

Supplementary Information

**On the importance of equatorial metal-centered excited states
in the photophysics of cyclometallated Ir(III) complexes**

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Table S1 Comparison between the bond distances (in Å) reported by Accorsi, Ortí and coworkers (reference 6) and those computed in this work (data within parentheses) for the coordination sphere of the Ir atom in the S_0 , $^3\text{MLCT}$ and $^3\text{MC}_{ax}$ minima of complexes **1–3**.

	Bond	(S_0)_{min}	($^3\text{MLCT}$)_{min}	($^3\text{MC}_{ax}$)_{min}
Complex 1	Ir–N _{1-bpy}	2.210(2.218)	2.196(2.203)	2.219(2.229)
	Ir–N _{2-bpy}	2.210(2.218)	2.196(2.203)	2.219(2.260)
	Ir–N _{3-ppy}	2.082(2.090)	2.081(2.090)	2.505(2.611)
	Ir–N _{6-ppy}	2.082(2.090)	2.081(2.090)	2.505(2.293)
	Ir–C _{4-ppy}	2.024(2.029)	1.999(2.007)	2.015(2.044)
	Ir–C _{5-ppy}	2.024(2.029)	1.999(2.007)	2.015(2.040)
Complex 2	Ir–N _{1-bpy}	2.360(2.358)	2.238(2.236)	2.515(2.297)
	Ir–N _{2-bpy}	2.207(2.214)	2.226(2.232)	2.226(2.247)
	Ir–N _{3-ppy}	2.093(2.099)	2.087(2.095)	2.204(2.295)
	Ir–N _{6-ppy}	2.079(2.083)	2.076(2.084)	2.604(2.646)
	Ir–C _{4-ppy}	2.013(2.018)	2.018(2.027)	2.033(2.036)
	Ir–C _{5-ppy}	2.028(2.034)	1.985(1.992)	2.042(2.049)
Complex 3	Ir–N _{1-bpy}	2.355(2.369)	2.301(2.305)	2.503(2.456)
	Ir–N _{2-bpy}	2.345(2.346)	2.233(2.238)	2.305(2.303)
	Ir–N _{3-ppy}	2.075(2.085)	2.071(2.083)	2.209(2.225)
	Ir–N _{6-ppy}	2.081(2.089)	2.096(2.100)	2.614(2.623)
	Ir–C _{4-ppy}	2.019(2.022)	1.990(1.996)	2.030(2.036)
	Ir–C _{5-ppy}	2.021(2.026)	2.011(2.020)	2.050(2.054)

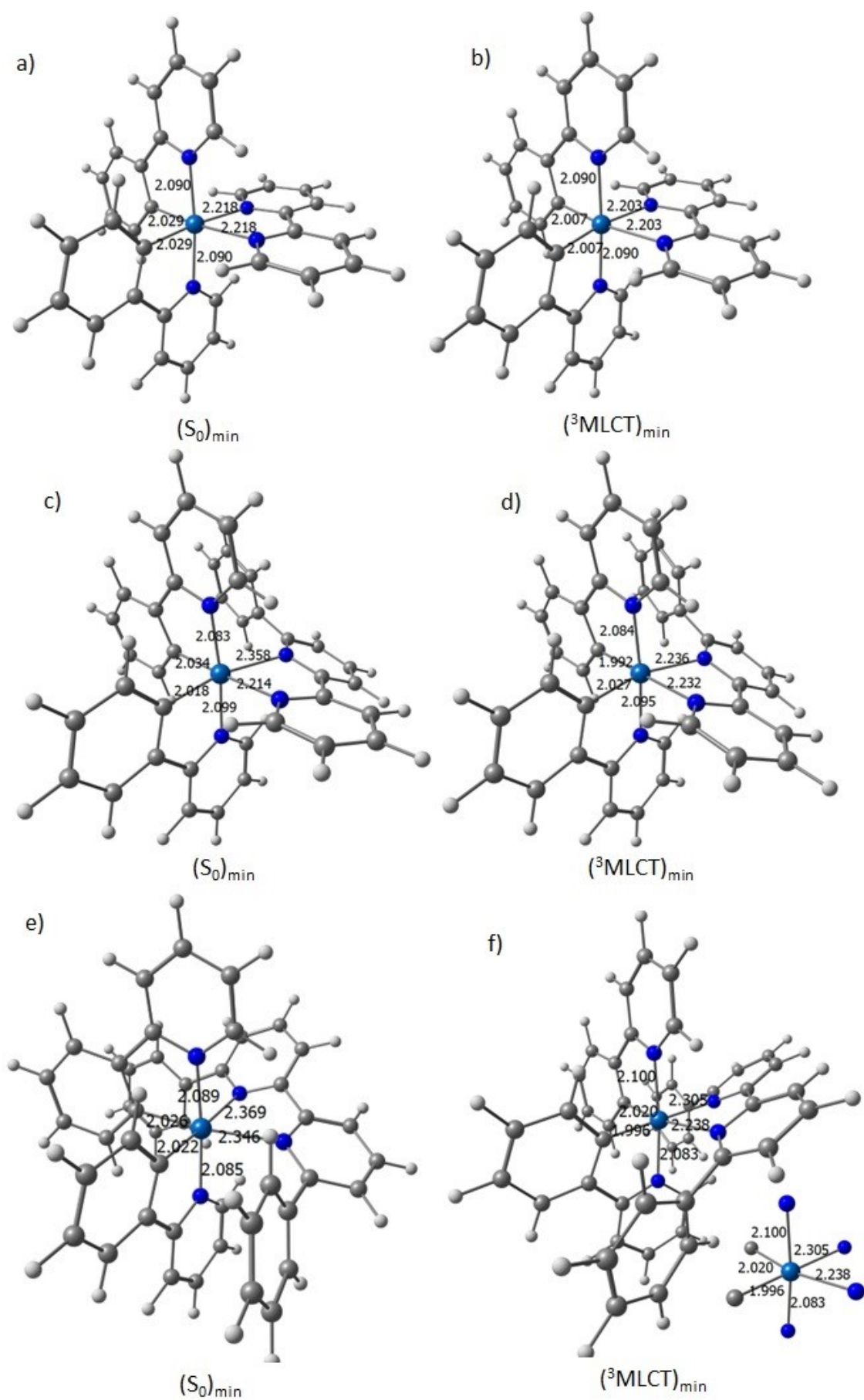


Fig. S1 B3LYP/DEF2-SVP-CPCM(CH_2Cl_2) (S_0)_{min} and (${}^3\text{MLCT}$)_{min} optimized structures calculated for complexes **1** (a and b), **2** (c and d) and **3** (e and f).

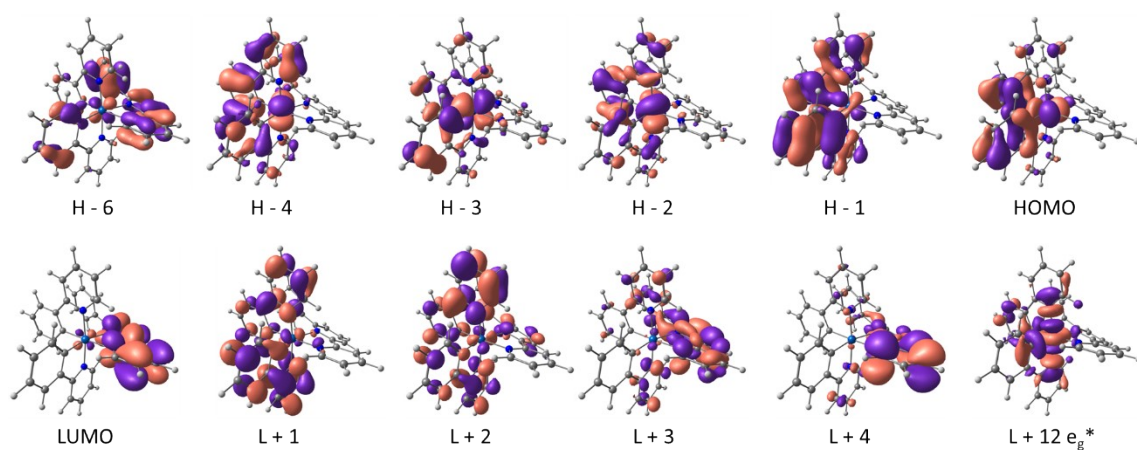


Fig. S2 Isosurface contour plots (± 0.03 a.u.) computed for the MOs of complex **2** at the DFT B3LYP/DEF2-SVP-CPCM(CH₂Cl₂) level.

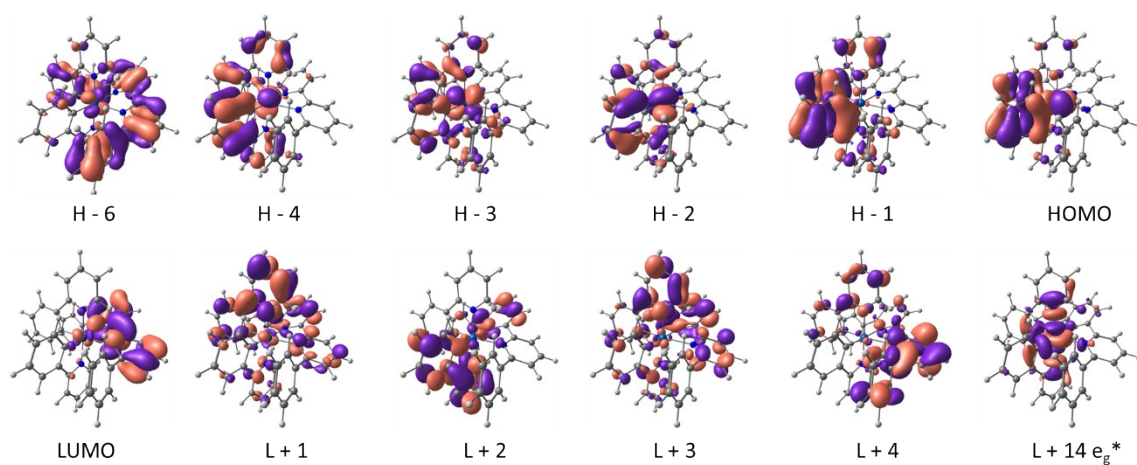
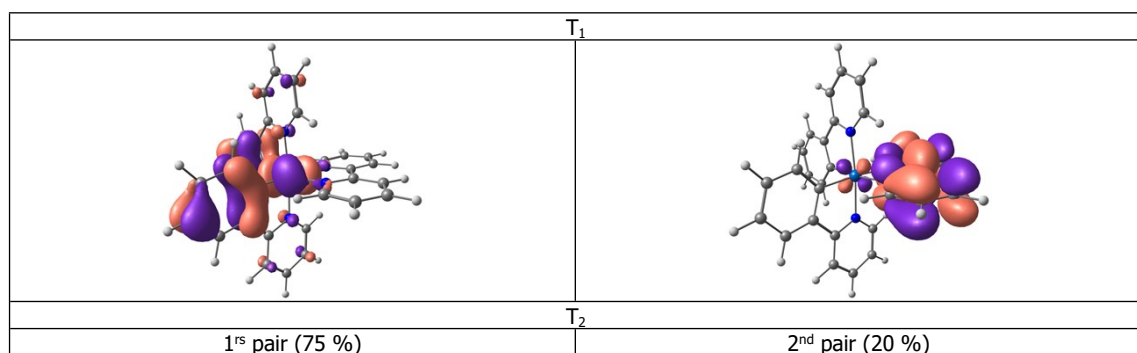


Fig. S3 Isosurface contour plots (± 0.03 a.u.) computed for the MOs of complex **3** at the DFT B3LYP/DEF2-SVP-CPCM(CH₂Cl₂) level.



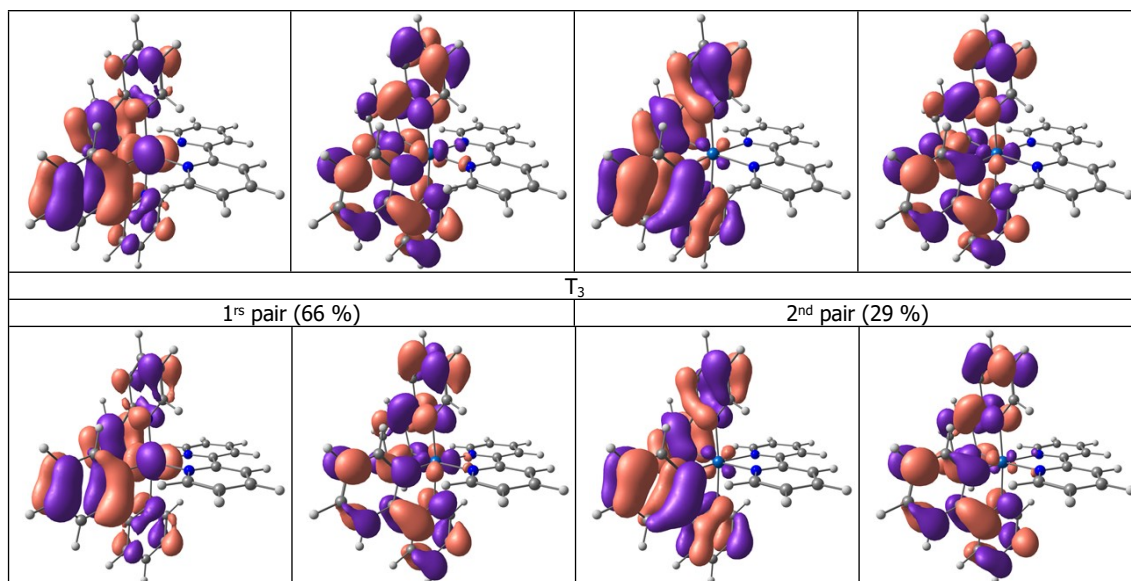


Fig. S4 Isosurface contour plots (± 0.03 a.u.) of the NTO pairs describing the electronic transitions to the three lowest triplet excited states (T_1 to T_3) computed for complex **1** at the DFT B3LYP/DEF2-SVP-PCM(CH_2Cl_2) level using the $(S_0)_{\text{min}}$ geometry.

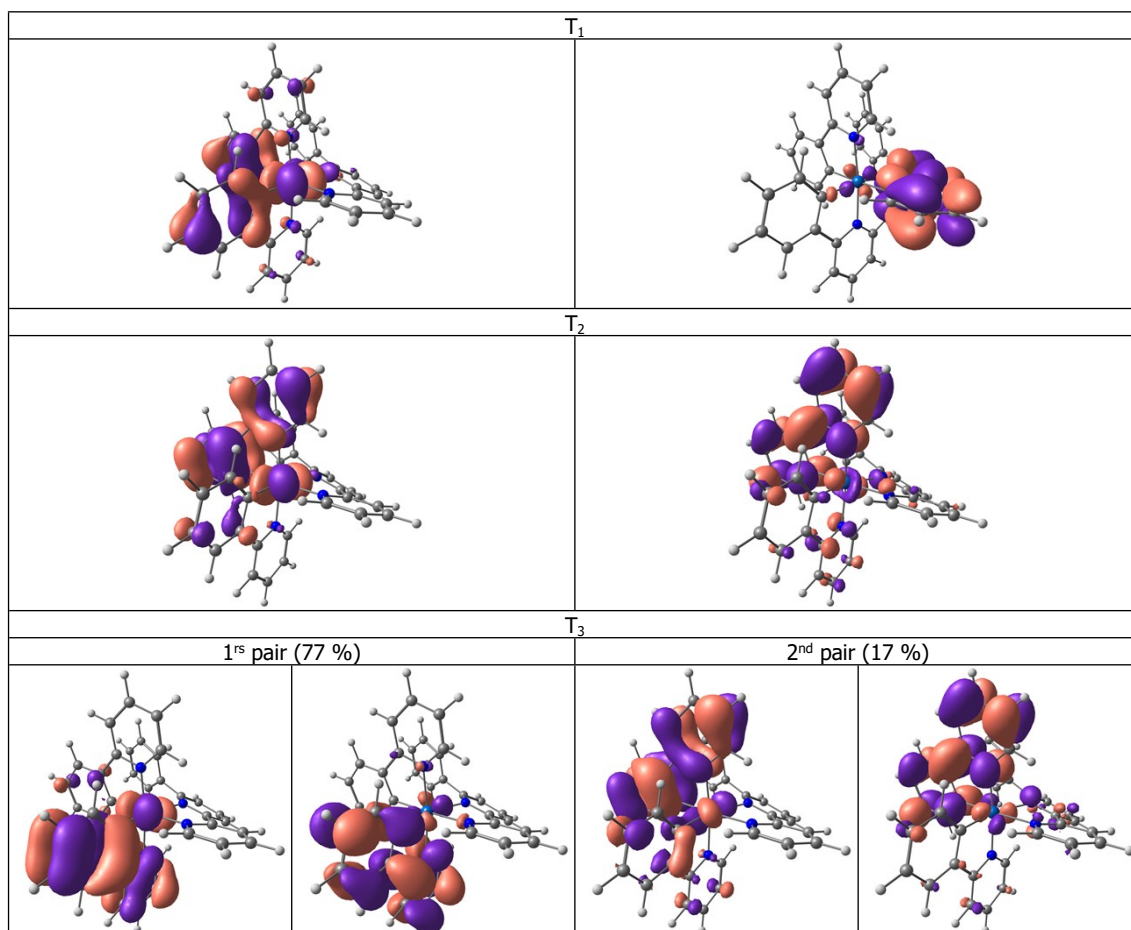


Fig. S5 Isosurface contour plots (± 0.03 a.u.) of the NTO pairs describing the electronic transitions to the three lowest triplet excited states (T_1 to T_3) computed for complex **2** at the DFT B3LYP/DEF2-SVP-CPCM(CH_2Cl_2) level using the $(S_0)_{\text{min}}$ geometry.

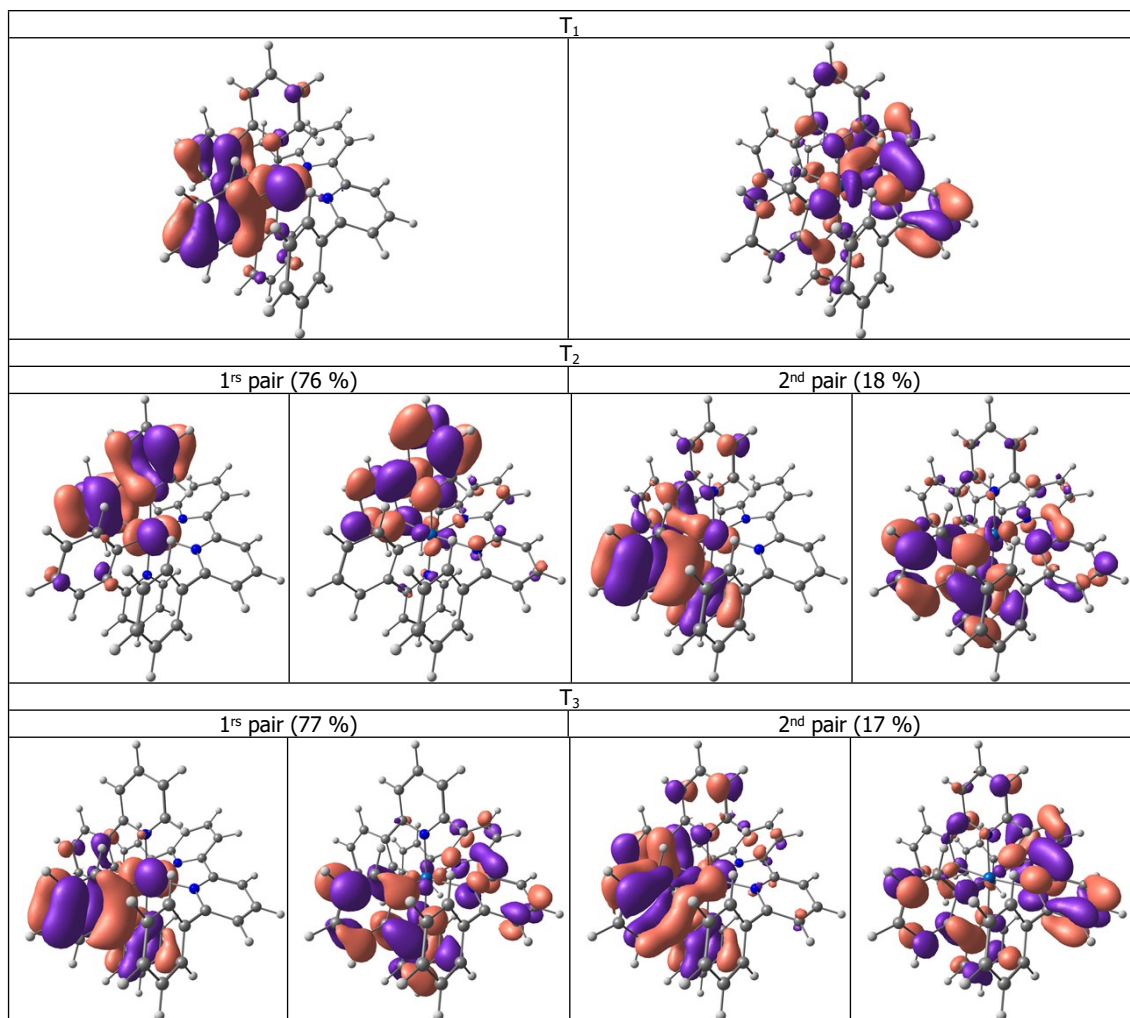


Fig. S6 Isosurface contour plots (± 0.03 a.u.) of the NTO pairs describing the electronic transitions to the three lowest triplet excited states (T₁ to T₃) computed for complex **3** at the DFT B3LYP/DEF2-SVP-PCM(CH₂Cl₂) level using the (S₀)_{min} geometry.

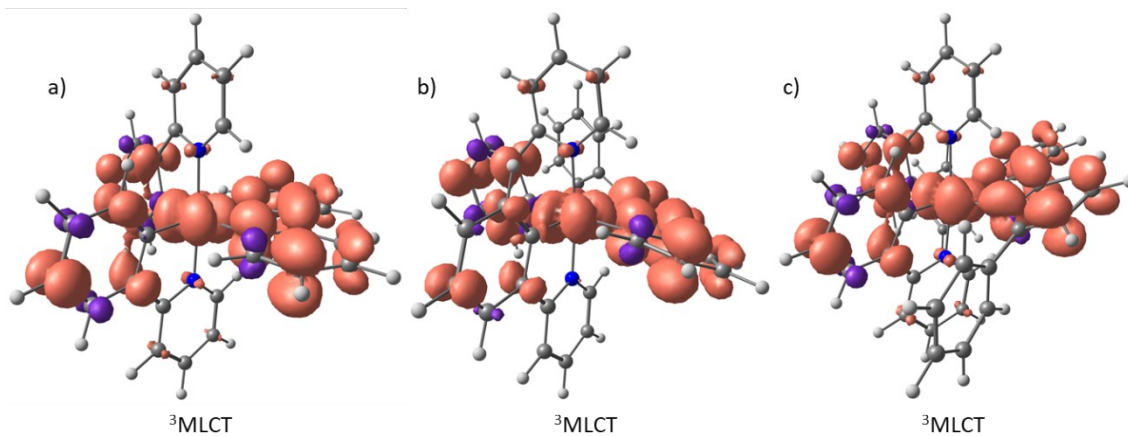


Fig. S7 B3LYP/DEF2-SVP-CPCM(CH₂Cl₂) isosurface contour plots (± 0.004 a.u.) of the unpaired-electron spin density computed at the (³MLCT)_{min} for complex **1** (a), **2** (b) and **3** (c).

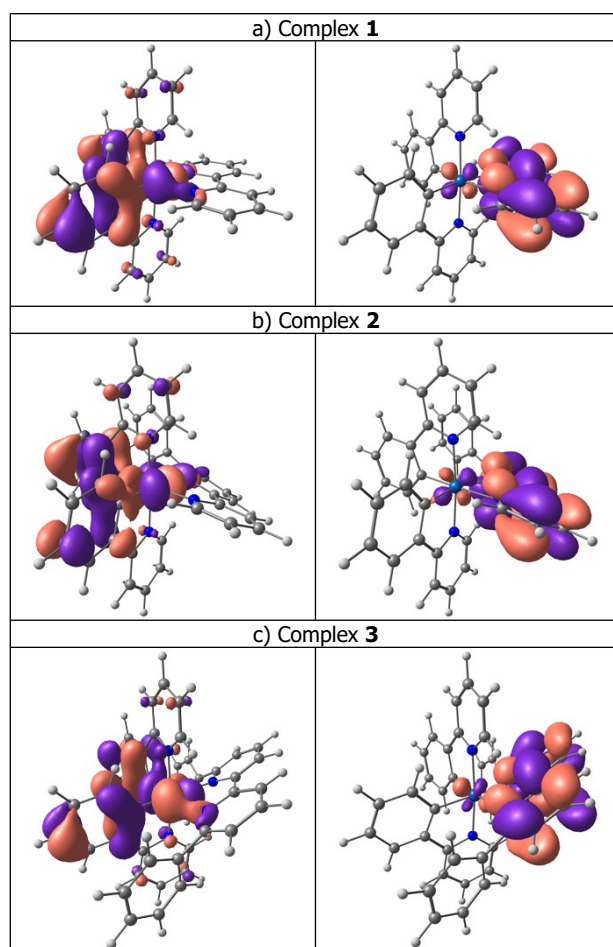


Fig. S8 B3LYP/DEF2-SVP-PCM(CH₂Cl₂) isosurface contour plots (± 0.03 a.u.) of the NTO pairs describing the electronic transition to the T₁ triplet computed at the optimized ³MLCT minima of complexes **1** (a), **2** (b) and **3** (c).

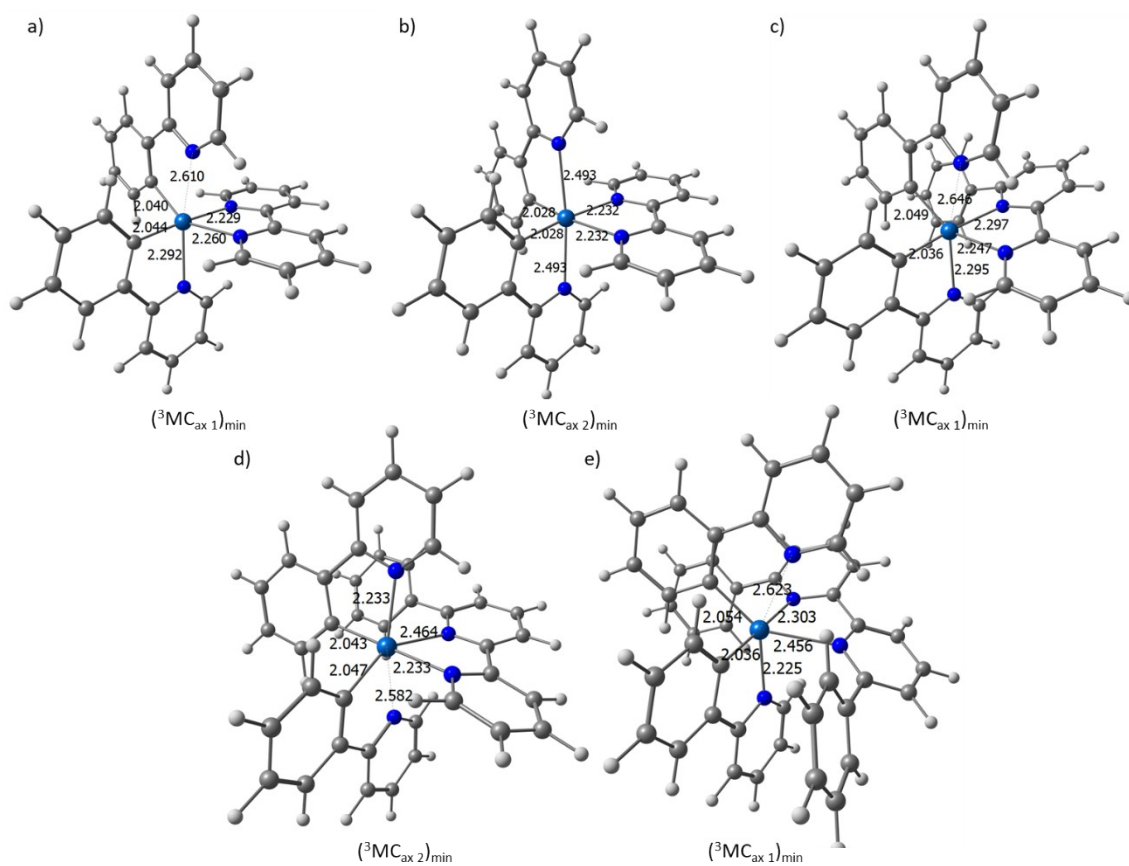


Fig. S9 B3LYP/DEF2-SVP-CPCM(CH₂Cl₂) optimized ³MC_{ax} minima calculated for complexes **1** (a and b), **2** (c and d) and **3** (e).

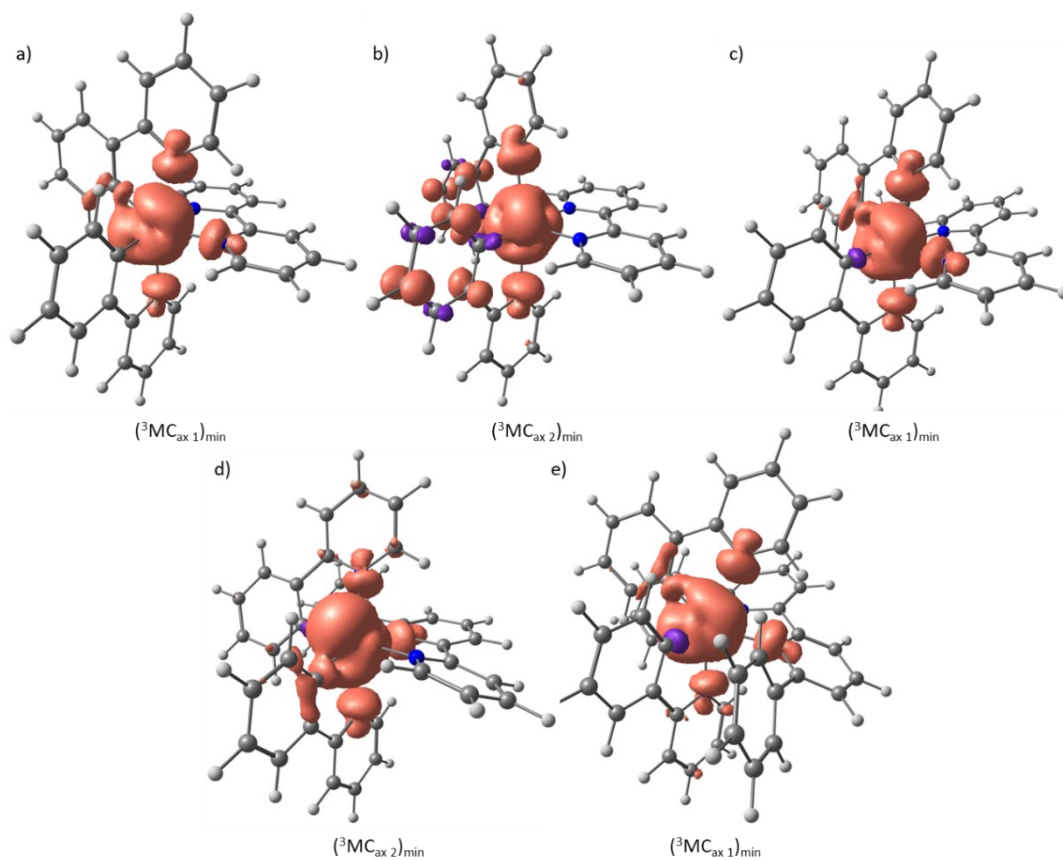


Fig. S10 B3LYP/DEF2-SVP-CPCM(CH₂Cl₂) isosurface contour plots (± 0.004 a.u.) of the unpaired-electron spin density computed at the optimized ³MC_{ax} minima for complex **1** (a and b), **2** (c and d) and **3** (e).

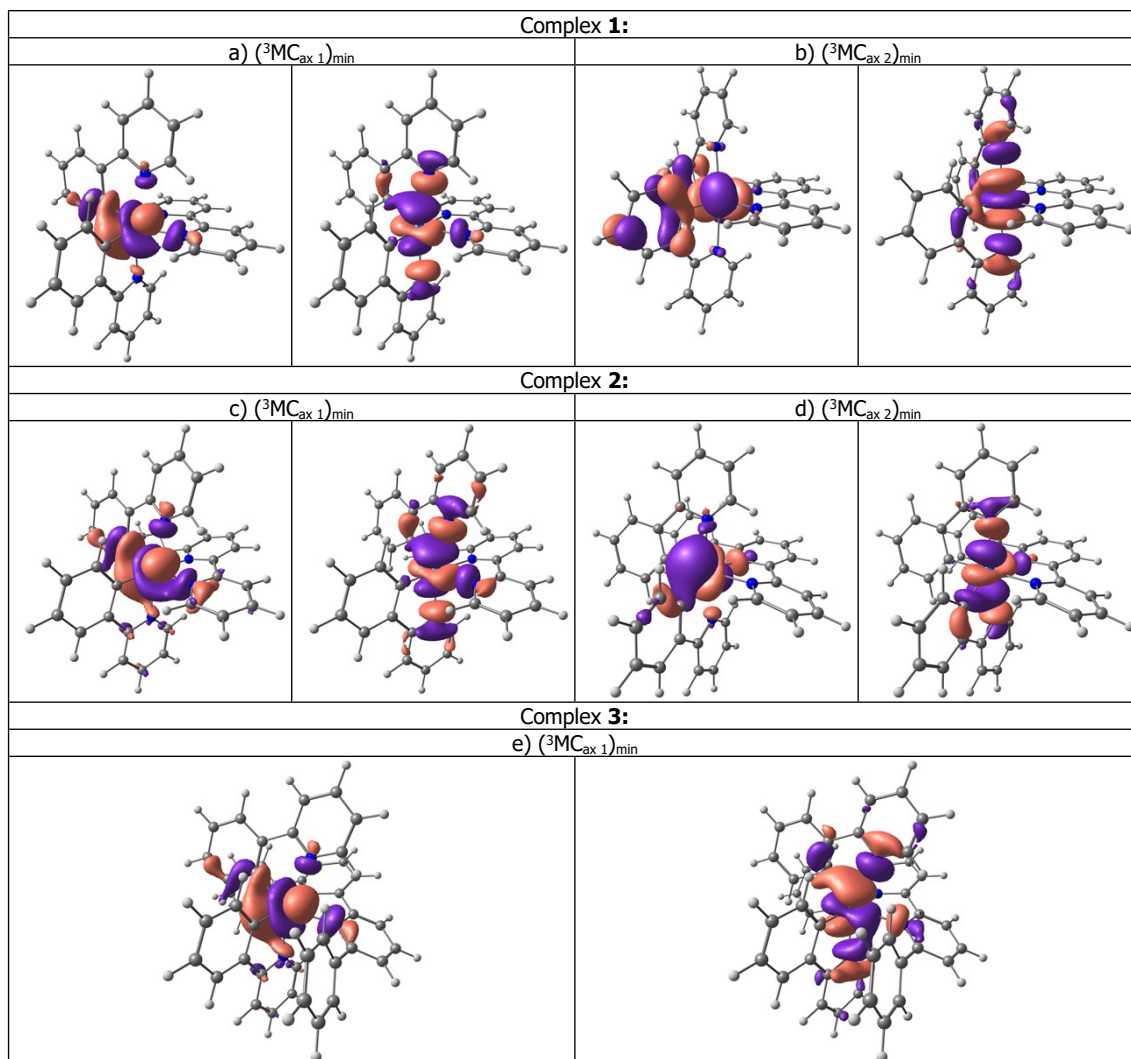


Fig. S11 B3LYP/DEF2-SVP-PCM(CH_2Cl_2) isosurface contour plots (± 0.03 a.u.) of the NTO pairs computed at the optimized ${}^3\text{MC}_{\text{ax}}$ minima of complexes **1** (a and b), **2** (c and d) and **3** (e).

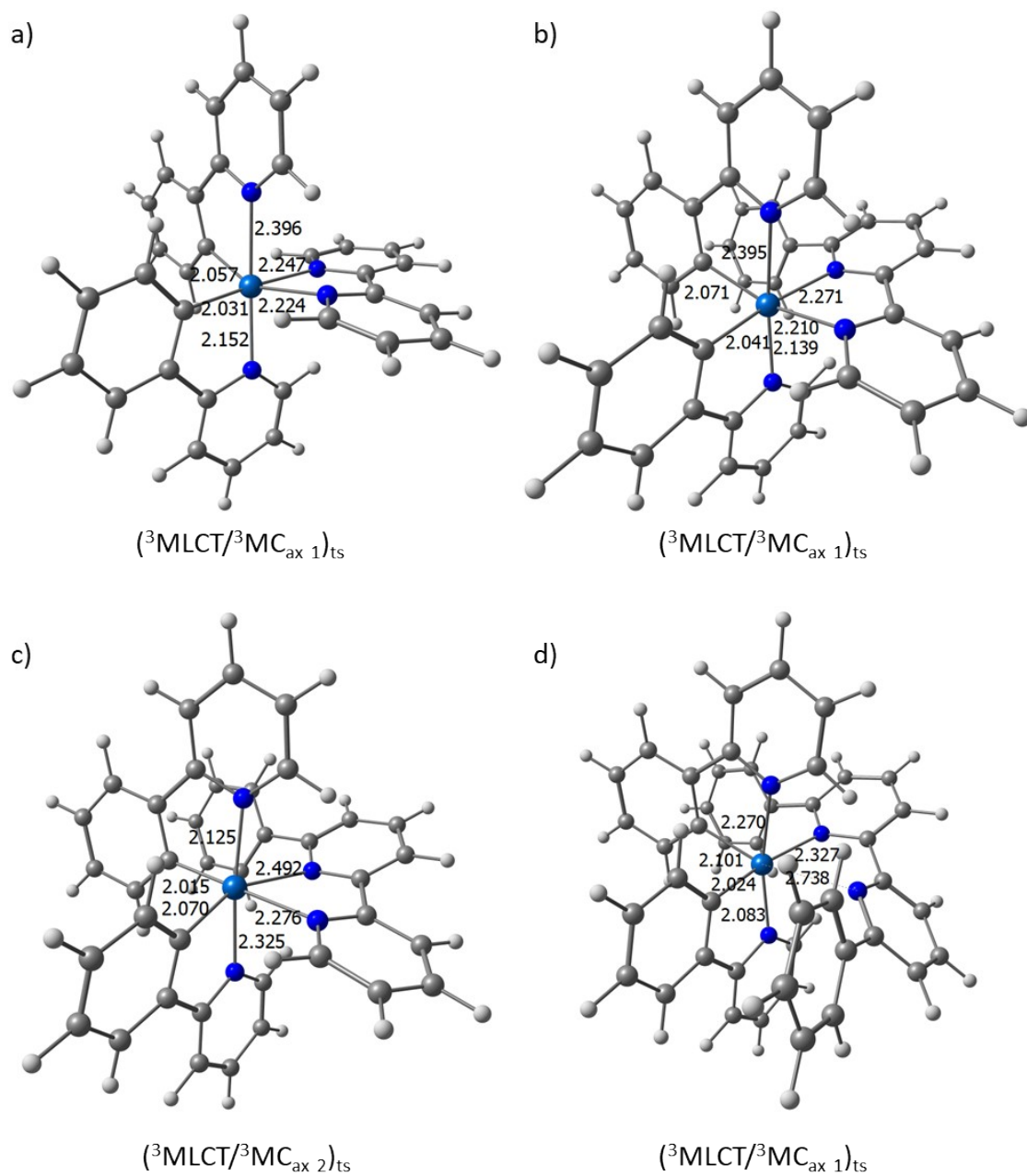


Fig. S12 B3LYP/DEF2-SVP-CPCM(CH_2Cl_2) transition state geometries connecting the ${}^3\text{MLCT}$ and ${}^3\text{MC}_{\text{ax}}$ minima for complexes **1** (a), **2** (b and c) and **3** (d).

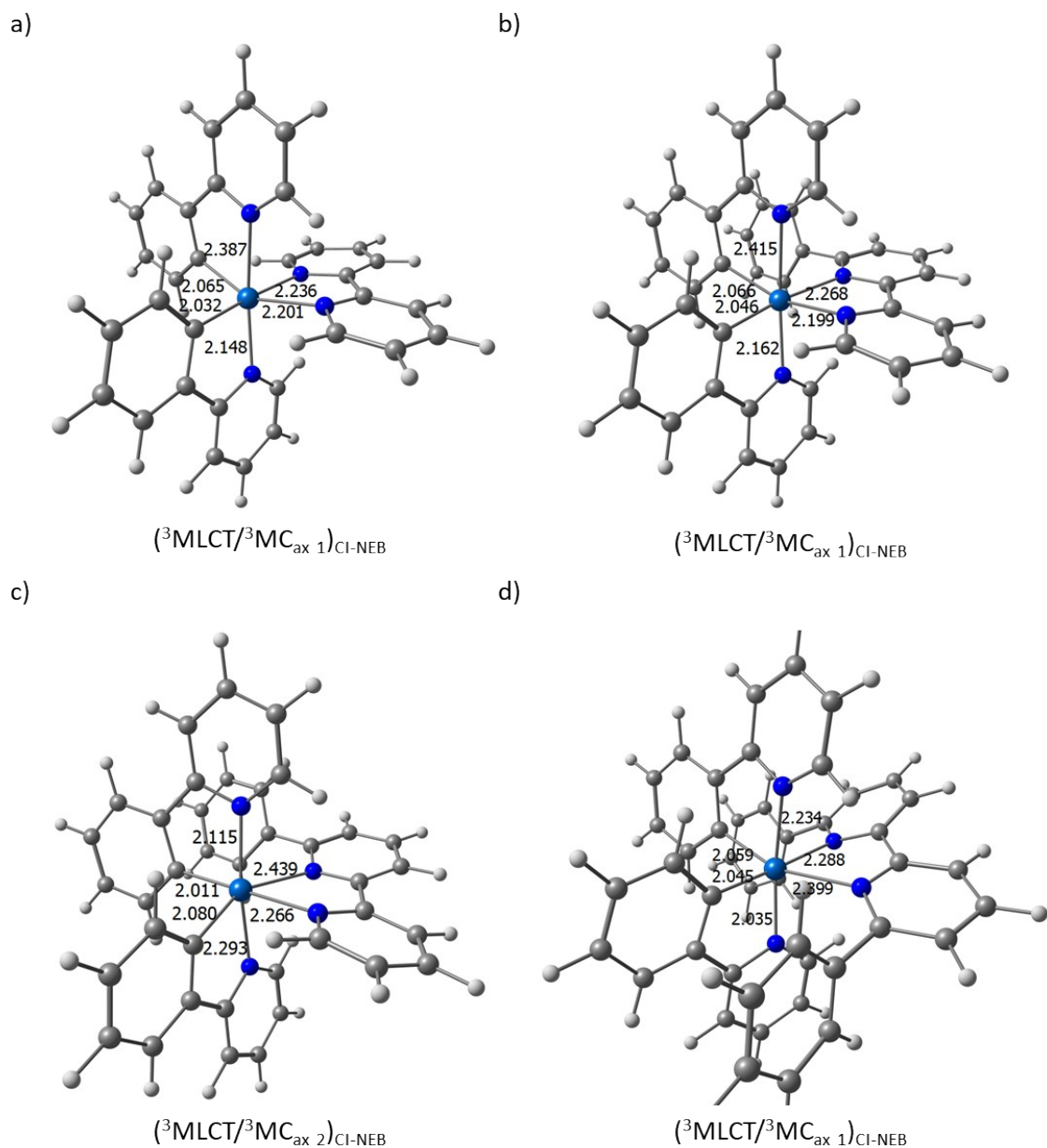


Fig. S13 B3LYP/DEF2-SVP-CPCM(CH_2Cl_2) geometries of the climbing image along the MEP obtained with the CI-NEB method connecting the ${}^3\text{MLCT}$ and ${}^3\text{MC}_{\text{ax}}$ minima for complexes **1** (a), **2** (b and c) and **3** (d).

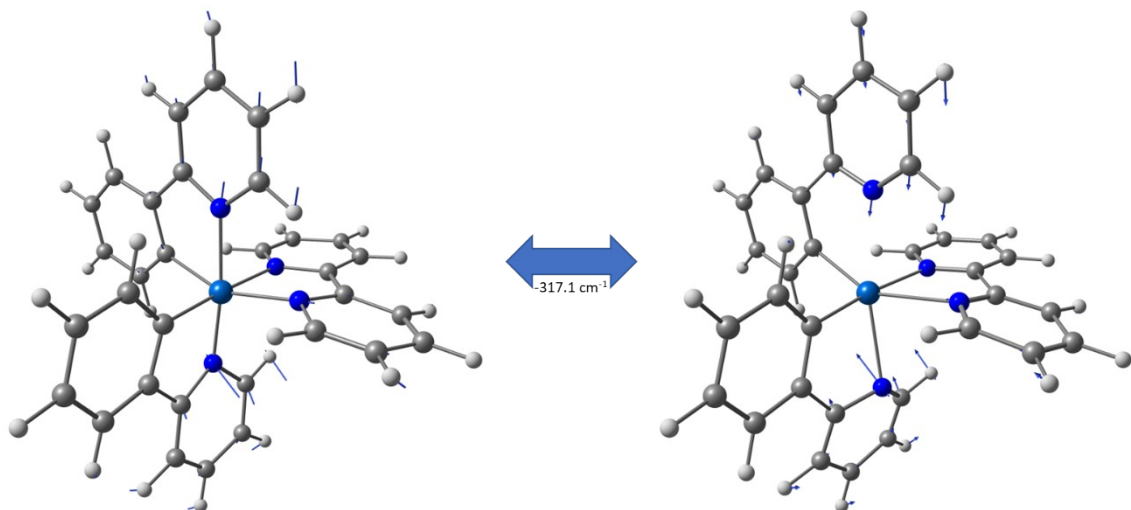


Fig. S14 Imaginary frequency characterizing the $({}^3\text{MLCT}/{}^3\text{MC}_{\text{ax}} 1)_{\text{ts}}$ transition state in complex **1**.

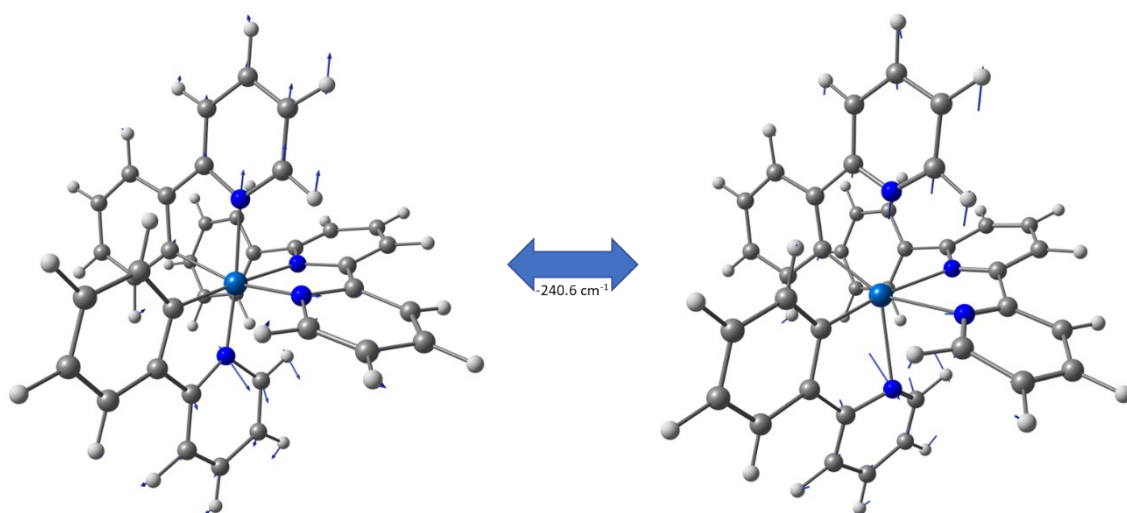


Fig. S15 Imaginary frequency characterizing the (${}^3\text{MLCT}/{}^3\text{MC}_{\text{ax}1}$)_{ts} transition state in complex 2.

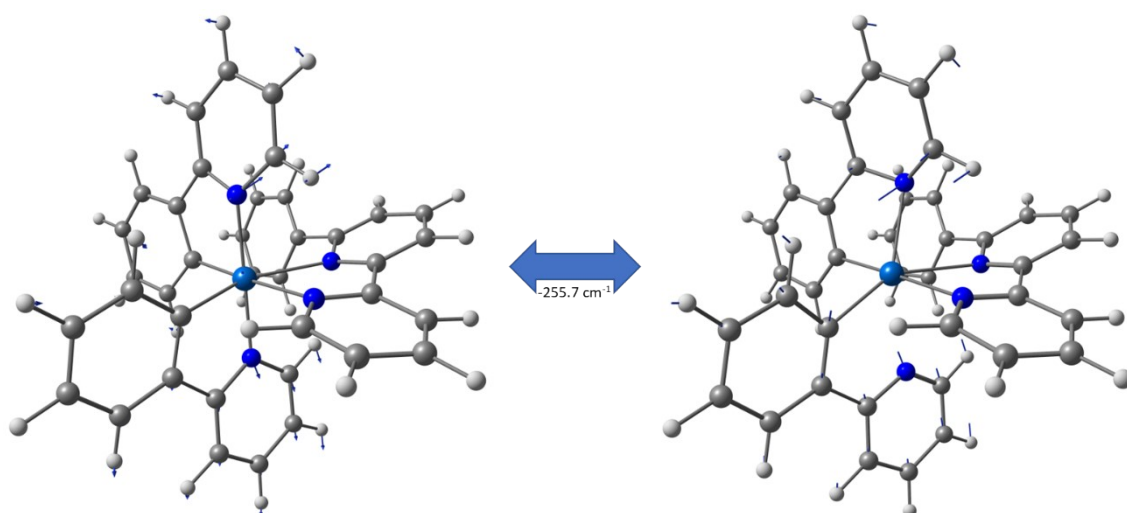


Fig. S16 Imaginary frequency characterizing the (${}^3\text{MLCT}/{}^3\text{MC}_{\text{ax}2}$)_{ts} transition state in complex 2.

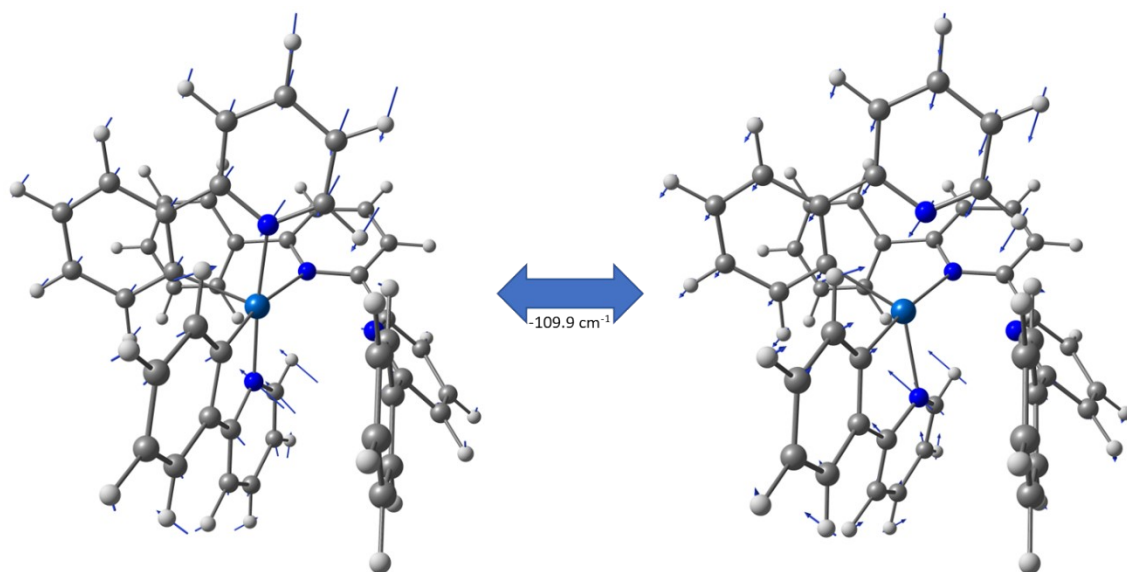


Fig. S17 Imaginary frequency characterizing the (${}^3\text{MLCT}/{}^3\text{MC}_{\text{ax}1}$)_{ts} transition state in complex 3.

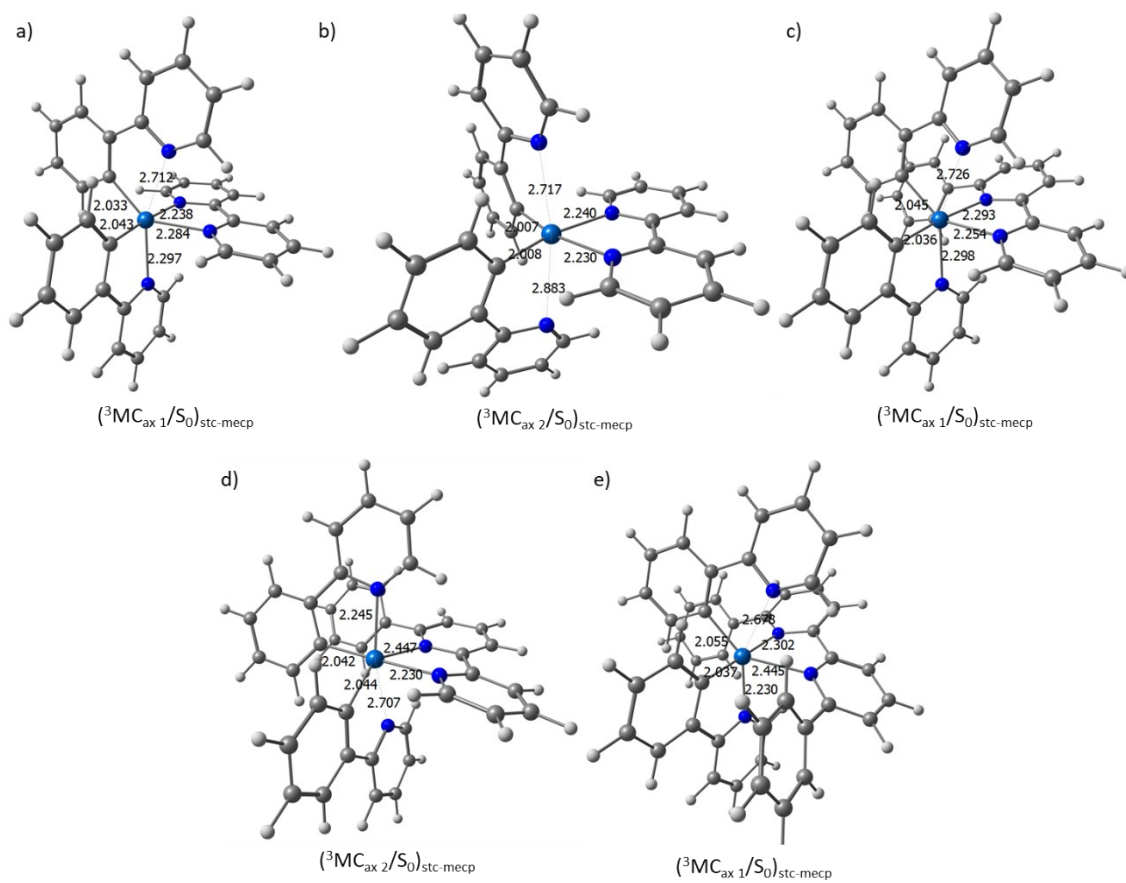


Fig. S18 B3LYP/DEF2-SVP-CPCM(CH_2Cl_2) minimum energy crossing point geometries between the ${}^3\text{MC}_{\text{ax}}$ and S_0 states ($({}^3\text{MC}_{\text{ax}}/S_0)_{\text{stc-mecp}}$) for complexes **1** (a and b), **2** (c and d) and **3** (e).

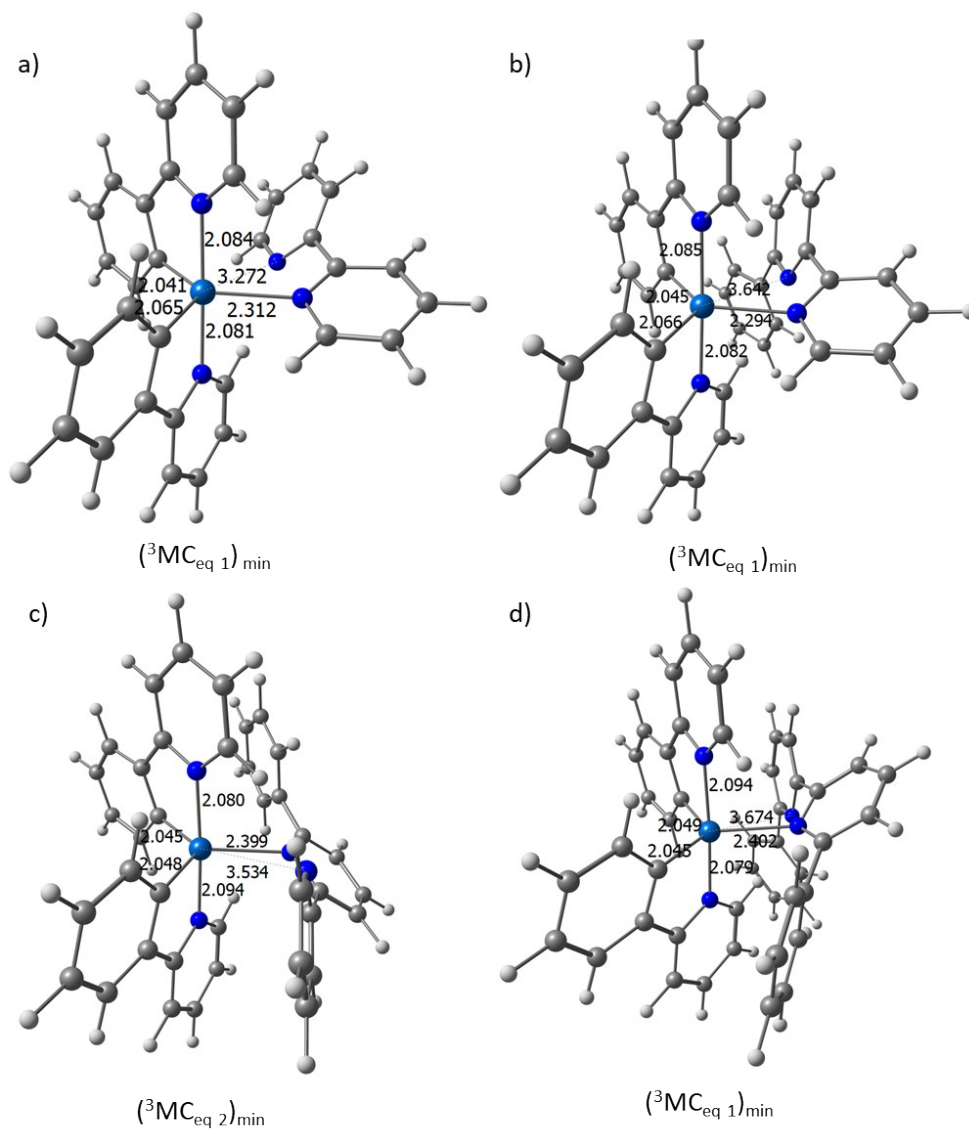


Fig. S19. B3LYP/DEF2-SVP-CPCM(CH_2Cl_2) optimized $^3MC_{eq}$ minima calculated for complexes **1** (a), **2** (b and c) and **3** (d).

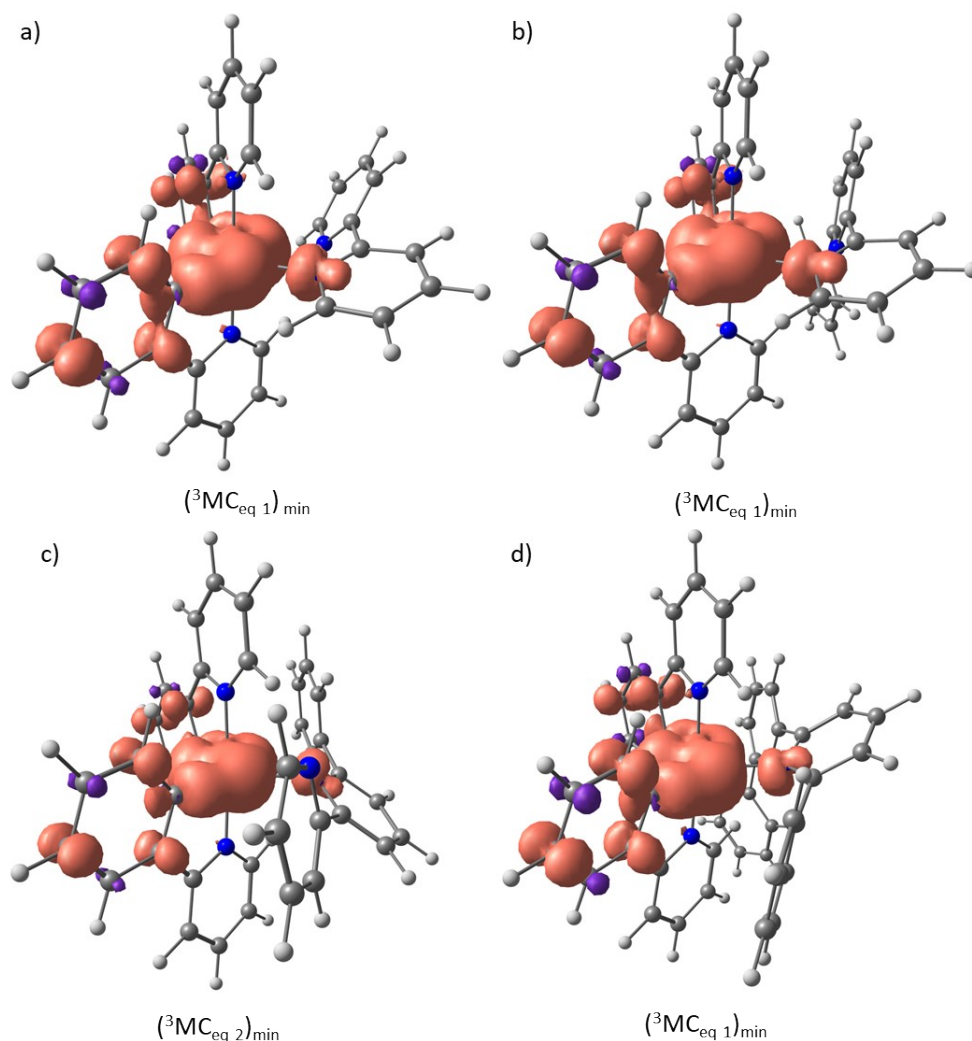


Fig. S20 B3LYP/DEF2-SVP-PCPM(CH_2Cl_2) isosurface contour plots (± 0.004 a.u.) of the unpaired-electron spin density computed at the optimized $^3\text{MC}_{\text{eq}}$ minima for complex **1** (a), **2** (b and c) and **3** (d).

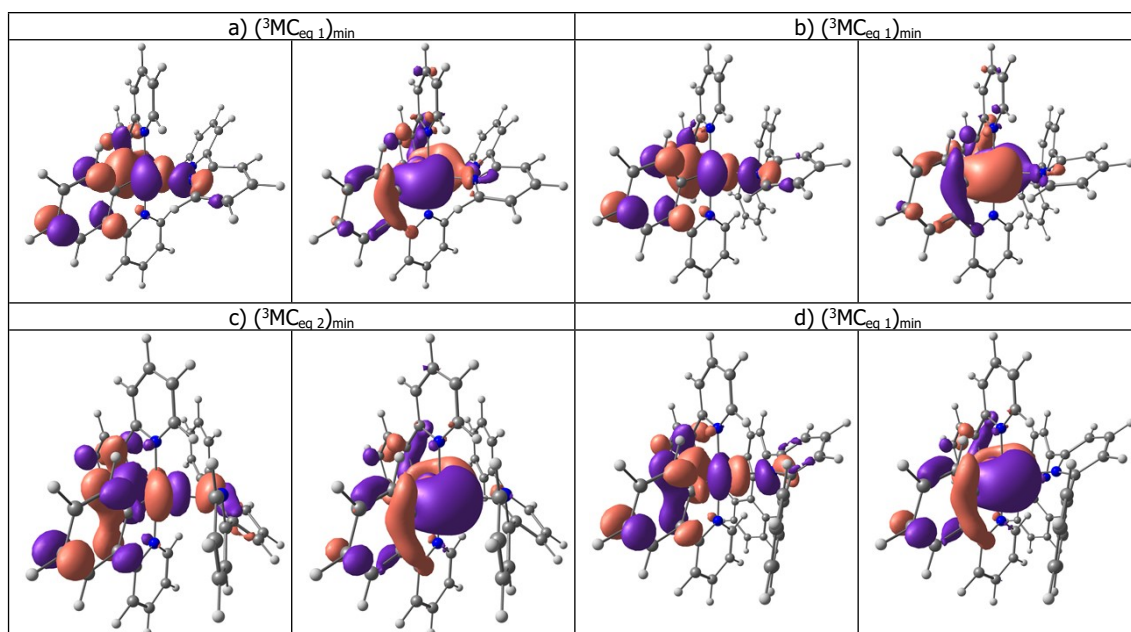


Fig. S21 B3LYP/DEF2-SVP-PCPM(CH_2Cl_2) isosurface contour plots (± 0.03 a.u.) of the NTO pairs computed at the optimized $^3\text{MC}_{\text{eq}}$ minima of complexes **1** (a), **2** (b and c) and **3** (d).

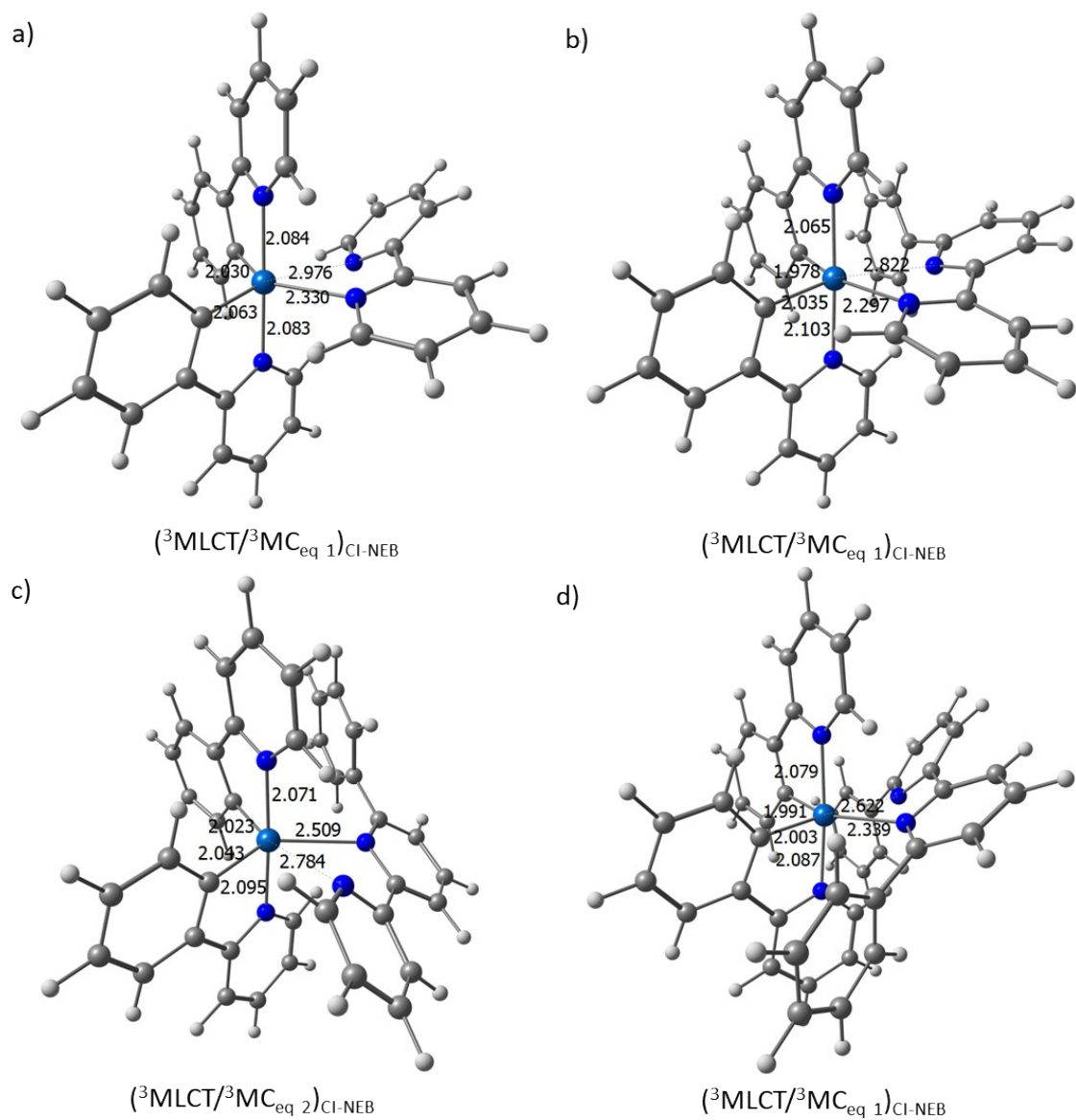


Fig. S22 B3LYP/DEF2-SVP-CPCM(CH_2Cl_2) geometries of the climbing image along the MEP obtained with the CI-NEB method connecting the ${}^3\text{MLCT}$ and ${}^3\text{MC}_{\text{eq}}$ minima for complexes **1** (a), **2** (b and c) and **3** (d).

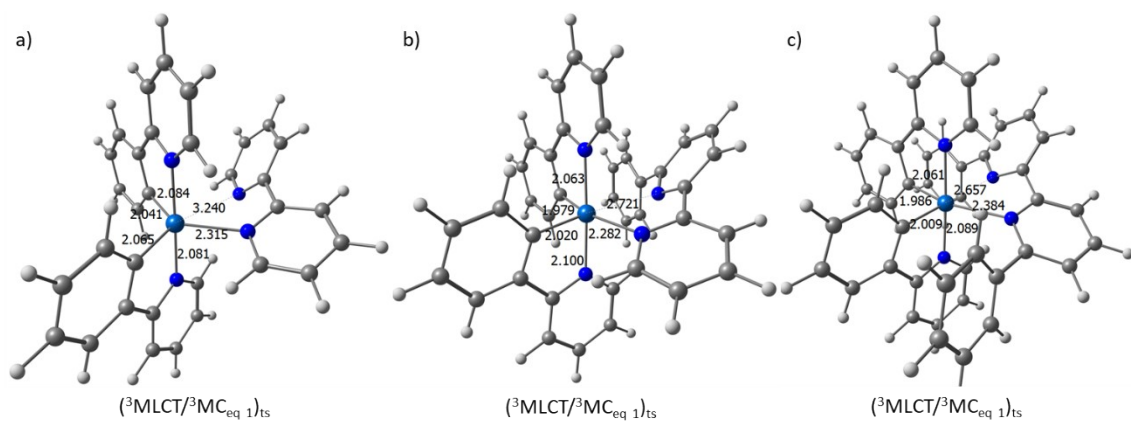


Fig. S23 B3LYP/DEF2-SVP-CPCM(CH_2Cl_2) transition state geometries connecting the ${}^3\text{MLCT}$ and ${}^3\text{MC}_{\text{eq}}$ minima for complexes **1** (a), **2** (b) and **3** (c).

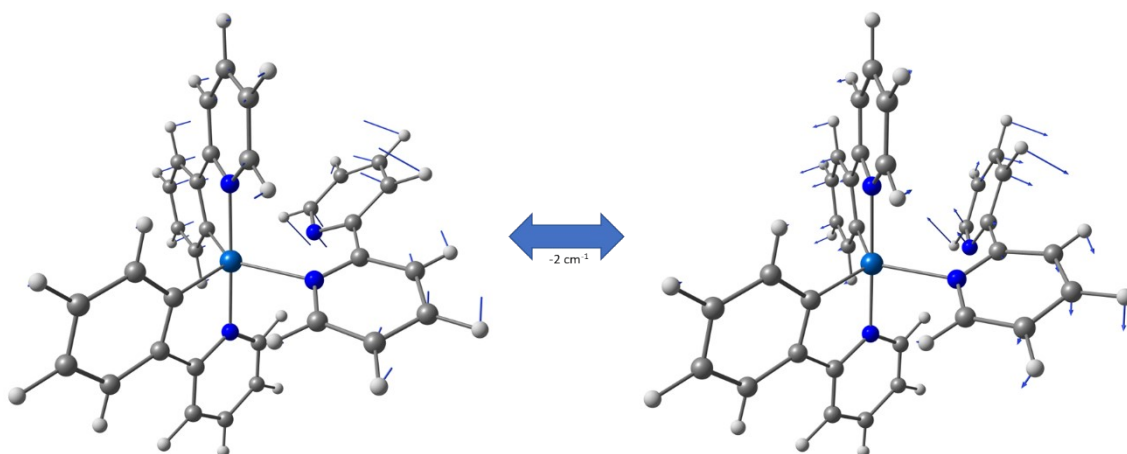


Fig. S24 Imaginary frequency characterizing the (${}^3\text{MLCT}/{}^3\text{MC}_{\text{eq}1}$)_{ts} transition state in complex **1**.

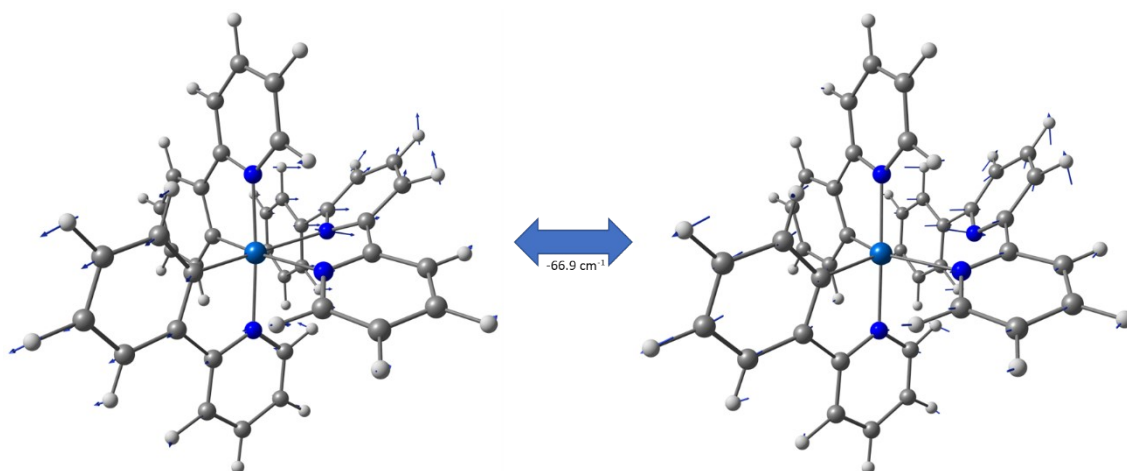


Fig. S25 Imaginary frequency characterizing the (${}^3\text{MLCT}/{}^3\text{MC}_{\text{eq}1}$)_{ts} transition state in complex **2**.

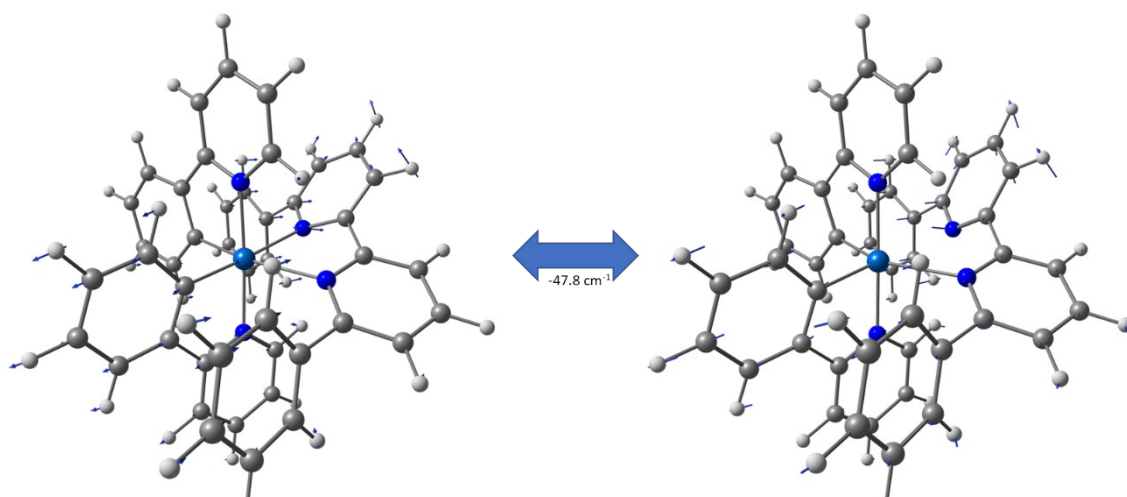


Fig. S26 Imaginary frequency characterizing the (${}^3\text{MLCT}/{}^3\text{MC}_{\text{eq}1}$)_{ts} transition state in complex **3**.

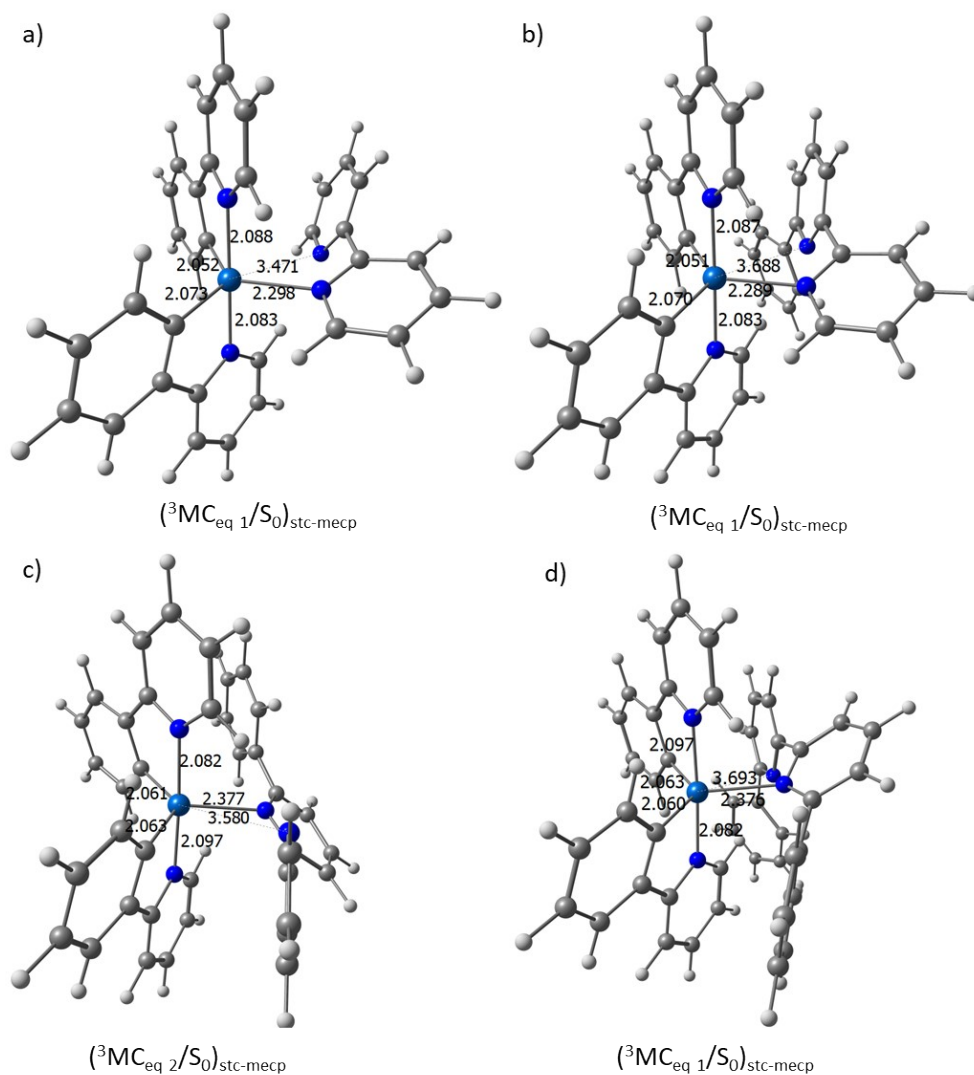


Fig. S27 B3LYP/DEF2-SVP-CPCM(CH₂Cl₂) minimum energy crossing point geometries between the ³MC_{eq} and S₀ states for complexes **1** (a), **2** (b and c) and **3** (d).

Table S2: DFT B3LYP/DEF2-SVP-CPCM(CH₂Cl₂) energy differences (eV) for evolving from the (MLCT)_{min} minimum to the (³MC_{ax})_{min} and the (³MC_{eq})_{min} minima for complexes **1**, **2** and **3**.

	Complex	ΔE^a	TS ^b	CI-NEB ^c
(³ MC _{ax 1}) _{min}	1	0.61	0.76	0.78
(³ MC _{ax 1}) _{min}	2	0.48	0.67	0.76
(³ MC _{ax 2}) _{min}	2	0.55	0.70	0.74
(³ MC _{ax 1}) _{min}	3	0.28	0.46	0.62
(³ MC _{eq 1}) _{min}	1	0.61	0.61	0.63
(³ MC _{eq 1}) _{min}	2	0.13	0.30	0.45
(³ MC _{eq 2}) _{min}	2	0.46	-	0.58
(³ MC _{eq 1}) _{min}	3	-0.18	0.16	0.31

^a Energy difference between the (MLCT)_{min} and the MC minimum.

^b Energy difference between the (MLCT)_{min} and the TS connecting the two minima.

^c Energy difference between the (MLCT)_{min} and the climbing image between the two minima.

```

!ZOOM-NEB-CI B3LYP DEF2-SVP SARC/J RIJCOSX RI-SOMF(1X) CPCM(CH2Cl2) UHF
%NEB
  PREOPT_ENDS FALSE
  NEB_END_XYZFILE "product.xyz"
  Restart_ALLXYZFile "orca_MEP.allxyz"
END
%SCF
  MAXITER 7500
END
%PAL
  NPROCS 64
END
%geom
  maxIter 950
end
* xyz 1 3

```

Fig. S28 Orca input file used in order to perform a CI-NEB calculation between two given minima belonging to the same spin multiplicity, so to obtain the corresponding climbing-image geometry.

```

!OPTTS slowConv tightscf B3LYP DEF2-SVP SARC/J RIJCOSX RI-SOMF(1X) CPCM(CH2Cl2) UHF FREQ
%SCF
  MAXITER 7500
END
%PAL
  NPROCS 12
END
%geom
  maxIter 950
  Calc_hess TRUE
end
%MAXCORE 4000
* xyz 1 3

```

Fig. S29 Orca input file used to localize the TS starting from the climbing image structure.

Table S3: Cartesian coordinates (*x*, *y*, *z*, in Å) of the optimized structures for the studied complexes. The level of theory employed in each optimization is specified.

Complex 1 in CH₂Cl₂.

(S₀)_{min} DFT B3LYP/DEF2-SVP CPCM

C	1.206330000	3.918871000	-1.328508000
C	1.067160000	2.692331000	-0.657390000
N	0.171109000	1.765914000	-1.113317000
C	-0.569112000	2.027845000	-2.208211000
C	1.820767000	2.280126000	0.532571000
C	1.518603000	0.979600000	1.028377000
C	2.223187000	0.541256000	2.165545000
C	3.178386000	1.353734000	2.788071000
C	3.461323000	2.633158000	2.288431000
C	2.782543000	3.094404000	1.161237000
Ir	0.068723000	0.000160000	0.000104000
N	0.177063000	-1.765190000	1.113539000
C	1.075834000	-2.688852000	0.657358000
C	1.219106000	-3.914873000	1.328566000
C	-0.456456000	-3.224330000	2.911053000
C	-0.561908000	-2.029301000	2.208751000
C	1.827771000	-2.274322000	-0.532858000
C	1.521569000	-0.974650000	-1.028405000
C	2.224575000	-0.533978000	-2.165640000
C	3.182087000	-1.343449000	-2.788527000
C	3.468930000	-2.622128000	-2.289212000
C	2.791788000	-3.085617000	-1.161949000
H	4.208447000	3.265103000	2.775372000
H	3.006396000	4.091363000	0.773487000

H	2.031644000	-0.452251000	2.579195000
H	3.710245000	0.984894000	3.670516000
H	2.029913000	0.459018000	-2.579055000
H	3.018623000	-4.082004000	-0.774473000
H	3.712660000	-0.972840000	-3.671005000
H	4.217794000	-3.251766000	-2.776470000
H	-1.259856000	1.246286000	-2.526266000
C	0.438726000	4.188394000	-2.457220000
H	1.920556000	4.656447000	-0.961844000
H	0.546082000	5.141206000	-2.981484000
C	-0.467667000	3.223277000	-2.910429000
H	-1.088753000	3.386429000	-3.792779000
C	0.452750000	-4.186673000	2.457585000
H	-1.254974000	-1.249869000	2.526979000
H	-1.076703000	-3.389318000	3.793651000
H	0.563267000	-5.139089000	2.981913000
H	1.935542000	-4.650243000	0.961762000
C	-2.746451000	-2.270055000	-2.671140000
C	-2.909651000	0.474851000	0.567441000
C	-4.088494000	0.974778000	1.139488000
C	-4.010634000	1.875803000	2.200801000
C	-2.754131000	2.261331000	2.670910000
C	-1.622196000	1.724014000	2.060035000
N	-1.695268000	0.853055000	1.040555000
H	-5.063301000	0.667380000	0.762434000
H	-4.923525000	2.271007000	2.652378000
H	-2.642099000	2.965296000	3.497610000
H	-0.618038000	1.993063000	2.394584000
C	-2.908020000	-0.484696000	-0.567160000
C	-4.085145000	-0.988591000	-1.139239000
C	-4.004248000	-1.889040000	-2.200815000
C	-1.616352000	-1.729007000	-2.060161000
N	-1.692368000	-0.858610000	-1.040413000
H	-5.060971000	-0.684637000	-0.762054000
H	-4.915796000	-2.287272000	-2.652441000
H	-2.632030000	-2.973366000	-3.498067000
H	-0.611287000	-1.994495000	-2.394834000

(³MLCT)_{min} DFT B3LYP/DEF2-SVP CPCM

C	-3.889732000	1.167016000	-1.477813000
C	-2.685158000	1.064891000	-0.768272000
N	-1.706642000	0.219188000	-1.204053000
C	-1.891717000	-0.523546000	-2.309070000
C	-2.349911000	1.800233000	0.458557000
C	-1.070547000	1.505908000	1.031979000
C	-0.705205000	2.167283000	2.225832000
C	-1.556133000	3.103224000	2.813270000
C	-2.799903000	3.393832000	2.227791000
C	-3.196259000	2.745628000	1.054095000
Ir	0.000019000	0.158314000	-0.000034000
N	1.706703000	0.218117000	1.204008000
C	2.685710000	1.063285000	0.768295000
C	3.890330000	1.164688000	1.477864000
C	3.067957000	-0.461798000	3.051006000
C	1.891335000	-0.524785000	2.308987000
C	2.350915000	1.798876000	-0.458507000
C	1.071400000	1.505307000	-1.031982000
C	0.706497000	2.166918000	-2.225840000

C	1.557999000	3.102369000	-2.813226000
C	2.801906000	3.392253000	-2.227683000
C	3.197833000	2.743801000	-1.053980000
H	-3.464202000	4.127594000	2.691137000
H	-4.165764000	2.987209000	0.613143000
H	0.257265000	1.955592000	2.696641000
H	-1.254906000	3.614920000	3.731339000
H	-0.256077000	1.955805000	-2.696701000
H	4.167456000	2.984818000	-0.612979000
H	1.257113000	3.614249000	-3.731304000
H	3.466651000	4.125640000	-2.690985000
H	-1.069001000	-1.178993000	-2.596992000
C	-4.083315000	0.401817000	-2.626236000
H	-4.671312000	1.841293000	-1.127543000
H	-5.019802000	0.476102000	-3.184123000
C	-3.068320000	-0.459858000	-3.051058000
H	-3.176727000	-1.078701000	-3.943296000
C	4.083450000	0.399325000	2.626256000
H	1.068241000	-1.179782000	2.596851000
H	3.175993000	-1.080746000	3.943217000
H	5.019965000	0.473056000	3.184169000
H	4.672300000	1.838533000	1.127636000
C	2.393315000	-2.645714000	-2.568201000
C	-0.483597000	-2.825895000	0.525755000
C	-1.033330000	-4.007595000	1.111214000
C	-1.972033000	-3.924923000	2.113783000
C	-2.394811000	-2.644419000	2.568149000
C	-1.832708000	-1.526791000	1.979792000
N	-0.902948000	-1.585143000	0.998371000
H	-0.705316000	-4.984596000	0.754824000
H	-2.387306000	-4.835054000	2.554022000
H	-3.136703000	-2.529254000	3.359795000
H	-2.124523000	-0.526170000	2.305501000
C	0.481995000	-2.826159000	-0.525816000
C	1.031171000	-4.008158000	-1.111198000
C	1.969927000	-3.925989000	-2.113760000
C	1.831744000	-1.527782000	-1.979913000
N	0.901949000	-1.585635000	-0.998495000
H	0.702695000	-4.984983000	-0.754751000
H	2.384776000	-4.836345000	-2.553934000
H	3.135265000	-2.530950000	-3.359852000
H	2.124034000	-0.527319000	-2.305678000

(³MC_{ax 1})_{min} DFT B3LYP/DEF2-SVP CPCM

Ir	-0.015920000	0.009100000	-0.431145000
N	-1.124490000	-0.925435000	1.739624000
N	1.711666000	0.703485000	-1.768586000
C	-3.119658000	-2.044054000	2.433299000
C	-2.324320000	-1.459774000	1.427251000
C	-0.681949000	-0.952771000	2.999530000
C	-2.714846000	-1.393571000	0.000638000
C	-1.828059000	-0.786120000	-0.924531000
C	-2.210525000	-0.717120000	-2.279035000
C	-3.426151000	-1.252245000	-2.720800000
C	-4.297074000	-1.852637000	-1.804392000
C	-3.942533000	-1.915312000	-0.457407000
C	2.425806000	-0.338750000	-2.266843000
C	3.410198000	-0.100481000	-3.242705000

C	2.888805000	2.254250000	-3.162439000
C	1.928764000	1.955283000	-2.199722000
C	2.077366000	-1.666019000	-1.720069000
C	0.957990000	-1.741445000	-0.838425000
C	0.635283000	-3.008015000	-0.313396000
C	1.375957000	-4.150319000	-0.635986000
C	2.471832000	-4.059263000	-1.503855000
C	2.818110000	-2.820635000	-2.042523000
H	-5.251983000	-2.267503000	-2.137025000
H	-4.637445000	-2.380896000	0.244410000
H	-1.548254000	-0.245371000	-3.013014000
H	-3.691706000	-1.195587000	-3.780399000
H	-0.216270000	-3.110364000	0.362997000
H	3.679285000	-2.757025000	-2.711954000
H	1.095531000	-5.118074000	-0.209181000
H	3.054853000	-4.948546000	-1.757094000
H	0.300221000	-0.510672000	3.188146000
C	-2.659978000	-2.070857000	3.747987000
H	-4.090166000	-2.477084000	2.191467000
H	-3.271158000	-2.523762000	4.533037000
C	-1.411936000	-1.516100000	4.046582000
H	-1.008826000	-1.517985000	5.061356000
C	3.641482000	1.198542000	-3.690138000
H	1.313967000	2.740464000	-1.751196000
H	3.040001000	3.285837000	-3.485660000
H	4.403852000	1.386706000	-4.450522000
H	3.985219000	-0.929679000	-3.655287000
C	3.166542000	0.966691000	2.636972000
C	-0.329720000	2.737979000	0.994422000
C	-0.845020000	3.990369000	1.357198000
C	-1.971265000	4.487715000	0.702903000
C	-2.557926000	3.721880000	-0.305367000
C	-1.999480000	2.481436000	-0.610321000
N	-0.918394000	1.996572000	0.021659000
H	-0.371442000	4.578327000	2.142746000
H	-2.380246000	5.462817000	0.977510000
H	-3.437078000	4.068815000	-0.851593000
C	0.886856000	2.161569000	1.619247000
C	1.633618000	2.824406000	2.604971000
C	2.781420000	2.220634000	3.117355000
C	2.376342000	0.360040000	1.662226000
N	1.271227000	0.943236000	1.174823000
H	1.328327000	3.804777000	2.969122000
H	3.370368000	2.728927000	3.884419000
H	4.059556000	0.460042000	3.007495000
H	2.626959000	-0.622659000	1.256133000
H	-2.433586000	1.846230000	-1.384917000

(³MC_{eq 1})_{min} DFT B3LYP/DEF2-SVP CPCM.

Ir	-0.309345000	0.455344000	0.153507000
N	0.684976000	-1.996816000	-1.770504000
N	-0.903296000	-1.726529000	0.637282000
N	1.444493000	0.304281000	1.269701000
N	-2.046210000	0.649088000	-0.976230000
C	1.636081000	-1.934383000	-2.706264000
C	3.090496000	-3.385941000	-1.466347000
C	2.098109000	-3.461383000	-0.486626000
C	0.903469000	-2.748791000	-0.681380000

C	-1.958648000	-1.829691000	1.467479000
C	-2.367008000	-3.037717000	2.028036000
C	-1.645010000	-4.191373000	1.718997000
C	-0.560711000	-4.088960000	0.849042000
C	-0.211717000	-2.841790000	0.306937000
C	2.855626000	-2.612227000	-2.604812000
C	3.879810000	0.153076000	2.606464000
C	-3.451005000	0.099447000	-2.835281000
C	-4.417464000	0.999966000	-2.373813000
C	3.342389000	2.028489000	-1.400285000
C	3.045050000	2.553587000	-2.659047000
C	1.747786000	2.429736000	-3.182159000
C	0.750261000	1.777793000	-2.452262000
C	1.025911000	1.229784000	-1.182478000
C	2.347528000	1.368196000	-0.658181000
C	1.519201000	-0.256802000	2.493332000
C	2.715240000	-0.355150000	3.194612000
C	3.804317000	0.732146000	1.342749000
C	2.571760000	0.800275000	0.675012000
C	-3.405482000	3.131923000	1.413558000
C	-2.994163000	3.679455000	2.631260000
C	-1.797093000	3.253145000	3.225408000
C	-1.009586000	2.278779000	2.603176000
C	-1.406871000	1.700798000	1.382118000
C	-2.623900000	2.147784000	0.784859000
C	-2.275470000	-0.047694000	-2.105819000
C	-2.986835000	1.512627000	-0.491300000
C	-4.184398000	1.706030000	-1.195419000
H	1.420193000	-1.312235000	-3.581790000
H	3.599428000	-2.528863000	-3.400443000
H	4.033898000	-3.923026000	-1.338864000
H	2.252786000	-4.050146000	0.419684000
H	-2.485769000	-0.901920000	1.700427000
H	-3.232035000	-3.060000000	2.693542000
H	-1.928873000	-5.160305000	2.137083000
H	0.004136000	-4.976343000	0.559316000
H	4.700654000	1.128601000	0.864953000
H	4.837742000	0.096364000	3.129042000
H	2.725625000	-0.817766000	4.182990000
H	0.583349000	-0.629294000	2.914304000
H	-3.598078000	-0.482500000	-3.746760000
H	-5.350110000	1.144646000	-2.924684000
H	-4.933674000	2.399758000	-0.812801000
H	-1.480967000	-0.735729000	-2.405588000
H	3.821985000	3.066106000	-3.231987000
H	1.516211000	2.845103000	-4.167417000
H	4.351881000	2.144241000	-0.998096000
H	-0.250911000	1.697543000	-2.882984000
H	-1.477861000	3.685243000	4.178401000
H	-0.077532000	1.967388000	3.082428000
H	-4.334910000	3.481771000	0.957672000
H	-3.605458000	4.444861000	3.116249000

(³MC_{ax 2})_{min} DFT B3LYP/DEF2-SVP CPCM.

C	-4.126579000	1.412473000	-1.472208000
C	-2.900943000	1.120724000	-0.839887000
N	-2.074729000	0.196799000	-1.373904000
C	-2.407099000	-0.454967000	-2.491104000

C	-2.434503000	1.773075000	0.410703000
C	-1.130051000	1.464310000	0.915921000
C	-0.711828000	2.116822000	2.098236000
C	-1.536013000	3.017465000	2.776714000
C	-2.810378000	3.306693000	2.272573000
C	-3.249107000	2.692076000	1.097536000
Ir	0.000073000	0.051955000	0.000024000
N	2.074936000	0.195433000	1.373897000
C	2.901488000	1.119261000	0.840243000
C	4.127016000	1.410667000	1.472923000
C	3.604215000	-0.223219000	3.168192000
C	2.406854000	-0.456528000	2.491116000
C	2.435642000	1.771709000	-0.410519000
C	1.131135000	1.463557000	-0.915938000
C	0.713454000	2.116165000	-2.098390000
C	1.538217000	3.016311000	-2.776821000
C	2.812650000	3.304919000	-2.272498000
C	3.250856000	2.690193000	-1.097327000
H	-3.463469000	4.013228000	2.791571000
H	-4.245044000	2.936488000	0.723286000
H	0.284523000	1.908963000	2.495947000
H	-1.185087000	3.499792000	3.693620000
H	-0.282939000	1.908776000	-2.496248000
H	4.246876000	2.934079000	-0.722949000
H	1.187691000	3.498741000	-3.693825000
H	3.466201000	4.011048000	-2.791470000
H	-1.685361000	-1.191934000	-2.860048000
C	-4.476400000	0.736938000	-2.640004000
H	-4.802234000	2.162684000	-1.061004000
H	-5.424831000	0.958635000	-3.136291000
C	-3.604619000	-0.221363000	-3.167789000
H	-3.842359000	-0.773484000	-4.079493000
C	4.476350000	0.734959000	2.640764000
H	1.684859000	-1.193374000	2.859796000
H	3.841568000	-0.775477000	4.079913000
H	5.424669000	0.956424000	3.137368000
H	4.802943000	2.160771000	1.061976000
C	2.683937000	-2.789532000	-2.243796000
C	-0.570747000	-2.947158000	0.473963000
C	-1.164821000	-4.125063000	0.950044000
C	-2.231836000	-4.046044000	1.843221000
C	-2.685737000	-2.788001000	2.243227000
C	-2.055657000	-1.657598000	1.727068000
N	-1.026899000	-1.731110000	0.865421000
H	-0.801192000	-5.099606000	0.626107000
H	-2.700834000	-4.957837000	2.220228000
H	-3.515909000	-2.673013000	2.942628000
H	-2.380845000	-0.655042000	2.011141000
C	0.569105000	-2.947469000	-0.474251000
C	1.162396000	-4.125712000	-0.950450000
C	2.229328000	-4.047313000	-1.843785000
C	2.054648000	-1.658767000	-1.727461000
N	1.025974000	-1.731674000	-0.865670000
H	0.798222000	-5.100047000	-0.626510000
H	2.697700000	-4.959380000	-2.220906000
H	3.514075000	-2.675021000	-2.943316000
H	2.380446000	-0.656401000	-2.011507000

(³MLCT/³MC_{ax 1})_{CI-NEB} DFT B3LYP/DEF2-SVP CPCM.

Ir	0.043970656	-0.049833869	-0.269752400
N	-1.149984932	-0.918437969	1.605485711
N	1.519468188	0.615355430	-1.681403247
C	-3.190253659	-1.965888371	2.290653856
C	-2.363298292	-1.427785502	1.287904511
C	-0.725646195	-0.931897484	2.874393727
C	-2.703088345	-1.363814159	-0.144026255
C	-1.759902248	-0.742878291	-0.997503193
C	-2.053775584	-0.628811672	-2.367265535
C	-3.241970855	-1.158127272	-2.889346048
C	-4.168146372	-1.778538718	-2.041760797
C	-3.901856245	-1.875443051	-0.675059545
C	2.285302384	-0.390464722	-2.206162488
C	3.193317618	-0.105119692	-3.235502460
C	2.504440605	2.206235718	-3.180444103
C	1.623920948	1.873282137	-2.157608438
C	2.054294805	-1.715694189	-1.607761793
C	1.010228257	-1.798218477	-0.639972679
C	0.760522331	-3.051306744	-0.050960738
C	1.508597544	-4.181157467	-0.401134470
C	2.533540537	-4.084026729	-1.351593879
C	2.805096361	-2.853836621	-1.953166295
H	-5.100695007	-2.181561329	-2.445052277
H	-4.634425378	-2.356426889	-0.022493247
H	-1.350321673	-0.135230593	-3.044933537
H	-3.445849980	-1.077106712	-3.961041666
H	-0.035274118	-3.155321068	0.689775296
H	3.609361314	-2.787146404	-2.689601066
H	1.287721456	-5.144799357	0.066877922
H	3.119859870	-4.965481891	-1.623617687
H	0.260943060	-0.509060165	3.065842388
C	-2.747941529	-1.982740585	3.611791717
H	-4.172337469	-2.366629636	2.037365687
H	-3.380622835	-2.401800459	4.398607803
C	-1.488551940	-1.458002258	3.915933285
H	-1.097502305	-1.451084896	4.935403904
C	3.306962017	1.196008385	-3.724842366
H	0.989090707	2.627479462	-1.689109901
H	2.564991488	3.238577987	-3.530068633
H	4.017477099	1.420712376	-4.524121990
H	3.810673926	-0.902106420	-3.651459708
C	3.295027065	0.956771867	2.590954793
C	-0.269653748	2.699486947	1.101838529
C	-0.794428546	3.955717320	1.467637297
C	-1.931380520	4.439728224	0.833983167
C	-2.534454257	3.663114593	-0.166746672
C	-1.979266614	2.424851413	-0.470259836
N	-0.884082862	1.942107520	0.144980752
H	-0.310779536	4.543502232	2.247536851
H	-2.344904295	5.411761416	1.113048350
H	-3.422941723	4.005091200	-0.700869883
C	0.960872329	2.148168134	1.669381853
C	1.833141899	2.872234870	2.508161961
C	2.994236455	2.277563080	2.981033169
C	2.407086099	0.291491186	1.762663982
N	1.258297685	0.858319212	1.324932519

H	1.597572825	3.900929287	2.781650956
H	3.667158677	2.830278654	3.640512424
H	4.196242570	0.448665775	2.938842628
H	2.588590534	-0.736384931	1.441165338
H	-2.424670245	1.784730169	-1.233717541

(³MLCT/³MC_{eq 1})_{CI-NEB} DFT B3LYP/DEF2-SVP CPCM.

Ir	-0.228945660	0.419112913	0.113849727
N	0.756240766	-1.849660969	-1.541606288
N	-0.875008183	-1.729348360	0.743942502
N	1.518636095	0.313116806	1.244064106
N	-1.962476734	0.561138914	-1.032830756
C	1.686034604	-1.787708813	-2.499140827
C	2.820010364	-3.722148245	-1.646609484
C	1.849406360	-3.791619381	-0.645517587
C	0.818097377	-2.836943970	-0.635820193
C	-1.892916385	-1.766581749	1.622876161
C	-2.361356373	-2.948809435	2.191862725
C	-1.753499588	-4.149109027	1.821576719
C	-0.710156412	-4.114642072	0.898468664
C	-0.280183881	-2.886239632	0.370685360
C	2.733164070	-2.708004537	-2.603456803
C	3.955999788	0.238992115	2.590180614
C	-3.357293193	-0.039964805	-2.884907662
C	-4.347103835	0.837801341	-2.428497998
C	3.315296261	2.303760982	-1.305102535
C	2.996211388	2.863059230	-2.542756449
C	1.719252476	2.663522142	-3.096195660
C	0.765422832	1.903904595	-2.416519552
C	1.064397555	1.316464698	-1.167225256
C	2.367635651	1.527169064	-0.615445899
C	1.622151380	-0.300875690	2.441195774
C	2.819058131	-0.364455087	3.144034675
C	3.850125277	0.878957988	1.359365560
C	2.618291395	0.907841749	0.686425491
C	-3.372703122	3.062805766	1.304500244
C	-2.980611303	3.639368659	2.514664231
C	-1.781974841	3.242297136	3.127342515
C	-0.975835493	2.266564657	2.532512454
C	-1.357261865	1.651810716	1.322890665
C	-2.575142206	2.072840368	0.706647185
C	-2.177208996	-0.150129788	-2.156473846
C	-2.922694692	1.408208439	-0.557789831
C	-4.127475634	1.562004668	-1.259208035
H	1.592216444	-0.965957970	-3.216995543
H	3.461953557	-2.623354419	-3.412730830
H	3.635693328	-4.449073842	-1.673967651
H	1.903295612	-4.564969810	0.122276898
H	-2.339741029	-0.805513255	1.886182725
H	-3.185655924	-2.915860995	2.906796592
H	-2.092665735	-5.101677211	2.235702082
H	-0.241671250	-5.040683175	0.563796283
H	4.722518174	1.351719419	0.907334629
H	4.914391984	0.208029114	3.114057389
H	2.852788226	-0.874882624	4.108177684
H	0.709263000	-0.747394606	2.839014187
H	-3.490482053	-0.632257348	-3.791882765
H	-5.286216585	0.950761145	-2.975623010

H	-4.892680206	2.238939047	-0.878712132
H	-1.366580174	-0.818427897	-2.454664141
H	3.739211754	3.460482772	-3.076912331
H	1.471959953	3.104856409	-4.066148602
H	4.304303590	2.482651460	-0.876076100
H	-0.221294809	1.769271837	-2.866850020
H	-1.478291176	3.698808701	4.074016057
H	-0.041463253	1.980382659	3.023834576
H	-4.298777717	3.394692451	0.828738325
H	-3.607659088	4.404956752	2.978654987

(³MLCT/³MC_{ax 2})_{CI-NEB} DFT B3LYP/DEF2-SVP CPCM.

C	-4.065958979	1.320726467	-1.494508912
C	-2.847487145	1.102276318	-0.823979199
N	-1.981487030	0.197172365	-1.322475918
C	-2.237226385	-0.489412818	-2.435152407
C	-2.413134017	1.792963404	0.422824007
C	-1.112681751	1.500968429	0.947447629
C	-0.714238706	2.155607376	2.136513757
C	-1.551992738	3.060436402	2.794016185
C	-2.814321883	3.350128667	2.259782358
C	-3.236745726	2.722429915	1.084033357
Ir	0.000053987	0.091072908	-0.000025859
N	1.981705396	0.195813579	1.322350613
C	2.848120958	1.100667144	0.824115289
C	4.066514516	1.318672051	1.494932421
C	3.419767825	-0.324085517	3.150774819
C	2.236930153	-0.490860621	2.435091102
C	2.414256643	1.791589062	-0.422719884
C	1.113672179	1.500330082	-0.947425835
C	0.715713515	2.155133536	-2.136563756
C	1.554057761	3.059426146	-2.794053277
C	2.816486121	3.348457341	-2.259698283
C	3.238440162	2.720586300	-1.083874513
H	-3.471015574	4.067295233	2.759512797
H	-4.225169557	2.965599482	0.689819540
H	0.271793966	1.950219163	2.562827797
H	-1.221871453	3.546570194	3.717596459
H	-0.270391055	1.950272704	-2.562965837
H	4.226961854	2.963223264	-0.689580398
H	1.224324341	3.545644388	-3.717726518
H	3.473636824	4.065217838	-2.759408505
H	-1.460538107	-1.192652997	-2.757781015
C	-4.348624161	0.601682546	-2.657272448
H	-4.788441898	2.043343377	-1.115205293
H	-5.294176560	0.761318900	-3.180299305
C	-3.420166993	-0.322195595	-3.150562564
H	-3.602143273	-0.900761259	-4.058501812
C	4.348668996	0.599475455	2.657725772
H	1.459885849	-1.193781912	2.757552145
H	3.601330252	-0.902741267	4.058740506
H	5.294158220	0.758761041	3.180973287
H	4.789313386	2.041095072	1.115858299
C	2.566730842	-2.745643558	-2.389504104
C	-0.546591463	-2.907830706	0.505769435
C	-1.116130418	-4.083284574	1.018185331
C	-2.135122288	-4.002209464	1.966889277
C	-2.568417850	-2.744237232	2.389189209

C	-1.964331739	-1.616120727	1.837335283
N	-0.983919357	-1.691729253	0.921487924
H	-0.772712180	-5.060077808	0.678582888
H	-2.586630159	-4.911202620	2.371813182
H	-3.362389608	-2.629423617	3.129642563
H	-2.273386190	-0.612703448	2.138317931
C	0.544913659	-2.908133394	-0.505979259
C	1.113787894	-4.083900827	-1.018419526
C	2.132769506	-4.003379159	-1.967181858
C	1.963310120	-1.617197877	-1.837597759
N	0.982901504	-1.692272796	-0.921705526
H	0.769862399	-5.060511867	-0.678803112
H	2.583751572	-4.912617893	-2.372139804
H	3.360713814	-2.631259249	-3.130011167
H	2.272910026	-0.613948093	-2.138577506

(³MLCT/³MC_{ax 1})_{ts} DFT B3LYP/DEF2-SVP CPCM.

Ir	0.061211000	-0.050083000	-0.199436000
N	-1.197092000	-0.950241000	1.630375000
N	1.544603000	0.620111000	-1.607172000
C	-3.250812000	-2.037370000	2.203589000
C	-2.385709000	-1.473748000	1.249042000
C	-0.835203000	-0.968038000	2.917765000
C	-2.668958000	-1.388772000	-0.195170000
C	-1.712934000	-0.720578000	-0.996685000
C	-1.965120000	-0.566759000	-2.371654000
C	-3.118514000	-1.111129000	-2.951652000
C	-4.052797000	-1.786458000	-2.156627000
C	-3.832166000	-1.917501000	-0.784359000
C	2.215849000	-0.406667000	-2.217160000
C	2.994392000	-0.151159000	-3.353532000
C	2.397583000	2.182050000	-3.215138000
C	1.634666000	1.875773000	-2.095023000
C	2.024010000	-1.723294000	-1.587109000
C	1.034688000	-1.795347000	-0.562203000
C	0.838728000	-3.035584000	0.073665000
C	1.582460000	-4.163995000	-0.290205000
C	2.546655000	-4.078956000	-1.303934000
C	2.765914000	-2.861493000	-1.950747000
H	-4.957917000	-2.204251000	-2.604746000
H	-4.573138000	-2.439094000	-0.174193000
H	-1.253289000	-0.031479000	-3.007863000
H	-3.289416000	-0.999820000	-4.026299000
H	0.088742000	-3.130639000	0.861976000
H	3.527348000	-2.801175000	-2.732259000
H	1.406739000	-5.117161000	0.217049000
H	3.129365000	-4.959384000	-1.586942000
H	0.134036000	-0.527692000	3.159623000
C	-2.872708000	-2.062260000	3.544246000
H	-4.212933000	-2.449458000	1.897654000
H	-3.536346000	-2.500503000	4.293973000
C	-1.639034000	-1.518514000	3.915413000
H	-1.300821000	-1.516812000	4.953467000
C	3.089367000	1.146550000	-3.857331000
H	1.086403000	2.650345000	-1.554977000
H	2.452197000	3.213565000	-3.568067000
H	3.695173000	1.348162000	-4.744038000
H	3.520330000	-0.970578000	-3.844920000

C	3.341637000	0.992538000	2.627909000
C	-0.219459000	2.735463000	1.130401000
C	-0.729337000	3.997392000	1.486998000
C	-1.888191000	4.468306000	0.880200000
C	-2.520448000	3.670922000	-0.081893000
C	-1.972736000	2.426170000	-0.378580000
N	-0.858972000	1.958100000	0.211408000
H	-0.223832000	4.598530000	2.242714000
H	-2.295376000	5.444514000	1.154130000
H	-3.427615000	3.999100000	-0.592473000
C	1.025125000	2.188189000	1.687121000
C	1.947437000	2.948112000	2.430646000
C	3.108000000	2.350466000	2.907817000
C	2.403983000	0.297414000	1.878772000
N	1.271101000	0.874272000	1.421266000
H	1.759611000	4.005099000	2.621275000
H	3.829141000	2.932643000	3.485976000
H	4.234378000	0.479452000	2.990309000
H	2.540740000	-0.758155000	1.632719000
H	-2.440741000	1.770907000	-1.115111000

(³MLCT/³MC_{eq 1})_{ts} DFT B3LYP/DEF2-SVP CPCM.

Ir	-0.302367000	0.452601000	0.146642000
N	0.703177000	-1.979909000	-1.743052000
N	-0.904102000	-1.727155000	0.642754000
N	1.453090000	0.303625000	1.259979000
N	-2.040494000	0.645308000	-0.981451000
C	1.659469000	-1.917635000	-2.673548000
C	3.076408000	-3.426972000	-1.459582000
C	2.078492000	-3.501753000	-0.485509000
C	0.899932000	-2.759952000	-0.669709000
C	-1.961920000	-1.823326000	1.470408000
C	-2.382285000	-3.029053000	2.027167000
C	-1.670411000	-4.188350000	1.716196000
C	-0.582953000	-4.093186000	0.849416000
C	-0.220766000	-2.847601000	0.312290000
C	2.863246000	-2.624393000	-2.582250000
C	3.891086000	0.157134000	2.592803000
C	-3.445828000	0.097289000	-2.840654000
C	-4.413148000	0.995731000	-2.376889000
C	3.336970000	2.059245000	-1.399266000
C	3.035299000	2.589689000	-2.654693000
C	1.738968000	2.458402000	-3.178637000
C	0.746779000	1.794259000	-2.452644000
C	1.026724000	1.241062000	-1.185847000
C	2.347738000	1.385982000	-0.661276000
C	1.532563000	-0.265031000	2.479880000
C	2.729989000	-0.361478000	3.178926000
C	3.810656000	0.744566000	1.333313000
C	2.576873000	0.810430000	0.667542000
C	-3.400553000	3.123919000	1.412458000
C	-2.989611000	3.669309000	2.631274000
C	-1.792847000	3.241811000	3.225249000
C	-1.005101000	2.268628000	2.601516000
C	-1.401897000	1.692706000	1.379274000
C	-2.618910000	2.140606000	0.782554000
C	-2.269707000	-0.049612000	-2.112153000
C	-2.981790000	1.507029000	-0.494512000

C	-4.180099000	1.700056000	-1.197463000
H	1.460997000	-1.271561000	-3.535690000
H	3.612093000	-2.540252000	-3.373032000
H	4.007531000	-3.986720000	-1.339673000
H	2.217557000	-4.112380000	0.408686000
H	-2.481465000	-0.891637000	1.704381000
H	-3.248832000	-3.045273000	2.690854000
H	-1.964275000	-5.155964000	2.130373000
H	-0.026163000	-4.985204000	0.558574000
H	4.704165000	1.149166000	0.857041000
H	4.850005000	0.101901000	3.113701000
H	2.744128000	-0.830652000	4.164155000
H	0.599336000	-0.645441000	2.899492000
H	-3.592725000	-0.483064000	-3.753161000
H	-5.346383000	1.140142000	-2.926808000
H	-4.930048000	2.392044000	-0.813045000
H	-1.474418000	-0.735656000	-2.414128000
H	3.808002000	3.112079000	-3.224420000
H	1.504100000	2.877586000	-4.161484000
H	4.345445000	2.181003000	-0.996319000
H	-0.253782000	1.708710000	-2.883713000
H	-1.474123000	3.672121000	4.179215000
H	-0.073254000	1.956161000	3.080535000
H	-4.329607000	3.474894000	0.956680000
H	-3.600956000	4.434018000	3.117284000

(³MC_{ax 1/S₀})_{stc-mecp} DFT B3LYP/DEF2-SVP CPCM.

Ir	0.392263000	-0.201739000	-0.118266000
N	-0.162184000	-1.047436000	2.398534000
N	1.892987000	0.500132000	-1.708804000
C	-1.946096000	-2.121887000	3.574153000
C	-1.384438000	-1.618301000	2.383053000
C	0.524040000	-0.964386000	3.540917000
C	-2.060151000	-1.679394000	1.067051000
C	-1.429038000	-1.103788000	-0.064772000
C	-2.089589000	-1.162899000	-1.308291000
C	-3.330518000	-1.794548000	-1.448532000
C	-3.948585000	-2.364192000	-0.330050000
C	-3.318022000	-2.299268000	0.911699000
C	2.582069000	-0.535847000	-2.253347000
C	3.421337000	-0.306570000	-3.358244000
C	2.812727000	2.027864000	-3.307783000
C	1.998683000	1.737454000	-2.216372000
C	2.366995000	-1.849557000	-1.611677000
C	1.382490000	-1.927612000	-0.581656000
C	1.190339000	-3.179178000	0.034813000
C	1.929391000	-4.306362000	-0.340789000
C	2.891572000	-4.213548000	-1.354436000
C	3.106902000	-2.988805000	-1.985609000
H	-4.920700000	-2.854973000	-0.423285000
H	-3.817557000	-2.746781000	1.773129000
H	-1.628305000	-0.715874000	-2.196462000
H	-3.812300000	-1.835509000	-2.429544000
H	0.445071000	-3.280399000	0.826752000
H	3.865916000	-2.923930000	-2.768846000
H	1.753235000	-5.263201000	0.159912000
H	3.473476000	-5.090632000	-1.649347000
H	1.511431000	-0.496787000	3.491194000

C	-1.229681000	-2.034729000	4.765548000
H	-2.935931000	-2.578028000	3.572734000
H	-1.658216000	-2.424594000	5.692585000
C	0.037986000	-1.445886000	4.757276000
H	0.638908000	-1.359117000	5.664878000
C	3.536069000	0.978081000	-3.885382000
H	1.412775000	2.519208000	-1.725267000
H	2.875098000	3.048126000	-3.690670000
H	4.185191000	1.159368000	-4.745966000
H	3.974437000	-1.131418000	-3.807694000
C	3.945536000	1.147464000	2.369399000
C	0.131191000	2.605240000	1.195301000
C	-0.406696000	3.845271000	1.567973000
C	-1.644490000	4.239978000	1.062247000
C	-2.318475000	3.385236000	0.189228000
C	-1.730947000	2.162457000	-0.131589000
N	-0.541829000	1.775740000	0.358002000
H	0.135388000	4.502702000	2.246935000
H	-2.071943000	5.204470000	1.346054000
H	-3.286934000	3.649584000	-0.239540000
C	1.461766000	2.139783000	1.660057000
C	2.307740000	2.910972000	2.472011000
C	3.558418000	2.408329000	2.829552000
C	3.052984000	0.431327000	1.572989000
N	1.849997000	0.917216000	1.237494000
H	2.000815000	3.897173000	2.818661000
H	4.225505000	3.000745000	3.460140000
H	4.917165000	0.718412000	2.621102000
H	3.300301000	-0.562472000	1.192141000
H	-2.232267000	1.460212000	-0.800240000

(³MC_{eq 1/S₀})_{stc-mecp} DFT B3LYP/DEF2-SVP CPCM.

Ir	-0.460030000	-0.212255000	-0.079492000
N	2.001279000	1.660634000	1.495092000
N	-1.801672000	0.673597000	1.245484000
N	0.881871000	-1.127075000	-1.391990000
C	2.701219000	-2.673097000	-1.626785000
C	1.750823000	-2.018889000	-0.828465000
C	0.949043000	-0.863127000	-2.711672000
C	1.584488000	-2.191362000	0.619883000
C	0.633443000	-1.332831000	1.246784000
C	0.413878000	-1.477988000	2.630504000
C	1.123549000	-2.426600000	3.373229000
C	2.066191000	-3.256734000	2.747741000
C	2.293541000	-3.141866000	1.375010000
C	-3.124869000	0.421814000	1.022250000
C	-4.094324000	0.978329000	1.869300000
C	-2.344763000	2.080480000	3.105452000
C	-1.421928000	1.493013000	2.245450000
C	-3.392300000	-0.420710000	-0.153511000
C	-2.258807000	-0.765150000	-0.948725000
C	-2.462472000	-1.574132000	-2.082258000
C	-3.744796000	-2.010396000	-2.433763000
C	-4.851297000	-1.656845000	-1.648522000
C	-4.676129000	-0.867246000	-0.509618000
H	2.618007000	-3.998581000	3.330672000
H	3.018710000	-3.803549000	0.895013000
H	-0.313714000	-0.844589000	3.143928000

H	0.942814000	-2.520804000	4.448098000
H	-1.617138000	-1.871970000	-2.708293000
H	-5.545193000	-0.607544000	0.099809000
H	-3.883690000	-2.630984000	-3.323915000
H	-5.851868000	-2.001897000	-1.921627000
H	0.227468000	-0.141976000	-3.100574000
C	2.767472000	-2.402136000	-2.991090000
H	3.389913000	-3.385306000	-1.171474000
H	3.507784000	-2.906897000	-3.616594000
C	1.877928000	-1.475007000	-3.546043000
H	1.893691000	-1.228389000	-4.609057000
C	-3.704122000	1.807947000	2.918435000
H	-0.346351000	1.672506000	2.330157000
H	-1.996680000	2.737872000	3.904096000
H	-4.455781000	2.246833000	3.579232000
H	-5.150251000	0.769638000	1.695051000
C	-0.492938000	3.603253000	-2.346614000
C	2.405141000	1.844250000	0.229061000
C	3.719225000	1.582334000	-0.190099000
C	4.639623000	1.110077000	0.748368000
C	4.221164000	0.927702000	2.067697000
C	2.890190000	1.217079000	2.387960000
H	4.009183000	1.735505000	-1.231700000
H	5.668000000	0.888818000	0.451103000
H	4.906759000	0.567875000	2.838195000
C	1.404821000	2.419856000	-0.720954000
C	1.741399000	3.556798000	-1.471634000
C	0.788256000	4.154243000	-2.295346000
C	-0.754763000	2.461178000	-1.593737000
N	0.171287000	1.871907000	-0.812660000
H	2.742969000	3.980424000	-1.379737000
H	1.039661000	5.044741000	-2.876803000
H	-1.283104000	4.038154000	-2.961529000
H	-1.737265000	1.984774000	-1.624503000
H	2.528201000	1.082996000	3.413319000

(³MC_{ax 2/S₀})_{stc-mecp} DFT B3LYP/DEF2-SVP CPCM.

C	3.883264000	2.027026000	1.282836000
C	3.004383000	1.173251000	0.586585000
N	2.655303000	-0.023952000	1.095018000
C	3.161062000	-0.411843000	2.268586000
C	2.419613000	1.560649000	-0.730376000
C	1.130871000	1.084504000	-1.151413000
C	0.656973000	1.502604000	-2.424753000
C	1.388995000	2.358190000	-3.245529000
C	2.641660000	2.816512000	-2.816324000
C	3.144783000	2.420408000	-1.572726000
Ir	0.002890000	-0.139972000	-0.029254000
N	-2.436887000	0.231008000	-1.166836000
C	-2.854994000	1.390155000	-0.621954000
C	-3.860180000	2.152866000	-1.249252000
C	-4.000738000	0.477340000	-2.973352000
C	-2.987694000	-0.210834000	-2.299476000
C	-2.202061000	1.816317000	0.649832000
C	-0.943899000	1.256443000	1.057698000
C	-0.386841000	1.697727000	2.287260000
C	-1.010945000	2.659637000	3.079556000
C	-2.236965000	3.198130000	2.666429000

C	-2.820789000	2.778164000	1.467063000
H	3.236015000	3.475699000	-3.454755000
H	4.134125000	2.771974000	-1.272210000
H	-0.318953000	1.149378000	-2.766678000
H	0.991077000	2.667292000	-4.215928000
H	0.566170000	1.276603000	2.617275000
H	-3.787332000	3.199927000	1.185599000
H	-0.551476000	2.987278000	4.016059000
H	-2.748751000	3.940986000	3.284107000
H	2.845728000	-1.396177000	2.634083000
C	4.408903000	1.617240000	2.508833000
H	4.136656000	3.009665000	0.882391000
H	5.087309000	2.271926000	3.062260000
C	4.047151000	0.368066000	3.018157000
H	4.434996000	0.004245000	3.972293000
C	-4.436880000	1.688891000	-2.431992000
H	-2.604159000	-1.160104000	-2.690636000
H	-4.426384000	0.074878000	-3.895148000
H	-5.215772000	2.274014000	-2.927916000
H	-4.179347000	3.108245000	-0.832048000
C	-2.334865000	-2.762356000	2.797997000
C	0.250508000	-3.196093000	-0.525286000
C	0.634904000	-4.414109000	-1.103123000
C	1.502911000	-4.414574000	-2.192863000
C	1.968303000	-3.192647000	-2.681118000
C	1.545502000	-2.019009000	-2.061612000
N	0.706022000	-2.015235000	-1.009504000
H	0.259163000	-5.356483000	-0.706052000
H	1.809766000	-5.357084000	-2.652009000
H	2.650788000	-3.136473000	-3.531163000
H	1.888651000	-1.047089000	-2.416424000
C	-0.661286000	-3.104747000	0.635015000
C	-1.201225000	-4.229506000	1.274282000
C	-2.046672000	-4.058578000	2.368442000
C	-1.765310000	-1.689151000	2.116650000
N	-0.947276000	-1.850469000	1.060432000
H	-0.961366000	-5.232521000	0.923161000
H	-2.472371000	-4.926882000	2.876497000
H	-2.991438000	-2.572260000	3.649059000
H	-1.969169000	-0.663412000	2.424254000

Complex 2 in CH₂Cl₂.

(S₀)_{min} DFT B3LYP/DEF2-SVP CPCM.

Ir	0.368764000	-0.157354000	0.103613000
N	-0.753324000	-0.794563000	1.739217000
N	1.466471000	0.258059000	-1.636883000
C	-2.551134000	-2.196959000	2.484634000
C	-1.766021000	-1.666596000	1.446771000
C	-0.525863000	-0.431418000	3.016838000
C	-1.940216000	-1.946837000	0.018365000
C	-1.061560000	-1.243139000	-0.852202000
C	-1.213861000	-1.458536000	-2.234595000
C	-2.186421000	-2.333419000	-2.732858000
C	-3.036031000	-3.028063000	-1.859771000
C	-2.913175000	-2.831285000	-0.484977000
C	2.385566000	-0.694557000	-1.977319000
C	3.183040000	-0.525665000	-3.121198000

C	2.072035000	1.560365000	-3.562252000
C	1.313871000	1.345943000	-2.416642000
C	2.425948000	-1.852258000	-1.077336000
C	1.490042000	-1.831276000	-0.006591000
C	1.483339000	-2.926199000	0.876364000
C	2.371529000	-3.995968000	0.709743000
C	3.291175000	-4.002021000	-0.347827000
C	3.316862000	-2.930323000	-1.239332000
H	-3.789079000	-3.717165000	-2.250796000
H	-3.578668000	-3.370159000	0.194214000
H	-0.561468000	-0.943614000	-2.944614000
H	-2.279243000	-2.481308000	-3.813307000
H	0.781365000	-2.956663000	1.712647000
H	4.035303000	-2.936654000	-2.062596000
H	2.343928000	-4.834401000	1.412307000
H	3.983119000	-4.838355000	-0.475466000
H	0.290614000	0.271630000	3.184528000
C	-2.309391000	-1.826722000	3.803566000
H	-3.353372000	-2.896389000	2.248188000
H	-2.919682000	-2.237595000	4.611663000
C	-1.278718000	-0.919956000	4.078148000
H	-1.054165000	-0.594989000	5.095497000
C	3.030522000	0.605365000	-3.917189000
H	0.550807000	2.061946000	-2.113612000
H	1.906346000	2.458949000	-4.158967000
H	3.647551000	0.738724000	-4.809210000
H	3.916330000	-1.288175000	-3.384759000
C	3.888539000	1.123817000	2.566932000
C	0.574491000	2.901985000	0.592079000
C	0.525008000	4.270880000	0.301717000
C	-0.591264000	4.789966000	-0.349198000
C	-1.651211000	3.936403000	-0.631281000
C	-1.562513000	2.573851000	-0.291415000
N	-0.434864000	2.054648000	0.250013000
H	1.358968000	4.922509000	0.558390000
H	-0.640689000	5.850273000	-0.607772000
H	-2.569677000	4.312391000	-1.084194000
C	1.753291000	2.321764000	1.287182000
C	2.681731000	3.116420000	1.978348000
C	3.760235000	2.512751000	2.622279000
C	2.926876000	0.395389000	1.870681000
N	1.885642000	0.976687000	1.249974000
H	2.556771000	4.197348000	2.030631000
H	4.486637000	3.121870000	3.165424000
H	4.714358000	0.603571000	3.055779000
H	2.983513000	-0.692581000	1.804005000
C	-3.405709000	1.173558000	0.663838000
C	-4.644801000	0.538478000	0.543136000
C	-2.789549000	1.746367000	-0.461679000
H	-5.120276000	0.108191000	1.428569000
C	-5.276050000	0.456633000	-0.702668000
C	-3.435951000	1.672466000	-1.708013000
H	-6.244671000	-0.041902000	-0.795163000
H	-2.969197000	2.122962000	-2.588016000
C	-4.665802000	1.020125000	-1.829309000
H	-5.152385000	0.957900000	-2.806306000
H	-2.925511000	1.252872000	1.641594000

(³MLCT)_{min} DFT B3LYP/DEF2-SVP CPCM.

Ir	0.424150000	-0.202187000	0.088337000
N	-0.788057000	-0.957374000	1.605802000
N	1.653131000	0.369969000	-1.508348000
C	-2.662905000	-2.362464000	2.106628000
C	-1.820581000	-1.739804000	1.175670000
C	-0.592266000	-0.749937000	2.919048000
C	-1.941886000	-1.827798000	-0.283908000
C	-0.973592000	-1.074436000	-1.031100000
C	-1.047609000	-1.114638000	-2.446078000
C	-2.027750000	-1.864485000	-3.090409000
C	-2.959877000	-2.603622000	-2.340366000
C	-2.918089000	-2.584388000	-0.941562000
C	2.630591000	-0.529698000	-1.822326000
C	3.542007000	-0.243931000	-2.849524000
C	2.420107000	1.851763000	-3.226331000
C	1.547588000	1.523076000	-2.193295000
C	2.609049000	-1.763076000	-1.024096000
C	1.592615000	-1.853722000	-0.029708000
C	1.522277000	-3.015076000	0.760292000
C	2.416949000	-4.069677000	0.557894000
C	3.409016000	-3.975743000	-0.429436000
C	3.504829000	-2.827502000	-1.218051000
H	-3.723319000	-3.196851000	-2.849981000
H	-3.651957000	-3.165000000	-0.378654000
H	-0.327085000	-0.555297000	-3.046055000
H	-2.071691000	-1.884866000	-4.182608000
H	0.763842000	-3.110102000	1.540036000
H	4.280182000	-2.769643000	-1.985029000
H	2.342237000	-4.970840000	1.172628000
H	4.110676000	-4.799368000	-0.582900000
H	0.244661000	-0.105017000	3.189027000
C	-2.455474000	-2.160430000	3.469937000
H	-3.480426000	-2.995113000	1.760354000
H	-3.108624000	-2.641362000	4.201952000
C	-1.408458000	-1.332738000	3.885586000
H	-1.215091000	-1.138733000	4.941883000
C	3.438704000	0.952523000	-3.554925000
H	0.735553000	2.190161000	-1.905031000
H	2.295028000	2.797352000	-3.756342000
H	4.144594000	1.179716000	-4.357395000
H	4.325803000	-0.961114000	-3.093038000
C	4.006894000	0.648260000	2.720673000
C	0.833766000	2.718006000	0.853922000
C	0.775109000	4.126951000	0.656732000
C	-0.330982000	4.707213000	0.085030000
C	-1.440423000	3.881881000	-0.242020000
C	-1.370279000	2.510091000	-0.027432000
N	-0.231570000	1.906949000	0.439168000
H	1.628789000	4.741896000	0.942794000
H	-0.372258000	5.785655000	-0.085078000
H	-2.375144000	4.315731000	-0.598816000
C	1.955740000	2.071745000	1.459527000
C	3.015835000	2.764414000	2.118183000
C	4.027591000	2.067184000	2.740566000
C	2.972429000	0.022849000	2.046816000
N	1.979542000	0.688099000	1.418360000

H	3.008349000	3.854041000	2.150989000
H	4.829107000	2.604241000	3.254369000
H	4.779264000	0.053079000	3.210163000
H	2.927984000	-1.066838000	1.996586000
C	-3.309782000	1.196407000	0.881241000
C	-4.580913000	0.633428000	0.733124000
C	-2.635536000	1.740205000	-0.226461000
H	-5.099227000	0.229716000	1.607179000
C	-5.193289000	0.596724000	-0.524975000
C	-3.262321000	1.705811000	-1.484706000
H	-6.188207000	0.157757000	-0.639179000
H	-2.753193000	2.137038000	-2.350531000
C	-4.528340000	1.130763000	-1.634403000
H	-4.999494000	1.106029000	-2.620837000
H	-2.848294000	1.246146000	1.870439000

($^3\text{MC}_{\text{ax } 1}$)_{min} DFT B3LYP/DEF2-SVP CPCM.

Ir	0.435646000	-0.212008000	-0.133198000
N	-0.270487000	-0.915497000	2.317654000
N	1.871767000	0.524099000	-1.765114000
C	-2.215888000	-1.724600000	3.447013000
C	-1.509991000	-1.446895000	2.258381000
C	0.306951000	-0.684590000	3.500499000
C	-2.029207000	-1.738979000	0.904118000
C	-1.280865000	-1.327453000	-0.228707000
C	-1.734740000	-1.714988000	-1.504500000
C	-2.915680000	-2.444102000	-1.670518000
C	-3.670433000	-2.817437000	-0.551567000
C	-3.223456000	-2.469866000	0.721013000
C	2.557024000	-0.499484000	-2.337617000
C	3.371434000	-0.248166000	-3.457591000
C	2.782148000	2.088039000	-3.334516000
C	1.986478000	1.775509000	-2.236496000
C	2.389315000	-1.815177000	-1.691087000
C	1.459155000	-1.905273000	-0.614638000
C	1.340333000	-3.146279000	0.038947000
C	2.095516000	-4.257054000	-0.351838000
C	2.995531000	-4.158901000	-1.421397000
C	3.140759000	-2.941638000	-2.084617000
H	-4.593432000	-3.390940000	-0.669854000
H	-3.805811000	-2.792441000	1.586504000
H	-1.160862000	-1.441238000	-2.394484000
H	-3.241930000	-2.725279000	-2.676053000
H	0.638774000	-3.251014000	0.869873000
H	3.855523000	-2.869355000	-2.907816000
H	1.977807000	-5.207166000	0.178043000
H	3.584964000	-5.025367000	-1.732181000
H	1.322384000	-0.278830000	3.484045000
C	-1.620082000	-1.470124000	4.679606000
H	-3.224473000	-2.135984000	3.408634000
H	-2.162396000	-1.682491000	5.604726000
C	-0.323716000	-0.947286000	4.716589000
H	0.189175000	-0.744708000	5.659029000
C	3.480062000	1.046555000	-3.958387000
H	1.427025000	2.550156000	-1.704954000
H	2.850900000	3.118778000	-3.687125000
H	4.110001000	1.244685000	-4.829407000
H	3.915137000	-1.064483000	-3.933336000

C	4.168972000	0.988468000	2.101514000
C	0.194508000	2.392915000	1.505966000
C	-0.367590000	3.412323000	2.282736000
C	-1.666326000	3.836882000	2.011855000
C	-2.344443000	3.266007000	0.942229000
C	-1.733655000	2.248536000	0.185514000
N	-0.502042000	1.784863000	0.507147000
H	0.193434000	3.861723000	3.100702000
H	-2.130440000	4.621808000	2.613385000
H	-3.337584000	3.617810000	0.660818000
C	1.592342000	1.941571000	1.744920000
C	2.501629000	2.674806000	2.524477000
C	3.797814000	2.192860000	2.703780000
C	3.222067000	0.315851000	1.332388000
N	1.977241000	0.785739000	1.161822000
H	2.211116000	3.622167000	2.976978000
H	4.512075000	2.758255000	3.307005000
H	5.172090000	0.573839000	2.216594000
H	3.458326000	-0.627600000	0.835459000
C	-3.820014000	1.452763000	-0.964345000
C	-4.521049000	1.099866000	-2.120002000
C	-2.446429000	1.752907000	-1.024205000
H	-5.585252000	0.858420000	-2.054475000
C	-3.865146000	1.057557000	-3.355782000
C	-1.796592000	1.705405000	-2.270286000
H	-4.416710000	0.790864000	-4.261309000
H	-0.741256000	1.969201000	-2.341643000
C	-2.501999000	1.363575000	-3.427016000
H	-1.984196000	1.344916000	-4.389695000
H	-4.341249000	1.482976000	-0.004206000

(³MC_{eq 1})_{min} DFT B3LYP/DEF2-SVP CPCM.

Ir	0.874471000	-0.938162000	0.240499000
N	1.814841000	1.027437000	0.958312000
N	-0.848752000	2.270900000	0.253875000
N	1.535843000	-0.533226000	-1.692015000
N	0.183176000	-1.385988000	2.156387000
C	-2.297139000	3.584731000	-3.519394000
C	-1.840125000	3.322193000	-2.225728000
C	-3.592315000	3.212003000	-3.898495000
C	-2.672267000	2.687411000	-1.283360000
C	-4.427858000	2.578436000	-2.971801000
C	-3.974216000	2.321640000	-1.674810000
C	3.162527000	1.034084000	0.961682000
C	3.231866000	3.017245000	2.306336000
C	1.837032000	3.021416000	2.286285000
C	1.147541000	2.022600000	1.584534000
C	-2.173852000	2.432853000	0.097707000
C	-3.048218000	2.398325000	1.203205000
C	-2.524190000	2.204180000	2.479263000
C	-1.143307000	2.060190000	2.634123000
C	-0.346030000	2.095033000	1.482097000
C	3.909296000	2.010970000	1.615486000
C	2.523156000	-0.105600000	-4.251489000
C	0.435907000	-1.625241000	4.529758000
C	-0.912430000	-1.984389000	4.642037000
C	3.781897000	-3.476839000	-1.620919000
C	4.124637000	-4.453822000	-0.683316000

C	3.572313000	-4.414435000	0.605204000
C	2.677176000	-3.398897000	0.958426000
C	2.324900000	-2.394938000	0.036787000
C	2.887907000	-2.450136000	-1.273028000
C	1.106050000	0.516670000	-2.418081000
C	1.574672000	0.765400000	-3.704138000
C	2.977454000	-1.181705000	-3.492217000
C	2.477302000	-1.383381000	-2.197526000
C	-3.187057000	-2.129390000	0.815541000
C	-3.787172000	-2.121289000	-0.445220000
C	-3.052892000	-1.711072000	-1.568724000
C	-1.723808000	-1.299957000	-1.432635000
C	-1.098140000	-1.285547000	-0.169747000
C	-1.850436000	-1.720721000	0.963392000
C	0.944183000	-1.338111000	3.267843000
C	-1.138390000	-1.724118000	2.246373000
C	-1.699098000	-2.034881000	3.494359000
H	-4.634861000	1.810980000	-0.970528000
H	-1.640801000	4.088887000	-4.234129000
H	-0.834881000	3.624653000	-1.926143000
H	-3.949543000	3.416001000	-4.911528000
H	-5.438550000	2.277377000	-3.260383000
H	3.655201000	0.214026000	0.434274000
H	4.999672000	1.968363000	1.584408000
H	3.780091000	3.795641000	2.842867000
H	1.270609000	3.808094000	2.788085000
H	-4.119858000	2.550543000	1.066826000
H	-3.184066000	2.178227000	3.350227000
H	-0.693568000	1.917332000	3.618633000
H	3.726350000	-1.863968000	-3.895455000
H	2.910852000	0.056195000	-5.260279000
H	1.196215000	1.625688000	-4.258779000
H	0.368567000	1.162798000	-1.936106000
H	1.090839000	-1.572044000	5.401085000
H	-1.346242000	-2.221454000	5.616452000
H	-2.752335000	-2.309211000	3.560347000
H	1.992083000	-1.065250000	3.127820000
H	4.819954000	-5.250821000	-0.958951000
H	3.841101000	-5.181804000	1.337032000
H	4.211580000	-3.524475000	-2.624559000
H	2.255442000	-3.396265000	1.966894000
H	-3.522938000	-1.710142000	-2.556388000
H	-1.176336000	-0.985063000	-2.324104000
H	-3.764932000	-2.463703000	1.680493000
H	-4.826100000	-2.442477000	-0.554980000

(³MC_{ax 2})_{min} DFT B3LYP/DEF2-SVP CPCM.

Ir	0.466432000	-0.536812000	0.395148000
N	-1.096878000	-0.646164000	1.985997000
N	1.587967000	0.528204000	-1.672233000
C	-3.117111000	-1.759108000	2.615221000
C	-2.139190000	-1.455310000	1.651823000
C	-0.983308000	-0.153613000	3.231266000
C	-2.125125000	-1.959379000	0.267163000
C	-1.008636000	-1.596150000	-0.539893000
C	-0.986220000	-2.073302000	-1.864556000
C	-2.011891000	-2.875206000	-2.373923000
C	-3.101520000	-3.227435000	-1.565273000

C	-3.156231000	-2.768274000	-0.249870000
C	2.473630000	-0.340301000	-2.207124000
C	3.210514000	0.016355000	-3.354009000
C	2.118804000	2.160379000	-3.350391000
C	1.424318000	1.737980000	-2.216801000
C	2.608253000	-1.638710000	-1.512646000
C	1.816846000	-1.875590000	-0.362826000
C	1.955182000	-3.104760000	0.309495000
C	2.847581000	-4.083825000	-0.141653000
C	3.626932000	-3.846425000	-1.280059000
C	3.506656000	-2.632402000	-1.954348000
H	-3.904280000	-3.856114000	-1.959293000
H	-4.011120000	-3.042279000	0.372797000
H	-0.146091000	-1.820603000	-2.516021000
H	-1.960010000	-3.232656000	-3.406867000
H	1.354509000	-3.314081000	1.200898000
H	4.125221000	-2.461007000	-2.837744000
H	2.930894000	-5.031944000	0.397376000
H	4.327381000	-4.604302000	-1.640000000
H	-0.115908000	0.480455000	3.430143000
C	-3.008395000	-1.239345000	3.902666000
H	-3.955733000	-2.405356000	2.355675000
H	-3.767232000	-1.474145000	4.653474000
C	-1.918410000	-0.421784000	4.225343000
H	-1.793825000	0.003654000	5.222737000
C	3.028440000	1.271056000	-3.929778000
H	0.709782000	2.404613000	-1.728468000
H	1.946615000	3.157513000	-3.760514000
H	3.595179000	1.552992000	-4.820934000
H	3.923375000	-0.682360000	-3.791640000
C	4.349811000	0.479389000	2.372680000
C	0.780557000	2.523749000	1.316859000
C	0.543194000	3.819299000	1.798214000
C	-0.691320000	4.416727000	1.564709000
C	-1.652219000	3.704838000	0.858110000
C	-1.365872000	2.406831000	0.392591000
N	-0.162599000	1.833665000	0.628264000
H	1.301627000	4.348009000	2.373164000
H	-0.898829000	5.424646000	1.931622000
H	-2.624195000	4.147569000	0.638292000
C	2.069235000	1.846327000	1.620905000
C	3.191169000	2.559432000	2.074469000
C	4.343756000	1.872524000	2.448852000
C	3.216540000	-0.161940000	1.878683000
N	2.111249000	0.499875000	1.492663000
H	3.171076000	3.647033000	2.127012000
H	5.221165000	2.420697000	2.800037000
H	5.218207000	-0.110003000	2.672775000
H	3.192309000	-1.247353000	1.774835000
C	-3.743212000	1.682772000	0.148046000
C	-4.805045000	1.168986000	-0.599678000
C	-2.439403000	1.720839000	-0.384601000
H	-5.807971000	1.137008000	-0.165652000
C	-4.585428000	0.706498000	-1.902284000
C	-2.227260000	1.235013000	-1.685043000
H	-5.417831000	0.318651000	-2.495565000
H	-1.229872000	1.263021000	-2.122493000
C	-3.295503000	0.743185000	-2.440672000

H	-3.115227000	0.384409000	-3.457062000
H	-3.925506000	2.053849000	1.159907000

(³MC_{eq 2})_{min} DFT B3LYP/DEF2-SVP CPCM.

Ir	-0.097498000	-0.412221000	0.142767000
N	-0.766091000	0.785076000	-3.113895000
N	0.295760000	1.838042000	-0.590621000
N	-1.768027000	0.345435000	1.152543000
N	1.523738000	-1.281442000	-0.828898000
H	-0.810068000	-0.532070000	-4.711742000
C	3.709508000	1.810697000	2.811708000
C	2.535672000	2.274622000	2.212244000
C	4.665618000	1.129212000	2.049786000
C	2.292252000	2.041556000	0.846082000
C	4.441427000	0.912823000	0.685356000
C	3.261918000	1.362832000	0.086387000
C	-1.417106000	0.113524000	-4.066414000
C	-3.534364000	1.031357000	-3.413664000
C	-2.861151000	1.741392000	-2.417345000
C	-1.469022000	1.590550000	-2.301156000
C	1.092804000	2.621260000	0.178463000
C	0.842471000	3.996197000	0.321499000
C	-0.220222000	4.577149000	-0.363037000
C	-0.982823000	3.778870000	-1.213571000
C	-0.694825000	2.411598000	-1.318661000
C	-2.799618000	0.203650000	-4.263856000
C	-4.099879000	1.230439000	2.388211000
C	2.865447000	-1.766720000	-2.751856000
C	3.690998000	-2.587345000	-1.974859000
C	-3.933467000	-2.187988000	-0.461677000
C	-3.751629000	-3.212780000	-1.392964000
C	-2.494435000	-3.410302000	-1.983832000
C	-1.419128000	-2.583439000	-1.646656000
C	-1.577777000	-1.536699000	-0.716718000
C	-2.859607000	-1.348789000	-0.119159000
C	-1.731699000	1.363946000	2.033831000
C	-2.872468000	1.840238000	2.670403000
C	-4.139333000	0.174767000	1.481035000
C	-2.958329000	-0.260792000	0.861341000
C	2.625714000	-2.836825000	2.344464000
C	2.230420000	-2.771840000	3.682291000
C	1.173405000	-1.930281000	4.062058000
C	0.508314000	-1.157146000	3.106413000
C	0.894385000	-1.195044000	1.751207000
C	1.972412000	-2.054195000	1.377647000
C	1.788381000	-1.131321000	-2.141634000
C	2.336775000	-2.048495000	-0.044360000
C	3.425743000	-2.724011000	-0.614259000
H	3.100990000	1.212565000	-0.982936000
H	3.879762000	1.986056000	3.877262000
H	1.795092000	2.811120000	2.811266000
H	5.588021000	0.773830000	2.516973000
H	5.192132000	0.396677000	0.081248000
H	-3.281227000	-0.365866000	-5.061826000
H	-4.618143000	1.124126000	-3.521635000
H	-3.407040000	2.392623000	-1.732114000
H	1.503879000	4.596760000	0.947657000
H	-0.430015000	5.645110000	-0.265186000

H	-1.780760000	4.210834000	-1.818943000
H	-5.085634000	-0.311272000	1.242430000
H	-5.017419000	1.575522000	2.870934000
H	-2.791049000	2.668716000	3.376032000
H	-0.751272000	1.798532000	2.236745000
H	3.045271000	-1.618476000	-3.818121000
H	4.539775000	-3.108911000	-2.424012000
H	4.067206000	-3.343829000	0.013026000
H	1.106005000	-0.474673000	-2.689369000
H	-4.589515000	-3.864215000	-1.654201000
H	-2.354165000	-4.214485000	-2.712073000
H	-4.914380000	-2.056353000	0.001562000
H	-0.450189000	-2.760284000	-2.119396000
H	0.867029000	-1.879679000	5.110993000
H	-0.316304000	-0.516622000	3.428563000
H	3.443550000	-3.502861000	2.059120000
H	2.743801000	-3.380431000	4.431095000

(³MLCT/³MC_{ax 1})_{CI-NEB} DFT B3LYP/DEF2-SVP CPCM.

Ir	0.483004861	-0.148434880	-0.022379854
N	-0.552242613	-0.887113394	2.030739427
N	1.757283266	0.464995007	-1.657438537
C	-2.432555261	-2.069465048	2.914574039
C	-1.675494240	-1.611284095	1.820887776
C	-0.134668470	-0.628542303	3.274104170
C	-1.989177947	-1.882078500	0.407268015
C	-1.107168524	-1.351398152	-0.563871505
C	-1.330653756	-1.655275552	-1.918281761
C	-2.442220726	-2.410598516	-2.308537506
C	-3.321350872	-2.920947265	-1.344538948
C	-3.089713316	-2.663921659	0.006457612
C	2.581119038	-0.515800575	-2.134229640
C	3.423416510	-0.246019919	-3.225854050
C	2.563466937	2.004738332	-3.306631898
C	1.749544439	1.687202959	-2.227173290
C	2.502808070	-1.791375778	-1.416476822
C	1.548635547	-1.861286972	-0.365830063
C	1.459085971	-3.061232251	0.359810425
C	2.275217679	-4.156254747	0.054345915
C	3.208339429	-4.078134063	-0.989636872
C	3.322864116	-2.897989678	-1.720616070
H	-4.179402818	-3.527593057	-1.645320891
H	-3.771686939	-3.080453485	0.751008146
H	-0.643691356	-1.289811148	-2.687245639
H	-2.614534145	-2.611912696	-3.369828663
H	0.737062599	-3.155192044	1.173936825
H	4.059187283	-2.838885945	-2.525836098
H	2.178117002	-5.080443297	0.631844134
H	3.844472942	-4.934549748	-1.227571069
H	0.793880111	-0.061976516	3.370845866
C	-2.007371339	-1.790692245	4.210818466
H	-3.343627440	-2.645347664	2.750510949
H	-2.588129545	-2.143565217	5.066696261
C	-0.828015468	-1.063605754	4.402147318
H	-0.447843838	-0.836965355	5.399687000
C	3.417762201	1.015315675	-3.812840742
H	1.078182090	2.427661300	-1.787311340
H	2.533439340	3.008310750	-3.734271713

H	4.075513989	1.228698129	-4.659063462
H	4.083922303	-1.025808711	-3.606050911
C	4.182598103	0.727565448	2.328943896
C	0.513618542	2.613187358	1.304189819
C	0.196600941	3.916678351	1.731789551
C	-1.007931355	4.493397261	1.363639448
C	-1.881262664	3.751459951	0.566505335
C	-1.528396345	2.460672026	0.153463452
N	-0.351201784	1.890244920	0.517978600
H	0.889492136	4.473719463	2.359044398
H	-1.265576625	5.503789291	1.688779016
H	-2.840547874	4.161736656	0.248268759
C	1.793942332	1.995057935	1.676246067
C	2.813654832	2.706949680	2.341405818
C	4.002277959	2.077680789	2.681617490
C	3.159942110	0.076001238	1.661010352
N	1.986540008	0.677539428	1.353610884
H	2.675879598	3.757569706	2.592964033
H	4.781816641	2.628827327	3.212234056
H	5.098046393	0.188500973	2.579196525
H	3.253272184	-0.971950011	1.370725886
C	-3.745245599	1.339949358	-0.125575203
C	-4.805147954	0.902231754	-0.924888889
C	-2.540916690	1.771602218	-0.708997193
H	-5.737650127	0.574662751	-0.456809569
C	-4.678575866	0.902907932	-2.318462291
C	-2.415307502	1.754505285	-2.107305935
H	-5.515729155	0.581883767	-2.944449549
H	-1.493827605	2.110155705	-2.575098327
C	-3.480580296	1.323835903	-2.906018102
H	-3.379234142	1.331245418	-3.994585058
H	-3.857327306	1.365426198	0.961731736

(³MLCT/³MC_{eq 1})_{CI-NEB} DFT B3LYP/DEF2-SVP CPCM.

Ir	0.552401146	-0.500123072	0.153739578
N	2.035138751	0.870399176	1.249684994
N	-0.409493327	2.135335741	0.457802605
N	1.573912133	0.002345916	-1.614880836
N	-0.482953111	-1.048567391	1.854241934
C	-3.460377261	1.946126090	-2.957166814
C	-2.448979235	2.287735246	-2.053148120
C	-4.657693332	1.387360308	-2.496699248
C	-2.628041444	2.082989060	-0.675403877
C	-4.840722897	1.168900906	-1.126808010
C	-3.836138187	1.523261585	-0.222738275
C	3.247012515	0.354632493	1.540119894
C	4.082864042	2.468045189	2.288676883
C	2.833595136	3.005452781	1.997569729
C	1.801751781	2.180989126	1.507795363
C	-1.657951876	2.631647442	0.323126430
C	-2.108659102	3.726675927	1.079964010
C	-1.256479167	4.320604846	2.007195115
C	0.028664426	3.808318828	2.144862303
C	0.426163947	2.721906217	1.344655929
C	4.289422879	1.102905616	2.075521284
C	3.068252759	0.515222192	-3.902262092
C	-0.746102100	-1.367568550	4.220822631
C	-1.929533191	-2.104797839	4.005335045

C	3.476287255	-3.173107225	-1.438573260
C	3.565416327	-4.235936096	-0.537484264
C	2.782700009	-4.239199854	0.628445124
C	1.907494439	-3.181771871	0.892912428
C	1.815037544	-2.089416100	0.008742461
C	2.614255668	-2.095325887	-1.172994090
C	1.409857910	1.154868739	-2.289401289
C	2.134807971	1.449720988	-3.439910411
C	3.250151936	-0.669895875	-3.193760072
C	2.494168435	-0.914506503	-2.037354596
C	-3.057281266	-2.645708474	-0.278933100
C	-3.299357708	-2.704541010	-1.647216229
C	-2.448128294	-2.031963504	-2.559652958
C	-1.360344472	-1.309797200	-2.094268948
C	-1.079095491	-1.220661089	-0.701889101
C	-1.972461451	-1.896441599	0.218832784
C	-0.059882005	-0.865100903	3.128386282
C	-1.640171549	-1.769628175	1.621196326
C	-2.367098676	-2.301053502	2.703312956
H	-3.992135535	1.374511148	0.848771930
H	-3.319639538	2.134581214	-4.024937526
H	-1.532249183	2.757901981	-2.416854739
H	-5.451651664	1.131187771	-3.202416629
H	-5.775055243	0.737067371	-0.757482032
H	3.377546660	-0.709245796	1.340384999
H	5.239478982	0.618097374	2.307063777
H	4.879871875	3.104105457	2.680871156
H	2.653840212	4.069429607	2.148696962
H	-3.116175439	4.111280815	0.914465001
H	-1.588076014	5.167945391	2.611859247
H	0.707539703	4.232966280	2.883542182
H	3.984527839	-1.403695092	-3.526976676
H	3.655765778	0.712317569	-4.802268332
H	1.963811102	2.393931509	-3.960005272
H	0.670674358	1.844749547	-1.880256883
H	-0.358737064	-1.190347853	5.225842014
H	-2.490273583	-2.517296156	4.846927471
H	-3.278594147	-2.867781358	2.507405840
H	0.866979983	-0.304372615	3.253468937
H	4.247218236	-5.065232994	-0.743335659
H	2.861222786	-5.071572259	1.333680531
H	4.085999825	-3.188875087	-2.345114134
H	1.303773799	-3.206375100	1.803998540
H	-2.656011572	-2.082495462	-3.631846726
H	-0.712104404	-0.802469323	-2.812056576
H	-3.716156737	-3.185879153	0.405400221
H	-4.153802881	-3.274767475	-2.021224122

(³MLCT/³MC_{ax 2})_{CI-NEB} DFT B3LYP/DEF2-SVP CPCM.

Ir	0.408554370	-0.400141292	0.219372241
N	-0.963592279	-0.672349713	1.806070177
N	1.513751154	0.379041456	-1.632681810
C	-2.915463533	-1.879882985	2.518998452
C	-2.016067739	-1.506261843	1.514800184
C	-0.787187423	-0.235231992	3.074881702
C	-2.069608214	-1.931719276	0.110905629
C	-1.012806064	-1.459717570	-0.729262417
C	-1.013146903	-1.865049933	-2.081635704

C	-2.008247427	-2.701942418	-2.587635646
C	-3.039561557	-3.155796417	-1.749182693
C	-3.070500846	-2.770567292	-0.407173120
C	2.468899739	-0.456611554	-2.112414249
C	3.258371921	-0.075516156	-3.211257027
C	2.086450836	2.022723315	-3.284497142
C	1.338373697	1.583320724	-2.194964975
C	2.592197183	-1.733354002	-1.392154091
C	1.773558074	-1.897783714	-0.249839443
C	1.866517633	-3.094641952	0.479866472
C	2.734524041	-4.116065267	0.072296602
C	3.543348911	-3.944336190	-1.059198630
C	3.476476719	-2.755059460	-1.785175223
H	-3.819896334	-3.812341249	-2.143111226
H	-3.880239926	-3.131095402	0.231824455
H	-0.214564503	-1.529389379	-2.747433239
H	-1.981055988	-3.013050289	-3.635750820
H	1.247893706	-3.246076088	1.369908370
H	4.112608342	-2.629513403	-2.664525858
H	2.780343406	-5.049287066	0.641053950
H	4.226460239	-4.736923190	-1.374847111
H	0.065148060	0.423520073	3.249269125
C	-2.744242869	-1.411483591	3.823308884
H	-3.754147329	-2.533513627	2.276045612
H	-3.451399300	-1.691729197	4.607327533
C	-1.652796491	-0.577405290	4.105511267
H	-1.480354219	-0.180262331	5.107763510
C	3.063745483	1.168858662	-3.804487079
H	0.575324193	2.221341486	-1.749508374
H	1.901323716	3.011972522	-3.707730990
H	3.672488592	1.472438693	-4.659799309
H	4.025317109	-0.749998392	-3.592592139
C	4.250832235	0.506947412	2.417858313
C	0.786972813	2.635635752	1.227457196
C	0.548521583	3.936148044	1.706580326
C	-0.677216898	4.539828935	1.464062220
C	-1.654843188	3.813236557	0.781755755
C	-1.375534043	2.515710210	0.327853038
N	-0.155377722	1.953365771	0.521106312
H	1.307983603	4.461429756	2.284496442
H	-0.877405084	5.555379104	1.812721610
H	-2.631532069	4.250206789	0.568967553
C	2.049039983	1.939215912	1.548326252
C	3.169273934	2.619898576	2.065368173
C	4.278485790	1.903351202	2.498294603
C	3.133346061	-0.100488971	1.854519167
N	2.066160419	0.587366934	1.408161931
H	3.172664249	3.707720659	2.124710830
H	5.150104846	2.426085566	2.899186139
H	5.082711482	-0.107228982	2.768005382
H	3.089678057	-1.184217853	1.745426835
C	-3.714847365	1.655901379	0.282287837
C	-4.815974979	1.096059984	-0.370158747
C	-2.480730719	1.799436753	-0.380971186
H	-5.762838437	0.983408994	0.164698942
C	-4.707899784	0.690767982	-1.705161889
C	-2.380712151	1.378162227	-1.716491217
H	-5.571627478	0.263181476	-2.221578349

H	-1.441324725	1.491868909	-2.258029954
C	-3.488937803	0.836407887	-2.374896997
H	-3.396160018	0.524147765	-3.418172065
H	-3.809610771	1.981945862	1.321269694

(³MLCT/³MC_{eq 2})_{CI-NEB} DFT B3LYP/DEF2-SVP CPCM.

Ir	-0.202007371	-0.412348446	-0.044122591
N	-1.112501254	0.645274185	-2.453339173
N	0.313070808	1.990946065	-0.546421234
N	-1.902993171	0.285334031	0.960530543
N	1.462054192	-1.198483218	-0.994631668
H	-1.417490478	-1.085644145	-3.546997963
C	3.701429020	1.571770099	2.854833505
C	2.548784459	2.100983647	2.268739716
C	4.668525250	0.944705380	2.060435861
C	2.335563106	1.987513307	0.882958491
C	4.471418700	0.842447115	0.678707986
C	3.310657806	1.355496770	0.092384378
C	-1.777796973	-0.068696376	-3.366478785
C	-3.321523900	1.717377590	-3.761664553
C	-2.620532319	2.469466892	-2.817453609
C	-1.495597469	1.903697919	-2.190501812
C	1.174507114	2.671334940	0.241767186
C	1.045574781	4.057732051	0.439818189
C	0.042717786	4.753638252	-0.225700595
C	-0.793422743	4.055206359	-1.093327720
C	-0.638126364	2.668791674	-1.234871421
C	-2.884538548	0.424551683	-4.059999742
C	-4.262746617	1.046962205	2.234280489
C	2.839449589	-1.651398876	-2.900605335
C	3.677289700	-2.450069438	-2.110761866
C	-3.823817454	-2.669789836	-0.175374688
C	-3.558094808	-3.792012902	-0.960350634
C	-2.303807931	-3.937627335	-1.578768385
C	-1.323678415	-2.955340135	-1.424067474
C	-1.571219261	-1.802473513	-0.648565622
C	-2.843519425	-1.674150905	-0.011463217
C	-1.948663617	1.404981023	1.711710223
C	-3.104373826	1.825098825	2.358018273
C	-4.218241966	-0.112127869	1.466317411
C	-3.026631435	-0.484687826	0.822747353
C	2.550944565	-2.705083873	2.202824494
C	2.134699453	-2.635707171	3.533571171
C	1.064263007	-1.798367473	3.895347988
C	0.411343217	-1.033958775	2.928624397
C	0.818799004	-1.068088419	1.574413727
C	1.912282629	-1.928306891	1.221703161
C	1.740102202	-1.046191244	-2.304304893
C	2.291879384	-1.934137060	-0.194082441
C	3.402104573	-2.586988137	-0.752531469
H	3.171464310	1.291038046	-0.988822489
H	3.847279805	1.653888691	3.935446012
H	1.799929739	2.596183569	2.892323478
H	5.577061708	0.542707235	2.516862264
H	5.229611201	0.366322672	0.051178316
H	-3.389991466	-0.196599234	-4.802046347
H	-4.199617295	2.138976359	-4.257148209
H	-2.955732712	3.477891246	-2.577881574

H	1.756733581	4.574153887	1.086728035
H	-0.069430833	5.832670608	-0.095573722
H	-1.549798655	4.590641227	-1.665370576
H	-5.107117284	-0.733894864	1.356733832
H	-5.188142502	1.342287453	2.734214151
H	-3.087166096	2.741163485	2.950710292
H	-1.019595028	1.968903412	1.801879214
H	3.025824737	-1.501432813	-3.965518117
H	4.541997910	-2.952674545	-2.550442525
H	4.053339707	-3.187072084	-0.116488590
H	1.044659884	-0.420738637	-2.865398001
H	-4.323703617	-4.561836186	-1.084921202
H	-2.097054497	-4.822660363	-2.187022557
H	-4.795593633	-2.579880061	0.316029563
H	-0.357585131	-3.088654312	-1.918257695
H	0.740938827	-1.749009228	4.938762626
H	-0.423658501	-0.398462359	3.233505993
H	3.371761356	-3.374732024	1.935167347
H	2.637449481	-3.240811328	4.292002830

(³MLCT/³MC_{ax 1})_{ts} DFT B3LYP/DEF2-SVP CPCM.

Ir	0.483824000	-0.169041000	0.024361000
N	-0.519875000	-0.845315000	2.091034000
N	1.714858000	0.444801000	-1.613791000
C	-2.468130000	-1.866418000	3.033259000
C	-1.684494000	-1.514345000	1.919557000
C	-0.097833000	-0.530185000	3.321664000
C	-2.013099000	-1.842506000	0.522348000
C	-1.121615000	-1.377908000	-0.473933000
C	-1.342037000	-1.761156000	-1.808380000
C	-2.463142000	-2.521331000	-2.159471000
C	-3.360589000	-2.951198000	-1.173128000
C	-3.131117000	-2.619170000	0.161903000
C	2.415421000	-0.569983000	-2.210600000
C	3.095106000	-0.330861000	-3.416421000
C	2.380712000	1.971142000	-3.339458000
C	1.714163000	1.682005000	-2.157571000
C	2.387968000	-1.837794000	-1.479119000
C	1.533550000	-1.879766000	-0.344039000
C	1.513202000	-3.054616000	0.424783000
C	2.301258000	-4.157792000	0.077051000
C	3.128316000	-4.112713000	-1.055296000
C	3.173092000	-2.955292000	-1.829453000
H	-4.228284000	-3.558428000	-1.443312000
H	-3.824297000	-2.977882000	0.926061000
H	-0.642028000	-1.459372000	-2.592770000
H	-2.627454000	-2.790843000	-3.206809000
H	0.868820000	-3.119631000	1.304872000
H	3.831453000	-2.917395000	-2.700831000
H	2.265116000	-5.063362000	0.689880000
H	3.739926000	-4.976761000	-1.327218000
H	0.862876000	-0.017029000	3.392030000
C	-2.038966000	-1.524438000	4.313338000
H	-3.404660000	-2.407452000	2.895920000
H	-2.643473000	-1.790402000	5.184226000
C	-0.825793000	-0.846132000	4.467646000
H	-0.443740000	-0.568514000	5.451957000
C	3.076199000	0.938383000	-3.986326000

H	1.175383000	2.455269000	-1.606766000
H	2.360316000	2.986711000	-3.738882000
H	3.604278000	1.127128000	-4.924153000
H	3.638292000	-1.143823000	-3.899524000
C	4.321559000	0.886811000	2.045392000
C	0.425775000	2.493754000	1.518947000
C	-0.028342000	3.619311000	2.229102000
C	-1.313800000	4.093644000	2.010042000
C	-2.105630000	3.463522000	1.047275000
C	-1.606696000	2.356115000	0.347041000
N	-0.377975000	1.845828000	0.618549000
H	0.616114000	4.096100000	2.967010000
H	-1.692543000	4.952892000	2.568407000
H	-3.102338000	3.837021000	0.809667000
C	1.788440000	1.975310000	1.717885000
C	2.829119000	2.767810000	2.240049000
C	4.097880000	2.227493000	2.410092000
C	3.269956000	0.158667000	1.514728000
N	2.031036000	0.679004000	1.354268000
H	2.644496000	3.812479000	2.491403000
H	4.908116000	2.840011000	2.811869000
H	5.297578000	0.414996000	2.173552000
H	3.395483000	-0.882757000	1.212234000
C	-3.777139000	1.416380000	-0.499086000
C	-4.612987000	1.017026000	-1.545798000
C	-2.447798000	1.799627000	-0.752661000
H	-5.640831000	0.712172000	-1.331495000
C	-4.138908000	1.013172000	-2.862631000
C	-1.980475000	1.789272000	-2.078213000
H	-4.796210000	0.710045000	-3.682019000
H	-0.964264000	2.117393000	-2.299172000
C	-2.821342000	1.402364000	-3.125256000
H	-2.445204000	1.412040000	-4.151789000
H	-4.156576000	1.425908000	0.525966000

(³MLCT/³MC_{eq 1})_{ts} DFT B3LYP/DEF2-SVP CPCM.

Ir	0.610011000	-0.416222000	0.132382000
N	2.125251000	1.014721000	1.061435000
N	-0.468870000	2.036646000	0.602148000
N	1.589995000	-0.035367000	-1.685419000
N	-0.401340000	-0.858912000	1.875372000
C	-2.843089000	2.153859000	-3.061677000
C	-2.073837000	2.348568000	-1.911626000
C	-4.135044000	1.625131000	-2.961799000
C	-2.584318000	2.025083000	-0.641626000
C	-4.654405000	1.300038000	-1.703071000
C	-3.889193000	1.505164000	-0.551881000
C	3.436971000	0.715982000	1.024463000
C	4.026618000	2.797771000	2.056320000
C	2.669269000	3.109705000	2.096903000
C	1.730272000	2.193995000	1.596095000
C	-1.792724000	2.323721000	0.582960000
C	-2.415115000	2.979384000	1.659739000
C	-1.653084000	3.398198000	2.749808000
C	-0.277284000	3.167721000	2.730634000
C	0.274083000	2.481087000	1.640673000
C	4.419997000	1.572063000	1.514476000
C	2.965678000	0.268418000	-4.081321000

C	-0.660928000	-0.994570000	4.260764000
C	-1.885292000	-1.680574000	4.105058000
C	3.223641000	-3.355135000	-1.486124000
C	3.302859000	-4.367242000	-0.527579000
C	2.642240000	-4.228162000	0.704488000
C	1.886251000	-3.084955000	0.973248000
C	1.797256000	-2.047036000	0.024803000
C	2.489202000	-2.187692000	-1.216487000
C	1.497634000	1.112401000	-2.380840000
C	2.168208000	1.306608000	-3.583685000
C	3.084906000	-0.908495000	-3.347101000
C	2.397242000	-1.044666000	-2.131010000
C	-3.062645000	-2.493214000	-0.125104000
C	-3.311737000	-2.646035000	-1.484074000
C	-2.441174000	-2.075156000	-2.447351000
C	-1.326433000	-1.359534000	-2.038197000
C	-1.037364000	-1.176755000	-0.658164000
C	-1.947409000	-1.748982000	0.314089000
C	0.044125000	-0.613465000	3.132249000
C	-1.596912000	-1.537885000	1.700543000
C	-2.339434000	-1.952839000	2.822201000
H	-4.302663000	1.243186000	0.425352000
H	-2.434614000	2.423906000	-4.039415000
H	-1.079314000	2.791092000	-1.991272000
H	-4.737351000	1.470769000	-3.861171000
H	-5.661765000	0.883969000	-1.616381000
H	3.704988000	-0.249791000	0.592532000
H	5.469453000	1.276125000	1.463846000
H	4.767267000	3.505984000	2.435760000
H	2.332157000	4.067992000	2.493885000
H	-3.482869000	3.200049000	1.612890000
H	-2.120172000	3.912719000	3.592780000
H	0.355113000	3.493493000	3.557843000
H	3.720164000	-1.719476000	-3.704713000
H	3.498801000	0.381204000	-5.028418000
H	2.059056000	2.252199000	-4.117447000
H	0.858865000	1.882444000	-1.947910000
H	-0.256831000	-0.765126000	5.248411000
H	-2.462141000	-1.997319000	4.976782000
H	-3.278687000	-2.487427000	2.671658000
H	1.006063000	-0.105727000	3.215300000
H	3.880817000	-5.270322000	-0.739786000
H	2.716169000	-5.020760000	1.454484000
H	3.736002000	-3.482605000	-2.442693000
H	1.364091000	-3.002957000	1.929853000
H	-2.653103000	-2.201067000	-3.512397000
H	-0.662610000	-0.931970000	-2.792601000
H	-3.735442000	-2.958984000	0.598988000
H	-4.185523000	-3.214970000	-1.812872000

(³MLCT/³MC_{ax 2})_{ts} DFT B3LYP/DEF2-SVP CPCM.

Ir	0.426881000	-0.386099000	0.257372000
N	-0.923639000	-0.616465000	1.881180000
N	1.545639000	0.306616000	-1.659393000
C	-2.731577000	-1.980594000	2.687796000
C	-1.940506000	-1.507862000	1.634478000
C	-0.684430000	-0.210657000	3.150260000
C	-2.064353000	-1.900206000	0.224665000

C	-1.050582000	-1.409638000	-0.653713000
C	-1.125429000	-1.769806000	-2.015223000
C	-2.149451000	-2.589787000	-2.492478000
C	-3.134081000	-3.071242000	-1.614768000
C	-3.091810000	-2.727023000	-0.262742000
C	2.409471000	-0.615124000	-2.154043000
C	3.174776000	-0.327633000	-3.297300000
C	2.188181000	1.865690000	-3.364521000
C	1.455355000	1.513376000	-2.232451000
C	2.490997000	-1.869148000	-1.384663000
C	1.741077000	-1.922247000	-0.185937000
C	1.838292000	-3.064802000	0.626279000
C	2.634007000	-4.150891000	0.238957000
C	3.360715000	-4.098811000	-0.957850000
C	3.294813000	-2.960044000	-1.763237000
H	-3.935743000	-3.714568000	-1.986880000
H	-3.866949000	-3.104731000	0.408448000
H	-0.364543000	-1.412405000	-2.712937000
H	-2.182195000	-2.861924000	-3.551325000
H	1.279930000	-3.122332000	1.565952000
H	3.872190000	-2.929340000	-2.690350000
H	2.688618000	-5.038998000	0.875298000
H	3.984717000	-4.943664000	-1.260417000
H	0.135058000	0.496670000	3.289989000
C	-2.492074000	-1.548688000	3.993571000
H	-3.531089000	-2.694098000	2.484020000
H	-3.109038000	-1.914488000	4.817537000
C	-1.443860000	-0.647107000	4.227497000
H	-1.220861000	-0.276186000	5.229771000
C	3.057417000	0.916850000	-3.911478000
H	0.777246000	2.224277000	-1.757561000
H	2.076062000	2.860656000	-3.799566000
H	3.648961000	1.148931000	-4.800705000
H	3.867681000	-1.071238000	-3.691915000
C	4.389924000	0.782381000	2.109797000
C	0.648498000	2.629992000	1.380287000
C	0.286294000	3.769047000	2.116557000
C	-1.002939000	4.274694000	1.993513000
C	-1.891922000	3.627247000	1.137258000
C	-1.477610000	2.494683000	0.417172000
N	-0.218596000	2.003628000	0.545174000
H	0.995892000	4.231164000	2.802535000
H	-1.313010000	5.155956000	2.559757000
H	-2.904967000	4.006241000	0.995582000
C	1.989725000	2.028901000	1.563158000
C	3.084501000	2.791661000	2.006095000
C	4.297853000	2.166120000	2.276741000
C	3.277111000	0.094284000	1.633429000
N	2.108301000	0.695547000	1.345717000
H	2.986630000	3.870858000	2.123997000
H	5.156840000	2.750428000	2.615252000
H	5.309736000	0.236695000	2.328080000
H	3.320595000	-0.982339000	1.467512000
C	-3.747843000	1.544359000	-0.027573000
C	-4.733513000	1.058080000	-0.890279000
C	-2.467705000	1.874541000	-0.512100000
H	-5.718169000	0.795273000	-0.494392000
C	-4.462363000	0.912506000	-2.255405000

C	-2.205750000	1.719860000	-1.883239000
H	-5.235778000	0.541119000	-2.933059000
H	-1.231936000	1.996294000	-2.286766000
C	-3.197258000	1.248608000	-2.748275000
H	-2.979014000	1.146548000	-3.814607000
H	-3.969407000	1.660399000	1.036467000

(³MC_{ax 1}/S₀)_{stc-mecp} DFT B3LYP/DEF2-SVP CPCM.

Ir	0.367502000	-0.129233000	0.138986000
N	-0.702714000	2.062702000	1.355535000
N	2.001509000	-1.244032000	-1.029694000
C	-2.792679000	2.624133000	2.373246000
C	-1.870958000	1.666629000	1.901158000
C	-0.396281000	3.361700000	1.297496000
C	-2.085663000	0.205542000	1.995096000
C	-1.182836000	-0.680687000	1.353067000
C	-1.352163000	-2.065230000	1.551010000
C	-2.404895000	-2.573292000	2.317446000
C	-3.312791000	-1.696659000	2.923163000
C	-3.145650000	-0.323144000	2.763896000
C	2.909838000	-1.823120000	-0.202315000
C	3.909938000	-2.652844000	-0.742398000
C	3.031087000	-2.238330000	-2.950635000
C	2.061912000	-1.435562000	-2.356604000
C	2.764817000	-1.496408000	1.229962000
C	1.650930000	-0.693681000	1.614726000
C	1.546185000	-0.336894000	2.972516000
C	2.488809000	-0.757270000	3.917007000
C	3.570065000	-1.558999000	3.528001000
C	3.705733000	-1.922840000	2.189190000
H	-4.135766000	-2.080878000	3.531298000
H	-3.841667000	0.350092000	3.268320000
H	-0.651579000	-2.771503000	1.095936000
H	-2.508065000	-3.654382000	2.447621000
H	0.707748000	0.281417000	3.301776000
H	4.559211000	-2.535663000	1.890563000
H	2.377181000	-0.461071000	4.964454000
H	4.306582000	-1.892852000	4.263408000
H	0.575192000	3.620565000	0.866018000
C	-2.477790000	3.978756000	2.301187000
H	-3.750438000	2.312851000	2.790365000
H	-3.187391000	4.726765000	2.664495000
C	-1.246501000	4.365386000	1.762991000
H	-0.949948000	5.414338000	1.698702000
C	3.967832000	-2.862221000	-2.117826000
H	1.309739000	-0.918264000	-2.958315000
H	3.048285000	-2.368441000	-4.034239000
H	4.742413000	-3.507492000	-2.540183000
H	4.637339000	-3.132241000	-0.087047000
C	3.423040000	3.070698000	-0.782998000
C	-0.457671000	1.874202000	-2.062149000
C	-1.258052000	2.676763000	-2.882745000
C	-2.513015000	2.214567000	-3.272355000
C	-2.911097000	0.946224000	-2.869414000
C	-2.067639000	0.173085000	-2.050274000
N	-0.881848000	0.661020000	-1.613537000
H	-0.916760000	3.659802000	-3.203598000
H	-3.159504000	2.829719000	-3.902317000

H	-3.860978000	0.527121000	-3.203152000
C	0.900102000	2.326532000	-1.653202000
C	1.559675000	3.399780000	-2.273703000
C	2.828716000	3.773970000	-1.833151000
C	2.721049000	2.005978000	-0.221466000
N	1.502304000	1.650084000	-0.652123000
H	1.098062000	3.934020000	-3.103238000
H	3.348475000	4.607761000	-2.311051000
H	4.412611000	3.332095000	-0.403704000
H	3.139236000	1.416264000	0.597155000
C	-3.799414000	-1.495184000	-1.327129000
C	-4.226676000	-2.812017000	-1.139726000
C	-2.481282000	-1.222746000	-1.737366000
H	-5.250402000	-3.006675000	-0.809254000
C	-3.350075000	-3.877179000	-1.376211000
C	-1.607929000	-2.299858000	-1.970924000
H	-3.688626000	-4.907654000	-1.239061000
H	-0.595616000	-2.108792000	-2.327605000
C	-2.040733000	-3.616804000	-1.794411000
H	-1.353511000	-4.443009000	-1.995080000
H	-4.491799000	-0.670714000	-1.139467000

(³MC_{eq 1}/S₀)_{stc-mecp} DFT B3LYP/DEF2-SVP CPCM.

Ir	-1.054245000	0.106003000	0.173587000
N	2.256279000	-0.561002000	-1.307853000
N	-0.636382000	2.128487000	-0.100730000
N	-1.473420000	-1.913947000	0.487943000
C	-0.962210000	-3.881591000	1.760643000
C	-0.761110000	-2.520896000	1.484004000
C	-2.353797000	-2.627178000	-0.241872000
C	0.184597000	-1.636242000	2.175319000
C	0.308152000	-0.315662000	1.647095000
C	1.178274000	0.582959000	2.294997000
C	1.916649000	0.185610000	3.413973000
C	1.796869000	-1.119148000	3.915742000
C	0.931352000	-2.026053000	3.300655000
C	-1.674028000	2.992300000	0.104669000
C	-1.478826000	4.370893000	-0.063180000
C	0.808165000	3.945873000	-0.689777000
C	0.564548000	2.589260000	-0.500393000
C	-2.940670000	2.341690000	0.472976000
C	-2.936930000	0.915295000	0.467703000
C	-4.122014000	0.243565000	0.821445000
C	-5.281373000	0.956290000	1.147122000
C	-5.274523000	2.358391000	1.139494000
C	-4.107313000	3.050118000	0.806945000
H	2.373248000	-1.426213000	4.792208000
H	0.835547000	-3.034704000	3.710269000
H	1.290118000	1.605969000	1.928201000
H	2.592039000	0.896527000	3.898775000
H	-4.152843000	-0.849016000	0.843687000
H	-4.112477000	4.142829000	0.815935000
H	-6.195899000	0.416897000	1.410640000
H	-6.179542000	2.913584000	1.399248000
H	-2.890679000	-2.085252000	-1.023110000
C	-1.875168000	-4.616734000	1.009068000
H	-0.394157000	-4.359781000	2.559076000
H	-2.032321000	-5.677576000	1.218828000

C	-2.582435000	-3.980181000	-0.017411000
H	-3.305489000	-4.515721000	-0.635035000
C	-0.232095000	4.851999000	-0.457529000
H	1.335644000	1.834113000	-0.673130000
H	1.797407000	4.276337000	-1.011045000
H	-0.075416000	5.925296000	-0.590497000
H	-2.306835000	5.060153000	0.105299000
C	-1.735826000	-0.082683000	-4.213683000
C	1.413496000	-1.511859000	-1.727342000
C	1.615067000	-2.875418000	-1.475591000
C	2.748452000	-3.244545000	-0.746993000
C	3.633169000	-2.257325000	-0.319509000
C	3.357914000	-0.907653000	-0.619542000
H	0.903676000	-3.620051000	-1.838133000
H	2.947049000	-4.296666000	-0.527099000
H	4.541848000	-2.532075000	0.217933000
C	0.267312000	-1.055584000	-2.579644000
C	0.224007000	-1.438941000	-3.927492000
C	-0.787031000	-0.951610000	-4.755425000
C	-1.649602000	0.236546000	-2.861045000
N	-0.681594000	-0.247569000	-2.057521000
H	1.000395000	-2.099535000	-4.318028000
H	-0.825663000	-1.237989000	-5.809425000
H	-2.540556000	0.340258000	-4.818082000
C	5.139819000	0.058817000	0.892462000
C	6.015833000	1.089718000	1.243592000
C	4.288908000	0.185968000	-0.222209000
H	6.661623000	0.975055000	2.118440000
C	6.062991000	2.264563000	0.484733000
C	4.343352000	1.374936000	-0.975513000
H	6.751245000	3.068845000	0.758528000
H	3.696711000	1.477540000	-1.849100000
C	5.223883000	2.401983000	-0.627655000
H	5.259809000	3.312886000	-1.231754000
H	5.107001000	-0.842413000	1.508920000
H	-2.388702000	0.890556000	-2.392717000

(³MC_{ax 2/S₀})_{stc-mecp} DFT B3LYP/DEF2-SVP CPCM.

Ir	-0.307224000	-0.184348000	-0.562711000
N	1.498383000	0.340741000	-1.788617000
N	-1.623069000	-0.113952000	1.802217000
C	3.486854000	-0.574214000	-2.749454000
C	2.383056000	-0.687990000	-1.886160000
C	1.659236000	1.454235000	-2.522240000
C	2.076141000	-1.866323000	-1.053227000
C	0.881195000	-1.820184000	-0.277712000
C	0.586308000	-2.939842000	0.524121000
C	1.423372000	-4.059116000	0.559272000
C	2.592118000	-4.090856000	-0.213600000
C	2.916002000	-2.996220000	-1.014852000
C	-2.712574000	-0.902923000	1.698573000
C	-3.619906000	-1.006046000	2.773114000
C	-2.258835000	0.529709000	4.027810000
C	-1.409087000	0.582428000	2.922532000
C	-2.882904000	-1.618627000	0.414727000
C	-1.947747000	-1.402291000	-0.626725000
C	-2.132735000	-2.081779000	-1.847206000
C	-3.204101000	-2.959850000	-2.042370000

C	-4.124009000	-3.172807000	-1.009487000
C	-3.961108000	-2.504328000	0.202199000
H	3.248477000	-4.964708000	-0.190697000
H	3.831937000	-3.027704000	-1.609393000
H	-0.321373000	-2.942987000	1.132479000
H	1.161801000	-4.914296000	1.189820000
H	-1.425042000	-1.933741000	-2.670485000
H	-4.689246000	-2.681248000	0.996150000
H	-3.316258000	-3.475918000	-3.000149000
H	-4.965804000	-3.856074000	-1.147888000
H	0.904464000	2.234919000	-2.399988000
C	3.662176000	0.584521000	-3.502130000
H	4.201273000	-1.393138000	-2.833652000
H	4.519149000	0.675693000	-4.174467000
C	2.730728000	1.623805000	-3.393386000
H	2.829068000	2.547000000	-3.967269000
C	-3.388998000	-0.288382000	3.943654000
H	-0.518591000	1.215501000	2.946898000
H	-2.035833000	1.115054000	4.922188000
H	-4.087469000	-0.365035000	4.781049000
H	-4.502986000	-1.639580000	2.693584000
C	-3.626316000	2.385345000	-2.103719000
C	-0.232624000	2.876354000	0.402634000
C	0.153153000	4.148416000	0.848746000
C	1.354292000	4.294737000	1.535055000
C	2.136968000	3.168316000	1.754660000
C	1.702588000	1.909449000	1.296176000
N	0.531094000	1.779452000	0.632654000
H	-0.462613000	5.022099000	0.643053000
H	1.674606000	5.276952000	1.890300000
H	3.078637000	3.240270000	2.299960000
C	-1.469200000	2.712693000	-0.406634000
C	-2.410735000	3.745941000	-0.544690000
C	-3.501224000	3.580993000	-1.395437000
C	-2.674677000	1.390292000	-1.895530000
N	-1.633069000	1.538430000	-1.058097000
H	-2.300092000	4.675129000	0.011916000
H	-4.237985000	4.380110000	-1.505958000
H	-4.450435000	2.210423000	-2.797810000
H	-2.751814000	0.430599000	-2.408063000
C	3.949980000	0.824380000	1.250141000
C	4.842538000	-0.180166000	1.631159000
C	2.587496000	0.745777000	1.598956000
H	5.894456000	-0.108979000	1.341851000
C	4.392063000	-1.267198000	2.389103000
C	2.142442000	-0.359123000	2.342575000
H	5.092028000	-2.046549000	2.702079000
H	1.094360000	-0.436420000	2.630264000
C	3.042243000	-1.350717000	2.744264000
H	2.682140000	-2.195554000	3.336517000
H	4.312012000	1.678179000	0.671412000

(³MC_{eq 2/S₀})_{stc-mecp} DFT B3LYP/DEF2-SVP CPCM.

Ir	0.007485000	-0.314628000	0.291380000
N	-2.145476000	0.078369000	-2.541670000
N	-0.118396000	1.624772000	-1.077354000
N	-1.072507000	0.783361000	1.714308000
N	1.068641000	-1.496482000	-1.054603000

H	-2.832779000	-1.549804000	-3.621915000
C	4.520268000	2.269796000	0.110520000
C	3.169018000	2.623403000	0.081339000
C	5.032545000	1.372393000	-0.833764000
C	2.306378000	2.065393000	-0.879882000
C	4.185734000	0.829479000	-1.806606000
C	2.830815000	1.170381000	-1.829277000
C	-3.118359000	-0.749505000	-2.929247000
C	-4.762818000	0.394753000	-1.611150000
C	-3.752936000	1.268901000	-1.204237000
C	-2.451136000	1.075556000	-1.695997000
C	0.894429000	2.525274000	-0.993891000
C	0.647993000	3.905540000	-1.083472000
C	-0.646996000	4.362433000	-1.303882000
C	-1.661450000	3.425002000	-1.487994000
C	-1.367411000	2.059049000	-1.385027000
C	-4.445045000	-0.633793000	-2.499311000
C	-2.640834000	2.104998000	3.594733000
C	1.393646000	-2.580731000	-3.164458000
C	2.565443000	-3.174779000	-2.683097000
C	-3.628359000	-1.888668000	1.896168000
C	-3.853464000	-3.107994000	1.253279000
C	-3.006824000	-3.519237000	0.213996000
C	-1.936947000	-2.711605000	-0.185462000
C	-1.692838000	-1.472938000	0.437897000
C	-2.557553000	-1.070281000	1.498028000
C	-0.689522000	1.976922000	2.207468000
C	-1.444249000	2.673341000	3.145104000
C	-3.039290000	0.871714000	3.085118000
C	-2.243706000	0.217366000	2.132604000
C	3.691550000	-2.095184000	1.487437000
C	3.980587000	-1.614341000	2.766250000
C	3.165045000	-0.631395000	3.345713000
C	2.059670000	-0.131438000	2.649918000
C	1.752005000	-0.588157000	1.353709000
C	2.589744000	-1.589509000	0.776792000
C	0.670237000	-1.747374000	-2.316767000
C	2.231698000	-2.029174000	-0.579029000
C	2.987516000	-2.891778000	-1.386054000
H	2.178830000	0.763177000	-2.604580000
H	5.176769000	2.700149000	0.871389000
H	2.776471000	3.328912000	0.818322000
H	6.091937000	1.102641000	-0.816426000
H	4.582707000	0.141525000	-2.557618000
H	-5.202517000	-1.337311000	-2.851933000
H	-5.782958000	0.517358000	-1.238170000
H	-3.967271000	2.081570000	-0.507596000
H	1.484837000	4.601410000	-1.009543000
H	-0.857270000	5.432366000	-1.375161000
H	-2.674138000	3.740395000	-1.742161000
H	-3.973115000	0.415646000	3.414630000
H	-3.258959000	2.620171000	4.334007000
H	-1.091502000	3.637845000	3.514136000
H	0.257345000	2.375436000	1.838864000
H	1.037033000	-2.757786000	-4.180646000
H	3.152209000	-3.843462000	-3.317740000
H	3.910422000	-3.325813000	-1.000256000
H	-0.248203000	-1.244225000	-2.632447000

H	-4.685389000	-3.743104000	1.568320000
H	-3.182396000	-4.475813000	-0.286888000
H	-4.285323000	-1.588914000	2.716307000
H	-1.291735000	-3.059217000	-0.995753000
H	3.392337000	-0.255117000	4.347447000
H	1.438438000	0.627836000	3.131082000
H	4.326868000	-2.869170000	1.050213000
H	4.839717000	-2.009264000	3.314556000

Complex 3 in CH₂Cl₂.

(S₀)_{min} DFT B3LYP/DEF2-SVP CPCM.

Ir	0.054799000	0.016143000	0.100997000
N	0.530805000	-0.936489000	-1.690972000
N	-0.357905000	0.816440000	1.985880000
C	1.676638000	-2.780047000	-2.712829000
C	1.304044000	-2.057245000	-1.567079000
C	0.169015000	-0.501118000	-2.913129000
C	1.695545000	-2.373913000	-0.191185000
C	1.279397000	-1.436150000	0.794030000
C	1.636252000	-1.693230000	2.129364000
C	2.370649000	-2.831902000	2.476597000
C	2.773160000	-3.749898000	1.495918000
C	2.438729000	-3.516392000	0.162878000
C	-1.322943000	0.165125000	2.701041000
C	-1.682509000	0.630777000	3.976853000
C	-0.044980000	2.383154000	3.776854000
C	0.265055000	1.887263000	2.515446000
C	-1.878298000	-1.014983000	2.032497000
C	-1.363266000	-1.285095000	0.734788000
C	-1.828614000	-2.435285000	0.075852000
C	-2.767463000	-3.283091000	0.673519000
C	-3.272340000	-3.001685000	1.951604000
C	-2.829894000	-1.866095000	2.627447000
H	3.342587000	-4.641292000	1.771163000
H	2.751297000	-4.231719000	-0.601980000
H	1.334774000	-1.004035000	2.921436000
H	2.628773000	-3.008127000	3.525395000
H	-1.456218000	-2.682902000	-0.920826000
H	-3.220117000	-1.649684000	3.625186000
H	-3.108626000	-4.174312000	0.138032000
H	-4.004394000	-3.666929000	2.416619000
H	-0.413916000	0.420161000	-2.941704000
C	1.278354000	-2.343464000	-3.972526000
H	2.288197000	-3.676724000	-2.608401000
H	1.566985000	-2.903686000	-4.865374000
C	0.517764000	-1.172915000	-4.079242000
H	0.196895000	-0.781535000	-5.046142000
C	-1.045181000	1.743160000	4.517803000
H	1.039856000	2.348963000	1.902125000
H	0.489878000	3.252556000	4.162904000
H	-1.321247000	2.106596000	5.510827000
H	-2.458901000	0.113370000	4.540986000
C	-3.436616000	2.933617000	-0.174105000
C	0.697198000	2.846246000	-0.991883000
C	1.219091000	3.911641000	-1.735904000
C	2.541657000	3.855579000	-2.165295000
C	3.305818000	2.756188000	-1.796338000

C	2.740237000	1.729283000	-1.017450000
N	1.433635000	1.757148000	-0.654237000
H	0.582391000	4.753805000	-2.006400000
H	2.969239000	4.660982000	-2.767103000
H	4.358433000	2.689155000	-2.074304000
C	-0.740849000	2.882836000	-0.614068000
C	-1.351597000	4.100560000	-0.291072000
C	-2.719044000	4.115027000	-0.024837000
C	-2.770668000	1.741682000	-0.516391000
N	-1.420214000	1.712300000	-0.645800000
H	-0.761128000	5.015033000	-0.231074000
H	-3.222704000	5.042993000	0.256134000
H	-4.521929000	2.926292000	-0.066832000
C	4.457637000	-0.037942000	-1.481766000
C	5.455425000	-0.915568000	-1.050184000
C	3.673466000	0.665747000	-0.549333000
H	6.050001000	-1.464698000	-1.785284000
C	5.699808000	-1.080707000	0.318086000
C	3.915091000	0.482549000	0.821818000
H	6.490962000	-1.755088000	0.656723000
H	3.324198000	1.036356000	1.554405000
C	4.929070000	-0.378333000	1.250752000
H	5.116505000	-0.501651000	2.320409000
H	4.282784000	0.102663000	-2.551628000
C	-3.604463000	0.557940000	-0.863859000
C	-4.723551000	0.210262000	-0.084485000
H	-4.906748000	0.722787000	0.863068000
C	-5.597511000	-0.795499000	-0.503801000
H	-6.456049000	-1.059959000	0.119273000
C	-5.377747000	-1.459226000	-1.716376000
H	-6.068855000	-2.238480000	-2.048851000
C	-4.272447000	-1.116019000	-2.502307000
H	-4.099378000	-1.620866000	-3.456572000
C	-3.391502000	-0.118041000	-2.078247000
H	-2.551351000	0.165437000	-2.712356000

(³MLCT)_{min} DFT B3LYP/DEF2-SVP CPCM.

Ir	0.047003000	0.214113000	0.163565000
N	0.696096000	-1.366237000	-1.027329000
N	-0.605507000	1.683722000	1.514318000
C	1.887302000	-3.446188000	-1.044242000
C	1.476354000	-2.281946000	-0.380979000
C	0.412726000	-1.519844000	-2.330457000
C	1.861669000	-1.886213000	0.976325000
C	1.380158000	-0.605688000	1.401715000
C	1.773401000	-0.130963000	2.673397000
C	2.584456000	-0.904942000	3.501562000
C	3.021682000	-2.173295000	3.082561000
C	2.663890000	-2.662000000	1.821994000
C	-1.660003000	1.310148000	2.295796000
C	-2.222103000	2.222808000	3.200640000
C	-0.586129000	3.854250000	2.528397000
C	-0.075335000	2.914092000	1.637590000
C	-2.085244000	-0.082837000	2.119194000
C	-1.402641000	-0.827214000	1.109815000
C	-1.730881000	-2.187716000	0.945772000
C	-2.675357000	-2.798870000	1.768271000
C	-3.334917000	-2.057865000	2.762753000

C	-3.044351000	-0.703719000	2.935035000
H	3.648481000	-2.780198000	3.740686000
H	3.017810000	-3.646589000	1.508808000
H	1.433044000	0.844754000	3.025682000
H	2.875344000	-0.528277000	4.485898000
H	-1.245508000	-2.781284000	0.169661000
H	-3.555335000	-0.142513000	3.720115000
H	-2.906500000	-3.859131000	1.636488000
H	-4.077738000	-2.539646000	3.403512000
H	-0.152068000	-0.713045000	-2.796557000
C	1.547843000	-3.634222000	-2.382486000
H	2.488571000	-4.186640000	-0.516301000
H	1.866537000	-4.537294000	-2.908570000
C	0.821512000	-2.641574000	-3.047491000
H	0.564861000	-2.728391000	-4.104586000
C	-1.686813000	3.503771000	3.314720000
H	0.787390000	3.140902000	1.013160000
H	-0.121335000	4.839258000	2.595086000
H	-2.119524000	4.219227000	4.018159000
H	-3.072788000	1.925471000	3.814061000
C	-3.648030000	1.974443000	-1.916938000
C	0.479445000	2.700993000	-1.512738000
C	1.078712000	3.947372000	-1.861543000
C	2.433676000	4.133811000	-1.743358000
C	3.235948000	3.044275000	-1.319951000
C	2.637701000	1.832324000	-0.997252000
N	1.276495000	1.663542000	-1.017715000
H	0.457683000	4.764194000	-2.224624000
H	2.889647000	5.091407000	-2.006002000
H	4.323143000	3.123348000	-1.296299000
C	-0.931631000	2.476905000	-1.632542000
C	-1.812344000	3.505119000	-2.082357000
C	-3.159251000	3.269777000	-2.202807000
C	-2.770239000	0.982986000	-1.483534000
N	-1.437535000	1.224980000	-1.281941000
H	-1.417330000	4.489022000	-2.328184000
H	-3.835598000	4.058815000	-2.540528000
H	-4.696266000	1.723810000	-2.079904000
C	3.751208000	-0.323981000	-1.655910000
C	4.765527000	-1.273208000	-1.496664000
C	3.580536000	0.705555000	-0.714283000
H	4.892727000	-2.059643000	-2.245489000
C	5.622940000	-1.210299000	-0.392260000
C	4.455519000	0.767824000	0.385190000
H	6.418400000	-1.950664000	-0.270752000
H	4.348843000	1.576694000	1.112425000
C	5.463116000	-0.187813000	0.549695000
H	6.131102000	-0.127727000	1.413340000
H	3.106825000	-0.361339000	-2.537398000
C	-3.374627000	-0.380275000	-1.350000000
C	-4.496470000	-0.574084000	-0.522523000
H	-4.832321000	0.239404000	0.124906000
C	-5.180744000	-1.792356000	-0.517950000
H	-6.045439000	-1.924803000	0.138102000
C	-4.765980000	-2.837604000	-1.350893000
H	-5.305999000	-3.788382000	-1.352653000
C	-3.662557000	-2.651936000	-2.190648000
H	-3.341689000	-3.452851000	-2.862588000

C	-2.977311000	-1.433525000	-2.191899000
H	-2.153884000	-1.284283000	-2.889272000

(³MC_{ax 1})_{min} DFT B3LYP/DEF2-SVP CPCM.

Ir	-0.114698000	-0.194612000	0.015964000
N	0.899257000	-1.311046000	-1.619657000
N	-0.344016000	1.881557000	1.603136000
C	2.286708000	-3.204990000	-2.072494000
C	1.695391000	-2.314334000	-1.158320000
C	0.676165000	-1.164023000	-2.937405000
C	1.863543000	-2.361329000	0.303362000
C	1.158621000	-1.386601000	1.066032000
C	1.335685000	-1.402293000	2.462093000
C	2.159591000	-2.344621000	3.084751000
C	2.835074000	-3.308437000	2.323343000
C	2.688934000	-3.311880000	0.937176000
C	-1.394667000	1.680362000	2.427296000
C	-1.862986000	2.726747000	3.247806000
C	-0.128332000	4.145952000	2.374288000
C	0.268506000	3.070324000	1.580248000
C	-1.974488000	0.321756000	2.419047000
C	-1.500859000	-0.618849000	1.471683000
C	-1.991629000	-1.936550000	1.537523000
C	-2.950181000	-2.313170000	2.481692000
C	-3.436313000	-1.373108000	3.398815000
C	-2.946575000	-0.069841000	3.365278000
H	3.474735000	-4.050299000	2.808433000
H	3.224916000	-4.060069000	0.348612000
H	0.813809000	-0.668161000	3.080401000
H	2.272471000	-2.332184000	4.173118000
H	-1.625518000	-2.691777000	0.836800000
H	-3.313589000	0.647698000	4.101939000
H	-3.312338000	-3.344976000	2.504045000
H	-4.182255000	-1.658368000	4.145106000
H	0.030800000	-0.333571000	-3.233550000
C	2.056862000	-3.054224000	-3.436990000
H	2.922944000	-4.013383000	-1.712074000
H	2.514672000	-3.745984000	-4.148685000
C	1.235862000	-2.012166000	-3.886299000
H	1.032936000	-1.855879000	-4.947239000
C	-1.226620000	3.964522000	3.220232000
H	1.115764000	3.174444000	0.898695000
H	0.408896000	5.095070000	2.322550000
H	-1.584164000	4.779960000	3.854388000
H	-2.721918000	2.573367000	3.900940000
C	-3.805443000	1.972970000	-1.475817000
C	0.388392000	2.372152000	-1.777604000
C	0.875431000	3.250866000	-2.755766000
C	2.245563000	3.303830000	-2.996913000
C	3.086183000	2.498212000	-2.238839000
C	2.546771000	1.642216000	-1.259461000
N	1.209745000	1.571512000	-1.060249000
H	0.188150000	3.859676000	-3.342442000
H	2.650385000	3.971129000	-3.761482000
H	4.167700000	2.540438000	-2.372073000
C	-1.083666000	2.273995000	-1.570201000
C	-1.901228000	3.387449000	-1.800386000
C	-3.283729000	3.239353000	-1.714691000

C	-2.938992000	0.889076000	-1.245979000
N	-1.594250000	1.070802000	-1.214663000
H	-1.460925000	4.357609000	-2.029363000
H	-3.945086000	4.094749000	-1.871329000
H	-4.882627000	1.804551000	-1.493365000
C	4.566628000	0.179734000	-1.039822000
C	5.562697000	-0.430739000	-0.274468000
C	3.510137000	0.875450000	-0.420343000
H	6.369548000	-0.976734000	-0.770583000
C	5.531330000	-0.334744000	1.121683000
C	3.477538000	0.948906000	0.982137000
H	6.318578000	-0.798704000	1.722009000
H	2.673153000	1.491390000	1.479954000
C	4.488054000	0.357269000	1.745143000
H	4.457447000	0.437549000	2.834623000
H	4.604348000	0.110142000	-2.129944000
C	-3.515017000	-0.477644000	-1.136908000
C	-4.722557000	-0.696881000	-0.448312000
H	-5.193930000	0.122781000	0.099058000
C	-5.311454000	-1.962928000	-0.431347000
H	-6.241894000	-2.118741000	0.120947000
C	-4.712779000	-3.028216000	-1.113929000
H	-5.178296000	-4.017433000	-1.104831000
C	-3.519402000	-2.818222000	-1.813423000
H	-3.052193000	-3.640163000	-2.362369000
C	-2.924575000	-1.554137000	-1.824164000
H	-2.010731000	-1.393551000	-2.396567000

(${}^3\text{MC}_{\text{eq } 1}$)_{min} DFT B3LYP/DEF2-SVP CPCM.

Ir	-0.795149000	0.302301000	-0.500973000
N	2.336911000	0.469312000	1.413002000
N	-0.600602000	0.365084000	1.892392000
N	-1.385632000	2.308307000	-0.398514000
N	-0.217677000	-1.681644000	-0.733444000
C	4.225915000	-1.701630000	1.454853000
C	5.002759000	-2.843785000	1.245812000
C	5.947589000	-2.874086000	0.212703000
C	6.111301000	-1.751930000	-0.607230000
C	5.339583000	-0.606032000	-0.394727000
C	4.384274000	-0.565124000	0.638695000
C	-4.812670000	-1.970561000	1.767800000
C	-3.977096000	-0.901097000	2.099924000
C	-4.269004000	-3.236930000	1.522640000
C	-2.582847000	-1.079157000	2.166921000
C	-2.885122000	-3.427477000	1.608435000
C	-2.045695000	-2.356189000	1.925105000
C	3.558844000	0.651083000	0.884651000
C	3.254128000	3.047665000	0.887425000
C	1.991452000	2.850030000	1.449056000
C	1.571776000	1.533199000	1.691836000
C	-1.698314000	0.031796000	2.617432000
C	-1.999481000	0.686426000	3.823213000
C	-1.144727000	1.673527000	4.303420000
C	0.019107000	1.953977000	3.589726000
C	0.273437000	1.272640000	2.392606000
C	4.052227000	1.941679000	0.605629000
C	-2.045895000	5.011597000	-0.413435000
C	1.275615000	-3.529418000	-0.435426000

C	0.430632000	-4.341892000	-1.199782000
C	1.236724000	3.239579000	-2.841346000
C	2.258716000	2.570524000	-3.518443000
C	2.484528000	1.206737000	-3.278502000
C	1.691316000	0.510479000	-2.361386000
C	0.660860000	1.164256000	-1.656938000
C	0.437565000	2.549927000	-1.914089000
C	-2.409337000	2.766871000	0.347700000
C	-2.769935000	4.109528000	0.373927000
C	-0.988643000	4.539423000	-1.187018000
C	-0.660490000	3.175445000	-1.166823000
C	-3.270041000	-2.369896000	-2.710821000
C	-4.416440000	-1.655136000	-3.064979000
C	-4.595581000	-0.342062000	-2.603735000
C	-3.629726000	0.258261000	-1.790999000
C	-2.469254000	-0.444471000	-1.408593000
C	-2.298498000	-1.780062000	-1.884918000
C	0.916576000	-2.201531000	-0.226672000
C	-1.072115000	-2.464024000	-1.456273000
C	-0.749493000	-3.805085000	-1.709243000
H	3.494402000	-1.674100000	2.265111000
H	4.874171000	-3.713137000	1.896589000
H	6.554333000	-3.768548000	0.047734000
H	6.840867000	-1.769307000	-1.421444000
H	5.466948000	0.254718000	-1.055369000
H	-0.968869000	-2.513579000	2.012500000
H	-5.892893000	-1.815092000	1.704284000
H	-4.407810000	0.084230000	2.296733000
H	-4.923677000	-4.075890000	1.271975000
H	-2.455792000	-4.417629000	1.434894000
H	5.055786000	2.075095000	0.199111000
H	3.616722000	4.057999000	0.681655000
H	1.341413000	3.694045000	1.686120000
H	-2.889204000	0.393517000	4.382575000
H	-1.363306000	2.194125000	5.239058000
H	0.745830000	2.676735000	3.963417000
H	-0.409103000	5.226014000	-1.804708000
H	-2.303519000	6.073456000	-0.423300000
H	-3.606648000	4.431795000	0.995924000
H	-2.957914000	2.024849000	0.930517000
H	2.205207000	-3.908325000	-0.007923000
H	0.686289000	-5.386934000	-1.391120000
H	-1.429784000	-4.424585000	-2.294237000
H	1.534379000	-1.516925000	0.360359000
H	2.877010000	3.111010000	-4.239709000
H	3.284511000	0.684659000	-3.811407000
H	1.063695000	4.298649000	-3.046727000
H	1.887753000	-0.551095000	-2.194079000
H	-5.494133000	0.215951000	-2.882766000
H	-3.791831000	1.284649000	-1.453386000
H	-3.137136000	-3.387263000	-3.086900000
H	-5.170069000	-2.119521000	-3.706074000

(³MLCT/³MC_{ax 1})_{CI-NEB} DFT B3LYP/DEF2-SVP CPCM.

Ir	-0.041703508	0.032719000	0.061944177
N	0.829747834	-1.228699434	-1.275477795
N	-0.453500772	1.656477642	1.539356896
C	1.927647110	-3.363815333	-1.544085609

C	1.539165186	-2.293929495	-0.725060398
C	0.581171447	-1.207561150	-2.622550552
C	1.823004023	-2.132062749	0.690065557
C	1.235451097	-0.985471900	1.292077761
C	1.477282207	-0.749267063	2.653385696
C	2.280180801	-1.619188594	3.400060410
C	2.848331315	-2.755354191	2.801199242
C	2.621602433	-3.011696014	1.451954618
C	-1.517271953	1.401793130	2.351876112
C	-2.006685890	2.404237439	3.205158281
C	-0.270786730	3.876603826	2.428085488
C	0.162740510	2.850236031	1.595582763
C	-2.040741909	0.033174278	2.272716547
C	-1.453399500	-0.809301129	1.302115601
C	-1.820365868	-2.160754188	1.258412654
C	-2.799422133	-2.653727964	2.127471176
C	-3.405253560	-1.811018079	3.069866205
C	-3.022256234	-0.473790888	3.147281499
H	3.472661020	-3.433382378	3.388641762
H	3.075412266	-3.889328108	0.984702649
H	1.032002425	0.114066808	3.152963114
H	2.460713249	-1.413313893	4.459312528
H	-1.356275080	-2.839524735	0.538210604
H	-3.475694382	0.171413632	3.903218212
H	-3.090649971	-3.706293916	2.069900738
H	-4.165204007	-2.201705439	3.751294140
H	0.074097791	-0.320273934	-3.004217940
C	1.650145511	-3.348050115	-2.907719213
H	2.471695237	-4.200855463	-1.103178260
H	1.965799377	-4.175746073	-3.547004638
C	0.967883936	-2.235722985	-3.454404817
H	0.753905048	-2.169697739	-4.522967347
C	-1.389582260	3.651536372	3.236364014
H	1.037765083	2.977658481	0.960016623
H	0.263529553	4.828182455	2.435563069
H	-1.770515594	4.438518311	3.891838673
H	-2.867797698	2.200670154	3.841867769
C	-3.737632846	2.005660331	-1.676378194
C	0.442517214	2.598784032	-1.677604987
C	0.966756412	3.629925228	-2.480257814
C	2.339771536	3.771777403	-2.609110764
C	3.168642203	2.845643141	-1.971854342
C	2.605652000	1.821275470	-1.200764620
N	1.264549879	1.725668197	-1.026116153
H	0.299234327	4.302185344	-3.016704083
H	2.761250764	4.579877040	-3.211214419
H	4.254436594	2.913010713	-2.050420195
C	-1.021749371	2.429110110	-1.572563653
C	-1.881859640	3.504195808	-1.863748318
C	-3.252833595	3.296676657	-1.893323375
C	-2.849734208	0.966699535	-1.364712618
N	-1.511753004	1.194382962	-1.250686546
H	-1.476793327	4.497436143	-2.051015968
H	-3.935941873	4.121204716	-2.109611290
H	-4.801128022	1.786134735	-1.772306894
C	4.218177142	-0.071798376	-1.418111183
C	5.244226711	-0.878883308	-0.918230528
C	3.568293974	0.854825572	-0.584260514

H	5.736553340	-1.599488935	-1.577066377
C	5.646135358	-0.753547594	0.416061791
C	3.970011338	0.969089240	0.755305361
H	6.457945757	-1.374156417	0.805201184
H	3.484314415	1.698588374	1.408011796
C	5.007479632	0.171307873	1.249610834
H	5.318848575	0.273279406	2.292481843
H	3.922475802	-0.153721023	-2.467409110
C	-3.420889557	-0.405560414	-1.246848045
C	-4.595826895	-0.616383768	-0.500163106
H	-5.015635972	0.201893590	0.089881127
C	-5.220440280	-1.864967705	-0.491242327
H	-6.125503071	-2.012709651	0.104111256
C	-4.691426704	-2.922246513	-1.240704762
H	-5.187408301	-3.896778713	-1.241844768
C	-3.529282169	-2.721877073	-1.992767333
H	-3.116941397	-3.537547202	-2.592848030
C	-2.897491010	-1.474576877	-1.994817482
H	-2.011829138	-1.322142660	-2.611795401

(³MLCT/³MC_{eq 1})_{CI-NEB} DFT B3LYP/DEF2-SVP CPCM.

Ir	-0.285594523	0.211020771	-0.129660269
N	1.792437864	0.815649378	1.349908223
N	-0.850293890	0.314341338	2.137666404
N	-0.618509676	2.257980372	-0.281019670
N	0.000442767	-1.855790426	-0.112664149
C	3.982135928	-1.171076562	0.484151163
C	4.815344607	-2.041841696	-0.224623544
C	5.522329468	-1.584409172	-1.341994081
C	5.395136273	-0.248265550	-1.739351777
C	4.560174552	0.620116542	-1.031258800
C	3.830090609	0.168405891	0.084346622
C	-4.981001180	-1.950242187	1.127809655
C	-4.152092686	-0.914624845	1.568794456
C	-4.524399404	-3.273287440	1.146734567
C	-2.846791363	-1.186926747	2.016050354
C	-3.232590106	-3.553617630	1.604770137
C	-2.397460627	-2.518327170	2.036568910
C	3.049722136	1.126070483	0.922722009
C	3.076959316	3.161759835	2.237103492
C	1.825090752	2.809411428	2.728909889
C	1.220548115	1.618006521	2.291011840
C	-2.029696903	-0.111065167	2.658069147
C	-2.518489486	0.402388467	3.868855090
C	-1.750903104	1.312882695	4.593571645
C	-0.508349615	1.680422902	4.095460097
C	-0.079295349	1.186557785	2.851679167
C	3.703974554	2.291940653	1.339001115
C	-0.978681286	4.997151473	-0.730577006
C	1.070227161	-3.886605822	0.568081823
C	0.280057245	-4.612302903	-0.333974339
C	1.449317157	2.338358796	-3.355723303
C	2.132039413	1.388120342	-4.108852141
C	2.165676094	0.037425691	-3.697277695
C	1.529322580	-0.351136559	-2.523874238
C	0.833383176	0.591161571	-1.731644944
C	0.795722481	1.963860744	-2.164238915
C	-1.435016419	2.989347906	0.514692660

C	-1.638346086	4.347479720	0.330194534
C	-0.161442011	4.247204923	-1.568337054
C	0.012502119	2.870391423	-1.345236132
C	-2.835828863	-2.227610664	-2.460482344
C	-3.838587326	-1.385042756	-2.943935314
C	-3.882951570	-0.034826549	-2.551873004
C	-2.915247753	0.478397533	-1.689083511
C	-1.901624490	-0.355271709	-1.168479082
C	-1.876885419	-1.734078784	-1.561201334
C	0.895929731	-2.509235182	0.646492835
C	-0.836014079	-2.553441521	-0.941294455
C	-0.683611536	-3.941817774	-1.082196733
H	3.481413073	-1.521031712	1.387566354
H	4.926310258	-3.077077054	0.109746242
H	6.179388726	-2.263069779	-1.892906484
H	5.949584248	0.120171924	-2.606815191
H	4.464327176	1.659370922	-1.355119488
H	-1.401685191	-2.748719184	2.421771405
H	-5.990639845	-1.723391654	0.774844079
H	-4.519344194	0.114772445	1.566103049
H	-5.176958087	-4.084695521	0.813107923
H	-2.873721311	-4.585740016	1.636373523
H	4.721208858	2.485814521	0.994527708
H	3.571049619	4.077914619	2.567266440
H	1.318724567	3.462566550	3.438480575
H	-3.480256777	0.050726564	4.244322637
H	-2.106058416	1.709004978	5.547791272
H	0.132323383	2.349175673	4.667904075
H	0.347620600	4.722379179	-2.407701624
H	-1.116263103	6.067032445	-0.902150644
H	-2.312377562	4.884197755	1.000526469
H	-1.960594226	2.453584294	1.304667291
H	1.819780155	-4.372651618	1.194912657
H	0.403233788	-5.693092804	-0.436939204
H	-1.335537157	-4.492254128	-1.760963983
H	1.480005845	-1.888737186	1.323144025
H	2.639856249	1.691336542	-5.028009830
H	2.703665140	-0.701198344	-4.296961221
H	1.412631340	3.373761382	-3.703041512
H	1.569610549	-1.398619393	-2.218891973
H	-4.675164555	0.616454099	-2.931178441
H	-2.952062492	1.535609084	-1.417417566
H	-2.808319969	-3.270046910	-2.786437549
H	-4.590610036	-1.778558041	-3.632313016

(³MLCT/³MC_{ax1})_{ts} DFT B3LYP/DEF2-SVP CPCM.

Ir	-0.180514000	-0.215473000	-0.040746000
N	0.660428000	-1.300930000	-1.606500000
N	-0.621562000	1.339176000	1.553845000
C	2.011156000	-3.216094000	-2.175387000
C	1.552434000	-2.283610000	-1.230637000
C	0.245114000	-1.238564000	-2.899773000
C	1.918955000	-2.240756000	0.177378000
C	1.203991000	-1.294774000	0.967097000
C	1.515841000	-1.201496000	2.335684000
C	2.497326000	-2.015377000	2.904793000
C	3.190325000	-2.953134000	2.119554000
C	2.904065000	-3.064052000	0.762509000

C	-1.508488000	0.943770000	2.504840000
C	-1.941917000	1.853249000	3.485798000
C	-0.572817000	3.553341000	2.472866000
C	-0.176454000	2.605666000	1.533917000
C	-1.956257000	-0.452994000	2.400468000
C	-1.502688000	-1.180558000	1.276076000
C	-1.854734000	-2.534061000	1.158726000
C	-2.684046000	-3.140710000	2.108180000
C	-3.143081000	-2.410842000	3.214681000
C	-2.775975000	-1.074220000	3.363608000
H	3.954368000	-3.591104000	2.571230000
H	3.452536000	-3.786561000	0.153301000
H	0.985679000	-0.489138000	2.971328000
H	2.724651000	-1.924813000	3.970937000
H	-1.485995000	-3.128620000	0.317424000
H	-3.122167000	-0.519929000	4.239171000
H	-2.964563000	-4.191862000	1.992592000
H	-3.776380000	-2.889723000	3.965890000
H	-0.443306000	-0.430462000	-3.149232000
C	1.577159000	-3.149246000	-3.494360000
H	2.708989000	-3.993829000	-1.862721000
H	1.931830000	-3.873756000	-4.231013000
C	0.674814000	-2.135205000	-3.862310000
H	0.314781000	-2.035286000	-4.888033000
C	-1.472259000	3.163049000	3.471327000
H	0.526701000	2.852420000	0.736819000
H	-0.179150000	4.570080000	2.419301000
H	-1.808134000	3.875900000	4.228616000
H	-2.651916000	1.532489000	4.248388000
C	-3.501143000	2.482714000	-1.614970000
C	0.694000000	2.143366000	-2.095497000
C	1.190281000	2.504946000	-3.355885000
C	2.555783000	2.360981000	-3.604122000
C	3.377302000	1.902211000	-2.578910000
C	2.819245000	1.583875000	-1.326036000
N	1.486264000	1.674508000	-1.111399000
H	0.514668000	2.869593000	-4.131074000
H	2.973481000	2.618759000	-4.580339000
H	4.455604000	1.827815000	-2.726176000
C	-0.775621000	2.278743000	-1.849299000
C	-1.407124000	3.474233000	-2.213364000
C	-2.786529000	3.591128000	-2.056147000
C	-2.822181000	1.295668000	-1.290710000
N	-1.467059000	1.228134000	-1.336040000
H	-0.813372000	4.304462000	-2.597749000
H	-3.299520000	4.522701000	-2.307097000
H	-4.589843000	2.507985000	-1.553653000
C	4.857737000	0.416923000	-0.421473000
C	5.749219000	0.139680000	0.617741000
C	3.719706000	1.216552000	-0.198841000
H	6.621085000	-0.492337000	0.428514000
C	5.527880000	0.667887000	1.894955000
C	3.503097000	1.732755000	1.091518000
H	6.230388000	0.457860000	2.705977000
H	2.638332000	2.370077000	1.278346000
C	4.402353000	1.465934000	2.126964000
H	4.223877000	1.887414000	3.119895000
H	5.039407000	-0.007146000	-1.412089000

C	-3.630564000	0.078427000	-1.005947000
C	-4.716809000	0.129557000	-0.113656000
H	-4.901416000	1.038230000	0.464917000
C	-5.552698000	-0.977938000	0.048977000
H	-6.385897000	-0.928241000	0.754984000
C	-5.328158000	-2.144316000	-0.691943000
H	-5.990160000	-3.006126000	-0.572186000
C	-4.256099000	-2.200921000	-1.588466000
H	-4.080450000	-3.104604000	-2.178090000
C	-3.410415000	-1.099471000	-1.742628000
H	-2.593392000	-1.143982000	-2.464632000

(³MLCT/³MC_{eq 1})_{ts} DFT B3LYP/DEF2-SVP CPCM.

Ir	-0.248744000	0.091252000	-0.081826000
N	1.804849000	0.940335000	1.374652000
N	-0.850063000	0.123563000	2.224530000
N	-0.471662000	2.119141000	-0.378012000
N	-0.020126000	-1.972823000	0.143695000
C	4.029362000	-0.546590000	0.134357000
C	4.949731000	-1.233860000	-0.660404000
C	5.651453000	-0.560341000	-1.666628000
C	5.428080000	0.807208000	-1.867759000
C	4.514510000	1.496478000	-1.067062000
C	3.798129000	0.828996000	-0.054361000
C	-5.019151000	-0.752064000	0.713654000
C	-3.854519000	-0.261453000	1.310480000
C	-5.329332000	-2.114506000	0.788284000
C	-2.993890000	-1.128094000	2.004540000
C	-4.472336000	-2.986016000	1.470040000
C	-3.317946000	-2.494230000	2.085671000
C	2.903544000	1.567672000	0.874952000
C	2.550751000	3.471890000	2.335754000
C	1.492627000	2.774354000	2.922811000
C	1.156324000	1.516393000	2.410965000
C	-1.856835000	-0.581868000	2.799920000
C	-1.920105000	-0.759740000	4.192706000
C	-0.971608000	-0.162882000	5.016600000
C	0.020994000	0.612961000	4.426549000
C	0.059932000	0.729101000	3.030678000
C	3.271583000	2.850432000	1.316655000
C	-0.685836000	4.836898000	-1.010720000
C	0.964581000	-3.944974000	1.080807000
C	0.134073000	-4.745287000	0.283184000
C	1.466757000	1.837010000	-3.527327000
C	2.103636000	0.797254000	-4.194163000
C	2.148761000	-0.501468000	-3.630849000
C	1.550363000	-0.747018000	-2.402394000
C	0.896822000	0.289244000	-1.691998000
C	0.867525000	1.613373000	-2.268610000
C	-1.186957000	2.957114000	0.411272000
C	-1.315176000	4.307797000	0.137524000
C	0.038655000	3.982839000	-1.830474000
C	0.150922000	2.616132000	-1.511694000
C	-2.727930000	-2.514183000	-2.322160000
C	-3.613363000	-1.691319000	-3.019564000
C	-3.602354000	-0.300503000	-2.809273000
C	-2.700058000	0.267377000	-1.910415000
C	-1.805553000	-0.543164000	-1.181841000

C	-1.827381000	-1.956385000	-1.398232000
C	0.856132000	-2.563156000	0.978730000
C	-0.868778000	-2.734678000	-0.613309000
C	-0.787567000	-4.135396000	-0.562691000
H	3.504189000	-1.069669000	0.934548000
H	5.125457000	-2.299361000	-0.488219000
H	6.372440000	-1.097048000	-2.289245000
H	5.967201000	1.340741000	-2.655269000
H	4.342664000	2.560881000	-1.244121000
H	-2.660401000	-3.174679000	2.632985000
H	-5.688122000	-0.065254000	0.188891000
H	-3.624952000	0.805411000	1.260793000
H	-6.240352000	-2.495953000	0.319262000
H	-4.707327000	-4.052031000	1.530844000
H	4.158435000	3.331283000	0.901137000
H	2.829132000	4.467183000	2.689766000
H	0.927465000	3.200415000	3.753347000
H	-2.742746000	-1.339450000	4.613395000
H	-1.011356000	-0.291930000	6.100953000
H	0.787309000	1.100352000	5.030286000
H	0.533361000	4.365269000	-2.724644000
H	-0.770078000	5.898556000	-1.253298000
H	-1.901706000	4.937864000	0.808584000
H	-1.673924000	2.508044000	1.278401000
H	1.693130000	-4.380421000	1.766810000
H	0.200457000	-5.834905000	0.330398000
H	-1.458224000	-4.738578000	-1.175594000
H	1.484069000	-1.891159000	1.565621000
H	2.569126000	0.983123000	-5.165831000
H	2.657696000	-1.308461000	-4.164339000
H	1.422329000	2.824644000	-3.992570000
H	1.584454000	-1.755448000	-1.985243000
H	-4.301100000	0.338272000	-3.356783000
H	-2.693035000	1.351211000	-1.773311000
H	-2.735741000	-3.590622000	-2.509530000
H	-4.312675000	-2.131095000	-3.735270000

(³MC_{ax 1/S₀})_{stc-mecp} DFT B3LYP/DEF2-SVP CPCM.

Ir	-0.073940000	-0.214818000	0.019566000
N	1.168785000	-1.255711000	-1.511648000
N	-0.524772000	1.904730000	1.593238000
C	2.667608000	-3.090793000	-1.832264000
C	1.941253000	-2.241175000	-0.978522000
C	1.096291000	-1.086812000	-2.843268000
C	1.941325000	-2.314395000	0.492334000
C	1.122557000	-1.378218000	1.186948000
C	1.143258000	-1.415672000	2.593712000
C	1.922358000	-2.344343000	3.290069000
C	2.709944000	-3.271322000	2.593513000
C	2.720950000	-3.251243000	1.199703000
C	-1.658878000	1.673151000	2.287027000
C	-2.257141000	2.708472000	3.034575000
C	-0.477713000	4.180479000	2.361006000
C	0.046587000	3.112913000	1.632381000
C	-2.190481000	0.295826000	2.222904000
C	-1.591100000	-0.636437000	1.339858000
C	-2.050830000	-1.967203000	1.365292000
C	-3.094510000	-2.366638000	2.203859000

C	-3.703543000	-1.435330000	3.053458000
C	-3.248140000	-0.119446000	3.061510000
H	3.315125000	-4.002942000	3.135146000
H	3.345423000	-3.969945000	0.663788000
H	0.532091000	-0.709628000	3.160645000
H	1.912050000	-2.350007000	4.384284000
H	-1.590063000	-2.717256000	0.716559000
H	-3.711588000	0.590733000	3.749297000
H	-3.427071000	-3.408566000	2.196631000
H	-4.517839000	-1.736899000	3.717383000
H	0.460223000	-0.272333000	-3.198395000
C	2.593119000	-2.917822000	-3.211461000
H	3.286061000	-3.884901000	-1.413982000
H	3.155469000	-3.577975000	-3.876755000
C	1.793587000	-1.894078000	-3.735176000
H	1.710283000	-1.721176000	-4.809612000
C	-1.662931000	3.966925000	3.071083000
H	0.966232000	3.240524000	1.056489000
H	0.030430000	5.146919000	2.363987000
H	-2.121346000	4.773895000	3.648791000
H	-3.183544000	2.531988000	3.581032000
C	-3.688040000	1.772176000	-1.864601000
C	0.482520000	2.408416000	-1.672569000
C	1.033020000	3.340830000	-2.563520000
C	2.417187000	3.465186000	-2.643774000
C	3.206105000	2.673093000	-1.818634000
C	2.602885000	1.760542000	-0.932040000
N	1.257070000	1.623913000	-0.888805000
H	0.388057000	3.935923000	-3.209215000
H	2.872455000	4.175983000	-3.337528000
H	4.292497000	2.768133000	-1.827585000
C	-0.995392000	2.227996000	-1.638586000
C	-1.843445000	3.296057000	-1.956385000
C	-3.215571000	3.068537000	-2.035050000
C	-2.793552000	0.736759000	-1.538583000
N	-1.474200000	0.993918000	-1.350977000
H	-1.437055000	4.292709000	-2.126207000
H	-3.902195000	3.886784000	-2.264565000
H	-4.744286000	1.543664000	-2.009211000
C	4.644462000	0.367330000	-0.534685000
C	5.578511000	-0.226033000	0.317692000
C	3.503537000	1.007724000	-0.013644000
H	6.452992000	-0.729858000	-0.102736000
C	5.399212000	-0.167132000	1.704648000
C	3.322773000	1.043438000	1.378966000
H	6.137748000	-0.617169000	2.373567000
H	2.449466000	1.541604000	1.801331000
C	4.271292000	0.470605000	2.230858000
H	4.124430000	0.521806000	3.312616000
H	4.798099000	0.328001000	-1.616143000
C	-3.299637000	-0.660896000	-1.497563000
C	-4.569999000	-0.949748000	-0.965151000
H	-5.152669000	-0.159612000	-0.485866000
C	-2.567890000	-1.701412000	-2.099249000
H	-1.600433000	-1.488609000	-2.554319000
C	-3.086936000	-2.997361000	-2.156170000
H	-2.508703000	-3.790481000	-2.637783000
C	-5.084596000	-2.246792000	-1.016612000

H	-6.067550000	-2.455877000	-0.586222000
C	-4.345712000	-3.275581000	-1.612376000
H	-4.752415000	-4.289446000	-1.657436000

(³MC_{eq 1}/S₀)_{stc-mecp} DFT B3LYP/DEF2-SVP CPCM.

Ir	-0.655870000	0.254485000	-0.478704000
N	2.498080000	0.339685000	1.441016000
N	-0.097333000	-1.733074000	-0.744764000
N	-1.227207000	2.266177000	-0.329728000
C	-0.795581000	4.514489000	-1.045788000
C	-0.480715000	3.147358000	-1.059671000
C	-2.254661000	2.713841000	0.417257000
C	0.629634000	2.534673000	-1.801747000
C	0.860174000	1.149147000	-1.554362000
C	1.902414000	0.512831000	-2.255481000
C	2.700347000	1.223897000	-3.158315000
C	2.466819000	2.587531000	-3.386839000
C	1.432486000	3.241152000	-2.713170000
C	-0.989258000	-2.510612000	-1.425092000
C	-0.680518000	-3.849941000	-1.703178000
C	1.404622000	-3.585146000	-0.527845000
C	1.057763000	-2.258044000	-0.294310000
C	-2.241434000	-1.827290000	-1.778407000
C	-2.403593000	-0.507702000	-1.259062000
C	-3.587982000	0.187611000	-1.571194000
C	-4.584866000	-0.403576000	-2.354032000
C	-4.413066000	-1.701497000	-2.856551000
C	-3.243250000	-2.409756000	-2.573382000
H	3.087488000	3.140150000	-4.096831000
H	1.251683000	4.300404000	-2.910839000
H	2.105918000	-0.549089000	-2.098903000
H	3.508890000	0.712589000	-3.688816000
H	-3.748047000	1.203522000	-1.202272000
H	-3.115225000	-3.414965000	-2.982385000
H	-5.500850000	0.151181000	-2.577451000
H	-5.189719000	-2.158943000	-3.474800000
H	-2.816356000	1.961550000	0.973776000
C	-1.859388000	4.975173000	-0.274081000
H	-0.199200000	5.212942000	-1.633352000
H	-2.106002000	6.039568000	-0.256887000
C	-2.601997000	4.059020000	0.478332000
H	-3.442473000	4.372053000	1.099952000
C	0.523386000	-4.390707000	-1.257154000
H	1.701342000	-1.580033000	0.271963000
H	2.352050000	-3.968397000	-0.145738000
H	0.768088000	-5.434625000	-1.468061000
H	-1.390798000	-4.466212000	-2.254851000
C	-1.831943000	0.580816000	3.833349000
C	1.747743000	1.414949000	1.714607000
C	2.197756000	2.725905000	1.496199000
C	3.476983000	2.904741000	0.966790000
C	4.260275000	1.786524000	0.691579000
C	3.735303000	0.502891000	0.942972000
H	1.559040000	3.579808000	1.728515000
H	3.864124000	3.909898000	0.781409000
H	5.275906000	1.905620000	0.311484000
C	0.437055000	1.169470000	2.397913000
C	0.189637000	1.841168000	3.601668000

C	-0.974706000	1.564176000	4.315568000
C	-1.539131000	-0.066865000	2.621668000
N	-0.448476000	0.276465000	1.888605000
H	0.924212000	2.552762000	3.981155000
H	-1.188554000	2.079950000	5.254929000
H	-2.716918000	0.282219000	4.397050000
C	5.528619000	-0.771773000	-0.301516000
C	6.280832000	-1.931182000	-0.510575000
C	4.540936000	-0.727302000	0.700892000
H	7.036439000	-1.950269000	-1.300632000
C	6.064702000	-3.064254000	0.281719000
C	4.329686000	-1.875095000	1.489050000
H	6.656131000	-3.969411000	0.119516000
H	3.571404000	-1.845522000	2.274269000
C	5.086754000	-3.031057000	1.283536000
H	4.916512000	-3.909163000	1.912609000
H	5.698543000	0.097412000	-0.941174000
C	-2.416634000	-1.189509000	2.188351000
C	-1.864677000	-2.459529000	1.943982000
H	-0.783592000	-2.598882000	2.006149000
C	-3.814700000	-1.034633000	2.154505000
H	-4.256372000	-0.054580000	2.352937000
C	-4.640438000	-2.120285000	1.852541000
H	-5.724308000	-1.982861000	1.814595000
C	-2.693963000	-3.547175000	1.657538000
H	-2.252774000	-4.531718000	1.481849000
C	-4.082389000	-3.380013000	1.605125000
H	-4.729338000	-4.231790000	1.378804000