Substituent regulated photoluminescent thermochromism in a rare type of octahedral Cu$_4$I$_4$ clusters

Ya-Dong Yu, Ling-Bin Meng, Qiu-Cheng Chen, Guang-Hui Chen and Xiao-Chun Huang*

Department of Chemistry and Key Laboratory for Preparation and Application of Ordered Structural Materials of Guangdong Province, Shantou University, Shantou, 515063, China.

Supporting Information

Contents

Scheme S1 Three-step syntheses of the ligands ................................................................. 3

Fig. S1 IR spectra of the five copper iodide clusters and the three proligands ....................... 3

Fig. S2–S9 The $^1$H NMR spectra of the three proligands and the five clusters ....................... 4

Fig. S10–S17 ESI-MS results of the five clusters ................................................................ 8

Fig. S18 PXRD patterns for clusters 1–5 ......................................................................... 12

Table S1 X-ray crystallographic data for clusters 1–5 ......................................................... 12

Fig. S19 Temperature dependence of solid-state luminescence spectra of cluster 1–5 from 300 to 80 K at $\lambda_{\text{ex}} = 330$ nm for 1 and $\lambda_{\text{ex}} = 340$ nm for 2–5 ................................................................................................................................. 14

Table S2 Photoluminescence CIE Coordinates, Peak Emission Wavelength ($\lambda_{\text{em}}$), and Lifetime ($\tau$) for Clusters 1–5 in the Solid State ............................................................. 15

Fig. S20 Temperature dependence of solid-state luminescence spectra of cluster 2 at different excitation wavelength .................................................................................. 16

Fig. S21 UV–vis absorption spectra of 1–4 in acetonitrile at different concentrations in CH$_3$CN at 298 K ..................................................................................................................... 16

Fig. S22 MALDI-TOF mass spectrum of complex 1 and 2 in acetonitrile solution ............. 17
**Fig. S23** Normalized emission spectra of the proligands in acetonitrile solution at room temperature ................................................................. 18

**Fig. S24** Luminescence spectra of clusters 1–4 in dry acetonitrile solution at RT and 77 K ........................................................................................................ 18

**Table S3** Emission wavelengths $\lambda_{em}$ for 2 based on $T_1$ optimized geometry in gas phase calculated with various functionals employing time-dependent density functional theory and the 6-31G(d) basis set ................................................................. 19

**Table S4** Relevant Computed Data for 1–4 ........................................................................................................... 19

**Fig. S25–S28** Isodensity surface plots of some molecular orbitals of complex 1–4 calculated for the singlet ground state at the $S_0$ optimized geometry ................................................................. 19

**Table S5–S12** Calculated TDDFT data at the $S_0$ optimized Geometry for Complex 1–4 ........ 21

**Table S13** Calculated TDDFT Singlet-Singlet Excitation Wavelengths and Transition Assignments for the Most Intense ($f > 0.1$) Transitions of Complex 1–4 at the $S_0$ Optimized Geometry in the Gas State ................................................................. 46

**Fig. S29** The density difference plots for the lowest triplet excitation of complex 2 and 3 in vacuo, calculated at the TDDFT optimized $T_1$ geometry ........................................................................ 47

**Table S14** Coordinates of geometry optimized structures ......................................................................................... 48-60
**Scheme S1** Three-step syntheses of the ligands.

**Fig. S1** IR spectra of the five copper iodide clusters and the three proligands.
Fig. S2 $^1$H NMR spectrum (400 MHz, CD$_3$CN) of proligand HL$_1$·I. The black circle shape and triangle shape denote the solvent residual signals of H$_2$O and CD$_3$CN, respectively.

Fig. S3 $^1$H NMR spectrum (400 MHz, CD$_3$CN) of proligand HL$_2$·I. The black circle shape and triangle shape denote the solvent residual signals of H$_2$O and CD$_3$CN, respectively.
Fig. S4 $^1$H NMR spectrum (400 MHz, CD$_3$CN) of proligand HL$_3$·I. The black circle shape and triangle shape denote the solvent residual signals of H$_2$O and CD$_3$CN, respectively.

Fig. S5 $^1$H NMR spectrum (400 MHz, CD$_3$CN) of the complex 1. The signals at 2.15, 2.09 and 1.94 ppm are the solvent residual signals of H$_2$O, acetone and CD$_3$CN, respectively.
Fig. S6 $^1$H NMR spectrum (400 MHz, CD$_3$CN) of the complex 2. The signals at 2.15, 2.09 and 1.94 ppm are the solvent residual signals of H$_2$O, acetone and CD$_3$CN, respectively.

Fig. S7 $^1$H NMR spectrum (400 MHz, CD$_3$CN) of the complex 3. The signals at 2.15, 2.09 and 1.94 ppm are the solvent residual signals of H$_2$O, acetone and CD$_3$CN, respectively.
Fig. S8 $^1$H NMR spectrum (400 MHz, CD$_3$CN) of the complex 4. The signals at 2.15, 2.09 and 1.94 ppm are the solvent residual signals of H$_2$O, acetone and CD$_3$CN, respectively.

Fig. S9 $^1$H NMR spectrum (400 MHz, CD$_3$CN) of the complex 5. The signals at 2.15, 2.09 and 1.94 ppm are the solvent residual signals of H$_2$O, acetone and CD$_3$CN, respectively.
Fig. S10 ESI-MS for complex 1 in acetonitrile at positive mode.

Fig. S11 ESI-MS for complex 1 in acetonitrile at negative mode.
Fig. S12 ESI-MS for complex 2 in acetonitrile at positive mode.

Fig. S13 ESI-MS for complex 2 in acetonitrile at negative mode.
Fig. S14 ESI-MS for complex 3 in acetonitrile at positive mode.

Fig. S15 ESI-MS for complex 3 in acetonitrile at negative mode.
Fig. S16 ESI-MS for complex 4 in acetonitrile at positive mode.

Fig. S17 ESI-MS for complex 4 in acetonitrile at negative mode.
Fig. S18 Comparison of the experimental PXRD patterns of complex 1–5 with the simulated patterns.

Table S1. X-ray Crystallographic Data for of Complex 1–5

<table>
<thead>
<tr>
<th></th>
<th>1 (293 K)</th>
<th>2 (293 K)</th>
<th>2 (100 K)</th>
</tr>
</thead>
<tbody>
<tr>
<td>formula</td>
<td>C₂₈H₃₇Cu₄I₄N₇</td>
<td>C₂₀H₁₆Cu₄F₆I₄N₆</td>
<td>C₂₀H₁₆Cu₄F₆I₄N₆</td>
</tr>
<tr>
<td>fw</td>
<td>1233.41</td>
<td>1216.15</td>
<td>1216.15</td>
</tr>
<tr>
<td>cryst syst</td>
<td>monoclinic</td>
<td>monoclinic</td>
<td>monoclinic</td>
</tr>
<tr>
<td>space group</td>
<td>P₂₁/n</td>
<td>P₂₁/n</td>
<td>P₂₁/n</td>
</tr>
<tr>
<td>a/Å</td>
<td>15.6308(10)</td>
<td>9.3659(3)</td>
<td>9.2037(7)</td>
</tr>
<tr>
<td>b/Å</td>
<td>11.7536(8)</td>
<td>9.8423(2)</td>
<td>9.8345(5)</td>
</tr>
<tr>
<td>c/Å</td>
<td>21.0207(14)</td>
<td>16.7265(4)</td>
<td>16.6471(9)</td>
</tr>
<tr>
<td>α/deg</td>
<td>90.00</td>
<td>90.00</td>
<td>90.00</td>
</tr>
<tr>
<td>β/deg</td>
<td>92.486(6)</td>
<td>102.865(3)</td>
<td>103.656(6)</td>
</tr>
<tr>
<td>γ/deg</td>
<td>90.00</td>
<td>90.00</td>
<td>90.00</td>
</tr>
<tr>
<td>V/Å³</td>
<td>3858.3(4)</td>
<td>1503.18(7)</td>
<td>1464.20(15)</td>
</tr>
<tr>
<td>Z</td>
<td>4</td>
<td>2</td>
<td>2</td>
</tr>
<tr>
<td>Dₐ₀/g·cm⁻³</td>
<td>2.123</td>
<td>2.687</td>
<td>2.758</td>
</tr>
<tr>
<td>reflns collected</td>
<td>20677</td>
<td>10017</td>
<td>7418</td>
</tr>
<tr>
<td>unique reflns</td>
<td>6787</td>
<td>2634</td>
<td>2557</td>
</tr>
<tr>
<td>GOF</td>
<td>1.055</td>
<td>1.036</td>
<td>1.041</td>
</tr>
<tr>
<td></td>
<td>3 (293 K)</td>
<td>3 (100 K)</td>
<td>4 (293 K)</td>
</tr>
<tr>
<td>------------</td>
<td>-----------</td>
<td>-----------</td>
<td>-----------</td>
</tr>
<tr>
<td>formula</td>
<td>C$<em>{30}$H$</em>{26}$Cu$_4$I$_4$N$_6$</td>
<td>C$<em>{30}$H$</em>{26}$Cu$_4$I$_4$N$_6$</td>
<td>C$<em>{30}$H$</em>{26}$Cu$_4$I$_4$N$_6$</td>
</tr>
<tr>
<td>fw</td>
<td>1232.33</td>
<td>1232.33</td>
<td>1232.33</td>
</tr>
<tr>
<td>cryst syst</td>
<td>orthorhombic</td>
<td>orthorhombic</td>
<td>triclinic</td>
</tr>
<tr>
<td>space group</td>
<td>Pnma</td>
<td>Pnma</td>
<td>P ̅1</td>
</tr>
<tr>
<td>a/Å</td>
<td>23.146(3)</td>
<td>22.6213(6)</td>
<td>8.3998(6)</td>
</tr>
<tr>
<td>b/Å</td>
<td>18.2397(18)</td>
<td>18.2046(5)</td>
<td>9.9053(5)</td>
</tr>
<tr>
<td>c/Å</td>
<td>9.1304(10)</td>
<td>9.0203(2)</td>
<td>10.7689(6)</td>
</tr>
<tr>
<td>α/deg</td>
<td>90.00</td>
<td>90.00</td>
<td>8.2740(6)</td>
</tr>
<tr>
<td>β/deg</td>
<td>90.00</td>
<td>90.00</td>
<td>9.9053(5)</td>
</tr>
<tr>
<td>γ/deg</td>
<td>90.00</td>
<td>90.00</td>
<td>10.7689(6)</td>
</tr>
<tr>
<td>V/Å$^3$</td>
<td>3854.6(8)</td>
<td>3714.67(16)</td>
<td>856.57(9)</td>
</tr>
<tr>
<td>Z</td>
<td>4</td>
<td>4</td>
<td>1</td>
</tr>
<tr>
<td>D$_{cal}$/g·cm$^{-3}$</td>
<td>2.123</td>
<td>2.204</td>
<td>2.389</td>
</tr>
<tr>
<td>reflns collected</td>
<td>14303</td>
<td>37092</td>
<td>7094</td>
</tr>
<tr>
<td>unique reflns</td>
<td>3499</td>
<td>3519</td>
<td>2999</td>
</tr>
<tr>
<td>GOF</td>
<td>1.009</td>
<td>1.015</td>
<td>1.007</td>
</tr>
<tr>
<td>$R_{int}$</td>
<td>0.1123</td>
<td>0.0580</td>
<td>0.0321</td>
</tr>
<tr>
<td>$R_1$ [I &gt; 2σ(I)]</td>
<td>0.0749</td>
<td>0.0372</td>
<td>0.0316</td>
</tr>
<tr>
<td>$wR_2$ (all data)</td>
<td>0.2097</td>
<td>0.0945</td>
<td>0.0596</td>
</tr>
</tbody>
</table>

$R_1 = \sum |F_o| - |F_c|/\sum |F_o|$. $wR_2 = \{\sum w(F_o^2 - F_c^2)^2/\sum w(F_o^2)^2\}^{1/2}$; $w = 1/\sigma^2(F_o^2) + (aP)^2 + bP$, where $P = \max(F_o^2,0) + 2F_c^2)/3$ for all data.
Fig. S19 Temperature dependence of solid-state luminescence spectra of cluster 1–5 from 300 to 80 K at $\lambda_{ex} = 330$ nm for 1 and $\lambda_{ex} = 340$ nm for 2–5.
Table S2. Photoluminescence CIE Coordinates, Peak Emission Wavelength ($\lambda_{em}$), and Lifetime ($\tau$) for Clusters 1–5 in the Solid State

<table>
<thead>
<tr>
<th>Compound</th>
<th>CIE$^a$</th>
<th>$\lambda_{em}$ (nm)</th>
<th>$\tau$ ($\mu$s)$^b$</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>80 K</td>
<td>300 K</td>
<td>80 K</td>
</tr>
<tr>
<td>1</td>
<td>(0.62, 0.37)</td>
<td>(0.61, 0.38)</td>
<td>633</td>
</tr>
<tr>
<td>2</td>
<td>(0.52, 0.46)</td>
<td>(0.58, 0.40)</td>
<td>597</td>
</tr>
<tr>
<td>3</td>
<td>(0.59, 0.39)</td>
<td>(0.60, 0.36)</td>
<td>607</td>
</tr>
<tr>
<td>4</td>
<td>(0.51, 0.48)</td>
<td>(0.54, 0.43)</td>
<td>577</td>
</tr>
<tr>
<td>5</td>
<td>(0.58, 0.40)</td>
<td>(0.62, 0.31)</td>
<td>644</td>
</tr>
</tbody>
</table>

$^a$CIE represents the Commission International d’Eclairage coordinates. $^b$For lifetime measurements, the pulsed excitation source of 337 nm generated from a nitrogen laser was used throughout.
Fig. S20 Temperature dependence of solid-state luminescence spectra of cluster 2 at $\lambda_{\text{ex}} = 340$ nm (left) and $\lambda_{\text{ex}} = 430$ nm (right).

Fig. S21 UV–vis absorption spectra of 1–4 in acetonitrile at different concentrations. The inset shows the apparent absorbance as a function of the concentration (1–10 $\mu$M) of 1 ($\lambda_{\text{abs}} = 370$ nm), 2 ($\lambda_{\text{abs}} = 360$ nm), 3 ($\lambda_{\text{abs}} = 368$ nm), 4 ($\lambda_{\text{abs}} = 368$ nm) in CH$_3$CN at 298 K.
Fig. S22 (a) MALDI-TOF mass spectrum of complex 1 and (b) of complex 2 in acetonitrile solution with experimental isotopic distribution pattern (black, inset) and simulated isotopic distribution pattern (red, inset).
Fig. S23 Normalized emission spectra of the proligands in acetonitrile solution at room temperature.

Fig. S24 Luminescence spectra of clusters 1–4 in dry acetonitrile solution (1 x 10⁻⁴ M) at RT (λₑₓ = 320 nm for 1, at 307 nm for 2, at 315 nm for 3, and at 310 nm for 4) and 77 K (λₑₓ = 330 nm for 1–4). Corresponding photos under UV irradiation at 254 nm (UV lamp) for RT and at 365 nm for 77 K are showed in the inset.
Table S3. Emission Wavelengths $\lambda_{em}$ for 2 Based on T$_1$ Optimized Geometry in Gas Phase Calculated with Various Functionals Employing Time-Dependent Density Functional Theory and the 6-31G(d) Basis Set

<table>
<thead>
<tr>
<th></th>
<th>$\lambda_{em}$ (nm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>PBE0</td>
<td>4055.5</td>
</tr>
<tr>
<td>M06-2X</td>
<td>902.4</td>
</tr>
<tr>
<td>wB97X-D</td>
<td>761.30</td>
</tr>
</tbody>
</table>

Table S4. Relevant Computed Data for 1–4

<table>
<thead>
<tr>
<th>$\lambda$</th>
<th>1$^\circ$</th>
<th>2$^\circ$</th>
<th>3$^\circ$</th>
<th>4$^\circ$</th>
</tr>
</thead>
<tbody>
<tr>
<td>S$^0$</td>
<td>T$^0$</td>
<td>S$^0$</td>
<td>T$^0$</td>
<td>S$^0$</td>
</tr>
<tr>
<td>PBE0</td>
<td>2.544-</td>
<td>2.552-</td>
<td>2.520-</td>
<td>2.669-</td>
</tr>
<tr>
<td>M06-2X</td>
<td>2.891</td>
<td>2.932</td>
<td>2.828</td>
<td>3.017</td>
</tr>
<tr>
<td>wB97X-D</td>
<td>2.473</td>
<td>2.596</td>
<td>2.514</td>
<td>2.560</td>
</tr>
</tbody>
</table>

Fig. S25 Isodensity surface plots of some molecular orbitals of complex 1 calculated for the singlet ground state at the $S_0$ optimized geometry.
**Fig. S26** Isodensity surface plots of some molecular orbitals of complex 2 calculated for the singlet ground state at the $S_0$ optimized geometry.

**Fig. S27** Isodensity surface plots of some molecular orbitals of complex 3 calculated for the singlet ground state at the $S_0$ optimized geometry.
**Fig. S28** Isodensity surface plots of some molecular orbitals of complex 4 calculated for the singlet ground state at the $S_0$ optimized geometry.

**Table S5.** Calculated TDDFT Singlet-Singlet Excitation Energies, Oscillator Strengths ($f$), Transition Assignments in Terms of Electronic Density Difference (EDD) Maps for the First 10 and Most Intense ($f > 0.03$) Transitions of Complex 1 at the $S_0$ Optimized Geometry in the Gas State$^a$

<table>
<thead>
<tr>
<th>Excited states</th>
<th>$\lambda$ (nm)</th>
<th>Energy (eV)</th>
<th>$f$</th>
<th>EDD</th>
<th>Assignment$^b$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$S_0 \rightarrow S_1$</td>
<td>423.1</td>
<td>2.929</td>
<td>0.0015</td>
<td>![EDD Map]</td>
<td>$^1$(X + M)LCT</td>
</tr>
<tr>
<td>$S_0 \rightarrow S_2$</td>
<td>422.6</td>
<td>2.933</td>
<td>0.0000</td>
<td>![EDD Map]</td>
<td>$^1$(X + M)LCT</td>
</tr>
<tr>
<td>Transition</td>
<td>$E$</td>
<td>$E/a.u.$</td>
<td>$\beta$</td>
<td>Notes</td>
<td></td>
</tr>
<tr>
<td>------------</td>
<td>-----</td>
<td>---------</td>
<td>--------</td>
<td>-------</td>
<td></td>
</tr>
<tr>
<td>$S_0 \rightarrow S_3$</td>
<td>401.4</td>
<td>3.088</td>
<td>0.0000</td>
<td>$^1(X + M)LCT$</td>
<td></td>
</tr>
<tr>
<td>$S_0 \rightarrow S_4$</td>
<td>400.2</td>
<td>3.097</td>
<td>0.0202</td>
<td>$^1(X + M)LCT$</td>
<td></td>
</tr>
<tr>
<td>$S_0 \rightarrow S_5$</td>
<td>381.4</td>
<td>3.250</td>
<td>0.0188</td>
<td>$^1(X + M)LCT$</td>
<td></td>
</tr>
<tr>
<td>$S_0 \rightarrow S_6$</td>
<td>380.3</td>
<td>3.259</td>
<td>0.0000</td>
<td>$^1(X + M)LCT$</td>
<td></td>
</tr>
<tr>
<td>$S_0 \rightarrow S_7$</td>
<td>370.5</td>
<td>3.346</td>
<td>0.4219</td>
<td>$^1(X + M)LCT/1ILCT$</td>
<td></td>
</tr>
<tr>
<td>$S_0 \rightarrow S_8$</td>
<td>370.4</td>
<td>3.346</td>
<td>0.0000</td>
<td>$^1(X + M)LCT/1ILCT$</td>
<td></td>
</tr>
<tr>
<td>$S_0 \rightarrow S_9$</td>
<td>357.0</td>
<td>3.472</td>
<td>f=0.0000</td>
<td>$^1(X + M)LCT$</td>
<td></td>
</tr>
<tr>
<td>$S_0 \rightarrow S_{10}$</td>
<td>356.1</td>
<td>3.481</td>
<td>0.0224</td>
<td>$^1(X + M)LCT$</td>
<td></td>
</tr>
<tr>
<td>------------------------</td>
<td>--------</td>
<td>--------</td>
<td>--------</td>
<td>----------------</td>
<td></td>
</tr>
<tr>
<td>$S_0 \rightarrow S_{14}$</td>
<td>338.0</td>
<td>3.667</td>
<td>0.0889</td>
<td>$^1(X + M)LCT$</td>
<td></td>
</tr>
<tr>
<td>$S_0 \rightarrow S_{16}$</td>
<td>325.4</td>
<td>3.810</td>
<td>0.3983</td>
<td>$^1(X + M)LCT/^3ILCT$</td>
<td></td>
</tr>
<tr>
<td>$S_0 \rightarrow S_{17}$</td>
<td>318.0</td>
<td>3.898</td>
<td>0.0793</td>
<td>$^1(X + M)LCT$</td>
<td></td>
</tr>
<tr>
<td>$S_0 \rightarrow S_{28}$</td>
<td>283.4</td>
<td>4.374</td>
<td>0.0562</td>
<td>$^1(X + M)LCT$</td>
<td></td>
</tr>
<tr>
<td>$S_0 \rightarrow S_{31}$</td>
<td>274.3</td>
<td>4.518</td>
<td>0.0349</td>
<td>$^1(X + M)LCT$</td>
<td></td>
</tr>
<tr>
<td>$S_0 \rightarrow S_{37}$</td>
<td>265.7</td>
<td>4.665</td>
<td>0.0510</td>
<td>$^3CC/^3(X + M)LCT$</td>
<td></td>
</tr>
<tr>
<td>Transition</td>
<td>Energy (eV)</td>
<td>Oscillator Strength</td>
<td>Assignment</td>
<td></td>
<td></td>
</tr>
<tr>
<td>------------</td>
<td>-------------</td>
<td>---------------------</td>
<td>-------------</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$S_0 \rightarrow S_{45}$</td>
<td>254.8</td>
<td>4.865</td>
<td>0.0801</td>
<td>$^1$CC</td>
<td></td>
</tr>
<tr>
<td>$S_0 \rightarrow S_{51}$</td>
<td>249.3</td>
<td>4.971</td>
<td>0.0429</td>
<td>$^1(\text{X} + \text{M})\text{LCT}$</td>
<td></td>
</tr>
<tr>
<td>$S_0 \rightarrow S_{59}$</td>
<td>242.2</td>
<td>5.117</td>
<td>0.1242</td>
<td>$^1(\text{CC}/(\text{X} + \text{M})\text{LCT}$</td>
<td></td>
</tr>
<tr>
<td>$S_0 \rightarrow S_{71}$</td>
<td>232.3</td>
<td>5.336</td>
<td>0.0411</td>
<td>$^1(\text{X} + \text{M})\text{LCT}$</td>
<td></td>
</tr>
<tr>
<td>$S_0 \rightarrow S_{74}$</td>
<td>229.6</td>
<td>5.398</td>
<td>0.0418</td>
<td>$^1$CC</td>
<td></td>
</tr>
<tr>
<td>$S_0 \rightarrow S_{81}$</td>
<td>225.57</td>
<td>5.4965</td>
<td>0.0376</td>
<td>$^1$CC</td>
<td></td>
</tr>
<tr>
<td>$S_0 \rightarrow S_{85}$</td>
<td>215.9</td>
<td>5.742</td>
<td>0.0727</td>
<td>$^1$CC</td>
<td></td>
</tr>
</tbody>
</table>
Table S6. Calculated TDDFT Singlet-Triplet Excitation Energies and Transition Assignments in Terms of Electronic Density Difference (EDD) Maps for the First 10 Transitions of Complex 1 at the $S_0$ Optimized Geometry in the Gas State

<table>
<thead>
<tr>
<th>Excited states</th>
<th>$\lambda$ (nm)</th>
<th>Energy (eV)</th>
<th>EDD</th>
<th>Assignment</th>
</tr>
</thead>
<tbody>
<tr>
<td>$S_0\to T_1$</td>
<td>524.9</td>
<td>2.361</td>
<td>$^3$ILCT</td>
<td></td>
</tr>
<tr>
<td>$S_0\to T_2$</td>
<td>524.9</td>
<td>2.361</td>
<td>$^3$ILCT</td>
<td></td>
</tr>
</tbody>
</table>

In the EDD maps (isovalue 0.005), Blue and purple represent zones of depletion and augmentation of electron density. Transitions with $f > 0.1$ are marked in orange (the same below). $^b$CC (cluster centered) is a combination of a halide-to-metal charge transfer (XMCT) and copper-centered transitions.
<table>
<thead>
<tr>
<th>State Transition</th>
<th>Energy (eV)</th>
<th>Oscillator Strength</th>
<th>Multiplicity</th>
</tr>
</thead>
<tbody>
<tr>
<td>$S_0 \rightarrow T_3$</td>
<td>434.0</td>
<td>2.856</td>
<td>$^3(X + M)LCT/ILCT$</td>
</tr>
<tr>
<td>$S_0 \rightarrow T_4$</td>
<td>432.9</td>
<td>2.863</td>
<td>$^3(X + M)LCT/ILCT$</td>
</tr>
<tr>
<td>$S_0 \rightarrow T_5$</td>
<td>428.5</td>
<td>2.893</td>
<td>$^3(X + M)LCT/ILCT$</td>
</tr>
<tr>
<td>$S_0 \rightarrow T_6$</td>
<td>428.2</td>
<td>2.895</td>
<td>$^3(X + M)LCT/ILCT$</td>
</tr>
<tr>
<td>$S_0 \rightarrow T_7$</td>
<td>400.8</td>
<td>3.093</td>
<td>$^3(X + M)LCT$</td>
</tr>
<tr>
<td>$S_0 \rightarrow T_8$</td>
<td>400.1</td>
<td>3.098</td>
<td>$^3(X + M)LCT$</td>
</tr>
<tr>
<td>$S_0 \rightarrow T_9$</td>
<td>375.4</td>
<td>3.301</td>
<td>$^3(X + M)LCT$</td>
</tr>
</tbody>
</table>
Table S7. Calculated TDDFT Singlet-Singlet Excitation Energies, Oscillator Strengths ($f$), Transition Assignments in Terms of Electronic Density Difference (EDD) Maps for the First 10 and Most Intense ($f > 0.03$) Transitions of Complex 2 at the $S_0$ Optimized Geometry in the Gas State.

<table>
<thead>
<tr>
<th>Excited states</th>
<th>$\lambda$ (nm)</th>
<th>Energy (eV)</th>
<th>$f$</th>
<th>EDD</th>
<th>Assignment</th>
</tr>
</thead>
<tbody>
<tr>
<td>$S_0 \rightarrow S_1$</td>
<td>436.9</td>
<td>2.837</td>
<td>0.0020</td>
<td><img src="image1" alt="Diagram" /></td>
<td>$^1(X + M)$LCT</td>
</tr>
<tr>
<td>$S_0 \rightarrow S_2$</td>
<td>435.9</td>
<td>2.843</td>
<td>0.0000</td>
<td><img src="image2" alt="Diagram" /></td>
<td>$^1(X + M)$LCT</td>
</tr>
<tr>
<td>$S_0 \rightarrow S_3$</td>
<td>417.1</td>
<td>2.972</td>
<td>0.0000</td>
<td><img src="image3" alt="Diagram" /></td>
<td>$^1(X + M)$LCT</td>
</tr>
<tr>
<td>$S_0 \rightarrow S_4$</td>
<td>415.6</td>
<td>2.982</td>
<td>0.0232</td>
<td><img src="image4" alt="Diagram" /></td>
<td>$^1(X + M)$LCT</td>
</tr>
<tr>
<td>$S_0 \rightarrow S_5$</td>
<td>393.5</td>
<td>3.150</td>
<td>0.0079</td>
<td><img src="image5" alt="Diagram" /></td>
<td>$^1(X + M)$LCT</td>
</tr>
<tr>
<td>Transition</td>
<td>Energy (eV)</td>
<td>Oscillator Strength</td>
<td>Intensity</td>
<td>Assignment</td>
<td></td>
</tr>
<tr>
<td>------------</td>
<td>------------</td>
<td>---------------------</td>
<td>-----------</td>
<td>------------</td>
<td></td>
</tr>
<tr>
<td>$S_0 \rightarrow S_6$</td>
<td>392.5</td>
<td>3.158</td>
<td>0.0000</td>
<td>$^1(X + M)$LCT</td>
<td></td>
</tr>
<tr>
<td>$S_0 \rightarrow S_7$</td>
<td>373.7</td>
<td>3.317</td>
<td>0.0000</td>
<td>$^1(X + M)$LCT</td>
<td></td>
</tr>
<tr>
<td>$S_0 \rightarrow S_8$</td>
<td>372.5</td>
<td>3.327</td>
<td>0.1132</td>
<td>$^1(X + M)$LCT</td>
<td></td>
</tr>
<tr>
<td>$S_0 \rightarrow S_9$</td>
<td>362.6</td>
<td>3.419</td>
<td>0.0000</td>
<td>$^1(X + M)$LCT</td>
<td></td>
</tr>
<tr>
<td>$S_0 \rightarrow S_{10}$</td>
<td>362.2</td>
<td>3.422</td>
<td>0.0595</td>
<td>$^1(X + M)$LCT</td>
<td></td>
</tr>
<tr>
<td>$S_0 \rightarrow S_{14}$</td>
<td>345.0</td>
<td>3.593</td>
<td>0.0435</td>
<td>$^1(X + M)$LCT</td>
<td></td>
</tr>
<tr>
<td>$S_0 \rightarrow S_{16}$</td>
<td>325.4</td>
<td>3.809</td>
<td>0.0995</td>
<td>$^1(X + M)$LCT</td>
<td></td>
</tr>
<tr>
<td>$S_0 \rightarrow S_{17}$</td>
<td>322.6</td>
<td>3.842</td>
<td>0.3446</td>
<td>$^1(X + M)LCT/ILCT$</td>
<td></td>
</tr>
<tr>
<td>------------------------</td>
<td>-------</td>
<td>-------</td>
<td>--------</td>
<td>-----------------</td>
<td></td>
</tr>
<tr>
<td>$S_0 \rightarrow S_{20}$</td>
<td>310.0</td>
<td>3.999</td>
<td>0.0806</td>
<td>$^1(X + M)LCT$</td>
<td></td>
</tr>
<tr>
<td>$S_0 \rightarrow S_{21}$</td>
<td>308.8</td>
<td>4.014</td>
<td>0.0563</td>
<td>$^1(X + M)LCT$</td>
<td></td>
</tr>
<tr>
<td>$S_0 \rightarrow S_{23}$</td>
<td>296.7</td>
<td>4.177</td>
<td>0.0603</td>
<td>$^1(X + M)LCT$</td>
<td></td>
</tr>
<tr>
<td>$S_0 \rightarrow S_{32}$</td>
<td>277.2</td>
<td>4.472</td>
<td>0.0440</td>
<td>$^1(X + M)LCT$</td>
<td></td>
</tr>
<tr>
<td>$S_0 \rightarrow S_{33}$</td>
<td>276.3</td>
<td>4.486</td>
<td>0.0840</td>
<td>$^1(X + M)LCT$</td>
<td></td>
</tr>
<tr>
<td>$S_0 \rightarrow S_{45}$</td>
<td>258.1</td>
<td>4.802</td>
<td>0.03040</td>
<td>$^1(X + M)LCT$</td>
<td></td>
</tr>
<tr>
<td>$S_0 \rightarrow S$</td>
<td>$E$ (cm$^{-1}$)</td>
<td>$\Delta E$ (cm$^{-1}$)</td>
<td>$\Delta E/E$ (%)</td>
<td>Decay Pathway</td>
<td></td>
</tr>
<tr>
<td>------------------</td>
<td>----------------</td>
<td>-----------------</td>
<td>----------------</td>
<td>----------------</td>
<td></td>
</tr>
<tr>
<td>$S_0 \rightarrow S_{53}$</td>
<td>251.7</td>
<td>4.924</td>
<td>0.0322</td>
<td>$^1CC/(X + M)LCT$</td>
<td></td>
</tr>
<tr>
<td>$S_0 \rightarrow S_{56}$</td>
<td>249.4</td>
<td>4.969</td>
<td>0.0683</td>
<td>$^1(X + M)LCT/ILCT$</td>
<td></td>
</tr>
<tr>
<td>$S_0 \rightarrow S_{63}$</td>
<td>241.5</td>
<td>5.133</td>
<td>0.1302</td>
<td>$^1CC$</td>
<td></td>
</tr>
<tr>
<td>$S_0 \rightarrow S_{75}$</td>
<td>231.1</td>
<td>5.364</td>
<td>0.0515</td>
<td>$^1CC$</td>
<td></td>
</tr>
<tr>
<td>$S_0 \rightarrow S_{81}$</td>
<td>227.0</td>
<td>5.460</td>
<td>0.0309</td>
<td>$^1CC$</td>
<td></td>
</tr>
<tr>
<td>$S_0 \rightarrow S_{93}$</td>
<td>220.1</td>
<td>5.631</td>
<td>0.0391</td>
<td>$^1(X + M)LCT/CC$</td>
<td></td>
</tr>
<tr>
<td>$S_0 \rightarrow S_{100}$</td>
<td>214.9</td>
<td>5.767</td>
<td>0.0449</td>
<td>$^1CC/(X + M)LCT$</td>
<td></td>
</tr>
</tbody>
</table>
Table S8. Calculated TDDFT Singlet-Triplet Excitation Energies and Transition Assignments in Terms of Electronic Density Difference (EDD) Maps for the First 10 Transitions of Complex 2 at the S₀ Optimized Geometry in the Gas State.

<table>
<thead>
<tr>
<th>Excited states</th>
<th>λ (nm)</th>
<th>Energy (eV)</th>
<th>EDD</th>
<th>Assignment</th>
</tr>
</thead>
<tbody>
<tr>
<td>S₀→T₁</td>
<td>470.6</td>
<td>2.634</td>
<td></td>
<td>^3ILCT/^3(X + M)LCT</td>
</tr>
<tr>
<td>S₀→T₂</td>
<td>470.3</td>
<td>2.636</td>
<td></td>
<td>^3ILCT/^3(X + M)LCT</td>
</tr>
<tr>
<td>$S_0 \rightarrow T_3$</td>
<td>441.9</td>
<td>2.805</td>
<td>$^3(X + M)LCT$</td>
<td></td>
</tr>
<tr>
<td>---------------------</td>
<td>------</td>
<td>-------</td>
<td>----------------</td>
<td></td>
</tr>
<tr>
<td>$S_0 \rightarrow T_4$</td>
<td>440.6</td>
<td>2.813</td>
<td>$^3(X + M)LCT$</td>
<td></td>
</tr>
<tr>
<td>$S_0 \rightarrow T_5$</td>
<td>423.0</td>
<td>2.930</td>
<td>$^3(X + M)LCT$</td>
<td></td>
</tr>
<tr>
<td>$S_0 \rightarrow T_6$</td>
<td>422.8</td>
<td>2.931</td>
<td>$^3(X + M)LCT$</td>
<td></td>
</tr>
<tr>
<td>$S_0 \rightarrow T_7$</td>
<td>398.9</td>
<td>3.107</td>
<td>$^3(X + M)LCT$</td>
<td></td>
</tr>
<tr>
<td>$S_0 \rightarrow T_8$</td>
<td>398.1</td>
<td>3.113</td>
<td>$^3(X + M)LCT$</td>
<td></td>
</tr>
<tr>
<td>$S_0 \rightarrow T_9$</td>
<td>385.0</td>
<td>3.219</td>
<td>$^3(X + M)LCT$</td>
<td></td>
</tr>
</tbody>
</table>
Table S9. Calculated TDDFT Singlet-Singlet Excitation Energies, Oscillator Strengths ($f$), Transition Assignments in Terms of Electronic Density Difference (EDD) Maps for the First 10 and Most Intense ($f > 0.03$) Transitions of Complex 3 at the $S_0$ Optimized Geometry in the Gas State

<table>
<thead>
<tr>
<th>Excited states</th>
<th>$\lambda$ (nm)</th>
<th>Energy (eV)</th>
<th>$f$</th>
<th>EDD</th>
<th>Assignment</th>
</tr>
</thead>
<tbody>
<tr>
<td>$S_0 \rightarrow S_1$</td>
<td>450.2</td>
<td>2.753</td>
<td>0.0000</td>
<td></td>
<td>$^1(X + M)LCT$</td>
</tr>
<tr>
<td>$S_0 \rightarrow S_2$</td>
<td>449.7</td>
<td>2.757</td>
<td>0.0008</td>
<td></td>
<td>$^1(X + M)LCT$</td>
</tr>
<tr>
<td>$S_0 \rightarrow S_3$</td>
<td>433.4</td>
<td>2.860</td>
<td>0.0029</td>
<td></td>
<td>$^1(X + M)LCT$</td>
</tr>
<tr>
<td>$S_0 \rightarrow S_4$</td>
<td>432.2</td>
<td>2.868</td>
<td>0.0039</td>
<td></td>
<td>$^1(X + M)LCT$</td>
</tr>
<tr>
<td>$S_0 \rightarrow S_5$</td>
<td>426.0</td>
<td>2.910</td>
<td>0.0192</td>
<td></td>
<td>$^1(X + M)LCT$</td>
</tr>
<tr>
<td>$S_0 \rightarrow S_n$</td>
<td>$\Delta E$</td>
<td>$\Delta E'$</td>
<td>$\Delta E''$</td>
<td>Type</td>
<td></td>
</tr>
<tr>
<td>---------------------</td>
<td>----------</td>
<td>------------</td>
<td>-------------</td>
<td>------</td>
<td></td>
</tr>
<tr>
<td>$S_0 \rightarrow S_6$</td>
<td>423.1</td>
<td>2.930</td>
<td>0.0099</td>
<td>$^1(X + M)\text{LCT}$</td>
<td></td>
</tr>
<tr>
<td>$S_0 \rightarrow S_7$</td>
<td>416.0</td>
<td>2.980</td>
<td>0.0003</td>
<td>$^1(X + M)\text{LCT}$</td>
<td></td>
</tr>
<tr>
<td>$S_0 \rightarrow S_8$</td>
<td>414.3</td>
<td>2.992</td>
<td>0.0002</td>
<td>$^1(X + M)\text{LCT}$</td>
<td></td>
</tr>
<tr>
<td>$S_0 \rightarrow S_9$</td>
<td>391.4</td>
<td>3.167</td>
<td>0.1587</td>
<td>$^1(X + M)\text{LCT} / ^1\text{ILCT}$</td>
<td></td>
</tr>
<tr>
<td>$S_0 \rightarrow S_{10}$</td>
<td>385.4</td>
<td>3.216</td>
<td>0.3375</td>
<td>$^1(X + M)\text{LCT} / ^1\text{ILCT}$</td>
<td></td>
</tr>
<tr>
<td>$S_0 \rightarrow S_{15}$</td>
<td>348.0</td>
<td>3.563</td>
<td>0.0353</td>
<td>$^1(X + M)\text{LCT} / ^1\text{ILCT}$</td>
<td></td>
</tr>
<tr>
<td>$S_0 \rightarrow S_{16}$</td>
<td>344.0</td>
<td>3.605</td>
<td>0.4853</td>
<td>$^1(X + M)\text{LCT} / ^1\text{ILCT}$</td>
<td></td>
</tr>
<tr>
<td>$S_0 \rightarrow S_n$</td>
<td>$E$ (eV)</td>
<td>$\Delta E$ (meV)</td>
<td>$\Delta A$ (ps^-1)</td>
<td>$^1(X + M)\text{LCT}$</td>
<td></td>
</tr>
<tr>
<td>---------------------</td>
<td>--------</td>
<td>----------------</td>
<td>------------------</td>
<td>-------------------</td>
<td></td>
</tr>
<tr>
<td>$S_0 \rightarrow S_{26}$</td>
<td>298.0</td>
<td>4.160</td>
<td>0.1426</td>
<td>$^1(X + M)\text{LCT}$</td>
<td></td>
</tr>
<tr>
<td>$S_0 \rightarrow S_{27}$</td>
<td>296.3</td>
<td>4.185</td>
<td>0.0830</td>
<td>$^1(X + M)\text{LCT}$</td>
<td></td>
</tr>
<tr>
<td>$S_0 \rightarrow S_{31}$</td>
<td>285.3</td>
<td>4.345</td>
<td>0.0576</td>
<td>$^1(X + M)\text{LCT}$</td>
<td></td>
</tr>
<tr>
<td>$S_0 \rightarrow S_{44}$</td>
<td>273.0</td>
<td>4.541</td>
<td>0.0510</td>
<td>$^1(X + M)\text{LCT}$</td>
<td></td>
</tr>
<tr>
<td>$S_0 \rightarrow S_{45}$</td>
<td>271.8</td>
<td>4.561</td>
<td>0.0621</td>
<td>$^1(X + M)\text{LCT}$</td>
<td></td>
</tr>
<tr>
<td>$S_0 \rightarrow S_{55}$</td>
<td>251.1</td>
<td>4.937</td>
<td>0.0494</td>
<td>$^1\text{CC}$</td>
<td></td>
</tr>
<tr>
<td>$S_0 \rightarrow S_{62}$</td>
<td>246.5</td>
<td>5.030</td>
<td>0.0423</td>
<td>$^1(X + M)\text{LCT}/^1\text{CC}$</td>
<td></td>
</tr>
<tr>
<td>Transition</td>
<td>Energy (eV)</td>
<td>Oscillator Strength</td>
<td>Type</td>
<td></td>
<td></td>
</tr>
<tr>
<td>------------</td>
<td>------------</td>
<td>---------------------</td>
<td>------</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$S_0 \rightarrow S_{65}$</td>
<td>244.4</td>
<td>5.073</td>
<td>0.2277</td>
<td>$^1(X + M)LCT/ILCT$</td>
<td></td>
</tr>
<tr>
<td>$S_0 \rightarrow S_{74}$</td>
<td>235.6</td>
<td>5.263</td>
<td>0.0583</td>
<td>$^1CC$</td>
<td></td>
</tr>
<tr>
<td>$S_0 \rightarrow S_{79}$</td>
<td>233.0</td>
<td>5.321</td>
<td>0.0802</td>
<td>$^1(X + M)LCT/ILCT$</td>
<td></td>
</tr>
<tr>
<td>$S_0 \rightarrow S_{81}$</td>
<td>231.9</td>
<td>5.347</td>
<td>0.0638</td>
<td>$^1CC$</td>
<td></td>
</tr>
<tr>
<td>$S_0 \rightarrow S_{86}$</td>
<td>228.7</td>
<td>5.422</td>
<td>0.0927</td>
<td>$^1(X + M)LCT$</td>
<td></td>
</tr>
<tr>
<td>$S_0 \rightarrow S_{90}$</td>
<td>228.2</td>
<td>5.433</td>
<td>0.1045</td>
<td>$^1(X + M)LCT/ILCT$</td>
<td></td>
</tr>
<tr>
<td>$S_0 \rightarrow S_{93}$</td>
<td>225.4</td>
<td>5.501</td>
<td>0.0488</td>
<td>$^1(X + M)LCT/ILCT$</td>
<td></td>
</tr>
</tbody>
</table>
### Table S10. Calculated TDDFT Singlet-Triplet Excitation Energies and Transition Assignments in Terms of Electronic Density Difference (EDD) Maps for the First 10 Transitions of Complex 3 at the S₀ Optimized Geometry in the Gas State

<table>
<thead>
<tr>
<th>Excited states</th>
<th>λ (nm)</th>
<th>Energy (eV)</th>
<th>EDD</th>
<th>Assignment</th>
</tr>
</thead>
<tbody>
<tr>
<td>S₀→T₁</td>
<td>566.1</td>
<td>2.190</td>
<td></td>
<td>³ILCT</td>
</tr>
<tr>
<td>S₀→S₉₈</td>
<td>222.1</td>
<td>5.581</td>
<td>0.0848</td>
<td>^1CC</td>
</tr>
<tr>
<td>S₀→S₁₀₅</td>
<td>219.0</td>
<td>5.661</td>
<td>0.0357</td>
<td>^1(X + M)LCT</td>
</tr>
<tr>
<td>S₀→S₁₁₇</td>
<td>213.6</td>
<td>5.804</td>
<td>0.1404</td>
<td>^1(X + M)LCT</td>
</tr>
<tr>
<td>S₀→S₁₁₈</td>
<td>213.5</td>
<td>5.807</td>
<td>0.0309</td>
<td>^1(X + M)LCT</td>
</tr>
<tr>
<td>S₀→S₁₄₆</td>
<td>204.1</td>
<td>6.075</td>
<td>0.0416</td>
<td>^1(X + M)LCT</td>
</tr>
<tr>
<td>$S_0 \rightarrow T$</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>---</td>
<td>---</td>
<td>---</td>
<td>---</td>
<td></td>
</tr>
<tr>
<td></td>
<td>566.1</td>
<td>2.190</td>
<td>$^3\text{ILCT}$</td>
<td></td>
</tr>
<tr>
<td>$S_0 \rightarrow T_2$</td>
<td>474.5</td>
<td>2.613</td>
<td>$^3(\text{X + M})\text{LCT}/^3\text{ILCT}$</td>
<td></td>
</tr>
<tr>
<td>$S_0 \rightarrow T_3$</td>
<td>474.0</td>
<td>2.616</td>
<td>$^3(\text{X + M})\text{LCT}/^3\text{ILCT}$</td>
<td></td>
</tr>
<tr>
<td>$S_0 \rightarrow T_4$</td>
<td>458.5</td>
<td>2.704</td>
<td>$^3(\text{X + M})\text{LCT}$</td>
<td></td>
</tr>
<tr>
<td>$S_0 \rightarrow T_5$</td>
<td>457.9</td>
<td>2.708</td>
<td>$^3(\text{X + M})\text{LCT}$</td>
<td></td>
</tr>
<tr>
<td>$S_0 \rightarrow T_6$</td>
<td>435.5</td>
<td>2.847</td>
<td>$^3(\text{X + M})\text{LCT}$</td>
<td></td>
</tr>
<tr>
<td>$S_0 \rightarrow T_7$</td>
<td>434.4</td>
<td>2.854</td>
<td>$^3(\text{X + M})\text{LCT}$</td>
<td></td>
</tr>
</tbody>
</table>
Table S11. Calculated TDDFT Singlet-Singlet Excitation Energies, Oscillator Strengths ($f$), Transition Assignments in Terms of Electronic Density Difference (EDD) Maps for the First 10 and Most Intense ($f > 0.03$) Transitions of Complex 4 at the $S_0$ Optimized Geometry in the Gas State.

<table>
<thead>
<tr>
<th>Excited states</th>
<th>$\lambda$ (nm)</th>
<th>Energy (eV)</th>
<th>$f$</th>
<th>EDD</th>
<th>Assignment</th>
</tr>
</thead>
<tbody>
<tr>
<td>$S_0 \rightarrow S_1$</td>
<td>424.2</td>
<td>2.923</td>
<td>0.0009</td>
<td>1</td>
<td>$^1(X + M)$LCT</td>
</tr>
<tr>
<td>$S_0 \rightarrow S_2$</td>
<td>423.7</td>
<td>2.926</td>
<td>0.0000</td>
<td>1</td>
<td>$^1(X + M)$LCT</td>
</tr>
<tr>
<td>$S_0 \rightarrow S_3$</td>
<td>403.7</td>
<td>3.071</td>
<td>0.0000</td>
<td>1</td>
<td>$^1(X + M)$LCT</td>
</tr>
<tr>
<td>$S_0 \rightarrow S_4$</td>
<td>402.4</td>
<td>3.081</td>
<td>0.0255</td>
<td>1</td>
<td>$^1(X + M)$LCT</td>
</tr>
<tr>
<td>( S_0 \rightarrow S )</td>
<td>E (kcal/mol)</td>
<td>IP (eV)</td>
<td>( \Delta E ) (eV)</td>
<td>Description</td>
<td></td>
</tr>
<tr>
<td>-----------------</td>
<td>-------------</td>
<td>---------</td>
<td>-----------------</td>
<td>-------------</td>
<td></td>
</tr>
<tr>
<td>( S_0 \rightarrow S_5 )</td>
<td>383.4</td>
<td>3.234</td>
<td>0.1647</td>
<td>( ^1(X + M)\text{LCT/ILCT} )</td>
<td></td>
</tr>
<tr>
<td>( S_0 \rightarrow S_6 )</td>
<td>381.9</td>
<td>3.246</td>
<td>0.0000</td>
<td>( ^1(X + M)\text{LCT/ILCT} )</td>
<td></td>
</tr>
<tr>
<td>( S_0 \rightarrow S_7 )</td>
<td>379.5</td>
<td>3.267</td>
<td>0.0000</td>
<td>( ^1(X + M)\text{LCT/ILCT} )</td>
<td></td>
</tr>
<tr>
<td>( S_0 \rightarrow S_8 )</td>
<td>378.4</td>
<td>3.276</td>
<td>0.3081</td>
<td>( ^1(X + M)\text{LCT/ILCT} )</td>
<td></td>
</tr>
<tr>
<td>( S_0 \rightarrow S_9 )</td>
<td>361.5</td>
<td>3.430</td>
<td>0.0000</td>
<td>( ^1(X + M)\text{LCT} )</td>
<td></td>
</tr>
<tr>
<td>( S_0 \rightarrow S_{10} )</td>
<td>360.5</td>
<td>3.440</td>
<td>0.0084</td>
<td>( ^1(X + M)\text{LCT} )</td>
<td></td>
</tr>
<tr>
<td>( S_0 \rightarrow S_{14} )</td>
<td>339.9</td>
<td>3.648</td>
<td>0.0552</td>
<td>( ^1(X + M)\text{LCT} )</td>
<td></td>
</tr>
<tr>
<td>( S_0 \rightarrow S )</td>
<td>( \Delta E )</td>
<td>( \Delta )</td>
<td>( \delta )</td>
<td>( \text{Type} )</td>
<td></td>
</tr>
<tr>
<td>--------------------------</td>
<td>-------</td>
<td>-----</td>
<td>-----</td>
<td>----------------</td>
<td></td>
</tr>
<tr>
<td>( S_0 \rightarrow S_{16} )</td>
<td>324.5</td>
<td>3.821</td>
<td>0.2890</td>
<td>(^1)(X + M)LCT/ILCT</td>
<td></td>
</tr>
<tr>
<td>( S_0 \rightarrow S_{17} )</td>
<td>321.4</td>
<td>3.858</td>
<td>0.0916</td>
<td>(^1)(X + M)LCT</td>
<td></td>
</tr>
<tr>
<td>( S_0 \rightarrow S_{20} )</td>
<td>316.9</td>
<td>3.912</td>
<td>0.1112</td>
<td>(^1)(X + M)LCT/ILCT</td>
<td></td>
</tr>
<tr>
<td>( S_0 \rightarrow S_{21} )</td>
<td>305.8</td>
<td>4.055</td>
<td>0.0516</td>
<td>(^1)(X + M)LCT</td>
<td></td>
</tr>
<tr>
<td>( S_0 \rightarrow S_{28} )</td>
<td>285.7</td>
<td>4.341</td>
<td>0.0579</td>
<td>(^1)(X + M)LCT</td>
<td></td>
</tr>
<tr>
<td>( S_0 \rightarrow S_{32} )</td>
<td>276.3</td>
<td>4.488</td>
<td>0.0403</td>
<td>(^1)(X + M)LCT/ILCT</td>
<td></td>
</tr>
<tr>
<td>( S_0 \rightarrow S_{33} )</td>
<td>275.6</td>
<td>4.498</td>
<td>0.0371</td>
<td>(^1)(X + M)LCT</td>
<td></td>
</tr>
<tr>
<td>Transition</td>
<td>$S_0 \rightarrow S_{39}$</td>
<td>Energy (kcal/mol)</td>
<td>$\Delta E$ (kcal/mol)</td>
<td>RCCA</td>
<td></td>
</tr>
<tr>
<td>-------------</td>
<td>-----------------</td>
<td>--------------------</td>
<td>---------------------</td>
<td>-------</td>
<td></td>
</tr>
<tr>
<td></td>
<td>266.0</td>
<td>4.661</td>
<td>0.0438</td>
<td>$^1CC$</td>
<td></td>
</tr>
<tr>
<td>$S_0 \rightarrow S_{45}$</td>
<td>255.3</td>
<td>4.857</td>
<td>0.0812</td>
<td>$^1CC$</td>
<td></td>
</tr>
<tr>
<td>$S_0 \rightarrow S_{51}$</td>
<td>251.9</td>
<td>4.922</td>
<td>0.1280</td>
<td>$^1(X + M)LCT$</td>
<td></td>
</tr>
<tr>
<td>$S_0 \rightarrow S_{60}$</td>
<td>244.6</td>
<td>5.069</td>
<td>0.1193</td>
<td>$^1(X + M)LCT$</td>
<td></td>
</tr>
<tr>
<td>$S_0 \rightarrow S_{63}$</td>
<td>241.8</td>
<td>5.127</td>
<td>0.1273</td>
<td>$^1CC$</td>
<td></td>
</tr>
<tr>
<td>$S_0 \rightarrow S_{69}$</td>
<td>237.6</td>
<td>5.217</td>
<td>0.0317</td>
<td>$^1(X + M)LCT$/$^1ILCT$</td>
<td></td>
</tr>
<tr>
<td>$S_0 \rightarrow S_{72}$</td>
<td>235.6</td>
<td>5.263</td>
<td>0.1066</td>
<td>$^1(X + M)LCT$/$^1ILCT$</td>
<td></td>
</tr>
<tr>
<td>$S_0 \rightarrow S_78$</td>
<td>232.5</td>
<td>5.333</td>
<td>0.2441</td>
<td>$^1(X + M)LCT$</td>
<td></td>
</tr>
<tr>
<td>----------------------</td>
<td>-------</td>
<td>-------</td>
<td>--------</td>
<td>----------------</td>
<td></td>
</tr>
<tr>
<td>$S_0 \rightarrow S_{80}$</td>
<td>231.4</td>
<td>5.357</td>
<td>0.1094</td>
<td>$^1(X + M)LCT/!^1ILCT$</td>
<td></td>
</tr>
<tr>
<td>$S_0 \rightarrow S_{87}$</td>
<td>226.8</td>
<td>5.466</td>
<td>0.0341</td>
<td>$^1CC$</td>
<td></td>
</tr>
<tr>
<td>$S_0 \rightarrow S_{88}$</td>
<td>226.2</td>
<td>5.480</td>
<td>0.1239</td>
<td>$^1CC /^1(X + M)LCT/!^1ILCT$</td>
<td></td>
</tr>
<tr>
<td>$S_0 \rightarrow S_{90}$</td>
<td>224.5</td>
<td>5.523</td>
<td>0.0574</td>
<td>$^1ILCT /^1CC /^1(X + M)LCT$</td>
<td></td>
</tr>
<tr>
<td>$S_0 \rightarrow S_{105}$</td>
<td>217.4</td>
<td>5.702</td>
<td>0.0384</td>
<td>$^1(X + M)LCT/!^1ILCT$</td>
<td></td>
</tr>
<tr>
<td>$S_0 \rightarrow S_{107}$</td>
<td>216.8</td>
<td>5.719</td>
<td>0.0413</td>
<td>$^1(X + M)LCT/!^1ILCT$</td>
<td></td>
</tr>
<tr>
<td>Transition</td>
<td>Energy (THz)</td>
<td>Oscillator Strength</td>
<td>Type</td>
<td></td>
<td></td>
</tr>
<tr>
<td>------------</td>
<td>--------------</td>
<td>---------------------</td>
<td>------</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$S_0 \rightarrow S_{109}$</td>
<td>216.2</td>
<td>5.734</td>
<td>0.1040</td>
<td>$^1\text{CC}$</td>
<td></td>
</tr>
<tr>
<td>$S_0 \rightarrow S_{118}$</td>
<td>212.4</td>
<td>5.836</td>
<td>0.0688</td>
<td>$^1(X + M)\text{LCT/CC}$</td>
<td></td>
</tr>
<tr>
<td>$S_0 \rightarrow S_{119}$</td>
<td>212.1</td>
<td>5.845</td>
<td>0.1212</td>
<td>$^1(X + M)\text{LCT/ILCT}$</td>
<td></td>
</tr>
<tr>
<td>$S_0 \rightarrow S_{122}$</td>
<td>210.6</td>
<td>5.886</td>
<td>0.0455</td>
<td>$^1(X + M)\text{LCT}$</td>
<td></td>
</tr>
<tr>
<td>$S_0 \rightarrow S_{126}$</td>
<td>208.5</td>
<td>5.945</td>
<td>0.0405</td>
<td>$^1(X + M)\text{LCT}$</td>
<td></td>
</tr>
<tr>
<td>$S_0 \rightarrow S_{128}$</td>
<td>208.1</td>
<td>5.958</td>
<td>0.0643</td>
<td>$^1(X + M)\text{LCT/CC}$</td>
<td></td>
</tr>
<tr>
<td>$S_0 \rightarrow S_{133}$</td>
<td>206.4</td>
<td>6.007</td>
<td>0.0927</td>
<td>$^1(X + M)\text{LCT/CC}$</td>
<td></td>
</tr>
</tbody>
</table>
Table S12. Calculated TDDFT Singlet-Triplet Excitation Energies and Transition Assignments in Terms of Electronic Density Difference (EDD) Maps for the First 10 Transitions of Complex 4 at the S₀ Optimized Geometry in the Gas State

<table>
<thead>
<tr>
<th>Excited states</th>
<th>$\lambda$ (nm)</th>
<th>Energy (eV)</th>
<th>EDD</th>
<th>Assignment</th>
</tr>
</thead>
<tbody>
<tr>
<td>$S_0 \rightarrow T_1$</td>
<td>519.1</td>
<td>2.388</td>
<td></td>
<td>$^3$ILCT</td>
</tr>
<tr>
<td>$S_0 \rightarrow T_2$</td>
<td>519.1</td>
<td>2.388</td>
<td></td>
<td>$^3$ILCT</td>
</tr>
<tr>
<td>$S_0 \rightarrow T_3$</td>
<td>437.1</td>
<td>2.835</td>
<td></td>
<td>$^3(X + M)LCT/^3$ILCT</td>
</tr>
<tr>
<td>$S_0 \rightarrow T_4$</td>
<td>437.1</td>
<td>2.835</td>
<td></td>
<td>$^3(X + M)LCT/^3$ILCT</td>
</tr>
<tr>
<td>$S_0 \rightarrow T_5$</td>
<td>436.3</td>
<td>2.841</td>
<td></td>
<td>$^3(X + M)LCT$</td>
</tr>
</tbody>
</table>
### Table S13. Calculated TDDFT Singlet-Singlet Excitation Wavelengths and Transition Assignments for the Most Intense ($f > 0.1$) Transitions of Complex 1–4 at the $S_0$ Optimized Geometry in the Gas State

<table>
<thead>
<tr>
<th>$S_0 \rightarrow T_6$</th>
<th>$\lambda$ (nm)</th>
<th>$f$</th>
<th>Assignment</th>
</tr>
</thead>
<tbody>
<tr>
<td>$S_0 \rightarrow T_7$</td>
<td>430.6</td>
<td>2.878</td>
<td>$^3(X + M)\text{LCT}$</td>
</tr>
<tr>
<td>$S_0 \rightarrow T_8$</td>
<td>430.1</td>
<td>2.882</td>
<td>$^3(X + M)\text{LCT}$</td>
</tr>
<tr>
<td>$S_0 \rightarrow T_9$</td>
<td>402.5</td>
<td>3.080</td>
<td>$^3(X + M)\text{LCT}$</td>
</tr>
<tr>
<td>$S_0 \rightarrow T_{10}$</td>
<td>401.8</td>
<td>3.085</td>
<td>$^3(X + M)\text{LCT}$</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>$S_0 \rightarrow T_{10}$</th>
<th>$\lambda$ (nm)</th>
<th>$f$</th>
<th>Assignment</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.4219</td>
<td>370.5</td>
<td></td>
<td>$^1(X + M)\text{LCT}$ $/^1\text{ILCT}$</td>
</tr>
<tr>
<td>0.3983</td>
<td>325.4</td>
<td></td>
<td>$^1(X + M)\text{LCT}$ $/^1\text{ILCT}$</td>
</tr>
<tr>
<td>0.1242</td>
<td>242.2</td>
<td></td>
<td>$^1\text{CC}^2(X + M)\text{LCT}$</td>
</tr>
<tr>
<td>0.1132</td>
<td>372.5</td>
<td></td>
<td>$^1(X + M)\text{LCT}$</td>
</tr>
<tr>
<td>0.3446</td>
<td>322.6</td>
<td></td>
<td>$^1(X + M)\text{LCT}$ $/^1\text{ILCT}$</td>
</tr>
</tbody>
</table>
The density difference plots (isovalue 0.0005) for the lowest triplet excitation of complex 2 and 3 in vacuo, calculated at the TDDFT optimized $T_1$ geometry. Blue and purple represent zones of depletion and augmentation of electron density in the $T_1$ excited state versus the $S_0$ ground state. The calculated emission wavelengths together with the experimental ones at 300 K are also listed for the sake of comparison.
### Table S14. Coordinates of geometry optimized structures

(1) XYZ coordinates of $S_0$ optimized geometry for complex 1

<table>
<thead>
<tr>
<th>Atom</th>
<th>X</th>
<th>Y</th>
<th>Z</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cu</td>
<td>-1.37745500</td>
<td>-0.27037100</td>
<td>-0.39713800</td>
</tr>
<tr>
<td>Cu</td>
<td>-0.13535800</td>
<td>2.37744300</td>
<td>-0.17963700</td>
</tr>
<tr>
<td>Cu</td>
<td>0.13535600</td>
<td>-2.37743500</td>
<td>0.17962900</td>
</tr>
<tr>
<td>Cu</td>
<td>1.37745100</td>
<td>0.27037100</td>
<td>0.39714600</td>
</tr>
<tr>
<td>I</td>
<td>2.03095900</td>
<td>2.90943300</td>
<td>1.14893600</td>
</tr>
<tr>
<td>I</td>
<td>0.43389700</td>
<td>0.64056800</td>
<td>-2.26780100</td>
</tr>
<tr>
<td>I</td>
<td>-0.43388800</td>
<td>-0.64057500</td>
<td>2.26781000</td>
</tr>
<tr>
<td>I</td>
<td>-2.03097300</td>
<td>-2.90942500</td>
<td>-1.14892600</td>
</tr>
<tr>
<td>N</td>
<td>-2.70655100</td>
<td>1.30665100</td>
<td>-0.05895800</td>
</tr>
<tr>
<td>N</td>
<td>-2.12981800</td>
<td>2.49012200</td>
<td>-0.16127500</td>
</tr>
<tr>
<td>N</td>
<td>-6.62417000</td>
<td>-1.80411600</td>
<td>0.50525500</td>
</tr>
<tr>
<td>C</td>
<td>-5.30085100</td>
<td>-1.90963400</td>
<td>0.79449400</td>
</tr>
<tr>
<td>C</td>
<td>-7.12589700</td>
<td>-0.61386300</td>
<td>0.09115200</td>
</tr>
<tr>
<td>C</td>
<td>-7.47342000</td>
<td>-2.98825900</td>
<td>0.57471900</td>
</tr>
<tr>
<td>C</td>
<td>-4.04985700</td>
<td>1.50046800</td>
<td>0.00291400</td>
</tr>
<tr>
<td>C</td>
<td>-3.07061500</td>
<td>3.47973000</td>
<td>-0.16751200</td>
</tr>
<tr>
<td>C</td>
<td>-4.45612800</td>
<td>-0.84448700</td>
<td>0.66663800</td>
</tr>
<tr>
<td>C</td>
<td>-1.88654000</td>
<td>5.29466600</td>
<td>1.03857300</td>
</tr>
<tr>
<td>C</td>
<td>-2.67319400</td>
<td>4.92974900</td>
<td>-0.23042900</td>
</tr>
<tr>
<td>C</td>
<td>-6.32376600</td>
<td>0.48377900</td>
<td>-0.06237200</td>
</tr>
<tr>
<td>C</td>
<td>-4.93423800</td>
<td>0.40015500</td>
<td>0.19361900</td>
</tr>
<tr>
<td>C</td>
<td>-4.31867900</td>
<td>2.88306300</td>
<td>-0.08382500</td>
</tr>
<tr>
<td>C</td>
<td>-1.79053000</td>
<td>5.16905200</td>
<td>-1.46474500</td>
</tr>
<tr>
<td>C</td>
<td>-3.92325000</td>
<td>5.80695100</td>
<td>-0.32502100</td>
</tr>
<tr>
<td>N</td>
<td>2.12981500</td>
<td>-2.49011600</td>
<td>0.16125700</td>
</tr>
<tr>
<td>N</td>
<td>2.70655500</td>
<td>-1.30664600</td>
<td>0.05896200</td>
</tr>
<tr>
<td>C</td>
<td>3.07060700</td>
<td>-3.47973000</td>
<td>0.16747200</td>
</tr>
<tr>
<td>C</td>
<td>4.04986100</td>
<td>-1.50046900</td>
<td>-0.00291500</td>
</tr>
<tr>
<td>C</td>
<td>4.31867300</td>
<td>-2.88307000</td>
<td>0.08377000</td>
</tr>
<tr>
<td>C</td>
<td>2.67317700</td>
<td>-4.92974800</td>
<td>0.23036100</td>
</tr>
<tr>
<td>C</td>
<td>4.93424900</td>
<td>-0.40015600</td>
<td>-0.19359500</td>
</tr>
<tr>
<td>C</td>
<td>1.88650700</td>
<td>-5.29462900</td>
<td>-1.03864100</td>
</tr>
<tr>
<td>C</td>
<td>1.79052600</td>
<td>-5.16907700</td>
<td>1.46468100</td>
</tr>
<tr>
<td>C</td>
<td>3.92322900</td>
<td>-5.80695900</td>
<td>0.32491700</td>
</tr>
<tr>
<td>C</td>
<td>6.32377800</td>
<td>-0.48379400</td>
<td>0.06239100</td>
</tr>
<tr>
<td>C</td>
<td>4.45614900</td>
<td>0.84449600</td>
<td>-0.66659700</td>
</tr>
<tr>
<td>C</td>
<td>7.12591700</td>
<td>0.61384400</td>
<td>-0.09111600</td>
</tr>
<tr>
<td>C</td>
<td>5.30087900</td>
<td>1.90964000</td>
<td>-0.79443600</td>
</tr>
<tr>
<td>N</td>
<td>6.62419700</td>
<td>1.80410800</td>
<td>-0.50520000</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>---</td>
<td>---</td>
<td>---</td>
<td>---</td>
</tr>
<tr>
<td>C</td>
<td>7.4734560000</td>
<td>2.9882460000</td>
<td>-0.5746460000</td>
</tr>
<tr>
<td>H</td>
<td>-4.9513170000</td>
<td>-2.8827170000</td>
<td>1.1195390000</td>
</tr>
<tr>
<td>H</td>
<td>-8.1883710000</td>
<td>-0.5928130000</td>
<td>-0.1215130000</td>
</tr>
<tr>
<td>H</td>
<td>-7.3317590000</td>
<td>-3.6074430000</td>
<td>-0.3152980000</td>
</tr>
<tr>
<td>H</td>
<td>-8.5177840000</td>
<td>-2.6828710000</td>
<td>0.6419660000</td>
</tr>
<tr>
<td>H</td>
<td>-7.2177140000</td>
<td>-3.5683190000</td>
<td>1.4628150000</td>
</tr>
<tr>
<td>H</td>
<td>-3.4123320000</td>
<td>-0.9659920000</td>
<td>0.9360730000</td>
</tr>
<tr>
<td>H</td>
<td>-2.4977310000</td>
<td>5.1450140000</td>
<td>1.9346610000</td>
</tr>
<tr>
<td>H</td>
<td>-1.5781430000</td>
<td>6.3458340000</td>
<td>1.0033450000</td>
</tr>
<tr>
<td>H</td>
<td>-0.9870350000</td>
<td>4.6779910000</td>
<td>1.1364070000</td>
</tr>
<tr>
<td>H</td>
<td>-6.7651380000</td>
<td>1.4089140000</td>
<td>-0.4142190000</td>
</tr>
<tr>
<td>H</td>
<td>-5.2788590000</td>
<td>3.3761090000</td>
<td>-0.0390270000</td>
</tr>
<tr>
<td>H</td>
<td>-1.4910050000</td>
<td>6.2219780000</td>
<td>-1.5150770000</td>
</tr>
<tr>
<td>H</td>
<td>-2.3230830000</td>
<td>4.9148370000</td>
<td>-2.3869480000</td>
</tr>
<tr>
<td>H</td>
<td>-0.8806370000</td>
<td>4.5601920000</td>
<td>-1.4247000000</td>
</tr>
<tr>
<td>H</td>
<td>-4.5659530000</td>
<td>5.6817490000</td>
<td>0.5532500000</td>
</tr>
<tr>
<td>H</td>
<td>-4.5104270000</td>
<td>5.5706580000</td>
<td>-1.2191960000</td>
</tr>
<tr>
<td>H</td>
<td>-3.6365140000</td>
<td>6.8621460000</td>
<td>-0.3796620000</td>
</tr>
<tr>
<td>H</td>
<td>5.2788480000</td>
<td>-3.3761210000</td>
<td>0.0389430000</td>
</tr>
<tr>
<td>H</td>
<td>2.4976880000</td>
<td>-5.1449570000</td>
<td>-1.9347330000</td>
</tr>
<tr>
<td>H</td>
<td>1.5781040000</td>
<td>-6.3457950000</td>
<td>-1.0034350000</td>
</tr>
<tr>
<td>H</td>
<td>0.9870040000</td>
<td>-4.6779460000</td>
<td>-1.1364480000</td>
</tr>
<tr>
<td>H</td>
<td>1.4909990000</td>
<td>-6.2220040000</td>
<td>1.5149920000</td>
</tr>
<tr>
<td>H</td>
<td>2.3230890000</td>
<td>-4.9148850000</td>
<td>2.3868840000</td>
</tr>
<tr>
<td>H</td>
<td>0.8806330000</td>
<td>-4.5602150000</td>
<td>1.4246600000</td>
</tr>
<tr>
<td>H</td>
<td>4.5659230000</td>
<td>-5.6817400000</td>
<td>-0.5533590000</td>
</tr>
<tr>
<td>H</td>
<td>4.5104180000</td>
<td>-5.5706900000</td>
<td>1.2190910000</td>
</tr>
<tr>
<td>H</td>
<td>3.6364880000</td>
<td>-6.8621530000</td>
<td>0.3795370000</td>
</tr>
<tr>
<td>H</td>
<td>6.7651450000</td>
<td>-1.4089390000</td>
<td>0.4142210000</td>
</tr>
<tr>
<td>H</td>
<td>3.4123540000</td>
<td>0.9660110000</td>
<td>-0.9360330000</td>
</tr>
<tr>
<td>H</td>
<td>8.1883900000</td>
<td>0.5927830000</td>
<td>0.1215460000</td>
</tr>
<tr>
<td>H</td>
<td>4.9513510000</td>
<td>2.8827300000</td>
<td>-1.1194670000</td>
</tr>
<tr>
<td>H</td>
<td>7.3318010000</td>
<td>3.6074170000</td>
<td>0.3153820000</td>
</tr>
<tr>
<td>H</td>
<td>8.5178180000</td>
<td>2.6828530000</td>
<td>-0.6419000000</td>
</tr>
<tr>
<td>H</td>
<td>7.2177520000</td>
<td>3.5683230000</td>
<td>-1.4627320000</td>
</tr>
</tbody>
</table>

(2) XYZ coordinates of UDFT optimized T1 geometry for complex I

<p>| | | | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Cu</td>
<td>-1.4483490000</td>
<td>-0.4280290000</td>
<td>-0.2726370000</td>
</tr>
<tr>
<td>Cu</td>
<td>-0.3668870000</td>
<td>2.1806540000</td>
<td>-0.1051970000</td>
</tr>
<tr>
<td>Cu</td>
<td>0.3673890000</td>
<td>-2.1846720000</td>
<td>0.1039920000</td>
</tr>
<tr>
<td>Cu</td>
<td>1.4486850000</td>
<td>0.4265410000</td>
<td>0.2720090000</td>
</tr>
<tr>
<td>I</td>
<td>0.4564350000</td>
<td>0.7436280000</td>
<td>-2.2176420000</td>
</tr>
<tr>
<td>I</td>
<td>-0.4543070000</td>
<td>-0.7491550000</td>
<td>2.2168370000</td>
</tr>
<tr>
<td></td>
<td>X</td>
<td>Y</td>
<td>Z</td>
</tr>
<tr>
<td>---</td>
<td>----------------</td>
<td>----------------</td>
<td>----------------</td>
</tr>
<tr>
<td>I</td>
<td>-1.52825200</td>
<td>-2.91844600</td>
<td>-1.32645100</td>
</tr>
<tr>
<td>I</td>
<td>1.52331900</td>
<td>2.91596100</td>
<td>1.33036000</td>
</tr>
<tr>
<td>N</td>
<td>-2.86878600</td>
<td>1.02582400</td>
<td>-0.16496800</td>
</tr>
<tr>
<td>N</td>
<td>-2.30120000</td>
<td>2.25450300</td>
<td>-0.31995800</td>
</tr>
<tr>
<td>N</td>
<td>-6.91450400</td>
<td>-1.98414600</td>
<td>0.41392000</td>
</tr>
<tr>
<td>C</td>
<td>-5.57654300</td>
<td>-2.27795000</td>
<td>0.21155300</td>
</tr>
<tr>
<td>C</td>
<td>-7.35805100</td>
<td>-0.72356800</td>
<td>0.47936400</td>
</tr>
<tr>
<td>C</td>
<td>-7.90664700</td>
<td>-3.10693000</td>
<td>0.62953700</td>
</tr>
<tr>
<td>C</td>
<td>-4.18900100</td>
<td>1.20624600</td>
<td>-0.07045900</td>
</tr>
<tr>
<td>C</td>
<td>-3.26400300</td>
<td>3.20340800</td>
<td>-0.33078300</td>
</tr>
<tr>
<td>C</td>
<td>-4.68363000</td>
<td>-1.23598800</td>
<td>0.14811500</td>
</tr>
<tr>
<td>C</td>
<td>-2.36536900</td>
<td>5.10326000</td>
<td>0.92823700</td>
</tr>
<tr>
<td>C</td>
<td>-2.94805100</td>
<td>4.67782600</td>
<td>-0.37974300</td>
</tr>
<tr>
<td>C</td>
<td>-6.50363700</td>
<td>0.32980000</td>
<td>0.38099900</td>
</tr>
<tr>
<td>C</td>
<td>-5.13185800</td>
<td>0.08316100</td>
<td>0.15800500</td>
</tr>
<tr>
<td>C</td>
<td>-4.48203100</td>
<td>2.58327200</td>
<td>-0.17905700</td>
</tr>
<tr>
<td>C</td>
<td>-1.92202100</td>
<td>4.93062400</td>
<td>-1.47991700</td>
</tr>
<tr>
<td>C</td>
<td>-4.20419900</td>
<td>5.43947800</td>
<td>-0.70479400</td>
</tr>
<tr>
<td>N</td>
<td>2.29946400</td>
<td>-2.25221900</td>
<td>0.31805800</td>
</tr>
<tr>
<td>N</td>
<td>2.86654900</td>
<td>-1.02324500</td>
<td>0.16338000</td>
</tr>
<tr>
<td>C</td>
<td>3.26355800</td>
<td>-3.19897700</td>
<td>0.32911800</td>
</tr>
<tr>
<td>C</td>
<td>4.18716700</td>
<td>-1.19931600</td>
<td>0.06812500</td>
</tr>
<tr>
<td>C</td>
<td>4.48048700</td>
<td>-2.57625400</td>
<td>0.17672000</td>
</tr>
<tr>
<td>C</td>
<td>2.95035200</td>
<td>-4.67388600</td>
<td>0.37853800</td>
</tr>
<tr>
<td>C</td>
<td>5.13102200</td>
<td>-0.07544000</td>
<td>-0.16068300</td>
</tr>
<tr>
<td>C</td>
<td>2.36825400</td>
<td>-5.10098500</td>
<td>-0.92919600</td>
</tr>
<tr>
<td>C</td>
<td>1.92498800</td>
<td>-4.92818300</td>
<td>1.47898200</td>
</tr>
<tr>
<td>C</td>
<td>4.20807500</td>
<td>-5.43293500</td>
<td>0.70354400</td>
</tr>
<tr>
<td>C</td>
<td>6.50362000</td>
<td>-0.32399100</td>
<td>-0.38386800</td>
</tr>
<tr>
<td>C</td>
<td>4.68432900</td>
<td>1.24444700</td>
<td>-0.15085200</td>
</tr>
<tr>
<td>C</td>
<td>7.35930100</td>
<td>0.72759500</td>
<td>-0.48240700</td>
</tr>
<tr>
<td>C</td>
<td>5.57788300</td>
<td>2.28576200</td>
<td>-0.21442200</td>
</tr>
<tr>
<td>N</td>
<td>6.91723300</td>
<td>1.99001300</td>
<td>-0.41663600</td>
</tr>
<tr>
<td>C</td>
<td>7.91052600</td>
<td>3.11113700</td>
<td>-0.63322000</td>
</tr>
<tr>
<td>H</td>
<td>-5.28177700</td>
<td>-3.24883000</td>
<td>0.10868700</td>
</tr>
<tr>
<td>H</td>
<td>-8.35743800</td>
<td>-0.55973000</td>
<td>0.60556900</td>
</tr>
<tr>
<td>H</td>
<td>-8.36324500</td>
<td>-3.33513200</td>
<td>-0.26883500</td>
</tr>
<tr>
<td>H</td>
<td>-8.61262800</td>
<td>-2.80121800</td>
<td>1.31642900</td>
</tr>
<tr>
<td>H</td>
<td>-7.40331300</td>
<td>-3.93423700</td>
<td>0.98469200</td>
</tr>
<tr>
<td>H</td>
<td>-3.68549000</td>
<td>-1.43611800</td>
<td>0.09212700</td>
</tr>
<tr>
<td>H</td>
<td>-3.11692600</td>
<td>5.39237400</td>
<td>1.57824800</td>
</tr>
<tr>
<td>H</td>
<td>-1.72505300</td>
<td>5.90234000</td>
<td>0.78983400</td>
</tr>
<tr>
<td>H</td>
<td>-1.83643300</td>
<td>4.32688100</td>
<td>1.35818000</td>
</tr>
<tr>
<td>H</td>
<td>-6.85125700</td>
<td>1.28461700</td>
<td>0.46838000</td>
</tr>
<tr>
<td>Atom</td>
<td>X</td>
<td>Y</td>
<td>Z</td>
</tr>
<tr>
<td>------</td>
<td>-------------</td>
<td>-------------</td>
<td>-------------</td>
</tr>
<tr>
<td>H</td>
<td>-5.40332200</td>
<td>3.02083400</td>
<td>-0.15257900</td>
</tr>
<tr>
<td>H</td>
<td>-1.17411100</td>
<td>5.54942700</td>
<td>-1.13027000</td>
</tr>
<tr>
<td>H</td>
<td>-2.37355700</td>
<td>5.37456600</td>
<td>-2.29536100</td>
</tr>
<tr>
<td>H</td>
<td>-1.49473200</td>
<td>4.03940200</td>
<td>-1.78406900</td>
</tr>
<tr>
<td>H</td>
<td>-4.94028600</td>
<td>5.19724300</td>
<td>-0.01908000</td>
</tr>
<tr>
<td>H</td>
<td>-4.53422500</td>
<td>5.17618900</td>
<td>-1.64897600</td>
</tr>
<tr>
<td>H</td>
<td>-4.01612200</td>
<td>6.45026100</td>
<td>-0.66900100</td>
</tr>
<tr>
<td>H</td>
<td>5.40231600</td>
<td>-3.01251900</td>
<td>0.14996000</td>
</tr>
<tr>
<td>H</td>
<td>3.12018300</td>
<td>-5.38890100</td>
<td>-1.57925300</td>
</tr>
<tr>
<td>H</td>
<td>1.72952800</td>
<td>-5.90125900</td>
<td>-0.79031100</td>
</tr>
<tr>
<td>H</td>
<td>1.83778400</td>
<td>-4.32580300</td>
<td>-1.35942400</td>
</tr>
<tr>
<td>H</td>
<td>1.17820600</td>
<td>-5.54856200</td>
<td>1.12966400</td>
</tr>
<tr>
<td>H</td>
<td>2.37739600</td>
<td>-5.37092000</td>
<td>2.29454600</td>
</tr>
<tr>
<td>H</td>
<td>1.49610500</td>
<td>-4.03761600</td>
<td>1.78298500</td>
</tr>
<tr>
<td>H</td>
<td>4.94355700</td>
<td>-5.18953700</td>
<td>0.01761600</td>
</tr>
<tr>
<td>H</td>
<td>4.53781100</td>
<td>-5.16700000</td>
<td>1.64754200</td>
</tr>
<tr>
<td>H</td>
<td>4.02190300</td>
<td>-6.44407100</td>
<td>0.66810400</td>
</tr>
<tr>
<td>H</td>
<td>6.85020100</td>
<td>-1.27919800</td>
<td>-0.47122000</td>
</tr>
<tr>
<td>H</td>
<td>3.68660600</td>
<td>1.44617300</td>
<td>-0.09480900</td>
</tr>
<tr>
<td>H</td>
<td>8.35836400</td>
<td>0.56201700</td>
<td>-0.60866100</td>
</tr>
<tr>
<td>H</td>
<td>5.28384100</td>
<td>3.25678100</td>
<td>-0.11160600</td>
</tr>
<tr>
<td>H</td>
<td>8.36777000</td>
<td>3.33927100</td>
<td>0.26490500</td>
</tr>
<tr>
<td>H</td>
<td>8.61608200</td>
<td>2.80445800</td>
<td>-1.32018800</td>
</tr>
<tr>
<td>H</td>
<td>7.40823800</td>
<td>3.93904800</td>
<td>-0.98856000</td>
</tr>
</tbody>
</table>

(3) XYZ coordinates of S0 optimized geometry for complex 2

<table>
<thead>
<tr>
<th>Atom</th>
<th>X</th>
<th>Y</th>
<th>Z</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cu</td>
<td>-1.34762600</td>
<td>-0.23351400</td>
<td>-0.37981300</td>
</tr>
<tr>
<td>Cu</td>
<td>-0.01567700</td>
<td>2.46511200</td>
<td>-0.15658800</td>
</tr>
<tr>
<td>Cu</td>
<td>0.01584400</td>
<td>-2.46468600</td>
<td>0.15548200</td>
</tr>
<tr>
<td>Cu</td>
<td>1.34739200</td>
<td>0.23365400</td>
<td>0.38051000</td>
</tr>
<tr>
<td>I</td>
<td>0.43194900</td>
<td>0.68002900</td>
<td>-2.26932300</td>
</tr>
<tr>
<td>I</td>
<td>-2.18371200</td>
<td>-2.78661800</td>
<td>-1.17623400</td>
</tr>
<tr>
<td>I</td>
<td>-0.43174100</td>
<td>-0.68100700</td>
<td>2.26976600</td>
</tr>
<tr>
<td>I</td>
<td>2.18293300</td>
<td>2.78701300</td>
<td>1.17672500</td>
</tr>
<tr>
<td>N</td>
<td>-2.61803800</td>
<td>1.39976400</td>
<td>-0.00689700</td>
</tr>
<tr>
<td>N</td>
<td>-2.00926900</td>
<td>2.56373400</td>
<td>-0.11897100</td>
</tr>
<tr>
<td>N</td>
<td>-6.54048500</td>
<td>-1.67562900</td>
<td>0.52859200</td>
</tr>
<tr>
<td>N</td>
<td>2.00937100</td>
<td>-2.56336100</td>
<td>0.11809800</td>
</tr>
<tr>
<td>N</td>
<td>2.61833100</td>
<td>-1.39939500</td>
<td>0.00708500</td>
</tr>
<tr>
<td>C</td>
<td>-7.38222800</td>
<td>-2.86811300</td>
<td>0.59099400</td>
</tr>
<tr>
<td>C</td>
<td>-7.02937400</td>
<td>-0.50911500</td>
<td>0.04231100</td>
</tr>
<tr>
<td>C</td>
<td>-5.23907100</td>
<td>-1.75977000</td>
<td>0.89844800</td>
</tr>
<tr>
<td>C</td>
<td>-3.95725000</td>
<td>1.62252800</td>
<td>0.04137800</td>
</tr>
</tbody>
</table>
(4) XYZ coordinates of UDFT optimized T₁ geometry for complex 2

Cu  1.71040800  0.41968700  -0.20987700
Cu  0.25217800  -2.36987900  -0.05854300
<table>
<thead>
<tr>
<th>Element</th>
<th>X</th>
<th>Y</th>
<th>Z</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cu</td>
<td>-0.25220100</td>
<td>2.36998300</td>
<td>0.05878600</td>
</tr>
<tr>
<td>Cu</td>
<td>-1.71043400</td>
<td>-0.41962400</td>
<td>0.20991100</td>
</tr>
<tr>
<td>I</td>
<td>-0.18213500</td>
<td>-0.38940700</td>
<td>-2.09283900</td>
</tr>
<tr>
<td>I</td>
<td>2.12137800</td>
<td>3.04025300</td>
<td>-0.63036100</td>
</tr>
<tr>
<td>I</td>
<td>0.18213100</td>
<td>0.38930000</td>
<td>2.09288800</td>
</tr>
<tr>
<td>I</td>
<td>-2.12143900</td>
<td>-3.04016600</td>
<td>0.63046500</td>
</tr>
<tr>
<td>N</td>
<td>2.89237900</td>
<td>-1.22935800</td>
<td>0.02010400</td>
</tr>
<tr>
<td>N</td>
<td>2.21809300</td>
<td>-2.37530200</td>
<td>-0.04948900</td>
</tr>
<tr>
<td>N</td>
<td>7.18342300</td>
<td>1.51856600</td>
<td>0.34577000</td>
</tr>
<tr>
<td>N</td>
<td>-2.21813000</td>
<td>2.37536500</td>
<td>0.04964000</td>
</tr>
<tr>
<td>N</td>
<td>5.89718500</td>
<td>1.75499500</td>
<td>0.75799100</td>
</tr>
<tr>
<td>C</td>
<td>4.21980500</td>
<td>-1.51090800</td>
<td>0.01724100</td>
</tr>
<tr>
<td>C</td>
<td>3.09505700</td>
<td>-3.39064800</td>
<td>-0.11079300</td>
</tr>
<tr>
<td>C</td>
<td>6.56710500</td>
<td>-0.70262500</td>
<td>-0.26931100</td>
</tr>
<tr>
<td>C</td>
<td>5.22569600</td>
<td>-0.48597300</td>
<td>0.13351100</td>
</tr>
<tr>
<td>C</td>
<td>4.93544100</td>
<td>0.79128300</td>
<td>0.67286800</td>
</tr>
<tr>
<td>C</td>
<td>4.38970200</td>
<td>-2.90322700</td>
<td>-0.07849400</td>
</tr>
<tr>
<td>C</td>
<td>2.61847300</td>
<td>-4.79895400</td>
<td>-0.13352300</td>
</tr>
<tr>
<td>C</td>
<td>-3.30951160</td>
<td>3.39068200</td>
<td>0.11086400</td>
</tr>
<tr>
<td>C</td>
<td>-4.21979300</td>
<td>1.51091100</td>
<td>-0.01736500</td>
</tr>
<tr>
<td>C</td>
<td>-4.38974500</td>
<td>2.90322000</td>
<td>0.07840800</td>
</tr>
<tr>
<td>C</td>
<td>-2.61857800</td>
<td>4.79900200</td>
<td>0.13368800</td>
</tr>
<tr>
<td>C</td>
<td>-5.22561600</td>
<td>0.48592900</td>
<td>-0.13378300</td>
</tr>
<tr>
<td>F</td>
<td>-1.51260600</td>
<td>4.93041000</td>
<td>0.89045400</td>
</tr>
<tr>
<td>F</td>
<td>-3.55991100</td>
<td>5.61478600</td>
<td>0.62924100</td>
</tr>
<tr>
<td>F</td>
<td>-2.30290100</td>
<td>5.25010100</td>
<td>-1.09164000</td>
</tr>
<tr>
<td>F</td>
<td>1.51239500</td>
<td>-4.93034300</td>
<td>-0.89013900</td>
</tr>
<tr>
<td>F</td>
<td>3.55971800</td>
<td>-5.61477900</td>
<td>-0.62917700</td>
</tr>
<tr>
<td>F</td>
<td>2.30294400</td>
<td>-5.25009000</td>
<td>1.09185900</td>
</tr>
<tr>
<td>C</td>
<td>-6.56708200</td>
<td>0.70248700</td>
<td>0.26890000</td>
</tr>
<tr>
<td>C</td>
<td>-4.93521400</td>
<td>-0.79130100</td>
<td>-0.67312600</td>
</tr>
<tr>
<td>C</td>
<td>-7.50169200</td>
<td>-0.28719500</td>
<td>0.16452100</td>
</tr>
<tr>
<td>C</td>
<td>-5.89689000</td>
<td>-1.75507100</td>
<td>-0.75838100</td>
</tr>
<tr>
<td>N</td>
<td>-7.18319100</td>
<td>-1.51873000</td>
<td>-0.34630400</td>
</tr>
<tr>
<td>C</td>
<td>-8.15882700</td>
<td>-2.59243500</td>
<td>-0.34333600</td>
</tr>
<tr>
<td>H</td>
<td>-5.30713800</td>
<td>3.47216300</td>
<td>0.08537700</td>
</tr>
<tr>
<td>H</td>
<td>7.96884100</td>
<td>3.26146900</td>
<td>1.18396700</td>
</tr>
<tr>
<td>H</td>
<td>8.10998800</td>
<td>3.16864400</td>
<td>-0.58813300</td>
</tr>
<tr>
<td>H</td>
<td>9.16245800</td>
<td>2.17614900</td>
<td>0.45178600</td>
</tr>
<tr>
<td>H</td>
<td>8.52999200</td>
<td>0.15625300</td>
<td>-0.48058100</td>
</tr>
<tr>
<td>H</td>
<td>5.69575000</td>
<td>2.74190500</td>
<td>1.15712800</td>
</tr>
<tr>
<td>Atom</td>
<td>X</td>
<td>Y</td>
<td>Z</td>
</tr>
<tr>
<td>------</td>
<td>--------------</td>
<td>--------------</td>
<td>--------------</td>
</tr>
<tr>
<td>H</td>
<td>6.86847600</td>
<td>-1.65496800</td>
<td>-0.69119100</td>
</tr>
<tr>
<td>H</td>
<td>3.94117300</td>
<td>1.02076100</td>
<td>1.03811900</td>
</tr>
<tr>
<td>H</td>
<td>5.30707400</td>
<td>-3.47220100</td>
<td>-0.08553900</td>
</tr>
<tr>
<td>H</td>
<td>-6.86557000</td>
<td>1.65480100</td>
<td>0.69077200</td>
</tr>
<tr>
<td>H</td>
<td>-3.94088400</td>
<td>-1.02071100</td>
<td>-1.03825400</td>
</tr>
<tr>
<td>H</td>
<td>-8.52994000</td>
<td>-0.15651900</td>
<td>0.47992700</td>
</tr>
<tr>
<td>H</td>
<td>-5.69534800</td>
<td>-2.74196300</td>
<td>-1.15751100</td>
</tr>
<tr>
<td>H</td>
<td>-8.10979200</td>
<td>-3.16884900</td>
<td>0.58749200</td>
</tr>
<tr>
<td>H</td>
<td>-9.16217000</td>
<td>-2.17643800</td>
<td>-0.45260100</td>
</tr>
</tbody>
</table>

(5) XYZ coordinates of $S_0$ optimized geometry for complex 3
<table>
<thead>
<tr>
<th></th>
<th>X</th>
<th>Y</th>
<th>Z</th>
</tr>
</thead>
<tbody>
<tr>
<td>C</td>
<td>4.25075700</td>
<td>-5.02428300</td>
<td>0.67653200</td>
</tr>
<tr>
<td>H</td>
<td>3.02982500</td>
<td>-3.32039600</td>
<td>1.14633400</td>
</tr>
<tr>
<td>C</td>
<td>5.41532200</td>
<td>-5.48279300</td>
<td>0.06664900</td>
</tr>
<tr>
<td>H</td>
<td>3.57804500</td>
<td>-5.72018200</td>
<td>1.16889600</td>
</tr>
<tr>
<td>C</td>
<td>6.26360300</td>
<td>-4.57827700</td>
<td>-0.56918300</td>
</tr>
<tr>
<td>H</td>
<td>5.65879800</td>
<td>-6.54136600</td>
<td>0.08082400</td>
</tr>
<tr>
<td>H</td>
<td>7.16881900</td>
<td>-4.92958100</td>
<td>-1.05671400</td>
</tr>
<tr>
<td>H</td>
<td>6.59327400</td>
<td>-2.52735600</td>
<td>-1.12035200</td>
</tr>
<tr>
<td>H</td>
<td>-3.02910500</td>
<td>3.32080800</td>
<td>1.14686500</td>
</tr>
<tr>
<td>H</td>
<td>-3.18066600</td>
<td>0.85332300</td>
<td>0.02807800</td>
</tr>
<tr>
<td>N</td>
<td>-3.18887200</td>
<td>0.46386900</td>
<td>0.01918400</td>
</tr>
<tr>
<td>H</td>
<td>-2.79711500</td>
<td>3.05391600</td>
<td>0.05741100</td>
</tr>
<tr>
<td>C</td>
<td>-3.93499000</td>
<td>3.67078700</td>
<td>0.66053500</td>
</tr>
<tr>
<td>C</td>
<td>-4.46431400</td>
<td>-1.32594800</td>
<td>-0.00051500</td>
</tr>
<tr>
<td>C</td>
<td>-4.48613200</td>
<td>0.88502000</td>
<td>-0.01832000</td>
</tr>
<tr>
<td>C</td>
<td>-3.85641200</td>
<td>3.28914700</td>
<td>0.01719200</td>
</tr>
<tr>
<td>C</td>
<td>-4.77783000</td>
<td>-2.75605500</td>
<td>0.01875700</td>
</tr>
<tr>
<td>C</td>
<td>-4.24963800</td>
<td>-5.02500700</td>
<td>0.67718900</td>
</tr>
<tr>
<td>C</td>
<td>-5.32757400</td>
<td>-0.24547700</td>
<td>-0.03404200</td>
</tr>
<tr>
<td>C</td>
<td>-4.83244000</td>
<td>2.26366500</td>
<td>-0.02658800</td>
</tr>
<tr>
<td>C</td>
<td>-4.22062100</td>
<td>4.60319700</td>
<td>0.00454100</td>
</tr>
<tr>
<td>C</td>
<td>-5.94511800</td>
<td>-3.22716100</td>
<td>-0.59630800</td>
</tr>
<tr>
<td>H</td>
<td>-3.57680700</td>
<td>-5.72068900</td>
<td>1.16969900</td>
</tr>
<tr>
<td>C</td>
<td>-5.41405900</td>
<td>-5.48385200</td>
<td>0.06728600</td>
</tr>
<tr>
<td>H</td>
<td>-6.40734800</td>
<td>-0.27861300</td>
<td>-0.02973500</td>
</tr>
<tr>
<td>C</td>
<td>-6.18231900</td>
<td>2.69695800</td>
<td>-0.08193200</td>
</tr>
<tr>
<td>H</td>
<td>-3.48424800</td>
<td>5.39870800</td>
<td>0.03697000</td>
</tr>
<tr>
<td>N</td>
<td>-5.52611500</td>
<td>4.98199200</td>
<td>-0.05119800</td>
</tr>
<tr>
<td>C</td>
<td>-6.26248500</td>
<td>-4.57959500</td>
<td>-0.56872500</td>
</tr>
<tr>
<td>H</td>
<td>-6.59256500</td>
<td>-2.52883100</td>
<td>-1.12019300</td>
</tr>
<tr>
<td>H</td>
<td>-5.65731100</td>
<td>-6.54247400</td>
<td>0.08158300</td>
</tr>
<tr>
<td>C</td>
<td>-6.49063500</td>
<td>4.02838700</td>
<td>-0.09037400</td>
</tr>
<tr>
<td>H</td>
<td>-6.99229100</td>
<td>1.97890800</td>
<td>-0.12376400</td>
</tr>
<tr>
<td>C</td>
<td>-5.87625600</td>
<td>6.39653000</td>
<td>-0.00369900</td>
</tr>
<tr>
<td>H</td>
<td>-7.16759200</td>
<td>-4.93115100</td>
<td>-1.05627600</td>
</tr>
<tr>
<td>H</td>
<td>-7.51286700</td>
<td>4.38650000</td>
<td>-0.13116600</td>
</tr>
<tr>
<td>H</td>
<td>-6.87270200</td>
<td>6.53822300</td>
<td>-0.42298400</td>
</tr>
<tr>
<td>H</td>
<td>-5.86266600</td>
<td>6.75977100</td>
<td>1.02790500</td>
</tr>
<tr>
<td>H</td>
<td>-5.16151500</td>
<td>6.96806900</td>
<td>-0.59780200</td>
</tr>
</tbody>
</table>

(6) XYZ coordinates of UDFT optimized T₁ geometry for complex 3

<table>
<thead>
<tr>
<th></th>
<th>X</th>
<th>Y</th>
<th>Z</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cu</td>
<td>1.45057500</td>
<td>-1.74862100</td>
<td>-0.02438000</td>
</tr>
<tr>
<td>Cu</td>
<td>-1.45050700</td>
<td>-1.74863100</td>
<td>-0.02439200</td>
</tr>
</tbody>
</table>

55
<table>
<thead>
<tr>
<th>Atom</th>
<th>X-coordinate</th>
<th>Y-coordinate</th>
<th>Z-coordinate</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cu</td>
<td>1.31763700</td>
<td>1.29226100</td>
<td>0.08910900</td>
</tr>
<tr>
<td>Cu</td>
<td>-1.31770200</td>
<td>1.29228100</td>
<td>0.08906600</td>
</tr>
<tr>
<td>I</td>
<td>-0.00003700</td>
<td>3.60243200</td>
<td>0.29028300</td>
</tr>
<tr>
<td>I</td>
<td>0.00005100</td>
<td>-3.89821200</td>
<td>-0.19206500</td>
</tr>
<tr>
<td>I</td>
<td>-0.00000300</td>
<td>-0.43388200</td>
<td>2.08649900</td>
</tr>
<tr>
<td>I</td>
<td>0.00001300</td>
<td>-0.21751200</td>
<td>-2.01136100</td>
</tr>
<tr>
<td>C</td>
<td>6.09917600</td>
<td>6.42611100</td>
<td>-0.13225800</td>
</tr>
<tr>
<td>N</td>
<td>3.17766800</td>
<td>-0.78619700</td>
<td>0.05347800</td>
</tr>
<tr>
<td>N</td>
<td>3.18887400</td>
<td>0.54827800</td>
<td>0.03169700</td>
</tr>
<tr>
<td>N</td>
<td>5.67488400</td>
<td>5.04156400</td>
<td>-0.18735300</td>
</tr>
<tr>
<td>H</td>
<td>6.97855500</td>
<td>6.56586600</td>
<td>-0.76429500</td>
</tr>
<tr>
<td>H</td>
<td>6.34600600</td>
<td>6.72816500</td>
<td>0.89246700</td>
</tr>
<tr>
<td>H</td>
<td>5.30050000</td>
<td>7.06859700</td>
<td>-0.50742300</td>
</tr>
<tr>
<td>C</td>
<td>6.59299900</td>
<td>4.03544400</td>
<td>-0.34699600</td>
</tr>
<tr>
<td>C</td>
<td>6.22369900</td>
<td>2.72283200</td>
<td>-0.31367300</td>
</tr>
<tr>
<td>H</td>
<td>7.61694600</td>
<td>4.35059090</td>
<td>-0.50994000</td>
</tr>
<tr>
<td>C</td>
<td>4.87255100</td>
<td>2.34019800</td>
<td>-0.10200700</td>
</tr>
<tr>
<td>H</td>
<td>6.99174100</td>
<td>1.97346700</td>
<td>-0.46605100</td>
</tr>
<tr>
<td>C</td>
<td>3.95424500</td>
<td>3.40695800</td>
<td>0.07113400</td>
</tr>
<tr>
<td>C</td>
<td>4.48046200</td>
<td>0.95714700</td>
<td>-0.06722300</td>
</tr>
<tr>
<td>C</td>
<td>4.36197700</td>
<td>4.70656300</td>
<td>0.02988600</td>
</tr>
<tr>
<td>H</td>
<td>2.90136700</td>
<td>3.21010700</td>
<td>0.23872300</td>
</tr>
<tr>
<td>H</td>
<td>3.67253500</td>
<td>5.53254200</td>
<td>0.16012900</td>
</tr>
<tr>
<td>C</td>
<td>5.31025600</td>
<td>-0.17832400</td>
<td>-0.11287400</td>
</tr>
<tr>
<td>C</td>
<td>4.44280800</td>
<td>-1.25868400</td>
<td>-0.02540500</td>
</tr>
<tr>
<td>H</td>
<td>6.38902300</td>
<td>-0.21783900</td>
<td>-0.14855200</td>
</tr>
<tr>
<td>C</td>
<td>4.73041300</td>
<td>-2.69447900</td>
<td>0.00520300</td>
</tr>
<tr>
<td>C</td>
<td>3.96444500</td>
<td>-3.55915500</td>
<td>0.79790800</td>
</tr>
<tr>
<td>C</td>
<td>5.77998700</td>
<td>-3.22708500</td>
<td>-0.75330900</td>
</tr>
<tr>
<td>C</td>
<td>4.22830200</td>
<td>-4.92490200</td>
<td>0.81315500</td>
</tr>
<tr>
<td>H</td>
<td>3.17512400</td>
<td>-3.15230500</td>
<td>1.42599900</td>
</tr>
<tr>
<td>C</td>
<td>5.27203100</td>
<td>-5.44482000</td>
<td>0.05245300</td>
</tr>
<tr>
<td>H</td>
<td>3.62146900</td>
<td>-5.58113800</td>
<td>1.43035000</td>
</tr>
<tr>
<td>C</td>
<td>6.04989200</td>
<td>-4.59032500</td>
<td>-0.72685500</td>
</tr>
<tr>
<td>H</td>
<td>5.48017800</td>
<td>-6.51075700</td>
<td>0.06749500</td>
</tr>
<tr>
<td>H</td>
<td>6.86346900</td>
<td>-4.99021000</td>
<td>-1.32579000</td>
</tr>
<tr>
<td>H</td>
<td>6.36888000</td>
<td>-2.56545800</td>
<td>-1.38269400</td>
</tr>
<tr>
<td>H</td>
<td>-3.17497600</td>
<td>-3.15230000</td>
<td>1.42614200</td>
</tr>
<tr>
<td>N</td>
<td>-3.17763100</td>
<td>-0.78626100</td>
<td>0.05346800</td>
</tr>
<tr>
<td>N</td>
<td>-3.18888900</td>
<td>0.54821200</td>
<td>0.03162400</td>
</tr>
<tr>
<td>H</td>
<td>-2.90143500</td>
<td>3.21008000</td>
<td>0.23825800</td>
</tr>
<tr>
<td>C</td>
<td>-3.96429400</td>
<td>-3.55921000</td>
<td>0.79808500</td>
</tr>
<tr>
<td>C</td>
<td>-4.44275700</td>
<td>-1.25880000</td>
<td>-0.02533900</td>
</tr>
<tr>
<td>C</td>
<td>-4.48049600</td>
<td>0.95703000</td>
<td>-0.06726500</td>
</tr>
</tbody>
</table>
(7) XYZ coordinates of $S_0$ optimized geometry for complex 4

<table>
<thead>
<tr>
<th>Element</th>
<th>X</th>
<th>Y</th>
<th>Z</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cu</td>
<td>-1.0378400</td>
<td>-0.91677400</td>
<td>0.3884300</td>
</tr>
<tr>
<td>Cu</td>
<td>1.03792500</td>
<td>0.91665900</td>
<td>-0.38841400</td>
</tr>
<tr>
<td>Cu</td>
<td>1.33515800</td>
<td>-1.99879100</td>
<td>-0.15435100</td>
</tr>
<tr>
<td>Cu</td>
<td>-1.33499500</td>
<td>1.99883900</td>
<td>0.15459900</td>
</tr>
<tr>
<td>I</td>
<td>-0.29344700</td>
<td>-3.50607500</td>
<td>1.20978500</td>
</tr>
<tr>
<td>I</td>
<td>0.29353500</td>
<td>3.50590200</td>
<td>-1.20992200</td>
</tr>
<tr>
<td>I</td>
<td>0.00337800</td>
<td>-0.81564600</td>
<td>-2.26718800</td>
</tr>
<tr>
<td>I</td>
<td>-0.00335500</td>
<td>0.81548400</td>
<td>2.26729900</td>
</tr>
<tr>
<td>N</td>
<td>3.10512600</td>
<td>-1.06483600</td>
<td>-0.07596200</td>
</tr>
<tr>
<td>N</td>
<td>-2.97965000</td>
<td>-0.24573900</td>
<td>-0.00821300</td>
</tr>
<tr>
<td>C</td>
<td>-4.74899500</td>
<td>-6.41049600</td>
<td>-0.62274100</td>
</tr>
<tr>
<td>N</td>
<td>-4.65816000</td>
<td>-4.95532900</td>
<td>-0.55851600</td>
</tr>
<tr>
<td>H</td>
<td>-5.79710300</td>
<td>-6.70754800</td>
<td>-0.66133800</td>
</tr>
<tr>
<td>H</td>
<td>-4.27606400</td>
<td>-6.85595200</td>
<td>0.25660200</td>
</tr>
<tr>
<td>H</td>
<td>-4.24721200</td>
<td>-6.76740600</td>
<td>-1.52351200</td>
</tr>
<tr>
<td>C</td>
<td>-5.71099500</td>
<td>-4.21299100</td>
<td>-0.13500500</td>
</tr>
</tbody>
</table>


<table>
<thead>
<tr>
<th></th>
<th>X</th>
<th>Y</th>
<th>Z</th>
</tr>
</thead>
<tbody>
<tr>
<td>C</td>
<td>-5.61223300</td>
<td>-2.85584700</td>
<td>0.01252900</td>
</tr>
<tr>
<td>H</td>
<td>-6.61946800</td>
<td>-4.75898400</td>
<td>0.09058400</td>
</tr>
<tr>
<td>C</td>
<td>-4.39384700</td>
<td>-2.19193800</td>
<td>-0.26008600</td>
</tr>
<tr>
<td>H</td>
<td>-6.47247600</td>
<td>-2.30449900</td>
<td>0.37386200</td>
</tr>
<tr>
<td>C</td>
<td>-3.33263800</td>
<td>-2.99191600</td>
<td>-0.74138200</td>
</tr>
<tr>
<td>C</td>
<td>-4.22506800</td>
<td>-0.78691100</td>
<td>-0.07543400</td>
</tr>
<tr>
<td>C</td>
<td>-3.48463800</td>
<td>-4.34430100</td>
<td>-0.86345300</td>
</tr>
<tr>
<td>H</td>
<td>-2.38676500</td>
<td>-2.54085700</td>
<td>-1.02334100</td>
</tr>
<tr>
<td>H</td>
<td>-2.67583700</td>
<td>-4.98499300</td>
<td>-1.19487300</td>
</tr>
<tr>
<td>C</td>
<td>-5.17922300</td>
<td>0.24497900</td>
<td>-0.00823300</td>
</tr>
<tr>
<td>C</td>
<td>-4.42452300</td>
<td>1.40719100</td>
<td>0.06643200</td>
</tr>
<tr>
<td>H</td>
<td>-6.25380500</td>
<td>0.16704700</td>
<td>-0.09179000</td>
</tr>
<tr>
<td>N</td>
<td>-3.10497300</td>
<td>1.06484200</td>
<td>0.07614000</td>
</tr>
<tr>
<td>C</td>
<td>-4.86537300</td>
<td>2.80300200</td>
<td>0.11157100</td>
</tr>
<tr>
<td>C</td>
<td>-6.10281100</td>
<td>3.13478500</td>
<td>0.67784600</td>
</tr>
<tr>
<td>C</td>
<td>-4.06928200</td>
<td>3.82758100</td>
<td>-0.41717300</td>
</tr>
<tr>
<td>C</td>
<td>-6.53414600</td>
<td>4.45550900</td>
<td>0.71492700</td>
</tr>
<tr>
<td>H</td>
<td>-6.71806400</td>
<td>2.35088500</td>
<td>1.11142700</td>
</tr>
<tr>
<td>C</td>
<td>-5.73307100</td>
<td>5.46860000</td>
<td>0.19240800</td>
</tr>
<tr>
<td>H</td>
<td>-7.49452900</td>
<td>4.69616500</td>
<td>1.16250000</td>
</tr>
<tr>
<td>C</td>
<td>-4.49999000</td>
<td>5.14887800</td>
<td>-0.37069500</td>
</tr>
<tr>
<td>H</td>
<td>-6.06840000</td>
<td>6.50137600</td>
<td>0.22495000</td>
</tr>
<tr>
<td>H</td>
<td>-3.86972000</td>
<td>5.92951300</td>
<td>-0.78726000</td>
</tr>
<tr>
<td>H</td>
<td>-3.11489000</td>
<td>3.58495700</td>
<td>-0.87868300</td>
</tr>
<tr>
<td>H</td>
<td>3.11507200</td>
<td>-3.58493000</td>
<td>0.87841900</td>
</tr>
<tr>
<td>N</td>
<td>2.97970300</td>
<td>0.24574000</td>
<td>0.00833500</td>
</tr>
<tr>
<td>C</td>
<td>4.42470800</td>
<td>-1.40706200</td>
<td>-0.06641200</td>
</tr>
<tr>
<td>H</td>
<td>2.38677700</td>
<td>2.54045000</td>
<td>1.02402800</td>
</tr>
<tr>
<td>C</td>
<td>4.06956400</td>
<td>-3.82747700</td>
<td>0.41707600</td>
</tr>
<tr>
<td>C</td>
<td>4.22508200</td>
<td>0.78701500</td>
<td>0.07538600</td>
</tr>
<tr>
<td>C</td>
<td>5.17932300</td>
<td>-0.24478500</td>
<td>0.00819500</td>
</tr>
<tr>
<td>C</td>
<td>4.86566900</td>
<td>-2.80283300</td>
<td>-0.11151800</td>
</tr>
<tr>
<td>C</td>
<td>3.33241300</td>
<td>2.99177700</td>
<td>0.74167400</td>
</tr>
<tr>
<td>C</td>
<td>4.50036800</td>
<td>-5.14874400</td>
<td>0.37063400</td>
</tr>
<tr>
<td>C</td>
<td>4.39364000</td>
<td>2.19208200</td>
<td>0.25995800</td>
</tr>
<tr>
<td>H</td>
<td>6.25390100</td>
<td>-0.16673600</td>
<td>0.09168900</td>
</tr>
<tr>
<td>C</td>
<td>6.10321100</td>
<td>-3.13452400</td>
<td>-0.67762400</td>
</tr>
<tr>
<td>C</td>
<td>3.48412500</td>
<td>-4.34420700</td>
<td>0.86366200</td>
</tr>
<tr>
<td>C</td>
<td>5.73355500</td>
<td>-5.46837300</td>
<td>-0.19228600</td>
</tr>
<tr>
<td>H</td>
<td>3.87007500</td>
<td>-5.92942700</td>
<td>0.78707400</td>
</tr>
<tr>
<td>C</td>
<td>5.61176600</td>
<td>2.85626600</td>
<td>-0.01309700</td>
</tr>
<tr>
<td>H</td>
<td>6.71848000</td>
<td>-2.35058000</td>
<td>-1.11110100</td>
</tr>
<tr>
<td>C</td>
<td>6.53464000</td>
<td>-4.45521600</td>
<td>-0.71466500</td>
</tr>
<tr>
<td>H</td>
<td>2.67530200</td>
<td>4.98471600</td>
<td>1.19537600</td>
</tr>
</tbody>
</table>
(8) XYZ coordinates of UDFT optimized $T_1$ geometry for complex 4

<table>
<thead>
<tr>
<th>Element</th>
<th>X</th>
<th>Y</th>
<th>Z</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cu</td>
<td>1.57735800</td>
<td>0.75358400</td>
<td>0.19465800</td>
</tr>
<tr>
<td>Cu</td>
<td>-1.57734400</td>
<td>-0.75368500</td>
<td>-0.19465600</td>
</tr>
<tr>
<td>Cu</td>
<td>-0.76954800</td>
<td>2.24482500</td>
<td>0.01052800</td>
</tr>
<tr>
<td>Cu</td>
<td>0.76961100</td>
<td>-2.24495300</td>
<td>-0.01051800</td>
</tr>
<tr>
<td>I</td>
<td>1.42008000</td>
<td>3.40012200</td>
<td>0.69597500</td>
</tr>
<tr>
<td>I</td>
<td>-1.42001200</td>
<td>-3.40025200</td>
<td>-0.69601400</td>
</tr>
<tr>
<td>I</td>
<td>0.05475000</td>
<td>0.46589900</td>
<td>-2.09659600</td>
</tr>
<tr>
<td>I</td>
<td>-0.05471800</td>
<td>-0.46601800</td>
<td>2.09660000</td>
</tr>
<tr>
<td>N</td>
<td>-2.69677000</td>
<td>1.85669900</td>
<td>0.04781100</td>
</tr>
<tr>
<td>N</td>
<td>3.07682700</td>
<td>-0.57807100</td>
<td>-0.09928300</td>
</tr>
<tr>
<td>C</td>
<td>7.28980100</td>
<td>4.38330000</td>
<td>-0.41518500</td>
</tr>
<tr>
<td>N</td>
<td>6.59739500</td>
<td>3.10949400</td>
<td>-0.41916800</td>
</tr>
<tr>
<td>H</td>
<td>8.36434600</td>
<td>4.21718100</td>
<td>-0.51413800</td>
</tr>
<tr>
<td>H</td>
<td>7.09779600</td>
<td>4.93698100</td>
<td>0.51123600</td>
</tr>
<tr>
<td>H</td>
<td>6.95390800</td>
<td>4.98485300</td>
<td>-1.26224100</td>
</tr>
<tr>
<td>C</td>
<td>7.19266700</td>
<td>1.99096500</td>
<td>0.10612400</td>
</tr>
<tr>
<td>C</td>
<td>6.51682100</td>
<td>0.81019800</td>
<td>0.21349000</td>
</tr>
<tr>
<td>H</td>
<td>8.22011200</td>
<td>2.10919300</td>
<td>0.42922200</td>
</tr>
<tr>
<td>C</td>
<td>5.16447900</td>
<td>0.69971300</td>
<td>-0.19901200</td>
</tr>
<tr>
<td>H</td>
<td>7.02945900</td>
<td>-0.04204600</td>
<td>0.64553400</td>
</tr>
<tr>
<td>C</td>
<td>4.58657400</td>
<td>1.86941000</td>
<td>-0.75300100</td>
</tr>
<tr>
<td>C</td>
<td>4.43205500</td>
<td>-0.53350600</td>
<td>-0.08256700</td>
</tr>
<tr>
<td>C</td>
<td>5.29404600</td>
<td>3.03197400</td>
<td>-0.84113500</td>
</tr>
<tr>
<td>H</td>
<td>3.56986900</td>
<td>1.85356400</td>
<td>-1.12814600</td>
</tr>
<tr>
<td>H</td>
<td>4.86894600</td>
<td>3.94069200</td>
<td>-1.25024200</td>
</tr>
<tr>
<td>C</td>
<td>4.92456500</td>
<td>-1.84536700</td>
<td>0.00586600</td>
</tr>
<tr>
<td>C</td>
<td>3.78985400</td>
<td>-2.65110800</td>
<td>0.01055900</td>
</tr>
<tr>
<td>H</td>
<td>5.95456500</td>
<td>-2.17057100</td>
<td>-0.01932000</td>
</tr>
<tr>
<td>N</td>
<td>2.69683100</td>
<td>-1.85676200</td>
<td>-0.04782300</td>
</tr>
<tr>
<td>C</td>
<td>3.69179900</td>
<td>-4.11278900</td>
<td>0.05128800</td>
</tr>
<tr>
<td>C</td>
<td>4.62816200</td>
<td>-4.86145400</td>
<td>0.77522100</td>
</tr>
</tbody>
</table>
C 2.67437600 -4.78962300 -0.63352600
C 4.54460800 -6.24830900 0.81982600
H 5.41149100 -4.34448400 1.32277900
C 3.52038200  6.91125100 0.14682100
H 5.27590300  8.13633400 1.39089500
C 2.58556100  6.17658600 -0.57808400
H 3.52729000 -7.99467400 0.18612600
H 4.54460800 -6.24830900 0.81982600
C -2.67437600  6.17658600 -0.57808400
H -3.52038200  8.13633400 1.39089500
H -4.54460800 -6.24830900 0.81982600
C -3.78972800  2.65110500 0.09930400
H -3.52038200 -2.64830900 0.81982600
C -4.54460800 -6.24830900 0.81982600
N -3.07682400  3.57802500 0.09930400
C -3.78972800  2.65110500 0.09930400
H -3.52038200 -2.64830900 0.81982600
C -4.54460800 -6.24830900 0.81982600
C -3.78972800  2.65110500 0.09930400
H -3.52038200 -2.64830900 0.81982600
C -4.54460800 -6.24830900 0.81982600
N -6.59812500  3.10895500 0.41998400
H -3.45191400  7.99458100 -0.18736500
C -7.19311800 -1.99045500 -0.10567100
H -7.02947200  0.04239100  0.64155800
H -5.27553000  6.81360900 -1.39150000
C -7.29078500 -4.38262500  0.41628700
H -8.22055900  2.10856400  0.22883000
H -8.36530900 -4.21626600  0.51507500
H -7.09878600 -4.93660200  0.50995800
H -9.55104000 -4.98400600  1.26354900