000 -0.0495670000
CARBON 6.0 -5.5643760000 -1.2513050000 0.5364680000
HYDROGEN 1.0 -6.3769580000 -1.9356570000 0.7724650000
CARBON 6.0 -7.2534470000 0.4336500000 -0.3309540000
HYDROGEN 1.0 -7.2782870000 1.2200040000 -1.0918720000
HYDROGEN 1.0 -7.8703360000 -0.3985180000 -0.6902090000
HYDROGEN 1.0 -7.7455220000 0.8346250000 0.5661650000
$END

Structure	$Mg(H_2O)_2\_bdt\_2$
E_{HF} / Hartree	-2408.3617957
E_{HOMO} / Hartree	0.081
E_{LUMO} / Hartree	0.134

Cartesian Coordinates
MgC12H12S4O2
C1
MAGNESIUM 12.0 -0.0000480000 0.1932410000 -0.0009340000
OXYGEN 8.0 -2.5208590000 2.3241320000 2.3201430000
OXYGEN 8.0 2.5232800000 2.3335760000 -2.3103350000
HYDROGEN 1.0 -2.2514520000 1.4000070000 2.4519520000
HYDROGEN 1.0 -2.4125850000 2.4099630000 1.3584150000
HYDROGEN 1.0 2.2549990000 1.4099130000 -2.4474850000
HYDROGEN 1.0 2.4137830000 2.4141180000 -1.3482610000
SULFUR 16.0 -1.9474660000 1.3558420000 -0.9981660000
SULFUR 16.0 -1.6212570000 -0.9671020000 1.4814390000
CARBON 6.0 -3.0775920000 -0.7936930000 0.4714990000
CARBON 6.0 -3.2138530000 0.1796470000 -0.5635470000
CARBON 6.0 -4.4259750000 0.2261870000 -1.2775960000
CARBON 6.0 -4.1629510000 -1.6546110000 0.7214170000
CARBON 6.0 -5.3545440000 -1.5851590000 0.0052170000
CARBON 6.0 -5.4878200000 -0.6324060000 -1.0073880000
HYDROGEN 1.0 -4.5182770000 0.9668980000 -2.0653620000
HYDROGEN 1.0 -4.0484910000 -2.3938900000 1.5076410000

HYDROGEN 1.0 -6.1665980000 -2.2704940000 0.2344140000
HYDROGEN 1.0 -6.4058340000 -0.5589880000 -1.5848420000
SULFUR 16.0 1.6222700000 -0.9616650000 -1.4863330000
SULFUR 16.0 1.9465270000 1.3523380000 1.0019330000
CARBON 6.0 3.2131060000 0.1775020000 0.5642420000
CARBON 6.0 3.0776840000 -0.7920230000 -0.4744780000
CARBON 6.0 4.1631930000 -1.6521230000 -0.7265700000
CARBON 6.0 4.4245570000 0.2212550000 1.2796120000
CARBON 6.0 5.4865320000 -0.6364610000 1.0072390000
CARBON 6.0 5.3541010000 -1.5854430000 -0.0090020000
HYDROGEN 1.0 4.0493830000 -2.3884620000 -1.5156400000
HYDROGEN 1.0 4.5161780000 0.9590220000 2.0702070000
HYDROGEN 1.0 6.4039990000 -0.5652650000 1.5858440000
HYDROGEN 1.0 6.1662720000 -2.2700350000 -0.2399970000
$END

Structure	$Mg(H_2O)_2\_Cl_2\_bdt\_2$
E_{HF} / Hartree	-4246.8548525
E_{HOMO} / Hartree	0.057
E_{LUMO} / Hartree	0.127

Cartesian Coordinates
MgC12H8S4O2Cl4
C1
MAGNESIUM 12.0 -0.0000950000 0.0003210000 -0.8926850000
OXYGEN 8.0 0.9218800000 1.2769220000 -2.7116980000
OXYGEN 8.0 -0.9222210000 -1.2791370000 -2.7115120000
HYDROGEN 1.0 -1.2920490000 -1.8474210000 -2.0096940000
HYDROGEN 1.0 -1.5722860000 -0.5527590000 -2.7609370000
HYDROGEN 1.0 1.2922120000 1.8466170000 -2.0113400000
HYDROGEN 1.0 1.5720690000 0.5505190000 -2.7603360000
SULFUR 16.0 -2.1742030000 1.2774890000 -1.2412180000
SULFUR 16.0 -1.4968080000 -1.5793220000 0.4260730000
CARBON 6.0 -3.0645280000 -0.7758200000 0.4883540000
CARBON 6.0 -3.3543170000 0.4558340000 -0.2220930000
CARBON 6.0 -4.6505770000 0.9870650000 -0.0796510000
CARBON 6.0 -4.1079150000 -1.3310020000 1.2547760000
CHLORINE 17.0 -5.1154810000 2.4912770000 -0.9153910000
CHLORINE 17.0 -3.8663050000 -2.8478600000 2.1576800000
CARBON 6.0 -5.3761330000 -0.7717530000 1.3690600000
CARBON 6.0 -5.6522760000 0.4065000000 0.6910530000

HYDROGEN 1.0 -6.6269840000 0.8729670000 0.7572980000
HYDROGEN 1.0 -6.1293180000 -1.2530080000 1.9799450000
SULFUR 16.0 1.4969050000 1.5796190000 0.4256440000
SULFUR 16.0 2.1740200000 -1.2780620000 -1.2404540000
CARBON 6.0 3.3543120000 -0.4558390000 -0.2219370000
CARBON 6.0 3.0645750000 0.7760860000 0.4880830000
CARBON 6.0 4.1080250000 1.3315010000 1.2542500000
CARBON 6.0 4.6506220000 -0.9869300000 -0.0795180000
CHLORINE 17.0 3.8664430000 2.8485890000 2.1568360000
CHLORINE 17.0 5.1154800000 -2.4914720000 -0.9147510000
CARBON 6.0 5.6523930000 -0.4061120000 0.6909140000
CARBON 6.0 5.3762690000 0.7723150000 1.3686100000
HYDROGEN 1.0 6.1294650000 1.2537620000 1.9793310000
HYDROGEN 1.0 6.6271220000 -0.8725300000 0.7571760000
$END

Structure	$Mg(H_2O)_2\_edt\_2$
E_{HF} / Hartree	-2100.9657637
E_{HOMO} / Hartree	0.115
E_{LUMO} / Hartree	0.146

Cartesian Coordinates
MgC4H8S4O2
C1
MAGNESIUM 12.0 -0.0006160000 -0.1761330000 -0.0026240000
OXYGEN 8.0 3.1307620000 1.8204520000 1.6023090000
OXYGEN 8.0 -3.1237210000 1.8809830000 -1.5350060000
HYDROGEN 1.0 2.7596450000 1.9469170000 0.7123310000
HYDROGEN 1.0 2.8760530000 0.8974920000 1.7744470000
HYDROGEN 1.0 -2.8719270000 0.9645960000 -1.7422420000
HYDROGEN 1.0 -2.7524990000 1.9719110000 -0.6405960000
SULFUR 16.0 1.6222120000 1.0331830000 -1.4729490000
SULFUR 16.0 1.9403230000 -1.4249480000 0.9949930000
CARBON 6.0 3.0223480000 -1.1447210000 -0.3853220000
CARBON 6.0 2.8993530000 -0.1947960000 -1.3362280000
HYDROGEN 1.0 3.8806030000 -1.8135810000 -0.4419620000
HYDROGEN 1.0 3.6648170000 -0.1459690000 -2.1099890000
SULFUR 16.0 -1.6249050000 0.9810810000 1.5071450000
SULFUR 16.0 -1.9394910000 -1.3917490000 -1.0434510000
CARBON 6.0 -3.0236690000 -1.1581930000 0.3437130000
CARBON 6.0 -2.9021180000 -0.2412260000 1.3266590000

HYDROGEN 1.0 -3.8823830000 -1.8281100000 0.3760700000

HYDROGEN 1.0 -3.6689410000 -0.2185870000 2.1002570000

$END

Structure	$Mg(H_2O)_2\_mdt\_{-2}$
E_{HF} / Hartree	-2258.2591155
E_{HOMO} / Hartree	0.103
E_{LUMO} / Hartree	0.140

Cartesian Coordinates

MgC8H16S4O2

C1

MAGNESIUM 12.0 0.1324470000 0.0441920000 0.1924580000

OXYGEN 8.0 -2.2653610000 -1.7646180000 2.1963540000

OXYGEN 8.0 0.4186980000 -0.9253530000 2.1522040000

HYDROGEN 1.0 -2.3769710000 -0.7897950000 2.1580310000

HYDROGEN 1.0 -2.2022360000 -1.9671280000 1.2377900000

HYDROGEN 1.0 -0.4033110000 -1.4311310000 2.3211870000

HYDROGEN 1.0 1.0915490000 -1.5244880000 1.7658080000

SULFUR 16.0 -1.9587580000 1.3241790000 1.0508150000

SULFUR 16.0 -1.6507780000 -1.3177240000 -1.0192640000

CARBON 6.0 -3.1924040000 0.8428750000 -0.1521490000

CARBON 6.0 -3.0704690000 -0.2244060000 -0.9831390000

CARBON 6.0 -4.3983080000 1.7632560000 -0.1272750000

CARBON 6.0 -4.1187860000 -0.6345550000 -1.9996790000

HYDROGEN 1.0 -4.8342790000 1.7854060000 0.8797710000

HYDROGEN 1.0 -5.1873800000 1.4807040000 -0.8295760000

HYDROGEN 1.0 -4.0937340000 2.7930860000 -0.3527700000

HYDROGEN 1.0 -4.4529690000 -1.6626610000 -1.8076030000

HYDROGEN 1.0 -5.0018040000 0.0102410000 -2.0095800000

HYDROGEN 1.0 -3.6876600000 -0.6358010000 -3.0086900000

SULFUR 16.0 2.1178000000 -1.5935170000 -0.3510600000

SULFUR 16.0 1.8319250000 1.8064200000 -0.1894980000

CARBON 6.0 3.4946450000 -0.4509050000 -0.3238620000

CARBON 6.0 3.3728580000 0.9026560000 -0.2780530000

CARBON 6.0 4.5587290000 1.8519240000 -0.2890640000

CARBON 6.0 4.8256270000 -1.1784160000 -0.3853690000

HYDROGEN 1.0 4.8647580000 -1.8214930000 -1.2743080000

HYDROGEN 1.0 4.9341790000 -1.8464090000 0.4795750000

HYDROGEN 1.0 5.6955830000 -0.5160500000 -0.4090940000

HYDROGEN 1.0 5.5275310000 1.3539550000 -0.3837960000

HYDROGEN 1.0 4.5742740000 2.4528140000 0.6296990000

HYDROGEN 1.0 4.4620340000 2.5639350000 -1.1187540000

$END

Structure	$Mg(H_2O)_2\_tfd\_2$
E_{HF} / Hartree	-3449.5853981
E_{HOMO} / Hartree	0.070
E_{LUMO} / Hartree	0.128

Cartesian Coordinates

MgC8H4S4O2F12

C1

MAGNESIUM 12.0 -0.0017840000 -0.0700460000 0.8820300000

OXYGEN 8.0 0.9718950000 -1.4347260000 2.5539190000

OXYGEN 8.0 -0.9704770000 0.9906590000 2.7541720000

HYDROGEN 1.0 1.6074070000 -0.7016460000 2.6685200000

HYDROGEN 1.0 1.3653930000 -1.9526500000 1.8261540000

HYDROGEN 1.0 -1.3831870000 1.6062560000 2.1185260000

HYDROGEN 1.0 -1.5958380000 0.2412050000 2.7713650000

SULFUR 16.0 2.1302130000 1.2701770000 1.3119810000

SULFUR 16.0 1.5609200000 -1.4737620000 -0.5708070000

CARBON 6.0 3.3267630000 0.5188710000 0.2502390000

CARBON 6.0 3.1127340000 -0.6366320000 -0.4647100000

CARBON 6.0 4.6472820000 1.2621740000 0.2532130000

CARBON 6.0 4.1966670000 -1.3141850000 -1.2821840000

FLUORINE 9.0 5.5435460000 0.7715500000 1.1725760000

FLUORINE 9.0 5.3044440000 1.2525320000 -0.9420580000

FLUORINE 9.0 4.5246630000 2.5776730000 0.5572840000

FLUORINE 9.0 5.4327460000 -1.2911560000 -0.6975430000

FLUORINE 9.0 3.9603580000 -2.6307550000 -1.5050790000

FLUORINE 9.0 4.3637100000 -0.7706580000 -2.5281070000

SULFUR 16.0 -2.1318960000 -1.4660570000 1.0809740000

SULFUR 16.0 -1.5604740000 1.5466330000 -0.3326980000

CARBON 6.0 -3.3438530000 -0.5284340000 0.2011590000

CARBON 6.0 -3.0958450000 0.6764760000 -0.4142290000

CARBON 6.0 -4.6983880000 -1.2102970000 0.1703610000

CARBON 6.0 -4.1447200000 1.4319010000 -1.2072630000

FLUORINE 9.0 -4.8741460000 -2.1089340000 1.1712170000

FLUORINE 9.0 -4.9276130000 -1.9180150000 -0.9802460000

FLUORINE 9.0 -5.7586910000 -0.3563260000 0.2984100000

FLUORINE 9.0 -4.9849160000 0.6394050000 -1.9337390000

FLUORINE 9.0 -4.9585440000 2.2091670000 -0.4185070000

FLUORINE 9.0 -3.6219740000 2.2887220000 -2.1169150000

$END

Structure	$Mg(H_2O)_2\_mnt\_2$
E_{HF} / Hartree	-2470.1081147
E_{HOMO} / Hartree	0.033
E_{LUMO} / Hartree	0.120

Cartesian Coordinates

MgC8N4H4S4O2

C1

MAGNESIUM 12.0 -0.0623840000 -0.1052630000 0.6622720000

OXYGEN 8.0 0.9986340000 0.7336180000 2.5200010000

OXYGEN 8.0 -0.7213420000 -1.9298210000 1.9436050000

HYDROGEN 1.0 -0.0107440000 -2.5825000000 1.9205580000

HYDROGEN 1.0 -1.3060340000 -2.1592830000 1.1884960000

HYDROGEN 1.0 1.6796040000 0.0392590000 2.4417910000

HYDROGEN 1.0 1.3630770000 1.4633110000 1.9845280000

SULFUR 16.0 2.1464170000 -1.5505300000 0.6193200000

SULFUR 16.0 1.5058940000 1.6426680000 -0.4841930000

CARBON 6.0 3.3067980000 -0.4869020000 -0.1669230000

CARBON 6.0 3.0404880000 0.7981730000 -0.6043990000

CARBON 6.0 4.6120380000 -1.0361820000 -0.3287910000

CARBON 6.0 4.0901420000 1.5502750000 -1.2157660000

NITROGEN 7.0 4.9211370000 2.1922240000 -1.7100890000

NITROGEN 7.0 5.6634430000 -1.5173190000 -0.4365410000

SULFUR 16.0 -2.1164550000 1.2885390000 1.1389940000

SULFUR 16.0 -1.6094640000 -1.3730700000 -0.9872620000

CARBON 6.0 -3.1239600000 -0.4934060000 -0.7749990000

CARBON 6.0 -3.3127250000 0.5833850000 0.0729520000

CARBON 6.0 -4.6001120000 1.2004140000 0.1336400000

CARBON 6.0 -4.2091080000 -0.9688550000 -1.5656350000

NITROGEN 7.0 -5.6327820000 1.7245500000 0.2124120000

NITROGEN 7.0 -5.0716950000 -1.3896170000 -2.2203130000

$END

Structure	$Ca(H_2O)_2\_tdt\_2$
E_{HF} / Hartree	-2964.5399496
E_{HOMO} / Hartree	0.066
E_{LUMO} / Hartree	0.116

Cartesian Coordinates

CaC14H16S4O2

C1

CALCIUM	20.0	-0.0804180000	-0.3278140000	0.6143150000
OXYGEN	8.0	1.1399990000	-2.1377600000	2.0210840000
OXYGEN	8.0	-0.5040720000	1.4702270000	2.3798700000
HYDROGEN	1.0	1.7692630000	-1.4184710000	2.2400090000
HYDROGEN	1.0	1.4976320000	-2.4385230000	1.1598660000
HYDROGEN	1.0	0.3197610000	1.9652300000	2.2650930000
HYDROGEN	1.0	-1.1244100000	1.8256190000	1.6983000000
SULFUR	16.0	2.5004730000	0.7206160000	1.4651400000
SULFUR	16.0	1.8716120000	-1.5471100000	-1.0734350000
CARBON	6.0	3.6751550000	0.2581510000	0.2109270000
CARBON	6.0	3.4109580000	-0.6863900000	-0.8269760000
CARBON	6.0	4.9517070000	0.8532130000	0.2652190000
CARBON	6.0	4.4570580000	-0.9630280000	-1.7298420000
CARBON	6.0	5.9733350000	0.5735050000	-0.6408780000
CARBON	6.0	5.7076070000	-0.3585710000	-1.6507820000
HYDROGEN	1.0	5.1308470000	1.5661660000	1.0651450000
HYDROGEN	1.0	4.2589190000	-1.6840000000	-2.5163020000
HYDROGEN	1.0	6.4761540000	-0.6128590000	-2.3784320000
CARBON	6.0	7.3076640000	1.2806300000	-0.5542200000
HYDROGEN	1.0	7.3487870000	2.1649470000	-1.2054920000
HYDROGEN	1.0	8.1308770000	0.6220560000	-0.8551400000
HYDROGEN	1.0	7.5096680000	1.6227470000	0.4658880000
SULFUR	16.0	-1.8088740000	1.6566880000	-0.4787410000
SULFUR	16.0	-2.5761640000	-1.5449550000	0.6161310000
CARBON	6.0	-3.4395940000	0.9347720000	-0.4844120000
CARBON	6.0	-3.7479930000	-0.3882890000	-0.0415520000
CARBON	6.0	-4.4921180000	1.7233300000	-0.9837380000
CARBON	6.0	-5.0925380000	-0.8122250000	-0.1308030000
HYDROGEN	1.0	-4.2477000000	2.7229860000	-1.3288330000
HYDROGEN	1.0	-5.3126640000	-1.8213540000	0.2063410000
CARBON	6.0	-6.1268190000	-0.0174660000	-0.6207530000
CARBON	6.0	-5.8082360000	1.2739660000	-1.0565910000
HYDROGEN	1.0	-6.5819880000	1.9270570000	-1.4560220000
CARBON	6.0	-7.5516160000	-0.5258600000	-0.6482240000
HYDROGEN	1.0	-8.1136000000	-0.2270890000	0.2479510000
HYDROGEN	1.0	-8.0993620000	-0.1371080000	-1.5148250000
HYDROGEN	1.0	-7.5814160000	-1.6191260000	-0.6972490000

$END

Structure	$Ca(H_2O)_2\_bdt_{-2}$
E_{HF} / Hartree	-2885.8905419
E_{HOMO} / Hartree	0.076
E_{LUMO} / Hartree	0.114

Cartesian Coordinates

CaC12H12S4O2

C1

CALCIUM 20.0 0.0000140000 0.5659610000 0.0005740000

OXYGEN 8.0 -1.2949680000 2.3942720000 1.3013150000

OXYGEN 8.0 1.2946980000 2.3965590000 -1.2970990000

HYDROGEN 1.0 -1.6735160000 1.6416490000 1.8016960000

HYDROGEN 1.0 -1.8720290000 2.4103290000 0.5095170000

HYDROGEN 1.0 1.6732740000 1.6448390000 -1.7988230000

HYDROGEN 1.0 1.8718880000 2.4113400000 -0.5053810000

SULFUR 16.0 -2.4484630000 1.0021330000 -1.3831310000

SULFUR 16.0 -1.9542730000 -0.7564610000 1.5749880000

CARBON 6.0 -3.4704850000 -0.7304840000 0.6400860000

CARBON 6.0 -3.6739190000 -0.0080430000 -0.5773380000

CARBON 6.0 -4.9409740000 -0.0920830000 -1.1912460000

CARBON 6.0 -4.5487140000 -1.4832930000 1.1497750000

CARBON 6.0 -5.7895210000 -1.5481920000 0.5234140000

CARBON 6.0 -5.9887950000 -0.8415100000 -0.6653780000

HYDROGEN 1.0 -5.0830910000 0.4598040000 -2.1148270000

HYDROGEN 1.0 -4.3813220000 -2.0297660000 2.0723070000

HYDROGEN 1.0 -6.5872670000 -2.1458240000 0.9575920000

HYDROGEN 1.0 -6.9459090000 -0.8744210000 -1.1801330000

SULFUR 16.0 1.9543520000 -0.7534280000 -1.5764330000

SULFUR 16.0 2.4485030000 0.9997130000 1.3849140000

CARBON 6.0 3.6739370000 -0.0090560000 0.5773520000

CARBON 6.0 3.4705290000 -0.7292410000 -0.6414170000

CARBON 6.0 4.5487490000 -1.4811350000 -1.1524580000

CARBON 6.0 4.9409550000 -0.0943020000 1.1911590000

CARBON 6.0 5.9887720000 -0.8427990000 0.6639500000

CARBON 6.0 5.7895300000 -1.5472490000 -0.5261660000

HYDROGEN 1.0 4.3813850000 -2.0258770000 -2.0760180000

HYDROGEN 1.0 5.0830660000 0.4558540000 2.1157740000

HYDROGEN 1.0 6.9458530000 -0.8766870000 1.1787010000

HYDROGEN 1.0 6.5872640000 -2.1441040000 -0.9614330000

$END

Structure	$Ca(H_2O)_2\_Cl_2\_bdt_{-2}$
E_{HF} / Hartree	-4724.3956941
E_{HOMO} / Hartree	0.243
E_{LUMO} / Hartree	0.245

Cartesian Coordinates

CaC12H8S4O2Cl4

C1

CALCIUM 20.0 -0.0770250000 0.0738760000 0.4007660000

OXYGEN 8.0 -0.4448630000 -0.6355340000 2.6925000000

OXYGEN 8.0 2.1574950000 -1.5221700000 2.9616530000

HYDROGEN 1.0 2.2207500000 -1.9115450000 2.0662120000

HYDROGEN 1.0 2.3993350000 -0.5942470000 2.7652450000

HYDROGEN 1.0 0.3560460000 -1.1267170000 2.9807370000

HYDROGEN 1.0 -1.1699210000 -1.2583630000 2.5202410000

SULFUR 16.0 2.3302840000 1.3257490000 1.2131040000

SULFUR 16.0 2.0169270000 -1.6373260000 -0.3795280000

CARBON 6.0 3.4720780000 -0.6381570000 -0.4747170000

CARBON 6.0 3.6042920000 0.6373540000 0.2016140000

CARBON 6.0 4.8231150000 1.3253490000 0.0412730000

CARBON 6.0 4.5759740000 -1.0806990000 -1.2300550000

CHLORINE 17.0 5.0955500000 2.8966520000 0.8318190000

CHLORINE 17.0 4.5275780000 -2.6360090000 -2.0933000000

CARBON 6.0 5.7617420000 -0.3668440000 -1.3648960000

CARBON 6.0 5.8870710000 0.8546420000 -0.7202640000

HYDROGEN 1.0 6.7946630000 1.4386020000 -0.8054400000

HYDROGEN 1.0 6.5689560000 -0.7637750000 -1.9672530000

SULFUR 16.0 -2.0680910000 1.6879900000 -0.5883270000

SULFUR 16.0 -2.3106630000 -1.6074430000 0.2138710000

CARBON 6.0 -3.7082430000 -0.5740930000 -0.0825790000

CARBON 6.0 -3.5995170000 0.8282920000 -0.4460040000

CARBON 6.0 -4.8056620000 1.5145700000 -0.6978440000

CARBON 6.0 -5.0064870000 -1.1143260000 0.0039730000

CHLORINE 17.0 -4.7967920000 3.2338670000 -1.1664270000

CHLORINE 17.0 -5.2572310000 -2.8200150000 0.4581460000

CARBON 6.0 -6.1714650000 -0.3960300000 -0.2439120000

CARBON 6.0 -6.0682300000 0.9393270000 -0.6039230000

HYDROGEN 1.0 -6.9513770000 1.5313980000 -0.8081650000

HYDROGEN 1.0 -7.1370990000 -0.8774660000 -0.1560880000

$END

Structure	$Ca(H_2O)_2\_edt\_2$
E_{HF} / Hartree	-2578.4983212
E_{HOMO} / Hartree	0.041
E_{LUMO} / Hartree	0.128

Cartesian Coordinates

CaC4H8S4O2

C1

CALCIUM 20.0 0.0000850000 0.0126190000 -0.0000450000

OXYGEN 8.0 -4.2565380000 -1.4193170000 1.1509440000

OXYGEN 8.0 4.2569780000 -1.4200540000 -1.1501420000

HYDROGEN 1.0 3.7275090000 -1.6671960000 -0.3700400000

HYDROGEN 1.0 3.8041380000 -0.5965160000 -1.4085890000

HYDROGEN 1.0 -3.8036310000 -0.5956480000 1.4088900000

HYDROGEN 1.0 -3.7271410000 -1.6669350000 0.3709310000

SULFUR 16.0 1.9821950000 -1.3154830000 1.3972690000

SULFUR 16.0 2.1806500000 1.2955930000 -1.1334160000

CARBON 6.0 2.4757750000 1.3809330000 0.6184940000

CARBON 6.0 2.4020380000 0.4053360000 1.5640860000

HYDROGEN 1.0 2.7219200000 2.3768710000 0.9870010000

HYDROGEN 1.0 2.5969470000 0.7255670000 2.5876850000

SULFUR 16.0 -1.9824180000 -1.3163130000 -1.3965060000

SULFUR 16.0 -2.1806000000 1.2961510000 1.1326880000

CARBON 6.0 -2.4759460000 1.3805190000 -0.6192470000

CARBON 6.0 -2.4023050000 0.4043790000 -1.5642770000

HYDROGEN 1.0 -2.7221470000 2.3762520000 -0.9882620000

HYDROGEN 1.0 -2.5974110000 0.7240240000 -2.5880280000

$SEND

Structure	$Ca(H_2O)_2\_mdt\_2$
E_{HF} / Hartree	-2735.7940180
E_{HOMO} / Hartree	0.063
E_{LUMO} / Hartree	0.123

Cartesian Coordinates

CaC8H16S4O2

C1

CALCIUM 20.0 0.1311900000 0.1335450000 0.1347560000

OXYGEN 8.0 0.4482290000 -1.3262820000 2.0893990000

HYDROGEN 1.0 -2.4056440000 -1.1894210000 1.9994970000

HYDROGEN 1.0 -2.2366590000 -2.1793950000 0.8800480000

HYDROGEN 1.0 -0.3732470000 -1.8619500000 2.1129260000

HYDROGEN 1.0 1.1486590000 -1.8193060000 1.6164080000

SULFUR 16.0 -2.2723930000 1.1228420000 1.2976380000

SULFUR 16.0 -1.9635860000 -1.1297580000 -1.2809740000

CARBON 6.0 -3.5000970000 0.8318720000 0.0212250000

CARBON 6.0 -3.3803110000 -0.0647430000 -0.9931830000

CARBON 6.0 -4.7181060000 1.7161900000 0.2231780000

CARBON 6.0 -4.4545660000 -0.2957400000 -2.0418110000

HYDROGEN 1.0 -5.1425300000 1.5486480000 1.2211190000

HYDROGEN 1.0 -5.5109020000 1.5605430000 -0.5135850000

HYDROGEN 1.0 -4.4252360000 2.7729060000 0.1888500000

HYDROGEN 1.0 -4.7440360000 -1.3539390000 -2.0531870000

HYDROGEN 1.0 -5.3587240000 0.3008870000 -1.8940100000

HYDROGEN 1.0 -4.0609490000 -0.0753420000 -3.0420140000

SULFUR 16.0 2.3337470000 -1.5340920000 -0.4982500000

SULFUR 16.0 2.2029680000 1.9245280000 -0.1943390000

CARBON 6.0 3.7423230000 -0.4363020000 -0.3255180000

CARBON 6.0 3.6868700000 0.9191580000 -0.2231650000

CARBON 6.0 4.9233570000 1.7975830000 -0.1149350000

CARBON 6.0 5.0416400000 -1.2243030000 -0.3339840000

HYDROGEN 1.0 5.1139300000 -1.8211390000 -1.2522890000

HYDROGEN 1.0 5.0539210000 -1.9409130000 0.4974370000

HYDROGEN 1.0 5.9409490000 -0.6069950000 -0.2590280000

HYDROGEN 1.0 5.8692620000 1.2524540000 -0.1760170000

HYDROGEN 1.0 4.9113130000 2.3526790000 0.8318400000

HYDROGEN 1.0 4.9141290000 2.5514710000 -0.9118820000

$END

Structure	$Ca(H_2O)_2\_tfd\_{-2}$
E_{HF} / Hartree	-3927.1233053
E_{HOMO} / Hartree	0.065
E_{LUMO} / Hartree	0.112

Cartesian Coordinates

CaC8H4S4O2F12

C1

CALCIUM 20.0 -0.0003210000 -0.0898700000 -0.7005250000

OXYGEN 8.0 -1.2269620000 -1.5802750000 -2.3788650000

OXYGEN 8.0 1.2499260000 0.9845790000 -2.6525740000

HYDROGEN 1.0 -1.8310150000 -0.8215600000 -2.5092580000

HYDROGEN 1.0 -1.6403860000 -2.0382760000 -1.6215120000

HYDROGEN 1.0 1.6744990000 1.5682170000 -1.9924670000

HYDROGEN 1.0 1.8393930000 0.2053660000 -2.6437240000

SULFUR 16.0 -2.4286780000 1.2376140000 -1.2871260000

SULFUR 16.0 -1.9939630000 -1.4470480000 0.7703340000

CARBON 6.0 -3.6781970000 0.5348640000 -0.2526660000

CARBON 6.0 -3.5222870000 -0.5959220000 0.5147250000

CARBON 6.0 -4.9854010000 1.3043140000 -0.3364880000

CARBON 6.0 -4.6677090000 -1.2398980000 1.2783440000

FLUORINE 9.0 -5.8484360000 0.8066750000 -1.2807860000

FLUORINE 9.0 -5.6924180000 1.3411630000 0.8300060000

FLUORINE 9.0 -4.8216490000 2.6080410000 -0.6670230000

FLUORINE 9.0 -5.8703950000 -1.1888580000 0.6318900000

FLUORINE 9.0 -4.4785800000 -2.5607610000 1.5185350000

FLUORINE 9.0 -4.8816040000 -0.6830780000 2.5109410000

SULFUR 16.0 2.4321670000 -1.5150060000 -0.9358950000

SULFUR 16.0 1.9746480000 1.5616500000 0.4582410000

CARBON 6.0 3.6958010000 -0.5523340000 -0.1614140000

CARBON 6.0 3.4955550000 0.6595860000 0.4578120000

CARBON 6.0 5.0553290000 -1.2295530000 -0.2265620000

CARBON 6.0 4.5974350000 1.4083450000 1.1883180000

FLUORINE 9.0 5.1670520000 -2.1194970000 -1.2427010000

FLUORINE 9.0 5.3628610000 -1.9426720000 0.9017950000

FLUORINE 9.0 6.0995890000 -0.3693480000 -0.4208870000

FLUORINE 9.0 5.4796870000 0.6079440000 1.8532450000

FLUORINE 9.0 5.3586470000 2.1911700000 0.3561820000

FLUORINE 9.0 4.1352790000 2.2556050000 2.1385480000

$END

Structure	$Ca(H_2O)_2\_mnt_{-2}$
E_{HF} / Hartree	-2947.6497886
E_{HOMO} / Hartree	0.005
E_{LUMO} / Hartree	0.118

Cartesian Coordinates

CaC8N4H4S4O2

C1

CALCIUM 20.0 -0.0656750000 -0.0256810000 -0.5268560000

OXYGEN 8.0 1.2253720000 -1.1196340000 -2.4208670000

OXYGEN 8.0 -0.6973900000 2.0907870000 -1.7064560000

HYDROGEN 1.0 -0.0216280000 2.7679090000 -1.5804650000

HYDROGEN 1.0 -1.3629120000 2.2357040000 -0.9955380000

HYDROGEN 1.0 1.8431880000 -0.3620160000 -2.3974650000

HYDROGEN 1.0 1.6350300000 -1.7404990000 -1.7901250000

SULFUR 16.0 2.4145010000 1.4405140000 -0.8308120000

SULFUR 16.0 1.9368920000 -1.6399310000 0.7388230000

CARBON 6.0 3.6192560000 0.5232850000 0.0685440000

CARBON 6.0 3.4235180000 -0.7008150000 0.6815540000

CARBON 6.0 4.9069020000 1.1368750000 0.1256220000

CARBON 6.0 4.5264670000 -1.3173260000 1.3508250000

NITROGEN 7.0 5.4007280000 -1.8487010000 1.8985310000

NITROGEN 7.0 5.9389280000 1.6682370000 0.1459790000

SULFUR 16.0 -2.4268670000 -1.4660710000 -0.9506760000

SULFUR 16.0 -2.0042010000 1.3642710000 1.0626220000

CARBON 6.0 -3.5153370000 0.5119760000 0.7347290000

CARBON 6.0 -3.6689690000 -0.6137810000 -0.0538170000

CARBON 6.0 -4.9760140000 -1.1796000000 -0.1913720000

CARBON 6.0 -4.6557560000 1.0758900000 1.3794100000

NITROGEN 7.0 -6.0204570000 -1.6665440000 -0.3286690000

NITROGEN 7.0 -5.5605760000 1.5675440000 1.9165910000

$END

Structure ligand	_tdt
E_{HF} / Hartree	-1066.8364333
E_{HOMO} / Hartree	0.147
E_{LUMO} / Hartree	0.147

Cartesian Coordinates

C7H6S2

C1

SULFUR 16.0 -2.4309670000 -1.2373940000 0.0123580000
SULFUR 16.0 -1.3780170000 2.0942050000 -0.0025850000
CARBON 6.0 -0.3054210000 0.6876990000 -0.0036570000
CARBON 6.0 -0.7437320000 -0.6979680000 0.0010610000
CARBON 6.0 1.0925210000 0.9216610000 -0.0134270000
HYDROGEN 1.0 1.4034940000 1.9641490000 -0.0186140000
CARBON 6.0 0.2704870000 -1.6837190000 -0.0097620000
HYDROGEN 1.0 -0.0600980000 -2.7187990000 -0.0157830000
CARBON 6.0 2.0722570000 -0.0750060000 -0.0179430000
CARBON 6.0 1.6398360000 -1.4061510000 -0.0189720000
HYDROGEN 1.0 2.3621720000 -2.2240630000 -0.0293410000
CARBON 6.0 3.5432940000 0.2784710000 0.0278210000
HYDROGEN 1.0 3.9063020000 0.4588930000 1.0530750000
HYDROGEN 1.0 4.1598040000 -0.5287480000 -0.3904860000
HYDROGEN 1.0 3.7566220000 1.1896680000 -0.5459480000
$END

Structure ligand	_bdt
E_{HF} / Hartree	-1027.5097086
E_{HOMO} / Hartree	0.150
E_{LUMO} / Hartree	0.200

Cartesian Coordinates
C6H4S2
C1
SULFUR 16.0 1.5588880000 -1.7461280000 -0.0000010000
SULFUR 16.0 1.5587920000 1.7461930000 -0.0000160000
CARBON 6.0 0.1115150000 0.7268610000 0.0000150000
CARBON 6.0 0.1115520000 -0.7268530000 0.0000250000
CARBON 6.0 -1.1514480000 1.3699580000 0.0000420000
HYDROGEN 1.0 -1.1389760000 2.4565760000 0.0000660000
CARBON 6.0 -1.1513790000 -1.3700020000 0.0000020000
HYDROGEN 1.0 -1.1388330000 -2.4566140000 -0.0000030000
CARBON 6.0 -2.3757670000 0.6997160000 -0.0000260000
HYDROGEN 1.0 -3.3088070000 1.2634670000 -0.0000310000
CARBON 6.0 -2.3757270000 -0.6998220000 -0.0000100000
HYDROGEN 1.0 -3.3087310000 -1.2636250000 -0.0000500000
$END

Structure ligand	Cl_2_bdt
E_{HF} / Hartree	-1946.7751014
E_{HOMO} / Hartree	0.137
E_{LUMO} / Hartree	0.197

Cartesian Coordinates

C6H2S2Cl2

C1

SULFUR 16.0 -1.6744910000 1.9874590000 0.0003050000

SULFUR 16.0 1.6742380000 1.9875930000 -0.0002920000

CARBON 6.0 0.7439540000 0.5141110000 -0.0001280000

CARBON 6.0 -0.7439710000 0.5140100000 0.0001260000

CARBON 6.0 1.3570390000 -0.7571330000 -0.0000780000

CARBON 6.0 -1.3569230000 -0.7571930000 -0.0000340000

CARBON 6.0 0.6941230000 -1.9852470000 -0.0000030000

CARBON 6.0 -0.6939190000 -1.9853410000 0.0000740000

HYDROGEN 1.0 -1.2542470000 -2.9127380000 -0.0001020000

CHLORINE 17.0 -3.1569490000 -0.9128660000 -0.0001630000

CHLORINE 17.0 3.1570630000 -0.9127060000 0.0001630000

HYDROGEN 1.0 1.2545390000 -2.9126230000 0.0001320000

$END

Structure Ligand	_edt
E_{HF} / Hartree	-873.8012831
E_{HOMO} / Hartree	0.163
E_{LUMO} / Hartree	0.247

Cartesian Coordinates

C2H2S2

C1

SULFUR 16.0 -1.9237940000 -0.4315890000 0.0000240000

SULFUR 16.0 1.9237140000 -0.4316540000 -0.0000020000

CARBON 6.0 0.6829950000 0.8420530000 -0.0000380000

CARBON 6.0 -0.6828620000 0.8420380000 -0.0000940000

HYDROGEN 1.0 1.1086310000 1.8536060000 0.0004850000

HYDROGEN 1.0 -1.1081500000 1.8537400000 -0.0000450000

$END

Structure ligand	_mdt
E_{HF} / Hartree	-952.4487945
E_{HOMO} / Hartree	0.169
E_{LUMO} / Hartree	0.207

Cartesian Coordinates

C4H6S2

C1

SULFUR 16.0 -1.7987940000 -1.1028300000 0.0086590000

SULFUR 16.0 1.7988120000 -1.1028160000 -0.0086310000

CARBON 6.0 0.6861680000 0.2905030000 0.0045580000

CARBON 6.0 -0.6861730000 0.2904810000 -0.0047150000

CARBON 6.0 1.3974010000 1.6481410000 0.0182940000

HYDROGEN 1.0 1.2547480000 2.2108290000 -0.9234100000

HYDROGEN 1.0 1.0444030000 2.3101520000 0.8288830000

HYDROGEN 1.0 2.4684100000 1.4924770000 0.1497390000

CARBON 6.0 -1.3974360000 1.6481260000 -0.0182640000

HYDROGEN 1.0 -1.2553020000 2.2103760000 0.9237910000

HYDROGEN 1.0 -1.0439630000 2.3105300000 -0.8283170000

HYDROGEN 1.0 -2.4683560000 1.4924700000 -0.1503710000

$END

Structure ligand	_tfd
E_{HF} / Hartree	-1548.1417725
E_{HOMO} / Hartree	0.146
E_{LUMO} / Hartree	0.225

Cartesian Coordinates

C4S2F6

C1

SULFUR 16.0 -1.6922420000 2.0234200000 -0.1721110000

SULFUR 16.0 1.6923770000 2.0232960000 0.1721050000

CARBON 6.0 0.6974350000 0.5812950000 0.0169710000

CARBON 6.0 -0.6974370000 0.5813020000 -0.0168430000

CARBON 6.0 1.5068860000 -0.6882950000 -0.0672960000

CARBON 6.0 -1.5069170000 -0.6882790000 0.0673440000

FLUORINE 9.0 -2.7443060000 -0.5367930000 0.6241740000

FLUORINE 9.0 -1.7718400000 -1.2941610000 -1.1547810000

FLUORINE 9.0 -0.9514220000 -1.6946930000 0.8315150000

FLUORINE 9.0 0.9510380000 -1.6949340000 -0.8310490000

FLUORINE 9.0 1.7722770000 -1.2939740000 1.1547850000

FLUORINE 9.0 2.7440330000 -0.5369550000 -0.6247500000

$END

Structure ligand	_mnt
E_{HF} / Hartree	-1058.4186354
E_{HOMO} / Hartree	0.121
E_{LUMO} / Hartree	0.212

Cartesian Coordinates

C4N2S2

C1

SULFUR 16.0 -1.7804170000 -1.4187250000 0.0000310000

SULFUR 16.0 1.7793310000 -1.4198360000 -0.0000780000

CARBON 6.0 0.7001590000 -0.0379120000 0.0000470000

CARBON 6.0 -0.7002890000 -0.0375970000 0.0000660000

CARBON 6.0 1.3725840000 1.2225590000 0.0000580000

CARBON 6.0 -1.3719660000 1.2233180000 0.0001370000

NITROGEN 7.0 1.9652940000 2.2273910000 0.0000610000

NITROGEN 7.0 -1.9632310000 2.2290050000 -0.0002180000

$END

Structure	_H_2O
E_{HF} / Hartree	-76.458425
E_{HOMO} / Hartree	-0.323
E_{LUMO} / Hartree	0.023

Cartesian Coordinates

H2O

Cs

OXYGEN 8.0 0.0000000000 0.1169140000 0.0000000000

HYDROGEN 1.0 0.7638620000 -0.4676570000 0.0000000000

HYDROGEN 1.0 -0.7638620000 -0.4676570000 0.0000000000

$END

Structure aquacomplexe	$Mg(H_2O)_6$
E_{HF} / Hartree	-658.5082646
E_{HOMO} / Hartree	-0.668
E_{LUMO} / Hartree	-0.322

Cartesian Coordinates

MgH12O6

C1

MAGNESIUM 12.0 0.0000480000 0.0000940000 -0.0000520000

OXYGEN 8.0 -1.4124420000 -0.1833330000 -1.5598020000

OXYGEN 8.0 0.2196300000 2.0548690000 -0.4385680000

OXYGEN 8.0 -1.5602470000 0.4547250000 1.3504230000

OXYGEN 8.0 1.4124490000 0.1839630000 1.5597370000

OXYGEN 8.0 -0.2196430000 -2.0547750000 0.4385940000

OXYGEN 8.0 1.5602040000 -0.4554120000 -1.3503610000

HYDROGEN 1.0 -2.3699820000 -0.0688210000 -1.4861880000

HYDROGEN 1.0 -1.2303960000 -0.3955350000 -2.4857000000

HYDROGEN 1.0 -0.2373250000 2.5506990000 -1.1319150000

HYDROGEN 1.0 0.7948170000 2.6845830000 0.0175470000

HYDROGEN 1.0 -2.0626990000 -0.1743610000 1.8863840000

HYDROGEN 1.0 -1.9074440000 1.3331610000 1.5582140000

HYDROGEN 1.0 1.2307280000 0.4007890000 2.4846290000

HYDROGEN 1.0 2.3694550000 0.0642680000 1.4874020000

HYDROGEN 1.0 -0.7981050000 -2.6835180000 -0.0147160000

HYDROGEN 1.0 0.2406860000 -2.5516560000 1.1289540000

HYDROGEN 1.0 1.9018410000 -1.3348080000 -1.5632440000

HYDROGEN 1.0 2.0682210000 0.1737820000 -1.8809190000

$END

Structure aquacomplexe	$Ca(H_2O)_6$
E_{HF} / Hartree	-1136.0583615
E_{HOMO} / Hartree	-0.671
E_{LUMO} / Hartree	-0.320

Cartesian Coordinates

CaH12O6

C1

CALCIUM 20.0 -0.0000600000 -0.0000500000 0.0000670000

OXYGEN 8.0 -1.7889790000 -0.1679970000 -1.5986860000

OXYGEN 8.0 0.9818760000 1.7815920000 -1.2818340000

OXYGEN 8.0 -1.2760750000 1.6064530000 1.2546360000
OXYGEN 8.0 1.7886320000 0.1679060000 1.5989620000
OXYGEN 8.0 -0.9817080000 -1.7820560000 1.2817390000
OXYGEN 8.0 1.2763660000 -1.6058420000 -1.2549400000
HYDROGEN 1.0 -2.6333600000 0.3039670000 -1.5846250000
HYDROGEN 1.0 -1.8174550000 -0.7208320000 -2.3921160000
HYDROGEN 1.0 0.6509270000 2.1619130000 -2.1074860000
HYDROGEN 1.0 1.7925100000 2.2699420000 -1.0811940000
HYDROGEN 1.0 -1.8979530000 1.4287000000 1.9740820000
HYDROGEN 1.0 -1.2761040000 2.5679580000 1.1475810000
HYDROGEN 1.0 1.8182700000 0.7230590000 2.3907260000
HYDROGEN 1.0 2.6316930000 -0.3064600000 1.5867190000
HYDROGEN 1.0 -1.7935250000 -2.2689660000 1.0823420000
HYDROGEN 1.0 -0.6496150000 -2.1638590000 2.1062560000
HYDROGEN 1.0 1.2710960000 -2.5679250000 -1.1533950000
HYDROGEN 1.0 1.9038160000 -1.4269580000 -1.9692400000
$END