**Supporting Information for**

# Deep-Blue Thermally Activated Delayed Fluorescence from a CF3-substituted Carbene-Metal-Amide Complex

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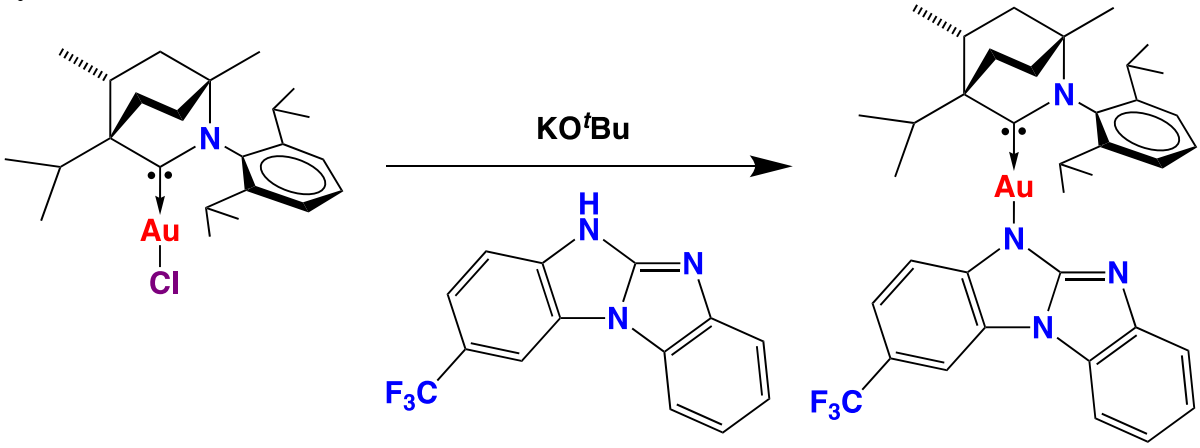
**General Considerations.**

All reactions were performed under a $N_2$ atmosphere in dry solvents. Potassium tert-butoxide was purchased from Merck and used as received. (BiCAAC)AuCl,[1] benzoguaidine and derivatives[2] were prepared according to literature procedures. $^1$H and $^{13}$C{$^1$H} NMR spectra were recorded using a Bruker AVIII HD 500 MHz NMR spectrometer. $^1$H NMR spectra (500.19 MHz) and $^{13}$C{$^1$H} (125.79 MHz) were referenced to $CD_2Cl_2$ at δ 5.32 ($^{13}$C, δ 53.84). All electrochemical experiments were performed using an Autolab PGSTAT 302N computer-controlled potentiostat. Cyclic voltammetry (CV) was performed using a three-electrode configuration consisting of a glassy carbon macrodisk working electrode (GCE) (diameter of 3 mm; BASi, Indiana, U.S.A.) combined with a Pt wire counter electrode (99.99%; GoodFellow, Cambridge, U.K.) and an Ag wire pseudoreference electrode (99.99%; GoodFellow, Cambridge, U.K.). The GCE was polished between experiments using alumina slurry (0.3 μm), rinsed in distilled water and subjected to brief sonication to remove any adhering alumina microparticles. The metal electrodes were then dried in an oven at 100 °C to remove residual traces of water, the GCE was left to air dry and residual traces of water were removed under vacuum. The Ag wire pseudoreference electrodes were calibrated to the ferrocene/ferrocenium couple in THF at the end of each run to allow for any drift in potential, following IUPAC recommendations.[3] All electrochemical measurements were performed at ambient temperatures under an inert $N_2$ atmosphere in THF containing the complex under study (1.4 mM) and the supporting electrolyte [*n*-$Bu_4N$][$PF_6$] (0.13 M). Data were recorded with Autolab NOVA software (v. 1.11). Elemental analyses were performed by the Microanalysis Laboratory at the University of Manchester. Mass spectrometry data were obtained by the Mass Spectrometry Laboratory at the University of Manchester. Thermogravimetric analysis was performed with a TA Instruments SDT650 simultaneous thermal analyser under a stream of nitrogen.

**Synthetic Procecures.**




**Synthesis of (BiCAAC)AuBGCF3**

To a solid mixture of (BiCAAC)AuCl (200 mg, 350 µmol), KO$^t$Bu (41.2 mg, 367 µmol) and BGCF3 (2-(trifluoromethyl)-5H-benzo[d]benzo[4,5]imidazo[1,2-a]imidazole) (96.2 mg, 350 µmol) was added THF (25 ml) at −78°C under $N_2$. The reaction mixture was allowed to reach RT slowly and stir for 4 hrs. The reaction mixture was dried under vacuum. The crude product was extracted with DCM and filtered through a pad of Celite® in a glass frit and dried under vacuum. The crude product was purified by column chromatography (eluent 1:4 ethyl acetate:hexane) to give the pure product as a white crystalline powder in 49% yield (140 mg, 173 µmol). $^1$H NMR (500 MHz, $CD_2Cl_2$) δ 7.91 (s, 0.6H, BGCF3 Ar-H *isomer a*), 7.81 (s, 0.4H, BGCF3 Ar-H *isomer b*), 7.71 (d, *J* = 7.7 Hz, 0.4H, BGCF3 Ar-H *isomer b*), 7.68 – 7.61 (m, 1.4H, *p*-CH Dipp and BGCF3 Ar-H *isomer a*), 7.55 (t, *J* = 7.1 Hz, 1H, BGCF3 Ar-H *isomer a+b*), 7.48 – 7.39 (m, 2.4H, *m*-CH Dipp and BGCF3 Ar-H *isomer b*), 7.32 – 7.16 (m, 1H, BGCF3 Ar-H *isomer a+b*), 7.10 (t, *J* = 7.5 Hz, 0.4H, BGCF3 Ar-H *isomer b*), 7.03 (t, *J* = 7.3 Hz, 0.6H. BGCF3 Ar-H *isomer a*), 6.97 (t, *J* = 8.0 Hz, 0.6H, BGCF3 Ar-H *isomer a*), 6.02 (d, *J* = 7.8 Hz, 0.6H, BGCF3 Ar-H, *isomer a*), 5.94 (d, *J* = 8.3 Hz, 0.4H, BGCF3 Ar-H *isomer b*), 3.31 – 3.21 (m, 1H, CH *i*Pr Carbene), 3.13 – 3.05 (m, 1H, CH *i*Pr Dipp), 2.71 – 2.63 (m, 1H, CH *i*Pr Dipp), 2.42 – 2.32 (m, 1H, C<u>H</u>($CH_3$) Carbene), 2.19 (dd, *J* = 13.6, 10.5 Hz, 1H, CH Carbene), 1.92 – 1.78 (m, 3H, CH Carbene), 1.68 (d, *J* = 6.5 Hz, 3H, CH Carbene), 1.39 – 1.30 (m, 12H, $CH_3$ *i*Pr Dipp), 1.15 (d, *J* = 6.6 Hz, 3H, CH(C<u>H</u>$_3$)), 0.88 (s, 3H, CH(C<u>H</u>$_3$)). $^{13}$C NMR (126 MHz, $CD_2Cl_2$) δ 245.50 (C:), 151.56 (Ar-<u>C</u>(NNN) BGCF3), 145.87 (Ar-<u>C</u> BGCF3), 145.77 (*o*-CH Dipp), 145.33 (Ar-<u>C</u> BGCF3), 145.01 (Ar-<u>C</u> BGCF3), 144.92 (*o*-CH Dipp), 142.32 (*i*-CH Dipp), 129.98 (Ar-<u>C</u> BGCF3), 127.97 (Ar-<u>C</u> BGCF3), 127.02 (Ar-<u>C</u> BGCF3), 125.58 (*m*-C Dipp), 121.96 (Ar-<u>C</u> BGCF3), 118.74 (Ar-<u>C</u> BGCF3), 116.39 (Ar-<u>C</u> BGCF3), 114.53 (Ar-<u>C</u> BGCF3 *isomer a*), 113.34 (Ar-<u>C</u> BGCF3 *isomer b*), 109.79 (Ar-<u>C</u> BGCF3),

106.75 (Ar-C BGCF3), 64.92 (C(CCN) Carbene), 55.83 (C(CCC) Carbene), 44.54 (CH Carbene), 34.84 (CH($CH_3$) Carbene), 32.99 (CH Carbene), 32.22 (CH *i*Pr Carbene), 29.61 (CH *i*Pr Dipp), 29.06 (CH *i*Pr Dipp), 25.34 ($CH_3$ *i*Pr Dipp), 25.09 ($CH_3$ *i*Pr Dipp), 24.20 ($CH_3$ *i*Pr Carbene), 24.02 ($CH_3$ *i*Pr Carbene), 23.37 ($CH_3$ *i*Pr Dipp), 21.48 (CH Carbene), 20.65 (CH Carbene), 19.67 (CH($CH_3$)), 16.48 ($CH_3$ *i*Pr Dipp). $^{19}F$ NMR (376 MHz, $CD_2Cl_2$) δ -59.50 (isomer a), -59.88 (*isomer b*). HRMS $C_{38}H_{44}AuN_4F_3$ theoretical $[M]^+$ = 810.3178, HRMS (APCI): = 810.3188.

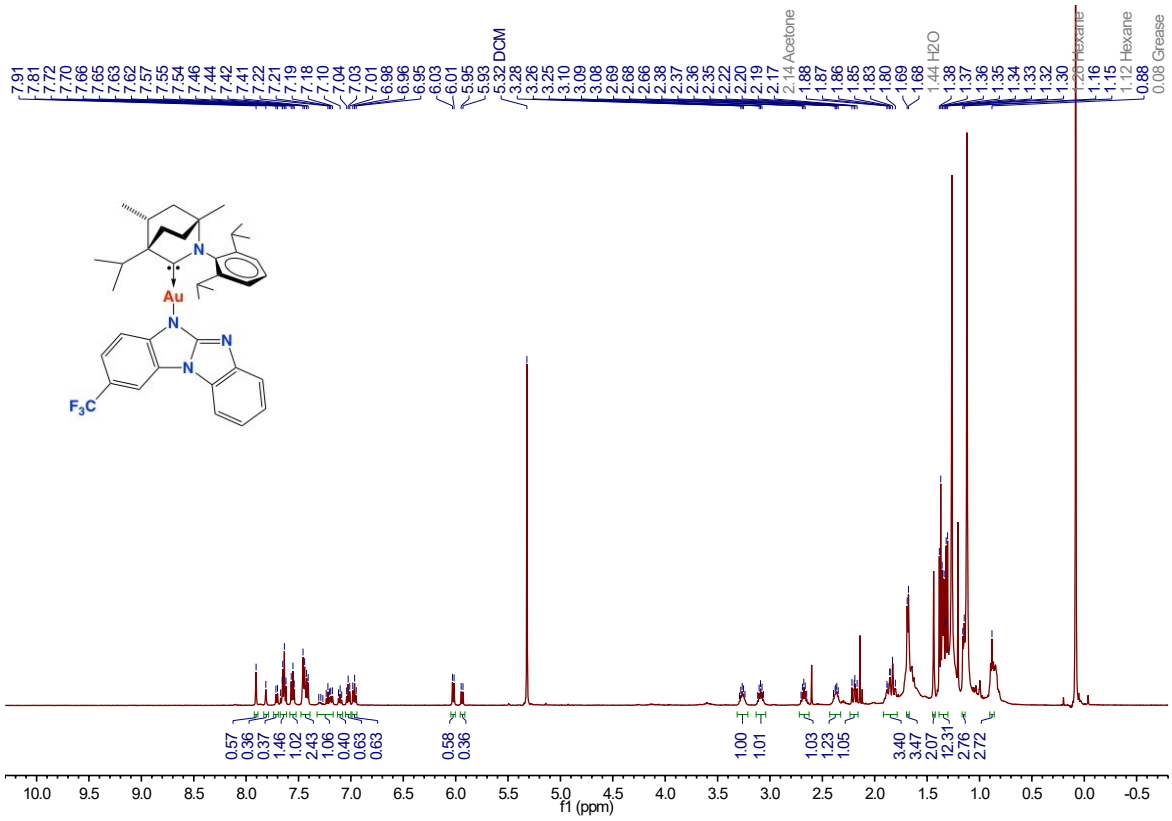



**Figure S1**. $^1H$ NMR (500 MHz, $CD_2Cl_2$)

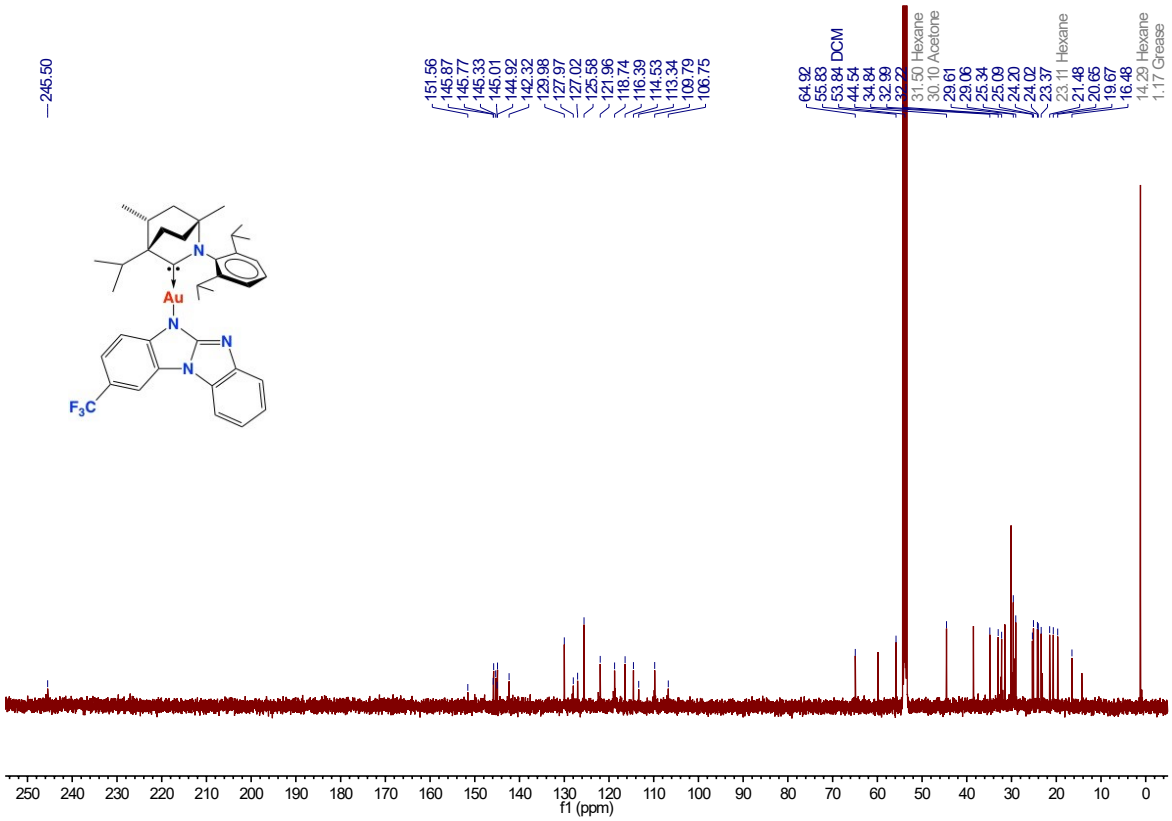



**Figure S2**. $^{13}C\{^{1}H\}$ NMR (126 MHz, $CD_2Cl_2$)

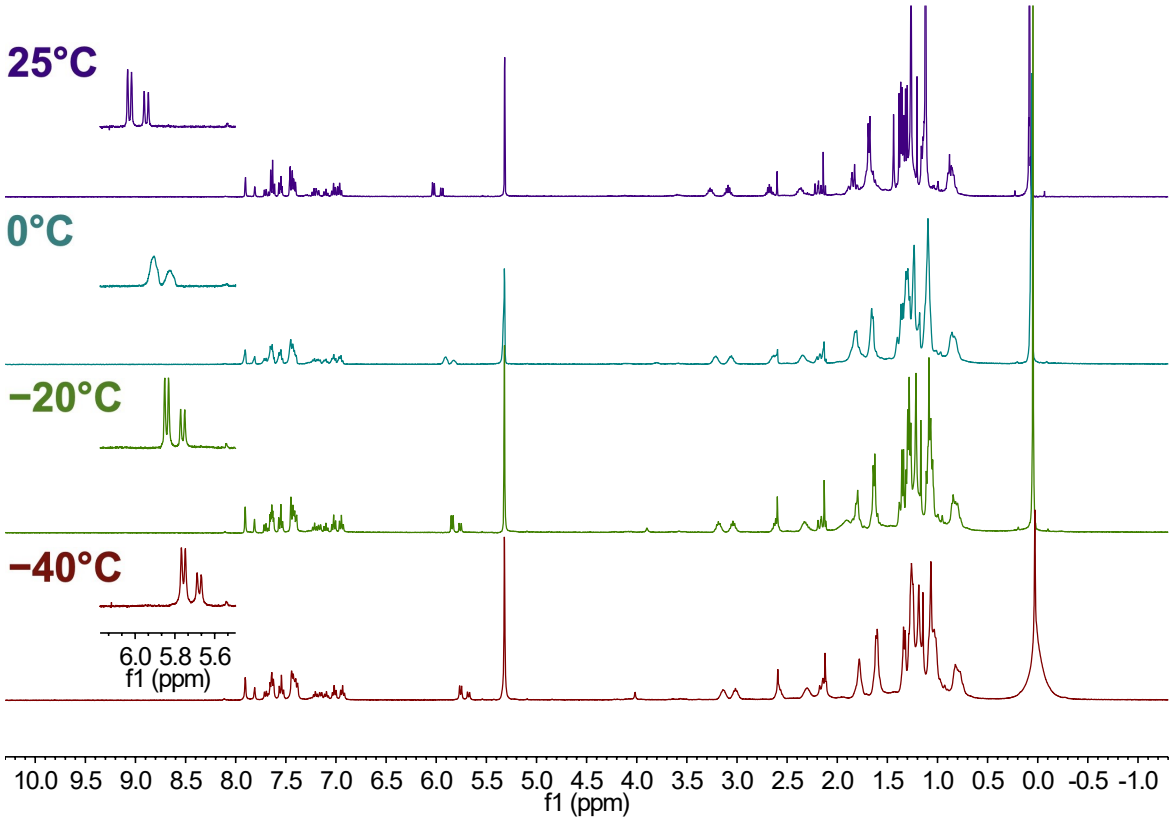



**Figure S3**. Variable Temperature $^{1}H$ NMR (400 MHz, $CD_2Cl_2$)

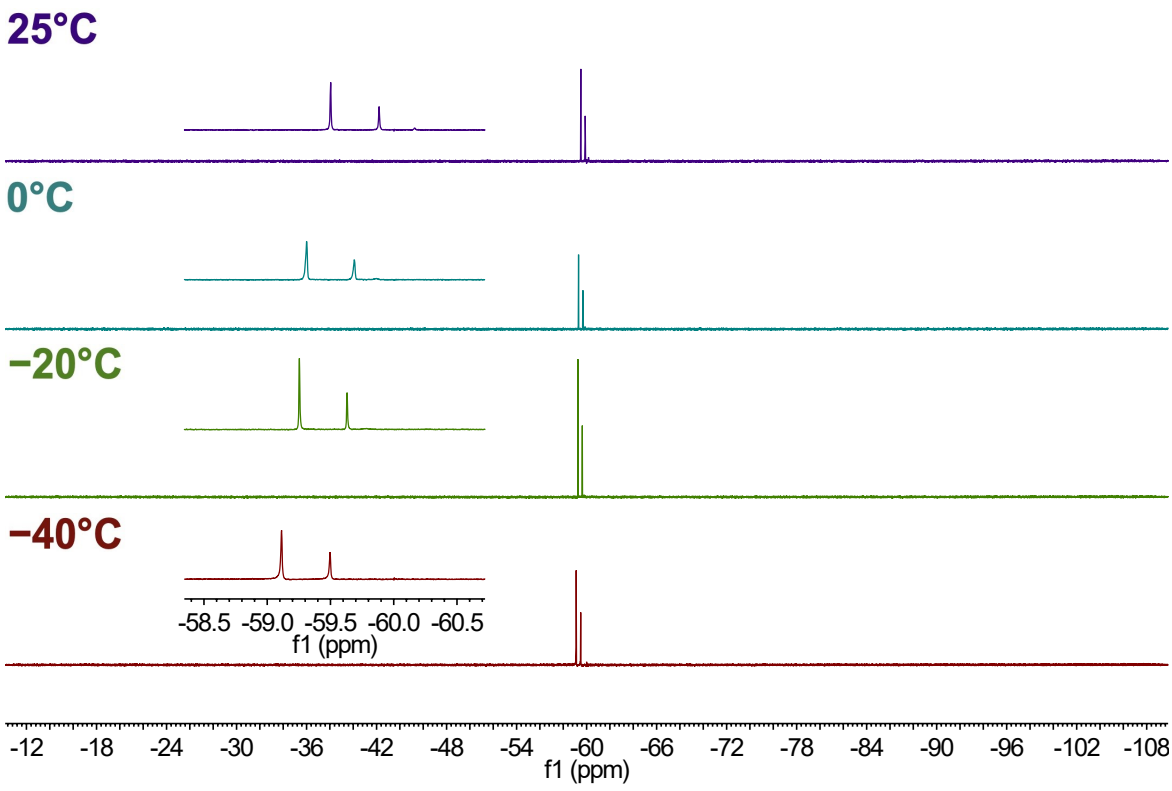



**Figure S4**. Variable Temperature $^{19}F\{^{1}H\}$ NMR (376 MHz, $CD_2Cl_2$)

**X-ray Crystallography.**

Crystals suitable for X-ray diffraction study were obtained by layering the dichloromethane solution of gold complexes with pentane at room temperature. Crystals were mounted in oil on glass fiber and fixed on the diffractometer in a cold nitrogen stream. Data was collected using Rigaku Oxford Diffraction XtaLAB Synergy-S diffractometer at 100 K. Data were processed using the CrystAlisPro-CCD and –RED software.[4] The structure was solved by intrinsic phasing or direct method 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 $U_{iso}(H)$ parameters equal to $1.2U_{eq}(C_i)$, for methyl groups equal to $1.5U_{eq}(C_{ii})$, where $U(C_i)$ and $U(C_{ii})$ 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.[5,6] OLEX2 software was used as graphical user interface.[7] To model disorder the library of the idealized fragments was used.[8]

**Crystal Data** for CCDC 2427966. $C_{38}H_{44}AuF_3N_4$ ($M$ =810.74 g/mol): monoclinic, space group $P2_1/n$ (no. 14), $a$ = 10.1448(3) Å, $b$ = 15.7992(4) Å, $c$ = 22.5860(6) Å, $\beta$ = 96.966(3)°, $V$ = 3593.36(16) Å$^3$, $Z$ = 4, $T$ = 99.97(18) K, μ(Cu Kα) = 8.074 mm$^{-1}$, *Dcalc* = 1.499 g/cm$^3$, 20361 reflections measured (6.844° ≤ 2Θ ≤ 152.174°), 7256 unique ($R_{int}$ = 0.0363, $R_{sigma}$ = 0.0423) which were used in all calculations. The final $R_1$ was 0.0731 (I > 2σ(I)) and $wR_2$ was 0.1553 (all data).

**Photophysical Characterisation.**

**Experimental Methods for Spectroscopy**

*Sample Preparation*

Samples for photophysics were made from powders stored in a glovebox. Solutions were made and kept in the glovebox until measured. Prior to measuring, solutions were transferred into 1mm path length quartz cuvettes which were sealed with a screw-top cap, parafilm and Teflon tape. Cuvettes were taken out of the glovebox immediately prior to experiments to minimize oxygen ingress.

Films were made from chlorobenzene solutions of polystyrene and CMA at 20mg/ml mixed in the appropriate ratio. Solution was drop-cast onto quartz substrates heated to 80°C or spin coated at 1500 rpm depending on the desired thickness. Films were made and stored in a glovebox. For transient absorption, films were encapsulated inside the glovebox using a coverslip, spacer tape and epoxy.

*Photoluminescence Quantum Yield*

Quantum yields have been measured in air for solid samples and under nitrogen for solutions. Photoluminescence quantum yields were recorded using a Hamamatsu Quantaurus-QY C11347-11. Quantum yields have been measured in air for solid samples and under nitrogen for solutions.

*Steady-state Photoluminescence*

Steady-state PL spectra were recorded using an Edinburg Instruments FLS980 spectrofluorimeter. The light source was a monochromated Xenon arc lamp; excitation wavelength varied. Samples were measured in air or under flowing nitrogen, at room temperature.

*Time-Correlated Single Photon Counting*

Time resolved luminescence data were collected on a time-correlated single photon counting (TCSPC) Edinburgh Instruments FLS980 spectrometer using F-900 software. A xenon flash lamp and EPL pulsed diode lasers were used as excitation sources. The collected data were analysed using F-900 software.

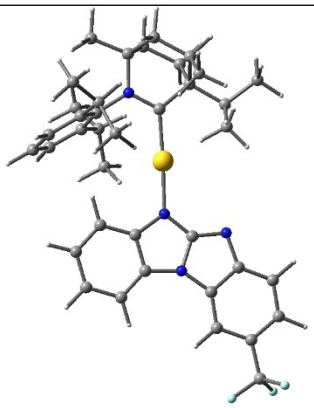
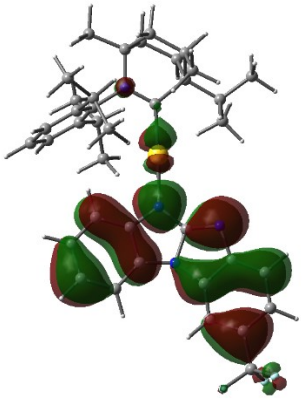
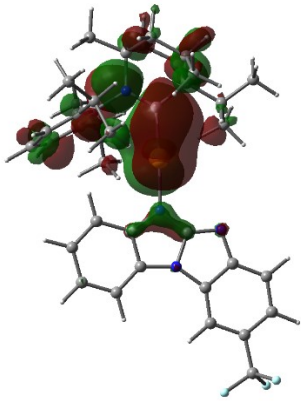
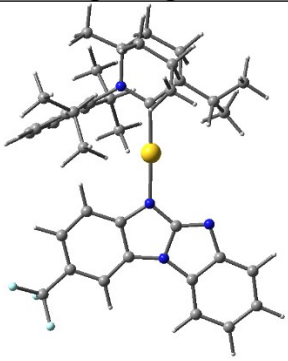
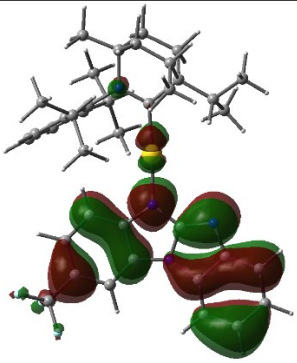
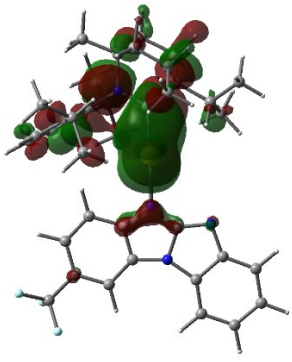
*UV-Vis Absorption*

UV-Vis spectra were measured using a Varian Cary 5000 UV-Vis-NIR spectrometer and Shimadzu UV-3600 Plus UV-VIS-NIR spectrophotometer. The spectrometer has a PMT detector for wavelength ranges from UV to visible, as well as InGaAs and PbS detectors for NIR. The light source used was a deuterium lamp for wavelengths less than 280nm and a tungsten halogen lamp for higher wavelengths.

**Computational Details**

The ground states of the complexes were studied by density functional theory (DFT) and the excited states by time-dependent DFT (TD-DFT) using the Tamm-Dancoff approximation.[9,10] Calculations were carried by the global hybrid MN15 functional of the Minnesota series by Truhlar and coworkers, which has especially good performance for noncovalent interactions and excitation energies.[11] The def2-TZVP basis set[12,13] was employed with relativistic effective core potential of 60 electrons for description of the core electrons of Au.[14] We have previously employed the selected methodology with success for closely related molecules.[15,16] Gold metal contributions to HOMO and LUMO were calculated by the Mulliken population analysis and HOMO-LUMO overlap integrals were calculated using Multiwfn program.[17] All calculations were carried out by Gaussian 16.[18]

**Table S1:** Optimised gas phase structures and molecular orbital distribution of the HOMO (middle) and LUMO (right) for gold complex involved in vertical excitation ($S_0 \rightarrow S_1$), including the contributions of the metal.

| | HOMO | LUMO |
|---|---|---|
|  **BICAuBGCF3** (isomer **A**) Overlap integral: 0.30 |  1.9%Au |  10.5%Au |
|  **BICAuBGCF3** (isomer **B**) Overlap integral: 0.29 |  1.7%Au |  10.5%Au |

| | | |
|---|---|---|
| ΔE = 2.55 kJ/mol | | |

**Table S2**: Dipole moments for $S_0$ and lowest singlet vertical excitation.

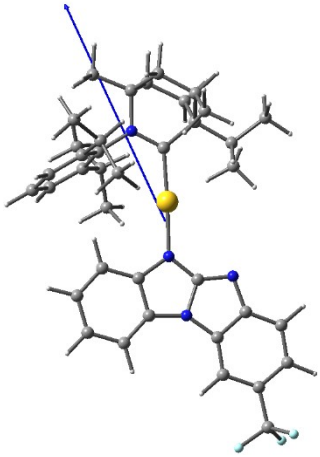
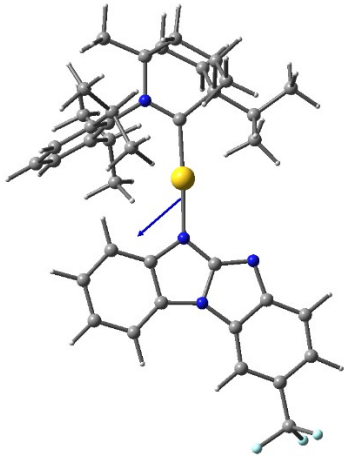
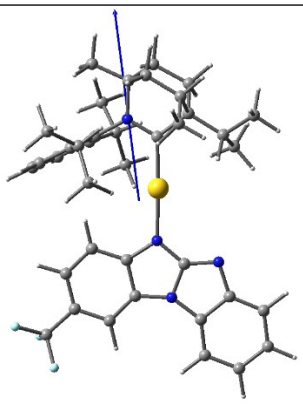
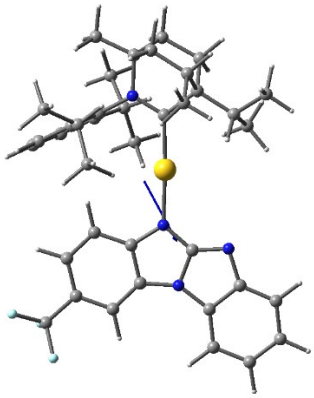
| | $S_0$ | $S_1@S_0$ |
|---|---|---|
| **BICAuBGCF3** (isomer **A**) |  15.8D |  (-)3.5D |
| **BICAuBGCF3** (isomer **B**) |  13.4D |  (-)4.5D |

**Table S3**: Bond dissociation energies in optimized $S_0$ geometry

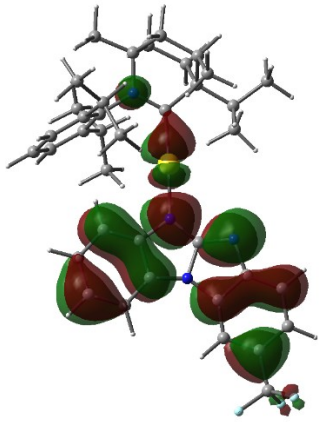
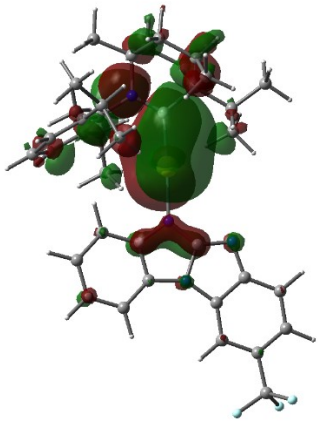
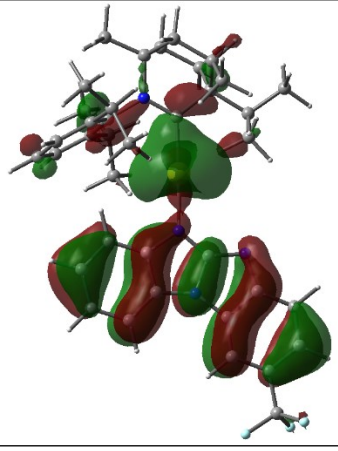
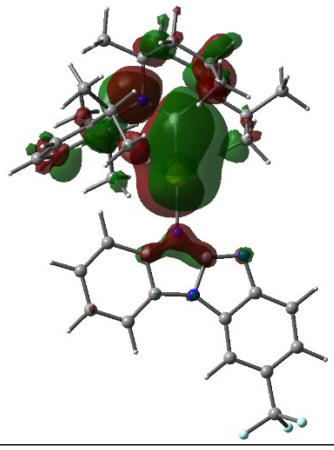
| | Au-C | | Au-N | |
|---|---|---|---|---|
| | kJ/mol | eV | kJ/mol | eV |
| **BICAuBGCF3** (isomer **A**) | 419.6 | 4.35 | 376.8 | 3.91 |
| **BICAuBGCF3** (isomer **B**) | 421.9 | 4.37 | 374.3 | 3.88 |

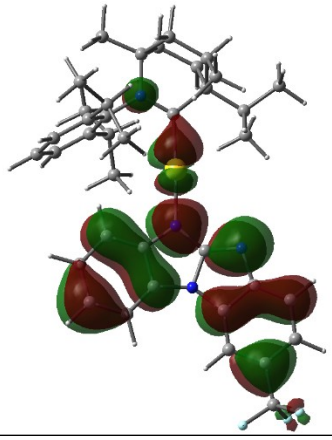
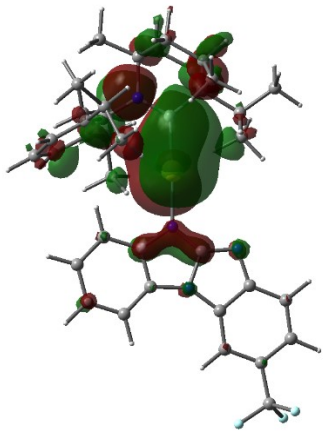
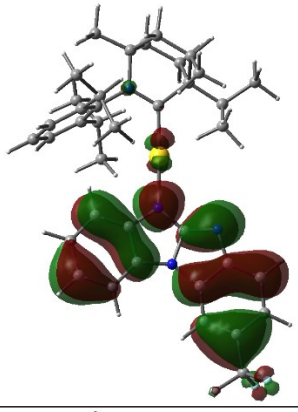
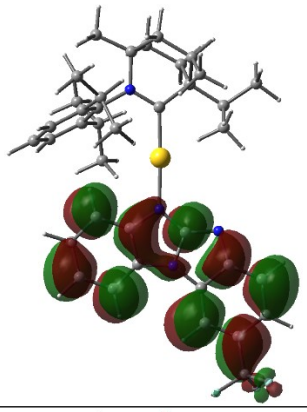
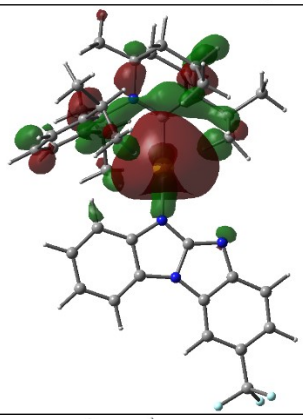
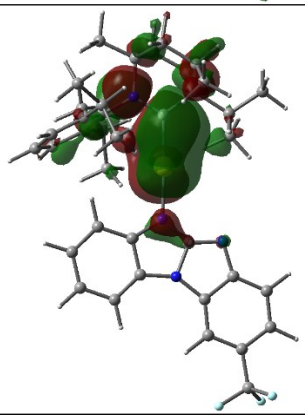
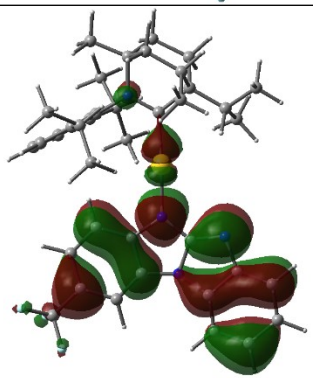
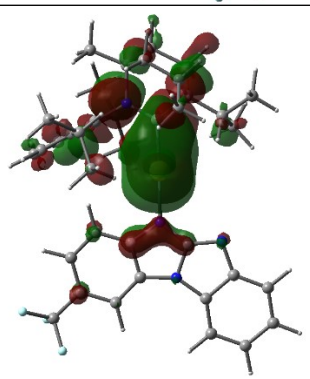
**Table S4:** Theoretically calculated $S_1$ and $T_n$ energy levels, orbital (HOMO, LUMO) contributions to vertical excitations ($S_0 \rightarrow S_1$ and $S_0 \rightarrow T_n$) and oscillator strength coefficients.

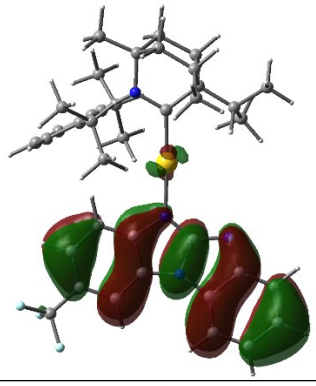
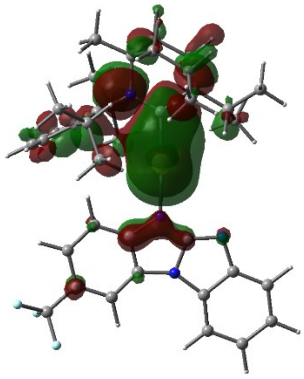
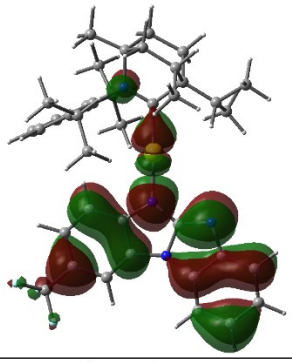
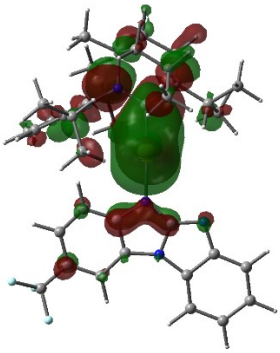
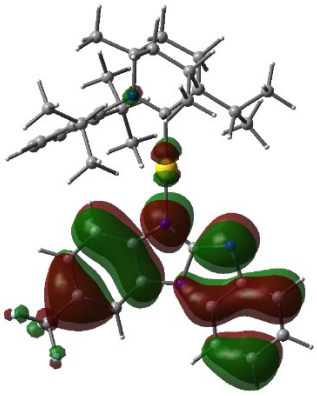
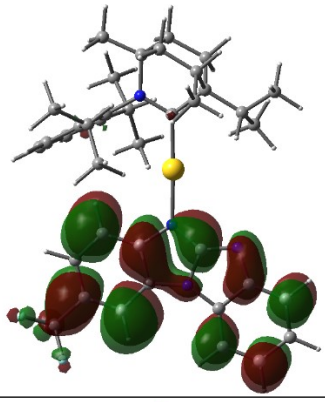
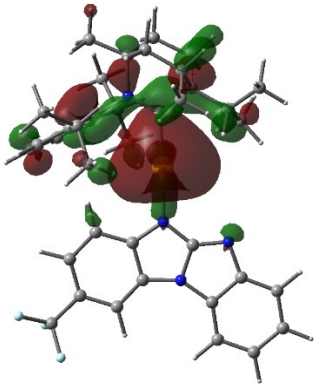
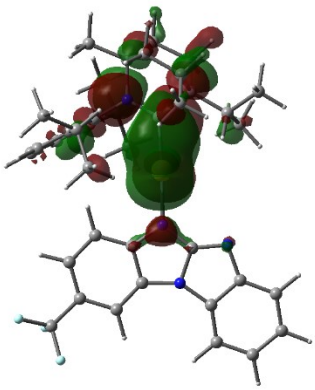
| | Excitation energy | Character | Oscillator strength |
|---|---|---|---|
| **BICAuBGCF3** (isomer **A**) | $S_1$ ($^1$CT): 3.22eV = 385nm | HOMO – LUMO (97%) | 0.2001 |
| | $S_2$ (mixed $^1$CT and $^1$LE(C)): | HOMO-1 – LUMO (65%) | 0.0141 |

| | | | |
|---|---|---|---|
| | 4.04eV = 307nm | HOMO-3 – LUMO (30%) | |
| | $T_1$ ($^3$CT): 3.00eV = 413nm | HOMO – LUMO (93%) | |
| | $T_2$ ($^3$LE(A)): 3.60eV = 345nm | HOMO – LUMO+3 (59%)<br>HOMO – LUMO+4 (20%) | |
| | $T_3$ ($^3$LE(C)): 3.69eV = 336nm | HOMO-3 – LUMO (81%) | |
| **BICAuBGCF3** (isomer **B**) | $S_1$ ($^1$CT): 3.19eV = 389nm | HOMO – LUMO (97%) | 0.1763 |
| | $S_2$ ($^1$CT): 4.00eV = 310nm | HOMO-1 – LUMO (97%) | 0.0122 |
| | $T_1$ ($^3$CT): 2.98eV = 416nm | HOMO – LUMO (93%) | |
| | $T_2$ ($^3$LE(A)): 3.53eV = 351nm | HOMO – LUMO+3 (59%)<br>HOMO – LUMO+4 (15%) | |
| | $T_3$ ($^3$LE(C)): 3.69eV = 336nm | HOMO-3 – LUMO (78%) | |

**Table S5.** Natural transition orbitals for vertical excited states.

| | | HONTO | LUNTO |
|---|---|---|---|
| **BICAuBGCF3** (isomer **A**) | $S_1$ |  |  |
| | $S_2$ |  |  |

| | | | |
|---|---|---|---|
| | $T_1$ |  |  |
| | $T_2$ |  |  |
| | $T_3$ |  |  |
| **BICAuBGCF3** (isomer **B**) | $S_1$ |  |  |

| | | | |
|---|---|---|---|
| | $S_2$ |  |  |
| | $T_1$ |  |  |
| | $T_2$ |  |  |
| | $T_3$ |  |  |

**Coordinates for the isomers A and B for complex Au2.**

90
BICAuBGCF3 (isomer A)

| | | | |
|---|---|---|---|
| Au | 0.59758900 | -0.35384500 | 0.05828500 |
| N | -1.24698400 | 0.43505300 | 0.11671200 |
| N | -3.47208700 | 0.72479100 | 0.10830600 |
| F | -8.98606400 | -0.85546900 | -1.07076100 |
| F | -9.01140200 | -0.92244000 | 1.07228900 |
| F | -8.63669600 | 0.94422100 | 0.06225600 |
| C | 3.27322300 | 1.18959800 | -0.20722800 |
| C | -4.64935700 | -0.00024900 | 0.07540000 |
| C | 2.97323900 | 1.69745300 | -1.47798400 |
| C | 4.83747800 | -0.83784600 | -0.09035300 |
| C | 3.37410600 | 2.01777000 | 0.91636100 |
| C | -1.53082800 | 1.79368800 | 0.14330700 |
| C | -2.92659700 | 2.00118700 | 0.13873300 |
| C | 4.97166500 | -1.75365300 | 1.12896200 |
| H | 5.08142100 | -1.15595600 | 2.03741700 |
| H | 5.90386100 | -2.31112400 | 1.00764300 |
| N | -2.83925200 | -1.45376200 | 0.05160100 |
| C | -5.98164800 | 0.36658000 | 0.07163600 |
| H | -6.29740600 | 1.40065200 | 0.09778000 |
| C | 2.76446200 | 0.83346700 | -2.70447700 |
| H | 2.80134000 | -0.21693400 | -2.40452600 |
| C | 2.83781600 | 3.07892400 | -1.60857400 |
| H | 2.61125800 | 3.49384600 | -2.58370200 |
| C | 2.97119500 | 3.92267600 | -0.51849000 |
| H | 2.85888300 | 4.99232200 | -0.64283800 |
| C | -0.66433400 | 2.87662000 | 0.16816600 |
| H | 0.41018500 | 2.71694400 | 0.17170100 |
| C | -2.44308600 | -0.20186500 | 0.09177000 |
| C | 3.21958300 | 3.38965700 | 0.73682200 |
| H | 3.28101900 | 4.04499900 | 1.59746500 |
| C | 5.92263500 | 0.21641500 | -0.11974400 |
| H | 5.83520000 | 0.85802600 | -0.99865000 |
| H | 6.88996200 | -0.28782000 | -0.15257400 |
| H | 5.89288900 | 0.84552800 | 0.77168600 |
| C | -3.47687100 | 3.26931900 | 0.15902500 |
| H | -4.54873700 | 3.41964000 | 0.15558600 |
| C | -1.21566700 | 4.15425300 | 0.18667100 |
| H | -0.55703700 | 5.01440300 | 0.20535200 |
| C | -5.17674100 | -2.36411800 | 0.00295400 |
| H | -4.87176600 | -3.40191700 | -0.02288000 |
| C | -6.91070900 | -0.66555700 | 0.03246900 |
| C | -4.21459500 | -1.35356300 | 0.04130900 |
| C | 1.38530800 | 1.08192700 | -3.31733300 |
| H | 0.59395900 | 0.96184900 | -2.57360200 |
| H | 1.20380200 | 0.38123900 | -4.13438000 |
| H | 1.31594000 | 2.09279200 | -3.72516300 |

| | | | |
|---|---|---|---|
| C | 3.54526600 | 1.46504300 | 2.31331900 |
| H | 3.85125600 | 0.42111700 | 2.22727800 |
| C | 3.86023700 | 1.08471200 | -3.74019300 |
| H | 3.81168600 | 2.11520400 | -4.10041800 |
| H | 3.73511500 | 0.42341500 | -4.59983200 |
| H | 4.85833500 | 0.92727200 | -3.32403800 |
| C | -8.37659800 | -0.36917200 | 0.02442100 |
| C | -6.51378100 | -2.00794400 | -0.00112200 |
| H | -7.27878300 | -2.77471500 | -0.03066100 |
| C | 4.60821000 | 2.20447000 | 3.12218300 |
| H | 5.56334900 | 2.25325400 | 2.59503400 |
| H | 4.76709300 | 1.70215700 | 4.07790400 |
| H | 4.29452800 | 3.22687900 | 3.34211200 |
| C | -2.59710600 | 4.34996500 | 0.18293000 |
| H | -2.99466700 | 5.35642100 | 0.19866700 |
| C | 2.20016000 | 1.50106100 | 3.04123500 |
| H | 1.85574200 | 2.53423800 | 3.13974700 |
| H | 2.29089300 | 1.07290500 | 4.04191100 |
| H | 1.43519200 | 0.94717800 | 2.49039900 |
| C | 3.76197000 | -2.69820800 | 1.24084600 |
| H | 4.11545100 | -3.73271200 | 1.20505000 |
| C | 3.72304900 | -2.73677100 | -1.26499900 |
| H | 3.09776000 | -2.63947900 | -2.15308800 |
| H | 4.08276600 | -3.76850300 | -1.24077800 |
| C | 2.85481900 | -2.50678100 | -0.00505500 |
| C | 3.00793100 | -2.47368600 | 2.54884300 |
| H | 3.68698500 | -2.58205700 | 3.39686300 |
| H | 2.18801200 | -3.17961800 | 2.68051800 |
| H | 2.58275400 | -1.46543500 | 2.58554900 |
| C | 1.95326500 | -4.88102100 | 0.36986700 |
| H | 2.70105000 | -5.29235200 | -0.31466400 |
| H | 1.05532900 | -5.49307600 | 0.27202000 |
| H | 2.32333000 | -4.99964500 | 1.38892900 |
| C | 1.61925600 | -3.43441600 | 0.01496600 |
| H | 0.95026800 | -3.03457100 | 0.78599900 |
| C | 0.85468400 | -3.42020700 | -1.30926500 |
| H | 0.77662100 | -2.41551000 | -1.73468500 |
| H | -0.16103400 | -3.78666500 | -1.15808900 |
| H | 1.34274000 | -4.06625600 | -2.04482500 |
| C | 2.44713400 | -1.05652100 | -0.01079600 |
| C | 4.88655300 | -1.74030000 | -1.32458600 |
| H | 5.85519900 | -2.24507700 | -1.32552500 |
| H | 4.84338800 | -1.12610300 | -2.22623700 |
| N | 3.47416300 | -0.23854200 | -0.05833400 |

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BICAuBGCF3 (isomer B)

| | | | |
|---|---|---|---|
| Au | 0.48767500 | 0.73469700 | -0.04951500 |
| N | -1.51986600 | 0.72926000 | -0.09559400 |
| N | -3.68664300 | 1.32737300 | -0.09396900 |
| C | 2.34078700 | -1.73611700 | 0.21455100 |

| | | | |
|---|---|---|---|
| C | -4.49468600 | 2.45316300 | -0.07612300 |
| C | 1.88026600 | -2.07577100 | 1.49343300 |
| C | 4.57636800 | -0.49036600 | 0.06199600 |
| C | 2.09364200 | -2.54483800 | -0.90057000 |
| C | -2.30335000 | -0.40676900 | -0.10475600 |
| C | -3.67530500 | -0.05717000 | -0.10351800 |
| C | 5.04538000 | 0.29284500 | -1.16712700 |
| H | 4.89921600 | -0.30387800 | -2.07106500 |
| H | 6.12325800 | 0.43814900 | -1.05988500 |
| N | -2.25757100 | 3.08777200 | -0.06209600 |
| C | -5.86748100 | 2.63237300 | -0.07469000 |
| H | -6.55158700 | 1.79314000 | -0.08973700 |
| C | 2.04388000 | -1.19115300 | 2.71214100 |
| H | 2.48924900 | -0.24288900 | 2.40048700 |
| C | 1.21291700 | -3.29117100 | 1.64038900 |
| H | 0.85318500 | -3.57668500 | 2.62193600 |
| C | 0.98969500 | -4.12680500 | 0.55864100 |
| H | 0.46669100 | -5.06480900 | 0.69587200 |
| C | -1.92244700 | -1.74158300 | -0.11636100 |
| H | -0.87045600 | -2.01028300 | -0.12203500 |
| C | -2.37812200 | 1.78707600 | -0.08427900 |
| C | 1.41292800 | -3.74344400 | -0.70459900 |
| H | 1.20115300 | -4.37615600 | -1.55826900 |
| C | 5.15846200 | -1.88675600 | 0.09146200 |
| H | 4.83657400 | -2.43703400 | 0.97768100 |
| H | 6.24653700 | -1.80445000 | 0.10996000 |
| H | 4.87187400 | -2.45813900 | -0.79318700 |
| C | -4.66912200 | -1.01274700 | -0.11276400 |
| H | -5.71821800 | -0.74885200 | -0.11775100 |
| C | -2.91976100 | -2.70848200 | -0.12313400 |
| H | -2.65280600 | -3.75776400 | -0.13567900 |
| C | -4.06757600 | 4.83293400 | -0.03692900 |
| H | -3.38342600 | 5.67170200 | -0.02275500 |
| C | -6.33275300 | 3.94176400 | -0.05372500 |
| C | -3.57279600 | 3.53126600 | -0.05732400 |
| C | 0.68615300 | -0.86987700 | 3.33853400 |
| H | 0.00055600 | -0.44570100 | 2.60113800 |
| H | 0.80659100 | -0.15332000 | 4.15308900 |
| H | 0.22460100 | -1.76902200 | 3.75250800 |
| C | 2.45309900 | -2.11471700 | -2.30493600 |
| H | 3.14796400 | -1.27630700 | -2.23288300 |
| C | 2.96295400 | -1.84803000 | 3.74193400 |
| H | 2.51418100 | -2.77153200 | 4.11573200 |
| H | 3.12132400 | -1.18420600 | 4.59410200 |
| H | 3.93623500 | -2.10314400 | 3.31556800 |
| C | -5.44303400 | 5.02086700 | -0.03527100 |
| H | -5.83990400 | 6.02854600 | -0.01943700 |
| C | 3.12758700 | -3.22010200 | -3.11373900 |
| H | 3.99044600 | -3.64027600 | -2.59271300 |
| H | 3.46276900 | -2.82796800 | -4.07541000 |

| | | | |
|---|---|---|---|
| H | 2.43206200 | -4.03562900 | -3.32153900 |
| C | -4.26717900 | -2.34959800 | -0.12428700 |
| C | 1.19497700 | -1.62170500 | -3.02241400 |
| H | 0.46917300 | -2.43540200 | -3.10562500 |
| H | 1.43591900 | -1.27321200 | -4.02906700 |
| H | 0.71780300 | -0.80530700 | -2.47350200 |
| C | 4.30468000 | 1.63727800 | -1.27618500 |
| H | 5.03759400 | 2.44893900 | -1.25299900 |
| C | 4.31506900 | 1.69980500 | 1.22926500 |
| H | 3.71330500 | 1.86161200 | 2.12413800 |
| H | 5.05215700 | 2.50584400 | 1.19155600 |
| C | 3.41098500 | 1.82459800 | -0.02010700 |
| C | 3.50733900 | 1.72191300 | -2.57493800 |
| H | 4.16420600 | 1.55197100 | -3.43028700 |
| H | 3.02856800 | 2.69245400 | -2.70437800 |
| H | 2.72040600 | 0.96106400 | -2.59947600 |
| C | 3.51305600 | 4.36039600 | -0.40635800 |
| H | 4.37078300 | 4.44587800 | 0.26736700 |
| H | 2.93029100 | 5.27716300 | -0.30442300 |
| H | 3.88719100 | 4.32013600 | -1.43004700 |
| C | 2.64035800 | 3.16381800 | -0.03655400 |
| H | 1.85909900 | 3.05718800 | -0.79823100 |
| C | 1.94741300 | 3.45704700 | 1.29472200 |
| H | 1.48470800 | 2.56613200 | 1.72925600 |
| H | 1.15673600 | 4.19372400 | 1.14991200 |
| H | 2.65910100 | 3.86126500 | 2.02048400 |
| C | 2.46516200 | 0.65257900 | 0.00238100 |
| C | 4.99218600 | 0.32570400 | 1.28724000 |
| H | 6.08128600 | 0.40780200 | 1.27431000 |
| H | 4.72167300 | -0.21761400 | 2.19482000 |
| N | 3.08670900 | -0.50383600 | 0.04840800 |
| H | -7.39902300 | 4.12808000 | -0.05189200 |
| C | -5.30946900 | -3.42278800 | -0.07355700 |
| F | -4.91607300 | -4.54267400 | -0.69709800 |
| F | -5.61074800 | -3.78250800 | 1.18774400 |
| F | -6.46177100 | -3.03802800 | -0.63929600 |

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