Structural Characterization and Lifetimes of Triple-Stranded Helical Coinage Metal Complexes: Synthesis, Spectroscopy and Quantum Chemical Calculations

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# Supporting Information

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Refinement details of 1,3 and 4

Crystal data collection and processing parameters are given below. In order to avoid quality degradation, the single crystals were mounted in perfluoropolyalkylether oil on top of an open Mark tube and then brought into the cold nitrogen stream of a low-temperature device (Oxford Cryosystems Cryostream unit) so that the oil solidified. Diffraction data were measured using a Stoe IPDS II diffractometer and graphite-monochromated MoKα (0.71073 Å) radiation. The structures were solved by dual-space direct methods with SHELXT, followed by full-matrix least-squares refinement using SHELXL-2014/7. All non-hydrogen atoms were refined anisotropically. The contribution of the hydrogen atoms, in their calculated positions, was included in the refinement using a riding model.

Crystallographic data (excluding structure factors) for the structures in this paper have been deposited with the Cambridge Crystallographic Data Centre as supplementary publication nos. CCDC 1862546-1862548. Copies of the data can be obtained from https://summary.ccdc.cam.ac.uk/structure-summary-form.

| Compound | Formula | 1 | 3 | 4 |
|----------|---------|---|---|---|
|          | C_{24}H_{21}N_9Ru_2P_2F_{12}·3 MeCN | C_{48}H_{36}Ag_3F_6N_{18}PRu_2 | C_{48}H_{36}Au_3F_6N_{18}PRu_2 |
| D\text{calc}/ g cm\textsuperscript{-3} | 1.702 | 1.482 | 2.153 |
| µ/mm\textsuperscript{-1} | 0.613 | 1.348 | 8.518 |
| Formula Weight | 949.68 | 1535.67 | 1802.96 |
| Colour | clear yellow | clear red | clear red |
| Shape | irregular | irregular | block |
| Size/mm\textsuperscript{3} | 0.20×0.10×0.10 | 0.2×0.05×0.05 | 0.30×0.20×0.15 |
| T/K | 200 | 293(2) | 200 |
| Crystal System | trigonal | monoclinic | monoclinic |
| Space Group | P-3c1 | C2/c | C2/c |
| a/Å | 13.7710(19) | 20.851(4) | 19.982 |
| b/Å | 13.7710(19) | 13.021(3) | 12.988 |
| c/Å | 22.570(5) | 27.401(6) | 21.632 |
| α/° | 90 | 90 | 90 |
| β/° | 90 | 112.28(3) | 97.88 |
| γ/° | 120 | 90 | 90 |
| V/Å\textsuperscript{3} | 3706.7(13) | 6884(3) | 5561.0 |
| Z | 4 | 4 | 4 |
| Z' | 0.33333 | 0.5 | 0.5 |
| Wavelength/Å | 0.71073 | 0.71073 | 0.71073 |
| Radiation type | MoKα | MoKα | MoKα |
| θ\text{max}/° | 1.708 | 1.606 | 1.875 |
| θ\text{max}/° | 25.984 | 27.000 | 26.140 |
| Measured Refl. | 39031 | 53994 | 19460 |
| Independent Refl. | 2434 | 7516 | 5481 |
| Reflections Used | 1850 | 5386 | 4237 |
| R\text{int} | 0.0887 | 0.0938 | 0.0484 |
| Parameters | 179 | 354 | 384 |
| Restraints | 12 | 0 | 145 |
| Largest Peak | 1.507 | 2.432 | 2.471 |
| Deepest Hole | -1.811 | -1.356 | -2.003 |
| Goof | 1.109 | 1.005 | 1.121 |
| wR\text{2} (all data) | 0.2421 | 0.2305 | 0.2154 |
| wR\text{2} | 0.2267 | 0.2186 | 0.1875 |
| R\text{1} (all data) | 0.0908 | 0.0923 | 0.1006 |
| R\text{1} | 0.0787 | 0.0773 | 0.0738 |
Synthesis of the compounds

The copper complex 2 was already described in the literature before.\[^{[S1-2]}\] However, the adapted synthesis and a complete characterisation are added for completeness.

[S1] M. H. W. Lam, S. T. C. Cheung, K.-M. Fung, W.-T. Wong, *Inorg. Chem.* **1997**, *36*, 4618-4619.

[S2] A. J. Metherell, W. Cullen, A. Stephenson, C. A. Hunter, M. D. Ward, *Dalton Trans.* **2014**, *43*, 71-84.

Synthesis of 2 [{Ru(pypz)$_3$)$_2$Cu$_3$}(PF$_6$)$_2$. To a solution of 200 mg of the pure fac-isomer (0.252 mmol) of [{Ru(pypzH)$_3$}](PF$_6$)$_2$ and 230 mg copper(II) tetrafluoroborate in methanol 0.15 mL of triethylamine were added. The solution immediately turned from yellow to red. Afterwards the solution was stirred at room temperature for three days. The orange precipitate was filtered off and washed with methanol. The crude product was dissolved in dichloromethane and the precipitate of excess copper salt was filtered of via celite before the solvent was removed *in vacuo*. The product was obtained as red powder. The product was crystallized from dichloromethane/diethylether to form orange-red crystals.

Yields: 122 mg (72 %)

Mp = 280 °C (decomposition).

$^1$H NMR (CD$_2$Cl$_2$, 300 MHz): $\delta$/ppm = 6.87 (d, 6H, pz-H, $^3$J$_{HH} = 2.4$ Hz), 6.91 (ddd, 6H, py-H, $^3$J$_{HH} = 8.0$, 7.4 ,1.5 Hz), 6.99 (d, 6H, pz-H, $^3$J$_{HH} = 2.4$ Hz), 7.11 (ddd, 6H, py-H, $^3$J$_{HH} = 5.7$, 1.5, 0.8 Hz), 7.69 (ddd, 6H, py-H, $^3$J$_{HH} = 8.0$, 7.4, 1.5 Hz), 7.83 (ddd, 6H, py-H, $^3$J$_{HH} = 7.9$, 1.5, 0.8 Hz).

$^{13}$C NMR (CD$_2$Cl$_2$, 75.5 MHz): $\delta$/ppm = 101.37 (s, 6 C, pz-CH), 120.47 (s, 6 C, py-CH), 122.55 (s, 6 , py-CH), 135. 41 (s, 6 C, py-CH), 142.78 (s, 6 C, py-CH), 150.70 (s, 6 C, pz-C$_a$), 150.90 (s, 6 C, py-CH), 157.60 (s, 6 C, py-C$_a$).

ESI-MS (m/z, %) 1258.933 (100) [M−PF6]$^+$.  

Elemental analysis (%): Calcd. for C$_{48}$H$_{36}$Cu$_3$F$_6$N$_{18}$PRu$_2$: C 41.10, H 2.59, N 17.97. Found: C 40.52, N 17.63, H 2.66.

IR (solid, attenuated total reflection (ATR) cm$^{-1}$: $\bar{\nu} = 390$ (vw), 411 (w), 427 (w), 451 (vw), 507 (w), 555 (m), 642 (m), 693 (w), 707 (m), 748 (vs), 835 (s), 879 (vw), 950 (vw), 986 (vw), 1018 (vw), 1050 (vw), 1136 (vw), 1149 (vw), 1212 (vw), 1359 (vw), 1445 (vw), 1527 (vw), 1604 (vw).
Synthesis of 3 [(Ru(pypz)$_3$)$_2$Ag$_3$(PF$_6$)]. To a solution of 150 mg of the isolated fac-isomer (0.181 mmol) of [Ru(pypzH)$_3$(PF$_6$)$_2$] and 80 mg silver tetrafluoroborate (4.11 mmol) in methanol 0.1 mL of triethylamine (0.72 mmol) were added. The solution immediately turned from yellow to red. Afterwards the solution was stirred at room temperature for three days. The orange precipitate was filtered off and washed with methanol. The crude product was dissolved in dichloromethane and the precipitate of excess silver salt was filtered of via celite before the solvent was removed in vacuo. The crude product was recrystallized from dichloromethane/diethyl ether to form orange-red needles.

Yields: 95 mg (68 %).

Mp = 290°C (decomposition).

$^1$H NMR (CD$_2$Cl$_2$, 300 MHz): δ/ppm = 6.85 (ddd, 6H, py-H, $^3$J$_{HH}$ = 7.4, 5.7, 1.5 Hz), 6.90-6.93 (m, 6H, pz-H), 7.11 (ddd, 6H, py-H, $^3$J$_{HH}$ = 5.7, 1.5, 0.8 Hz), 7.14 (d, 6H, pz-H, $^3$J$_{HH}$ = 2.37 Hz), 7.66 (ddd, 6H, py-H, $^3$J$_{HH}$ = 8.0, 7.4, 1.5 Hz), 7.80 (ddd, 6H, py-H, $^3$J$_{HH}$ = 7.9, 1.5, 0.8 Hz).

$^{13}$C NMR (CD$_2$Cl$_2$, 75.5 MHz): δ/ppm = 78.11 (s, 6 C, pz-C$_q$), 103.53 (d, 6 C, pz-CH, $^2$J$_{CAg}$ = 1.61 Hz), 120.37 (s, 6 C, py-CH), 122.50 (s, 6 C, py-CH), 135.43 (s, 6 C, py-CH), 143.73 (d, 6 C, pz-CH, $^3$J$_{CAg}$ = 0.4 Hz), 150.92 (s, 6 C, py-CH), 157.76 (s, 6 C, py-C$_q$).

ESI-MS (m/z, %) 1390.861 (100) [M−PF$_6$]+.

Elemental analysis (%): Calcd. for C$_{48}$H$_{36}$Ag$_3$F$_6$N$_{18}$PRu$_2$: C 37.54, H 2.36, N 16.42. Found: C 37.50, H 2.50, N 16.02.

IR (solid, attenuated total reflection (ATR) cm$^{-1}$: $\tilde{\nu}$ = 397 (vw), 413 (w), 444 (vw), 506 (w), 555 (w), 612 (vw), 640 (w), 749 (vs), 838 (s), 881 (vw), 946 (vw), 981 (w), 1018 (w), 1053 (w), 1094 (vw), 1132 (vw), 1231 (vw), 1355 (w), 1446 (w), 1527 w, 1604 (w).

Synthesis of 4 [(Ru(pypz)$_3$)$_2$Au$_3$](PF$_6$). To a solution of 128 mg of the isolated fac-isomer (0.155 mmol) of [Ru(pypzH)$_3$](PF$_6$)$_2$ and 150 mg chloro(tetrahydrothiophene)gold(I) (0.47 mmol) in methanol 0.1 mL of triethylamine (0.72 mmol) were added. The solution immediately turned from yellow to red. Afterwards the solution was heated to reflux for 16 h. The resulting orange precipitate of the crude complex was filtered off and washed with methanol. The crude product was dissolved in dichloromethane and the precipitate of elemental gold was filtered of via celite before the solvent was removed in vacuo. The crude product was recrystallized from dichloromethane/hexane 4 was obtained as orange-red needles.

Yields: 90 mg (64 %).

Mp = 260-295°C (decomposition).

$^1$H NMR (CD$_2$Cl$_2$, 300 MHz): δ/ppm = 6.88 (ddd, 6H, py-H, $^3$J$_{HH}$ = 7.4, 5.8, 1.5 Hz), 6.91 (d, 6H, pz-H, $^3$J$_{HH}$ = 2.5), 7.06 (d, 6H, pz-H, $^3$J$_{HH}$ = 2.4 Hz), 7.08 (ddd, 6H, py-H, $^3$J$_{HH}$ = 5.68, 1.5,
0.8 Hz), 7.69 (ddd, 6H, py-H, $^3\text{J}_{HH} = 8.0, 7.5, 1.5$ Hz), 7.82 (ddd, 6H, py-H, $^3\text{J}_{HH} = 7.9, 1.5, 0.8$ Hz).

$^{13}$C NMR (CD$_2$Cl$_2$, 75.5 MHz): $\delta$/ppm = 103.77 (s, 6 C, pz-CH), 120.64 (s, 6 C, py-CH), 122.72 (s, 6 C, py-CH), 135.71 (s, 6 C, py-CH), 143.30 (s, 6 C, pz-CH), 150.33 (s, 6 C, py-CH).

ESI-MS (m/z, %) 1658.572 (100) [M−PF6]+.

Elemental analysis: Calcd. for C$_{48}$H$_{36}$Au$_3$F$_6$N$_{18}$PRu$_2$: C 31.98, H 2.01, N 13.98. Found: C 32.49, H 2.14, N 13.93.

IR (solid, attenuated total reflection (ATR) cm$^{-1}$: $\tilde{\nu}$ = 388 (vw), 419 (w), 451 (w), 506 (vw), 523 (vw), 555 (s), 642 (w), 708 (m), 748 (vs), 834 (vs), 879 (vw), 951 (vw), 987 (vw), 1018 (vw), 1074 (vw), 1137 (vw), 1156 (vw), 1362 (vw), 1445 (w), 1528 (vw), 1605 (vw).
NMR spectra

$^1$H NMR spectroscopic investigations of crystalline 3 show the expected pattern, very similar to the spectrum of 2. A slight difference could be observed for the multiplet with a chemical shift of $\delta = 6.90$-$6.93$ ppm, which is correlated to the pyrazolyl CH group next to the coordinating nitrogen atom. In 2, this signal appears as a regular doublet ($\delta^{1}\text{H} = 6.87$ ppm) with a coupling constant of 2.4 Hz that superimposes the signal at $\delta^{1}\text{H} = 6.91$ ppm (ddd) of a pyridine CH group. In 3, however, the doublet is replaced by the already described multiplet slightly shifted to higher frequencies. This kind of splitting in 3 as compared to 2 is caused by coupling to $^{109}\text{Ag}$ and therefore neither observable in the copper complex nor in the gold complex. Both the $^1$H NMR spectra and crystal structures are consistent proving that all six 3-(pyridine-2-yl)pyrazolyl ligands are equivalent in solid state and in solution. In the $^{13}$C NMR spectrum of 3, coupling of the carbon atoms of the CH-groups in the pyrazole rings to the silver atoms are observable. This correlation leads to two doublets with chemical shifts of $\delta^{13}\text{C} = 103.5$ and 143.8 ppm and coupling constants of 1.61 and $= 0.4$ Hz, respectively. The chemical shift with the larger coupling constant can be assigned to the carbon atoms right next to the coordinating nitrogen atoms. Furthermore, a $^{109}\text{Ag},^1\text{H}$ correlation spectrum clearly demonstrates that the silver cations of the complex 3 are coordinated to the deprotonated nitrogen atom of the pyrazolyl rings.

$^1$H-NMR

![NMR spectrum](image)

*Figure SI-1*: $^1$H-NMR-spectrum (300 MHz, CD$_2$Cl$_2$) of 2. Impurities of solvents are marked with a diamond sign. The residual CDHCl$_2$ peak is marked with an asterisk.
$^{13}$C-$^1$H-NMR

*Figure SI-2: $^{13}$C-$^1$H-NMR-spectrum (75 MHz, CD$_2$Cl$_2$) of 2. The CD$_2$Cl$_2$ peak is marked with an asterisk.*
Figure SI-3: $^1$H-NMR-spectrum (300 MHz, CD$_2$Cl$_2$) of 3. Impurities of solvents are marked with a diamond sign. The residual CDCl$_2$ peak is marked with an asterisk.

Figure SI-4: $^{109}$Ag/$^1$H-NMR spectrum of 3.
$^{13}$C-{$^1$H}-NMR

Figure SI-5: $^{13}$C-{$^1$H}-NMR-spectrum (75 MHz, CD$_2$Cl$_2$) of 3. The CD$_2$Cl$_2$ peak is marked with an asterisk.
Figure SI-6. $^1$H-NMR-spectrum (300 MHz, CD$_2$Cl$_2$) of 4. Impurities of solvents are marked with a diamond sign. The residual CDHC$_2$ peak is marked with an asterisk.
Figure SI-7: $^{13}$C($^1$H)-NMR-spectrum (75 MHz, CD$_2$Cl$_2$) of 4. The CD$_2$Cl$_2$ peak is marked with an asterisk. Due to low solubility of 4 quaternery carbon atoms could not be observed. The peak with a chemical shift of 150.33 ppm could only be observed with the help of hetero nuclear correlation spectra.
Figure SI-8: HMQC-spectrum of 4.

$$\text{[(Ru(pypz)₃Au)₂(PF₆)]}$$ 4

$$\text{[(Ru(pypz)₃Ag)₂(PF₆)]}$$ 3

$$\text{[(Ru(pypz)₃Cu)₂(PF₆)]}$$ 2

Figure SI-9: $^1$H NMR spectra of 2, 3 and 4 in CD₂Cl₂. For better gratitude of the essential peaks, residual solvent peaks of CDHCl₂ and trace amounts of CHCl₃ between 7.3 and 7.5 ppm were cleared out.
Additional crystallographic data

*Figure SI-10:* Molecular structure of $\text{fac-Ru(pypzH)_3}(\text{PF}_6)_2$ (1). The anion $[\text{PF}_6]^-$, solvent molecule (MeCN) and hydrogen atoms except of H1-H1'' have been omitted for clarity, displacement ellipsoids are drawn at the 30 % probability level. Selected bond lengths [pm] and angles [°]: Ru1−N2'' 207.2(4); Ru1−N2 204.6(4); N3−N3' 417.4; N1−Ru1−N1' 95.3(7); N1−Ru1−N2' 171.6(1); N1−Ru1−N2 77.0(0); N1−Ru1−N2' 88.9(0); N2−Ru1−N2' 99.1(2). Equivalent atoms denoted with primes are generated by (i) $−y, x−y, z$ and (ii) $−x+y, −x, z$. 
Additional computational data

Figure SI-11: Computed UV/Vis spectrum of 3, obtained from TDDFT calculations at the M06/def2-TZVP level (def2-SV(P) for H).

Figure SI-12: Computed UV/Vis spectrum of 4, obtained from TDDFT calculations at the M06/def2-TZVP level (def2-SV(P) for H).
Figure SI-13: Weighted average transition densities of 3 for the bands A through C of Figure 6. Green corresponds to a gain while orange indicates a loss of electron density (iso-value: ±0.005 $\AA^3$).

Figure SI-14: Weighted average transition densities of 4 for the bands A through C of Figure 6. Green corresponds to a gain while orange indicates a loss of electron density (iso-value: ±0.005 $\AA^3$).
Table SI1. Type of electronic excitations for 2, 3 and 4.

| Excitation | Compound | $\Delta E$ /eV | $\lambda$ /nm | $f_{osc}$ | Character     |
|------------|----------|----------------|-------------|--------|---------------|
| 4e         | 2        | 2.725          | 455.0       | 0.0316 | M(Ru)LCT      |
|            | 3        | 2.744          | 451.8       | 0.0252 |               |
|            | 4        | 2.769          | 447.8       | 0.0244 |               |
| 5e         | 2        | 2.860          | 433.5       | 0.0695 | M(Ru)LCT      |
|            | 3        | 2.880          | 430.5       | 0.0696 |               |
|            | 4        | 2.898          | 427.8       | 0.0923 |               |
| 6e         | 2        | 2.880          | 430.5       | 0.2332 | M(Ru)LCT      |
|            | 3        | 2.897          | 427.9       | 0.2395 |               |
|            | 4        | 2.914          | 425.5       | 0.2033 |               |
| 5a_2       | 2        | 3.281          | 377.9       | 0.0338 | M(Ru)LCT      |
|            | 3        | 3.291          | 376.7       | 0.0405 |               |
|            | 4        | 3.314          | 374.1       | 0.0397 |               |
| 13e        | (10e)    | 3.336          | 371.7       | 0.0323 | M(Ru)LCT      |
|            | (11e)    | 3.338          | 371.4       | 0.0758 |               |
| 14e        | (11e)    | 3.337          | 371.5       | 0.0502 | M(Ru)LCT      |
|            | (12e)    | 3.345          | 370.7       | 0.0108 |               |
| 9a_2       | 2        | 3.540          | 350.2       | 0.0421 | M(Ru)LCT      |
|            | 3        | 3.550          | 349.3       | 0.0432 |               |
|            | 4        | 3.579          | 346.4       | 0.0358 |               |
| 16a_2      | (15a_2)  | 2              | 4.264       | 290.8  | M(Cu/Ag/Au)LCT|
|            | 3        | 4.355          | 284.7       | 1.0686 |               |
|            | 4        | 4.293          | 288.8       | 1.1058 |               |
Figure SI-15: Transition densities of 2 for the substantial transitions shown in Figure 6 (blue sticks). Green corresponds to a gain while orange indicates a loss of electron density (iso-value: ±0.0025 \(a_0^{-3}\)).
Figure SI-16: Transition densities of 3 for the substantial transitions. Green corresponds to a gain while orange indicates a loss of electron density (iso-value: ±0.0025 $\text{a}_0^{-3}$).
Figure SI-17: Transition densities of 4 for the substantial transitions. Green corresponds to a gain while orange indicates a loss of electron density (iso-value: ±0.0025 $a_0^{-3}$).
Figure SI-18: Computed absorption spectrum of the Ru metalloligand $[\text{Ru(pypzH)}_3]^{2+}$ in comparison with the compounds 2, 3, and 4.

$3e$ ($\lambda = 385.0$ nm, $f_{osc} = 0.2515$)

$7e$ ($\lambda = 314.2$ nm, $f_{osc} = 0.0664$)

Figure SI-19: Transition densities of the Ru metalloligand $[\text{Ru(pypzH)}_3]^{2+}$. Green corresponds to a gain while orange indicates a loss of electron density (iso-value: $\pm 0.0025 \, \alpha_0^{-3}$).
Figure SI-20: Spin densities of the lowest triplet state of 2, 3, and 4 (iso-value: ±0.01 $a_0^{-3}$).
Figure SI-21: Frontier molecular orbitals and spin density of 2 in the lowest triplet state $T_1$: a) Singly occupied molecular orbital (SOMO) and b) lowest unoccupied molecular orbital (LUMO).

Figure SI-22: Frontier molecular orbitals and spin density of 3 in the lowest triplet state $T_1$: a) Singly occupied molecular orbital (SOMO) and b) lowest unoccupied molecular orbital (LUMO).
Figure SI-23: Frontier molecular orbitals and spin density of 4 in the lowest triplet state $T_1$: a) Singly occupied molecular orbital (SOMO) and lowest unoccupied molecular orbital (LUMO).
**Additional information Step-Scan FTIR**

![Image](image_url)

*Figure SI-24*: Step-scan FTIR spectrum 0 to 500 ns after irradiation of 2 and the ground state FTIR spectrum (black) in comparison. The negative bands correlate to the absorption bands of the ground state.

![Image](image_url)

*Figure SI-25*: Comparison of calculated ground state (green) and excited state (orange) IR spectrum with the Step-Scan difference spectrum of \([\text{Ru(pypz)}_3\text{Cu}]^+\) (2).
Figure SI-26: Decay curves obtained from a global fit of eight bands of (2). A bi-exponential fit yields two time constants.

Table SI2. Type of vibrations of 2.

|ν/cm⁻¹ ground state | ν/cm⁻¹ excited state | Character of the vibration                                      |
|--------------------|----------------------|-----------------------------------------------------------------|
| 1609               | 1600                 | C-C stretching in pyridine                                      |
| 1557               | 1522                 | C-C stretching in pyridine and C-H-bending                     |
| 1531               | 1531                 | C-C stretching between pyridine and pyrazole                   |
| 1448               | 1448                 | C-C stretching in pyridine accompanied with C-H-wagging        |
| 1363               | 1355                 | N₂-C stretching in pyrazole                                    |
| 1215               | 1215                 | C-H wagging                                                    |
| 1150               | 1131                 | N-N stretching in pyrazole accompanied with breathing of both rings |
Figure SI-27: Step-scan FTIR spectrum 0 to 500 ns after irradiation of 3 and the ground state FTIR spectrum (black) in comparison. The negative bands correlate to the absorption bands of the ground state.

Figure SI-28: Comparison of calculated ground state (green) and excited state (orange) IR spectrum with the Step-Scan difference spectrum of [(Ru(pyz)₃)₂Ag₃]⁺ (3).
Figure SI-29: Decay curves obtained from a global fit of eight bands of (3). A bi-exponential fit yields two time constants.

Table SI3. Type of vibrations of 3.

| 𝜈/cm⁻¹ ground state | 𝜈/cm⁻¹ excited state | Character of the vibration                        |
|---------------------|----------------------|--------------------------------------------------|
| 1609                | 1601                 | C-C stretching in pyridine                       |
| 1558                | 1522                 | C-C stretching in pyridine and C-H-bending       |
| 1531                | 1522                 | C-C stretching between pyridine and pyrazole     |
| 1447                | 1442                 | C-C stretching in pyridine accompanied with C-H-wagging |
| 1359                | 1351                 | N₂-C stretching in pyrazole                      |
| 1217                |                      | C-H wagging                                      |
| 1149 - 1135         | 1118                 | N-N stretching in pyrazole accompanied with breathing of both rings |
Figure SI-30: Step-scan FTIR spectrum 0 to 500 ns after irradiation of 3 and the ground state FTIR spectrum (black) in comparison. The negative bands correlate to the absorption bands of the ground state.

Figure SI-31: Comparison of calculated ground state (green) and excited state (orange) IR spectrum with the Step-Scan difference spectrum of [[Ru(pypz)3]2Au3]+ (4).
Figure SI-32: Decay curves obtained from a global fit of eight bands of (4). A bi-exponential fit yields two time constants.

Table SI4. Type of vibrations of 4.

| \( \tilde{\nu} / \text{cm}^{-1} \) ground state | \( \tilde{\nu} / \text{cm}^{-1} \) excited state | Character of the vibration                                      |
|-----------------------------------------------|-----------------------------------------------|---------------------------------------------------------------|
| 1609                                         | 1601                                         | C-C stretching in pyridine                                    |
| 1557                                         | 1551                                         | C-C stretching in pyridine and C-H-bending                    |
| 1532                                         | 1524                                         | C-C stretching between pyridine and pyrazole                 |
| 1448                                         | 1443                                         | C-C stretching in pyridine accompanied with C-H-wagging       |
| 1433                                         | 1426                                         | C-C stretching in pyridine accompanied with C-H-bending       |
| 1365                                         | 1359                                         | N\(_2\)-C stretching in pyrazole                             |
| 1225                                         |                                              | C-H wagging                                                   |
| 1161                                         |                                              | N-N stretching in pyrazole accompanied with breathing of both rings |
Figure SI-33: Comparison of obtained FTIR spectra of the excited state (normalized) of 2, 3 and 4.

Figure SI-34: Comparison of calculated IR spectra of the singlet ground state of 2, 3 and 4. A Gaussian convolution of 10 cm\(^{-1}\) was used to broaden the bands. (scal. 0.965).
Figure SI-35: Comparison of calculated IR spectra of the excited triplet state of 2, 3 and 4. A Gaussian convolution of 10 cm$^{-1}$ was used to broaden the bands. (scal. 0.965).
Geometrical information of calc. structures

Figure SI-36: Structural definitions of the calculated ground state of [(Ru(pypz)_3)_2M_3]^+ (M = Cu, Ag, Au). H atoms are omitted for clarity. Calculation method: M06/def2-TZVP [def2-ecp pseudo-potentials for Ru, Ag, and Au, def2-SV(P) for H].

Table SI5. Structural characterisation of 2 in the $D_3$-symmetrical ground state.

| involved atoms | distances / Å |
|----------------|---------------|
| Cu-Cu          | 3.479         |
| $\angle$ Cu-Cu-Cu / ° | 60.0         |
| N$_1$-Ru       | 2.102         |
| N$_2$-Ru       | 2.061         |
| A(Cu$_{\text{triangle}}$)-Ru | 3.095       |
| Cu-Ru          | 3.857         |
| N$_3$-Cu       | 1.880         |
| N$_1$-C$_1$     | 1.355         |
| C$_1$-C$_2$     | 1.387         |
| C$_2$-C$_3$     | 1.377         |
| C$_3$-C$_4$     | 1.385         |
| C$_4$-C$_5$     | 1.377         |
| C$_5$-N$_1$     | 1.336         |
| C$_1$-C$_6$     | 1.441         |
| C$_6$-N$_2$     | 1.344         |
| N$_2$-N$_3$     | 1.336         |
| N$_3$-C$_8$     | 1.348         |
| C$_8$-C$_7$     | 1.377         |
| C$_7$-C$_6$     | 1.395         |
Figure SI-37: Structural definitions of the calculated excited ($T_1$) state of $\left[[\text{Ru(pypz)}_2]_2M_3\right]^+$ ($M = \text{Cu, Ag, Au}$). H atoms are omitted for clarity.
Table S16. Structural characterisation of 2 in the excited state (T₁).

| involved atoms | distances / Å | In. Atoms | d / Å | In. Atoms | d / Å |
|----------------|---------------|-----------|-------|-----------|-------|
| Cu₁-Cu₂        | 3.551         |           |       |           |       |
| Cu₂-Cu₃        | 3.880         |           |       |           |       |
| Cu₃-Cu₁        | 3.621         |           |       |           |       |
| N₁ₐ-Ru₁        | 2.648         | N₁₀-Ru₁   | 2.123 | N₁₆-Ru₁   | 2.160 |
| N₂ₐ-Ru₁        | 2.100         | N₂₂-Ru₁   | 2.053 | N₂₆-Ru₁   | 2.338 |
| ∠ Cu₁-Cu₂-Cu₃ / ° | 58.1         |           |       |           |       |
| ∠ Cu₂-Cu₃-Cu₁ / ° | 56.4         |           |       |           |       |
| ∠ Cu₃-Cu₁-Cu₂ / ° | 65.5         |           |       |           |       |
| Cu₁-Ru₁        | 3.620         | Cu₂-Ru₁   | 3.772 | Cu₃-Ru₁   | 3.875 |
| N₃ₐ-Cu₁        | 1.886         | N₃₀-Cu₂   | 1.886 | N₃₆-Cu₃   | 1.883 |
| N₁₉-C₁ₐ        | 1.339         | N₁₀-C₁₉   | 1.354 | N₁₆-C₁₆   | 1.352 |
| C₁₈-C₂₈        | 1.391         | C₁₉-C₂₉   | 1.388 | C₁₆-C₂₆   | 1.389 |
| C₂₉-C₃₉        | 1.378         | C₂₀-C₃₀   | 1.376 | C₂₀-C₃₀   | 1.377 |
| C₃₉-C₄₉        | 1.384         | C₃₀-C₄₀   | 1.386 | C₃₀-C₄₀   | 1.385 |
| C₄₉-C₅₉        | 1.381         | C₴₀-C₵₀   | 1.376 | C₴₀-C₵₀   | 1.377 |
| C₅₉-N₁₉        | 1.326         | C₵₀-N₁₀   | 1.336 | C₵₀-N₁₀   | 1.336 |
| C₁₉-C₆₉        | 1.456         | C₁₉-C₆₉   | 1.440 | C₁₆-C₆₆   | 1.449 |
| C₆₉-N₂₉        | 1.343         | C₆₀-N₂₀   | 1.347 | C₆₀-N₂₀   | 1.339 |
| N₂₉-N₃₉        | 1.341         | N₂₀-N₃₀   | 1.337 | N₂₀-N₃₀   | 1.335 |
| N₃₉-C₈₉        | 1.342         | N₃₀-C₸₀   | 1.345 | N₃₀-C₸₀   | 1.345 |
| C₸₉-C₇₉        | 1.378         | C₸₀-C₇₀   | 1.380 | C₸₀-C₇₀   | 1.381 |
| C₇₉-C₆₉        | 1.395         | C₇₀-C₶₀   | 1.392 | C₇₀-C₆₀   | 1.397 |
Table SI7. Structural characterisation of 3 in the $D_3$-symmetrical ground state.

| involved atoms | distances / Å |
|----------------|---------------|
| Ag-Ag          | 3.290         |
| $\angle$ Ag-Ag-Ag / ° | 60.0          |
| N$_1$-Ru       | 2.101         |
| N$_2$-Ru       | 2.063         |
| A(Ag$_{\text{triangle}}$)-Ru | 3.392         |
| Ag-Ru          | 4.030         |
| N$_3$-Ag       | 2.113         |
| N$_1$-C$_1$    | 1.355         |
| C$_1$-C$_2$    | 1.388         |
| C$_2$-C$_3$    | 1.377         |
| C$_3$-C$_4$    | 1.385         |
| C$_4$-C$_5$    | 1.377         |
| C$_5$-N$_1$    | 1.336         |
| C$_1$-C$_6$    | 1.441         |
| C$_6$-N$_2$    | 1.345         |
| N$_2$-N$_3$    | 1.334         |
| N$_3$-C$_8$    | 1.348         |
| C$_8$-C$_7$    | 1.378         |
| C$_7$-C$_6$    | 1.395         |
Table S18. Structural characterisation of 3 in the excited state (T₁).

| involved atoms | distances / Å | In. Atoms | d / Å | In. Atoms | d / Å |
|----------------|---------------|-----------|-------|-----------|-------|
| Ag₁–Ag₂        | 3.298         |           |       |           |       |
| Ag₂–Ag₃        | 3.603         |           |       |           |       |
| Ag₃–Ag₁        | 3.479         |           |       |           |       |
| N₁₁a–Ru₁       | 2.623         | N₁₁b–Ru₁ | 2.121 | N₁₁c–Ru₁ | 2.152 |
| N₂₂a–Ru₁       | 2.104         | N₂₂b–Ru₁ | 2.055 | N₂₂c–Ru₁ | 2.354 |
| ∡Ag₁–Ag₂–Ag₃ / ° | 60.4         |           |       |           |       |
| ∡Ag₂–Ag₃–Ag₁ / ° | 55.5         |           |       |           |       |
| ∡Ag₃–Ag₁–Ag₂ / ° | 64.2         |           |       |           |       |
| Ag₁–Ru₁       | 3.779         | Ag₂–Ru₁  | 3.940 | Ag₃–Ru₁  | 4.108 |
| N₃₃a–Ag₁       | 2.113         | N₃₃b–Ag₂ | 2.116 | N₃₃c–Ag₃ | 2.106 |
| N₁₁a–C₁₁a      | 1.339         | N₁₁b–C₁₁b| 1.354 | N₁₁c–C₁₁c| 1.352 |
| C₁₁a–C₂₂a      | 1.391         | C₁₁b–C₂₂b| 1.388 | C₁₁c–C₂₂c| 1.389 |
| C₂₂a–C₃₃a      | 1.378         | C₂₂b–C₃₃b| 1.376 | C₂₂c–C₃₃c| 1.377 |
| C₃₃a–C₄₄a      | 1.385         | C₃₃b–C₄₄b| 1.386 | C₃₃c–C₄₄c| 1.385 |
| C₄₄a–C₅₅a      | 1.381         | C₄₄b–C₅₅b| 1.376 | C₄₄c–C₅₅c| 1.376 |
| C₅₅a–N₅₅a      | 1.326         | C₅₅b–N₅₅b| 1.336 | C₅₅c–N₅₅c| 1.336 |
| C₁₁a–C₆₆a      | 1.456         | C₁₁b–C₆₆b| 1.440 | C₁₁c–C₆₆c| 1.449 |
| C₆₆a–N₆₆a      | 1.344         | C₆₆b–N₆₆b| 1.348 | C₆₆c–N₆₆c| 1.341 |
| N₂₂a–N₂₂a      | 1.338         | N₂₂b–N₂₂b| 1.336 | N₂₂c–N₂₂c| 1.334 |
| N₃₃a–C₈₈a      | 1.342         | N₃₃b–C₈₈b| 1.344 | N₃₃c–C₈₈c| 1.344 |
| C₈₈a–C₇₇a      | 1.378         | C₈₈b–C₇₇b| 1.381 | C₈₈c–C₇₇c| 1.382 |
| C₇₇a–C₆₆a      | 1.395         | C₇₇b–C₆₆b| 1.392 | C₇₇c–C₆₆c| 1.397 |
Table S19. Structural characterisation of 4 in the $D_3$-symmetrical ground state.

| involved atoms         | distances / Å |
|------------------------|---------------|
| Au-Au                  | 3.542         |
| $\angle$ Au-Au-Au / °  | 60.0          |
| N$_1$-Ru               | 2.095         |
| N$_2$-Ru               | 2.075         |
| A(Au$_{\text{triangle}}$)-Ru | 3.274     |
| Au-Ru                  | 4.026         |
| N$_3$-Au               | 2.048         |
| N$_1$-C$_1$            | 1.354         |
| C$_1$-C$_2$            | 1.388         |
| C$_2$-C$_3$            | 1.377         |
| C$_3$-C$_4$            | 1.385         |
| C$_4$-C$_5$            | 1.377         |
| C$_5$-N$_1$            | 1.337         |
| C$_1$-C$_6$            | 1.440         |
| C$_6$-N$_2$            | 1.344         |
| N$_2$-N$_3$            | 1.335         |
| N$_3$-C$_8$            | 1.349         |
| C$_8$-C$_7$            | 1.376         |
| C$_7$-C$_6$            | 1.394         |
Table S110. Structural characterisation of 4 in the excited state (T₁).

| involved atoms | distances / Å | In. Atoms d / Å | In. Atoms | d / Å |
|----------------|--------------|-----------------|-----------|-------|
| Au₁-Au₂        | 3.478        |                 |           |       |
| Au₂-Au₃        | 3.859        |                 |           |       |
| Au₃-Au₁        | 3.781        |                 |           |       |
| N₁₁a-Ru₁       | 2.624        | N₁b-Ru₁         | 2.135     | N₁c-Ru₁ | 2.156 |
| N₂₁a-Ru₁       | 2.109        | N₂b-Ru₁         | 2.068     | N₂c-Ru₁ | 2.334 |
| 4 Au₁-Au₂-Au₃ / ° | 61.8       |                 |           |       |
| 4 Au₂-Au₃-Au₁ / ° | 54.2       |                 |           |       |
| 4 Au₃-Au₁-Au₂ / ° | 64.1       |                 |           |       |
| Au₁-Ru₁        | 3.738        | Au₂-Ru₁         | 3.971     | Au₃-Ru₁ | 4.071 |
| N₃₁a-Au₁       | 2.045        | N₃b-Au₂         | 2.044     | N₃c-Au₃ | 2.039 |
| N₁₁a-C₁a       | 1.340        | N₁b-C₁b         | 1.352     | N₁c-C₁c | 1.353 |
| C₁₁a-C₂a       | 1.391        | C₁b-C₂b         | 1.389     | C₁c-C₂c | 1.389 |
| C₂₁a-C₃a       | 1.378        | C₂b-C₃b         | 1.376     | C₂c-C₃c | 1.376 |
| C₃₁a-C₄a       | 1.384        | C₃b-C₄b         | 1.387     | C₃c-C₄c | 1.385 |
| C₄₁a-C₅a       | 1.381        | C₄b-C₅b         | 1.376     | C₄c-C₅c | 1.377 |
| C₅₁a-N₁₁a      | 1.326        | C₅b-N₁b         | 1.336     | C₅c-N₁c | 1.336 |
| C₁₁a-C₆a       | 1.457        | C₁b-C₆b         | 1.439     | C₁c-C₆c | 1.447 |
| C₆₁a-N₂₁a      | 1.344        | C₆b-N₂b         | 1.347     | C₆c-N₂c | 1.336 |
| N₂₁a-N₃₁a      | 1.337        | N₂b-N₃b         | 1.335     | N₂c-N₃c | 1.329 |
| N₃₁a-C₈a       | 1.343        | N₃b-C₈b         | 1.345     | N₃c-C₈c | 1.347 |
| C₈₁a-C₇a       | 1.377        | C₈b-C₇b         | 1.378     | C₈c-C₇c | 1.379 |
| C₇₁a-C₆a       | 1.396        | C₇b-C₆b         | 1.392     | C₇c-C₆c | 1.399 |
XYZ coordinates of calculated (DFT) structures

Singlet ground state of [{Ru(pypz)$_3$)$_2$Cu$_3$} (2):

| Atom | X          | Y          | Z          |
|------|------------|------------|------------|
| H    | -4.8360851 | -1.8788285 | 6.2116582  |
| H    | -4.8360851 | 1.8788285  | -6.2116582 |
| C    | -3.9597409 | -1.5050774 | 5.6936121  |
| H    | -3.8627511 | -3.1342586 | 4.2924632  |
| H    | -3.7497200 | -0.2676018 | -6.9079420 |
| C    | -3.9597409 | 1.5050774  | -5.6936121 |
| H    | -3.7497200 | 0.2676018  | 6.9079420  |
| C    | -3.4243233 | 2.2037250  | 4.6347267  |
| C    | -3.3623906 | 0.3174944  | -6.0827377 |
| C    | -3.3623906 | -0.3174944 | 6.0827377  |
| H    | -3.8627511 | 3.1342586  | -4.2924632 |
| H    | -3.4136410 | -2.7178206 | -0.4869979 |
| H    | -2.5808209 | -4.3382570 | 2.4101516  |
| C    | -3.4243233 | 2.2037250  | -4.6347267 |
| C    | -2.6588327 | -2.5422346 | -1.2402168 |
| H    | -2.4666303 | -4.4041850 | -2.4101516 |
| H    | -3.4136410 | 2.7178206  | 0.4869979  |
| C    | -1.8520275 | -3.5703709 | 2.2073103  |
| C    | -2.3035790 | -1.7082901 | 3.9842878  |
| C    | -2.1660182 | -3.3890883 | 2.2073103  |
| C    | -2.2497642 | 0.1201247  | 5.3995036  |
| C    | -2.2497642 | -0.1201247 | -5.3995036 |
| C    | -2.3035790 | 1.7082901  | -3.9842878 |
| H    | -1.7521659 | -1.0451317 | 5.6782869  |
| C    | -2.6588327 | 2.5422346  | 1.2402168  |
| N    | -2.0410199 | -1.3460679 | -1.3124293 |
| C    | -1.6628229 | -2.3568956 | 2.8685340  |
| H    | -0.7829720 | -4.9123699 | -4.2924632 |
| Cu   | -2.0085367 | 0.0000000  | 0.0000000  |
| H    | -2.4666303 | 4.4041850  | 2.4101516  |
| H    | -1.7521659 | 1.0451317  | 5.6782869  |
| N    | -1.7161888 | -0.5508456 | 4.3743677  |
| H    | -2.5808209 | 4.3382570  | -2.4101516 |
| N    | -2.0410199 | 1.3460679  | 1.3124293  |
| C    | -2.1660182 | 3.3890883  | 2.2073103  |
| H    | -0.6468812 | -4.3152101 | 0.4869979  |
| N    | -1.7161888 | 0.5508456  | -4.3743677 |
| C    | -0.8722234 | 3.5737340  | 1.2402168  |
| C    | -1.2097208 | 2.6184952  | 2.8685340  |
| C    | -0.1963201 | -4.0674135 | -4.6347267 |
| N    | -1.1582176 | -1.3960014 | 2.3134554  |
| C    | -1.8520275 | 3.5703709  | -2.2073103 |
| C    | -1.6628229 | 2.3568956  | 2.8685340  |
| C    | -0.3276331 | 2.8491029  | -3.984278  |
| N    | -0.6298639 | -1.7010465 | 2.3134554  |
| N    | -1.1582176 | 1.3960014  | 2.3134554  |
| C    | -1.2097208 | 2.6184952  | 2.8685340  |
| H    | 0.7909293  | -5.1275868 | 6.2116582  |
| H    | -0.0290277 | -2.0399860 | 5.6782869  |
| C    | 0.6764352  | -4.1817749 | -5.6936121 |
| N    | -0.1452191 | -2.4406090 | 1.3124293  |
| N    | -0.6298639 | 1.7010465  | 2.3134554  |
| C    | -0.8722234 | 3.5737340  | -1.2402168 |
| N    | 0.3810482  | -1.761859 | -4.3743677 |
| Ru   | -0.0000000 | 0.0000000  | 3.2921770  |
| H    | -0.6468812 | 4.3152101  | -0.4869979 |
| Ru   | -0.0000000 | 0.0000000  | -3.2921770 |
|   |   |   |   |
|---|---|---|---|
| H | -0.782972 | 4.9123699 | 4.2924632 |
| C | 1.4062371 | -3.0706629 | -6.0827377 |
| C | -0.3276331 | 2.8491029 | 3.9842878 |
| H | -0.0290277 | 2.0399860 | -5.6782869 |
| C | 1.0208511 | -2.0084153 | 5.3995036 |
| C | -0.1963201 | 4.0674135 | 4.6347267 |
| N | -0.1452191 | 2.4406090 | -1.3124293 |
| H | 2.1066099 | -3.1135519 | -6.9079420 |
| N | 0.3810482 | 1.7616859 | 4.3743677 |
| C | 1.2289131 | -1.8882906 | -5.3995036 |
| H | 1.6431100 | -3.3811537 | 6.9079420 |
| Cu | 1.0042683 | -1.7394438 | 0.0000000 |
| N | 1.3351407 | -1.2108404 | 4.3743677 |
| C | 1.9561536 | -2.7531685 | 6.0827377 |
| C | 1.0208511 | 2.0084153 | -5.3995036 |
| H | 1.7811936 | -0.9948543 | -5.6782869 |
| C | 0.6764352 | 4.1817749 | 5.6936121 |
| C | 1.2289131 | 1.8882906 | 5.3995036 |
| H | 0.7909293 | 5.1275868 | 6.2116582 |
| N | 1.3351407 | 2.1084040 | -4.3743677 |
| H | 1.7811936 | 0.9948543 | 5.6782869 |
| H | 1.6431100 | 3.3811537 | -6.9079420 |
| Cu | 1.0042683 | 1.7394438 | 0.0000000 |
| C | 1.4062371 | 3.0706629 | 6.0827377 |
| N | 1.7880815 | 0.3050451 | 2.3134554 |
| N | 1.7880815 | -0.3050451 | -2.3134554 |
| C | 1.9561536 | 2.7531685 | 6.0827377 |
| N | 2.1862390 | -1.0945411 | -1.3124293 |
| C | 3.2833057 | -2.6769757 | 5.6936121 |
| C | 2.6312121 | -1.1408129 | 3.9842878 |
| N | 2.1862390 | 1.0945411 | 1.3124293 |
| C | 2.1066099 | 3.1135519 | 6.9079420 |
| H | 4.0451558 | -3.2487583 | 6.2116582 |
| C | 2.6312121 | 1.1408129 | -3.9842878 |
| C | 2.8725437 | -0.2615987 | 2.8685340 |
| C | 2.8725437 | 0.2615987 | -2.8685340 |
| C | 3.6206434 | -1.8636885 | 4.6347267 |
| C | 3.2833057 | 2.6769757 | 5.6936121 |
| C | 3.5310561 | -1.0314994 | -1.2402168 |
| C | 3.6206434 | 1.8636885 | -4.6347267 |
| C | 3.5310561 | 1.0314994 | 1.2402168 |
| H | 4.6457232 | -1.7781113 | 4.2924632 |
| H | 4.0605222 | -1.5973895 | -0.4869979 |
| C | 4.0180456 | 0.1812826 | 2.2073103 |
| C | 4.0180456 | -0.1812826 | -2.2073103 |
| H | 4.0451558 | 3.2487583 | 6.2116582 |
| H | 4.0605222 | 1.5973895 | 4.8669979 |
| H | 4.6457232 | 1.7781113 | -4.2924632 |
| H | 5.0474512 | -0.0659280 | 2.4101516 |
| H | 5.0474512 | 0.0659280 | -2.4101516 |
Excited triplet state of [(Ru(pypz)₃)Cu] (2):

| Element | X      | Y      | Z      |
|---------|--------|--------|--------|
| H       | -5.9639415 | -4.0078589 | 3.4761896 |
| H       | 5.9067358  | -5.6938104 | -0.0062625 |
| C       | -5.4755723  | 3.2966848  | 2.818846 |
| H       | -4.0464098  | 2.6404488  | 4.2865081 |
| H       | 6.9379777   | -4.0093540 | 1.5263673 |
| C       | 5.5474000   | 4.6700257  | 0.0140811 |
| H       | -6.7314433  | -3.7067444 | 1.110829 |
| C       | -4.4163194  | 2.5422912  | 3.2720815 |
| H       | 6.1224958   | -3.7415585 | 0.8649420 |
| H       | -5.9038335  | -3.1341311 | 1.5113345 |
| H       | 4.0246789   | -4.9913718 | -1.4672908 |
| H       | 0.7060859   | -2.4699151 | 3.8242271 |
| C       | -2.1776014  | -0.8958199 | 4.9464664 |
| C       | 4.5064674   | -4.2832599 | -0.8022376 |
| H       | 1.3875327   | -1.751972 | 3.3817444 |
| H       | 2.5193206   | -0.8353709 | 5.0419069 |
| C       | -0.3804530  | -4.2261998 | -1.3183948 |
| C       | -2.0155846  | -0.943827 | 3.9778158 |
| H       | -3.804537   | 1.6380161  | 2.4161776 |
| C       | 2.3006556   | -0.9194033 | 3.9896055 |
| C       | -5.2558248  | -2.2202139 | 0.7106369 |
| C       | 5.6285153   | -2.4521926 | 0.8475655 |
| H       | 4.0635875   | -2.9650657 | -0.7544345 |
| H       | 6.0513726   | -1.6841121 | 1.4961982 |
| C       | -1.1318685  | -3.4560862 | -1.4209548 |
| N       | 1.4083063   | -1.5807497 | 2.0487409 |
| N       | -2.6993072  | -0.7908791 | 2.7872119 |
| H       | 4.2058819   | 1.1234437  | 4.9071659 |
| Cu      | 0.0868748   | 2.0042714  | 0.7718946 |
| H       | -2.2918998  | -3.9212732 | 3.2415187 |
| H       | -5.5606720  | -2.0628030 | -0.3208293 |
| N       | -4.2320126  | -1.4769777 | 1.1402544 |
| C       | 2.5481407   | -4.0208662 | -3.1458554 |
| N       | -1.2072419  | -2.4590870 | -0.5161405 |
| C       | -2.0912135  | -3.2862209 | -2.3938248 |
| H       | -0.3436780  | 0.9064024  | 4.2415538 |
| N       | 4.6380555   | -2.0600445 | 0.0550310 |
| C       | -1.0927659  | 0.4178462  | 3.6347969 |
| C       | 2.8660633   | -0.2169035 | 2.9295385 |
| C       | 4.4259610   | 1.4754041  | 3.9058559 |
| N       | 2.3228946   | -0.6453665 | 1.7739246 |
| C       | 2.3215303   | -3.0806575 | -2.6700645 |
| C       | 2.9531213   | -2.4964125 | -1.5717395 |
| C       | 3.8236864   | 0.8530369  | 2.8209713 |
| N       | -2.1955696  | -0.0130560 | 1.8139061 |
| N       | -2.1999591  | -1.6428358 | -0.8803315 |
| C       | -2.7493775  | -2.1177617 | -2.0113364 |
| H       | 5.7500884   | 3.0378037  | 4.5276413 |
| H       | -5.5568728  | 0.6358752  | 1.9175026 |
| C       | 5.2775528   | 2.5350576  | 3.6906467 |
| N       | -1.1213762  | 0.7309864  | 2.3291409 |
| N       | 2.3809603   | -1.3078133 | -1.3191751 |
| C       | 1.3577130   | -2.1658596 | 3.0346465 |
| N       | 4.0766801   | 1.2558384  | 1.5528384 |
| Ru      | -3.1819393  | -0.0542093 | 0.0046340 |
| H       | 0.6267102   | -2.2075496 | 3.8297096 |
| Ru      | 3.1259453   | 0.1073412  | 0.0411818 |
| H       | -4.1421815  | -2.5059208 | 4.357114 |
| C       | 5.5162686   | 2.9563195  | 2.3918788 |
| Element | X-Coordinate | Y-Coordinate | Z-Coordinate |
|---------|--------------|--------------|--------------|
| C       | -3.8594911   | -1.3709769   | -2.5469804   |
| H       | 5.2962075    | -0.6225235   | -2.0067090   |
| C       | -5.2996040   | 1.6049049    | 1.4974859    |
| C       | -4.4919559   | -1.6650075   | 3.7465265    |
| N       | 1.4026472    | -1.1050678   | -2.2131022   |
| H       | 6.1704987    | 3.7927334    | 2.1790772    |
| N       | -4.2609905   | -0.3318737   | 1.7760775    |
| C       | 4.9003837    | 2.2891137    | 1.3583002    |
| H       | -6.8301682   | 2.6643560    | 2.5368857    |
| Cu      | -0.1121955   | 1.8368132    | 1.2804527    |
| N       | -4.2747173   | 1.6201201    | 0.6401142    |
| C       | -6.0053780   | 2.7368674    | 1.8385420    |
| C       | 5.0147347    | 0.3585837    | -2.3813338   |
| H       | 5.0621512    | 2.5824948    | 0.3247887    |
| C       | -5.5429560   | -0.8823453   | 4.1701735    |
| C       | -5.2812262   | 0.4204930    | -2.1992499   |
| H       | -6.0437432   | -1.0956500   | -5.1082271   |
| N       | 4.0739325    | 0.9993517    | -1.6827400   |
| H       | -5.5699860   | 1.2444696    | -1.5520533   |
| H       | 6.3778882    | 0.338519     | -4.0218557   |
| Cu      | 0.1185311    | 0.2546468    | -1.9680466   |
| C       | -5.9457804   | 0.1827945    | -3.3813966   |
| N       | -2.2104422   | 1.5075940    | -0.9292804   |
| N       | 1.9466909    | 2.0620536    | -0.4622421   |
| C       | 5.6135304    | 0.985023     | -3.4970157   |
| N       | 1.0962365    | 2.8252194    | 0.2280718    |
| C       | -5.6381153   | 3.9471934    | 1.2724082    |
| C       | -3.9024250   | 2.8037808    | 0.0944682    |
| N       | -1.1882222   | 1.6030868    | -1.7824821   |
| H       | -6.7656434   | 0.8270593    | -3.6744554   |
| H       | -6.1750009   | 4.8572927    | 1.5163919    |
| C       | 3.6699521    | 2.2215879    | -2.0955526   |
| C       | -2.777113    | 2.7204046    | -0.8022772   |
| C       | 2.6274789    | 2.8463697    | -1.3073275   |
| C       | -4.5762040   | 3.9787243    | 0.3962137    |
| C       | 5.2162903    | 2.1567635    | -3.9182233   |
| C       | 1.2248390    | 4.0970183    | -0.1902710   |
| C       | 4.237525     | 2.8202925    | -3.2131342   |
| C       | -1.1091365   | 2.8827019    | -2.1980103   |
| H       | -4.2507881   | 4.9052222    | -0.0631808   |
| H       | 0.6147675    | 4.8821395    | 0.2346618    |
| C       | -2.0997095   | 3.6354955    | 1.6064343    |
| C       | 2.1930442    | 4.1673569    | -1.1729169   |
| H       | 5.6632688    | 2.6113079    | -4.7958473   |
| H       | -0.3284128   | 3.1823923    | -2.8834364   |
| H       | 3.8856362    | 3.7985021    | -3.5207897   |
| H       | -2.2998885   | 4.6862055    | 1.7406538    |
| H       | 2.5447669    | 5.0476185    | -1.6876582   |
Singlet ground state of \([\{\text{Ru}(\text{pypz})_3\}_2\text{Ag}_3\} (3):

\[
\begin{array}{ccc}
\text{H} & -4.9253045 & -1.6625718 \\
\text{H} & -4.9253040 & 1.6625725 \\
\text{C} & -4.0306443 & -1.3308918 \\
\text{H} & -4.0148115 & -2.9557182 \\
\text{H} & -3.7331717 & 0.4221603 \\
\text{C} & -4.0306440 & 1.3308917 \\
\text{H} & -3.7331709 & 0.4221617 \\
\text{C} & -3.5305017 & 2.0479197 \\
\text{C} & -3.3746906 & 0.1765766 \\
\text{H} & -3.3746903 & 0.1765776 \\
\text{H} & -4.0148111 & 2.9557180 \\
\text{H} & -3.1938844 & -2.9054389 \\
\text{C} & -2.0544836 & -3.4591279 \\
\text{C} & -2.3866366 & -1.6066215 \\
\text{C} & -1.9590827 & -3.5022487 \\
\text{H} & -2.2420015 & 0.2095504 \\
\text{H} & -2.2420014 & -0.2095507 \\
\text{C} & -2.3866364 & 1.6066217 \\
\text{H} & -1.6993557 & -1.1084965 \\
\text{C} & -2.4773898 & 2.6840199 \\
\text{N} & -1.9497807 & -1.4473347 \\
\text{C} & -1.7844401 & -2.2755738 \\
\text{H} & -0.5409909 & -4.9454793 \\
\text{Ag} & -1.9009742 & 0.0000002 \\
\text{H} & -2.1934828 & 4.5374766 \\
\text{H} & -1.6993567 & 1.1084962 \\
\text{N} & -1.7429648 & -0.4816749 \\
\text{H} & -2.8286614 & 4.1839059 \\
\text{N} & -1.9497804 & 1.4473343 \\
\text{C} & -1.9590828 & 3.5022493 \\
\text{H} & -0.9073589 & -4.2347227 \\
\text{N} & -1.7429663 & 0.4816749 \\
\text{C} & -1.0813403 & -3.5000545 \\
\text{C} & -1.0813057 & -2.6714544 \\
\text{C} & 0.0031223 & -4.0720762 \\
\text{H} & -1.1084884 & -1.4437778 \\
\text{C} & -2.0544834 & 3.4591285 \\
\text{C} & -1.7844402 & 2.2755737 \\
\text{C} & -0.1962757 & -2.8586484 \\
\text{N} & -0.7163783 & -1.6726929 \\
\text{N} & -1.0984847 & 1.4437774 \\
\text{C} & -1.0813054 & 2.6714540 \\
\text{H} & 1.0647846 & -5.0900149 \\
\text{H} & -0.1158045 & -2.0277588 \\
\text{C} & 0.8926286 & -4.1473976 \\
\text{N} & -0.2847900 & -2.4179680 \\
\text{N} & -0.7163781 & 1.6726930 \\
\text{C} & -1.0813197 & 3.5000549 \\
\text{N} & 0.4572759 & -1.7385152 \\
\text{Ru} & -0.0081337 & -0.0032999 \\
\text{H} & -0.9073583 & 4.2347227 \\
\text{Ru} & -0.0081341 & 0.0032998 \\
\text{H} & -0.5409915 & 4.9454790 \\
\text{C} & 1.5674942 & -3.0021038
\end{array}
\]
| Atom | X-Coordinate | Y-Coordinate | Z-Coordinate |
|------|--------------|--------------|--------------|
| C    | -0.1962759   | 2.8586475    | 4.2382653    |
| H    | -0.1158053   | 2.0477905    | -5.9446077   |
| C    | 0.9327862    | -2.0478905   | 5.6589360    |
| C    | 0.0031220    | 4.0720759    | 4.8810838    |
| N    | -0.2847897   | 2.4179682    | -1.5501568   |
| H    | 2.2800913    | -3.0147642   | -7.1353650   |
| N    | 0.4572756    | 1.7385140    | 4.6316008    |
| C    | 1.3202903    | -1.8259267   | -5.6481002   |
| H    | 1.5017452    | -3.4459453   | 7.1654074    |
| Ag   | 0.9367307    | -1.6518419   | 0.0062513    |
| N    | 1.2771373    | -1.2688508   | 4.6289689    |
| C    | 1.8371061    | -2.8354311   | 6.3359930    |
| C    | 0.9327856    | 2.0478905    | -5.6589362   |
| H    | 1.8278044    | -0.9055939   | -5.9253945   |
| C    | 0.8926284    | 4.1473973    | 5.9297266    |
| C    | 1.3202896    | 1.8259263    | 5.6480997    |
| H    | 1.0647843    | 5.0900151    | 6.4375381    |
| N    | 1.2771374    | 1.2688518    | -4.6289694   |
| C    | 1.8278042    | 0.9055945    | 5.5253950    |
| H    | 1.5017451    | 3.4459447    | 7.1654070    |
| Ag   | 0.9367311    | 1.6518415    | -0.0062514   |
| C    | 1.5674939    | -3.0021037   | 6.3199473    |
| N    | 1.7846175    | 0.2203298    | 2.5559793    |
| N    | 1.7846177    | -0.2203305   | 2.5559789    |
| C    | 1.8371055    | 2.8354315    | -6.3359937   |
| N    | 2.2097440    | 0.9659553    | -1.5341839   |
| C    | 3.1629376    | -2.8243269   | 5.9341566    |
| C    | 2.5706549    | -1.2632506   | 4.2254025    |
| N    | 2.2097432    | 0.9659546    | 1.5341840    |
| H    | 2.2800909    | 3.0147644    | 7.1353653    |
| H    | 3.9012353    | -3.4313123   | 6.4464837    |
| C    | 2.5706549    | 1.2632514    | -4.2254030   |
| C    | 2.8427739    | -0.4068475   | 3.0989034    |
| C    | 2.8427751    | 0.4068470    | -3.0989022   |
| C    | 3.5297702    | 2.0317500    | 4.8694865    |
| C    | 3.1629380    | 2.8243267    | -5.9341557   |
| C    | 3.5450459    | -0.8114557   | -1.4317301   |
| C    | 3.5297694    | 2.0317503    | -4.8694888   |
| C    | 3.5450466    | 0.8114580    | 1.4317265    |
| H    | 4.5547960    | -1.9978090   | 4.5185675    |
| H    | 4.0906977    | -1.3296153   | -0.6555084   |
| C    | 3.9991653    | -0.0525697   | 2.4039988    |
| C    | 3.9991613    | 0.0525679    | -2.4039971   |
| H    | 3.9012348    | 3.4313121    | -6.4464832   |
| H    | 4.0906972    | 1.3296140    | 0.6555087    |
| H    | 4.5547956    | 1.9978089    | -4.5185668   |
| H    | 5.0140068    | -0.3657208   | 2.5890252    |
| H    | 5.0140074    | 0.3657223    | -2.5890252   |
Excited triplet state of \([\text{Ru}(\text{pypz})_3]_2\text{Ag}_3\) (3):

$$
\begin{array}{ccc}
\text{H} & -4.8614947 & -1.6452597 & 6.4879065 \\
\text{H} & -5.4181596 & 1.9054716 & -6.2351396 \\
\text{C} & -3.9791281 & -1.3148801 & 5.9508253 \\
\text{H} & -3.9954796 & -2.9447350 & 4.5483349 \\
\text{H} & -4.2814446 & -0.0437298 & -7.3126965 \\
\text{C} & -4.4598888 & 1.5511405 & -5.8697588 \\
\text{H} & -3.6552483 & 0.4432547 & 7.1609371 \\
\text{C} & -3.5031204 & -2.0373616 & 4.8796140 \\
\text{C} & -3.8354770 & 0.4705360 & -6.4696400 \\
\text{C} & -3.3146689 & -0.1590383 & 6.3276595 \\
\text{H} & -4.3280536 & 3.0070322 & -4.2960962 \\
\text{H} & -3.3212294 & -2.9865821 & -0.7499564 \\
\text{H} & -2.8673469 & -4.1731388 & 2.6018203 \\
\text{C} & -3.8562311 & 2.1687707 & -4.7961146 \\
\text{C} & -2.5780841 & -2.7557866 & -1.5006165 \\
\text{H} & -2.1772533 & -4.6277557 & 2.6080904 \\
\text{H} & -3.3008984 & 2.8200219 & 0.5998767 \\
\text{C} & -2.0818149 & -3.4631152 & 2.4003248 \\
\text{C} & -2.3722860 & -1.5982431 & 4.2054702 \\
\text{C} & -1.9869548 & -3.5805681 & -2.4370113 \\
\text{C} & -2.1967768 & 0.2235322 & 5.6202272 \\
\text{C} & -2.6180822 & 0.0617109 & -5.9626328 \\
\text{C} & -2.6295188 & 1.6929364 & -4.3438133 \\
\text{H} & -2.0865464 & -0.7838469 & 6.4009318 \\
\text{C} & -2.5636991 & 2.6191893 & 1.3648476 \\
\text{N} & -2.0909529 & -1.5071666 & 1.6043665 \\
\text{C} & -1.7899447 & -2.2784947 & 3.0765585 \\
\text{H} & -0.4507874 & -5.0203625 & -4.4817921 \\
\text{Ag} & -2.0030746 & -0.0723150 & -0.0512006 \\
\text{H} & -2.2791141 & 4.4929437 & 2.4998605 \\
\text{H} & -1.6485658 & 1.1238783 & 5.8859358 \\
\text{N} & -1.7190467 & -0.4730181 & 4.5843276 \\
\text{H} & -2.9349360 & 4.2251823 & -2.7257232 \\
\text{N} & -2.0155224 & 1.3918039 & 1.4704096 \\
\text{C} & -2.0338191 & 3.4587309 & 2.3198029 \\
\text{H} & -0.9473120 & -4.2775043 & 0.6596558 \\
\text{C} & -2.0227131 & 0.6575153 & -4.9381990 \\
\text{C} & -1.1134378 & -3.5298099 & 1.4226392 \\
\text{C} & -1.0998517 & -2.7424258 & -3.1056749 \\
\text{C} & 0.1271358 & -4.1493895 & -4.7687218 \\
\text{N} & -1.1928684 & -1.4988545 & -2.5934217 \\
\text{C} & -2.1840150 & 3.4796632 & -2.5206446 \\
\text{C} & -1.9477727 & 2.2850469 & -3.2021257 \\
\text{C} & -0.1223021 & -2.9342077 & -4.1452273 \\
\text{N} & -0.7147840 & 1.6965592 & 2.5165155 \\
\text{N} & -1.1378095 & 1.4155356 & 2.4746381 \\
\text{C} & -1.1269168 & 2.6510023 & 3.0055508 \\
\text{H} & 1.3181006 & -5.1708313 & -6.2233362 \\
\text{H} & -0.0383176 & -1.9287642 & 5.9233534 \\
\text{C} & 1.1076845 & -4.2274238 & -5.7312410 \\
\text{N} & -0.2982229 & -2.4600199 & 1.5052713 \\
\text{N} & -0.8955803 & 1.6635261 & -2.6434074 \\
\text{C} & -1.2111303 & 3.5117396 & -1.5448243 \\
\text{N} & 0.5822809 & -1.8243189 & -4.4693365 \\
\text{Ru} & -0.0047058 & -0.0006898 & 3.4597524 \\
\text{H} & -1.0142906 & 4.2521676 & -0.7816678 \\
\text{Ru} & 0.0067163 & -0.0613849 & -3.4405121 \\
\text{H} & -0.6032038 & 4.9501498 & 4.3943288 \\
\text{C} & 1.8235437 & -3.0868725 & -6.0607181 \\
\end{array}
$$
Singlet ground state of \([\{\text{Ru(pypz}_3\}\}_2\text{Au}_3]\) (4):

|   |   |   |   |   |   |   |
|---|---|---|---|---|---|---|
| H | -4.8445048 | -1.8043999 | 6.4394398 |
| H | -4.8445182 | 1.8044101 | -6.4394425 |
| C | -3.9640464 | -1.4512448 | 5.9140433 |
| H | -3.9150598 | 3.0844018 | 4.5157565 |
| H | -3.7034556 | 0.3167590 | 7.1260598 |
| C | -3.9640176 | 1.4512094 | 5.9140422 |
| H | -3.7034576 | 0.3167518 | 7.1260563 |
| C | -3.4531924 | -2.1627862 | 4.8515841 |
| C | -3.3377648 | 0.2762193 | 6.2967882 |
| C | -3.3377437 | -0.2761768 | 6.2968020 |
| H | -3.9150506 | 3.0843893 | -4.5157512 |
| H | -3.3346286 | 2.8467891 | 0.6341871 |
| H | -2.7129978 | -4.2951240 | 2.6154737 |
| C | -3.4532178 | 2.1628036 | 4.8515881 |
| C | -2.6044571 | -2.6365510 | -1.4022882 |
| H | -2.3375500 | -4.4801414 | -2.5850969 |
| H | -3.3346216 | 2.8467876 | 0.6341983 |
| C | -1.9600115 | -3.5541218 | 2.4026538 |
| H | -2.3282036 | -1.6914147 | 4.1901417 |
| C | -2.0859331 | -3.4519672 | 2.3814653 |
| C | -2.2258926 | 0.1399919 | 5.5996688 |
| C | -2.2258819 | -0.1399945 | 5.5996716 |
| C | -2.3281697 | 1.6913917 | 4.1901318 |
| H | -1.7089158 | -1.0574398 | 5.8675649 |
| C | -2.6044821 | 2.6365459 | 1.4022535 |
| N | -2.0474481 | -1.4110981 | 1.4868617 |
| C | -1.7129931 | -2.3540212 | 3.0689343 |
| H | -0.6668422 | -4.9188566 | -4.4657357 |
| Au | -2.0638328 | -0.0000134 | 0.0001030 |
| H | -2.3375486 | 4.4801243 | 2.5850947 |
| H | -1.7089058 | 1.0574458 | 5.8675490 |
| N | -1.7176695 | -0.5433894 | 4.5696072 |
| H | -2.7130039 | 4.2951273 | 2.6154740 |
| N | -2.0474365 | 1.4110874 | 1.4868662 |
| C | -2.0859541 | 3.4520049 | 2.3814859 |
| H | -0.8127723 | -4.3239052 | 0.6488977 |
| N | -1.7176677 | 0.5434047 | 4.5696109 |
| C | -1.0028979 | -3.5860344 | 1.4147938 |
| C | -1.1800883 | -2.6324418 | 3.0540079 |
| C | -0.1046762 | -4.0562805 | -4.8040952 |
| N | -1.1765658 | -1.4085147 | -2.4983654 |
| C | -1.9599959 | 3.5541147 | -2.4026384 |
| C | -1.7130053 | 2.3540277 | -3.0689370 |
| C | -0.2847339 | -2.8384368 | -4.1636746 |
| N | -0.6693518 | -1.7263790 | 2.5008293 |
| N | -1.1765671 | 1.4085255 | 2.4983670 |
| C | -1.1800888 | 2.6324123 | 3.0539977 |
| H | 0.9458068 | -5.0961513 | 6.3532856 |
| H | -0.0617676 | 2.0262692 | 5.8606164 |
| C | 0.7888218 | -4.1497118 | 5.8476327 |
| N | -0.2358384 | -2.4794292 | 1.4883142 |
| N | -0.6693437 | 1.7263765 | 2.5008259 |
| C | -1.0029044 | 3.5860086 | -1.4148219 |
| N | 0.3965804 | -1.7338068 | -4.5500814 |
| Ru | -0.0153123 | -0.0114113 | 3.4678506 |
| H | -0.8127703 | 4.3239134 | -6.468873 |
| Ru | -0.0153136 | 0.0114103 | -3.4678566 |
| H | -0.6668485 | 4.9188734 | 4.4657416 |
| C | 1.4856862 | -3.0175306 | -6.2367085 |
Excited triplet state of \([\text{Ru(pypz)}_3]^{2+}\text{Au}\) (4):

\[
\begin{align*}
H & \quad -4.8492022 & -1.8838409 & 6.3271043 \\
H & \quad -5.0264566 & 2.0387580 & -5.8634844 \\
C & \quad -3.9727420 & -1.5094508 & 5.8095566 \\
H & \quad -3.8155321 & -3.1865222 & 4.4725092 \\
H & \quad -4.0852026 & -0.2084732 & -6.4593006 \\
C & \quad -4.1194614 & 1.6714504 & -5.3953801 \\
H & \quad -3.8218267 & 0.3129101 & 6.9584472 \\
C & \quad -3.4044262 & -2.2336756 & 4.7858402 \\
C & \quad -3.6046097 & 0.4293471 & -5.7275887 \\
C & \quad -3.4087410 & -0.2941650 & 6.1622943 \\
H & \quad -3.8453588 & 3.4031634 & -4.1518866 \\
H & \quad -3.1598145 & -3.1235590 & 0.7206748 \\
H & \quad -2.5550255 & -4.3856696 & 2.6173856 \\
C & \quad -3.4670692 & 2.4328010 & -4.4528183 \\
C & \quad -2.4460702 & -2.8779533 & -1.4937408 \\
H & \quad -2.2059673 & -4.6561510 & 2.7749300 \\
H & \quad -3.2155658 & 2.6762033 & 0.2868536 \\
C & \quad -1.8159634 & -3.6302251 & 2.4067875 \\
C & \quad -2.2851851 & -1.7358803 & 4.1343541 \\
C & \quad -1.9468270 & -3.6399669 & 2.5261348 \\
C & \quad -2.2968656 & 0.1448079 & 5.4793158 \\
C & \quad -2.4516343 & 0.0653632 & -5.1054477 \\
C & \quad -2.3091333 & 1.9496663 & -3.8568433 \\
H & \quad -2.0068882 & -0.9571418 & -5.3380569 \\
C & \quad -2.5497707 & 2.5067807 & 1.1210939 \\
N & \quad -1.8987450 & -1.6525383 & -1.5411653 \\
C & \quad -1.6183748 & -2.4086830 & 3.0501567 \\
H & \quad -0.4950633 & -5.1492668 & -4.4153116 \\
Au & \quad -1.9421137 & -0.1890034 & -0.1140365 \\
H & \quad -2.4264466 & 4.3873298 & 2.2679431 \\
H & \quad -1.8280704 & 1.0927179 & 5.7287821 \\
N & \quad -1.7318627 & -0.5513274 & 4.4875501 \\
H & \quad -2.3708031 & 4.7740176 & -2.6397356 \\
N & \quad -1.9681419 & 1.3014007 & 1.2849685 \\
C & \quad -2.1370386 & 3.3599691 & 2.1182788 \\
H & \quad -0.6054008 & -4.4073531 & 0.6996821 \\
N & \quad -1.8031502 & 0.7420882 & -4.1977376 \\
C & \quad -0.8336796 & -3.6585885 & 1.4446622 \\
N & \quad -1.0669198 & -2.7875243 & -3.1947942 \\
C & \quad -0.0423049 & -4.2896207 & -4.8961597 \\
N & \quad -1.0569169 & -1.5941179 & 2.5776995 \\
C & \quad -1.7008298 & 3.9857163 & -2.3358670 \\
C & \quad -1.5921190 & 2.6842176 & 2.8368155 \\
C & \quad -0.2476051 & -3.0147316 & -4.3777184 \\
N & \quad -0.5787515 & -1.7649033 & 2.4937759 \\
N & \quad -1.1804785 & 1.3486632 & 2.3600266 \\
C & \quad -1.2654433 & 2.5849007 & 2.8819448 \\
H & \quad 0.9260919 & -5.4259692 & -6.4303310 \\
H & \quad -0.0809547 & -1.9115706 & 5.9090421 \\
C & \quad 0.7516320 & -4.4397381 & -6.0126445 \\
N & \quad -0.0988110 & -2.5297792 & 1.5122574 \\
N & \quad -0.6149760 & 2.0358696 & -2.1967300 \\
N & \quad -0.7260392 & 4.0472288 & -1.3624540 \\
N & \quad 0.3036099 & -1.9352295 & 4.9479939 \\
Ru & \quad -0.0119963 & 0.0022014 & 3.4250540 \\
H & \quad -0.4465163 & 4.8575597 & -0.7040037 \\
Ru & \quad 0.0287210 & 0.0715618 & -3.2801217 \\
H & \quad -0.9970169 & 4.8962177 & 4.3190117 \\
C & \quad 1.3282843 & -3.3213426 & -6.5898373
\end{align*}
\]
| Element | x     | y     | z     |
|---------|-------|-------|-------|
| C       | -0.4537777 | 2.8480431 | 4.0422278 |
| H       | -0.0545631 | 2.2462862 | -5.5769889 |
| C       | 0.9681382  | -1.9211708 | 5.6260566 |
| C       | -0.3978209 | 4.0739395  | 4.6913785 |
| N       | -0.0850202 | 2.8643480  | -1.3024229 |
| H       | 1.9599379  | -3.3977634 | -7.4667309 |
| N       | 0.2738183  | 1.7902790  | 4.4739371 |
| C       | 1.0737913  | 0.9681382  | -1.9211708 |
| C       | 0.3978209  | 4.0739395  | -5.5769889 |
| N       | 0.0850202  | 2.8643480  | -1.3024229 |
| H       | 1.5011179  | 1.1808687  | -6.4381535 |
| C       | 0.4170657  | 4.2232786  | 5.7907085 |
| C       | 1.0706806  | 1.9518268  | 5.5351549 |
| H       | 0.4687047  | 5.1742950  | 6.3091638 |
| N       | 1.3573659  | 1.2994112  | -4.4129168 |
| C       | 1.6433605  | 1.0749542  | 5.8395817 |
| H       | 1.6037403  | 3.4468479  | -6.9704716 |
| Au      | 1.1113340  | 2.0288123  | 0.1213451 |
| C       | 1.1713252  | 3.1426594  | 6.2189621 |
| N       | 1.8241068  | 0.3262670  | 2.4955406 |
| C       | 1.8806862  | -0.3799509 | 2.4779553 |
| C       | 1.9365717  | 2.7899962  | -6.1762740 |
| N       | 2.3258619  | -1.1232731 | -1.4623911 |
| C       | 3.2082567  | -2.6569296 | 5.9306622 |
| C       | 2.6004774  | -1.1421046 | 4.1868304 |
| N       | 2.2821608  | 1.0874970  | 1.5006203 |
| H       | 1.8314382  | 3.2177459  | 7.0741637 |
| H       | 3.9527211  | -3.2415195 | 6.4594889 |
| C       | 2.6698504  | 1.1062851  | -4.1508360 |
| C       | 2.8770917  | -0.2904518 | 3.0598081 |
| C       | 2.9437907  | 0.2068461  | -3.0620760 |
| C       | 3.5679985  | -1.8820024 | 4.8516282 |
| C       | 3.2838933  | 2.600311   | -5.9087092 |
| C       | 3.6661138  | -1.0179147 | -1.4078136 |
| C       | 3.6523684  | 1.7522062  | -4.8896497 |
| C       | 3.6205693  | 0.9477691  | 1.4265343 |
| H       | 4.5940639  | -1.8379648 | 4.5050713 |
| H       | 4.2179510  | -1.5436960 | -0.6420175 |
| C       | 4.0497566  | 0.0780683  | 2.4019108 |
| C       | 4.1101537  | -0.1858248 | 2.4117914 |
| H       | 4.0397923  | 3.1124540  | 6.4939557 |
| H       | 4.1777868  | 1.4850640  | 0.6727129 |
| H       | 4.6948653  | 1.5752877  | 4.6517423 |
| H       | 5.0609575  | -0.2290975 | 2.6130027 |
| H       | 5.1266946  | 0.0951314  | -2.6335189 |