# Electronic Supplementary Information: Thermally Activated Delayed Fluorescence of a Ir(III) Complex: Absorption and Emission Properties, Nonradiative Rates, and Mechanism

Ling-Ya Peng#, Zi-Wen Li#, Guang-Ning Pan, Wen-Kai Chen, Yuan-Jun Gao* and Ganglong Cui*

Key Laboratory of Theoretical and Computational Photochemistry, Ministry of Education, College of Chemistry, Beijing Normal University, Beijing 100875, China.

E-mail: yuanjun.gao@mail.bnu.edu.cn and ganglong.cui@bnu.edu.cn

## Table of content

**I Tables**

8. **Table S8** Calculated Forward and Reverse Intersystem Crossing Rates at Different Temperatures.

**II Figures**

9. **Fig. S1** Selected geometric parameters at the $T_2$ minima of the Ir(III) complex in toluene solution.
10. **Fig. S2** Spatial overlap of the optimized $S_0$, $S_1$, $T_1$ and $T_2$ structures in solution.
11. **Fig. S3** Geometric modifications between $S_1$, $T_1$, $T_2$ and $S_0$.
12. **Fig. S4** Duschinsky matrices of the Ir(III) complex in the forward and reverse intersystem crossing processes.
13. **Fig. S5** Calculated Huang-Rhys factor of each vibrational mode of the Ir(III) complex for the forward and reverse intersystem crossing processes in solution.

**III Cartesian Coordinates of Optimized Structures**

## I Tables

**Table S1** Selected Geometric Parameters of the Ir(III) Complex at the $S_0$, $S_1$, $T_1$ and $T_2$ Minima.

| **Bond Length (Å)** | **Exp.** | **$S_0$** | **$S_1$** | **$T_1$** | **$T_2$** |
|---|---|---|---|---|---|
| Ir-C9 | 1.928 | 1.920 | 1.955 | 1.933 | 1.938 |
| Ir-C6 | 2.071 | 2.075 | 2.061 | 2.065 | 2.070 |
| Ir-C1 | 2.070 | 2.075 | 2.061 | 2.065 | 2.070 |
| Ir-N1 | 2.069 | 2.086 | 2.120 | 2.141 | 2.138 |
| Ir-N2 | 2.049 | 2.056 | 2.065 | 2.067 | 2.059 |
| Ir-N3 | 2.049 | 2.056 | 2.081 | 2.076 | 2.060 |
| **Bond Angle (°)** | **Exp.** | **$S_0$** | **$S_1$** | **$T_1$** | **$T_2$** |
| C1-Ir-N1 | 79.2 | 78.6 | 76.6 | 75.8 | 75.9 |
| C1-Ir-C6 | 158.2 | 157.3 | 150.6 | 150.7 | 151.8 |
| N2-Ir-N3 | 160.1 | 159.5 | 160.3 | 161.1 | 160.6 |
| N2-Ir-C9 | 79.9 | 79.8 | 80.1 | 80.3 | 80.2 |
| C1-Ir-C9 | 102.2 | 101.4 | 103.7 | 104.3 | 104.6 |
| N1-Ir-N2 | 104.4 | 100.2 | 97.3 | 96.9 | 99.0 |
| N1-Ir-C9 | 175.6 | 179.9 | 177.5 | 177.7 | 179.2 |
| **Torsion Angle (°)** | **Exp.** | **$S_0$** | **$S_1$** | **$T_1$** | **$T_2$** |
| C1-C2-C3-N1 | 6.6 | 0.0 | 0.8 | 1.5 | 0.6 |
| C2-C3-N1-C4 | 176.8 | -180.0 | 177.2 | 178.6 | 179.8 |
| N2-C7-C8-C9 | 0.9 | 0.2 | -0.0 | -0.2 | 0.5 |
| C7-C8-C9-C10 | 179.0 | -180.0 | 180.0 | 179.9 | -179.6 |
| C8-C9-Ir-C6 | -91.6 | -89.9 | -84.2 | -86.3 | -88.9 |
| C3-N1-Ir-N2 | 92.8 | 90.0 | 92.1 | 92.2 | 90.6 |
| C3-N1-Ir-N3 | -89.1 | -90.0 | -87.9 | -87.8 | -89.6 |
| C1-C9-Ir-N1 | 73.9 | 179.9 | 95.4 | 93.4 | 126.3 |

**Table S2** Calculated Energies of the $S_1$ and $T_1$ Minima (kcal/mol) Relative to the $S_0$ Minimum at M11-L/6-31G*&SDD(Ir) level.

| $S_1$ | $T_1$ |
|---|---|
| 55.1 | 51.1 |

**Table S3** Calculated Energy Gaps between the $S_2$ State and the $S_1$, $T_1$ and $T_2$ States ($\Delta E_{S2\text{-}S1}$, $\Delta E_{S2\text{-}T1}$, $\Delta E_{S2\text{-}T2}$) at the $S_0$, $S_1$, and $T_1$ Minima in Solution Computed at MS-CASPT2/PCM level.

| | $\Delta E_{S2\text{-}S1}$ | | $\Delta E_{S2\text{-}T1}$ | | $\Delta E_{S2\text{-}T2}$ | |
|---|---|---|---|---|---|---|
| | kcal/mol | eV | kcal/mol | eV | kcal/mol | eV |
| **At $S_0$-Min** | 16.0 | 0.69 | 15.9 | 0.69 | 13.0 | 0.56 |
| **At $S_1$-Min** | 13.9 | 0.60 | 14.8 | 0.64 | 6.8 | 0.29 |
| **At $T_1$-Min** | 16.1 | 0.70 | 16.2 | 0.70 | 7.4 | 0.32 |

**Table S4** Calculated Vertical Excitation Energies ($E_\perp$), Wavelength ($\lambda$), Main Electronic Configurations of the Ir(III) Complex in Solution.

| **MS-CASPT2** | **$E_\perp$ (kcal/mol)** | **$E_\perp$ (eV)** | **$\lambda$ (nm)** | ***f*** | **Configurations** |
|---|---|---|---|---|---|
| $S_1$ | 60.9 | 2.64 | 470 | 0.1544 | $d_2$ -> $\pi_3$* (77.9%) |
| $S_2$ | 76.9 | 3.33 | 372 | 0.1192 | $d_2$ -> $\pi_4$* (85.9%) |
| $S_3$ | 82.4 | 3.57 | 347 | 0.0177 | $d_3$ -> $\pi_3$* (90.0%) |
| $S_4$ | 95.6 | 4.15 | 299 | 0.0106 | $d_3$ -> $\pi_4$* (93.5%) |
| $S_5$ | 96.9 | 4.20 | 295 | 0.0000 | $d_1$ -> $\pi_3$* (94.7%) |
| $S_6$ | 106.6 | 4.62 | 268 | 0.0000 | $d_1$ -> $\pi_4$* (95.5%) |
| $S_7$ | 107.9 | 4.68 | 265 | 0.0378 | $\pi_1$ -> $\pi_3$* (66.3%)<br>$d_2$ -> $\pi_3$* (14.6%) |

**Table S5** Calculated Vertical Emission Energies ($E_\perp$), Wavelengths (λ), Oscillator Strengths (ƒ), and Electronic Configurations at the $S_1$ and $T_1$ Minima in Solution.

| | **$S_1$** | | | | |
|---|---|---|---|---|---|
| | **$E_\perp$ (kcal/mol)** | **$E_\perp$ (eV)** | **λ (nm)** | **ƒ** | **Configurations** |
| **MS-CASPT2** | 57.0 | 2.47 | 501 | 0.1080 | $d_2$ -> $\pi_3$* (82.7%) |
| **Exp.** | 53.2 | 2.31 | 537 | | |
| | **$T_1$** | | | | |
| | **$E_\perp$ (kcal/mol)** | **$E_\perp$ (eV)** | **λ (nm)** | **ƒ** | **Configurations** |
| **MS-CASPT2** | 55.0 | 2.38 | 520 | 0.0000 | $d_2$ -> $\pi_3$* (79.5%) |
| **Exp.** | 52.9 | 2.30 | 540 | | |

**Table S6** Calculated Spin-Orbit Couplings (SOCs) and Reorganization Energy ($\lambda_{reog}$) in the Forward and Reverse Intersystem Crossing Processes.

| | **$S_1$ -> $T_1$** | **$T_1$ -> $S_1$** |
|---|---|---|
| **SOC ($cm^{-1}$)** | 45.43 | 34.68 |
| **$\lambda_{reog}$ (eV)** | 0.04 | 0.02 |

**Table S7** Calculated Spin-Orbit Couplings (SOCs) using Different Software and Corresponding (Reverse) Intersystem Crossing Rates ($k_{(r)ISC}$).

| | | SOC ($S_1$, $cm^{-1}$) | SOC ($T_1$, $cm^{-1}$) | $k_{ISC}$ ($s^{-1}$) | $k_{rISC}$ ($s^{-1}$) |
|---|---|---|---|---|---|
| **M11-L/TZP** | **ADF** | 45.43 | 34.68 | $4.86x10^{11}$ | $2.29x10^{9}$ |
| **M06/ DKH-def2-TZVP& SARC-DKH-TZVP(Ir)** | **ORCA** | 74.67 | 41.81 | $1.31x10^{12}$ | $3.33x10^{9}$ |
| **B3LYP/ DKH-def2-TZVP& SARC-DKH-TZVP(Ir)** | **ORCA** | 86.42 | 50.91 | $1.76x10^{12}$ | $4.93x10^{9}$ |
| **M11-L/ 6-31G*&SDD(Ir)** | **PySOC** | 61.73 | 41.87 | $9.27x10^{11}$ | $3.34x10^{9}$ |

**Note:** For SOC calculations with MS-CASPT2, the present OPENMOLCAS version does not support the combination of using the atomic mean-field approximation and the effective core potential. The present work started two years ago, when our ADF license is valid. However, we did not extend the ADF license because we prefer using free ORCA now (see our recent works, refs. 31-32). Unfortunately, the latest ORCA does not support the M11-L functional. Instead, we checked SOC using ORCA with several functionals, which give similar values (same order of the magnitude). Importantly, with PySOC, the same M11-L functional gave much close results (see Table S7).

**Table S8** Temperature Dependence of the (Reverse) Intersystem Crossing Rates ($k_{(r)ISC}$).

| | **77 K** | **100 K** | **150 K** | **200 K** | **250 K** | **300 K** |
|---|---|---|---|---|---|---|
| $k_{ISC(S1-T1)}$ | $3.36x10^{11}$ | $3.53x10^{11}$ | $4.00x10^{11}$ | $4.42x10^{11}$ | $4.72x10^{11}$ | $4.86x10^{11}$ |
| $k_{rISC(T1-S1)}$ | $2.22x10^{3}$ | $2.59x10^{5}$ | $2.41x10^{7}$ | $2.38x10^{8}$ | $9.36x10^{8}$ | $2.29x10^{9}$ |

## II Figures

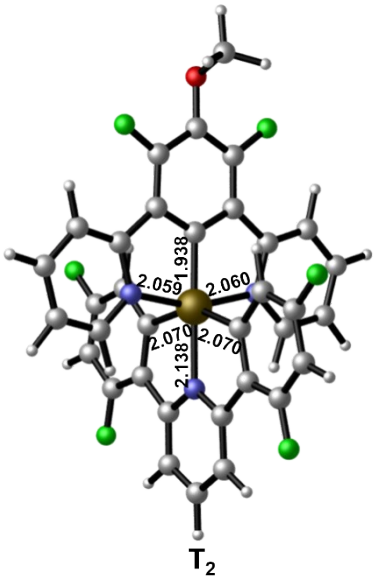


**Fig. S1** Selected geometric parameters of the $T_2$ minimum of the Ir(III) complex in toluene solution.

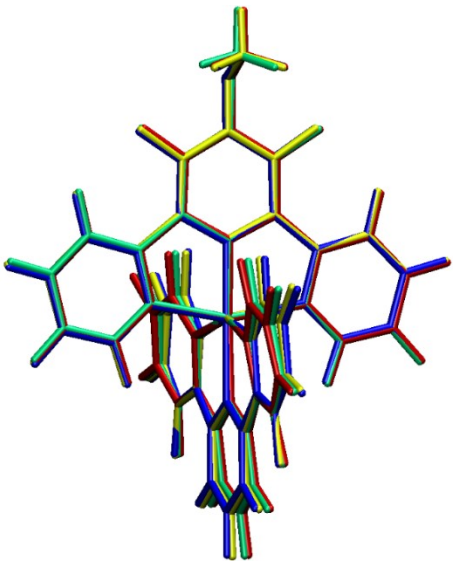

**Fig. S2** Spatial overlap of the optimized $S_0$ (blue), $S_1$ (red), $T_1$ (green) and $T_2$ (yellow) structures in solution.

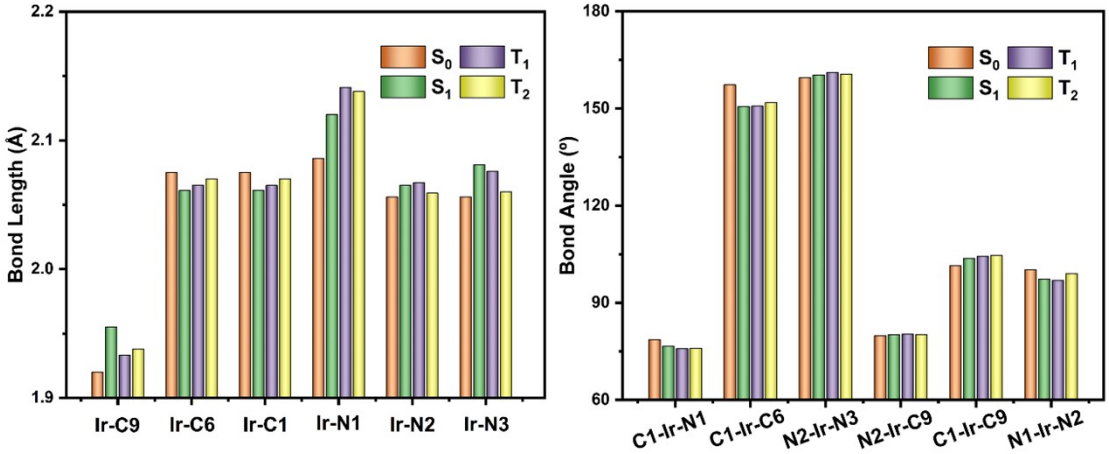


**Fig. S3** Geometric changes including (left) bond lengths (in Å) of Ir-C9, Ir-C6, Ir-C1, Ir-N1, Ir-N2 and Ir-N3; and (right) angles of C1-Ir-N1, C1-Ir-C6, N2-Ir-N3, N2-Ir-C9, C1-Ir-C9 and N1-Ir-N2 between $S_1$, $T_1$, $T_2$ and $S_0$.

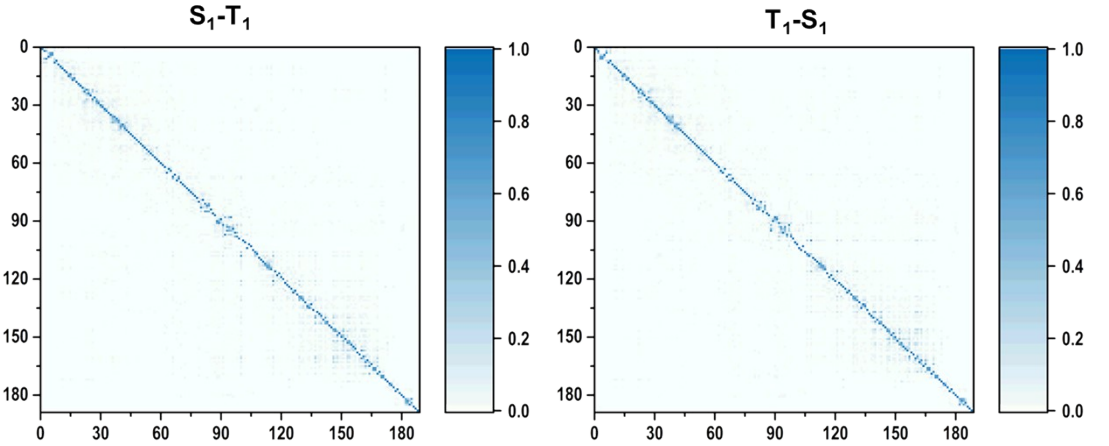


**Fig. S4** Duschinsky matrices of the Ir(III) complex for the (left) forward and (right) reverse intersystem crossing processes.

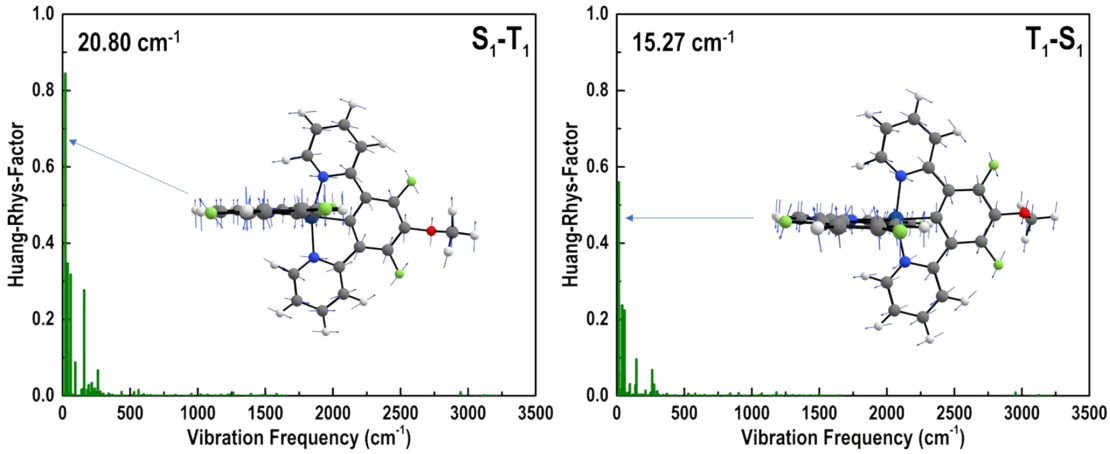


**Fig. S5** Calculated Huang-Rhys factor of each vibrational mode of the Ir(III) complex for the (left) forward and (right) reverse intersystem crossing processes in solution.

## III Cartesian Coordinates of Optimized Structures

$S_0$.xyz

| | | | |
|---|---|---|---|
| C | -2.135288000 | -4.529926000 | -0.000021000 |
| C | -0.765833000 | -4.370657000 | -0.000019000 |
| C | -2.899003000 | -3.387089000 | -0.000017000 |
| C | -2.354662000 | -2.105702000 | -0.000010000 |
| C | -0.164135000 | -3.130040000 | -0.000013000 |
| C | -0.937723000 | -1.975754000 | -0.000009000 |
| C | -3.143773000 | -0.874934000 | -0.000006000 |
| C | -4.530577000 | -0.744013000 | -0.000001000 |
| N | -2.381713000 | 0.230533000 | -0.000005000 |
| C | -2.884285000 | 1.475593000 | 0.000001000 |
| C | -4.266049000 | 1.650548000 | 0.000006000 |
| C | -5.069797000 | 0.527335000 | 0.000005000 |
| C | -1.845559000 | 2.504644000 | 0.000002000 |
| C | -0.491180000 | 2.068936000 | 0.000002000 |
| C | -2.097770000 | 3.873720000 | 0.000002000 |
| C | -1.103562000 | 4.822945000 | 0.000002000 |
| C | 0.198183000 | 4.369336000 | 0.000002000 |
| C | 0.515090000 | 3.027387000 | 0.000002000 |
| F | -0.015125000 | -5.458811000 | -0.000024000 |
| F | -4.216525000 | -3.559888000 | -0.000019000 |
| F | 1.168135000 | 5.268267000 | 0.000002000 |
| F | -3.345805000 | 4.329794000 | 0.000001000 |
| C | 0.765374000 | -0.115541000 | 4.690751000 |
| C | -0.561559000 | 0.028527000 | 4.320782000 |
| C | 1.728495000 | -0.219616000 | 3.712414000 |
| C | 1.365541000 | -0.180049000 | 2.369237000 |
| N | 0.054366000 | -0.038024000 | 2.023417000 |
| C | -0.863339000 | 0.061028000 | 2.978270000 |
| C | 2.259288000 | -0.275010000 | 1.235855000 |
| C | 3.637090000 | -0.421861000 | 1.200134000 |
| C | 1.599795000 | -0.205594000 | 0.000004000 |
| C | 2.259297000 | -0.275002000 | -1.235842000 |
| C | 3.637099000 | -0.421854000 | -1.200112000 |
| C | 4.332891000 | -0.500764000 | 0.000014000 |
| C | 1.365558000 | -0.180036000 | -2.369230000 |
| C | 1.728522000 | -0.219595000 | -3.712405000 |
| N | 0.054381000 | -0.038013000 | -2.023417000 |
| C | -0.863318000 | 0.061043000 | -2.978276000 |
| C | -0.561529000 | 0.028550000 | -4.320787000 |
| C | 0.765407000 | -0.115514000 | -4.690747000 |
| H | 1.050084000 | -0.146605000 | -5.746449000 |

| | | | |
|---|---|---|---|
| Ir | -0.308530000 | 0.002053000 | -0.000002000 |
| H | -1.361367000 | 0.114979000 | -5.058580000 |
| F | 4.360623000 | -0.496410000 | 2.302815000 |
| F | 4.360640000 | -0.496397000 | -2.302787000 |
| O | 5.663713000 | -0.706218000 | 0.000018000 |
| C | 6.393676000 | 0.486937000 | 0.000026000 |
| H | -2.600794000 | -5.515236000 | -0.000027000 |
| H | 0.930225000 | -3.079075000 | -0.000012000 |
| H | -5.177894000 | -1.618354000 | -0.000001000 |
| H | -4.707335000 | 2.644863000 | 0.000011000 |
| H | -6.158073000 | 0.647602000 | 0.000009000 |
| H | -1.343285000 | 5.885921000 | 0.000002000 |
| H | 1.571959000 | 2.738371000 | 0.000002000 |
| H | 1.050043000 | -0.146638000 | 5.746454000 |
| H | -1.361402000 | 0.114952000 | 5.058570000 |
| H | 2.779917000 | -0.335332000 | 3.977148000 |
| H | -1.894350000 | 0.172538000 | 2.625136000 |
| H | 2.779945000 | -0.335308000 | -3.977132000 |
| H | -1.894331000 | 0.172550000 | -2.625148000 |
| H | 6.179219000 | 1.092084000 | 0.899335000 |
| H | 6.179224000 | 1.092092000 | -0.899280000 |
| H | 7.454400000 | 0.203949000 | 0.000028000 |

$S_1$.xyz

| | | | |
|---|---|---|---|
| C | -2.045930000 | -4.510001000 | -0.294442000 |
| C | -0.693179000 | -4.286128000 | -0.451139000 |
| C | -2.854643000 | -3.415603000 | -0.104254000 |
| C | -2.364684000 | -2.114328000 | -0.054161000 |
| C | -0.138595000 | -3.022292000 | -0.419310000 |
| C | -0.969545000 | -1.940201000 | -0.180042000 |
| C | -3.166498000 | -0.908033000 | 0.075639000 |
| C | -4.548559000 | -0.804408000 | 0.203136000 |
| N | -2.414760000 | 0.200037000 | 0.034314000 |
| C | -2.942832000 | 1.430341000 | 0.078959000 |
| C | -4.319332000 | 1.590224000 | 0.207562000 |
| C | -5.106188000 | 0.457055000 | 0.277079000 |
| C | -1.927142000 | 2.463268000 | -0.049883000 |
| C | -0.590382000 | 2.028193000 | -0.177470000 |
| C | -2.162574000 | 3.833618000 | -0.100340000 |
| C | -1.162204000 | 4.755693000 | -0.293294000 |
| C | 0.123514000 | 4.280036000 | -0.451755000 |
| C | 0.429338000 | 2.934328000 | -0.418914000 |
| F | 0.089430000 | -5.328319000 | -0.637392000 |

| | | | |
|---|---|---|---|
| F | -4.152393000 | -3.641874000 | 0.025915000 |
| F | 1.089066000 | 5.155623000 | -0.640527000 |
| F | -3.393913000 | 4.301189000 | 0.031553000 |
| C | 0.584604000 | -0.098018000 | 4.776578000 |
| C | -0.736821000 | 0.036857000 | 4.374794000 |
| C | 1.582626000 | -0.195656000 | 3.834859000 |
| C | 1.270820000 | -0.160393000 | 2.472085000 |
| N | -0.041763000 | -0.029663000 | 2.099583000 |
| C | -0.988485000 | 0.064106000 | 3.017631000 |
| C | 2.211838000 | -0.247431000 | 1.385538000 |
| C | 3.617664000 | -0.379033000 | 1.426913000 |
| C | 1.639518000 | -0.188002000 | 0.121472000 |
| C | 2.328243000 | -0.246337000 | -1.093081000 |
| C | 3.723062000 | -0.381445000 | -0.981344000 |
| C | 4.351471000 | -0.450497000 | 0.258079000 |
| C | 1.489359000 | -0.163708000 | -2.249902000 |
| C | 1.903593000 | -0.195925000 | -3.589192000 |
| N | 0.138145000 | -0.040223000 | -1.981050000 |
| C | -0.729240000 | 0.043032000 | -2.973984000 |
| C | -0.373187000 | 0.015820000 | -4.303714000 |
| C | 0.989562000 | -0.107812000 | -4.605927000 |
| H | 1.326136000 | -0.134144000 | -5.646806000 |
| Ir | -0.304215000 | -0.001863000 | 0.035184000 |
| H | -1.138450000 | 0.089053000 | -5.077150000 |
| F | 4.282117000 | -0.438136000 | 2.579818000 |
| F | 4.503310000 | -0.453508000 | -2.059216000 |
| O | 5.686666000 | -0.629255000 | 0.322479000 |
| C | 6.393028000 | 0.572026000 | 0.232619000 |
| H | -2.465220000 | -5.515146000 | -0.332717000 |
| H | 0.941628000 | -2.907264000 | -0.548916000 |
| H | -5.176356000 | -1.692797000 | 0.239537000 |
| H | -4.767657000 | 2.581153000 | 0.248367000 |
| H | -6.190654000 | 0.560467000 | 0.381180000 |
| H | -1.384343000 | 5.821822000 | -0.332134000 |
| H | 1.467724000 | 2.616476000 | -0.550925000 |
| H | 0.838687000 | -0.126892000 | 5.840995000 |
| H | -1.558742000 | 0.118240000 | 5.087008000 |
| H | 2.624242000 | -0.302498000 | 4.137988000 |
| H | -2.009412000 | 0.167575000 | 2.631297000 |
| H | 2.968501000 | -0.293989000 | -3.807156000 |
| H | -1.779138000 | 0.138116000 | -2.668896000 |
| H | 6.126815000 | 1.258212000 | 1.057511000 |
| H | 6.209648000 | 1.081053000 | -0.730823000 |
| H | 7.458590000 | 0.316124000 | 0.306619000 |

$T_1$.xyz

| | | | |
|---|---|---|---|
| C | -2.045014000 | -4.519597000 | -0.259095000 |
| C | -0.686561000 | -4.297218000 | -0.340372000 |
| C | -2.859548000 | -3.420768000 | -0.131522000 |
| C | -2.370834000 | -2.118932000 | -0.075266000 |
| C | -0.132592000 | -3.032659000 | -0.297024000 |
| C | -0.975249000 | -1.943795000 | -0.141496000 |
| C | -3.173932000 | -0.911097000 | 0.016767000 |
| C | -4.558398000 | -0.811663000 | 0.112312000 |
| N | -2.419677000 | 0.196370000 | -0.010454000 |
| C | -2.956039000 | 1.423672000 | 0.034780000 |
| C | -4.334986000 | 1.580753000 | 0.131289000 |
| C | -5.121851000 | 0.447089000 | 0.174632000 |
| C | -1.943243000 | 2.463445000 | -0.040987000 |
| C | -0.604265000 | 2.033935000 | -0.111721000 |
| C | -2.182830000 | 3.833789000 | -0.079100000 |
| C | -1.179304000 | 4.764787000 | -0.194514000 |
| C | 0.114427000 | 4.296093000 | -0.282453000 |
| C | 0.424900000 | 2.950540000 | -0.255837000 |
| F | 0.107297000 | -5.340652000 | -0.465608000 |
| F | -4.163042000 | -3.643437000 | -0.068421000 |
| F | 1.087867000 | 5.176346000 | -0.397232000 |
| F | -3.422548000 | 4.293014000 | -0.010144000 |
| C | 0.543496000 | -0.143563000 | 4.762831000 |
| C | -0.779036000 | 0.001535000 | 4.342845000 |
| C | 1.547904000 | -0.232573000 | 3.831588000 |
| C | 1.253163000 | -0.179776000 | 2.464350000 |
| N | -0.060794000 | -0.042728000 | 2.074638000 |
| C | -1.014312000 | 0.043167000 | 2.985469000 |
| C | 2.199531000 | -0.254306000 | 1.387801000 |
| C | 3.599431000 | -0.378457000 | 1.425816000 |
| C | 1.634625000 | -0.183112000 | 0.109514000 |
| C | 2.337177000 | -0.229175000 | -1.100729000 |
| C | 3.731765000 | -0.364725000 | -0.989246000 |
| C | 4.344853000 | -0.435860000 | 0.255324000 |
| C | 1.508587000 | -0.138807000 | -2.266032000 |
| C | 1.939396000 | -0.153536000 | -3.599440000 |
| N | 0.162562000 | -0.025996000 | -2.006603000 |
| C | -0.699402000 | 0.060875000 | -3.002599000 |
| C | -0.330089000 | 0.047926000 | -4.331770000 |
| C | 1.030061000 | -0.060950000 | -4.622563000 |
| H | 1.374862000 | -0.073091000 | -5.661052000 |
| Ir | -0.287738000 | -0.003015000 | 0.011089000 |
| H | -1.089002000 | 0.122210000 | -5.111361000 |

| | | | |
|---|---|---|---|
| F | 4.266205000 | -0.428382000 | 2.576719000 |
| F | 4.515018000 | -0.460112000 | -2.065290000 |
| O | 5.674494000 | -0.609755000 | 0.348612000 |
| C | 6.401467000 | 0.558211000 | 0.095474000 |
| H | -2.463082000 | -5.524940000 | -0.302123000 |
| H | 0.953439000 | -2.925107000 | -0.366343000 |
| H | -5.182875000 | -1.702511000 | 0.137498000 |
| H | -4.784151000 | 2.571069000 | 0.172096000 |
| H | -6.208707000 | 0.547812000 | 0.254237000 |
| H | -1.404475000 | 5.830455000 | -0.223797000 |
| H | 1.472183000 | 2.644576000 | -0.329544000 |
| H | 0.784597000 | -0.186527000 | 5.829409000 |
| H | -1.609473000 | 0.078326000 | 5.045392000 |
| H | 2.586479000 | -0.346667000 | 4.144664000 |
| H | -2.031930000 | 0.152424000 | 2.590883000 |
| H | 3.006269000 | -0.240702000 | -3.809499000 |
| H | -1.751451000 | 0.146432000 | -2.703928000 |
| H | 6.137640000 | 1.354038000 | 0.815281000 |
| H | 6.237427000 | 0.929802000 | -0.930757000 |
| H | 7.460486000 | 0.296587000 | 0.218770000 |

$T_2$.xyz

| | | | |
|---|---|---|---|
| C | 2.077384000 | -4.537796000 | 0.161994000 |
| C | 0.715979000 | -4.327845000 | 0.217548000 |
| C | 2.885077000 | -3.430193000 | 0.070166000 |
| C | 2.387197000 | -2.131049000 | 0.030650000 |
| C | 0.153123000 | -3.067033000 | 0.184989000 |
| C | 0.991216000 | -1.968999000 | 0.086875000 |
| C | 3.179311000 | -0.915313000 | -0.056835000 |
| C | 4.563970000 | -0.807487000 | -0.135453000 |
| N | 2.415602000 | 0.187174000 | -0.055858000 |
| C | 2.945809000 | 1.417002000 | -0.124869000 |
| C | 4.324764000 | 1.581066000 | -0.205394000 |
| C | 5.120534000 | 0.453295000 | -0.210828000 |
| C | 1.928571000 | 2.455623000 | -0.102503000 |
| C | 0.591798000 | 2.024904000 | -0.026737000 |
| C | 2.160707000 | 3.827295000 | -0.143888000 |
| C | 1.150557000 | 4.758132000 | -0.111407000 |
| C | -0.142760000 | 4.287824000 | -0.032224000 |
| C | -0.445932000 | 2.941292000 | 0.013421000 |
| F | -0.072573000 | -5.380343000 | 0.305205000 |
| F | 4.191195000 | -3.643547000 | 0.020945000 |
| F | -1.124183000 | 5.167747000 | 0.000495000 |

| | | | |
|---|---|---|---|
| F | 3.399254000 | 4.290545000 | -0.216541000 |
| C | -0.875176000 | -0.258749000 | -4.675441000 |
| C | 0.467235000 | -0.132649000 | -4.323379000 |
| C | -1.818846000 | -0.309609000 | -3.652239000 |
| C | -1.425420000 | -0.236919000 | -2.334343000 |
| N | -0.094866000 | -0.112953000 | -2.004324000 |
| C | 0.806516000 | -0.064739000 | -2.996425000 |
| C | -2.300549000 | -0.279747000 | -1.168902000 |
| C | -3.678346000 | -0.384145000 | -1.103809000 |
| C | -1.640971000 | -0.197779000 | 0.061723000 |
| C | -2.253275000 | -0.209772000 | 1.319258000 |
| C | -3.632078000 | -0.318626000 | 1.312356000 |
| C | -4.346324000 | -0.409583000 | 0.119095000 |
| C | -1.332736000 | -0.101505000 | 2.444421000 |
| C | -1.671589000 | -0.100010000 | 3.779254000 |
| N | -0.017272000 | 0.004537000 | 2.053021000 |
| C | 0.924436000 | 0.110378000 | 3.002834000 |
| C | 0.639660000 | 0.116593000 | 4.344142000 |
| C | -0.686913000 | 0.008820000 | 4.758610000 |
| H | -0.952909000 | 0.008945000 | 5.817394000 |
| Ir | 0.289074000 | -0.022573000 | 0.017537000 |
| H | 1.458360000 | 0.205463000 | 5.062297000 |
| F | -4.436503000 | -0.463670000 | -2.180541000 |
| F | -4.348828000 | -0.341467000 | 2.420188000 |
| O | -5.676444000 | -0.573664000 | 0.146617000 |
| C | -6.378938000 | 0.639499000 | 0.170183000 |
| H | 2.503004000 | -5.540427000 | 0.191250000 |
| H | -0.935200000 | -2.968303000 | 0.233086000 |
| H | 5.193898000 | -1.694771000 | -0.138361000 |
| H | 4.766618000 | 2.573638000 | -0.263742000 |
| H | 6.207866000 | 0.560247000 | -0.275077000 |
| H | 1.370423000 | 5.824727000 | -0.145620000 |
| H | -1.493780000 | 2.633307000 | 0.074951000 |
| H | -1.184963000 | -0.316113000 | -5.720740000 |
| H | 1.255862000 | -0.086640000 | -5.078169000 |
| H | -2.879945000 | -0.409868000 | -3.885191000 |
| H | 1.849683000 | 0.033781000 | -2.677045000 |
| H | -2.722200000 | -0.187666000 | 4.060544000 |
| H | 1.952823000 | 0.192521000 | 2.634591000 |
| H | -6.167145000 | 1.241998000 | -0.730748000 |
| H | -6.130118000 | 1.230155000 | 1.069342000 |
| H | -7.444600000 | 0.379415000 | 0.190911000 |