Supporting Information for

Excited State Lifetime Modulation by Twisted and Tilted Molecular Design in Carbene-Metal-Amide Photoemitters

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NMR spectroscopy.
2-chloro-6-fluoro-N-(2-fluorophenyl)aniline.

\(^1\)H NMR (300 MHz, CDCl\(_3\))
$^{13}$C($^1$H) NMR (75 MHz, CDCl$_3$)

$^{19}$F NMR (282 MHz, CDCl$_3$)
1,8-difluoro-9H-carbazole (S2)

$^1$H NMR (300 MHz, CDCl$_3$)
$^{13}\text{C}\{^{1}\text{H}\}$ NMR (75 MHz, CDCl$_3$)

$^{19}\text{F}\{^{1}\text{H}\}$ NMR (282 MHz, CDCl$_3$)
$(\Lambda^d\text{CAAC})\text{Au}(1,8\text{-difluorocarbazole})$ (1).

$^1\text{H NMR (300 MHz, CD}_2\text{Cl}_2)$
$^{13}$C{$^{1}$H} NMR (75 MHz, CD$_2$Cl$_2$)
$^{19}$F$\{1H\}$ NMR (282 MHz, CD$_2$Cl$_2$)
(AdCAAC)Cu(1,8-difluorocarbazole) (2).

$^1$H NMR (300 MHz, CD$_2$Cl$_2$)
$^{13}$C\{H\} NMR (75 MHz, CD$_2$Cl$_2$)
$^{19}$F NMR (282 MHz, CD$_2$Cl$_2$)
($^\text{AdCAAC}$)Au(1,3,6,8-tetramethylcarbazole).

$^1$H NMR (300 MHz, CD$_2$Cl$_2$)
$^{13}$C($^{1}$H) NMR (75 MHz, CD$_2$Cl$_2$)
(AdCAAC)Au(5,12-dihydro-5-phenyl-indolo[3,2-a]carbazole) (4)

$^1\text{H} \text{NMR (300 MHz, CD}_2\text{Cl}_2$)
$^{13}\text{C}$\textsuperscript{(H)} NMR (75 MHz, CD$_2$Cl$_2$)
**Figure S1.** VT NMR $^{19}$F (282 MHz) in DCM-d$_2$ for complex 2.

**Figure S2.** NMR $^1$H{$^{19}$F} (bottom left) and $^1$H (top left) in DCM-d$_2$ (282 MHz) for complex 2 at 20 °C and NMR $^{19}$F{$^1$H} (bottom right) and $^{19}$F (top right). The spin-splitting of protons $H_a$ and $H_b$ is caused by $^{19}$F atoms.
Figure S3. TGA curves for the complexes 1–4.
Electrochemistry.

Figure S4. Full range cyclic voltammogram for gold 1 and copper complex 2. Recorded using a glassy carbon electrode in THF solution (1.4 mM) with [n-Bu₄N]PF₆ as supporting electrolyte (0.13 M), scan rate 0.1 Vs⁻¹.

Figure S5. Full range cyclic voltammogram for the gold complex 3 and 4. Recorded using a glassy carbon electrode in THF solution (1.4 mM) with [n-Bu₄N]PF₆ as supporting electrolyte (0.13 M), scan rate 0.1 Vs⁻¹.

X-Ray Crystallography.

Complex 1 crystallizes with two independent molecules in the unit cell. The atoms C3, C26 and C27 were disordered over two half-populated positions for complex 1. The unit cell for monoclinic polymorph of complex 2 contains two independent molecules whereas triclinic polymorph of 2 contains three independent molecules and one 2-methyl-pentane molecules as a solvate. Further analysis of the residual electron density for the triclinic polymorph of 2 indicates the presence of two additional and severely disordered 2-methylpentane molecules which
contribution was removed from the diffraction data with PLATON/SQUEEZE for the final refinement.1,2 The unit cell for of complex 3·Benzene contains two independent molecules of 3 and two co-crystallized benzene molecules. The unit cell for of complex 3·CH₂Cl₂ contains one independent molecule of 3 and one co-crystallized CH₂Cl₂ molecule. Crystals were mounted in oil on glass fiber and fixed on the diffractometer in a cold nitrogen stream. Data were collected using an Oxford Diffraction Xcalibur-3/Sapphire3-CCD diffractometer with graphite monochromated Mo Kα radiation (λ = 0.71073 Å) at 140 K. Data were processed using the CrystAlisPro-CCD and –RED software.3 The structure was solved by direct methods and refined by the full-matrix least-squares against F² in an anisotropic (for non-hydrogen atoms) approximation. All hydrogen atom positions were refined in isotropic approximation in a “riding” model with the Uiso(H) parameters equal to 1.2 Ueq(Ci), for methyl groups equal to 1.5 Ueq(Cii), where U(Ci) and U(Cii) are respectively the equivalent thermal parameters of the carbon atoms to which the corresponding H atoms are bonded. All calculations were performed using the SHELXTL software.4

The principal crystallographic data and refinement parameters:

Crystals suitable for X-ray diffraction study were obtained by layering the CH₂Cl₂ solution of complex 1 hexanes at room temperature followed by cooling at -20 °C. CCDC number 1956198, C₃₀H₄₅AuF₂N₂, Orthorhombic, space group P2₁2₁2₁, a = 9.4894(3) Å, b = 15.5514(6) Å, c = 21.9698(7) Å, V = 3242.16(19) Å³, Z = 4, dcalc = 1.591 g cm⁻³, μ = 4.580 mm⁻¹, colourless/block, crystal size 0.36 × 0.24 × 0.20 mm, F(000) = 1560, Tmin/Tmax 0.36383/1.00000, R₁ = 0.0289 (from 7835 unique reflections with I>2σ(I); Rint = 0.0482, Rsigma = 0.0422) and wR₂ = 0.0603 (from all 37125 reflections), GOF = 1.019, Δρmin/Δρmax = 0.99/–0.88. Another crystallization attempt by layering the toluene solution resulted in identical unit cell parameters and no inclusion of the solvated molecules: C₃₀H₄₅AuF₂N₂, Orthorhombic, space group P2₁2₁2₁, a = 9.4987(4) Å, b = 15.459(1) Å, c = 21.9894(8) Å, V = 3229.1(3) Å³, Z = 4, dcalc = 1.598 g cm⁻³, μ = 4.598 mm⁻¹, colourless/block, crystal size 0.21 × 0.17 × 0.16 mm, F(000) = 1560, Tmin/Tmax 0.32107/1.00000, R₁ = 0.0802 (from 6351 unique reflections with I>2σ(I); Rint = 0.1391, Rsigma = 0.0422) and wR₂ = 0.1901 (from all 30781 reflections), GOF = 1.138, Δρmin/Δρmax = 2.66/–3.88.

Crystals of complex 2 suitable for X-ray diffraction study were obtained by cooling a saturated CH₂Cl₂:2-methylpentane (1:9) solution at -20 °C to give a triclinic polymorph. CCDC
number 2027574, C_{41}H_{49.5}CuF_{2}N_{2}, Triclinic, space group \( P-1 \), \( a = 16.6891(7) \) Å, \( b = 17.6024(7) \) Å, \( c = 22.2861(6) \) Å, \( \alpha = 107.079(3)^{\circ} \), \( \beta = 105.291(3)^{\circ} \), \( \gamma = 90.672(3)^{\circ} \), \( V = 6008.4(4) \) Å\(^3\), \( Z = 6 \), \( d_{\text{calc}} = 1.114 \) g cm\(^{-3}\), \( \mu = 0.582 \) mm\(^{-1}\), colorless/plate, crystal size 0.19 × 0.15 × 0.03 mm, \( F(000) = 2140.0 \), \( T_{\text{min}}/T_{\text{max}} = 0.74046/1.00000 \), \( R_1 = 0.0750 \) (from 23619 unique reflections with \( I > 2\sigma(I) \)); \( R_{\text{int}} = 0.1000 \), \( R_{\text{sigma}} = 0.1297 \)) and \( wR_2 = 0.1894 \) (from all 76057 reflections), \( GOF = 1.024 \), \( \Delta\rho_{\text{min}}/\Delta\rho_{\text{max}} = 1.06/−0.47 \).

Crystals of complex 2 suitable for X-ray diffraction study were obtained by layering saturated CH\(_2\)Cl\(_2\) solution with hexanes at room temperature to give a monoclinic polymorph. CCDC number 1956197, C\(_{39}\)H\(_{45}\)CuF\(_2\)N\(_2\), Monoclinic, space group \( P2_1/c \), \( a = 18.3730(4) \) Å, \( b = 18.3497(4) \) Å, \( c = 19.5826(4) \) Å, \( \beta = 92.460(2)^{\circ} \), \( V = 6596.0(2) \) Å\(^3\), \( Z = 8 \), \( d_{\text{calc}} = 1.296 \) g cm\(^{-3}\), \( \mu = 0.703 \) mm\(^{-1}\), colorless/prism, crystal size 0.23 × 0.19 × 0.10 mm, \( F(000) = 2720.0 \), \( T_{\text{min}}/T_{\text{max}} = 0.86893/1.00000 \), \( R_1 = 0.0402 \) (from 15904 unique reflections with \( I > 2\sigma(I) \)); \( R_{\text{int}} = 0.0439 \), \( R_{\text{sigma}} = 0.0443 \)) and \( wR_2 = 0.1147 \) (from all 63044 reflections), \( GOF = 1.052 \), \( \Delta\rho_{\text{min}}/\Delta\rho_{\text{max}} = 0.47/−0.38 \).

Crystals of complex 3·Benzene suitable for X-ray diffraction study were obtained by slow layering saturated benzene solution with hexanes at room temperature, CCDC number 2027575, C\(_{49}\)H\(_{61}\)AuN\(_2\), Orthorhombic, space group \( P2_12_12_1 \), \( a = 18.6537(2) \) Å, \( b = 20.2335(2) \) Å, \( c = 21.4452(2) \) Å, \( V = 8094.05(14) \) Å\(^3\), \( Z = 8 \), \( d_{\text{calc}} = 1.436 \) g cm\(^{-3}\), \( \mu = 3.671 \) mm\(^{-1}\), yellow/prism, crystal size 0.37 × 0.29 × 0.23 mm, \( F(000) = 3584.0 \), \( T_{\text{min}}/T_{\text{max}} = 0.69359 /1.00000 \), \( R_1 = 0.0248 \) (from 20607 unique reflections with \( I > 2\sigma(I) \)); \( R_{\text{int}} = 0.0442 \), \( R_{\text{sigma}} = 0.0401 \)) and \( wR_2 = 0.1147 \) (from all 101737 unique reflections), \( GOF = 1.052 \), \( \Delta\rho_{\text{min}}/\Delta\rho_{\text{max}} = 0.86/−0.51 \), Flack parameter 0.018(4).

Crystals of complex 3·CH\(_2\)Cl\(_2\) suitable for X-ray diffraction study were obtained by layering saturated CH\(_2\)Cl\(_2\) solution with hexanes at room temperature followed by cooling at -20 °C, CCDC number 1956199, C\(_{44}\)H\(_{57}\)AuCl\(_2\)N\(_2\), Monoclinic, space group \( P2_1/n \), \( a = 13.3315(5) \) Å, \( b = 19.3773(5) \) Å, \( c = 15.9007(5) \) Å, \( \beta = 105.989(4)^{\circ} \), \( V = 3948.7(2) \) Å\(^3\), \( Z = 4 \), \( d_{\text{calc}} = 1.483 \) g cm\(^{-3}\), \( \mu = 3.894 \) mm\(^{-1}\), yellow/plate, crystal size 0.47 × 0.23 × 0.05 mm, \( F(000) = 1792 \), \( T_{\text{min}}/T_{\text{max}} = 0.37970/1.00000 \), \( R_1 = 0.0230 \) (from 7740 unique reflections with \( I > 2\sigma(I) \)); \( R_{\text{int}} = 0.0322 \), \( R_{\text{sigma}} = 0.0234 \)) and \( wR_2 = 0.0555 \) (from all 37479 unique reflections), \( GOF = 1.017 \), \( \Delta\rho_{\text{min}}/\Delta\rho_{\text{max}} = 1.49/−1.19 \).
Crystals of desolvated complex 3 suitable for X-ray diffraction study were obtained by layering saturated CH$_2$Cl$_2$ solution with hexanes followed by removal of the crystals from the mother solution and slow drying at room temperature, CCDC number 2180575, C$_{43}$H$_{55}$AuN$_2$, Monoclinic, space group $P2_1/c$, $a = 20.441(2)$ Å, $b = 19.513(4)$ Å, $c = 18.204(2)$ Å, $\beta = 93.390(11)^\circ$, $V = 7248(2)$ Å$^3$, $Z = 8$, $d_{\text{calc}} = 1.460$ g cm$^{-3}$, $\mu = 7.852$ mm$^{-1}$, yellow/prism, crystal size 0.03 × 0.06 × 0.10 mm, $F(000) = 3248$, $T_{\text{min}}/T_{\text{max}} = 0.5870/1.00000$, $R_1 = 0.0595$ (from 7317 unique reflections with $I > 2\sigma(I)$; $R_{\text{int}} = 0.210$) and $wR_2 = 0.1466$ (from all 12335 unique reflections), $GOF = 0.997$, $\Delta\rho_{\text{min}}/\Delta\rho_{\text{max}} = 0.80/-2.27$.

The crystals of complex 4 were obtained by layering chlorobenzene/dichloromethane (1:1) solution with hexane at room temperature. CCDC number 1956200, C$_{51}$H$_{54}$AuN$_3$, Triclinic, space group $P-1$, $a = 9.6336(8)$ Å, $b = 9.9583(6)$ Å, $c = 20.9277(10)$ Å, $\alpha = 91.113(4)^\circ$, $\beta = 100.183(5)^\circ$, $\gamma = 93.507(7)^\circ$, $V = 1971.4(2)$ Å$^3$, $Z = 2$, $d_{\text{calc}} = 1.526$ g cm$^{-3}$, $\mu = 3.772$ mm$^{-1}$, yellow/needle, crystal size 0.10 × 0.05 × 0.04 mm, $F(000) = 920$, $T_{\text{min}}/T_{\text{max}} = 0.30830/1.00000$, $R_1 = 0.0341$ (from 7736 unique reflections with $I > 2\sigma(I)$; $R_{\text{int}} = 0.0451$, $R_{\text{sigma}} = 0.0594$) and $wR_2 = 0.0795$ (from all 18480 unique reflections), $GOF = 1.025$, $\Delta\rho_{\text{min}}/\Delta\rho_{\text{max}} = 1.44/-1.28$.

**Powder X-ray diffraction.** The data was collected on the Rigaku Smartlab SE powder diffractometer in reflection mode with a Bragg-Brentano geometry using Cu Kα radiation ($\lambda = 1.54184$ Å) at 300 K. The crystals of complexes 1-4 were deposited intact on the Si zero-background sample holder. The sample spinning was applied to reduce the preferred orientation effects. The data was collected in the range of 6–60° with a 0.007 step size and speed 0.8° per min. The data was processed and analyzed with SMARTLAB STUDIO II software using different preferred orientation models – March$^5$ or spherical harmonics model$^6$ to account for the preferred crystallographic orientation. The whole-powder-pattern fitting (WPPF) technique was applied to reproduce the diffraction pattern, peak intensities and unit cell parameters for diffractograms presented on Fig. 2. The WPPF calculation including texture refinement allowed to estimate the concentration of the main phase as 95±10% where significant standard deviation originates due to severe preferred orientation of the polycrystalline material.
Figure S6. Crystal structures of complexes 1 (top left), 2 (top right), 3 (bottom left) and 4 (bottom right). Ellipsoids are shown at the 50% level. Hydrogen atoms and co-crystallized solvent molecules are omitted for clarity.
Figure S7. a) Overlap of independent molecules A, B and C for complexes 2 (Triclinic, P-1), 2 (Monoclinic, P2_1/c) and 3·Benzene. b) Packing diagram for 3·benzene (top); c) Packing diagram for 3·CH_2Cl_2 (bottom) complexes.
**Thin-film preparation**

The solid-state samples for steady-state UV-Vis, photoluminescence (PL) and time-resolved PL measurements were prepared on the pre-cleaned Quartz substrates. Solution-processed complex 3 and 4 were spin-coated inside a solvent glovebox from anhydrous chlorobenzene solutions in either pristine or blended conditions. The samples were then annealed in the hot plate at 90°C for 10 minutes to remove the remaining solvent. Vacuum-deposited pristine or doped thin films for complex 1 and 2 were prepared by thermal evaporation under high vacuum (10⁻⁷ torr). The thickness of all the thin-films is ca. 80–100 nm.

**Photophysical Characterisation**

Solution UV-visible absorption spectra were recorded using a Perkin-Elmer Lambda 35 UV/vis spectrometer. UV-vis spectra of solid films were recorded using an Agilent 8453 UV-visible spectrophotometer. Photoluminescence measurements for solid state, host-guest films, MeTHF solutions at 298 and 77K were recorded using an Edinburgh Instruments FLS980 and FS5 spectrometers. Absolute photoluminescent quantum yields was measured for toluene solutions using an Edinburgh Instruments FS5 spectrometer with excitation wavelength 400 nm for complex 1 (0.02 mg mL⁻¹), with 360 nm for 2 (0.02 mg mL⁻¹), with 415 nm for complex 3 (0.05 mg mL⁻¹), and 415 nm for complex 4 (0.03 mg mL⁻¹). Toluene solutions have been prepared in a nitrogen glovebox from freshly distilled toluene and measured in a 1 cm screw-cap quartz cuvette.

All excited state lifetimes for complexes 1–4 were measured on Edinburgh Instruments FS5 spectrometer with mono- and biexponential fitting provided by Edinburgh Instruments Fluoracle software v2.6.1. The crystalline, solution, neat film and host-guest time resolved fluorescence data at 77K were collected on an Edinburgh Instruments FS5 spectrofluorimeter using the 5 W microsecond Xe flash lamp with a repetition rate of 100 Hz (360 nm excitation wavelength).

**Temperature-dependent time-resolved photoluminescence measurements (cryogenic PL measurement)**

Solid-state samples were prepared using the same method as thin-film preparation for steady-state measurement. Time-resolved PL spectra were carried out by using an electrically-gated intensified CCD (ICCD) camera (AndoriStar DH740 CCI-010) coupled with an image identifier
tube, giving high sensitivity and low noise level. A calibrated grating spectrometer (Andor SR303i) is connected to the ICCD for spectrum calibration. Photoexcitation is at the wavelength of 400 nm, given by femtosecond laser pulses which were created by second harmonic generation (SHG) in a BBO crystal from the fundamental 800 nm output (pulse width = 80 fs) of a Ti:Sapphire laser system (Spectra Physics Solstice), at a repetition rate of 1 kHz and ca. 200 µm diameter spots size on a sample. A 425 nm long-pass filter was applied to avoid the scattered laser signals entering the camera. The minimum gate width of the ICCD was ca. 5 ns. The kinetics of PL emissions can be obtained by setting the gate delay steps with respect to the excitation pulse. The gate width used in the measurements was 200 µm. The iCCD gate duration was 5 ns for 0-100 ns region, 10 ns for 100-1000 ns, 1 µs for 1-100 µs region and 10 µs for 100-900 µs. Liquid helium was used for sample cooling and a temperature-controlled cryostat was used for temperature regulation.
Figure S9. Normalized UV-vis and emission spectra in toluene, THF and CH$_2$Cl$_2$ for complexes 1 (a, b), 2 (c, d), 3 (e, f) and 4 (g, h) showing negative and positive solvatochromism, respectively.
Figure S9. Normalized UV-vis and emission spectra in THF for complexes 1, 2 and ligands 1,8-difluorocarbazole and corresponding lithium salt (i, j); emission map for complex 3*DCM at room temperature (k) and 77 K (l).
Figure S10. Emission decay kinetics for complex 1 (a), 2 (b), 3 (c) and 4 (d) in toluene solution at 295 K.
Figure S11 Emission decay kinetics for crystals of complexes 1, 2 and 3 at 295 K (left panel), 77 K (middle), and photoluminescence profile after various delays at 77 K (right panel).
Figure S11 Continue. Emission decay kinetics for crystals of complexes 3 and 4 at 295 K (left panel), 77 K (middle), and photoluminescence profile after various delays at 77 K (right panel).
Fitting and calculation of the activation energy for reverse intersystem crossing (rISC), radiative ($k_r$) and non-radiative decay rate ($k_{nr}$)

As the non-radiative decay is no longer negligible for twisted/tilted complexes, we assume it follows the same rate equation of activation energy\(^7\)

$$
k_r = A_1 \times \exp\left(\frac{\Delta E_{A,r}}{k_B T}\right) + y_0 \quad (S1)$$

$$
k_{nr} = A_2 \times \exp\left(\frac{\Delta E_{A,nr}}{k_B T}\right) + y_1 \quad (S2)$$

Where $\Delta E_{A,r}$ and $\Delta E_{A,nr}$ are the activation energy for radiative decay and non-radiative decay respectively. $\Delta E_{A,r}$ is the activation energy for reverse intersystem crossing (rISC) from triplets to singlets. Both decay rates are related to the total PL intensity ($PL_{tot}$) and the absolute decay rate ($k_T$) with the following relationships:

$$
k_T = k_r + k_{nr} \quad (S3)$$

$$
PL_{tot} \propto \frac{k_r}{k_r + k_{nr}} \quad (S4)
$$

Where $PL_{tot}$ is the temperature dependent total PL intensities calculated by integrating the time-dependent decays over the complete measurement window and $k_T$ is the reciprocal of the corresponded decay time when the normalized PL integral equals to $\frac{1}{e}$.

The equations $S3$ and $S4$ were adopted as the constraints to get all the values ($A_1$, $A_2$, $\Delta E_{A,r}$, $\Delta E_{A,nr}$, $y_0$ and $y_1$) in equations $S1$ and $S2$. Because the non-radiative decay process becomes significant only at high temperature, below that temperature $T_1$, $PL_{tot}$ and $k_T$ increase with temperature. Consequently, the value of $\Delta E_{A,r}$ can be calculated by fitting the curve of $k_T$ VS. Temperature from 10 K to $K_1$.

We take complex 3 as the example to demonstrate the fitting process:
Figure S12. (a) Total PL intensity (black dots) and absolute decay rate (red dots) obtained from temperature-dependent time-resolved PL spectra by using an electrically gated ICCD, the red dash line is the fitting to the decay rate from 10 K to 175 K by using the rate equation; (b) experimental absolute decay rate $k_T$ and fitted $k_T$ using equation S3; (c) experimental total PL intensity $PL_{tot}$ and fitted $PL_{tot}$ using equation S4.

The total PL intensity begins to drop from 175 K, so we only fit the data of $PL_{tot}$ and $k_T$ below 175 K by using the rate equation (S1). The calculated average activation energy is 42.2 meV and we substitute this value as $\Delta E_{A,r}$ in equation S1. By fitting the $PL_{tot}$ and $k_T$ among the whole measurement window (10K to 100K) and applying equations S3 and S4, we obtained the optimised values for other constants in equations S1 and S2 and collected in Table S1.

Table S1. Optimized values for the rate equations of complexes 1–4.

|             | Complex 1   | Complex 2   | Complex 3   | Complex 4   |
|-------------|-------------|-------------|-------------|-------------|
| $A_1$       | $1.00 \times 10^{-2}$ | $4.00 \times 10^{-3}$ | $1.25 \times 10^{-2}$ | $9.40 \times 10^{-3}$ |
| $\Delta E_{A,r}$ | 58.11       | 136.40      | 42.22       | 41.80       |
| $y_0$       | $4.00 \times 10^{-5}$ | $2.00 \times 10^{-5}$ | $4.00 \times 10^{-5}$ | $3.00 \times 10^{-5}$ |
| $A_2$       | -           | 600.00      | 450.00      | 520.00      |
| $\Delta E_{A,\text{nr}}$ | -           | 323.13      | 327.45      | 344.68      |
| $y_1$       | -           | $5.00 \times 10^{-4}$ | $1.80 \times 10^{-5}$ | $1.00 \times 10^{-5}$ |
Figure S13. UV-Vis absorption spectra (a) (d), steady-state PL spectra (b) (e) and time-resolved PL decay at room temperature (c) (f) of thin-film pristine complexes 1 and 2, and 20% doped in o-CBP, TCP and TSPO1. Thin films were deposited via vacuum-deposition.
Figure S14. UV-Vis absorption spectra (a) (d), steady-state PL spectra (b) (e) and time-resolved PL spectra at room temperature (c) (f) of thin-film Pristine Complexes 3 and 4, and 20% doped in o-CBP and PVK. Thin films were spin-coated from chlorobenzene solutions.

Figure S15. (a) Complex 1 temperature-dependent total PL intensities calculated by integrating the time-dependent decays over the complete measurement window; (b) Temperature-dependent decay rate k and the fitting of ln (k) to 1/T.
Figure S16. (a) Absolute decay rate $K$ extracted from temperature-dependent time-resolved PL spectra and fitted decay rate of complex 2; (b) Normalised total PL intensity extracted from temperature-dependent time-resolved PL spectra and fitted total PL of complex 2; (c) Calculated radiative decay rate $K_r$ and non-radiative decay rate $K_{nr}$ or complex 2.

Figure S17. (a) (d) Absolute decay rate $K$ extracted from temperature-dependent time-resolved PL spectra and fitted decay rate of complex 3 and 4; (b) (e) Normalised total PL intensity extracted from temperature-dependent time-resolved PL spectra and fitted total PL of complex 3 and 4; (c) (f) Calculated radiative decay rate $K_r$ and non-radiative decay rate $K_{nr}$ or complex 3 and 4.
Table S2. Steady-state PL peak, decay lifetime and FWHM of solid-state pristine complexes 3 and 4 or 20% doped in o-CBP and PVK.

|                | Complex 3 |            | Complex 4 |            |
|----------------|-----------|------------|-----------|------------|
|                | $\lambda_{em}$ | $\tau$ (µs) | FWHM (nm) | $\lambda_{em}$ | $\tau$ (µs) | FWHM (nm) |
| Pristine       | 574       | 0.34       | 139       | 535        | 0.47       | 126       |
| o-CBP          | 551       | 0.50       | 130       | 520        | 0.56       | 108       |
| PVK            | 561       | 0.45       | 137       | 535        | 0.65       | 127       |

Solution-processing device fabrication

Devices were carried out by solution processing with a forward configuration as follows: ITO/PEDOT:PSS/Active Layer/ETL/LiF/Al. Indium tin-oxide (ITO; WF $\sim$ 4.8 eV) coated glass substrates were used and subsequently cleaned by sonication in acetone and 2-propanol for 10 minutes, followed by O$_2$ plasma treatment for 10 minutes. PEDOT: PSS (Clevios CH4083, LumTech Taiwan) was spin-casted on top of the ITO under ambient conditions and annealed on a hot plate at 160 °C for 20 minutes, forming a 40 nm-thick film. The PEDOT: PSS-coated substrates were then transferred to a nitrogen-filled glovebox to conduct the following solution processes.

For structure 1, first a 40 nm-thick emitting layer (EML) of o-CBP doped with 20 wt.% of complex 3 and 4 in chlorobenzene was spin-coated on top of the PEDOT: PSS layer and annealed on a hot plate at 60 °C for 5 min to remove residual solvent. Since o-CBP is sensitive to humidity and temperature, the glovebox atmosphere has to be stable to avoid crystallization. Samples were then transferred to a vacuum deposition system. 10 nm of TSPO1 doped with 10 wt.% of 1,3,5-tris(2-N-phenylbenzimidazole-1-yl)benzene (TPBi) was deposited, followed by 40 nm-thick of TSPO1 as the electron-transporting layer (ETL). For structure 2, instead, 10 nm-thick of UGH2: TPBi (9:1 in wt.%) and 40 nm-thick of TPBi were used as the hole blocking layer (HBL) and the ETL.

Similarly, for structure 3, 50 nm-thick EML of Poly(9-vinylcarbazone) (PVK, Sigma-Aldrich) doped with 20 wt.% of complex 3 and 4 in chlorobenzene was spin-coated on top of the PEDOT: PSS and annealed at 90°C for 10 min to remove any solvent present. Samples were then transferred to the vacuum deposition system for further deposition of 10 nm-thick of UGH2: TPBi (9:1 in wt.%) and 40 nm-thick of TPBi. For all samples, 0.8 nm-thick LiF (99.99%, Sigma-Aldrich) and 100 nm-thick aluminium were subsequently deposited by thermal evaporation under high vacuum (< $3 \times 10^{-6}$ mbar) as the electrode.
Vacuum thermal-evaporated device fabrication

Fully-evaporated devices were fabricated by high vacuum (10^{-7} Torr) thermal evaporation on ITO glass substrates. The optimum blue architecture for complex 1 and 2 devices comprised a 40 nm thick layer of 1,1-bis[4-[N,N-di(4-tolyl)amino]phenyl]-cyclohexane (TAPC) used as the electron blocking layer (EBL) and HTL. A 5 nm-thick of 9,9’-Biphenly-2,2’-diylbis-9H-carbazole (o-CBP) was deposited as an additional EBL to avoid triplet transfer towards anode or the formation of interfacial states between EML and HTL. The following layer is a 30 nm-thick of EML comprising either host free or 20 wt.% of complex 1 and 2 dispersed in a host material. o-CBP, 1,3,5-tris(carbazol-9-yl)benzene (TCP) and diphenyl-4-triphenylsilyl-phenylphosphine oxide (TSPO1) were used as the host materials. Then, a 40 nm layer of TSPO1 acting as the ETL and HBL was evaporated.

Another OLED architecture for complex 1 and 2 used TAPC as the EBL and HTL. A 20 nm of either host-free or 20 wt.% doped complex 1 and 2 in various host materials were evaporated on top of the TAPC. Same hosts were tested (i.e. o-CBP, TCP and TSPO1). A 10 nm of 1,4-bis(triphenylsilyl)benzene (UGH2) was deposited as the EBL. 40 nm-thick layer of TPBi was then evaporated as the ETL. For both structures, a 0.8 nm-thick LiF (99.99%, Sigma-Aldrich) and a 100 nm-thick aluminium were subsequently deposited as the cathode. Each substrate has eight 4.5 mm² pixels as defined by the overlap area of the shadow mask and ITO stripe.

OLED Characterisation.

The forward-viewing current–voltage–luminance characteristics of these OLED devices were measured using a Keithley 2400 source meter, Keithley 2000 multimeter and a calibrated Si photodiode (from RS components), which was placed at a distance of 4 cm from the devices. External quantum efficiencies were calculated from on-axis irradiance assuming a Lambertian emission profile and accounting for photodiode quantum efficiency across the electroluminescence spectrum. The electroluminescence spectra were obtained by a fibre spectrometer (Flame-S-VIS-NIR-ES, Ocean Optics). All the measurements were carried out at room temperature under ambient conditions.
Figure S18. Typical OLED performance of complex 1 in host free and different hosts in a normal structure (left); (a) Current-density vs. Voltage; (b) Luminance vs. Voltage; (c) external quantum efficiency (EQE) vs. luminance; (d) electroluminescence (EL) spectra.

Figure S19. Typical OLED performance of complex 1 in host free and different hosts in a blue structure (left); (a) Current-density vs. Voltage; (b) Luminance vs. Voltage; (c) external quantum efficiency (EQE) vs. luminance; (d) electroluminescence (EL) spectra.
Table S3. OLED performance summary of complex 1

|                  | Normal architecture |                  | Blue architecture |                  |
|------------------|---------------------|------------------|-------------------|------------------|
|                  | Turn-on (V)         | EQE (max. %)     | EQE % (100 cd/m²) | EQE % (1000 cd/m²)| EL peaks (nm) |
| Host-free        | 4.4                 | 11.5             | 11.0              | 6.6              | 485           |
| O-CBP            | 4.7                 | 6.8              | 4.2               | 1.2              | 485           |
| TCP              | 4.7                 | 5.2              | 3.5               | 1.5              | 485           |
| TSP01            | 4.7                 | 9.6              | 7.4               | 3.9              | 480           |
|                  |                     |                  |                   |                  |               |
| Host-free        | 3.0                 | 8.8              | 8.7               | 6.0              | 480           |
| O-CBP            | 3.2                 | 6.3              | 4.2               | -                | 480           |
| TCP              | 3.6                 | 5.3              | 2.6               | -                | 480           |
| TSP01            | 3.2                 | 11.3             | 10.5              | 5.9              | 475           |

Figure S20. Typical OLED performance of complex 2 in host free and different hosts in a normal structure (left); (a) Current-density vs. voltage; (b) Luminance vs. voltage; (c) external quantum efficiency (EQE) vs. luminance; (d) electroluminescence (EL) spectra.
Figure S21. Typical OLED performance of complex 2 in host free and different hosts in a blue structure (left); (a) current-density vs. voltage; (b) luminance vs. voltage; (c) external quantum efficiency (EQE) vs. luminance; (d) electroluminescence (EL) spectra.

Table S4. OLED performance summary of complex 2

|                         | Normal architecture |                     | Blue architecture |                     |
|-------------------------|---------------------|---------------------|-------------------|---------------------|
|                         | Turn-on (V)         | EQE (max. %)        | EQE % (100 cd/m²) | EQE % (1000 cd/m²) | EL peaks (nm) |
| o-CBP                   | 4.5                 | 7.3                 | 4.4               | -                   | 495           |
| TSPO1                   | 4.8                 | 10.5                | 6.4               | -                   | 492           |
| TCP                     | 4.5                 | 6.0                 | 3.5               | -                   | 495           |
| Host-free               | 4.4                 | 4.5                 | 2.9               | -                   | 495           |
|                         |                     |                     |                   |                     | 500           |
|                         | Turn-on (V)         | EQE (max. %)        | EQE % (100 cd/m²) | EQE % (1000 cd/m²) | EL peaks (nm) |
| o-CBP                   | 3.2                 | 21.3                | 10.6              | -                   | 500           |
| TSPO1                   | 3.1                 | 13.2                | 5.0               | -                   | 496           |
| TCP                     | 3.2                 | 9.3                 | 4.2               | -                   | 500           |
| Host-free               | 3.0                 | 9.6                 | 7.9               | -                   | 498           |
Figure S22. Typical OLED performance with complex 3 in host-free and host-guest stack; (a) current-density vs. voltage; (b) luminance vs. voltage; (c) external quantum efficiency (EQE) vs. luminance; (d) electroluminescence (EL) spectra; (e) Schematic of OLED stack of structure 1, 2 and 3 for Complex 3 and 4, host-free is in structure 1.
Table S5. OLED performance summary of complex 3

| Normal architecture | Turn-on (V) | EQE (max. %) | EQE % (100 cd/m²) | EQE % (1000 cd/m²) | EL peaks (nm) |
|---------------------|------------|--------------|-------------------|-------------------|--------------|
| Host-free           | 5.2        | 10.0         | 10.0              | 9.2               | 550          |
| Structure 1         | 4.3        | 14.1         | 14.1              | 12.5              | 540          |
| Structure 2         | 4.8        | 12.1         | 11.6              | 11.8              | 540          |
| Structure 3         | 4.4        | 10.2         | 10.1              | 9.5               | 550          |

Figure S23. Typical OLED performance of Complex 4 in host free and different structures; (a) current-density vs. voltage; (b) luminance vs. voltage; (c) external quantum efficiency (EQE) vs. luminance; (d) electroluminescence (EL) spectra.
Table S6. OLED performance summary of Complex 4

|               | Normal architecture |
|---------------|---------------------|
|               | Turn-on (V) | EQE (max. %) | EQE % (100 cd/m²) | EQE % (1000 cd/m²) | EL peaks (nm) |
| Host-free     | 3.5         | 11.0         | 10.8              | 9.9               | 535           |
| Structure 1   | 3.9         | 19.1         | 19.0              | 16.7              | 525           |
| Structure 2   | 4.5         | 18.2         | 18.2              | 16.4              | 525           |
| Structure 3   | 5.0         | 16.3         | 16.3              | 15.6              | 535           |

Figure S24 (a) Champion device structure for complex 3; (b) Current-density vs. Voltage; (c) Luminance vs. Voltage; (d) external quantum efficiency (EQE) vs. Luminance for OLED device with varied doping concentration from 10 wt. % to 50 wt. % for complex 3. OLED device with 20 wt.% doping concentration for complex 3 shows the best performance.
**Figure S25.** Maximum EQE histograms of the OLED devices based on complexes 1 (a), 2 (b), 3 (c) and 4 (d).
## Computational Details

### Compound 1 (Au):

| State | Character | Osc. Str. | Energy / eV | GS | S₁ | T₁ |
|-------|-----------|-----------|-------------|----|----|----|
| φ     | -         | -         |             | 149.92 | -116.09 | -139.74 |
| τ     | -         | -         |             | -76.11 | -88.06 | -80.59 |
|r₁    | 2.01      | 2.00      | 2.01        |    |    |    |
|r₂    | 2.07      | 2.11      | 2.08        |    |    |    |

### GS Electronic Structure:

| State | Character | Osc. Str. | Energy / eV |
|-------|-----------|-----------|-------------|
| GS    | -         | -         | 0.39        |
| T₁    | ³LE(D)    | -         | 3.14        |
| T₂    | ³CT       | -         | 3.27        |
| S₁    | ¹CT       | 0.141     | 3.40        |
| T₃    | ³LE(A)    | -         | 3.47        |
| T₄    | ³LE(D)    | -         | 3.60        |
| T₅    | ³LE(D)    | -         | 3.88        |
| S₂    | ¹LE(A)/¹LE(D) | -         | 3.92        |

### S₁ Electronic Structure:

| State | Character | Osc. Str. | Energy / eV |
|-------|-----------|-----------|-------------|
| GS    | -         | -         | 0.39        |
| T₁    | ³CT       | -         | 2.99        |
| S₁    | ¹CT       | 0.044     | 3.05        |
| T₂    | ³LE(D)    | -         | 3.43        |
| T₃    | ³LE(A)    | 0.006     | 3.44        |
| S₂    | ¹LE(A)    | -         | 3.83        |
| T₄    | ³LE(A)    | -         | 3.88        |

### T₁ Electronic Structure:

| State | Character | Osc. Str. | Energy / eV |
|-------|-----------|-----------|-------------|
| GS    | -         | -         | 0.21        |
| T₁    | ³LE(D)    | -         | 3.01        |
| T₂    | ³CT       | 0.027     | 3.41        |
| T₃    | ³CT/³LE(D)| -         | 3.43        |
| S₁    | ¹CT       | 0.120     | 3.52        |
| T₄    | ³LE(A)    | -         | 3.79        |
| S₂    | ³LE(D)    | 0.082     | 3.85        |

### SOC

| State | T₁    | T₂    | T₃    | T₄    | T₅    |
|-------|-------|-------|-------|-------|-------|
| GS    | 0.844 | 0.246 | 0.510 | 7.771 | 0.327 |
| S₁    | 0.845 | 7.543 | 1.056 | 0.597 | 0.052 |
| T₁    | 0.612 | 3.010 | 1.820 | 0.600 | 0.049 |
| S₂    | 0.146 | 0.550 | 0.715 | 1.582 | 0.182 |
| S₃    | 0.477 | 0.974 | 0.525 | 0.176 | 0.737 |
| T₂    | -     | 1.148 | 0.492 | 1.653 | 0.125 |
| S₄    | -     | -0.613| 12.713| 0.655 |       |
| T₃    | -     | -     | 0.769 | 0.031 |       |
| S₅    | -     | -     | -     | 0.477 |       |

### SOC

| State | T₁    | T₂    | T₃    | T₄    | T₅    |
|-------|-------|-------|-------|-------|-------|
| GS    | 0.223 | 1.071 | 7.976 | 0.626 | 2.198 |
| S₁    | 8.877 | 0.039 | 2.073 | 0.192 | 4.434 |
| T₁    | 0.712 | 0.071 | 1.161 | 0.622 | 0.535 |
| S₂    | 0.997 | 0.050 | 0.455 | 1.949 | 0.296 |
| S₃    | 0.487 | 0.006 | 0.633 | 0.038 | 0.865 |
| T₂    | -     | 1.236 | 12.179| 0.812 | 3.292 |
| S₄    | -     | -     | 0.066 | 0.099 | 0.173 |
| T₃    | -     | -     | 0.209 | 6.624 |       |
| S₅    | -     | -     | -     | 0.557 |       |

### SOC

| State | T₁    | T₂    | T₃    | T₄    | T₅    |
|-------|-------|-------|-------|-------|-------|
| GS    | 1.244 | 0.218 | 0.461 | 8.190 | 0.753 |
| S₁    | 0.362 | 1.643 | 1.426 | 0.774 | 0.667 |
| T₁    | 0.326 | 7.898 | 3.210 | 0.647 | 0.324 |
| S₂    | 0.207 | 0.861 | 0.978 | 1.800 | 0.582 |
| S₃    | 0.562 | 0.979 | 0.496 | 0.165 | 0.568 |
| T₂    | -     | 1.525 | 1.149 | 0.639 | 1.998 |
| S₄    | -     | -     | 0.436 | 12.078| 1.100 |
| T₃    | -     | -     | 4.806 | 0.329 |       |
| S₅    | -     | -     | -     | 0.415 |       |
Figure S26. The difference of electronic density associated with the singlet and triplet excited states in the ground state geometry for complex 1.
### Compound 2 (Cu)

|   | GS  | S1       | T1        |
|---|-----|----------|-----------|
| φ | 86.31 | 83.21 | 81.93 |
| τ | -83.84 | -86.38 | -84.86 |
| r1 | 1.92 | 1.90 | 1.88 |
| r2 | 1.93 | 1.91 | 1.94 |

### GS Electronic Structure:

| State | Character | Osc. Str. | Energy / eV |
|-------|-----------|-----------|-------------|
| GS    |           |           | -           |
| T1    | 3LE(A)    |           | 2.92        |
| T2    | 3CT       |           | 3.06        |
| S1    | 1CT       | 0.007     | 3.32        |
| T3    | 3LE(A)    |           | 3.35        |
| S2    | 1LE(A)/1CT| 0.005     | 3.39        |
| T4    |           |           | 3.48        |
| S3    | 1LE(A)    | 0.086     | 3.85        |

### S1 Electronic Structure:

| State | Character | Osc. Str. | Energy / eV |
|-------|-----------|-----------|-------------|
| GS    |           |           | -           |
| T1    | 3CT/3LE(A)|           | 2.71        |
| S1    | 1CT/1LE(A)| 0.003     | 3.01        |
| T2    | 3CT       |           | 3.23        |
| T3    | 3LE(D)    | 0.006     | 3.34        |
| S2    | 1LE(D)    |           | 3.37        |
| T4    | 3CT/3LE(D)|           | 3.82        |

### T1 Electronic Structure:

| State | Character | Osc. Str. | Energy / eV |
|-------|-----------|-----------|-------------|
| GS    |           |           | -           |
| T1    | 3LE(A)    |           | 2.68        |
| S1    | 1CT/1LE(A)| 0.005     | 3.07        |
| T2    | 3CT       |           | 3.23        |
| S2    | 1CT       | 0.005     | 3.31        |
| T3    | 3LE(D)    |           | 3.35        |
| T4    | 3LE(D)    |           | 3.78        |
Figure S27. The difference of electronic density associated with the singlet and triplet excited states in the ground state geometry for complex 2.
### Compound 3 PLANAR:

|         | GS   | S1   | T1   |
|---------|------|------|------|
| $\phi$  | 42.95| 74.87| 50.07|
| $\tau$  | -122.78| -108.36| -116.09|
| $r_1$   | 2.00 | 2.02 | 2.01 |
| $r_2$   | 2.06 | 2.17 | 2.16 |

#### GS Electronic Structure:

| State | Character | Osc. Str. | Energy / eV |
|-------|-----------|-----------|-------------|
| GS    | -         | -         | 0.03        |
| T1    | 3\text{CT} | -         | 2.95        |
| S1    | 1\text{CT} | 0.050     | 3.04        |
| T2    | 3\text{LE(D)} | -         | 3.10        |
| T3    | 3\text{LE(D)} | -         | 3.41        |
| T4    | 3\text{LE(A)} | -         | 3.58        |
| T5    | 3\text{CT} | 0.003     | 3.70        |

#### S1 Electronic Structure:

| State | Character | Osc. Str. | Energy / eV |
|-------|-----------|-----------|-------------|
| GS    | -         | -         | 0.64        |
| T1    | 3\text{CT} | -         | 2.69        |
| S1    | 1\text{CT} | 0.003     | 2.73        |
| T2    | 3\text{LE(A)} | -         | 3.50        |
| T3    | 3\text{LE(D)} | -         | 3.51        |
| T4    | 3\text{CT} | -         | 3.69        |
| S2    | 1\text{CT} | 0.003     | 3.69        |
| S3    | 1\text{LE(A)} | 0.009     | 3.95        |
| T5    | 3\text{LE(D)} | -         | 3.99        |

#### T1 Electronic Structure:

| State | Character | Osc. Str. | Energy / eV |
|-------|-----------|-----------|-------------|
| GS    | -         | -         | 0.48        |
| T1    | 3\text{CT} | -         | 2.65        |
| S1    | 1\text{CT} | 0.003     | 2.73        |
| T2    | 3\text{LE(D)} | -         | 3.37        |
| T3    | 3\text{LE(A)} | -         | 3.55        |
| T4    | 3\text{CT} | -         | 3.64        |
| S2    | 1\text{CT} | 0.003     | 3.65        |
| T5    | 3\text{CT} | -         | 3.83        |
### Compound 3 Orthogonal:

|       | GS  | S1   | T1   |
|-------|-----|------|------|
| ϕ     | 88.46 | 89.71 | 90.42 |
| τ     | -58.51 | -70.28 | -68.96 |
| r1    | 2.01  | 2.01  | 2.01  |
| r2    | 2.07  | 2.15  | 2.15  |

#### GS Electronic Structure:

| State | Character | Osc. Str. | Energy / eV |
|-------|-----------|-----------|-------------|
| GS    | -         | -         | -           |
| T1    | 3_CT      | -         | 2.91        |
| S1    | 1_CT      | 0.003     | 2.95        |
| T2    | 3_LE(D)   | -         | 3.06        |
| T3    | 3_LE(D)   | -         | 3.38        |
| T4    | 3_LE(A)   | -         | 3.57        |
| T5    | 3_CT      | -         | 3.66        |
| S2    | 1_CT      | 0.002     | 3.67        |

#### S1 Electronic Structure:

| State | Character | Osc. Str. | Energy / eV |
|-------|-----------|-----------|-------------|
| GS    | -         | -         | 0.41        |
| T1    | 3_CT      | -         | 2.65        |
| S1    | 1_CT      | 0.001     | 2.67        |
| T2    | 3_LE(D)   | -         | 3.29        |
| T3    | 3_LE(A)   | -         | 3.59        |
| T4    | 3_CT      | -         | 3.62        |
| S2    | 1_CT      | 0.002     | 3.63        |
| T5    | -         | -         | 3.76        |

#### T1 Electronic Structure:

| State | Character | Osc. Str. | Energy / eV |
|-------|-----------|-----------|-------------|
| GS    | -         | -         | 0.40        |
| T1    | 3_CT      | -         | 2.65        |
| S1    | 1_CT      | 0.003     | 2.67        |
| T2    | 3_LE(D)   | -         | 3.28        |
| T3    | 3_LE(A)   | -         | 3.59        |
| T4    | 3_CT      | -         | 3.62        |
| S2    | 1_CT      | 0.003     | 3.63        |
Figure S28. The difference of electronic density associated with the singlet and triplet excited states in the ground state geometry for complex 3.
### Compound 4:

|    | GS    | S1     | T1     |
|----|-------|--------|--------|
| $\phi$ | 172.19 | 93.78  | 125.14 |
| $\tau$ | -126.70 | -91.82 | -106.75 |
| r1  | 2.01  | 2.01  | 2.01  |
| r2  | 2.06  | 2.13  | 2.13  |

**GS Electronic Structure:**

| State | Character | Osc. Str. | Energy / eV |
|-------|-----------|-----------|-------------|
| GS    | -         | -         | 0.00        |
| T1    | $3\text{CT}^3\text{LE(D)}$ | - | 2.99 |
| T2    | $3\text{CT}^3\text{LE(D)}$ | - | 3.10 |
| T3    | $3\text{CT}^3\text{LE(D)}$ | - | 3.16 |
| S1    | $1\text{CT}$ | 0.131 | 3.21 |
| T4    | $3\text{LE(D)}$ | - | 3.35 |
| S2    | $1\text{CT}$ | - | 3.40 |
| T5    | $3\text{CT}$ | - | 3.50 |

**S1 Electronic Structure:**

| State | Character | Osc. Str. | Energy / eV |
|-------|-----------|-----------|-------------|
| GS    | -         | -         | 0.42        |
| T1    | $3\text{CT}$ | - | 2.72 |
| S1    | $1\text{CT}$ | 0.000 | 2.73 |
| T2    | $3\text{CT}$ | - | 3.19 |
| S2    | $1\text{CT}$ | 0.000 | 3.19 |
| T4    | $3\text{LE(D)}$ | - | 3.35 |
| T5    | $3\text{LE(A)}$ | - | 3.37 |

**T1 Electronic Structure:**

| State | Character | Osc. Str. | Energy / eV |
|-------|-----------|-----------|-------------|
| GS    | -         | -         | 0.39        |
| T1    | $3\text{CT}$ | - | 2.71 |
| S1    | $1\text{CT}$ | 0.027 | 2.77 |
| T2    | $3\text{CT}$ | - | 3.19 |
| S2    | $1\text{CT}$ | 0.000 | 3.21 |
| T3    | $3\text{LE(D)}$ | - | 3.31 |
| T4    | $3\text{LE(A)}$ | - | 3.39 |

**SOC**

| State | T1     | T2     | T3     | T4     | T5     |
|-------|--------|--------|--------|--------|--------|
| S1    | 0.460  | 0.516  | 0.882  | 0.578  | 1.574  |
| S2    | 0.581  | 0.719  | 0.167  | 0.300  | 0.298  |
| S3    | 1.093  | 1.627  | 0.422  | 1.424  | 1.106  |
| S4    | 1.073  | 0.736  | 1.076  | 0.491  | 0.123  |
| S5    | 3.739  | 1.714  | 4.447  | 1.769  | 0.826  |

| State | T1     | T2     | T3     | T4     | T5     |
|-------|--------|--------|--------|--------|--------|
| S1    | 0.041  | 0.826  | 2.783  | 5.224  | 0.351  |
| S2    | 0.790  | 0.030  | 0.076  | 2.470  | 2.425  |
| S3    | 5.645  | 2.376  | 0.252  | 1.935  | 0.155  |
| S4    | 2.635  | 0.728  | 0.704  | 0.394  | 1.663  |
| S5    | 0.977  | 0.849  | 0.390  | 3.092  | 0.454  |

| State | T1     | T2     | T3     | T4     | T5     |
|-------|--------|--------|--------|--------|--------|
| S1    | -      | 1.121  | 3.986  | 7.676  | 0.533  |
| S2    | -      | -      | 0.120  | 3.635  | 3.430  |
| S3    | -      | -      | -      | 0.123  | 0.572  |
| S4    | -      | -      | -      | -      | 0.059  |

| State | T1     | T2     | T3     | T4     | T5     |
|-------|--------|--------|--------|--------|--------|
| S1    | 0.426  | 1.142  | 2.016  | 5.169  | 0.484  |
| S2    | 1.108  | 0.331  | 0.129  | 2.237  | 2.087  |
| S3    | 5.444  | 2.298  | 1.069  | 1.659  | 0.643  |
| S4    | 1.990  | 0.471  | 0.925  | 0.510  | 1.988  |
| S5    | 0.947  | 0.917  | 0.527  | 3.070  | 0.260  |

| State | T1     | T2     | T3     | T4     | T5     |
|-------|--------|--------|--------|--------|--------|
| S1    | -      | 1.461  | 3.618  | 7.833  | 0.713  |
| S2    | -      | -      | 0.366  | 3.320  | 2.958  |
| S3    | -      | -      | -      | 1.487  | 1.493  |
| S4    | -      | -      | -      | -      | 0.781  |
Figure S29. The difference of electronic density associated with the singlet and triplet excited states in the ground state geometry for complex 4.

Table S7. Energy of the HOMO and LUMO (in eV) and their overlap (in %). Cartesian components of dipole moments for the ground ($\mu^{\text{GS}}$) and first excited state ($\mu^{\text{ES}}$) with their absolute value (in Debye). Values are provided for the optimised geometry of the ground state (GS), first singlet ($S_1$) and triplet ($T_1$) excited states.

|                | Complex 1 | Complex 2 | Complex 3 |
|----------------|-----------|-----------|-----------|
|                | GS  | $S_1$ | $T_1$ | GS  | $S_1$ | $T_1$ | GS  | $S_1$ | $T_1$ |
| HOMO           | -5.50 | -5.36 | -5.39 | -5.36 | -5.31 | -5.36 | -5.14 | -4.27 | -4.93 |
| LUMO           | -1.42 | -2.01 | -1.39 | -1.17 | -1.66 | -1.61 | -1.42 | -2.42 | -2.01 |
| Overlap        | 27.58 | 19.40 | 26.21 | 13.55 | 15.82 | 14.28 | 23.50 | 16.01 | 20.27 |
| $\mu_x^{\text{GS}}$ | -1.21 | -0.50 | -0.78 | 1.35  | 0.56  | 0.85  | 14.66 | 15.88 | 15.57 |
| $\mu_y^{\text{GS}}$ | 0.11  | -0.26 | -0.09 | 0.05  | -0.58 | -0.49 | -2.52 | -2.39 | -2.42 |
| $\mu_z^{\text{GS}}$ | 11.78 | 12.32 | 11.98 | 11.49 | 11.22 | 11.19 | 0.83  | 0.85  | 0.81  |
| $||\mu^{\text{GS}}||$ | 11.84 | 12.33 | 12.01 | 11.57 | 11.25 | 11.24 | 14.90 | 16.08 | 15.77 |
| $\mu_x^{\text{ES}}$ | -1.11 | 0.82  | -1.02 | 0.32  | -1.29 | -0.66 | -7.02 | -8.40 | -7.93 |
| $\mu_y^{\text{ES}}$ | -0.32 | -0.72 | -0.49 | -0.39 | -0.86 | -0.82 | 1.38  | 0.50  | 1.38  |
| $\mu_z^{\text{ES}}$ | 14.04 | -11.31 | 14.85 | 5.77  | 3.61  | 5.31  | -0.05 | -1.18 | -0.27 |
| $||\mu^{\text{ES}}||$ | 14.09 | 11.37 | 14.89 | 5.79  | 3.93  | 5.41  | 7.16  | 8.50  | 8.06  |
Table S8. Coordinates for ground and excited states (S1 and T1) geometries from TD-DFT calculations for complexes 1–4 and CMA1.

Complex CMA1, Ground state S0.

| Atom | X (Å)      | Y (Å)      | Z (Å)      |
|------|------------|------------|------------|
| C    | -2.1108263740 | -2.1790979610 | -4.8949238118 |
| C    | -1.2357550093 | -1.1577001007 | -5.2501914675 |
| C    | -0.5378942466 | -0.4767366696 | -4.2434549388 |
| C    | -0.7245353676 | -0.8313797228 | -2.8745792368 |
| C    | -1.6100301425 | -1.8647934925 | -2.5250323138 |
| C    | -2.2920748408 | -2.5245052975 | -3.5411902919 |
| N    | 0.0481046686  | -0.0442229528 | -2.050431442 |
| C    | 0.7349376741  | 0.8279496905 | -2.8648827682 |
| C    | 0.4141509591  | 0.6057808070 | -4.2373887132 |
| C    | 1.0061791700  | 1.3899556227 | -5.2368963768 |
| C    | 1.9074651158  | 2.3848506756 | -4.8725219769 |
| C    | 2.2184696135  | 2.6020624335 | -3.5160235875 |
| C    | 1.6432639786  | 1.8378774425 | -2.5074839095 |
| Au   | 0.0881351676  | -0.1478161779 | -0.0056032747 |
| C    | 0.0631170614  | -0.2784492290 | 1.9996800712 |
| N    | -0.7518707635 | -1.1138555121 | 2.6002180012 |
| C    | -0.6941253285 | -1.1067623627 | 1.092136685 |
| C    | 0.6080044470  | -0.3355933379 | 4.1356275480 |
| C    | 0.8611938114  | 0.9862514824  | 3.0410407076 |
| C    | 2.3857306477  | 0.5927487851  | 2.7478606390 |
| C    | 3.0703460176  | 1.2846242975  | 3.9379082676 |
| C    | 2.5426521507  | 2.7169466880  | 4.0855852007 |
| C    | 1.0277521759  | 2.6856331293  | 4.3098518337 |
| N    | 0.3387337340  | 1.9745698491  | 3.1360820343 |
| C    | 2.0918183403  | 1.3982163831  | 1.4860509736 |
| C    | 2.1625566196  | 2.8236066124  | 1.6216514372 |
| C    | 0.6510839803  | 2.7694940356  | 1.8600655776 |
| C    | 2.8452766774  | 3.5076619204  | 2.8097679226 |
| C    | -1.6482945831 | -1.9875553906 | 1.8731236515 |
| C    | -2.9438433284 | -1.5383517376 | 1.5317869743 |
| C    | -3.790679613  | -2.4313953738 | 0.8640909899 |
| C    | -3.3748462117 | -3.7123389913 | 0.5241846143 |
| C    | -2.0774412110 | -4.1128572286 | 0.8200538657 |
| C    | -1.1845008465 | -3.2661594527 | 1.4861119180 |
| C    | -3.4483199890 | -0.1232318800 | 1.7724771895 |
| C    | -3.5965780399 | 0.633719619  | 0.4482653163 |
| C    | 0.2467906712  | -3.7454089681 | 1.6785355437 |
| C    | 0.3234890725  | -5.0864592525 | 2.4057416203 |
| C    | -1.9055118681 | -0.3947273395 | 4.7074530222 |
| C    | -0.6267200698 | -2.5138998523 | 4.6879940082 |
| C    | -4.7671578784 | -0.0961551534 | 2.5484023588 |
| C    | 0.9735447914  | -3.8296630949 | 0.3319506179 |
| H    | -1.7851026072 | -0.3706093820 | 5.8002601449 |
| H    | -2.8356039272 | -0.9361837515 | 4.4876547534 |
| H    | -2.0030619397 | 0.6409640799  | 4.3558797581 |
| H    | 2.9152446954  | 0.7172154230  | 4.8695600224 |
|   |   |   |   |
|---|---|---|---|
| C | -1.7927260227 | 2.6075151888 | -4.7387665132 |
| C | -0.9271472128 | 1.6049078630 | -5.2141290935 |
| C | -0.3289331185 | 0.7609076231 | -4.2952528022 |
| C | -0.5971452248 | 0.9099305347 | -2.9037564718 |
| C | -1.4530279307 | 1.9160638881 | -2.4340243902 |
-2.0465699937  2.7609222224  -3.3718276497
0.0967880976  -0.0154536440  -2.1615599421
0.8416594392  -0.7603210547  -3.0438419761
0.6190323939  -0.3417649595  -4.3880060219
1.2776120958  -0.9684622026  -5.4311388568
2.1697328771  -2.0136340824  -5.1280964218
2.3967160245  -2.4163089298  -3.807899189
1.7369405681  -1.7971133352  -2.7463986186
0.0383754449  -0.2122873792  -0.0885965963
0.0273030880  -0.3267988108  1.9083111777
-0.8442085803  -1.1642183223  2.6141282326
-0.7042235506  -1.0800893114  4.0845236202
0.6455999376  -0.3654184722  4.1984912622
0.8553638710  0.4710707769  2.9172972684
2.3763766294  0.5598573492  2.5992265230
3.1214497302  1.2345149109  3.7632625706
2.6202992766  2.6720469282  3.9457503358
1.1148625648  2.6573540303  4.226811244
0.3761134110  1.9573325737  3.0762384153
2.6634287107  1.3711104061  1.3330373998
2.1467424632  2.8020055740  1.4992797056
0.6450979881  2.7582598877  1.796047789
2.8823513886  3.4691966022  2.6649930172
-1.7689200091  -2.0333808731  1.9676129015
-3.0769577417  -1.5887933063  1.6480341099
-3.9786052499  -2.4888714881  1.0652414027
-3.6111365255  -3.7969237387  0.7734770286
-2.3129888227  -4.2142357251  1.0417519213
-1.3747908854  -3.3530074022  1.6239929631
-3.5373574596  -0.1558615008  1.8571078940
-3.7888309471  0.5356931969  0.5149234123
0.0452429830  -3.8654101172  1.8031946243
0.1131126052  -5.1586145299  2.6191815661
-1.8343505872  -0.2802723230  4.7452378721
-0.6554364139  -2.4454698011  4.7683562579
-4.7861501647  -0.0568518423  2.7361291231
0.7202270262  -4.0703900276  0.4443911676
-1.6334484844  -0.1789974132  5.8231765928
-2.7961704705  -0.8016114916  4.6363206655
-1.9366511164  0.7283489286  4.3241978247
2.9964443467  0.6627831659  4.6972955490
4.2043418825  1.2423264518  3.5467344624
1.4424793190  -1.1271403662  4.2439409439
0.7046575782  0.2131935377  5.128972467
2.7538320800  -0.4698093048  2.4683006902
-0.7082846599  1.9675691005  3.2748494359
0.1792443160  -3.0549280267  4.4005290263
-1.5917602242  -3.0088601414  4.6288688275
-0.5153334469  -2.3015042675  5.8506834479
0.1024622629  2.3084004181  0.9470460429
0.2554380641  3.7839576424  1.9203440516
Complex CMA1, Excited state T1.

C  -1.9600266251 -2.3525284454 -4.8810646826
C  -1.1770973717 -1.2500273808 -5.2749728258
C  -0.5197852042 -0.5265622169 -4.2957077467
C  -0.6418112799 -0.9031003908 -2.9269139800
C  -1.4224024673 -2.0012378433 -2.5359810978
C  -2.0789183805 -2.7190359463 -3.5634666464
N   0.0788513056 -0.0630510962 -2.1157493931
C   0.6730087876  0.8714355230 -2.9268650880
C   0.3492319883  0.6448111306 -4.2958038978
C   0.8517410055  1.4835836827 -5.2752759072
C   1.6801201475  2.5521228041 -4.8820888807
C   1.9937562749  2.7743707533 -3.5370623415
C   1.4948584784  1.9384161834 -2.5376104008
Au  0.1433439387 -0.1646124230 -0.0480439596
C   0.1067290143 -0.2640190613  1.9473730788
Complex 1, Ground state S0.

| Atom | X          | Y          | Z          |
|------|------------|------------|------------|
| H    | 0.7114951596 | 3.6996616853 | 4.4705761262 |
| H    | 0.8564340217  | 2.161213407 | 5.3191826441 |
| H    | 3.1031741349  | 3.154895120 | 5.0118268513 |
| H    | 2.4251388979  | 3.4410489664 | 0.7680706158 |
| H    | -2.6493706120 | 0.4124392309 | 2.2903510324 |
| H    | -4.0960210619 | -4.3631516226 | -0.0604209396 |
| H    | -4.6603818659 | -0.6138531977 | 3.4655415648 |
| H    | -5.751729745 | -0.4733361351 | 1.9486473360 |
| H    | -4.9924700811 | 0.9901081088 | 2.7657617297 |
| H    | -0.3554372650 | -5.0534856316 | 3.4158345179 |
| H    | 1.2461186151  | -5.3935865280 | 2.7119167774 |
| H    | -0.2233815716 | -5.9302102634 | 1.8754671973 |
| H    | 0.9608487184  | -2.977959539 | -0.1674014698 |
| H    | 0.4681642065  | -4.6885514421 | -0.2656480953 |
| H    | 1.9778859213  | -4.246750943 | 0.5675374428 |
| H    | 1.7279713384  | 2.1047549342 | -1.4841213594 |
| H    | 2.6364764514  | 3.614410997 | -3.2651762149 |
| H    | -1.5116146773 | -2.2779050225 | -1.4826018121 |
| H    | -2.6957070254 | -3.5782196485 | -3.263782106 |
| H    | 0.6145147491  | 1.3279218122 | -6.3301703313 |
| H    | 2.0837950349  | 3.222760528 | -5.6444935068 |
| H    | -1.0971259472 | -0.978084154 | -6.3299360108 |
| H    | -2.4863636672 | -2.9315627587 | -5.6432959820 |

Complex 1, Ground state S0.

| Atom | X          | Y          | Z          |
|------|------------|------------|------------|
| C    | 0.0008842877 | -0.0289037376 | 1.9897406761 |
| N    | -0.8206722727 | -0.7652938102 | 2.7030423246 |
| F    | -2.697241816 | -1.2210475650 | -1.3008173214 |
| Au   | -0.0117985220 | -0.1213808109 | -0.0187781354 |
| N    | -0.0329282923 | -0.2408075728 | -2.0897035122 |
| F    | 2.8411368242  | 0.0359280924 | -1.4940723301 |
| C    | 0.8699056143  | 0.8106128189 | 2.9257920806 |
| C    | 0.7033617163  | 0.0518588859 | 4.2574660058 |
| H    | 1.5187538988  | -0.6850591570 | 4.3407381023 |
| H    | 0.7569556919  | 0.6919368474 | 5.1445253800 |
| C    | -0.6295398832 | -0.6896776604 | 4.2013375772 |
| C    | -1.8554297088 | -1.5960328813 | 2.1245298800 |
| C    | -1.5609355654 | -2.9400950951 | 1.7950771737 |
| C    | -2.6062231108 | -3.7381499283 | 1.3178935429 |
| H    | -2.4024943101 | -4.779571051 | 1.0572310134 |
| C    | -3.8904301741 | -3.2330645242 | 1.1575530194 |
| H    | -4.6920560474 | -3.8795111766 | 0.7909586090 |
| C    | -4.1437454799 | -1.8964872638 | 1.4359117290 |
| H    | -5.1448681977 | -1.4927961888 | 1.2662366183 |
| C    | -3.1399659894 | -1.0446643969 | 1.9097528236 |
| C    | -3.4796106225 | 0.4267191077 | 2.0958739779 |
| H    | -2.6275950340 | 0.9158672256 | 2.5844533377 |
| C    | -3.6811580100 | 1.1246596928 | 0.7465109647 |
| H    | -3.8993176722 | 2.1927511767 | 0.9053396785 |
| H    | -4.5279613926 | 0.6845902225 | 0.1968762748 |
Complex 1, Excited state S1.

C  -0.0880485129  0.1135338833  1.9105858429
N  -0.7486832468  -0.8446661733  2.6863233035
F  -2.8495459468  0.1241641442  -1.5890358834
Au -0.0673183845  -0.0320188951  -0.0859137478
N   0.0094841088  -0.1540360894  -2.1930947570
F   2.7910203815  -0.4221053635  -1.2282588848
C   0.7681557668  0.9724357995  2.8377023848
C   0.9228460001  0.0198549598  4.0448554223
H  -0.3211619419  -0.8775364208  4.1048480429
H   1.8047421381  -0.6158594487  3.8584655297
H   1.0904140824  0.5239071192  5.0059910355
C  -0.3211619419  -0.8775364208  4.1048480429
C   1.8454742245  -1.5939322033  2.1678407315
C   1.6419984293  -2.9038582144  1.6597548833
C   -2.7442780492  -3.6301439880  1.1899290018
H  -2.5899897866  -4.6435862708  0.8088318787
C   -4.0219370974  -3.0849930774  1.7996385733
H  -4.8690115392  -3.6691233150  0.8099303609
C   -4.2089057786  -1.7815961832  1.6270355225
H  -5.2078988888  -1.3419948934  1.5952980549
C   -3.1434130523  -1.0169045563  2.1155836060
C   -3.4330938958  0.4131794628  2.5404737789
H  -2.4999559702  0.8263890233  2.9427017468
C   -3.8370236330  1.2848486340  1.3481492719
H  -4.0061421027  2.3233479581  1.6760509008
H  -4.7722048979  0.9245218017  0.8886389616
H  -3.0622075911  1.2954259858  0.5690487258
C  -4.5059359675  0.4936310131  3.6289480061
H  -4.6140120644  1.5315458457  3.9826835714
H  -4.2622048106  -0.1359708897  4.4970849640
H  -5.4892620784  0.1737072108  3.2480951414
C  -0.2684059489  -3.5428680423  1.5314793431
H   0.4586126187  -2.8430059533  1.9670592376
C   0.1115246049  -3.7376080645  0.0597445452
H   1.1349349292  -4.1382095293  -0.0247116730
H   0.0748422399  -2.7840409572  -0.4910123699
Complex 1, Excited state T1.

C  -0.0532922913  0.0009834105  1.9899124346
N  -0.8271081480  -0.7669863954  2.7188054710
F  -2.8966034088  -0.7659755587  -1.3629414366
Au -0.1110534278  -0.0793386638  -0.0220570792
N  -0.1120119495  -0.1741959007  -2.1023290364
F  2.7268529082  -0.2658011963  -1.3200874809
C  0.8275004790  0.8524961060  2.8998896668
C  0.7255784400  0.0805461653  4.2315877098
C  -0.0532922913  0.0009834105  1.9899124346
Complex 2, Ground state S0.

Cu  -0.0030453697 -0.0119788752  -0.0202258960
F   -1.4723022664  2.4785124766  -0.7439338829
N   1.0220614171  0.3485150560  2.6586121866
F   0.7898055907  -2.5977281909  -1.5923783184
|   |     X       |     Y       |     Z       |
|---|------------|------------|------------|
| C | -1.1854379151 | -0.3146673283 | 2.7798106053 |
| N | -0.2032619805 | 0.1281051215 | -1.9300861487 |
| C | 0.0097497570 | 0.0129382320 | 1.8976890922 |
| C | -0.6450077219 | 1.2438909000 | -2.5906042449 |
| C | -0.7788835399 | 0.2823945746 | 4.1432021970 |
| H | -1.2275503315 | 1.8424566661 | 4.2360903182 |
| H | -1.1216622153 | -0.300881275 | 5.0063240930 |
| C | 0.7457475358 | 0.4167339746 | 4.1459809853 |
| C | -1.3176207296 | -1.8697752931 | 2.7975863114 |
| C | -0.4249720366 | -2.3450231351 | 3.1036004025 |
| C | 2.6583255312 | 1.9647981306 | 1.7570415349 |
| C | 1.6407636514 | 3.0879104425 | 1.6486697670 |
| H | 0.6845983402 | 2.7299750280 | 2.0582250459 |
| C | 2.3400763845 | 0.6432876362 | 2.1426493518 |
| C | -1.7730972883 | -2.3916122415 | 1.4097520689 |
| H | -0.9919017181 | -2.1704463203 | 0.6623227690 |
| H | -1.8664147398 | -3.4901535109 | 1.4549193821 |
| C | 2.9456527319 | -1.8641095072 | 2.2518340191 |
| H | 1.9797059216 | -1.9213089671 | 2.7671407081 |
| C | 0.1252055310 | -0.1423705800 | -4.2182543000 |
| C | -2.9578756998 | -0.2504832328 | 0.9213950078 |
| H | -2.2365997250 | 0.0401157550 | 0.1394119045 |
| H | -3.9175926369 | 0.2147586753 | 0.6380386679 |
| C | 3.9717534180 | 2.2319665959 | 1.3527283594 |
| H | 4.2361259053 | 3.2481619108 | 1.0499531114 |
| C | -0.8578502426 | 2.2043013551 | -4.8487843222 |
| H | -0.7113283693 | 2.1300344988 | -5.9295741800 |
| C | 3.2912510595 | -0.3986833731 | 2.0500594459 |
| C | -0.4628236114 | 1.1552862200 | -4.0029215596 |
| C | 0.5319890350 | -0.8560862598 | -5.3573768911 |
| C | 0.4448375106 | -0.4097764934 | -6.3515044560 |
| C | 1.4022665940 | 3.4210981390 | 0.1730926637 |
| H | 0.6149959228 | 4.1839037138 | 0.0723188643 |
| C | 1.0825833104 | 2.5302495107 | -0.3871239282 |
| H | 2.3187081264 | 3.8119096582 | -0.2969090530 |
| C | 0.2409648650 | -0.7120107130 | -2.9150182492 |
| C | -3.1052257863 | -1.7716811489 | 0.9764686153 |
| H | -3.3799069899 | -2.1529102062 | -0.0215740789 |
| C | 1.4313454887 | -0.7101617399 | 4.9156346642 |
| C | 2.5251458036 | -0.6590110092 | 4.8198407296 |
| H | 1.0875969823 | -1.7041276918 | 4.6004311270 |
| H | 1.1860299791 | -0.5929781534 | 5.9814859894 |
| C | 4.9364454768 | 1.2338366187 | 1.3112819890 |
| H | 5.9573652454 | 1.4682908338 | 0.9988671810 |
| H | -2.5324432593 | 0.2855879492 | 2.2912740327 |
| H | -2.4220972828 | 1.3825519274 | 2.2401653041 |
| C | -1.2555225722 | 2.3952303667 | -2.074024033 |
| C | 0.7299455620 | -2.022005187 | -2.8071345325 |
| C | -3.6279715672 | -0.0787911584 | 3.3048562254 |
| H | -3.3902772316 | 0.3215385254 | 4.3035490580 |
| H | -4.5753597201 | 0.3931631710 | 2.9941369752 |
Complex 2, Excited state S1.

Cu  -0.2517821910  0.0583903517  -0.0334966167
F   -1.5144277672  2.6273430626  -0.7937254081
N    1.0402985059  0.3598558469  2.6433325744
F    0.7071284541  -2.4505686786  -1.5267924062
C   -1.2175887245  -0.3318878184  2.7667658442
N   -0.2175469585  0.2803569236  -1.9285082267
C    0.0670188486  0.0767811535  1.8571009502
C   -0.6611898156  1.3861946277  -2.6127361061
C   -0.7875821262  0.3136891382  4.1018284455
H   -1.2349260339  1.3197351153  4.1542879921
H   -1.1289813641  -0.2332538864  4.9917561039
C    0.7452318256  0.4500522523  4.0963428657
C   -1.3672409131  -1.8863467037  2.8437829446
H   -0.4012171447  -2.3195267338  3.1516034479
| X         | Y         | Z         |
|-----------|-----------|-----------|
| H         | 2.228307127 -2.236691039 0.2011165599 |
| C         | -4.1782434294 -2.2545704478 2.0332252529 |
| H         | -4.2749873486 -3.3530842426 2.0795291454 |
| H         | -5.1567777631 -1.8567094630 1.7127150690 |
| C         | 2.1335799135 4.3021079326 2.3761015143 |
| H         | 1.3464479012 5.0727368606 2.3499241895 |
| H         | 3.0423564148 4.7498449774 1.9421841731 |
| H         | 2.3453663508 4.0712063323 3.4300721946 |
| C         | 1.0921002616 -2.6352056245 -3.8481809753 |
| H         | 1.4543994459 -3.6542626606 -3.6987235600 |
| C         | -3.8019340726 -1.7002080845 3.4101485703 |
| H         | -4.5812144728 -1.9711144656 4.1430053479 |
| C         | -1.6400315902 3.5697366500 -2.9556013874 |
| H         | -2.1151200383 4.4578938223 -2.5334084528 |
| C         | 1.1707027951 1.7911785685 4.6934069351 |
| H         | 2.2617785959 1.9303815560 4.6409490247 |
| H         | 0.8798781177 1.8287501215 5.7547305129 |
| H         | 0.6842065402 2.6312739607 4.1800281372 |
| C         | -1.4099188827 3.4538480162 -4.3360729240 |
| H         | -1.7062298850 4.2756726981 -4.9918242723 |
| C         | 3.8672560678 -2.5690587077 3.2461707891 |
| H         | 3.9103449517 -2.0305961417 4.2039472587 |
| H         | 4.8940921432 -2.6313908212 2.8515626153 |
| H         | 3.5335426825 -3.5987578345 3.4515915813 |

**Complex 2, Excited state T1.**

| X         | Y         | Z         |
|-----------|-----------|-----------|
| Cu        | -0.1595678670 0.1045486931 0.0242839298 |
| F         | -1.5449827827 2.6207933330 -0.7300248778 |
| N         | 1.0629672363 0.3626136833 2.6730357522 |
| F         | 0.7746378178 -2.3934215431 -1.5188174816 |
| C         | -1.2129814342 -0.3343224150 2.7703307514 |
| N         | -0.2648934880 0.2910989439 -1.9055379741 |
| C         | -0.0433092863 0.0842699719 1.8992476664 |
| C         | -0.7262612392 1.9393599232 -2.5766422122 |
| C         | -0.7938257073 0.3211292589 4.1072405634 |
| H         | -1.2614089862 1.3173492708 4.1591513366 |
| H         | -1.1335738697 -0.2390500505 4.9894912218 |
| C         | 0.7400243454 0.4856132257 4.1198034695 |
| C         | -1.3469803798 1.8860129604 2.8364211990 |
| H         | -0.3876306838 -2.3105368926 3.1751534505 |
| C         | 2.7122198073 1.8832407898 1.6501864381 |
| C         | 1.7300358992 3.0386261434 1.5622326726 |
| H         | 0.7762841385 2.6993125809 1.9923031253 |
| C         | 2.3557683561 0.5904141655 2.1135184954 |
| C         | -1.6793846718 -2.4302388110 1.4417817375 |
| H         | -0.8740244492 -2.1614996903 0.7288737336 |
| H         | -1.7183412806 -3.5325116236 1.4640502985 |
| C         | 2.9198715779 -1.9217110817 2.3209390958 |
| H         | 1.9057238813 -1.9199221908 2.7415339100 |
| C         | 0.0614297613 0.0032631837 -4.1879834632 |
Complex 3, Ground state S0.

Au  -0.0085593454 -0.0542653031 0.0557072463
N   -2.0633988127 -0.028450439 -0.0716508196
C   -4.8377816302 1.5653453686 1.6492068467
H   -5.6487977238 2.2454798095 1.3709717901
N   2.7251325691 -0.9252312723 0.6872185595
C   1.9939642810 -0.0471955162 0.0331015418
C   3.1281417400 2.2072129081 0.0534699075
H   3.4237232205 1.9664806524 1.0874422910
C   4.1975722424 -0.9226474971 0.3597082861
C   -4.7267516890 1.1122039746 2.9588189464
C   -3.796633872 1.358697053 -0.739362424
C   -3.916775163 1.1344353471 0.6861979458
C   1.4345149227 3.4546192965 -1.3257084755
H   0.5118261394 4.0554339963 -1.2820620891
C   2.9193580333 0.8792609227 -0.7565147916
C   3.8225158794 3.4048847310 -2.0412578647
H   4.6365488588 3.9714479645 -2.5238783950
C   1.8482528275 3.0556784921 0.0930807116
H   2.0404583131 3.955839028 0.7015800655
H   1.0268885015 2.5108246350 0.5845904830
C   -3.1426329973 1.2403091033 -3.4064509396
H   -2.9228014722 1.1635865609 -4.4771555564
C   -2.8563956064 0.2574161429 1.0325096101
C   4.1975353135 0.0185172066 -0.8465793352
C   5.1272927519 0.5973534939 -0.8956486099
H   4.1432320741 -0.5789460149 -1.7712920047
C   5.0590180546 -0.4185312559 1.5179408436
H   4.9439647033 -1.0543400674 2.4072054833
H   4.8423627053 0.6201698736 1.7948597663
H   6.1147176881 -0.4666711778 1.2128421019
C   1.7106135687 -3.1011943879 1.2995232032
C   -4.5572032436 2.0879343873 -1.6529341209
H   -5.4183315898 2.6730708969 -1.3159955129
C   2.4315056174 1.3086944822 -2.167764583
| Symbol | X       | Y       | Z       |
|--------|---------|---------|---------|
| H      | 2.231   | 0.397   | -2.758  |
| C      | -2.764  | -0.260  | 2.342   |
| C      | 3.551   | 2.123   | -2.839  |
| H      | 4.473   | 1.529   | -2.939  |
| C      | 3.237   | 2.383   | -3.864  |
| H      | 4.473   | 1.529   | -2.939  |
| H      | 3.237   | 2.383   | -3.864  |
| C      | 3.551   | 2.123   | -2.839  |
| H      | 4.473   | 1.529   | -2.939  |
| H      | 3.237   | 2.383   | -3.864  |
| C      | -4.223  | 2.053   | -3.002  |
| H      | -1.309  | -0.456  | -2.700  |
| H      | -1.521  | -1.480  | -2.699  |
| C      | 2.111   | 3.021   | 4.030   |
| C      | -5.682  | 2.164   | 4.800   |
| H      | -6.497  | 2.168   | 4.313   |
| H      | -5.176  | 2.161   | 4.313   |
| C      | -6.141  | 0.700   | 4.549   |
| C      | -2.671  | 0.601   | -1.449  |
| C      | 2.553   | 4.260   | -1.991  |
| H      | 2.250   | 4.557   | -3.009  |
| H      | 2.745   | 5.190   | 4.129   |
| C      | -4.998  | 2.835   | -4.026  |
| H      | -5.369  | 2.189   | -4.838  |
| H      | -4.375  | 3.615   | -4.496  |
| C      | -5.867  | 3.336   | -3.574  |
| C      | 2.431   | 0.044   | 3.452   |
| C      | 2.431   | 0.044   | 3.452   |
| H      | 4.379   | 0.964   | 4.098   |
| H      | 5.199   | 2.520   | 0.603   |
| C      | 4.684   | -2.318  | 0.013   |
| H      | 4.602   | -3.016  | 0.833   |
| H      | 5.745   | -2.253  | -0.295  |
| C      | 4.135   | 0.193   | 3.268   |
| H      | 1.174   | 2.186   | 2.135   |
| C      | 0.897   | 2.444   | 3.171   |
| H      | 0.314   | 1.643   | 0.171   |
| C      | -3.699  | 0.195   | 3.269   |
| H      | 3.647   | 0.202   | 4.288   |
| H      | 2.361   | 0.495   | 2.525   |
| C      | 2.176   | -1.822  | 1.680   |
| C      | 1.575   | -3.562  | -0.143  |
| H      | 2.005   | -2.782  | 0.789   |
| C      | 1.651   | 3.985   | 1.936   |
| H      | 1.593   | 5.028   | 0.414   |
| C      | 2.309   | 4.877   | 1.722   |
| H      | 2.252   | -5.131  | -1.484  |
| H      | 1.850   | 0.139   | 0.129   |
| H      | 3.370   | -0.835  | 0.129   |
Complex 3, Excited state S1.

Au  -0.0177198012  0.1300728145  0.0776107012
N   -2.1776490870  0.1802248448 -0.1028272440
C   -5.3147421236  1.3261236449  1.2577074056
H   -6.2641214054  1.6966898636  0.8614639591
N   2.6869957459 -0.9522219864  0.597863084
C   1.9958194490  0.1956518936  0.1912627861
C   3.6073866189  2.2216858374  0.3248345730
H   4.0355165519  1.775213692  1.2357314050
C   4.0495111356 -1.076925463  0.0313689894
C   -5.1319941539  1.2037457672  2.6501862182
C   -4.1648608872  0.9035109899 -1.0306823618
C   -4.2878912399  0.9585077579  0.4122645332
C   1.9519024061  3.9242083084 -0.4916868782
H   1.1809151259  4.6505068559 -0.1818629775
C   2.9772789108  1.0908559718 -0.5633137433
C   4.1256336170  3.628457590  -1.6849020253
H   4.9259010830  4.1429187204 -2.2450068361
C   2.5352374579  3.2329619977  0.7435112467
H   2.9820237901  3.9830474389  1.4196778754
H   1.7394114607  2.7200783865  1.3067821733
C   -3.3418609966  0.4877316516 -3.6266464824
H   -3.0359322716  0.3110307879 -4.6613833054
C   -3.0391140697  0.4783219866  0.9153785660
C   4.0263731652  0.0496112467 -1.0109341415
H   5.0362276838  0.4519697279 -1.1681041591
H   3.6950042189 -0.3681269005 -1.9764116410
C   5.1628940994 -0.8854397236  1.0712651161
H   5.0760514540 -1.6260262854  1.8807229930
H   5.1619812884  0.1162463671  1.5178456892
H   6.1435867524 -1.0324774426  0.5930930951
C   1.4960515961 -3.0066472851  1.2976022281
C   -5.0274723553  1.2241877442 -2.0586288661
Complex 3, Excited state T1.

Au  -0.0185654113 -0.0550227281 -0.0213968146
N   -2.1724365020  0.0827430891 -0.122834796
C   -5.0634498806  1.4140177081  1.5736244448
H   -5.9335293547  2.0195798565  1.3055824496
N   -5.7284705221 -0.9814540783  0.6756211496
C   -1.9888365625  0.0290866834  0.0515213050
C   -3.3471403546  2.2286185025  0.0865484578
H   -3.6750240447  1.945105337  1.1002922201
C   -4.1585900991 -0.1041838186  0.2997157976
C   -4.8919382089  0.9760585320  2.9036284762
C   -4.0249984058  1.2801804070 -0.8053276728
C   -4.1258771781  1.0588269507  0.6250940265
C   -1.6796146245  3.6142179276 -1.1830723312
C   -0.8069177672  4.2826407444 -1.0863144253
C   -2.9653022872  0.9274974054 -0.705893905
C   -4.0222098472  3.4138004111 -0.20195823030
H   -4.8466391877  3.9341406258 -2.5371406117
C   -2.1343868214  3.1586774777  0.2069759060
C   -2.4035523285  4.0341288429  0.8237607489
H   -1.3144575729  2.6338387129  0.7224075521
C   -3.3203880101  1.2158380445 -3.4713249936
C   -3.0740416189  1.1732878105 -4.5357876927
C   -2.9757263135  0.2854575279  0.9683873393
C   -4.1671646288 -0.0302166897 -0.8758600968
H   -5.1409554027  0.4707297667 -0.9575841846
H   -4.0186724554 -0.5964396804 -1.8103121449
C   -5.0912135831 -0.5707839592  1.4349850169
C   -4.9886112706 -1.2317741054  2.3085735500
H   -4.9017693825  0.4609290910  1.7568027746
H   -6.1373082067 -0.6282191882  1.0968623517
| C          | 1.6767817604 | -3.0997821643 | 1.3765953154 |
| C          | -4.8244829658 | 1.9381424646 | -1.7178349120 |
| H          | -5.7290887229 | 2.4624038272 | -1.3975751974 |
| C          | 2.4837761597  | 1.4210406589 | -2.0976070307 |
| H          | 2.1913452023  | 0.5351027800 | -2.6880139143 |
| C          | -2.8185719191 | -0.2168253707 | 2.2840595062 |
| C          | 3.6202622702  | 2.1655824156 | -2.8161111641 |
| H          | 4.4921407881  | 1.5078764866 | -2.9619129719 |
| H          | 3.2819143998  | 2.4608762679 | -3.8246981761 |
| C          | 3.4990849940  | 0.1143729899 | 4.5851814286 |
| H          | 3.8445715394  | 1.1463396275 | 4.7564410122 |
| H          | 4.3842318762  | -0.5105193534 | 4.3951380521 |
| H          | 3.0425729991  | -0.2332482000 | 5.5259412947 |
| C          | -1.3426609731 | -0.2804307282 | -3.0941484047 |
| H          | -1.2698255971 | -0.2051229960 | -4.1874832663 |
| H          | -1.4721447027 | -1.3409724950 | -2.8271624700 |
| C          | -0.3847573665 | 0.0307983057 | -2.6507752953 |
| C          | 2.1134824051  | -1.3421156123 | 3.0321357706 |
| C          | -5.8761929371 | 1.3742363008 | 3.9604260895 |
| H          | -6.9110841879 | 1.3117368890 | 3.5906327312 |
| H          | -5.7103274914 | 2.4190718538 | 4.274129815 |
| H          | -5.7901129621 | 0.7426392811 | 4.8552528449 |
| C          | -2.8268733134 | 0.6149594061 | -1.2071324999 |
| C          | 2.8182044156  | 4.3510132228 | -1.8933877167 |
| C          | 2.8480274446  | 4.6867868892 | -2.8919836384 |
| H          | 3.1005970082  | 5.2559900275 | -1.3275766000 |
| C          | -5.2923145502 | 2.6680739855 | -4.084580534 |
| H          | -5.0348235018 | 2.3872848520 | -5.1149846034 |
| H          | -5.1397581888 | 3.7564933714 | -3.9882337169 |
| H          | -6.3668814197 | 2.4818042963 | -3.9334708787 |
| C          | 2.5040597025  | 0.0725757932 | 3.4247083422 |
| H          | 2.9757771615  | 0.5306559652 | 2.5477760131 |
| C          | 4.4728628104  | 3.0004296457 | -0.6161838858 |
| H          | 4.7221137435  | 3.8987240283 | -0.0239405494 |
| H          | 5.3997504509  | 2.4069983922 | -0.6689572909 |
| C          | 4.6274001235  | -2.3984779255 | -0.1527786588 |
| H          | 4.5710784466  | -3.1311360147 | 0.6667127799 |
| H          | 5.6781484434  | -2.3416246695 | -0.4767832549 |
| H          | 4.0350582836  | -2.7677130370 | -1.0002126377 |
| C          | 1.2934592802  | 2.3789413298 | -1.9962773595 |
| H          | 0.9747694845  | 2.6757419046 | -3.0113696251 |
| H          | 0.4329976465  | 1.8784870009 | -1.5229762362 |
| C          | -3.7908269620 | 0.1656290324 | 3.2142486646 |
| H          | -3.6939733592 | -0.2083911262 | 4.2371795676 |
| C          | -2.4823461010 | 0.5367586934 | -2.5794032782 |
| C          | 2.1784781087  | -1.8112893673 | 1.6945121665 |
| C          | 1.5410968344  | -3.6068534750 | -0.0503427573 |
| H          | 1.9866880296  | -2.8463659401 | -0.7068932884 |
| C          | 1.6338234094  | -2.1990720975 | 4.0281654594 |
| H          | 1.5990019879  | -1.8473512318 | 5.0625497711 |
| Atoms | X         | Y         | Z         |
|-------|-----------|-----------|-----------|
| C     | 2.2535817542 | -4.9410992569 | -0.2812124266 |
| H     | 2.2067061567  | -5.2230892231 | -1.3452412811 |
| H     | 1.7774101543  | -5.7540606202 | 0.2899526698  |
| H     | 3.3118572551  | -4.9057577890 | 0.0129393898  |
| C     | -1.7413287559 | -1.1769906541 | 2.6641775265  |
| H     | -1.8130543623 | -1.4493637157 | 3.7249808543  |
| H     | -0.7371242408 | -0.7704877416 | 2.4775272547  |
| H     | -1.8148121167 | -2.0982448261 | 2.0659083994  |
| C     | 1.2041409594  | -3.4869254584 | 3.704051884   |
| H     | 0.8368792111  | -3.7335811002 | -0.4478460581 |
| H     | -0.0209681052 | -0.4610463448 | -1.4966934908 |
| H     | -0.457916834  | -2.7703358146 | -0.3510691554 |
| C     | 1.2123347965  | -4.751570507  | 0.1766528659  |
| C     | 1.2721168087  | 0.9205899557  | 3.7504051884  |
| H     | 0.6064808730  | 0.9978134120  | 2.877883501   |
| C     | 1.5734913686  | 1.9423715513  | 4.0324455433  |
| H     | 0.7017148955  | 0.4952158696  | 4.5919644854  |

Complex 3b, Ground state S0.

| Atoms | X         | Y         | Z         |
|-------|-----------|-----------|-----------|
| Au    | 0.0162917614 | -0.0398872099 | 0.0189820767 |
| N     | 2.7406304713  | -0.2261520145 | 1.0992587765 |
| C     | 4.3100344589  | 0.4718445514  | -0.4707018722 |
| H     | 5.1831692391  | 0.1137854062  | -1.0275977098 |
| H     | 4.4349538235  | 1.5593389805  | -0.3443555375 |
| N     | -2.0496811218 | -0.0063203894 | 0.0669418631  |
| C     | 2.1988265045  | -0.5091013142 | 2.4130124844  |
| C     | 1.6228730193  | 0.2522690753  | 4.6244509334  |
| H     | 1.4505157855  | 1.0658316700  | 5.3324736801  |
| C     | 1.9818378728  | 0.5624328864  | 3.3096946492  |
| H     | 2.0281856963  | -0.0283509514 | 0.0124997651  |
| C     | 4.2372235764  | -0.1775299686 | 0.9085378791  |
| C     | -2.7919952166 | -1.1536372771 | 0.3033448746  |
| C     | 2.9626872472  | 0.2126423333  | -1.1754822797 |
| C     | 1.9954690291  | 2.0277472978  | 2.9056358917  |
| H     | 2.3661362727  | 2.0967522612  | 1.8706763467  |
| C     | 1.9583970221  | -1.8478131812 | 2.7973761157  |
| C     | -3.8927254600 | -0.8836714084 | 1.1593285896  |
| C     | -2.7205074118 | 1.0217073643  | 0.7141068402  |
| C     | 2.8858267514  | 2.8984274712  | 3.7951086267  |
| H     | 3.9228730454  | 2.5371599753  | 3.8451662928  |
| H     | 2.5014523672  | 2.3961483876  | 4.8259141966  |
| H     | 2.9019428154  | 3.9325068869  | 3.4172938044  |
| C     | -2.4621015283 | 2.4106505597  | 0.6743315349  |
| C     | -4.5958883970 | -3.1893228895 | 1.0517624931  |
| C     | 1.6032312274  | -2.0925277686 | 4.1281222319  |
| H     | 1.4131040610  | -3.1206095241 | 4.4440719737  |
| C     | -2.6290681499 | -2.4436406985 | -0.2497374245 |
| Element | x          | y          | z          |
|---------|------------|------------|------------|
| C       | 0.5625602158 | 2.5734302204 | 2.9128975833 |
| H       | -0.1201225504 | 1.949625292  | 2.3191062638 |
| H       | 0.5340806794  | 3.5961405496 | 2.5057621469 |
| C       | -3.8464983097 | 0.5295832258 | 1.4255021280 |
| C       | 2.9859913980  | -1.0312874093 | -2.1304008345 |
| H       | -0.1201225504 | 1.9499625292 | 2.3191062638 |
| H       | 0.5340806794  | 3.5961405496 | 2.5057621469 |
| H       | 0.1608645266  | 2.6126068280 | 3.9376678662 |
| C       | -3.8464983097 | 0.5295832258 | 1.4255021280 |
| C       | 2.9859913980  | -1.0312874093 | -2.1304008345 |
| H       | -0.1201225504 | 1.9499625292 | 2.3191062638 |
| H       | 0.5340806794  | 3.5961405496 | 2.5057621469 |
| H       | 0.1608645266  | 2.6126068280 | 3.9376678662 |
| C       | -3.8464983097 | 0.5295832258 | 1.4255021280 |
| C       | 2.9859913980  | -1.0312874093 | -2.1304008345 |
| H       | -0.1201225504 | 1.9499625292 | 2.3191062638 |
| H       | 0.5340806794  | 3.5961405496 | 2.5057621469 |
| H       | 0.1608645266  | 2.6126068280 | 3.9376678662 |
| C       | -3.8464983097 | 0.5295832258 | 1.4255021280 |
| C       | 2.9859913980  | -1.0312874093 | -2.1304008345 |
| H       | -0.1201225504 | 1.9499625292 | 2.3191062638 |
| H       | 0.5340806794  | 3.5961405496 | 2.5057621469 |
| H       | 0.1608645266  | 2.6126068280 | 3.9376678662 |
| C       | -3.8464983097 | 0.5295832258 | 1.4255021280 |
| C       | 2.9859913980  | -1.0312874093 | -2.1304008345 |
| H       | -0.1201225504 | 1.9499625292 | 2.3191062638 |
| H       | 0.5340806794  | 3.5961405496 | 2.5057621469 |
| H       | 0.1608645266  | 2.6126068280 | 3.9376678662 |
| C       | -3.8464983097 | 0.5295832258 | 1.4255021280 |
| C       | 2.9859913980  | -1.0312874093 | -2.1304008345 |
| H       | -0.1201225504 | 1.9499625292 | 2.3191062638 |
| H       | 0.5340806794  | 3.5961405496 | 2.5057621469 |
| H       | 0.1608645266  | 2.6126068280 | 3.9376678662 |
| C       | -3.8464983097 | 0.5295832258 | 1.4255021280 |
| C       | 2.9859913980  | -1.0312874093 | -2.1304008345 |
| H       | -0.1201225504 | 1.9499625292 | 2.3191062638 |
| H       | 0.5340806794  | 3.5961405496 | 2.5057621469 |
| H       | 0.1608645266  | 2.6126068280 | 3.9376678662 |
| C       | -3.8464983097 | 0.5295832258 | 1.4255021280 |
### Complex 3b, Excited state S1.

| Element | X          | Y          | Z          |
|---------|------------|------------|------------|
| N       | 0.0067018784 | -0.0343843987 | 0.1142259628 |
| C       | 2.8258771082  | -0.2443860945 | 1.1599424659 |
| C       | 4.2566114535  | 0.5365553404  | -0.4870295271 |
| H       | 5.1451581949  | 0.2753213037  | -1.0760574166 |
| H       | 4.2946579694  | 1.6253991295  | -0.3171786205 |
| N       | -2.1372114144 | -0.0099618426 | 0.2579953910 |
| C       | 2.3526921344  | -0.5519298715 | 2.4686032668 |
| C       | 1.8208992789  | 0.1660246159  | 4.7270843195 |
| H       | 1.6654234450  | 0.9693575386  | 5.4520707737 |
| C       | 2.1299686301  | 0.4921476178  | 3.4022566218 |
| C       | 2.0126648427  | -0.0294785253 | 0.0364092471 |
| C       | 4.2730891802  | -0.1656373511 | 0.8721683069 |
| C       | -2.9281914037 | -1.1247059452 | 0.3800868874 |
| C       | 2.9140608536  | 0.2102388451  | -1.1776597053 |
| C       | 2.1240825427  | 1.9596993771  | 3.0107386231 |
| H       | 2.4611089420  | 2.0227813235  | 1.9655783827 |
| C       | 2.1462757830  | -1.8961369408 | 2.8671260927 |
| C       | -4.1247803777 | -0.8253514096 | 1.0988928833 |
| C       | -2.8498980242 | 1.0471616729  | 0.7645678908 |
| C       | 3.0358097994  | 2.8293469063  | 3.8786148796 |
| H       | 4.0718440331  | 2.4626716687  | 3.8948704413 |
| H       | 2.6829401958  | 2.8678976827  | 4.9215543388 |
| C       | 3.0475071854  | 3.8652036634  | 3.5033674099 |
| C       | -2.5494768294 | 2.4328895493  | 0.7080938922 |
| C       | -4.8349766497 | -3.1173642144 | 0.9254749126 |
| C       | 1.8400745352  | -2.1709972627 | 4.2048059619 |

---

Au 0.0067018784 -0.0343843987 0.1142259628
N 2.8258771082 -0.2443860945 1.1599424659
C 4.2566114535 0.5365553404 -0.4870295271
H 5.1451581949 0.2753213037 -1.0760574166
H 4.2946579694 1.6253991295 -0.3171786205
N -2.1372114144 -0.0099618426 0.2579953910
C 2.3526921344 -0.5519298715 2.4686032668
C 1.8208992789 0.1660246159 4.7270843195
H 1.6654234450 0.9693575386 5.4520707737
C 2.1299686301 0.4921476178 3.4022566218
C 2.0126648427 -0.0294785253 0.0364092471
C 4.2730891802 -0.1656373511 0.8721683069
C -2.9281914037 -1.1247059452 0.3800868874
C 2.9140608536 0.2102388451 -1.1776597053
C 2.1240825427 1.9596993771 3.0107386231
H 2.4611089420 2.0227813235 1.9655783827
C 2.1462757830 -1.8961369408 2.8671260927
C -4.1247803777 -0.8253514096 1.0988928833
C -2.8498980242 1.0471616729 0.7645678908
C 3.0358097994 2.8293469063 3.8786148796
H 4.0718440331 2.4626716687 3.8948704413
H 2.6829401958 2.8678976827 4.9215543388
C 3.0475071854 3.8652036634 3.5033674099
C -2.5494768294 2.4328895493 0.7080938922
C -4.8349766497 -3.1173642144 0.9254749126
C 1.8400745352 -2.1709972627 4.2048059619
| Atom | X   | Y   | Z   |
|------|-----|-----|-----|
| H    | 4.5462642953 | 1.8960618166 | -2.6916208811 |
| C    | 4.0751527220 | -0.7829240154 | -3.2395813031 |
| H    | 4.1342219598 | -1.6720353435 | -3.8921310327 |
| H    | 5.0805574555 | -0.6534080308 | -2.8074578502 |
| C    | 3.6973192494 | 0.4455419874  | -4.0711325758 |
| H    | 4.4778729921 | 0.6339783730  | -4.8282842321 |
| C    | -5.5130083191 | 3.8309055671  | 2.6930862776  |
| H    | -6.5681677633 | 3.5247382860  | 2.6404566897  |
| H    | -5.4225875832 | 4.8423489433  | 2.7275204153  |
| H    | -5.2478448853 | 3.8965721589  | 3.7624485473  |
| C    | 1.2846840614  | -0.0626287880 | -3.7042212455 |
| H    | 0.3144064780  | -2.543727493  | -4.1945556518 |
| C    | 3.087724622  | -4.1940686449 | 2.2801740798  |
| H    | 4.1233224787 | -3.8532427199 | 2.4194777442  |
| H    | 3.0926238794 | -4.9761264181 | 1.5038970111  |
| H    | 2.766930056  | -4.6716091767 | 3.2193701788  |
| C    | -4.6201915170| 2.8556229763  | 1.9894042608  |
| C    | 2.3587663859 | 0.1861370582  | -4.7668849213 |
| H    | 2.4445793436 | -0.6862797238 | -5.4380857716 |
| H    | 2.0826696787 | 1.0502576395  | -5.3964421080 |
| C    | -5.8149386972 | -4.206195939  | 1.2501410271  |
| H    | -6.8521020583 | -3.8632138708 | 1.1049662078  |
| H    | -5.7231273084 | -4.5081061525 | 2.3064101789  |
| H    | -5.6533477868 | -5.0955231817 | 0.6310764907  |

Complex 3b, Excited state T1.

| Au   | 0.0038701715 | -0.0334131018 | 0.0944233126 |
| N    | 2.8179380017 | -0.2538257918 | 1.1549144854 |
| C    | 4.2563423816 | 0.5360392265  | -0.4817357308 |
| H    | 5.1469755351 | 0.2767152594  | -1.0684086035 |
| H    | 4.2948287383 | 1.6239728030  | -0.3062987518 |
| N    | 2.1384472903  | 0.0069425518  | 0.2403548223  |
| C    | 2.3379515245 | -0.5065655701 | 2.4612495265  |
| C    | 1.7917353243 | 0.1575701076  | 4.7160404396  |
| H    | 1.6316353302 | 0.9609756120  | 5.4399359494  |
| C    | 2.1091943793 | 0.4837045320  | 3.3932482855  |
| C    | 2.0100083112 | -0.0314585979 | 0.0295037179  |
| C    | 2.4665484092 | -0.1733836232 | 0.8739804785  |
| C    | -2.9166090444 | -1.124072154 | 0.3850247156  |
| C    | 2.9166968589 | 0.2145929914  | -1.1795209290 |
| C    | 2.1071022037 | 1.9514462648  | 3.0022859263  |
| H    | 2.4508079265 | 2.0147331011  | 1.9592773110  |
| C    | 2.1303213895 | -1.9047690941 | 2.8588904179  |
| C    | -4.1075330883 | -0.8253884720 | 1.1221994113  |
| C    | -2.8467470607 | 1.0504121254  | 0.7549305998  |
| C    | 3.0141202636 | 2.8194658430  | 3.8767385104  |
| H    | 4.0496478889 | 2.4516835977  | 3.8966326053  |
| H    | 2.6544404233 | 2.8575640692  | 4.9173603470  |
| H    | 3.0293483949 | 3.8558703834  | 3.5023694659  |
| C    | -2.5505924447 | 2.4358582347 | 0.6873056119  |
Complex 4, Ground state $S_0$.

| Element | X         | Y         | Z         |
|---------|-----------|-----------|-----------|
| Au      | 0.0526217872 | 0.0291699945 | -0.0187305601 |
| N       | -1.9831919171 | -0.2792127015 | 0.0038900791 |
| C       | 2.0589772137 | 0.0787980067 | 0.0763039755 |
| N       | 2.6558826950 | -0.0120696233 | 1.2474966039 |
| C       | 2.8410967526 | -0.8853385947 | -2.1924629814 |
| H       | 2.7276169227 | -1.8954969009 | -1.7604707057 |
| C       | 1.9406475820 | -0.1427176700 | 2.4968817809 |
| C       | 3.1188618846 | 0.1116260623 | -1.0266638489 |
| C       | 0.6147989721 | -3.2845334058 | 1.6036721220 |
| H       | 0.1319590929 | -2.5789022524 | 0.9107373881 |
| H       | -0.1126682734 | -3.5079107758 | 2.3987719538 |
| H       | 0.8196177587 | -4.2169196308 | 1.0541788786 |
| C       | -2.5806736697 | 0.9943639147 | -4.3994051360 |
| C       | 1.5918481930 | -0.5259349549 | -3.0014505213 |
| H       | 1.4619382009 | -1.2724559978 | -3.8031781950 |
| H       | 0.6846255863 | -0.5834246438 | -2.3798247466 |
| C       | -1.4950800586 | 2.1623908625 | -2.5650290665 |
| H       | -1.2370106783 | 2.2349600860 | -1.5064816731 |
| N       | -3.3687544386 | -0.1292542291 | -4.5984752142 |
| C       | -3.6076604381 | -1.7294500543 | -0.7825541732 |
| C       | -4.3709733902 | -2.3558993318 | -1.7804741726 |
| H       | -5.0139018728 | -3.2019894922 | -1.5231740557 |
|     |            |            |            |
|-----|------------|------------|------------|
| C   | 4.1616574189 | 0.0164157659 | 1.2139006088 |
| C   | -3.9888908303 | -0.4805623795 | -5.8160432205 |
| C   | -3.4695334624 | -1.9443172805 | 0.6360604233 |
| C   | -5.9826480450 | -0.9516514861 | -7.1010670902 |
| H   | -7.0701421712 | -1.0469158749 | -7.1528794521 |
| C   | -4.3050711760 | -1.9233199080 | -3.0975007313 |
| H   | -4.8752185661 | -2.4248363741 | -3.8803951946 |
| C   | 1.6525446441 | -1.4422352175 | 2.9734168280 |
| C   | -2.7193569791 | -0.6640696044 | -1.0969981009 |
| C   | -2.1793538178 | 1.0365507052 | -3.0377003184 |
| C   | 1.5453669241 | 1.0128127733 | 3.2067559282 |
| C   | 4.4178931445 | 1.5619017132 | -2.6532969741 |
| H   | 4.4823822414 | 2.5723701314 | -3.099106929 |
| H   | 5.3778820132 | 1.3928782019 | -2.140155206 |
| C   | -2.256097196 | 2.0184314727 | -5.293810589 |
| H   | -2.5752043581 | 1.9794876622 | -6.3356980328 |
| C   | 0.6940611343 | -0.4336073136 | 4.9669143651 |
| H   | 0.2148372583 | -0.5472234057 | 5.9422963411 |
| C   | 1.0322836607 | -1.5550515871 | 4.2209353610 |
| H   | 0.7941239535 | -2.5484482132 | 4.6061604555 |
| C   | -5.2078357209 | -1.1613768336 | -8.2413842874 |
| H   | -5.6841792155 | -1.4280820008 | -9.1878055225 |
| C   | -2.7340886920 | -0.1345325548 | -2.4046501027 |
| C   | 0.9321422956 | 0.8334282404 | 4.4515591910 |
| H   | 0.6201539930 | 1.7113966384 | 5.0224499071 |
| H   | 1.9637867805 | 1.8778280461 | -2.4630933977 |
| H   | 1.0882583493 | 1.8992641180 | -1.7982548627 |
| H   | 2.0672374823 | 2.8947006427 | -2.8782257715 |
| C   | -4.0815498763 | -2.7996477882 | 1.5593734692 |
| H   | -4.8454539221 | -3.5113750133 | 1.2339618393 |
| C   | 3.2324140631 | 1.5290972800 | -1.6791674126 |
| H   | 3.3857274185 | 2.2854285102 | -0.8916945400 |
| C   | -1.5456826369 | 3.1107240451 | -4.8004655561 |
| H   | -1.2910728863 | 3.9295622835 | -5.4781848714 |
| C   | 4.3921807972 | -0.3015104699 | -0.2577611899 |
| H   | 4.5245980311 | -1.3996037064 | -0.3646278535 |
| H   | 5.3103100343 | 0.1590305457 | -0.6291212426 |
| C   | 1.6684952398 | 2.4257820695 | 2.6598224524 |
| H   | 2.2374947350 | 2.3758403059 | 1.7214816640 |
| C   | -2.4755600457 | -1.0244109253 | 1.0679408731 |
| H   | 4.0461038121 | -0.8655150224 | -3.1469232435 |
| C   | 4.9732009570 | -1.1670959817 | -2.6324229815 |
| H   | 3.8804505224 | -1.6098625239 | -3.9436985388 |
| C   | 2.9410179224 | 0.8946479306 | -4.5439734741 |
| H   | 2.7854961825 | 0.1827319984 | -5.3730953488 |
| H   | 3.0531695834 | 1.8941441634 | -4.9985185011 |
| C   | -1.1811228593 | 3.1912003792 | -3.4482731494 |
| H   | -0.6532240577 | 4.0757061937 | -3.0837495270 |
| C   | -3.5107988844 | -0.7985684761 | -3.3819447055 |
| C   | 1.9151396298 | -2.7142806384 | 2.1797406338 |
| H   | 2.5565756523 | -2.455934215 | 1.3246121551 |
| Element | x          | y          | z          |
|---------|------------|------------|------------|
| C       | -5.3809887396 | -0.6031138490 | -5.8943463203 |
| H       | -5.9835214752 | -0.4152005962 | -5.0033930535 |
| C       | -3.7137075101 | -2.7257649473 | 2.8988524717 |
| H       | -4.191256362 -3.3806394595 | 2.1457494379    |
| C       | 4.7967385667 -1.0079307067 | 1.8879331406    |
| H       | 4.5172830099 -2.0364440487 | 3.1972137165    |
| H       | 4.5355828480 -0.8212280398 | 3.1972137165    |
| C       | 5.8902940550 -0.9275475062 | 2.0549984666    |
| H       | 1.7397365894 0.8738621764 | -3.5971258518    |
| H       | 0.8210664882 1.1441129797 | -4.1417035094    |
| H       | -2.1119068118 -0.9526348167 | 2.4179098064    |
| C       | -1.3575173085 -0.2360268081 | 2.7535845312    |
| C       | -2.7397773287 -1.8044332806 | 3.3206706776    |
| H       | -2.4754552303 -1.7489371262 | 4.3803598736    |
| C       | 4.6876730547 1.4001848870 | 1.5979239679    |
| H       | 4.2907121312 2.1957027663 | 0.9540641466    |
| H       | 5.7832187296 1.4023898436 | 1.4988270742    |
| H       | 4.4503143758 1.6421451359 | 2.6428338497    |
| C       | 4.2063670601 0.5287407571 | -3.764211421    |
| C       | 5.0778407235 0.5323985834 | -4.4408752849    |
| C       | -3.2114421815 -0.6999278203 | -6.9588800326    |
| H       | -2.1246234796 -0.6184297921 | -6.8874758733    |
| C       | -3.8217903927 -1.0290011683 | -8.1668110778    |
| H       | -3.2063512324 -1.1975397703 | -9.0541008351    |
| C       | 2.4070479099 3.3674269787 | 3.6128370402    |
| H       | 3.3867465628 2.9732587634 | 3.9218021663    |
| H       | 1.8231169657 3.5509473708 | 4.5282985706    |
| H       | 2.5703871681 4.3450737071 | 3.1330833688    |
| C       | 0.2895341933 2.9981939971 | 2.3161528454    |
| H       | -0.2456887234 2.3612266161 | 1.5960799108    |
| H       | 0.3922510654 4.0021513746 | 1.8747984784    |
| H       | -0.3401889153 3.0911729526 | 3.2148634726    |
| C       | 2.6399998280 -3.7786821767 | 3.0074794548    |
| H       | 3.5449736987 -3.3875164698 | 3.4963197871    |
| H       | 2.9345438726 -4.6239597498 | 2.3662928333    |
| H       | 1.9876386185 -4.1861306704 | 3.7951328104    |

**Complex 4, Excited state S1.**

| Element | x          | y          | z          |
|---------|------------|------------|------------|
| Au      | 0.3236229354 | -0.9469901920 | -0.4432436056 |
| N       | -1.6479858000 | -1.6245156896 | -0.8687957214 |
| C       | 2.1905113423 | -0.3352153798 | -0.0223191111 |
| N       | 2.4230382457 | 0.4866432355 | 1.0859130762 |
| C       | 3.9599128905 | -2.0185791673 | -0.8920354394 |
| H       | 3.9816669250 | -2.4405268412 | 0.1272669247 |
| C       | 1.6201242394 | 0.4391816567 | 2.2611488036 |
| C       | 3.5059388023 | -0.5258618976 | -0.7854929573 |
| C       | 2.1834546619 | -3.0040323630 | 2.5446588922 |
| H       | 1.6315886649 | -2.8434152879 | 1.6066151525 |
| H       | 1.4825611121 | -3.3742225281 | 3.3110294792 |
| H       | 2.9381144159 | -3.7877229687 | 2.3685893763 |
|    |    |    |    |
|---|---|---|---|
| C | -2.6998664115 | 1.8312804414 | -3.8442154435 |
| C | 3.0047149629 | -2.8422564701 | -1.7579716307 |
| H | 3.3345715959 | -2.8422564701 | -1.7579716307 |
| H | 1.9923993191 | -2.8283690594 | -1.3205475484 |
| C | -0.6642235262 | 1.5461122345 | -2.5504289283 |
| H | -0.0546447264 | 0.9929490098 | -1.8322676249 |
| N | -3.9138923215 | 1.2163553212 | -4.0438287921 |
| C | -3.767092086 | -2.121350617 | -1.6137697038 |
| C | -4.9166641022 | -2.3603640923 |
| H | -5.7361269016 | -2.6639644392 | -2.2977254328 |
| C | 3.6962914187 | 1.2214284000 | 0.9796573516 |
| C | -4.9526926862 | 1.6914312009 | -4.8834217218 |
| C | -3.3847177463 | -3.1505261149 | -0.6729667585 |
| C | -7.1832034854 | 2.5746248726 | -5.1548921561 |
| H | -8.1294752019 | 2.9008360682 | -4.7168576135 |
| C | -5.0245906062 | -0.8348638782 | -3.2048531489 |
| H | -5.9177870566 | -0.6781767825 | -3.8113177575 |
| C | 1.8208698639 | -0.6044782068 | 3.2005134258 |
| C | -2.6399790168 | -1.2043456102 | -1.6755083738 |
| C | -1.9386550140 | 1.0724790263 | -2.9092424441 |
| C | 0.6200851097 | 1.4109680663 | 2.4967165865 |
| C | 4.8853400292 | -0.899572017 | -2.9009714672 |
| H | 4.8367217457 | 0.3070848294 | -3.9300695874 |
| C | 5.621198146 | 0.5329092280 | -2.3679143516 |
| C | -2.2308171652 | 3.0263390873 | -4.4037198988 |
| H | -2.8425877006 | 3.5957474671 | -5.1053649028 |
| C | 0.07530159 | 0.3337154845 | 4.607189745 |
| H | -0.5205782986 | 0.2970411020 | 5.5228269641 |
| C | 1.0388577139 | -0.6373411207 | 4.3577900092 |
| H | 1.1950909425 | -1.439509044 | 5.0833280513 |
| C | -6.9911672320 | 2.6382663169 | -6.5344543800 |
| H | -7.7893778136 | 3.0095810858 | -7.1813562335 |
| C | -2.7485664729 | -0.0586379223 | -2.5353209996 |
| C | -0.128235306 | 1.3444309229 | 3.6784417104 |
| H | -0.8979388498 | 2.0986196419 | 3.8638398152 |
| C | 2.5338232531 | -0.8180711327 | -3.1324047167 |
| H | 1.5053973558 | -0.7486174178 | -2.7424863653 |
| C | 2.5133695767 | -0.3929660545 | -4.1514844998 |
| C | -4.0099023104 | -4.2834144238 | -0.170311309 |
| H | -5.0156968023 | -4.5630643092 | -0.4944662241 |
| C | 3.4920333304 | 0.0034313915 | -2.2595363534 |
| H | 3.1606604157 | 1.0555097358 | -2.2606525156 |
| C | -0.9704135071 | 3.4565507961 | -4.0263635011 |
| H | -0.5741347477 | 4.3855125979 | -4.4436232257 |
| C | 4.5052073005 | 0.2436568556 | 0.1193901964 |
| H | 4.9978950919 | -0.776721486 | 0.7913653641 |
| H | 5.3010640408 | 0.7581971957 | -0.4347751750 |
| C | 0.2913342039 | 2.4967062094 | 1.4912085808 |
| H | 0.9547871079 | 2.3395757957 | 0.6296375959 |
| C | -2.0851430853 | -2.7952942965 | -0.2473785530 |
| C | 5.3648235818 | -2.1085747265 | -1.5076656819 |
| Atom | X | Y | Z |
|------|---|---|---|
| H    | 6.1020560923 | -1.5678820750 | -0.8916242816 |
| H    | 5.6902222850 | -3.1640400533 | -1.5247133366 |
| C    | 4.3822109195 | -2.3679030931 | -3.7892602488 |
| H    | 4.7141081292 | -3.4198921791 | -3.8386040208 |
| H    | 4.3754509265 | -1.9858570103 | -4.8253594123 |
| C    | -0.1935140952 | 2.7203087038 | -3.1092680335 |
| H    | 0.7963492776 | 3.0859857780 | -2.8286039667 |
| C    | -3.9623653141 | 0.0741876264 | -3.2611922992 |
| C    | 2.8497099536 | -1.7001761332 | 2.9849599898 |
| H    | 3.4903684262 | -1.3767635207 | 2.1536813481 |
| C    | -6.1643402390 | 2.1102990354 | -4.3261217723 |
| H    | -6.2955388280 | 2.0779472450 | -3.2421275537 |
| C    | -3.3239273200 | -5.0672338542 | 0.7694357354 |
| C    | -3.7999960078 | -5.9620785638 | 1.1761819410 |
| C    | 4.3498671509 | 1.4833024394 | 2.3318044266 |
| H    | 4.5755429930 | 0.5528707972 | 2.8709238685 |
| H    | 3.7032982432 | 2.1003308671 | 2.9742266072 |
| C    | 5.2966424447 | 2.0257120443 | 2.1858770452 |
| H    | 2.9793319296 | -2.2814918236 | -3.1821813778 |
| H    | 2.2712937664 | -2.8620905014 | -3.7980587453 |
| C    | -1.4057772998 | -3.5693933782 | 0.6895016689 |
| H    | -0.4091764492 | -3.2853749612 | 1.0266090024 |
| C    | -2.0436321493 | -4.7109579015 | 1.1909284206 |
| H    | -1.5257131794 | -5.3287178601 | 1.9276278741 |
| C    | 3.5195137164 | 2.5650930201 | 0.2552922443 |
| C    | 2.9356561537 | 2.4407913657 | -0.6677422110 |
| H    | 4.5006119973 | 2.9866166240 | -0.0141867090 |
| C    | 3.0059657400 | 3.2999497133 | 0.8905783480 |
| C    | 5.3513286000 | -1.5483760009 | -2.9329792000 |
| C    | 6.3662293596 | -1.6042655272 | -3.3635801486 |
| C    | -4.7600598911 | 1.7483477600 | -6.2664743270 |
| H    | -3.8114282148 | 1.4100616367 | -6.6892576191 |
| C    | -5.7779819749 | 2.2290028023 | -7.0870908869 |
| H    | -5.6246559695 | 2.2740831994 | -8.167823196 |
| C    | 0.5485351960 | 3.8969423563 | 2.0497067458 |
| H    | 1.5789689511 | 4.0074915529 | 2.4206524962 |
| H    | -0.1263744820 | 4.1244966366 | 2.8909020080 |
| C    | 0.3811815466 | 4.6633284853 | 1.2757446348 |
| C    | -1.1477475561 | 2.3692997733 | 0.9887780871 |
| C    | -1.3318571266 | 1.3620492658 | 0.5851432323 |
| H    | -1.3464203332 | 3.095104258 | 0.1883447193 |
| H    | -1.8778249185 | 2.5495407543 | 1.7945889756 |
| C    | 3.7410558379 | -1.9298176005 | 4.2060392522 |
| H    | 4.2162603898 | -0.9974518175 | 4.5473747072 |
| H    | 4.5372994310 | -2.6522810542 | 3.9663693506 |
| H    | 3.1750580128 | -2.3422424637 | 5.0566289213 |

**Complex 4, Excited state T1.**

| Atom | X | Y | Z |
|------|---|---|---|
| Au   | 0.1513781114 | -0.4979729407 | -0.1728199789 |
| N    | -1.8997638345 | -1.0328451714 | -0.3269268626 |
H  -1.3806718124    2.6610220454    2.8522398839
C   3.8939215712   -2.7142882543    3.6221590733
H   4.5043724089   -1.9015333004    4.0446754104
H   4.5732681820   -3.4409255382    3.1487338800
H   3.4049903981   -3.2292617685    4.4642116988

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