

Supplementary information

Functional investigation

In order to select the most accurate functional for structure optimization and electronic properties calculation, we referred to the Koopmans approach⁴⁶. This approach is based on the comparison of the computed electronic affinity and ionization potential to the HOMO and LUMO, analogs of IP and EA respectively according to equations 13 and 14⁴⁷:

$$\varepsilon_{LUMO} = -EA \quad (1)$$

$$\varepsilon_{HOMO} = -IP \quad (2)$$

$$\Delta = |IP + E_{HOMO}| + |EA + E_{LUMO}| \quad (3)$$

The functional which has the minimal Δ value (eq 15) is deemed the most appropriate for this type of calculations.

Table S1 Comparison of structural parameters calculated with different fonctionnal with DEF2-TZVP bases-set. Bond length in Angström and dihedral angle in degree.

Ru(S ₂ TTP) Cl ₂						
Bond	B3LYP	M05	M05-2x	CAMB3LYP	WB97XD	experimental value
Ru1—N1	2.088	2.092	2.092	2.080	2.077	2.082
Ru1—S1	2.254	2.250	2.258	2.246	2.250	2.251
Ru1—C11	2.458	2.449	2.454	2.438	2.439	2.399
S1—C4	1.746	1.733	1.734	1.731	1.731	1.750
S1—C1	1.746	1.733	1.734	1.731	1.731	1.755
N1—C6	1.385	1.378	1.368	1.375	1.375	1.393
Dihedral angle	12.374	11.951	12.206	12.143	12.123	12.700

Table S2 Comparison of structural parameters calculated at with B3LYP functional and different bases set bases-set / Bond length in Angström and dihedral angle in degree.

Bond	6-311LANL2DZ	6-311LANL2TZ	DEF2TZP	experimental
Ru1—N1	2,108	2,109	2,088	2.082
Ru1—S1	2,293	2,293	2,251	2.251
Ru1—C11	2,510	2,494	2,460	2.399
S1—C4	1,766	1,766	1,750	1.750
S1—C1	1.766	1,766	1,750	1.755
N1—C6	1,385	1,386	1,385	1.393
Dihedral angle	12.492	12.046	12.374	12.700

Table S3 calculation of Electronic properties : Ionisation Potential (IP), Electronic Affinity (EA), HOMO energy, LUMO energy, Koopmans condition: $\Delta = |IP + E_{HOMO}| + |EA + E_{LUMO}|$

Functional	IP(ev)	EA(ev)	E_{HOMO}	E_{LUMO}	IP+ E_{HOMO}	EA+ E_{LUMO}	Δ
B3LYP	4,98	3,74	-5,27	-3,70	-0,29	0,04	0,33
CAM-B3LYP	6,04	3,82	-6,65	-2,92	-0,61	0,90	1,51
M05	4,92	3,75	-5,38	-3,52	-0,46	0,23	0,68
M052X	5,99	4,00	-6,75	-3,26	-0,76	0,74	1,51
WB97XD	5,77	3,82	-7,19	-2,42	-1,42	1,40	2,82

The B3LYP functional showed the lowest Δ value. Consequently, all geometry optimizations and electronic property calculations were performed at B3LYP level.

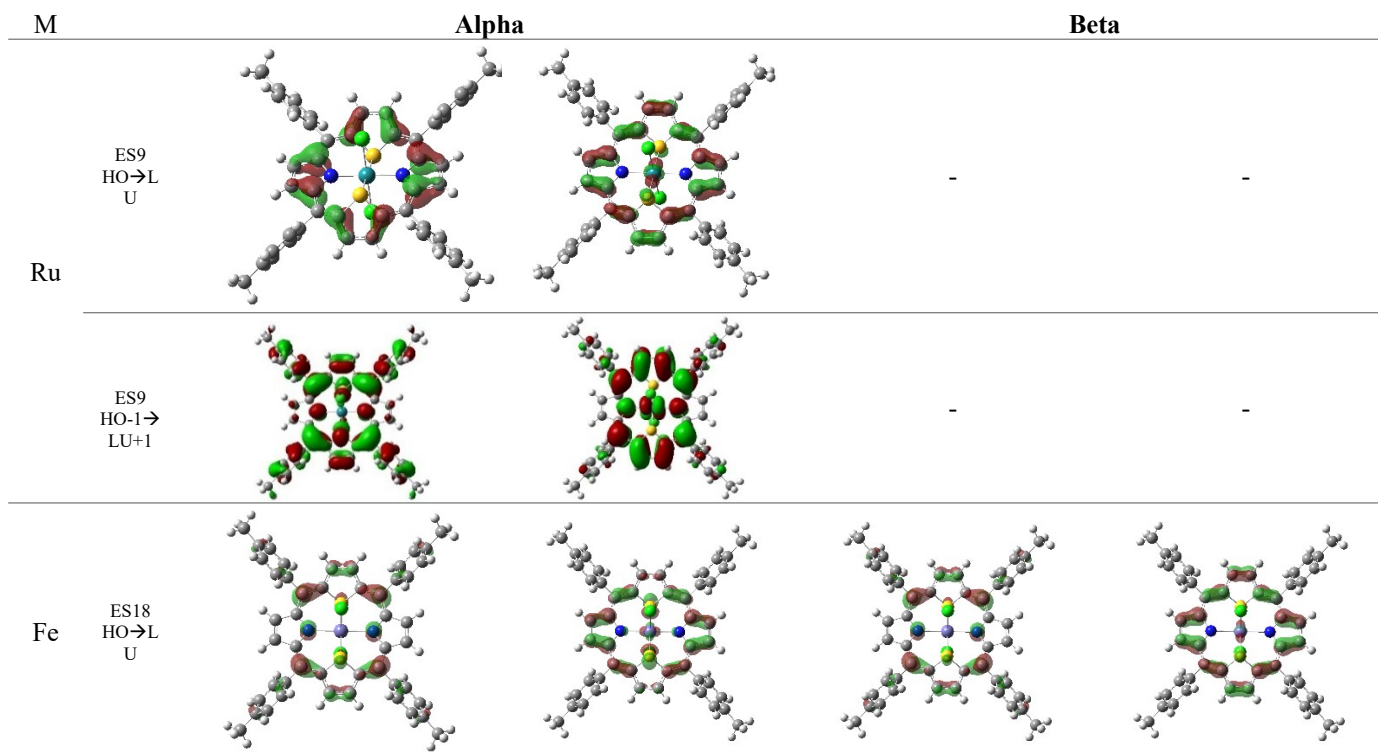
Table S4 Comparison of structural parameters calculated with different bases set with B3LYP functional. Bond length in Angström, RMSD Calculation

Bond	Bases set			
	exp	Def2tzvp	6-311LANL2DZ	6-311LANL2TZ
C7-C8	1,332	1,345	1,350	1,350
C2-C3	1,371	1,395	1,398	1,398
N1-C9	1,384	1,385	1,385	1,386
C1-C2	1,388	1,400	1,402	1,402
C3-C4	1,391	1,400	1,402	1,402
N1-C6	1,393	1,385	1,385	1,386
C9-C10	1,405	1,410	1,420	1,420
C1-C10i	1,410	1,410	1,409	1,411
C5-C6	1,410	1,420	1,419	1,419
C4-C5	1,418	1,410	1,409	1,411
C6-C7	1,442	1,451	1,454	1,454
C8-C9	1,456	1,451	1,454	1,454
C5-C11	1,493	1,490	1,491	1,491
S1-C4	1,749	1,750	1,766	1,766
S1-C1	1,754	1,750	1,766	1,766
Ru-N	2,083	2,088	2,108	2,109
Ru-S	2,251	2,250	2,293	2,293
Ru-Cl	2,399	2,460	2,510	2,494
r²	-	0,999	0,999	0,999
RMSD	-	0,028	0,069	0,067

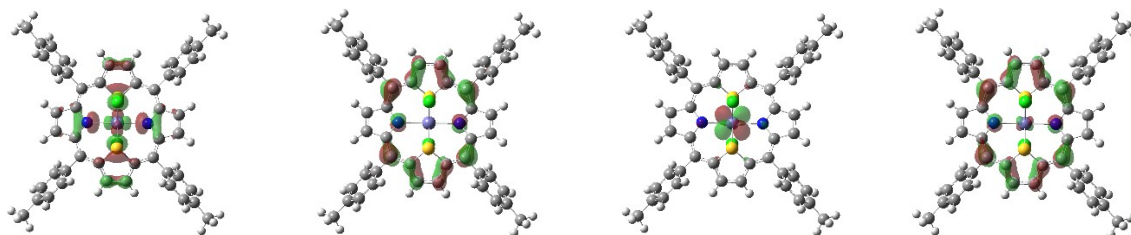
Table S5 Calculated angles for $M(S_2TTP)Cl_2$ Bond angles and dihedral angle in degrees ($^\circ$)

Bond angles	Ru exp	Ru sim	Mn	Fe II Q	Ni T	Cu D
N(1)-Mt-N (2)	180	180	180	180	180	180
S(1)-Mt- S(2)	180	180	180	180	180	180
N(1)-Mt- Cl(1)	88.49 (9)	90.003	90.035	90.000	90.000	89.996
N(1)-Mt- S(1A)	89.78 (9)	89.998	89.989	90.000	90.000	89.999
C(4) - S(1)-C(1)	91.8 (2)	93.431	93.339	93.247	93.120	92.778
C(1)-S(1)-Mt	108.21 (14)	108.927	102.276	104.400	106.610	104.714
C(9)-N(1)-Mt	127.3 (3)	126.483	126.083	126.234	126.415	126.396
S(1)-Mt-Cl(1)	89.25 (4)	92.332	94.280	93.753	93.449	94.031
N(1)-Mt-S(1)	90.22 (9)	90.002	90.011	90.000	90.000	89.998
C(4)-S(1)-Mt	108.07 (14)	108.927	102.276	104.400	106.610	104.715
C(9)-N(1)-C(6)	106.6 (3)	107.038	107.885	107.533	107.170	107.211
C(6)-N(1)-Mt	125.9 (3)	126.479	126.032	126.234	126.415	126.393
Dihedral angle	12.700	12.374	12.600	11.32	11.907	11.766

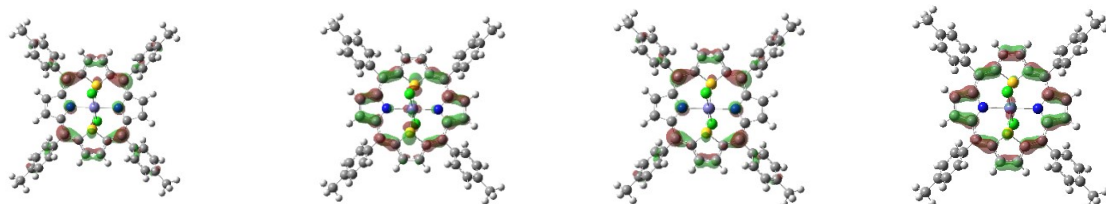
Scheme 1 Natural transition orbital analyses of the representative excited states HOMO, LUMO, HOMO-1 and LUMO+1 corresponding to transition with highest oscillator strength for $M(S_2TTP) Cl_2$ Isovalue: 0.04 u.a.(Green: Positive value/Red: Negative value).



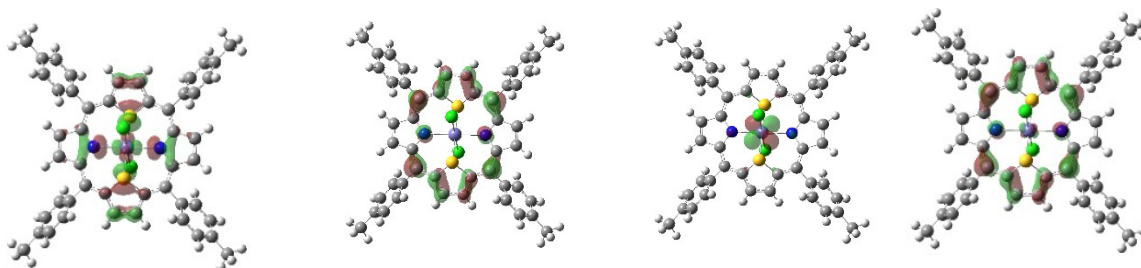
ES18
HO-
1→LU+
1



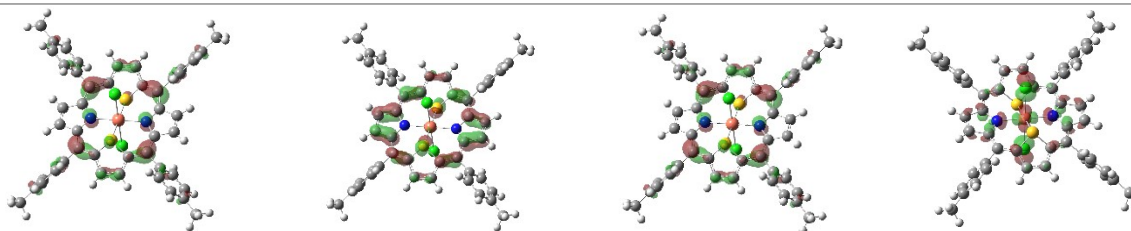
ES22
HO→L
U



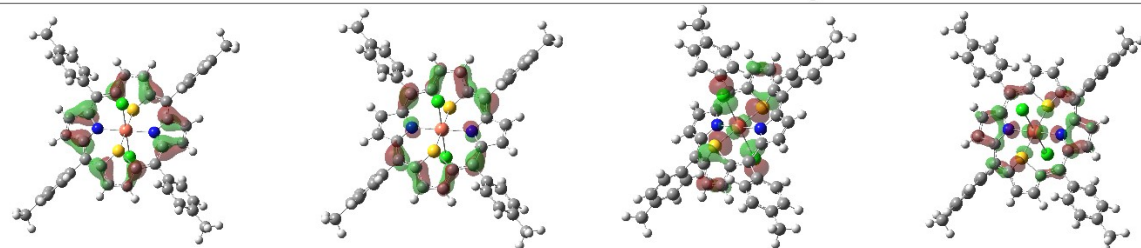
ES22
HO-
1→LU+
1



ES24
HO→L
U

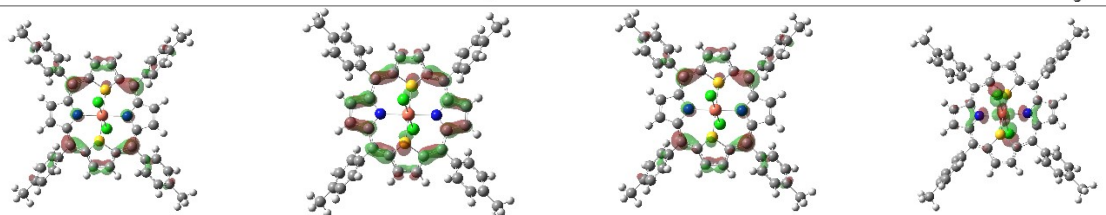


ES24H
O-1→
LU+1

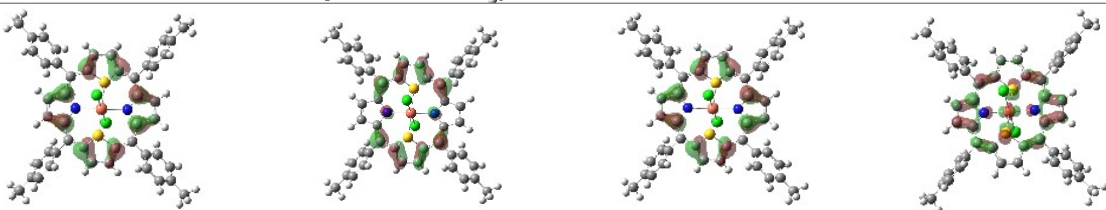


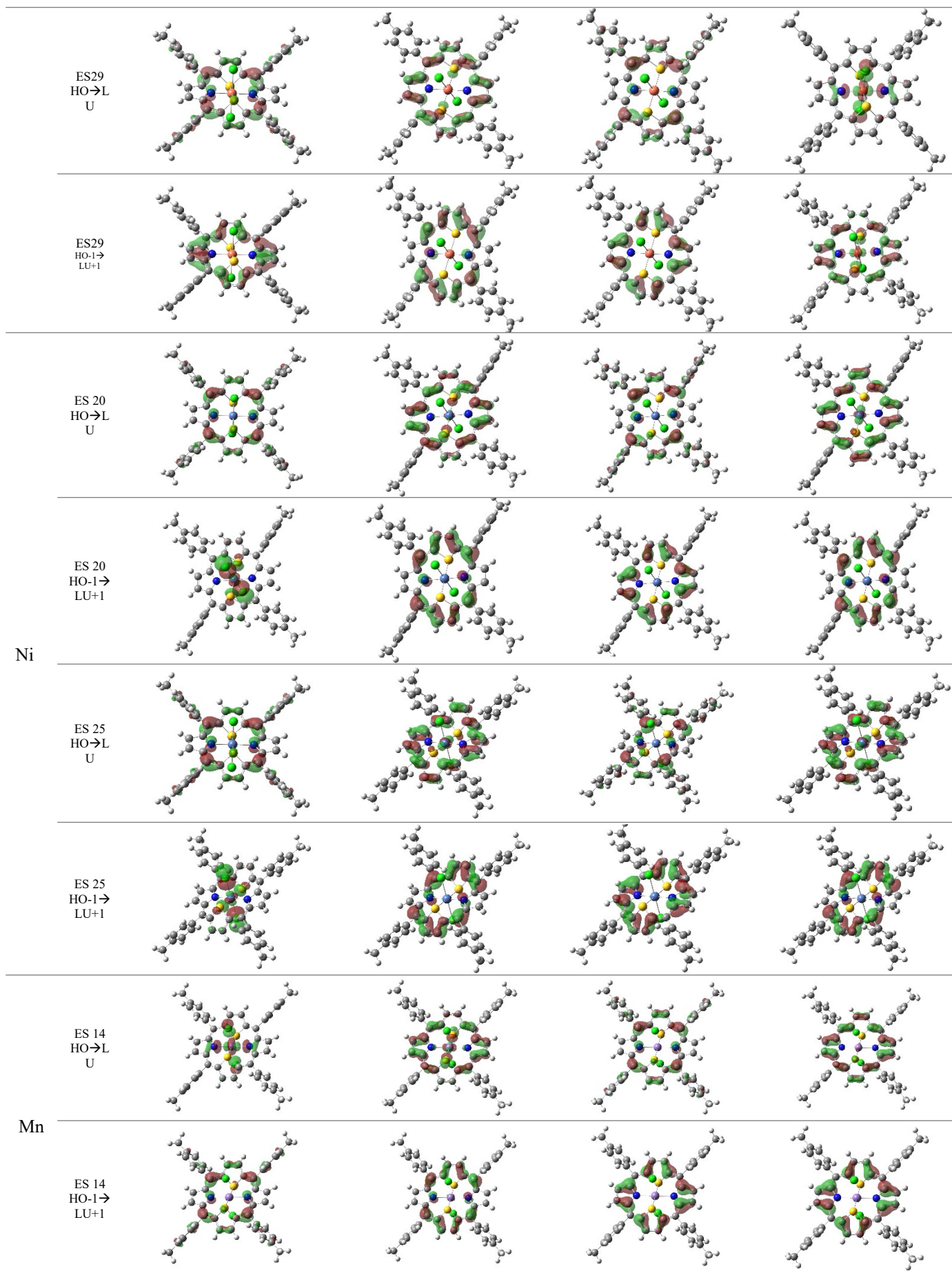
Cu

ES27
HO→L
U

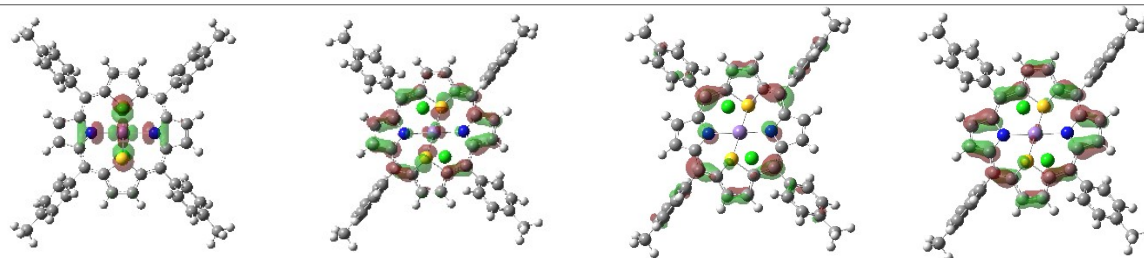


ES27
HO-1→
LU+1

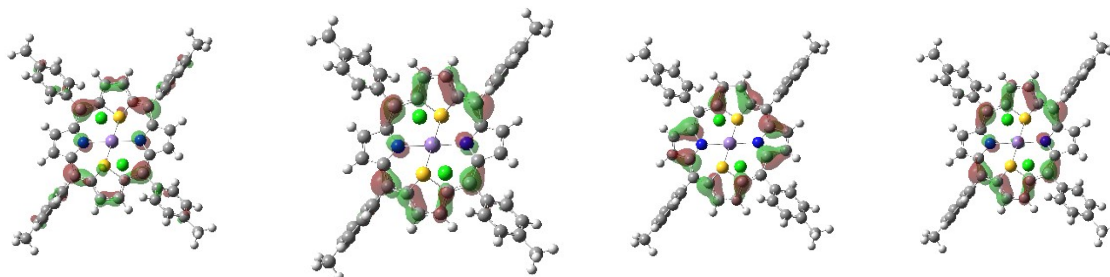




ES 20
HO→L
U



ES 20
HO-1→
LU+1



Cartesian Coordinates of Optimized structures (Å)

Optimized structure of Ru-Dithiaporphyrin Complex

6	0.327653000	2.462539000	2.566879000
6	0.167752000	1.099922000	2.913982000
6	0.561182000	2.946451000	1.265696000
7	0.000000000	0.000000000	2.088464000
6	0.099328000	0.665476000	4.297071000
16	1.184534000	1.918166000	0.000000000
6	0.241321000	4.185651000	0.697409000
44	0.000000000	0.000000000	0.000000000
6	-0.167752000	-1.099922000	2.913982000
6	-0.099328000	-0.665476000	4.297071000
1	0.207498000	1.308927000	5.152247000
6	0.561182000	2.946451000	-1.265696000
1	-0.101911000	5.025296000	1.283583000
6	0.241321000	4.185651000	-0.697409000

7	0.000000000	0.000000000	-2.088464000
16	-1.184534000	-1.918166000	0.000000000
17	2.147662000	-1.196399000	0.000000000
6	-0.327653000	-2.462539000	2.566879000
6	-0.167752000	-1.099922000	-2.913982000
6	-0.561182000	-2.946451000	1.265696000
17	-2.147662000	1.196399000	0.000000000
6	0.167752000	1.099922000	-2.913982000
6	0.099328000	0.665476000	-4.297071000
6	0.327653000	2.462539000	-2.566879000
1	0.207498000	1.308927000	-5.152247000
6	-0.099328000	-0.665476000	-4.297071000
6	-0.327653000	-2.462539000	-2.566879000
6	-0.241321000	-4.185651000	0.697409000
6	-0.241321000	-4.185651000	-0.697409000
1	0.101911000	-5.025296000	1.283583000
6	-0.561182000	-2.946451000	-1.265696000
1	0.101911000	-5.025296000	-1.283583000
1	-0.207498000	-1.308927000	-5.152247000
1	-0.207498000	-1.308927000	5.152247000
1	-0.101911000	5.025296000	-1.283583000
6	-0.142755000	-3.495239000	-3.623480000
6	-1.143771000	-4.438218000	-3.876892000
6	1.042315000	-3.577892000	-4.362543000
6	-0.971687000	-5.415296000	-4.848170000
1	-2.072617000	-4.392816000	-3.322281000
6	1.212948000	-4.564707000	-5.323019000
1	1.840802000	-2.872412000	-4.172105000
6	0.210234000	-5.500983000	-5.586623000
1	-1.771830000	-6.121286000	-5.036979000

1	2.143889000	-4.609626000	-5.875982000
6	-0.142755000	-3.495239000	3.623480000
6	-1.143771000	-4.438218000	3.876892000
6	1.042315000	-3.577892000	4.362543000
6	-0.971687000	-5.415296000	4.848170000
1	-2.072617000	-4.392816000	3.322281000
6	1.212948000	-4.564707000	5.323019000
1	1.840802000	-2.872412000	4.172105000
6	0.210234000	-5.500983000	5.586623000
1	-1.771830000	-6.121286000	5.036979000
1	2.143889000	-4.609626000	5.875982000
6	0.142755000	3.495239000	3.623480000
6	1.143771000	4.438218000	3.876892000
6	-1.042315000	3.577892000	4.362543000
6	0.971687000	5.415296000	4.848170000
1	2.072617000	4.392816000	3.322281000
6	-1.212948000	4.564707000	5.323019000
1	-1.840802000	2.872412000	4.172105000
6	-0.210234000	5.500983000	5.586623000
1	1.771830000	6.121286000	5.036979000
1	-2.143889000	4.609626000	5.875982000
6	0.142755000	3.495239000	-3.623480000
6	1.143771000	4.438218000	-3.876892000
6	-1.042315000	3.577892000	-4.362543000
6	0.971687000	5.415296000	-4.848170000
1	2.072617000	4.392816000	-3.322281000
6	-1.212948000	4.564707000	-5.323019000
1	-1.840802000	2.872412000	-4.172105000
6	-0.210234000	5.500983000	-5.586623000
1	1.771830000	6.121286000	-5.036979000

1	-2.143889000	4.609626000	-5.875982000
6	0.410502000	-6.583608000	-6.612507000
1	0.909058000	-7.450559000	-6.169155000
1	-0.541255000	-6.926958000	-7.018827000
1	1.034226000	-6.238318000	-7.437950000
6	0.410502000	-6.583608000	6.612507000
1	-0.541255000	-6.926958000	7.018827000
1	0.909058000	-7.450559000	6.169155000
1	1.034226000	-6.238318000	7.437950000
6	-0.410502000	6.583608000	6.612507000
1	0.541255000	6.926958000	7.018827000
1	-0.909058000	7.450559000	6.169155000
1	-1.034226000	6.238318000	7.437950000
6	-0.410502000	6.583608000	-6.612507000
1	-0.909058000	7.450559000	-6.169155000
1	0.541255000	6.926958000	-7.018827000
1	-1.034226000	6.238318000	-7.437950000

Optimized structure of Fe-Dithiaporphyrin Complex

6	0.338933000	2.455757000	2.552742000
6	0.163222000	1.089962000	2.894968000
6	0.593255000	2.918932000	1.258833000
7	0.000000000	0.000000000	2.066185000
6	0.095279000	0.666868000	4.278049000
16	1.166727000	1.857853000	0.000000000
6	0.322694000	4.177238000	0.692827000
6	-0.163222000	-1.089962000	2.894968000
6	-0.095279000	-0.666868000	4.278049000
1	0.202443000	1.313637000	5.130766000
6	0.593255000	2.918932000	-1.258833000

1	0.020145000	5.027931000	1.284654000
6	0.322694000	4.177238000	-0.692827000
7	0.000000000	0.000000000	-2.066185000
16	-1.166727000	-1.857853000	0.000000000
17	2.093215000	-1.190896000	0.000000000
6	-0.338933000	-2.455757000	2.552742000
6	-0.163222000	-1.089962000	-2.894968000
6	-0.593255000	-2.918932000	1.258833000
17	-2.093215000	1.190896000	0.000000000
6	0.163222000	1.089962000	-2.894968000
6	0.095279000	0.666868000	-4.278049000
6	0.338933000	2.455757000	-2.552742000
1	0.202443000	1.313637000	-5.130766000
6	-0.095279000	-0.666868000	-4.278049000
6	-0.338933000	-2.455757000	-2.552742000
6	-0.322694000	-4.177238000	0.692827000
6	-0.322694000	-4.177238000	-0.692827000
1	-0.020145000	-5.027931000	1.284654000
6	-0.593255000	-2.918932000	-1.258833000
1	-0.020145000	-5.027931000	-1.284654000
1	-0.202443000	-1.313637000	-5.130766000
1	-0.202443000	-1.313637000	5.130766000
1	0.020145000	5.027931000	-1.284654000
6	-0.145397000	-3.489923000	-3.604707000
6	-1.149496000	-4.424670000	-3.875490000
6	1.051247000	-3.579842000	-4.324121000
6	-0.968031000	-5.402497000	-4.844275000
1	-2.087784000	-4.371475000	-3.337746000
6	1.230668000	-4.567571000	-5.281854000
1	1.851310000	-2.880042000	-4.119943000

6	0.225666000	-5.496509000	-5.562497000
1	-1.770190000	-6.102136000	-5.047419000
1	2.170133000	-4.618784000	-5.819572000
6	-0.145397000	-3.489923000	3.604707000
6	-1.149496000	-4.424670000	3.875490000
6	1.051247000	-3.579842000	4.324121000
6	-0.968031000	-5.402497000	4.844275000
1	-2.087784000	-4.371475000	3.337746000
6	1.230668000	-4.567571000	5.281854000
1	1.851310000	-2.880042000	4.119943000
6	0.225666000	-5.496509000	5.562497000
1	-1.770190000	-6.102136000	5.047419000
1	2.170133000	-4.618784000	5.819572000
6	0.145397000	3.489923000	3.604707000
6	1.149496000	4.424670000	3.875490000
6	-1.051247000	3.579842000	4.324121000
6	0.968031000	5.402497000	4.844275000
1	2.087784000	4.371475000	3.337746000
6	-1.230668000	4.567571000	5.281854000
1	-1.851310000	2.880042000	4.119943000
6	-0.225666000	5.496509000	5.562497000
1	1.770190000	6.102136000	5.047419000
1	-2.170133000	4.618784000	5.819572000
6	0.145397000	3.489923000	-3.604707000
6	1.149496000	4.424670000	-3.875490000
6	-1.051247000	3.579842000	-4.324121000
6	0.968031000	5.402497000	-4.844275000
1	2.087784000	4.371475000	-3.337746000
6	-1.230668000	4.567571000	-5.281854000
1	-1.851310000	2.880042000	-4.119943000

6	-0.225666000	5.496509000	-5.562497000
1	1.770190000	6.102136000	-5.047419000
1	-2.170133000	4.618784000	-5.819572000
6	0.435225000	-6.579907000	-6.585608000
1	0.920420000	-7.450381000	-6.134417000
1	-0.512051000	-6.916494000	-7.007693000
1	1.074924000	-6.238564000	-7.400378000
6	0.435225000	-6.579907000	6.585608000
1	-0.512051000	-6.916494000	7.007693000
1	0.920420000	-7.450381000	6.134417000
1	1.074924000	-6.238564000	7.400378000
6	-0.435225000	6.579907000	6.585608000
1	0.512051000	6.916494000	7.007693000
1	-0.920420000	7.450381000	6.134417000
1	-1.074924000	6.238564000	7.400378000
6	-0.435225000	6.579907000	-6.585608000
1	-0.920420000	7.450381000	-6.134417000
1	0.512051000	6.916494000	-7.007693000
1	-1.074924000	6.238564000	-7.400378000
26	0.000000000	0.000000000	0.000000000

Optimized structure of Ni-Dithiaporphyrin Complex

6	0.364902000	2.450890000	2.563379000
6	0.180386000	1.087832000	2.929816000
6	0.611783000	2.911243000	1.263406000
7	0.000000000	0.000000000	2.113677000
6	0.105275000	0.667320000	4.312902000
16	1.264686000	1.898715000	0.000000000
6	0.242209000	4.146488000	0.690250000
6	-0.180386000	-1.087832000	2.929816000

6	-0.105275000	-0.667320000	4.312902000
1	0.226168000	1.309511000	5.167557000
6	0.611783000	2.911243000	-1.263406000
1	-0.141859000	4.963374000	1.281990000
6	0.242209000	4.146488000	-0.690250000
7	0.000000000	0.000000000	-2.113677000
16	-1.264686000	-1.898715000	0.000000000
17	2.168884000	-1.251583000	0.000000000
6	-0.364902000	-2.450890000	2.563379000
6	-0.180386000	-1.087832000	-2.929816000
6	-0.611783000	-2.911243000	1.263406000
17	-2.168884000	1.251583000	0.000000000
6	0.180386000	1.087832000	-2.929816000
6	0.105275000	0.667320000	-4.312902000
6	0.364902000	2.450890000	-2.563379000
1	0.226168000	1.309511000	-5.167557000
6	-0.105275000	-0.667320000	-4.312902000
6	-0.364902000	-2.450890000	-2.563379000
6	-0.242209000	-4.146488000	0.690250000
6	-0.242209000	-4.146488000	-0.690250000
1	0.141859000	-4.963374000	1.281990000
6	-0.611783000	-2.911243000	-1.263406000
1	0.141859000	-4.963374000	-1.281990000
1	-0.226168000	-1.309511000	-5.167557000
1	-0.226168000	-1.309511000	5.167557000
1	-0.141859000	4.963374000	-1.281990000
6	-0.161298000	-3.496309000	-3.600781000
6	-1.147857000	-4.459304000	-3.838229000
6	1.024162000	-3.570040000	-4.341164000
6	-0.961673000	-5.447052000	-4.795394000

1	-2.076900000	-4.419269000	-3.283712000
6	1.209025000	-4.568532000	-5.286295000
1	1.812417000	-2.850711000	-4.161188000
6	0.220700000	-5.524415000	-5.534308000
1	-1.750830000	-6.168018000	-4.973114000
1	2.139936000	-4.607450000	-5.839623000
6	-0.161298000	-3.496309000	3.600781000
6	-1.147857000	-4.459304000	3.838229000
6	1.024162000	-3.570040000	4.341164000
6	-0.961673000	-5.447052000	4.795394000
1	-2.076900000	-4.419269000	3.283712000
6	1.209025000	-4.568532000	5.286295000
1	1.812417000	-2.850711000	4.161188000
6	0.220700000	-5.524415000	5.534308000
1	-1.750830000	-6.168018000	4.973114000
1	2.139936000	-4.607450000	5.839623000
6	0.161298000	3.496309000	3.600781000
6	1.147857000	4.459304000	3.838229000
6	-1.024162000	3.570040000	4.341164000
6	0.961673000	5.447052000	4.795394000
1	2.076900000	4.419269000	3.283712000
6	-1.209025000	4.568532000	5.286295000
1	-1.812417000	2.850711000	4.161188000
6	-0.220700000	5.524415000	5.534308000
1	1.750830000	6.168018000	4.973114000
1	-2.139936000	4.607450000	5.839623000
6	0.161298000	3.496309000	-3.600781000
6	1.147857000	4.459304000	-3.838229000
6	-1.024162000	3.570040000	-4.341164000
6	0.961673000	5.447052000	-4.795394000

1	2.076900000	4.419269000	-3.283712000
6	-1.209025000	4.568532000	-5.286295000
1	-1.812417000	2.850711000	-4.161188000
6	-0.220700000	5.524415000	-5.534308000
1	1.750830000	6.168018000	-4.973114000
1	-2.139936000	4.607450000	-5.839623000
6	0.436700000	-6.618319000	-6.544553000
1	0.949348000	-7.470473000	-6.088749000
1	-0.509971000	-6.982622000	-6.944329000
1	1.054233000	-6.275438000	-7.375580000
6	0.436700000	-6.618319000	6.544553000
1	-0.509971000	-6.982622000	6.944329000
1	0.949348000	-7.470473000	6.088749000
1	1.054233000	-6.275438000	7.375580000
6	-0.436700000	6.618319000	6.544553000
1	0.509971000	6.982622000	6.944329000
1	-0.949348000	7.470473000	6.088749000
1	-1.054233000	6.275438000	7.375580000
6	-0.436700000	6.618319000	-6.544553000
1	-0.949348000	7.470473000	-6.088749000
1	0.509971000	6.982622000	-6.944329000
1	-1.054233000	6.275438000	-7.375580000
28	0.000000000	0.000000000	0.000000000

Optimized structure of Cu-Dithiaporphyrin Complex

6	0.408540000	2.457676000	2.538572000
6	0.204770000	1.088907000	2.880706000
6	0.684473000	2.943968000	1.254627000
7	0.000000000	0.000000000	2.062832000
6	0.119183000	0.665361000	4.257702000

16	1.375398000	1.959747000	0.000000000
6	0.259682000	4.170948000	0.687404000
6	-0.204770000	-1.088907000	2.880706000
6	-0.119183000	-0.665361000	4.257702000
1	0.253563000	1.304039000	5.112713000
6	0.684473000	2.943968000	-1.254627000
1	-0.172633000	4.960159000	1.283169000
6	0.259682000	4.170948000	-0.687404000
7	0.000000000	0.000000000	-2.062832000
16	-1.375398000	-1.959747000	0.000000000
17	2.155790000	-1.290822000	0.000000000
6	-0.408540000	-2.457676000	2.538572000
6	-0.204770000	-1.088907000	-2.880706000
6	-0.684473000	-2.943968000	1.254627000
17	-2.155790000	1.290822000	0.000000000
6	0.204770000	1.088907000	-2.880706000
6	0.119183000	0.665361000	-4.257702000
6	0.408540000	2.457676000	-2.538572000
1	0.253563000	1.304039000	-5.112713000
6	-0.119183000	-0.665361000	-4.257702000
6	-0.408540000	-2.457676000	-2.538572000
6	-0.259682000	-4.170948000	0.687404000
6	-0.259682000	-4.170948000	-0.687404000
1	0.172633000	-4.960159000	1.283169000
6	-0.684473000	-2.943968000	-1.254627000
1	0.172633000	-4.960159000	-1.283169000
1	-0.253563000	-1.304039000	-5.112713000

1	-0.253563000	-1.304039000	5.112713000
1	-0.172633000	4.960159000	-1.283169000
6	-0.178961000	-3.486307000	-3.587146000
6	-1.153936000	-4.454609000	-3.850361000
6	1.019700000	-3.544917000	-4.307807000
6	-0.944597000	-5.431540000	-4.813747000
1	-2.092076000	-4.426685000	-3.310633000
6	1.227886000	-4.532898000	-5.258884000
1	1.799929000	-2.822396000	-4.107080000
6	0.250698000	-5.493229000	-5.533104000
1	-1.725250000	-6.156465000	-5.011720000
1	2.168583000	-4.560409000	-5.796119000
6	-0.178961000	-3.486307000	3.587146000
6	-1.153936000	-4.454609000	3.850361000
6	1.019700000	-3.544917000	4.307807000
6	-0.944597000	-5.431540000	4.813747000
1	-2.092076000	-4.426685000	3.310633000
6	1.227886000	-4.532898000	5.258884000
1	1.799929000	-2.822396000	4.107080000
6	0.250698000	-5.493229000	5.533104000
1	-1.725250000	-6.156465000	5.011720000
1	2.168583000	-4.560409000	5.796119000
6	0.178961000	3.486307000	3.587146000
6	1.153936000	4.454609000	3.850361000
6	-1.019700000	3.544917000	4.307807000
6	0.944597000	5.431540000	4.813747000
1	2.092076000	4.426685000	3.310633000

6	-1.227886000	4.532898000	5.258884000
1	-1.799929000	2.822396000	4.107080000
6	-0.250698000	5.493229000	5.533104000
1	1.725250000	6.156465000	5.011720000
1	-2.168583000	4.560409000	5.796119000
6	0.178961000	3.486307000	-3.587146000
6	1.153936000	4.454609000	-3.850361000
6	-1.019700000	3.544917000	-4.307807000
6	0.944597000	5.431540000	-4.813747000
1	2.092076000	4.426685000	-3.310633000
6	-1.227886000	4.532898000	-5.258884000
1	-1.799929000	2.822396000	-4.107080000
6	-0.250698000	5.493229000	-5.533104000
1	1.725250000	6.156465000	-5.011720000
1	-2.168583000	4.560409000	-5.796119000
6	0.491987000	-6.575625000	-6.549925000
1	1.004676000	-7.427658000	-6.093920000
1	-0.445064000	-6.944129000	-6.968079000
1	1.119710000	-6.219745000	-7.367757000
6	0.491987000	-6.575625000	6.549925000
1	-0.445064000	-6.944129000	6.968079000
1	1.004676000	-7.427658000	6.093920000
1	1.119710000	-6.219745000	7.367757000
6	-0.491987000	6.575625000	6.549925000
1	0.445064000	6.944129000	6.968079000
1	-1.004676000	7.427658000	6.093920000
1	-1.119710000	6.219745000	7.367757000

6	-0.491987000	6.575625000	-6.549925000
1	-1.004676000	7.427658000	-6.093920000
1	0.445064000	6.944129000	-6.968079000
1	-1.119710000	6.219745000	-7.367757000
29	0.000000000	0.000000000	0.000000000

Optimized structure of Mn-Dithiaporphyrin Complex

6	0.393238000	2.450236000	2.574361000
6	0.199870000	1.088949000	2.962150000
6	0.640058000	2.918722000	1.270682000
7	0.000000000	0.000000000	2.153627000
6	0.117196000	0.667371000	4.342945000
16	1.381762000	1.968280000	0.000000000
6	0.179313000	4.123858000	0.688783000
6	-0.199870000	-1.088949000	2.962150000
6	-0.117196000	-0.667371000	4.342945000
1	0.251542000	1.303383000	5.200480000
6	0.640058000	2.918722000	-1.270682000
1	-0.280009000	4.902768000	1.278081000
6	0.179313000	4.123858000	-0.688783000
7	0.000000000	0.000000000	-2.153627000
16	-1.381762000	-1.968280000	0.000000000
17	2.235581000	-1.313550000	0.000000000
6	-0.393238000	-2.450236000	2.574361000
6	-0.199870000	-1.088949000	-2.962150000
6	-0.640058000	-2.918722000	1.270682000
17	-2.235581000	1.313550000	0.000000000
6	0.199870000	1.088949000	-2.962150000
6	0.117196000	0.667371000	-4.342945000
6	0.393238000	2.450236000	-2.574361000

1	0.251542000	1.303383000	-5.200480000
6	-0.117196000	-0.667371000	-4.342945000
6	-0.393238000	-2.450236000	-2.574361000
6	-0.179313000	-4.123858000	0.688783000
6	-0.179313000	-4.123858000	-0.688783000
1	0.280009000	-4.902768000	1.278081000
6	-0.640058000	-2.918722000	-1.270682000
1	0.280009000	-4.902768000	-1.278081000
1	-0.251542000	-1.303383000	-5.200480000
1	-0.251542000	-1.303383000	5.200480000
1	-0.280009000	4.902768000	-1.278081000
6	-0.176428000	-3.502732000	-3.601036000
6	-1.144612000	-4.490776000	-3.813479000
6	1.000738000	-3.560307000	-4.356861000
6	-0.950200000	-5.485252000	-4.761451000
1	-2.066536000	-4.463996000	-3.246539000
6	1.194504000	-4.566055000	-5.292136000
1	1.776643000	-2.823686000	-4.194894000
6	0.223644000	-5.545760000	-5.515635000
1	-1.725769000	-6.225152000	-4.919994000
1	2.119056000	-4.592513000	-5.856713000
6	-0.176428000	-3.502732000	3.601036000
6	-1.144612000	-4.490776000	3.813479000
6	1.000738000	-3.560307000	4.356861000
6	-0.950200000	-5.485252000	4.761451000
1	-2.066536000	-4.463996000	3.246539000
6	1.194504000	-4.566055000	5.292136000
1	1.776643000	-2.823686000	4.194894000
6	0.223644000	-5.545760000	5.515635000
1	-1.725769000	-6.225152000	4.919994000

1	2.119056000	-4.592513000	5.856713000
6	0.176428000	3.502732000	3.601036000
6	1.144612000	4.490776000	3.813479000
6	-1.000738000	3.560307000	4.356861000
6	0.950200000	5.485252000	4.761451000
1	2.066536000	4.463996000	3.246539000
6	-1.194504000	4.566055000	5.292136000
1	-1.776643000	2.823686000	4.194894000
6	-0.223644000	5.545760000	5.515635000
1	1.725769000	6.225152000	4.919994000
1	-2.119056000	4.592513000	5.856713000
6	0.176428000	3.502732000	-3.601036000
6	1.144612000	4.490776000	-3.813479000
6	-1.000738000	3.560307000	-4.356861000
6	0.950200000	5.485252000	-4.761451000
1	2.066536000	4.463996000	-3.246539000
6	-1.194504000	4.566055000	-5.292136000
1	-1.776643000	2.823686000	-4.194894000
6	-0.223644000	5.545760000	-5.515635000
1	1.725769000	6.225152000	-4.919994000
1	-2.119056000	4.592513000	-5.856713000
6	0.449759000	-6.646688000	-6.515745000
1	0.986516000	-7.482080000	-6.056645000
1	-0.494031000	-7.035948000	-6.898398000
1	1.048963000	-6.300785000	-7.358830000
6	0.449759000	-6.646688000	6.515745000
1	-0.494031000	-7.035948000	6.898398000
1	0.986516000	-7.482080000	6.056645000
1	1.048963000	-6.300785000	7.358830000
6	-0.449759000	6.646688000	6.515745000

1	0.494031000	7.035948000	6.898398000
1	-0.986516000	7.482080000	6.056645000
1	-1.048963000	6.300785000	7.358830000
6	-0.449759000	6.646688000	-6.515745000
1	-0.986516000	7.482080000	-6.056645000
1	0.494031000	7.035948000	-6.898398000
1	-1.048963000	6.300785000	-7.358830000
25	0.000000000	0.000000000	0.000000000

Optimized structure of Acceptor A1

6	2.386980000	0.324673000	0.024176000
7	0.873007000	1.982131000	0.064026000
6	0.156576000	0.802576000	0.034895000
6	1.073274000	-0.233316000	0.009488000
7	2.587272000	-1.889954000	-0.032706000
6	3.303304000	-0.710255000	-0.003722000
6	-1.282517000	0.788172000	0.029437000
6	4.743990000	-0.694716000	-0.003415000
6	2.271718000	1.781576000	0.066053000
8	3.075721000	2.692796000	0.099313000
6	1.188238000	-1.689463000	-0.033521000
8	0.384493000	-2.601417000	-0.066701000
16	5.670092000	-2.201906000	0.032853000
6	7.131524000	-1.268193000	0.010080000
6	6.797568000	0.118509000	-0.021763000
7	5.456728000	0.392185000	-0.028409000
6	8.441795000	-1.714969000	0.021080000
6	9.442016000	-0.745500000	-0.001217000
6	9.111532000	0.640623000	-0.033647000
6	7.803534000	1.088377000	-0.044365000

7	10.798037000	-1.017803000	0.005540000
6	11.483345000	0.074421000	-0.019625000
16	10.583911000	1.569938000	-0.054746000
16	-2.209842000	2.294392000	-0.012784000
6	-3.670634000	1.360698000	0.001581000
6	-3.335603000	-0.025447000	0.036915000
7	-1.997249000	-0.299066000	0.051586000
6	-4.981204000	1.807274000	-0.019768000
6	-5.984309000	0.838721000	-0.004868000
6	-5.649350000	-0.548632000	0.031907000
6	-4.344402000	-0.995987000	0.053270000
7	-7.329433000	1.111236000	-0.024805000
6	-8.044612000	0.025486000	-0.005846000
16	-7.117386000	-1.481943000	0.041382000
1	0.479479000	2.909162000	0.104583000
1	2.980659000	-2.816975000	-0.074782000
1	8.699826000	-2.764470000	0.045598000
1	7.544501000	2.137628000	-0.068737000
1	-5.238538000	2.856788000	-0.047748000
1	-4.085820000	-2.045280000	0.080321000
1	12.564342000	0.103899000	-0.019893000
6	-9.489474000	0.022585000	-0.022015000
6	-11.898518000	-0.558470000	-0.041636000
6	-11.684722000	0.793767000	-0.059612000
1	-12.838207000	-1.086689000	-0.044729000
1	-12.483267000	1.521067000	-0.080010000
16	-10.429074000	-1.436434000	-0.011334000
6	-10.313001000	1.127720000	-0.048641000
1	-9.928712000	2.136577000	-0.059414000

Optimized structure of Acceptor A2

6	-2.412691000	0.430565000	-0.018450000
7	-0.966372000	2.145022000	-0.110881000
6	-0.203242000	0.996756000	-0.038221000
6	-1.078148000	-0.073342000	0.021016000
7	-2.524408000	-1.787398000	0.114260000
6	-3.287417000	-0.639130000	0.041063000
6	1.234731000	1.038239000	-0.028788000
6	-4.726139000	-0.680388000	0.031029000
6	-2.355902000	1.888051000	-0.112736000
8	-3.195884000	2.764510000	-0.183405000
6	-1.134743000	-1.530444000	0.115570000
8	-0.294778000	-2.407199000	0.186059000
16	-5.595098000	-2.221439000	0.014357000
6	-7.090757000	-1.343692000	0.014520000
6	-6.808948000	0.054705000	0.023575000
7	-5.481113000	0.379111000	0.032538000
6	-8.383454000	-1.839927000	0.005773000
6	-9.421415000	-0.909049000	0.007207000
6	-9.141104000	0.489391000	0.016635000
6	-7.853006000	0.986267000	0.024762000
7	-10.757144000	-1.230291000	0.000992000
6	-11.514989000	-0.177187000	0.005071000
16	-10.642617000	1.364491000	0.016657000
16	2.104775000	2.578904000	-0.010189000
6	3.600018000	1.700799000	-0.013775000
6	3.317121000	0.302583000	-0.024984000
7	1.990269000	-0.021479000	-0.032862000
6	4.892701000	2.196801000	-0.005875000
6	5.932367000	1.266736000	-0.010947000

6	5.649029000	-0.132932000	-0.022981000
6	4.361982000	-0.629316000	-0.029689000
7	7.265453000	1.589798000	-0.005447000
6	8.021716000	0.530381000	-0.014049000
16	7.150529000	-1.011291000	-0.030246000
1	-0.610132000	3.084239000	-0.193777000
1	-2.880596000	-2.726692000	0.196486000
1	-8.600582000	-2.898835000	-0.001044000
1	-7.634607000	2.044955000	0.032020000
1	5.109745000	3.255685000	0.002860000
1	4.143534000	-1.687974000	-0.038890000
6	9.462683000	0.580859000	-0.012590000
6	11.917410000	0.085254000	-0.006485000
6	11.624917000	1.433323000	-0.031507000
1	12.385842000	2.198981000	-0.069563000
16	10.453467000	-0.842088000	0.021657000
6	10.247874000	1.714225000	-0.036585000
1	9.828881000	2.708874000	-0.066221000
6	13.231344000	-0.559977000	0.004446000
6	13.405701000	-1.878597000	-0.439081000
6	14.357183000	0.140646000	0.462871000
6	14.659216000	-2.474363000	-0.425341000
1	12.558158000	-2.437603000	-0.815675000
6	15.609981000	-0.455629000	0.468659000
1	14.247719000	1.151049000	0.833618000
6	15.768142000	-1.765802000	0.026051000
1	14.770433000	-3.492617000	-0.775527000
1	16.464792000	0.102402000	0.829104000
1	16.745790000	-2.230072000	0.034341000
6	-12.979448000	-0.219706000	0.000636000

6	-13.634076000	-1.459335000	-0.016678000
6	-13.747588000	0.950436000	0.013654000
6	-15.018908000	-1.520805000	-0.020770000
1	-13.044368000	-2.364946000	-0.026883000
6	-15.133795000	0.884319000	0.009562000
1	-13.266465000	1.920362000	0.027565000
6	-15.774205000	-0.350587000	-0.007646000
1	-15.512200000	-2.484220000	-0.034287000
1	-15.713757000	1.797921000	0.019966000
1	-16.855415000	-0.401347000	-0.010809000

Optimized structure of Acceptor A3

6	2.373814000	-0.295842000	0.030273000
7	0.991332000	-2.067208000	0.054435000
6	0.189304000	-0.945175000	0.053309000
6	1.023049000	0.159033000	0.043552000
7	2.404944000	1.927853000	0.114245000
6	3.207397000	0.806092000	0.069210000
6	-1.247491000	-1.035410000	0.072128000
6	4.644839000	0.894220000	0.081572000
6	2.371178000	-1.759803000	0.033796000
8	3.243300000	-2.604538000	0.022008000
6	1.024996000	1.620698000	0.093854000
8	0.152634000	2.466127000	0.115355000
16	5.457984000	2.442042000	0.344419000
6	6.982611000	1.627747000	0.192907000
6	6.747530000	0.234581000	-0.039116000
7	5.431462000	-0.127164000	-0.094385000
6	8.252404000	2.159389000	0.274435000
6	9.322478000	1.270421000	0.118387000

6	9.088783000	-0.120112000	-0.113610000
6	7.815267000	-0.651782000	-0.194734000
7	10.635536000	1.629581000	0.170073000
6	11.427050000	0.601034000	-0.007554000
16	10.609162000	-0.938823000	-0.261423000
16	-2.061543000	-2.592324000	0.270291000
6	-3.585553000	-1.772312000	0.164642000
6	-3.351590000	-0.373684000	-0.006168000
7	-2.036351000	-0.008151000	-0.053076000
6	-4.858779000	-2.308215000	0.229219000
6	-5.928353000	-1.418337000	0.118564000
6	-5.694823000	-0.019524000	-0.051624000
6	-4.424630000	0.516879000	-0.115892000
7	-7.248295000	-1.783128000	0.160017000
6	-8.035356000	-0.754997000	0.033020000
16	-7.223423000	0.800307000	-0.155628000
1	0.669280000	-3.021137000	0.002109000
1	2.726009000	2.883045000	0.084216000
1	8.439040000	3.209418000	0.449005000
1	7.628834000	-1.701811000	-0.369256000
1	-5.041555000	-3.365600000	0.357764000
1	-4.241162000	1.574123000	-0.244700000
6	-9.476625000	-0.872747000	0.043292000
6	-11.936457000	-0.510248000	0.006343000
6	-11.571626000	-1.847202000	0.135320000
1	-12.304656000	-2.637849000	0.210763000
16	-10.519512000	0.494999000	-0.088704000
6	-10.193022000	-2.052768000	0.156646000
1	-9.714536000	-3.015242000	0.249138000
6	-13.285706000	-0.073799000	-0.035202000

1	-14.008297000	-0.878123000	0.042441000
6	-13.812130000	1.182783000	-0.155025000
6	-13.033598000	2.368245000	-0.268121000
7	-12.411911000	3.335710000	-0.360354000
6	-15.226263000	1.359970000	-0.171095000
7	-16.369993000	1.508927000	-0.184745000
6	12.847708000	0.803110000	0.018486000
1	13.124595000	1.836052000	0.188560000
6	13.859219000	-0.091534000	-0.134279000
6	15.214667000	0.354046000	-0.066068000
7	16.310779000	0.705509000	-0.012341000
6	13.681079000	-1.487597000	-0.363869000
7	13.561652000	-2.618752000	-0.549841000

Optimized structure of Acceptor A4

6	2.373814000	-0.295842000	0.030273000
7	0.991332000	-2.067208000	0.054435000
6	0.189304000	-0.945175000	0.053309000
6	1.023049000	0.159033000	0.043552000
7	2.404944000	1.927853000	0.114245000
6	3.207397000	0.806092000	0.069210000
6	-1.247491000	-1.035410000	0.072128000
6	4.644839000	0.894220000	0.081572000
6	2.371178000	-1.759803000	0.033796000
8	3.243300000	-2.604538000	0.022008000
6	1.024996000	1.620698000	0.093854000
8	0.152634000	2.466127000	0.115355000
16	5.457984000	2.442042000	0.344419000
6	6.982611000	1.627747000	0.192907000
6	6.747530000	0.234581000	-0.039116000

7	5.431462000	-0.127164000	-0.094385000
6	8.252404000	2.159389000	0.274435000
6	9.322478000	1.270421000	0.118387000
6	9.088783000	-0.120112000	-0.113610000
6	7.815267000	-0.651782000	-0.194734000
7	10.635536000	1.629581000	0.170073000
6	11.427050000	0.601034000	-0.007554000
16	10.609162000	-0.938823000	-0.261423000
16	-2.061543000	-2.592324000	0.270291000
6	-3.585553000	-1.772312000	0.164642000
6	-3.351590000	-0.373684000	-0.006168000
7	-2.036351000	-0.008151000	-0.053076000
6	-4.858779000	-2.308215000	0.229219000
6	-5.928353000	-1.418337000	0.118564000
6	-5.694823000	-0.019524000	-0.051624000
6	-4.424630000	0.516879000	-0.115892000
7	-7.248295000	-1.783128000	0.160017000
6	-8.035356000	-0.754997000	0.033020000
16	-7.223423000	0.800307000	-0.155628000
1	0.669280000	-3.021137000	0.002109000
1	2.726009000	2.883045000	0.084216000
1	8.439040000	3.209418000	0.449005000
1	7.628834000	-1.701811000	-0.369256000
1	-5.041555000	-3.365600000	0.357764000
1	-4.241162000	1.574123000	-0.244700000
6	-9.476625000	-0.872747000	0.043292000
6	-11.936457000	-0.510248000	0.006343000
6	-11.571626000	-1.847202000	0.135320000
1	-12.304656000	-2.637849000	0.210763000
16	-10.519512000	0.494999000	-0.088704000

6	-10.193022000	-2.052768000	0.156646000
1	-9.714536000	-3.015242000	0.249138000
6	-13.269260560	-0.079118700	-0.034695620
8	-13.570828610	1.105160060	-0.148042660
1	-14.034366950	-0.880259830	0.042120240
6	12.847708000	0.803110000	0.018486000
8	13.315919750	1.955973220	0.206248360
1	13.508756810	-0.026497040	-0.121751760

Optimized structure of Acceptor A5

6	1.853620750	-0.165675460	0.092189490
7	0.382833590	-1.012502650	1.565025740
6	-0.357942140	-0.526876880	0.507846880
6	0.530586660	0.004650760	-0.410029030
7	1.994078600	0.934396260	-1.837306200
6	2.738493220	0.407978220	-0.801430910
6	-1.795323930	-0.606013110	0.484449670
6	4.174247880	0.513818200	-0.761866610
6	1.774863790	-0.837082740	1.390731270
8	2.600740050	-1.203765000	2.201771030
6	0.604805280	0.722704010	-1.681992000
8	-0.221947730	1.098310000	-2.489226510
16	5.046343590	1.490670070	-1.949829470
6	6.533542530	1.038748650	-1.178774300
6	6.243219010	0.182306500	-0.068716490
7	4.917174920	-0.083051020	0.124004950
6	7.820471120	1.403913980	-1.513637510
6	8.851267920	0.896405100	-0.713908700
6	8.562459870	0.041251330	0.393936020
6	7.271792790	-0.323709230	0.728718580

7	10.174427800	1.157280820	-0.906211680
6	10.921971990	0.555815480	-0.014375480
16	10.044941320	-0.409584780	1.170263440
16	-2.700766800	-1.178283670	1.891080420
6	-4.169219910	-0.951744680	0.997484630
6	-3.851789520	-0.450043700	-0.301595470
7	-2.519288720	-0.273578630	-0.544432970
6	-5.469922260	-1.189442910	1.402626110
6	-6.481677190	-0.917996850	0.480246080
6	-6.164711730	-0.415675430	-0.818747410
6	-4.867026500	-0.177587370	-1.224427020
7	-7.818446550	-1.099134940	0.719566750
6	-8.540449550	-0.767820760	-0.310767760
16	-7.637861070	-0.187934420	-1.711788690
1	0.016171710	-1.510529200	2.361244720
1	2.365534200	1.359938460	-2.672357580
1	8.048729090	2.049500270	-2.349690870
1	7.043733730	-0.969245280	1.564809700
1	-5.715737860	-1.569482730	2.384022230
1	-4.620510570	0.202180400	-2.205764480
6	-9.983122060	-0.867380930	-0.314039990
6	-12.412363100	-0.826030130	-0.843777940
6	-12.127150040	-1.313803630	0.428194250
1	-12.903643680	-1.638826350	1.106106610
16	-10.942039190	-0.393702570	-1.667506700
6	-10.765858150	-1.337538300	0.727497140
1	-10.345474880	-1.680854430	1.659844590
7	-13.655757770	-0.719217940	-1.325443970
8	-13.812494240	-0.179838290	-2.385124160
8	-14.559224770	-1.167524900	-0.676462460

7	12.386880120	0.677507250	-0.002744030
8	12.884539730	1.270649400	-0.910163720
8	12.985620560	-0.098091890	0.677578700

Optimized structure of Acceptor A6

6	1.853620750	-0.165675460	0.092189490
7	0.382833590	-1.012502650	1.565025740
6	-0.357942140	-0.526876880	0.507846880
6	0.530586660	0.004650760	-0.410029030
7	1.994078600	0.934396260	-1.837306200
6	2.738493220	0.407978220	-0.801430910
6	-1.795323930	-0.606013110	0.484449670
6	4.174247880	0.513818200	-0.761866610
6	1.774863790	-0.837082740	1.390731270
8	2.600740050	-1.203765000	2.201771030
6	0.604805280	0.722704010	-1.681992000
8	-0.221947730	1.098310000	-2.489226510
16	5.046343590	1.490670070	-1.949829470
6	6.533542530	1.038748650	-1.178774300
6	6.243219010	0.182306500	-0.068716490
7	4.917174920	-0.083051020	0.124004950
6	7.820471120	1.403913980	-1.513637510
6	8.851267920	0.896405100	-0.713908700
6	8.562459870	0.041251330	0.393936020
6	7.271792790	-0.323709230	0.728718580
7	10.174427800	1.157280820	-0.906211680
6	10.921971990	0.555815480	-0.014375480
16	10.044941320	-0.409584780	1.170263440
16	-2.700766800	-1.178283670	1.891080420
6	-4.169219910	-0.951744680	0.997484630

6	-3.851789520	-0.450043700	-0.301595470
7	-2.519288720	-0.273578630	-0.544432970
6	-5.469922260	-1.189442910	1.402626110
6	-6.481677190	-0.917996850	0.480246080
6	-6.164711730	-0.415675430	-0.818747410
6	-4.867026500	-0.177587370	-1.224427020
7	-7.818446550	-1.099134940	0.719566750
6	-8.540449550	-0.767820760	-0.310767760
16	-7.637861070	-0.187934420	-1.711788690
1	0.016171710	-1.510529200	2.361244720
1	2.365534200	1.359938460	-2.672357580
1	8.048729090	2.049500270	-2.349690870
1	7.043733730	-0.969245280	1.564809700
1	-5.715737860	-1.569482730	2.384022230
1	-4.620510570	0.202180400	-2.205764480
6	-9.983122060	-0.867380930	-0.314039990
6	-12.412363100	-0.826030130	-0.843777940
6	-12.127150040	-1.313803630	0.428194250
1	-12.903643680	-1.638826350	1.106106610
16	-10.942039190	-0.393702570	-1.667506700
6	-10.765858150	-1.337538300	0.727497140
1	-10.345474880	-1.680854430	1.659844590
6	12.456637650	0.683302100	-0.002190160
8	13.286557330	0.187326220	0.758600920
8	12.915427910	1.474877100	-1.004353070
1	13.884043460	1.538191260	-0.973757260
6	-13.826812210	-0.688652300	-1.437125270
8	-14.187025270	-0.274414510	-2.538131820
8	-14.789398020	-1.100891260	-0.574050780
1	-15.669849820	-1.003856670	-0.972233880

Optimized structure of Acceptor A7

6	1.853620750	-0.165675460	0.092189490
7	0.382833590	-1.012502650	1.565025740
6	-0.357942140	-0.526876880	0.507846880
6	0.530586660	0.004650760	-0.410029030
7	1.994078600	0.934396260	-1.837306200
6	2.738493220	0.407978220	-0.801430910
6	-1.795323930	-0.606013110	0.484449670
6	4.174247880	0.513818200	-0.761866610
6	1.774863790	-0.837082740	1.390731270
8	2.600740050	-1.203765000	2.201771030
6	0.604805280	0.722704010	-1.681992000
8	-0.221947730	1.098310000	-2.489226510
16	5.046343590	1.490670070	-1.949829470
6	6.533542530	1.038748650	-1.178774300
6	6.243219010	0.182306500	-0.068716490
7	4.917174920	-0.083051020	0.124004950
6	7.820471120	1.403913980	-1.513637510
6	8.851267920	0.896405100	-0.713908700
6	8.562459870	0.041251330	0.393936020
6	7.271792790	-0.323709230	0.728718580
7	10.174427800	1.157280820	-0.906211680
6	10.921971990	0.555815480	-0.014375480
16	10.044941320	-0.409584780	1.170263440
16	-2.700766800	-1.178283670	1.891080420
6	-4.169219910	-0.951744680	0.997484630
6	-3.851789520	-0.450043700	-0.301595470
7	-2.519288720	-0.273578630	-0.544432970
6	-5.469922260	-1.189442910	1.402626110

6	-6.481677190	-0.917996850	0.480246080
6	-6.164711730	-0.415675430	-0.818747410
6	-4.867026500	-0.177587370	-1.224427020
7	-7.818446550	-1.099134940	0.719566750
6	-8.540449550	-0.767820760	-0.310767760
16	-7.637861070	-0.187934420	-1.711788690
1	0.016171710	-1.510529200	2.361244720
1	2.365534200	1.359938460	-2.672357580
1	8.048729090	2.049500270	-2.349690870
1	7.043733730	-0.969245280	1.564809700
1	-5.715737860	-1.569482730	2.384022230
1	-4.620510570	0.202180400	-2.205764480
6	-9.983122060	-0.867380930	-0.314039990
6	-12.412363100	-0.826030130	-0.843777940
6	-12.127150040	-1.313803630	0.428194250
1	-12.903643680	-1.638826350	1.106106610
16	-10.942039190	-0.393702570	-1.667506700
6	-10.765858150	-1.337538300	0.727497140
1	-10.345474880	-1.680854430	1.659844590
6	-13.826812210	-0.688652300	-1.437125270
7	-14.892241410	-0.585172890	-1.884062220
6	12.456637650	0.683302100	-0.002190160
7	13.612619570	0.779330980	0.006988390