Supplementary Information (SI) for Inorganic Chemistry Frontiers.

Tunable Aurophilic Aggregates as the Basis of Mechano- and Thermochromism in Gold(I) Ethynyl Complexes

Juan Carlos Pérez-Sánchez[a], Jessica Cámara[a], M. Carmen Blanco[b], Lucía Aloras-Perún[a], María Gil-Moles[a], Rosa M. Gomila[c], Antonio Frontera[c], M. Concepción Gimeno[a]*

[a]Instituto de Síntesis Química y Catálisis Homogénea (ISQCH), Consejo Superior de Investigaciones Científicas (CSIC)-University of Zaragoza, Pedro Cerbuna 12, 50009, Zaragoza, Spain.

[b]Centro Universitario de la Defensa, Universidad de Zaragoza-Academia General Militar, 50090, Zaragoza, Spain.

[c]Departament de Química, Universitat de les Illes Balears, Crta de Valldemossa km 7.5, 07122 Palma de Mallorca (Baleares), Spain

gimeno@unizar.es

TABLE OF CONTENTS

1. Experimental Section

General Considerations and Materials: All experiments and manipulations were carried out under air, unless otherwise stated. All chemical reagents were purchased from commercial suppliers and used as received. The starting materials, [AuCl(tht)] (tht = tetrahydrothiophene),[1] [Au(C≡CR)$_n$] {R = 2-pyridine (**2**), 3-pyridine (**3**), 4-pyridine (**4**), phenyl (**5**)}[2] were prepared according to published procedures. All other reagents were commercially available and were used without further purification.

NMR Information: ^{1}H, ^{13}C{^{1}H} APT, ^{31}P{^{1}H} NMR spectra were recorded on a Bruker Avance 300 or 400 spectrometers, at the indicated frequencies, at 298.15 K, unless otherwise stated. Chemical shifts are reported in ppm and referenced to the residual internal signal of the deuterated solvent (^{1}H, ^{13}C) and external H_3PO_4 85% (^{31}P). Multiplicity of the observed signals is indicated as follows: s = singlet, d = doublet, dd = doublet of doublets, ddd = doublet of doublets of doublets, dt = doublet of triplets, m = multiplet, br = broad signal. *J* values are given in Hz.

HRMS and FTIR: A Bruker MicroToF-Qspectrometer was used for high-resolution mass spectra-ESI (HRMS-ESI) equipped with an API-ESI source and a QTOF mass analyzer, both allowing a maximum error in the measurement of 5 ppm. Infrared spectra were recorded (in solid) in the range 4000–280 cm^{-1} on a PerkinElmer Spectrum 100 FTIR spectrometer equipped with an ATR accessory.

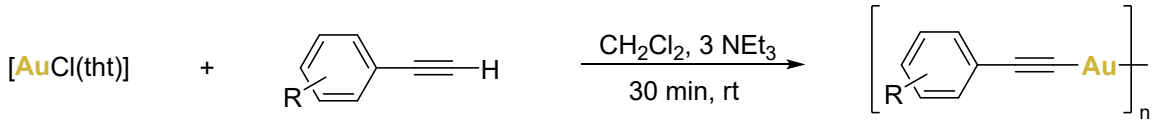
Steady-State Photoluminescence Studies and Lifetimes: Steady-state photoluminescence spectra and lifetime measurements were recorded with a FluoTime300 PicoQuant spectrometer as powder samples, placed in a quartz tube. A liquid nitrogen dewar assembly was used for the studies at 77 K. Quantum yields were measured by the absolute method using a Hamamatsu Quantaurus-QY C11347compact one-box absolute quantum yield measurement system. In order to prove the reproducibility of the measurements, three or more measurements were carried out for each compound with different amount of solid powder sample. Through studies carried out for different substances using both, the absolute method and the comparative one the relative uncertainty for the absolute method has been determined as less than 6%.[3] For film preparation, ca. 4 mg of compound and ca. 76 mg of PMMA were dissolved in 1 mL of CH_2Cl_2 in order to obtain films which contain about at 5 wt. % of the compound. The mixture was sonicated for 15–20 min. Films were prepared by drop casting the resulting solution. Two or three films of each complex were prepared as well as two or three reference samples. Each sample was measured using each reference in order to prove the reproducibility of the results.

Thermal analysis: Thermogravimetric and differential thermal analyses (TGA/DTA) were performed using a SDT 2960 instrument at a heating rate of 10 °C min^{-1} under N_2 atmosphere.

Crystallography: Crystals suitable for X-ray studies were obtained by vapor diffusion of n-hexane over a solution of the corresponding compound in dichloromethane. Crystals were mounted on a MiTeGen Crystal micromount and transferred to the cold gas stream of a Bruker D8 VENTURE diffractometer. Data were collected using monochromated MoK α radiation (λ = 0.71073 Å). Scan type ω. Absorption correction based on multiple scans were applied with the program ShelXT.[4] All non-hydrogen atoms were refined anisotropically. Hydrogen atoms were included using a riding model. CCDC deposition numbers 2441966 (**6**), 2441967 (**7**), 2441968 (**8**), 2441969 (**9**) contains the supplementary crystallographic data. These data can be obtained free of charge by The Cambridge Crystallography Data Center.

Powder X-ray Measurements: Data have been recorded at room temperature using a RIGAKU Ru2500 diffractometer provided with a rotating anode. Measurement conditions: Cu anode with a graphite monocromator, Cu Kα radiation, 40 kV and 80 mA, 2θ 3° to 50°, step = 0.03°, t = 1 s/step.

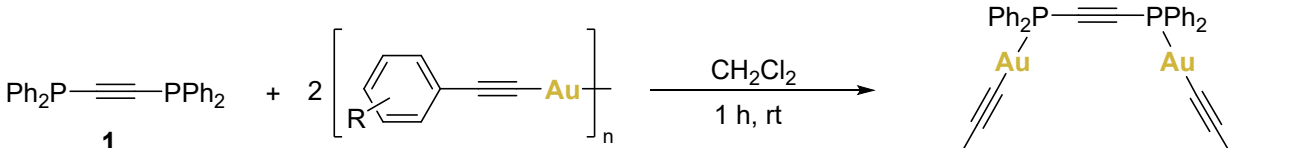
Synthetic procedures:



2-py, R = *o*-N
3-py, R = *m*-N
4-py, R = *p*-N
Ph, R = H

2, R = *o*-N
3, R = *m*-N
4, R = *p*-N
5, R = H

Synthesis of alkynyl gold(I) polymers (**2**–**5**): These compounds were prepared by following an experimental procedure previously described, with some modifications.[2] To a solution of the corresponding pyridineacetylene {101 µL (**2-py**), 103 mg (**3-py** and **4-py**), 1 mmol} or phenylacetylene **Ph** (110 µL, 1 mmol) in dichloromethane (15 mL), [AuCl(tht)] (321 mg, 1 mmol) and NEt_3 (415 µL, 3 mmol) were added. A solid immediately appeared, and the resulting suspension was stirred for 30 minutes. Ethanol (15 mL) was added, and the resulting yellow precipitate was filtered, washed with more ethanol (3 × 5 mL), acetone (3 × 5 mL), and diethyl ether (3 × 5 mL), and dried under vacuum. Yield: average 70% for all compounds. The high insolubility of these derivatives prevented characterization by solution NMR.

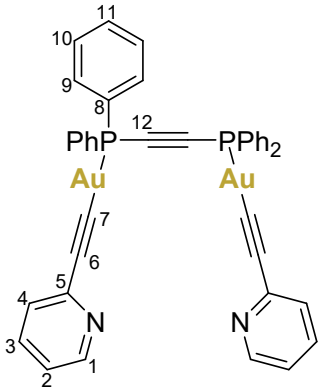


2, R = *o*-N
3, R = *m*-N
4, R = *p*-N
5, R = H

6, R = *ortho*-N
7, R = *meta*-N
8, R = *para*-N
9, R = H

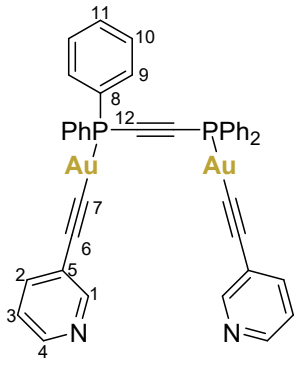
Synthesis of alkynyl-dppa gold(I) complexes (**6**–**9**): To a suspension of $[AuC{\equiv}CR]_n$ (150 mg, 0.5 mmol for **2**–**5**) in dichloromethane (20 mL), dppa **1** (96 mg, 0.25 mmol) was added. The resulting suspension was stirred for 1 hour until the solid completely dissolved, yielding a clear solution. If insoluble residues were observed (**8**), the reaction mixture was filtered through Celite®. The resulting colorless solution was then evaporated under reduced pressure to approximately 2-3 mL, followed by the addition of diethyl ether (10 mL), which precipitated a white solid. The solid was further washed with diethyl ether (2 × 5 mL) and dried under vacuum.

Characterization of the complexes:



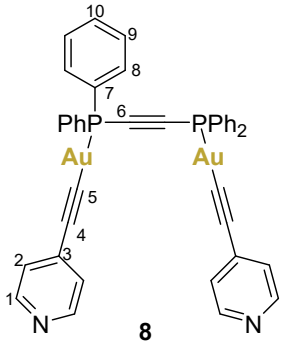
6

Complex **6**. Yield: 79%, 196 mg. **^{1}H NMR** (400 MHz, CD_2Cl_2) δ_H (ppm): 8.47 (d, $^{3}J_{H1}$-H_2 = 4.89 Hz, 2H, H_1), 7.67–7.76 (m, 8H, HPh), 7.81 (m, 8H, HPh), 7.35–7.54 (m, 14H, $2H_3$ + HPh), 7.34 (d, $^{3}J_{H4}$-H_3 = 7.84 Hz, 2H, H_4), 7.05 (ddd, $^{3}J_{H2}$-H_3 = 7.52 Hz, $^{3}J_{H2}$-H_1 = 4.89 Hz, $^{4}J_{H2}$-H_4 = 1.14 Hz, 2H, H_2). **^{13}C{^{1}H} APT NMR** (101 MHz, CD_2Cl_2) δ_C (ppm): 150.1 (s, 2C, C_1), 145.0 (s, 2C, C_5), 136.0 (s, 2C, C_3), 133.5 (d, $^{2}J_{CP}$ = 16.2 Hz, 8C, C_9), 132.83 (s, 2C, C_7), 131.6 (d, $^{4}J_{CP}$ = 1.5 Hz, 4C, C_{11}), 131.5 (d, $^{1}J_{CP}$ = 35.2 Hz, 4C, C_8), 129.7 (d, $^{3}J_{CP}$ = 10.5 Hz, 8C, C_{10}), 127.6 (s, 2C, C_4), 121.8 (s, 2C, C_2), 105.0 (s, 2C, C_{12}), 103.1 (s, 2C, C_6). **^{31}P{^{1}H} NMR** (162 MHz, CD_2Cl_2) δ_P (ppm): 15.6 (br s, 2P, PPh_2). **HRMS** (ESI-QTOF) m/z: $[M + Na]^+$ calculated for $C_{40}H_{28}Au_2N_2NaP_2$ 1015.0951, found 1015.0943. **IR** ν (cm^{-1}): 2101 (w, C≡C). **Elemental analysis** (%) calcd. for $C_{40}H_{28}Au_2N_2P_2$, C: 48.40, H: 2.84, N: 2.82; found C: 48.09, H: 2.84, N: 2.89.



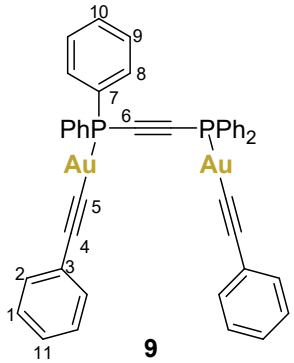
7

Complex **7**. Yield: 61%, 151 mg. **^{1}H NMR** (400 MHz, CD_2Cl_2) δ_H (ppm): 8.54 (dd, $^{4}J_{H1-H2}$ = 2.1 Hz, $^{5}J_{H1-H3}$ = 0.9 Hz, 2H, H_1), 8.38 (dd, $^{3}J_{H4-H3}$ = 4.9 Hz, $^{4}J_{H4-H2}$ = 1.7 Hz, 2H, H_4), 7.81 (m, 8H, HPh), 7.62 (dt, $^{3}J_{H2-H3}$ = 7.9 Hz, $^{4}J_{H2-H4,H1}$ = 1.9 Hz, 2H, H_2), 7.49 (m, 12H, HPh), 7.16 (ddd, $^{3}J_{H3-H2}$ = 7.9 Hz, $^{3}J_{H3-H4}$ = 4.9 Hz, $^{5}J_{H3-H1}$ = 0.9 Hz, 2H, H_1). **^{13}C{^{1}H} APT NMR** (101 MHz, CD_2Cl_2) δ_C (ppm): 150.0 (s, 2C, C_1), 147.4 (s, 2C, C_4), 139.0 (s, 2C, C_2), 135.7 (s, 2C, C_5), 133.8 (d, 2JCP = 16.2 Hz, 8C, C_9), 132.8 (d, $^{4}J_{CP}$ = 2.5 Hz, 4C, C_{11}), 130.0 (d, $^{3}J_{CP}$ = 12.4 Hz, 8C, C_{10}), 128.5 (d, $^{1}J_{CP}$ = 62.6 Hz, 4C, C_8), 123.1 (s, 2C, C_3), 122.33 (s, 2C, C_7), 102.4 (d, $^{1}J_{CP}$ = 75.8 Hz, 2C, C_{12}), 100.5 (s, 2C, C_6). **^{31}P{^{1}H} NMR** (162 MHz, CD_2Cl_2) δ_P (ppm): 14.8 (br s, 2P, PPh_2). **HRMS** (ESI-QTOF) m/z: $[M + Na]^+$ calculated for $C_{40}H_{28}Au_2N_2NaP_2$ 1015.0951, found 1015.0904. **IR** ν (cm^{-1}): 2158 (w, C≡C). **Elemental analysis** (%) calcd. for $C_{40}H_{28}Au_2N_2P_2$, C: 48.40, H: 2.84, N: 2.82; found C: 48.45, H: 2.72, N: 2.79.



8

Complex **8**. Yield: 59%. 146 mg. **^{1}H NMR** (400 MHz, CD_2Cl_2) δ_H (ppm): 7.78 (m, 8H, HPh), 7.52–7.46 (m, 16H, HPh), 7.14 (m, 4H, H_2), 7.15 (m, 4H, H_1). **^{13}C{^{1}H} APT NMR** (101 MHz, CD_2Cl_2) δ_C (ppm): 148.8 (s, 4C, C_1), 138.3 (s, 2C, C_3), 133.7 (d, $^{2}J_{CP}$ = 17.2 Hz, 8C, C_8), 133.4 (s, 2C, C_5), 132.5 (s, 4C, C_{10}), 129.9 (d, $^{3}J_{CP}$ = 12.0 Hz, 8C, C_9), 128.9 (s, 4C, C_7), 126.6 (s, 4C, C_2), 103.33 (s, 2C, C_6), 101.44 (s, 2C, C_4). **^{31}P{^{1}H} NMR** (162 MHz, CD_2Cl_2) δ_P (ppm): 10.5 (br s, 2P, PPh_2). **HRMS** (ESI-QTOF) m/z: $[M + H]^+$ calculated for $C_{40}H_{29}Au_2N_2P_2$ 993.1132, found 993.1120. **IR** ν (cm^{-1}): 2115 (w, C≡C). **Elemental analysis** (%) calcd. for $C_{40}H_{28}Au_2N_2P_2$, C: 48.40, H: 2.84, N: 2.82; found C: 48.30, H: 2.70, N: 2.59. **Note**: The obtained spectral data is consistent with previous reported values.[5]



9

Complex **9**. Yield: 81%, 200 mg. **^{1}H NMR** (400 MHz, CD_2Cl_2) δ_H (ppm): 7.85–7.78 (m, 8H, PPh), 7.58–7.49 (m, 12H, PPh), 7.44–7.36 (m, 4H, H_{Ar}), 7.29–7.16 (m, 6H, H_{Ar}). **^{13}C{^{1}H} APT NMR** (101 MHz, CD_2Cl_2) δ_C (ppm): 133.8 (d, $^{2}J_{CP}$ = 16.2 Hz 8C, C_8), 132.8 (br s, 4C, C_{10}), 132.4 (s, 4C, $C_{2/1}$), 130.0 (d, $^{3}J_{CP}$ = 12.3 Hz, 8C, C_9), 128.6 (d, $^{1}J_{CP}$ = 60.6 Hz, 4C, C_7), 128.5 (s, 4C, $C_{1/2}$), 127.2 (s, 2C, C_{11}), 125.4 (s, 2C, $C_{4/5/3}$), 103.6 (s, 2C, C_6) **^{31}P{^{1}H} NMR** (162 MHz, CD_2Cl_2) δ_P (ppm): 15.6 (br s, 2P, PPh_2). **HRMS** (ESI-QTOF) m/z: $[M + Na]^+$ calculated for $C_{42}H_{30}Au_2NaP_2$ 1013.1046, found 1013.1012. **IR** ν (cm^{-1}): 2100 (w, C≡C). **Elemental analysis** (%) calcd. for $C_{42}H_{30}Au_2N_2P_2$, C: 50.93, H: 3.05; found C: 50.81, H: 3.01.

2. NMR and FTIR Spectroscopy Data

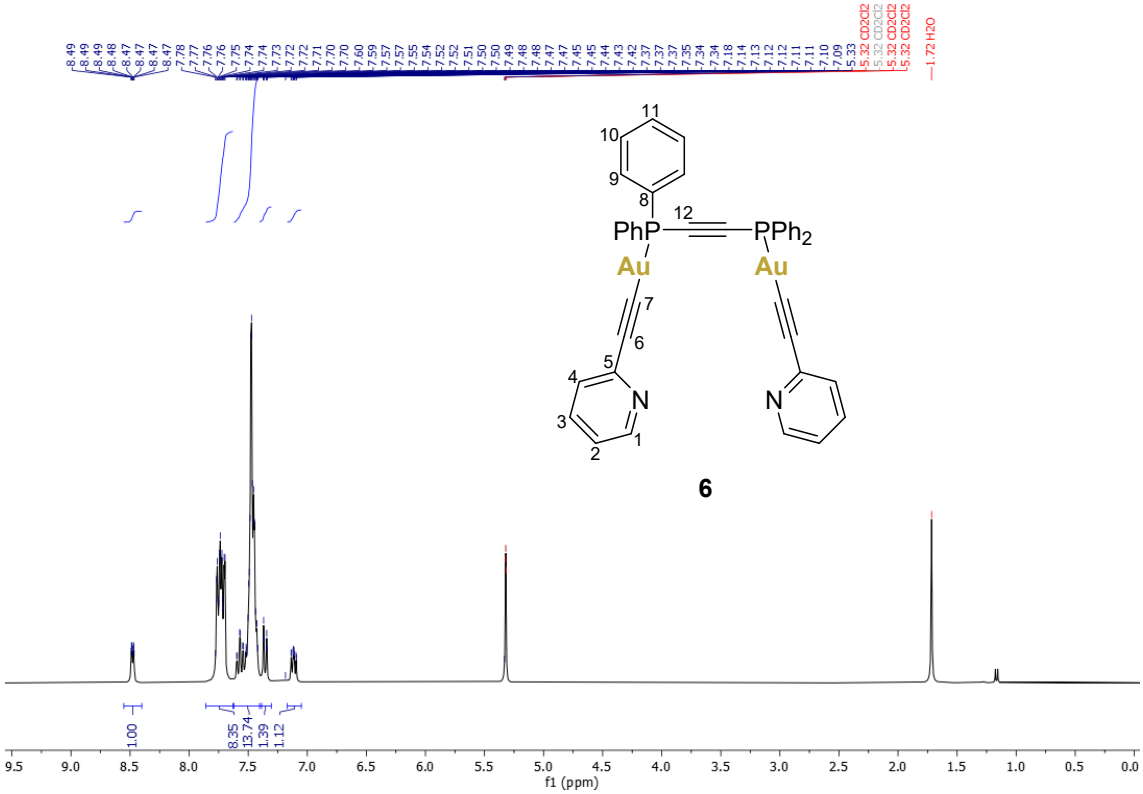


Figure S1. ^{1}H NMR (400 MHz, CD_2Cl_2) spectrum of complex **6**.

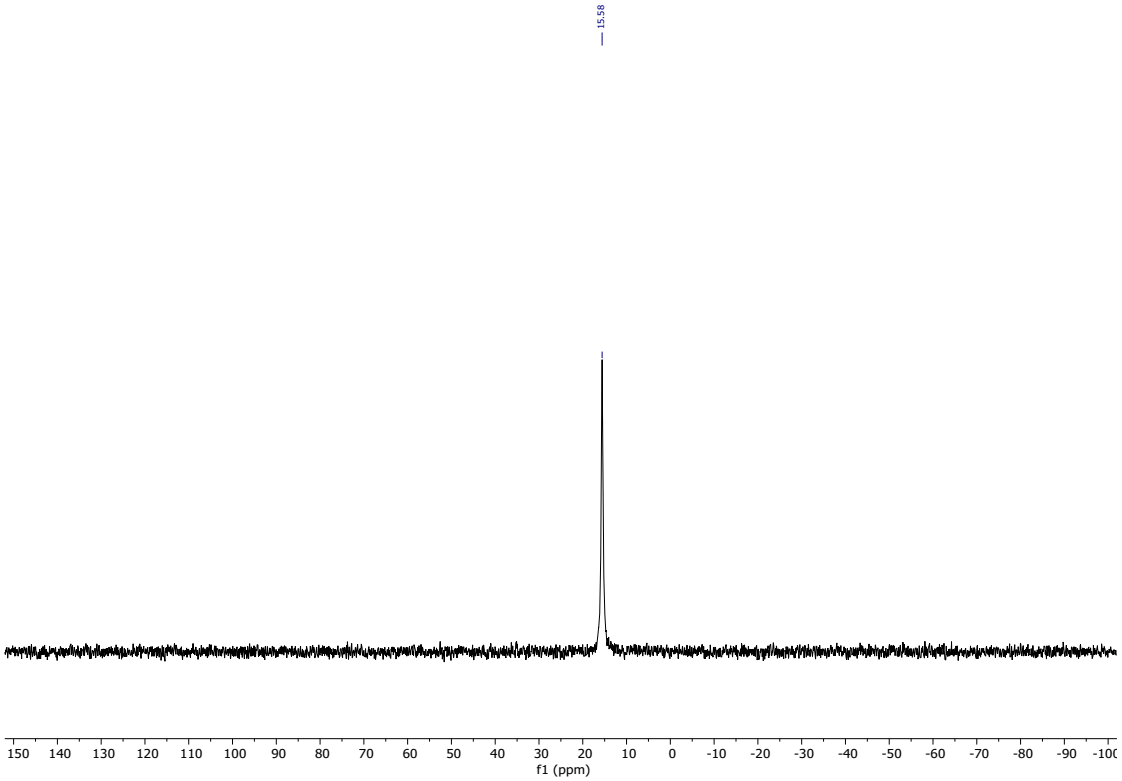


Figure S2. $^{31}P\{^{1}H\}$ NMR (162 MHz, CD_2Cl_2) spectrum of complex **6**.

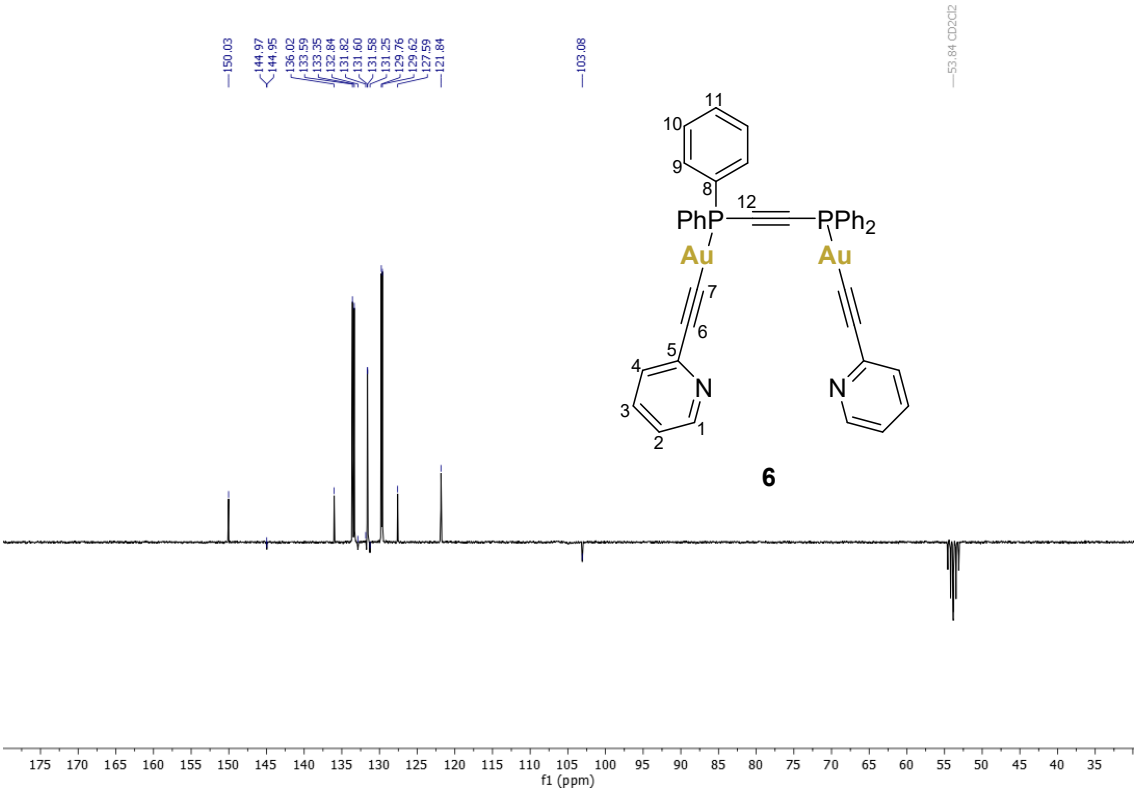


Figure S3. $^{13}C\{^{1}H\}$ APT NMR (101 MHz, CD_2Cl_2) spectrum of complex **6.**

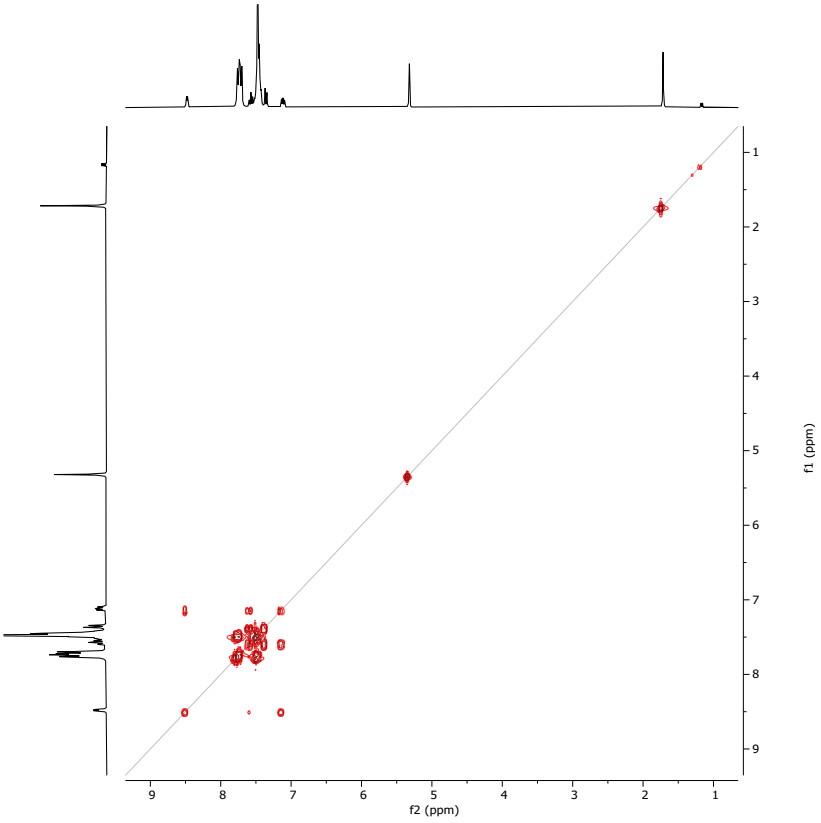


Figure S4. ^{1}H-^{1}H COSY NMR (400 MHz, CD_2Cl_2) spectrum of complex **6**.

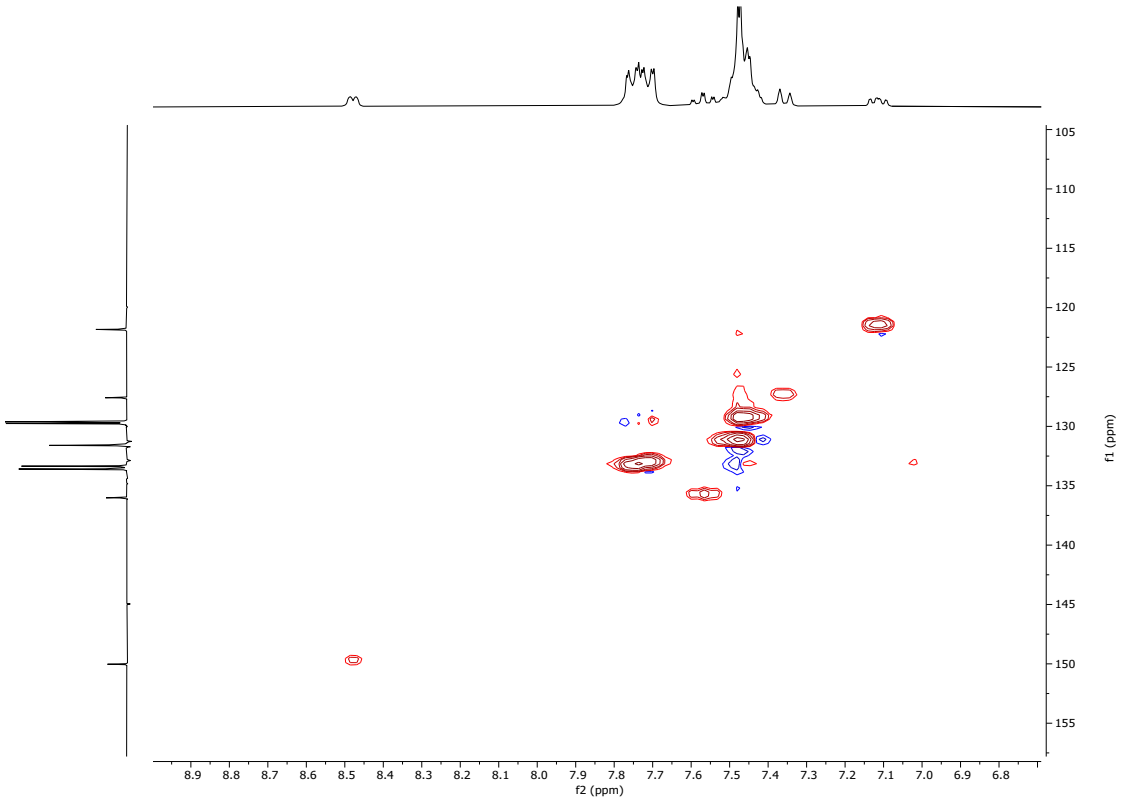


Figure S5. ^{1}H-$^{13}C\{^{1}H\}$ HSQC NMR (400 MHz, 101 MHz, CD_2Cl_2) spectrum of complex **6**.

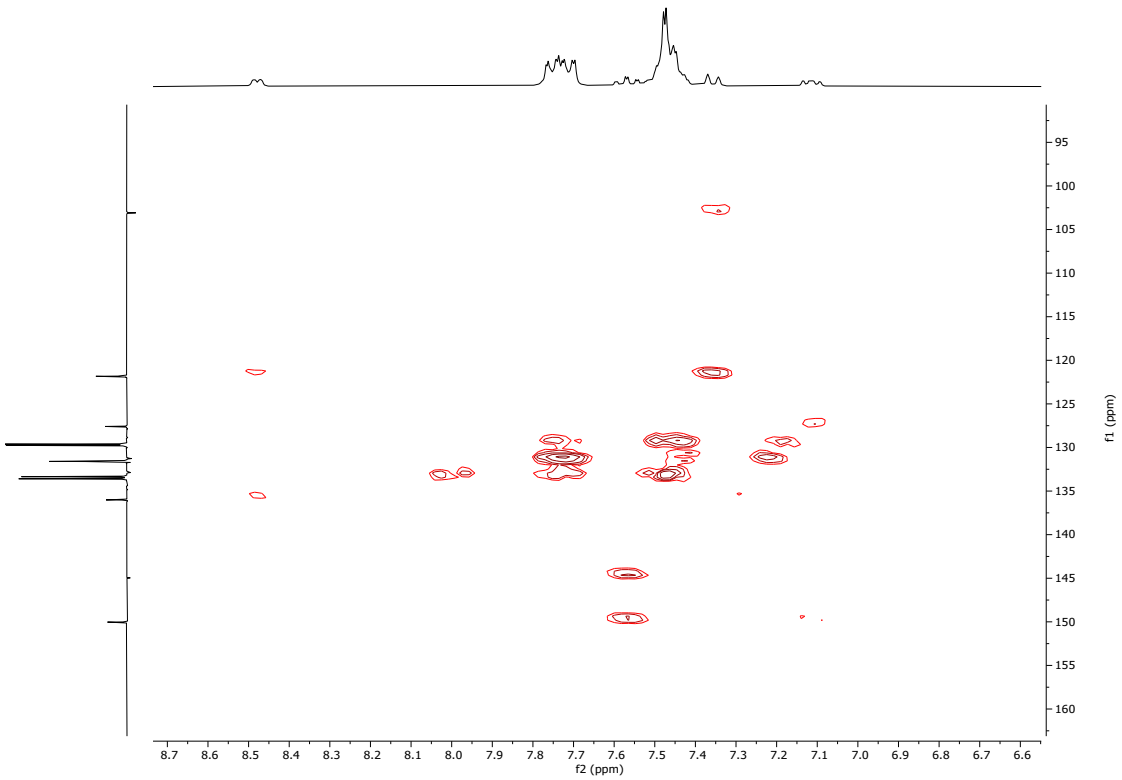


Figure S6. ^{1}H-$^{13}C\{^{1}H\}$ HMBC NMR (400 MHz, 101 MHz, CD_2Cl_2) spectrum of complex **6**.

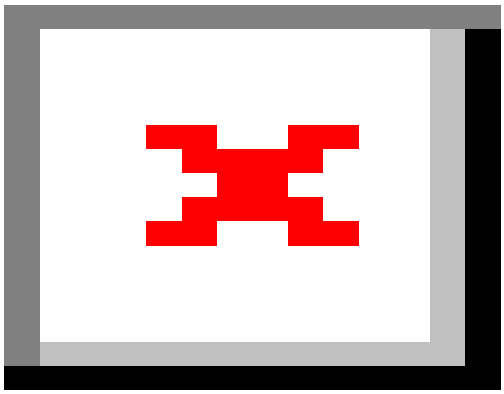


Figure S7. FT-IR ATR spectrum of complex **6**.

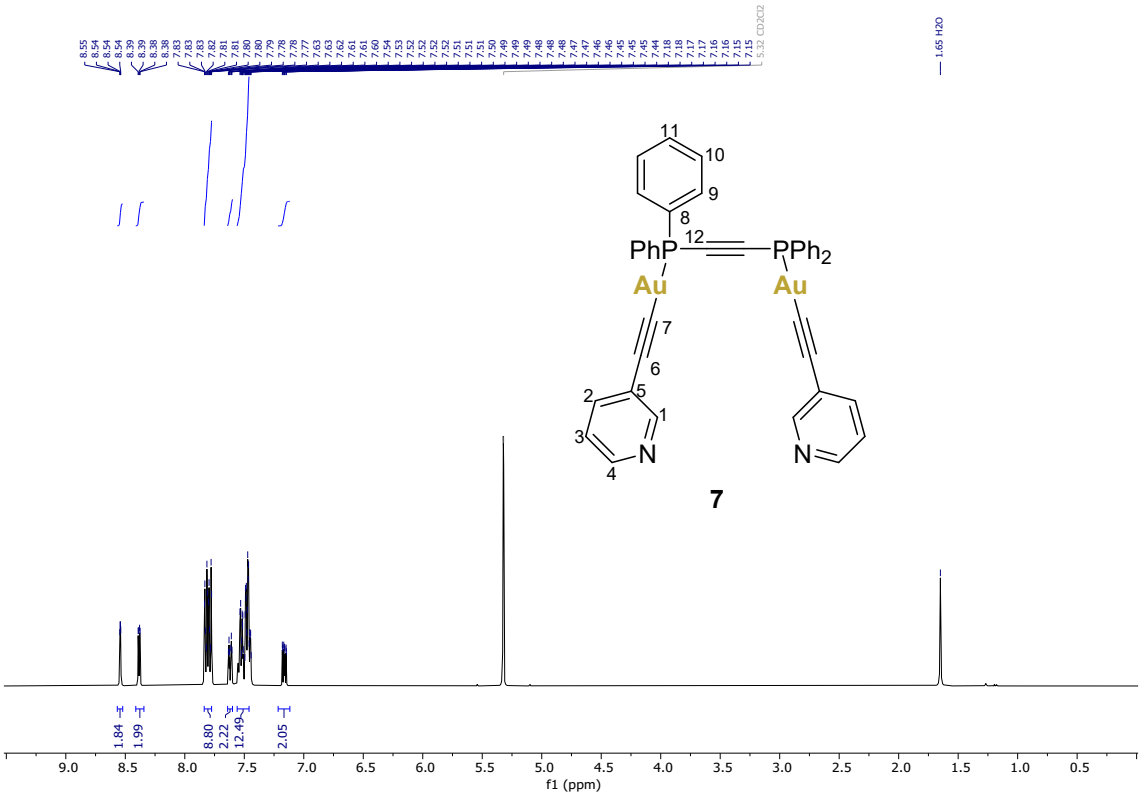


Figure S8. ^{1}H NMR (400 MHz, CD_2Cl_2) spectrum of complex **7**.

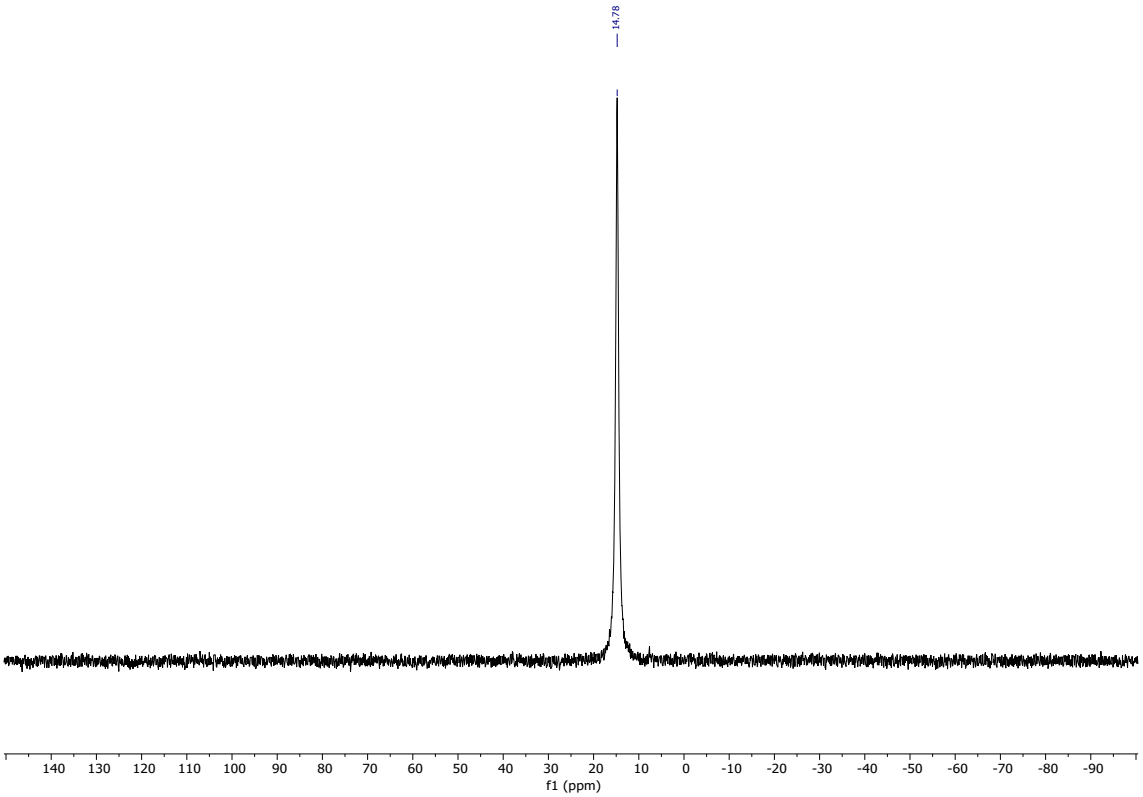


Figure S9. $^{31}P\{^{1}H\}$ NMR (162 MHz, CD_2Cl_2) spectrum of complex **7**.

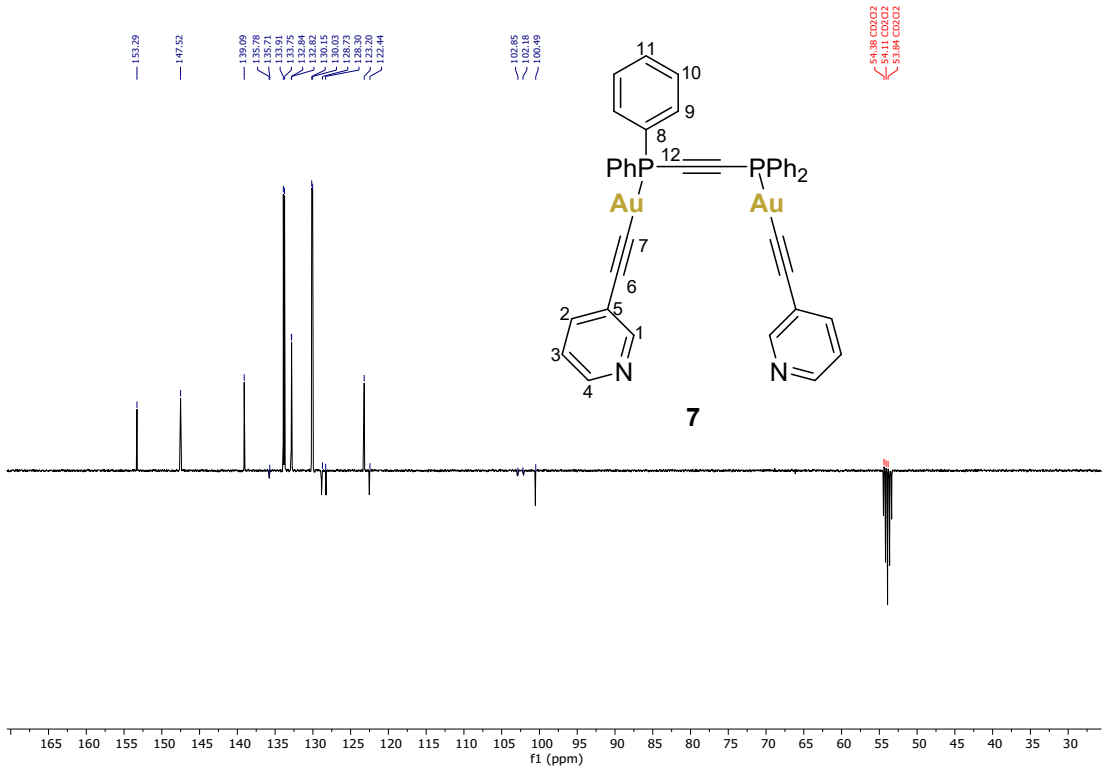


Figure S10. $^{13}C\{^{1}H\}$ APT NMR (101 MHz, CD_2Cl_2) spectrum of complex **7**.

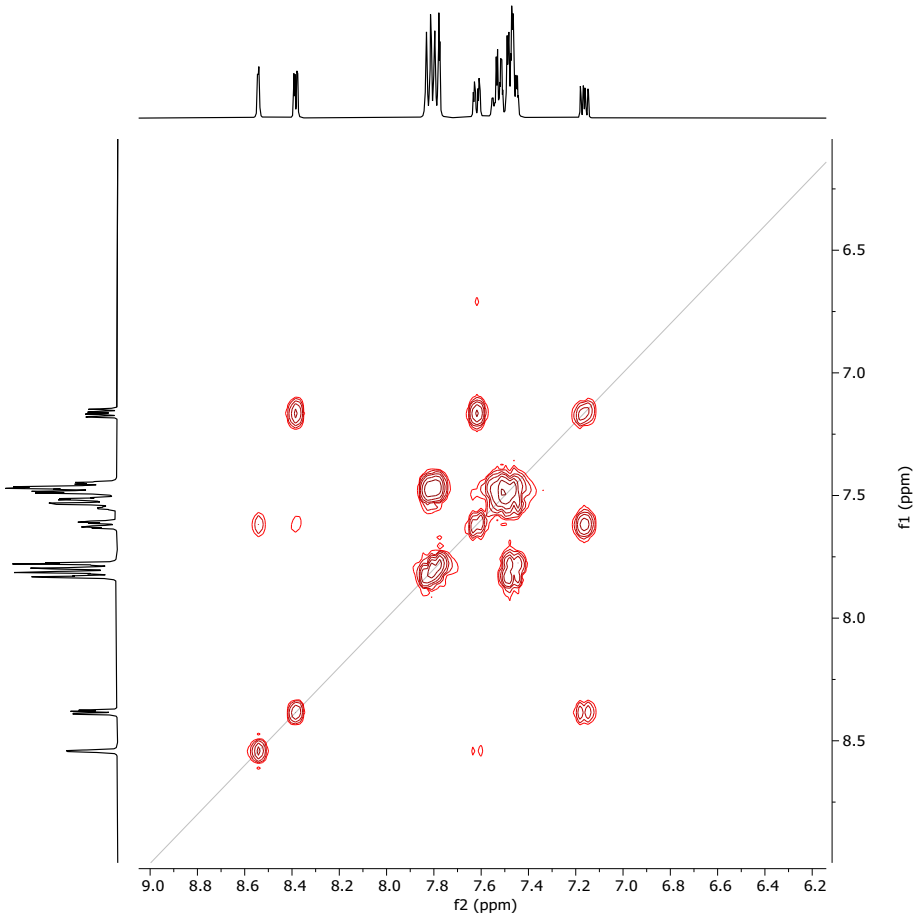


Figure S11. ^{1}H-^{1}H COSY NMR (400 MHz, CD_2Cl_2) spectrum of complex **7**.

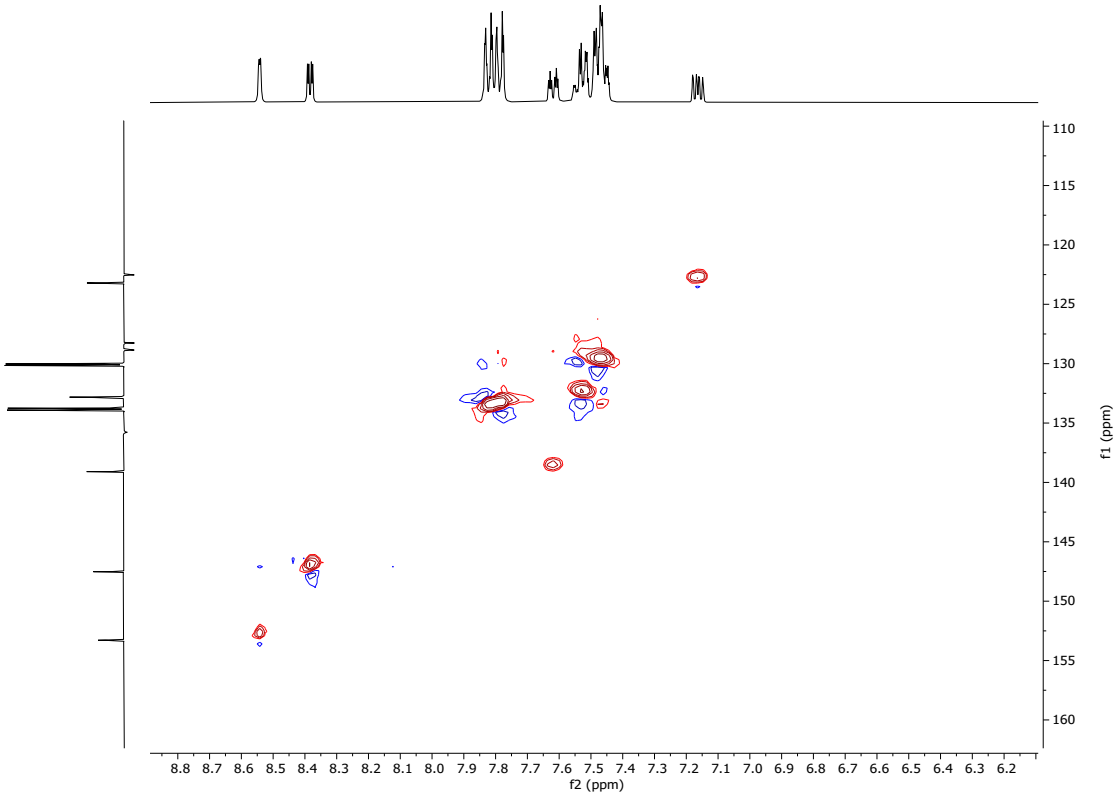


Figure S12. ^{1}H-$^{13}C\{^{1}H\}$ HSQC NMR (400 MHz, 101 MHz, CD_2Cl_2) spectrum of complex **7**.

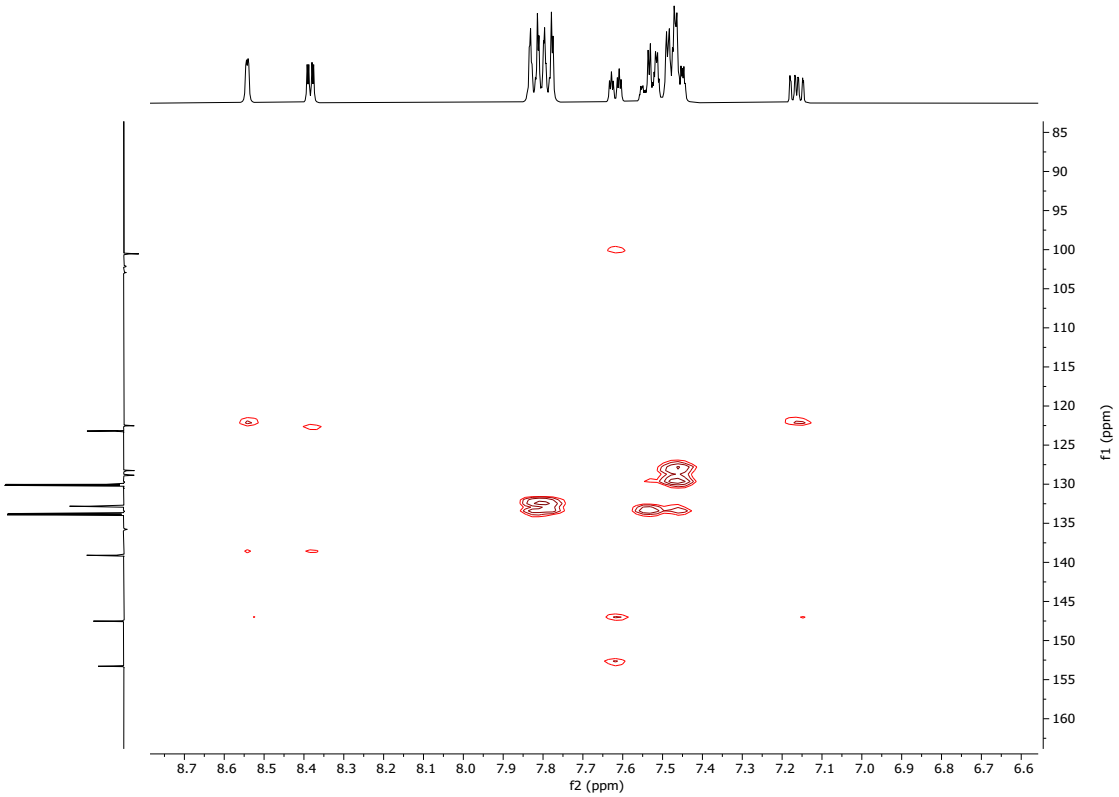


Figure S13. ^{1}H-$^{13}C\{^{1}H\}$ HMBC NMR (400 MHz, 101 MHz, CD_2Cl_2) spectrum of complex **7**.

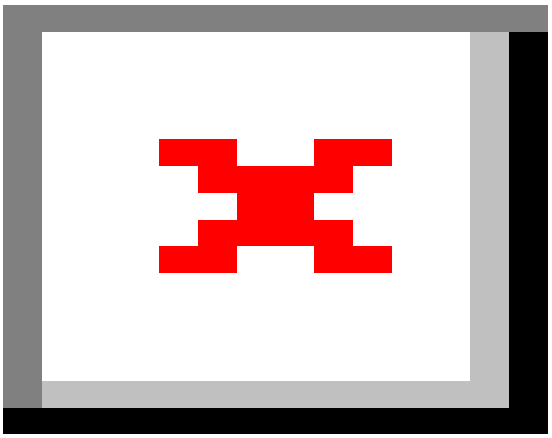


Figure S14-A. FT-IR ATR spectrum of complex **7**.

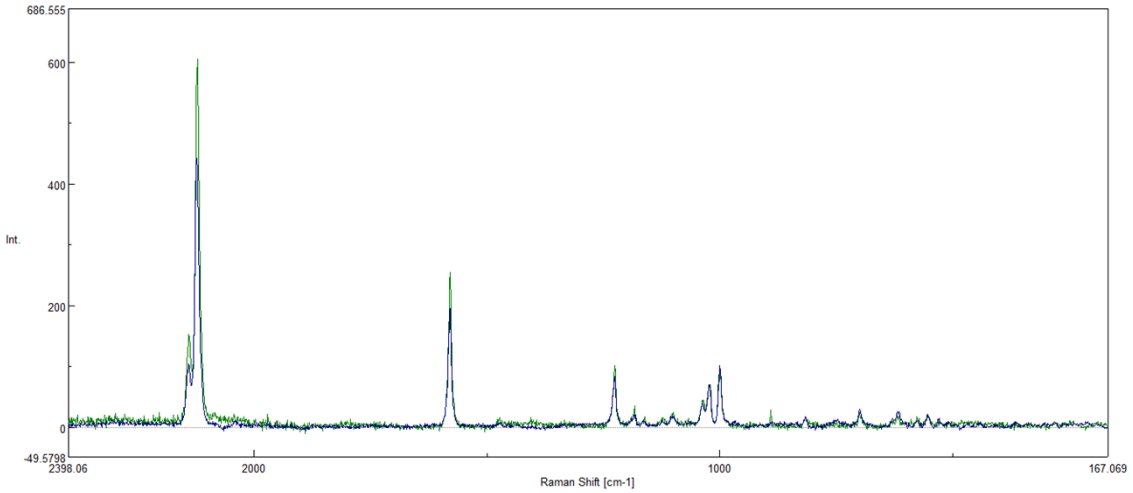


Figure S14-B. Raman spectra of complexes $\mathbf{7}_{\mathbf{pristine}}$ (green) and $\mathbf{7}_{\mathbf{ground}}$ (blue).

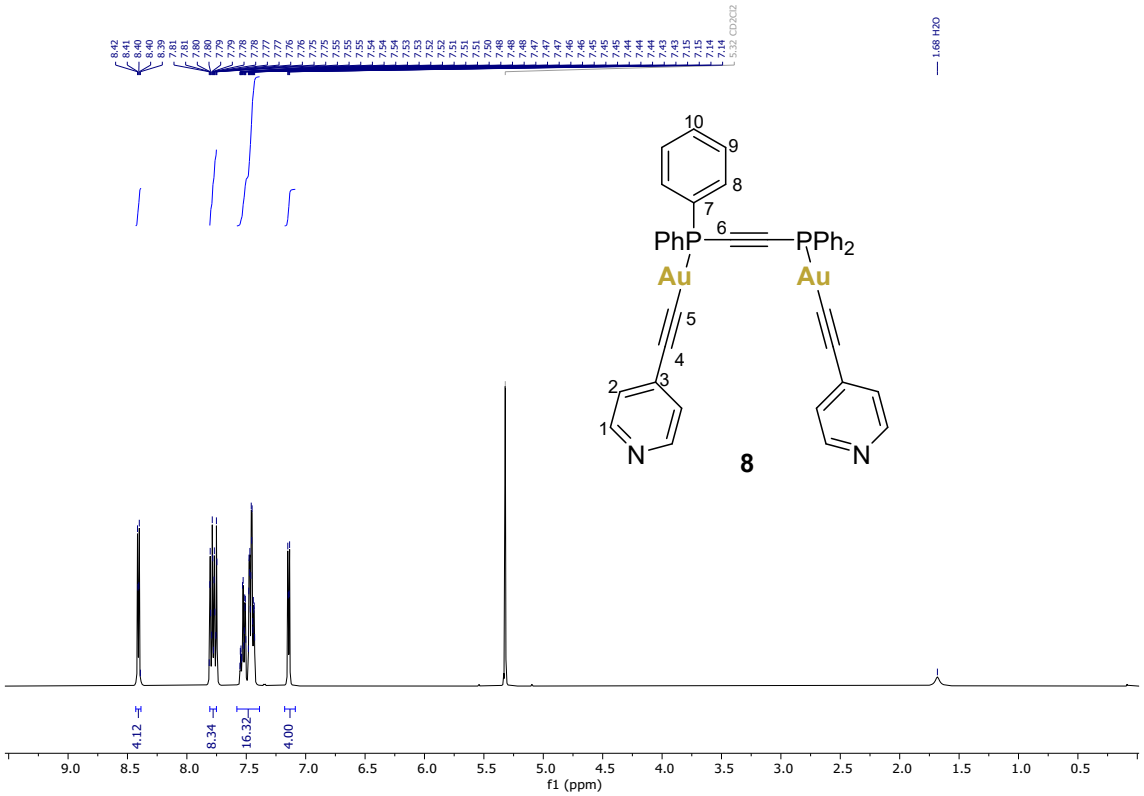


Figure S15. ^{1}H NMR (400 MHz, CD_2Cl_2) spectrum of complex **8**.

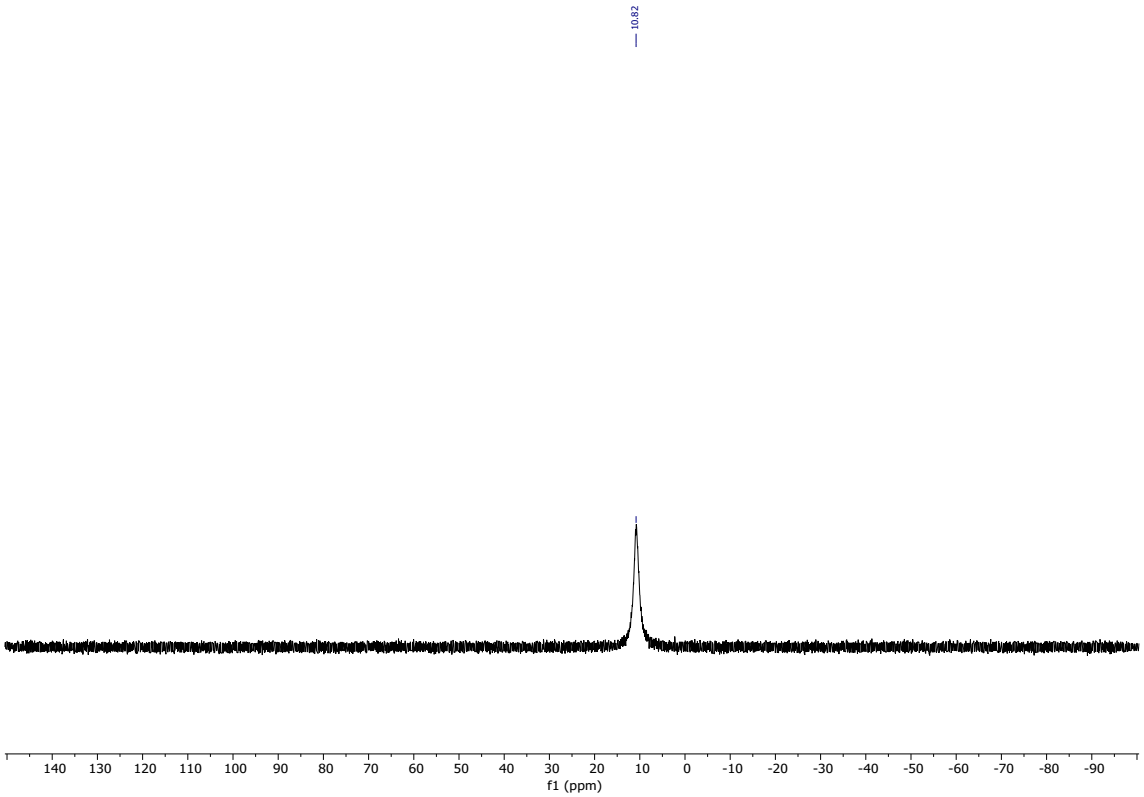


Figure S16. $^{31}P\{^{1}H\}$ NMR (400 MHz, CD_2Cl_2) spectrum of complex **8**.

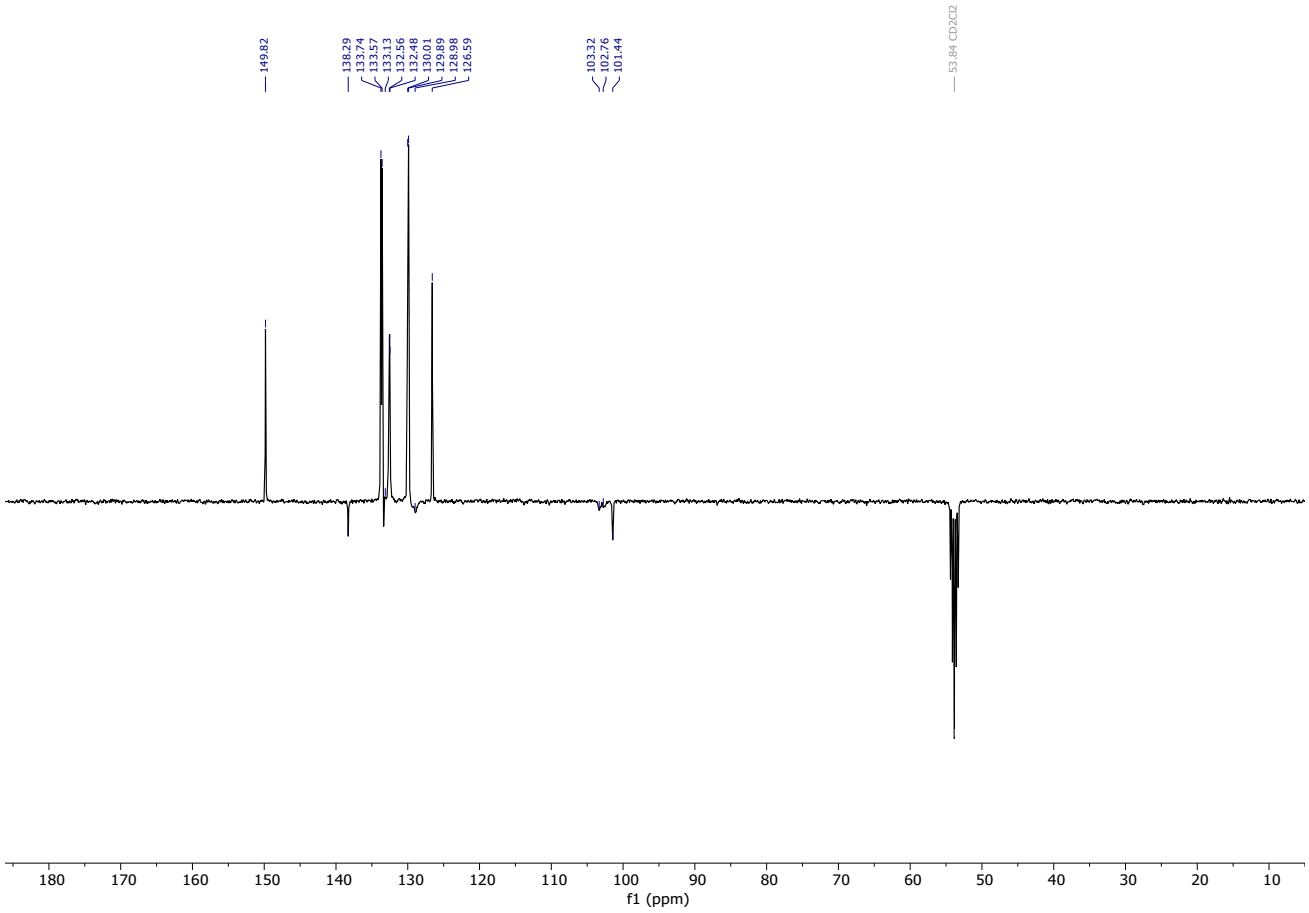


Figure S17. $^{13}C\{^{1}H\}$ APT NMR (101 MHz, CD_2Cl_2) spectrum of complex **8**.

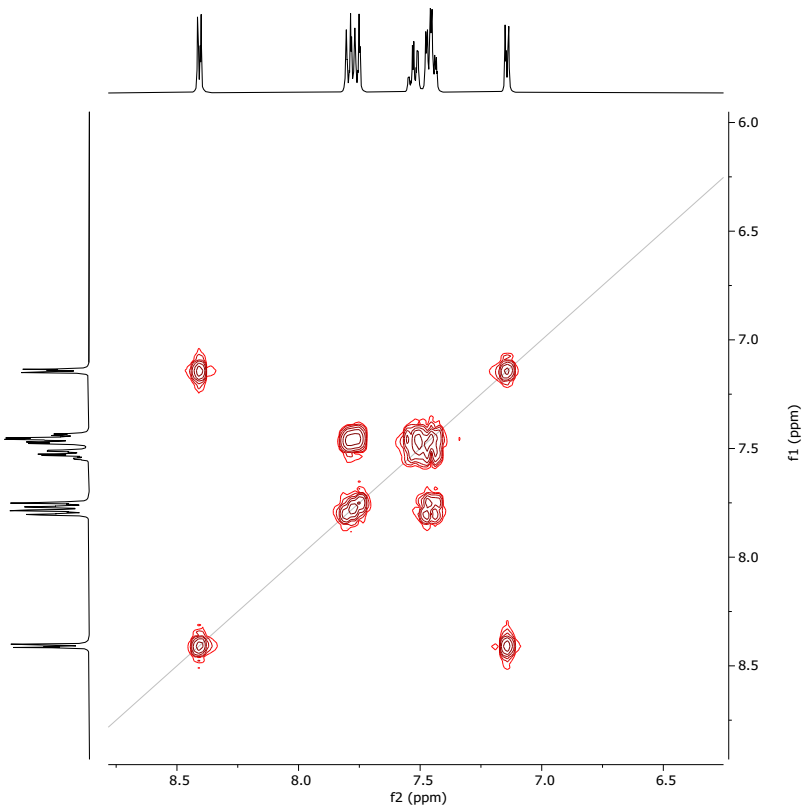


Figure S18. ^{1}H-^{1}H COSY NMR (400 MHz, CD_2Cl_2) spectrum of complex **8**.

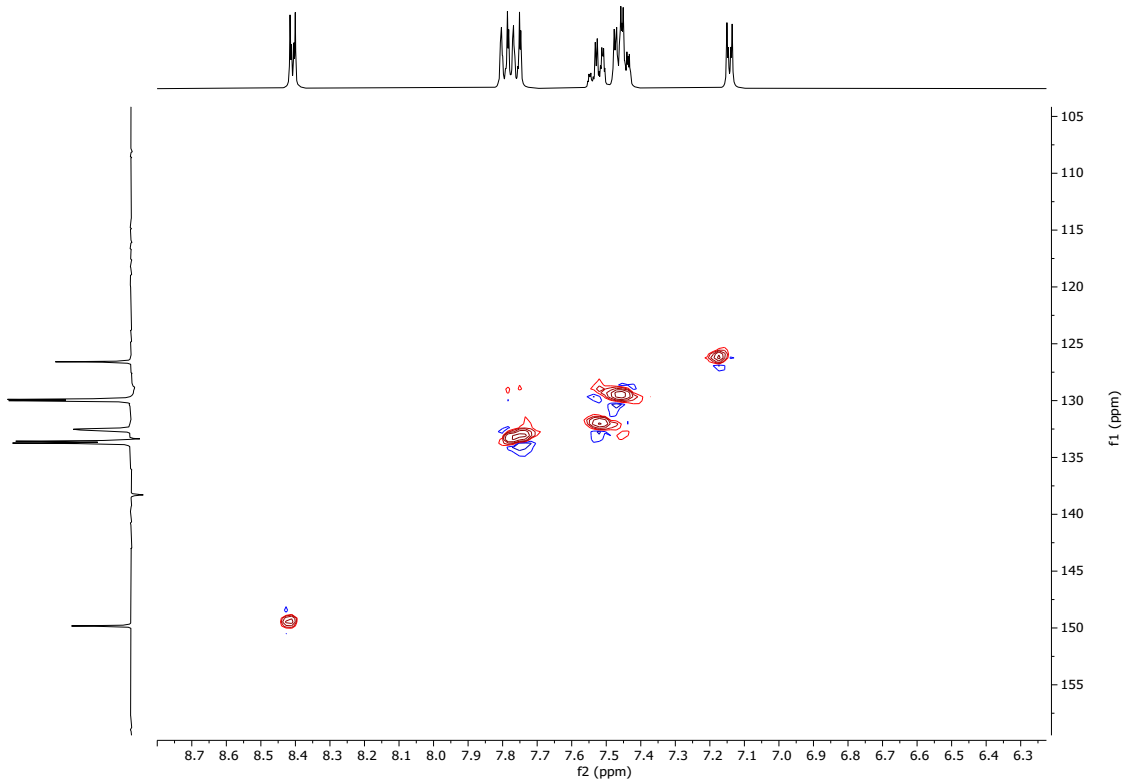


Figure S19. ^{1}H-$^{13}C\{^{1}H\}$ HSQC NMR (400 MHz, 101 MHz, CD_2Cl_2) spectrum of complex **8**.

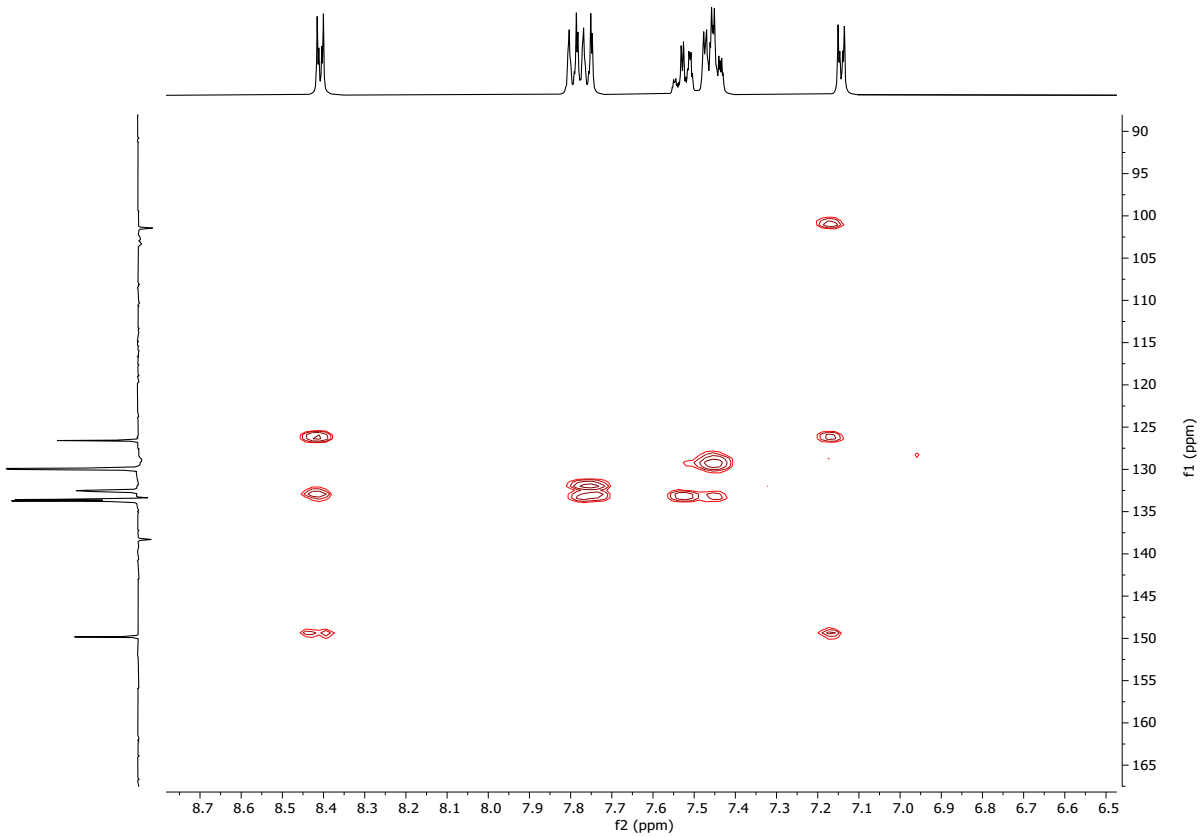


Figure S20. ^{1}H-$^{13}C\{^{1}H\}$ HMBC NMR (400 MHz, 101 MHz, CD_2Cl_2) spectrum of complex **8**.

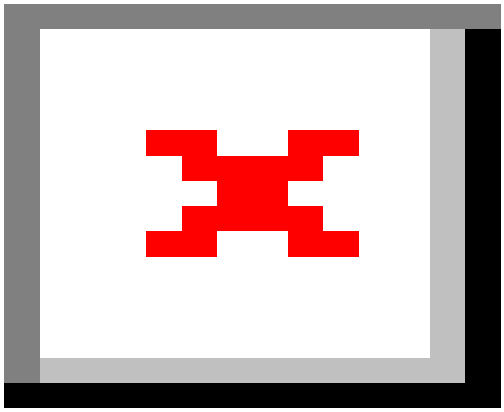


Figure S21. FT-IR ATR spectrum of complex **8**.

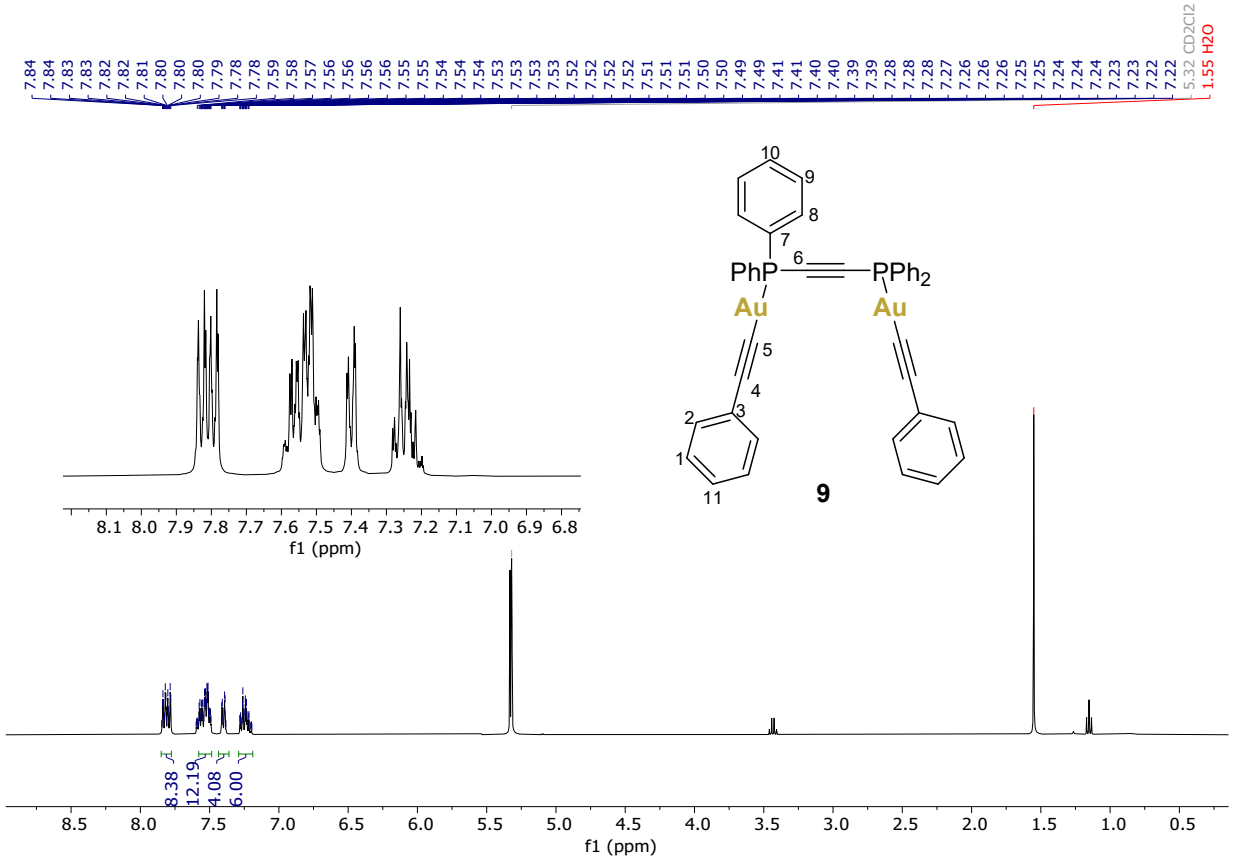


Figure S22. ^{1}H NMR (400 MHz, CD_2Cl_2) spectrum of complex **8**.

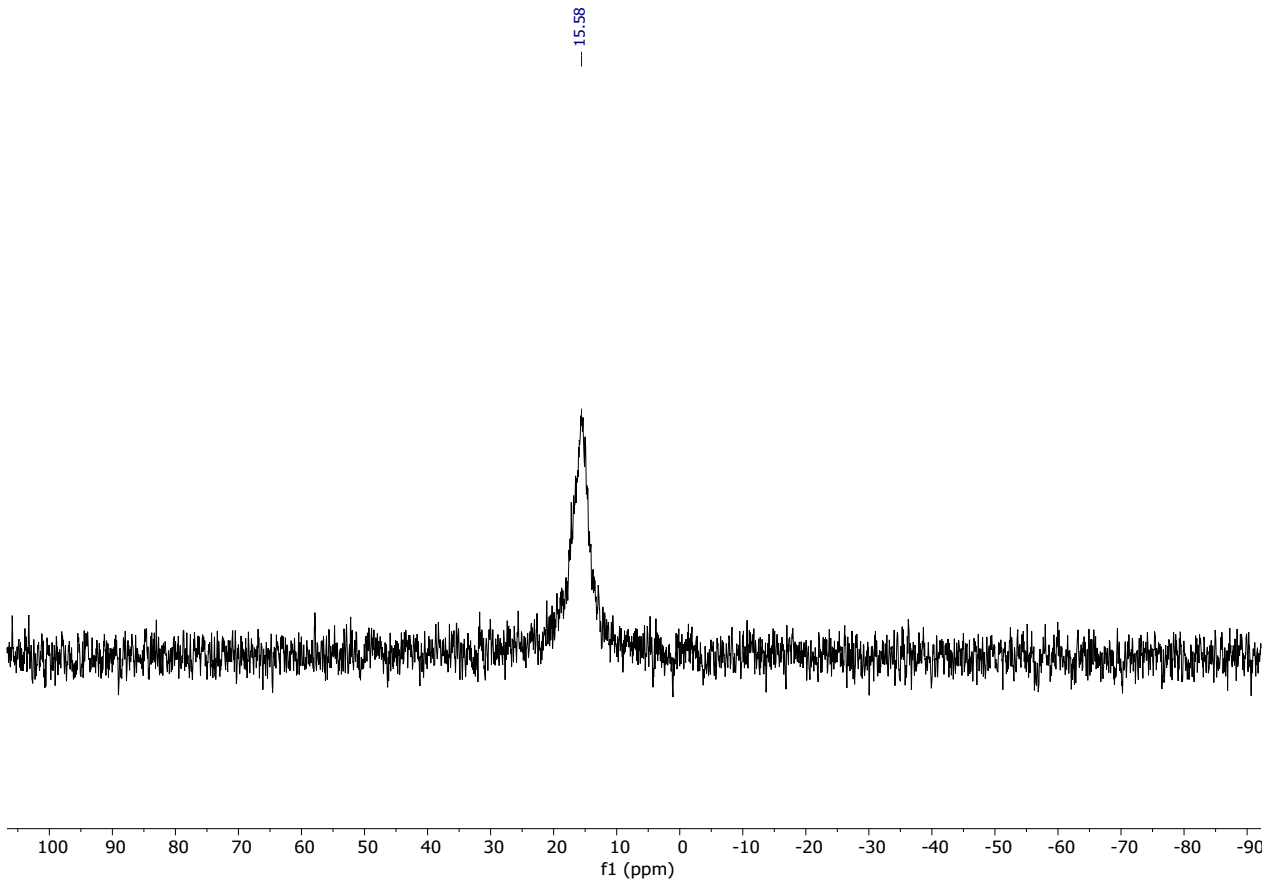


Figure S23. $^{31}P\{^{1}H\}$ NMR (162 MHz, CD_2Cl_2) spectrum of complex **9**.

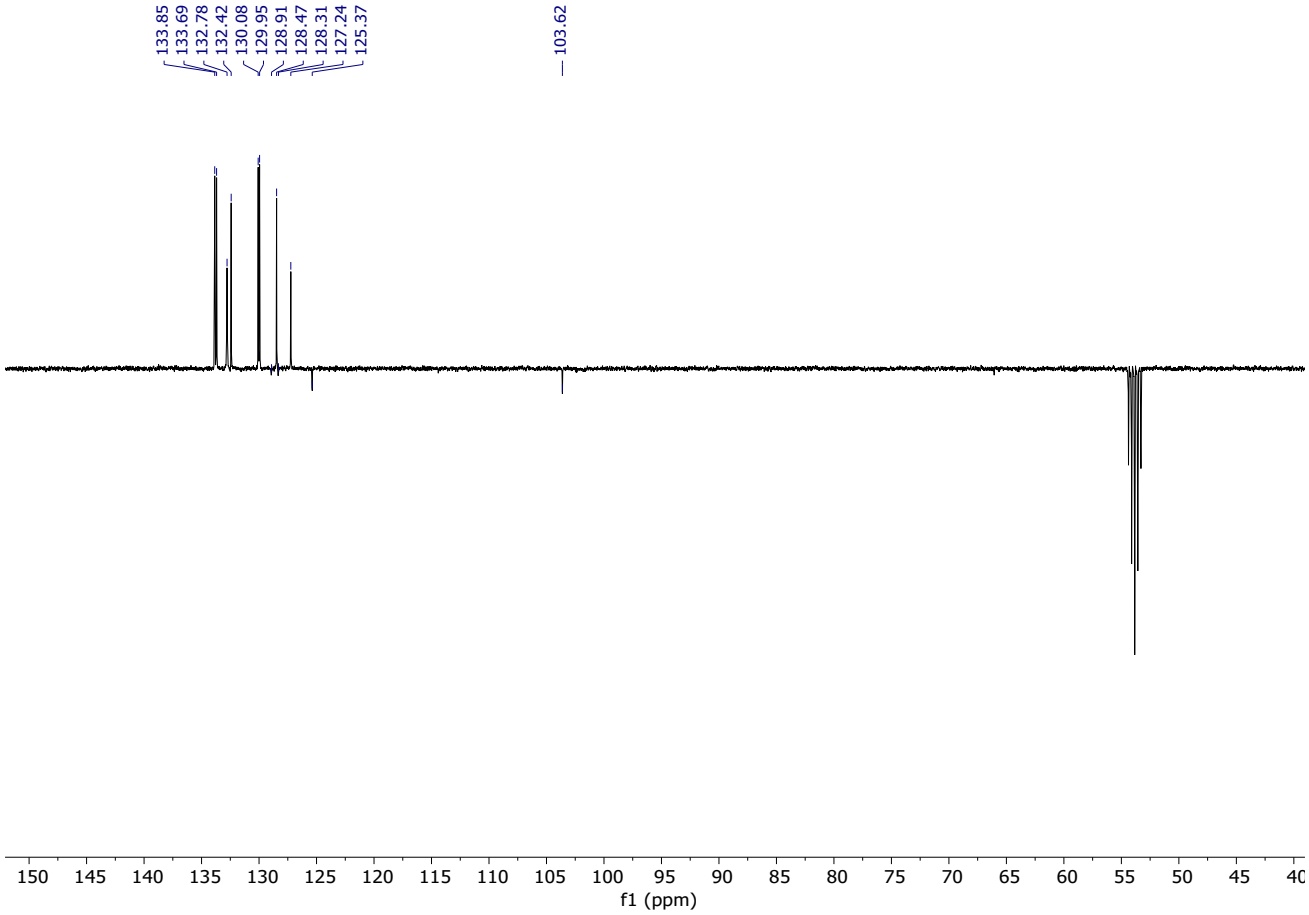


Figure S24. $^{13}C\{^{1}H\}$ APT NMR (101 MHz, CD_2Cl_2) spectrum of complex **9**.

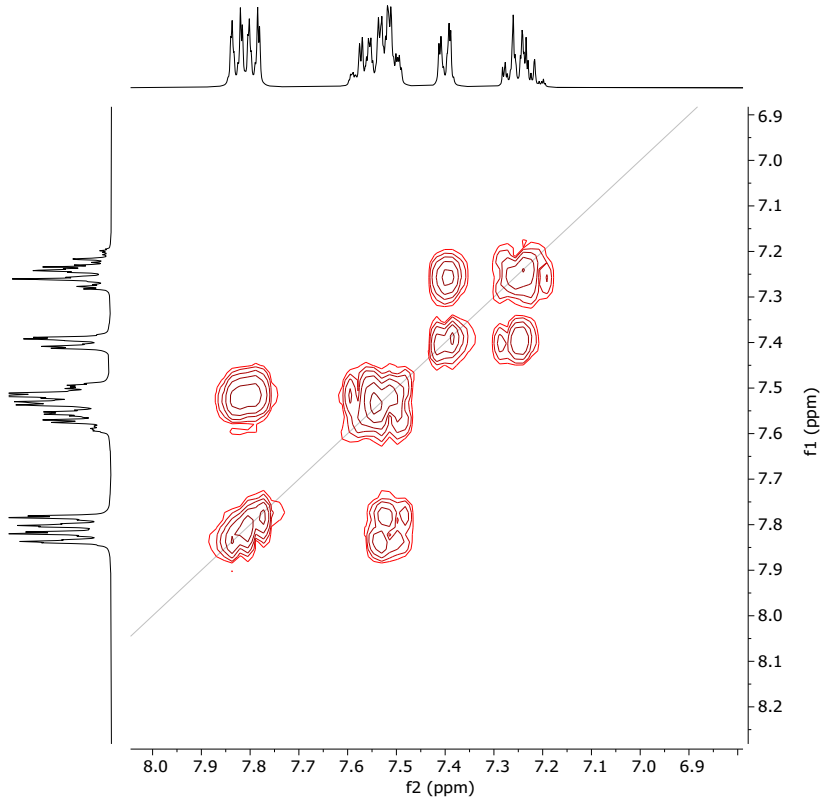


Figure S25. ^{1}H-^{1}H COSY NMR (400 MHz, CD_2Cl_2) spectrum of complex **9.**

3. THERMAL ANALYSIS: THERMOGRAVIMETRIC ANALYSIS TGA-DTA

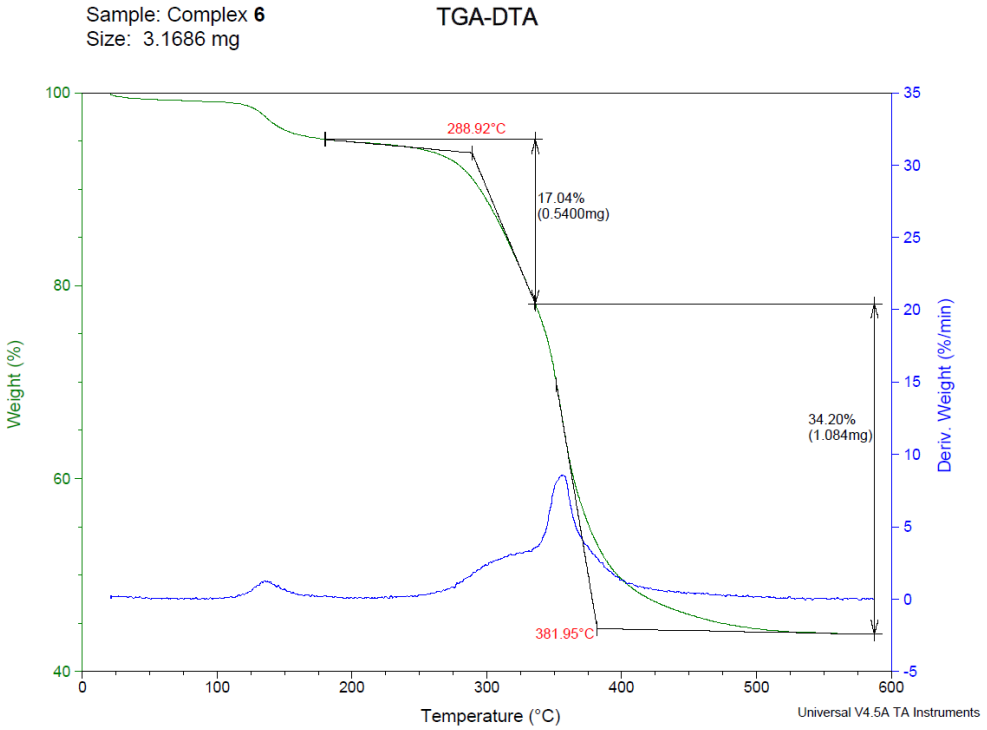


Figure S26. TGA (green trace, vertical scale on the left) and 1st derivative of the weight loss curve (blue trace, vertical scale on the right) of complex **6** recorded on heating at 10 ºC min^{-1}.

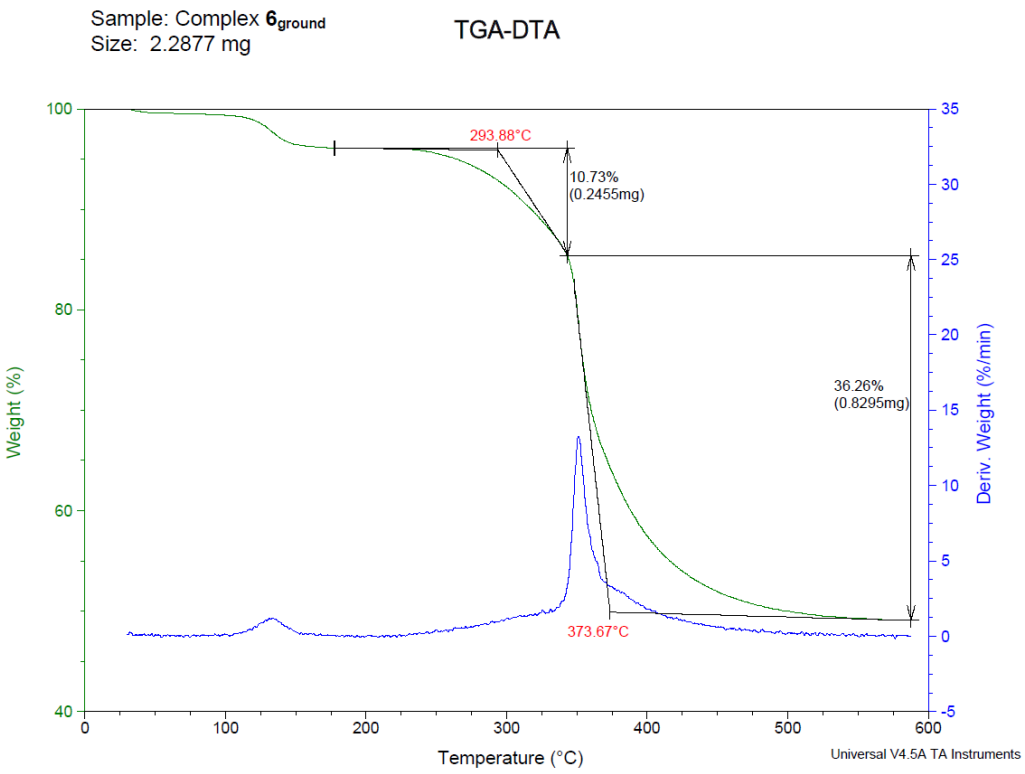


Figure S27. TGA (green trace, vertical scale on the left) and 1st derivative of the weight loss curve (blue trace, vertical scale on the right) of complex **6$_{ground}$** recorded on heating at 10 ºC min^{-1}.

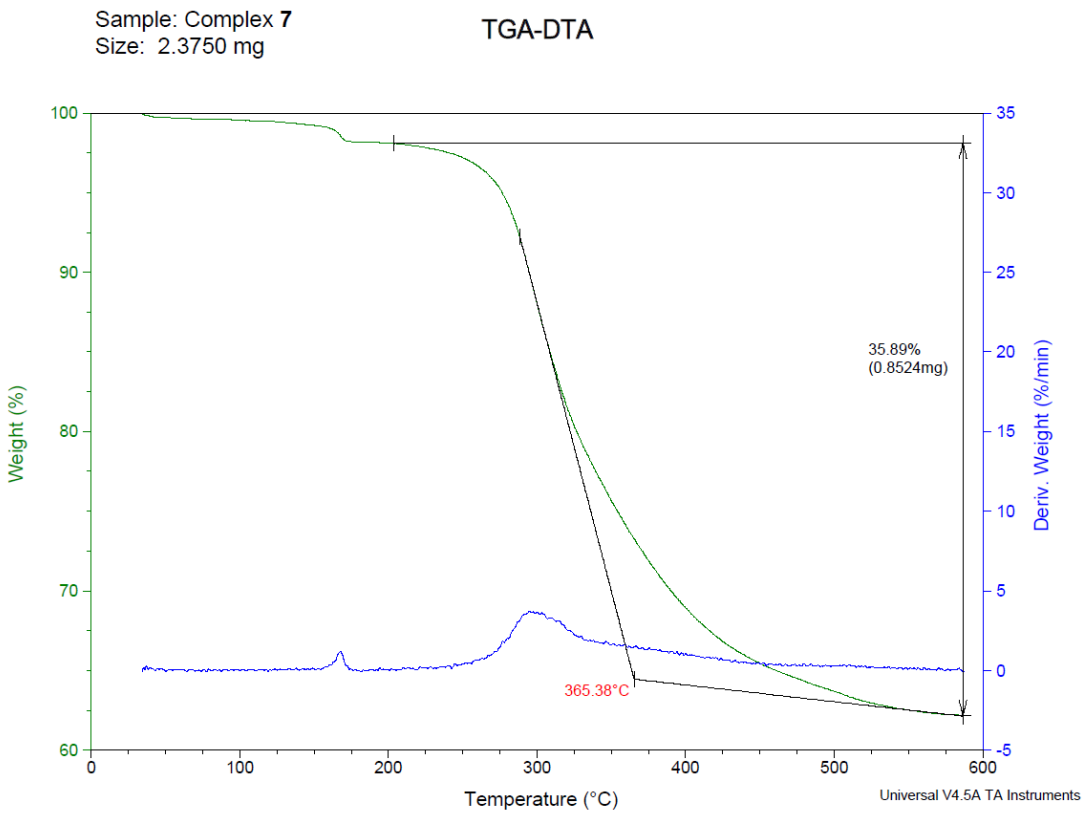


Figure S28. TGA (green trace, vertical scale on the left) and 1st derivative of the weight loss curve (blue trace, vertical scale on the right) of complex **7** recorded on heating at 10 ºC min^{-1}.

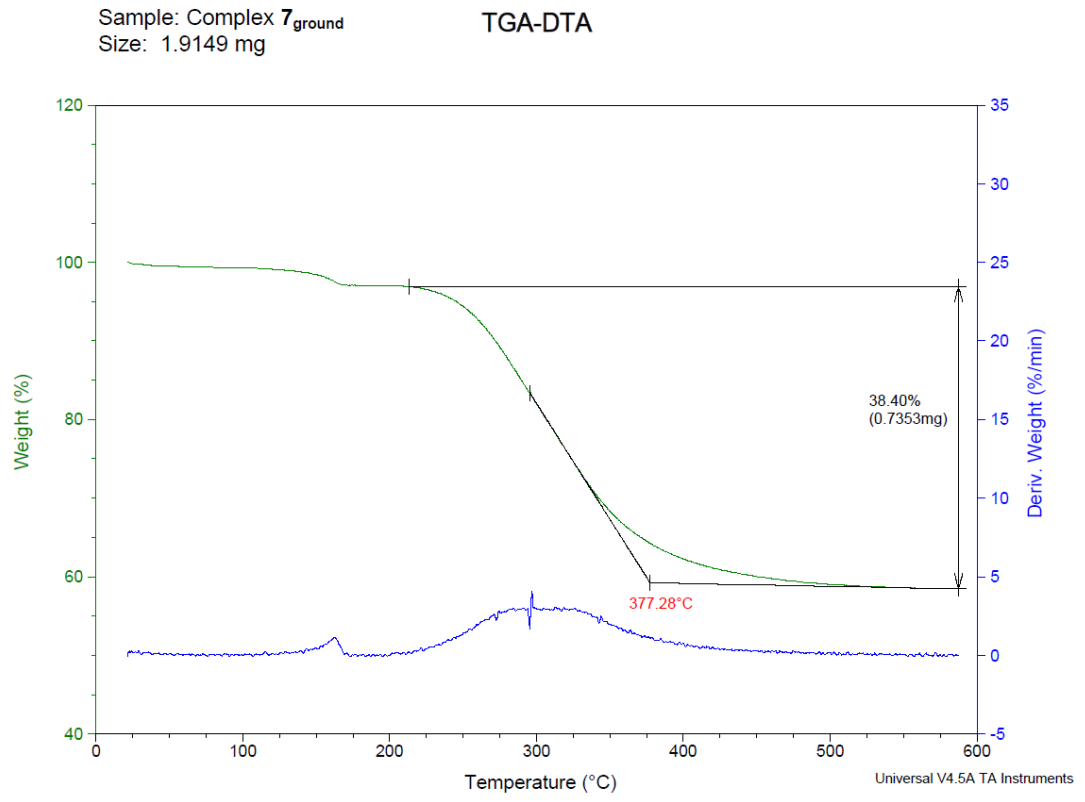


Figure S29. TGA (green trace, vertical scale on the left) and 1st derivative of the weight loss curve (blue trace, vertical scale on the right) of complex $\mathbf{7}_{\mathbf{ground}}$ recorded on heating at 10 ºC min^{-1}.

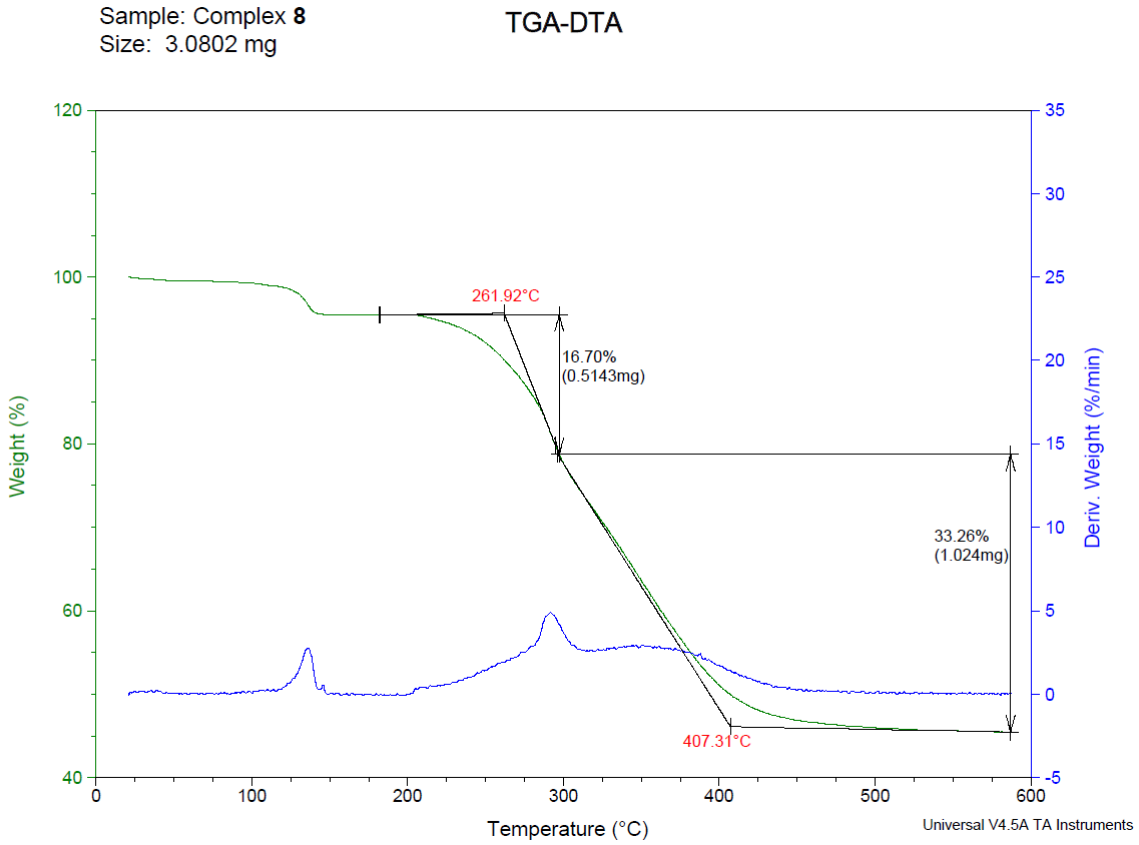


Figure S30. TGA (green trace, vertical scale on the left) and 1st derivative of the weight loss curve (blue trace, vertical scale on the right) of complex **8** recorded on heating at 10 ºC min^{-1}.

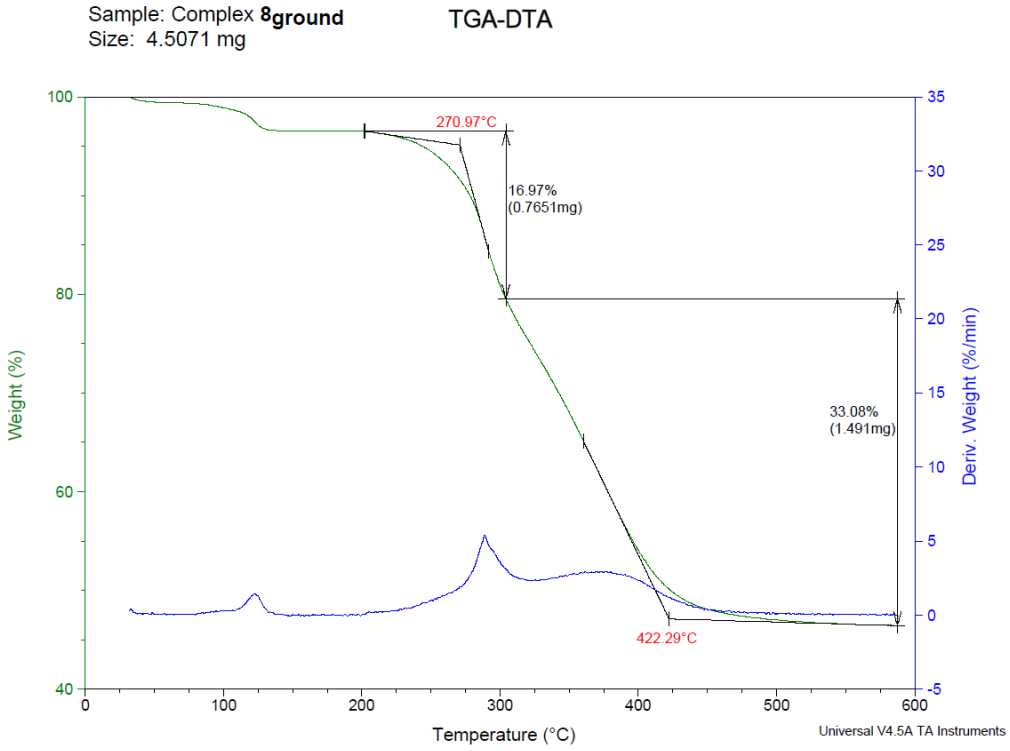


Figure S31. TGA (green trace, vertical scale on the left) and 1st derivative of the weight loss curve (blue trace, vertical scale on the right) of complex $\mathbf{8}_{\mathbf{ground}}$ recorded on heating at 10 ºC min^{-1}.

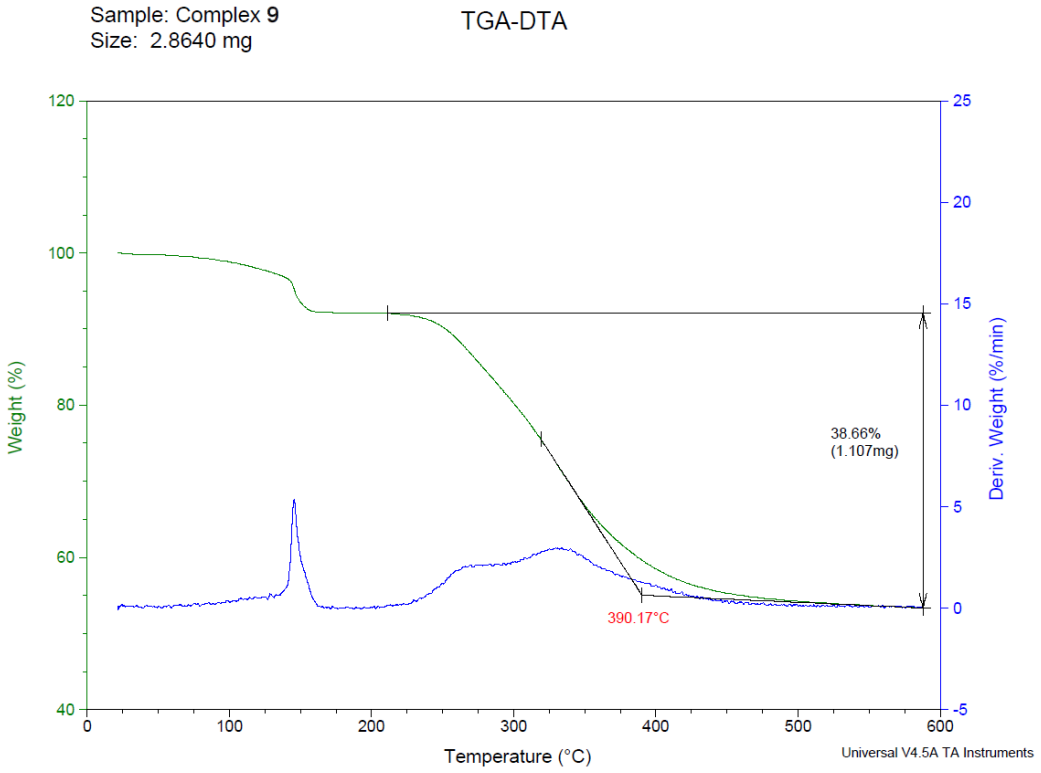


Figure S32. TGA (green trace, vertical scale on the left) and 1st derivative of the weight loss curve (blue trace, vertical scale on the right) of complex **9** recorded on heating at 10 ºC min^{-1}.

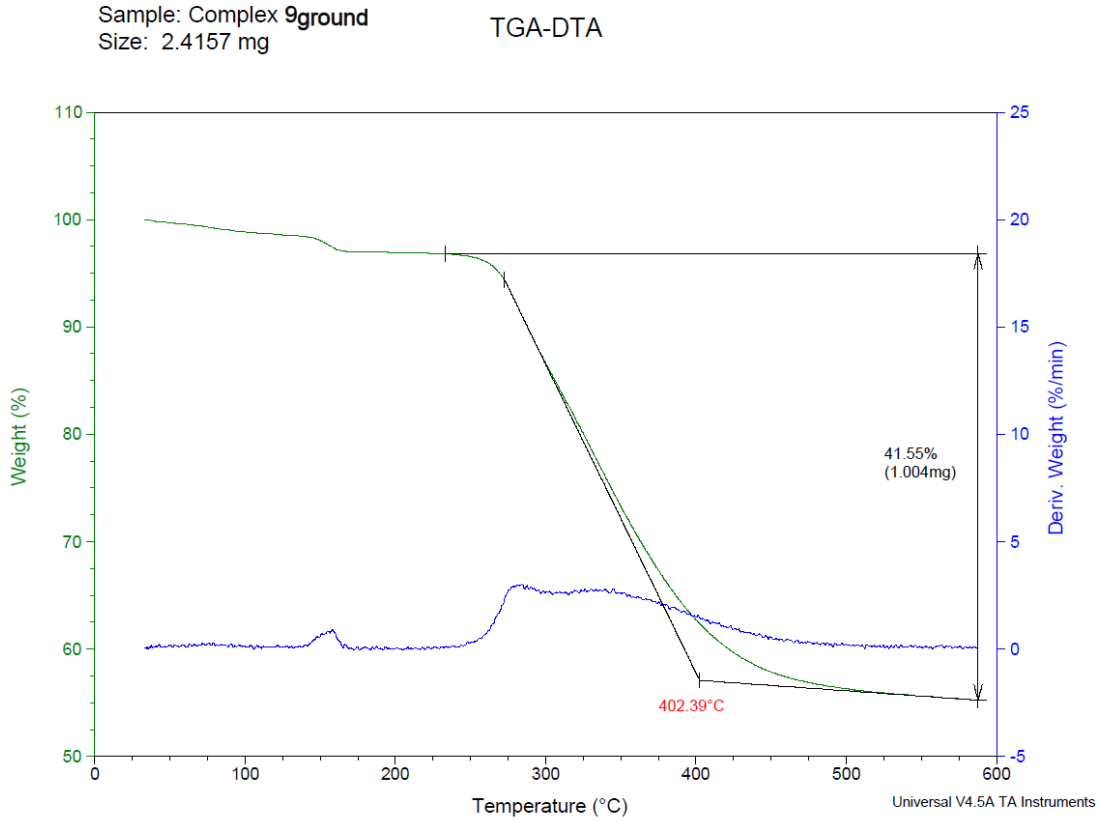


Figure S33. TGA (green trace, vertical scale on the left) and 1st derivative of the weight loss curve (blue trace, vertical scale on the right) of complex $\mathbf{9}_{\mathbf{ground}}$ recorded on heating at 10 ºC min^{-1}.

4. PHOTOPHYSICAL MEASUREMENTS

4.1. Solid State Photophysical Measurements

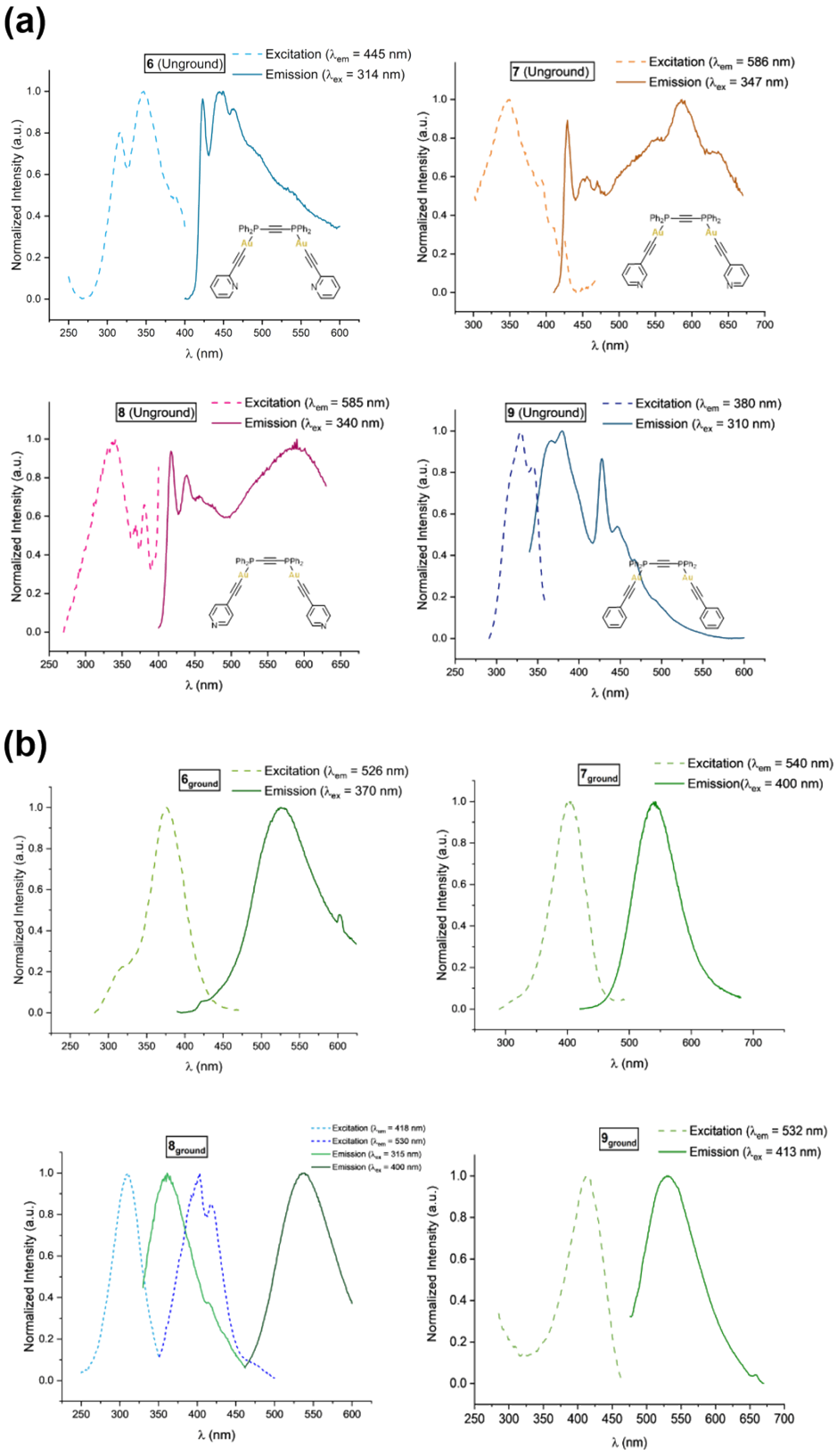


Figure S34. (a) Excitation and emission spectra of complexes **6**–**9** at room temperature as pristine solids. (b) Excitation and emission spectra of complexes **6**–**9** at room temperature as ground solids.

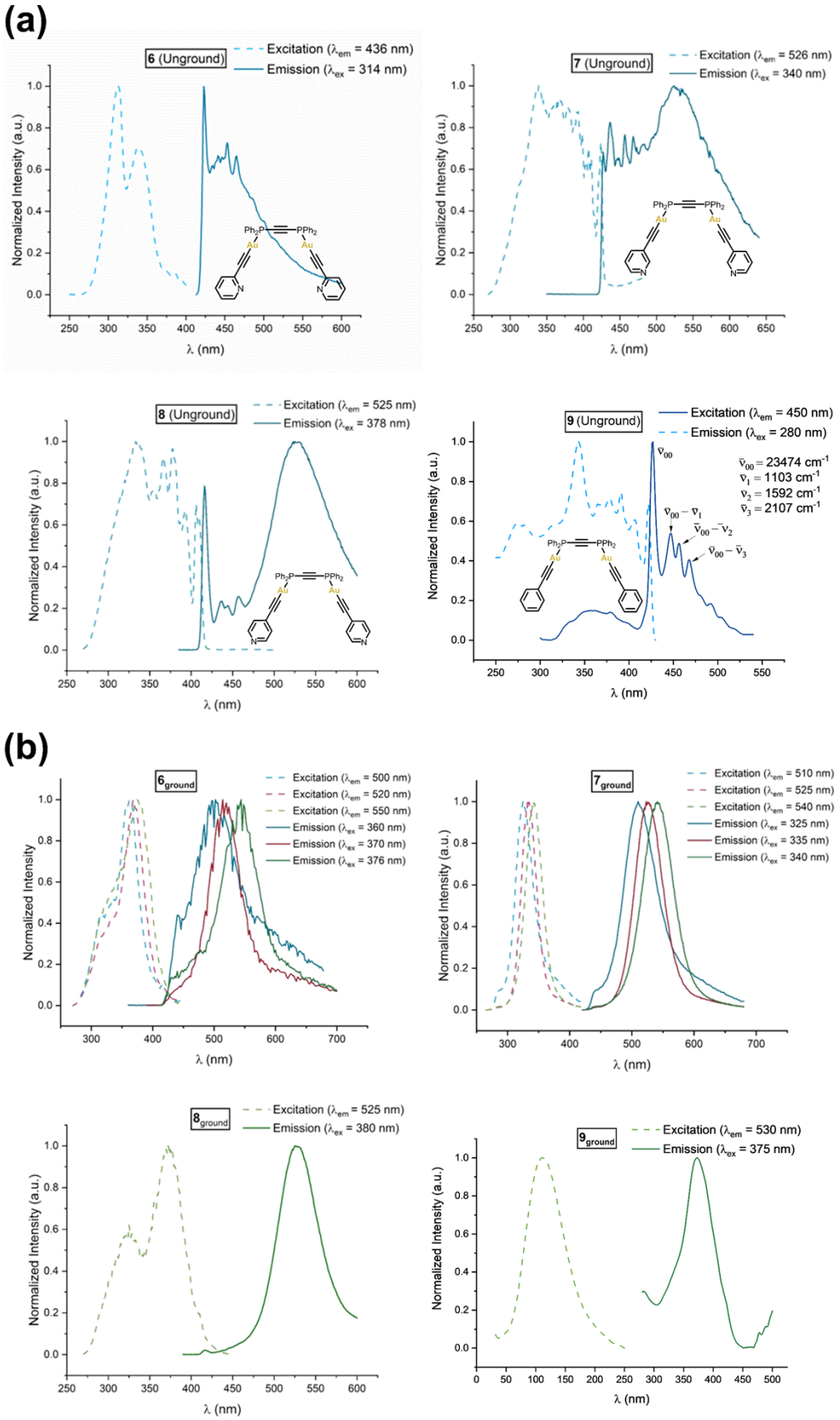


Figure S35. (a) Excitation and emission spectra of complexes **6**–**9** at 77 K as pristine solids. (b) Excitation and emission spectra of complexes **6**–**9** at 77 K as ground solids.

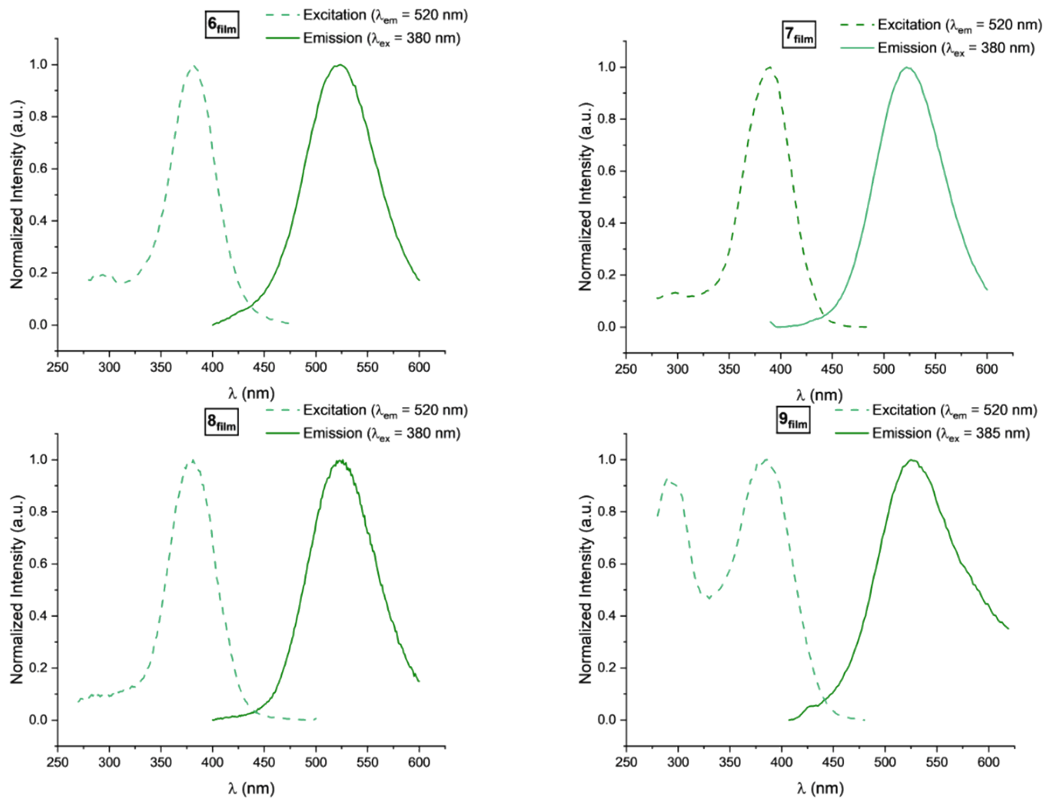


Figure S36. Excitation and emission spectra of complexes **6**–**9** as PMMA films (5% w/w).

4.2. Variable Temperature Measurements (Solid State)

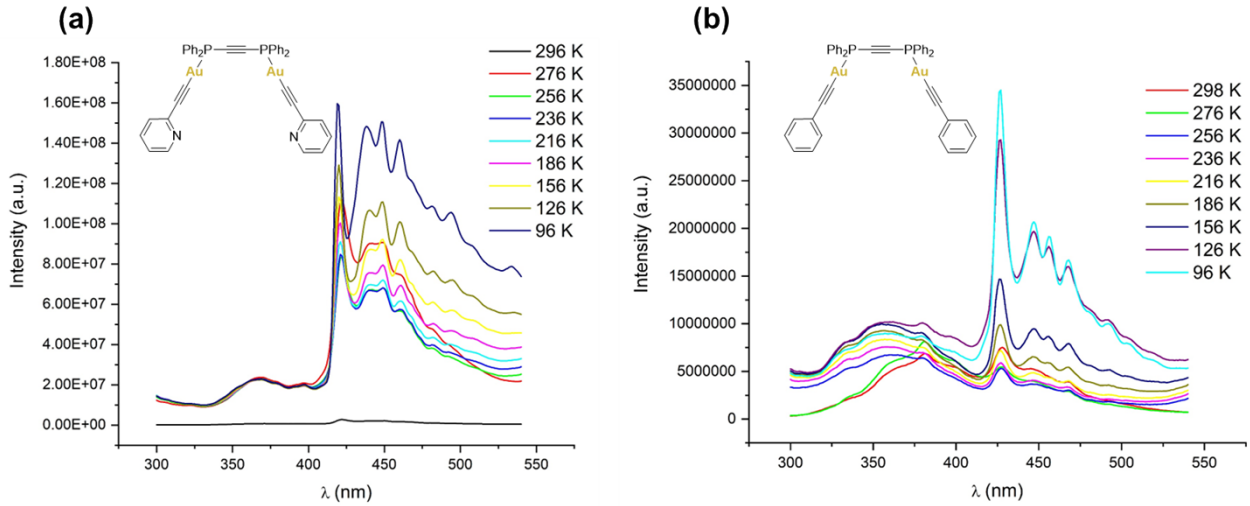


Figure S37. (a) Emission spectra of complex **6** at different temperatures (λ_{ex} = 315 nm) as a pristine solid. (b) . Emission spectra of complex **9** at different temperatures (λ_{ex} = 280 nm) as a pristine solid.

4.3. Solution State Photophysical Measurements

Complex 6

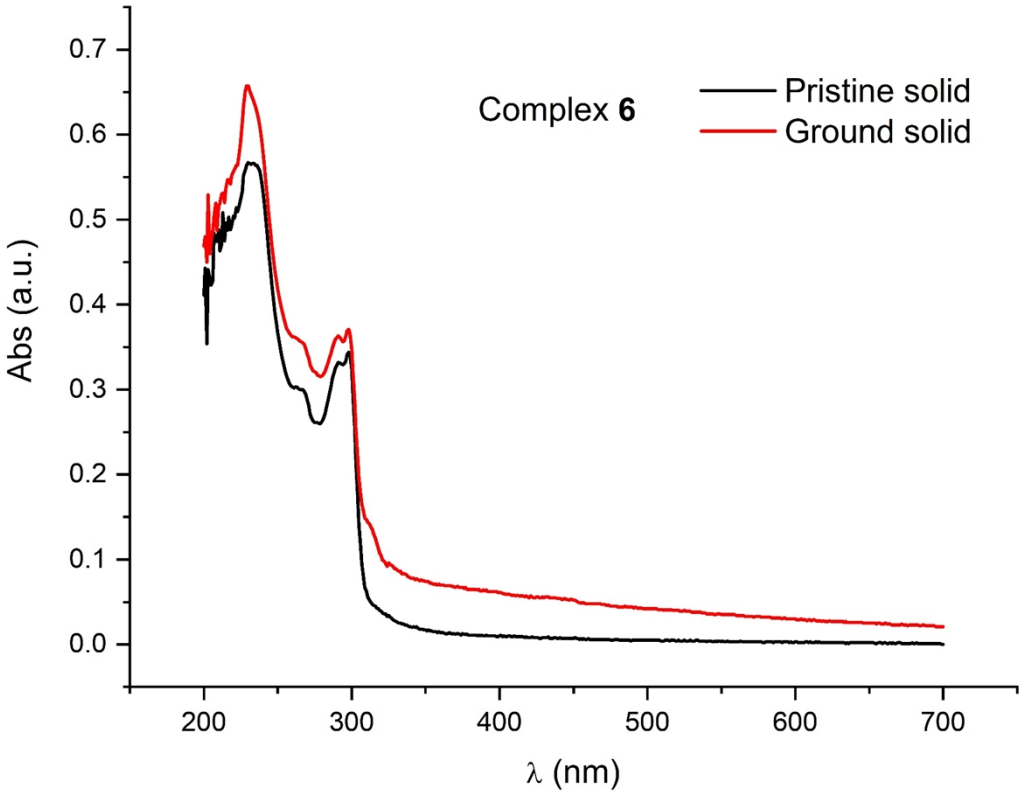


Figure S38. Absorption spectra of complex **6** as a pristine solid (black) and after being ground (red), in CH_2Cl_2 ($5 \cdot 10^{-4}$ M).

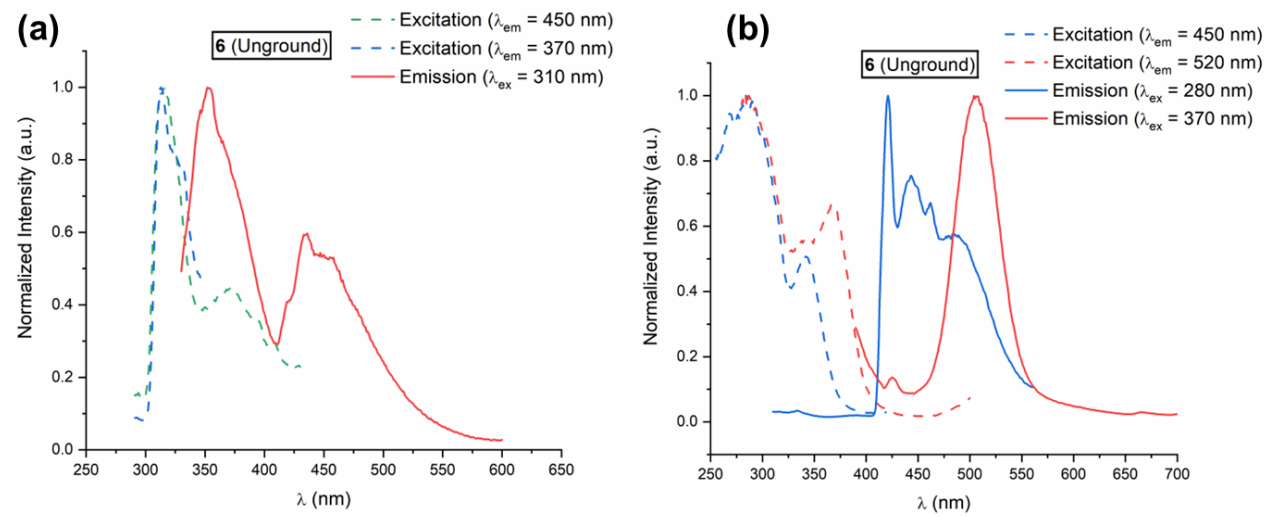


Figure S39. (**a**) Excitation and emission spectra of complex **6**, in CH_2Cl_2 ($5 \cdot 10^{-4}$ M), at room temperature. (**b**) Excitation and emission spectra of complex **6**, in CH_2Cl_2 ($5 \cdot 10^{-4}$ M), vitrificated solution (77 K).

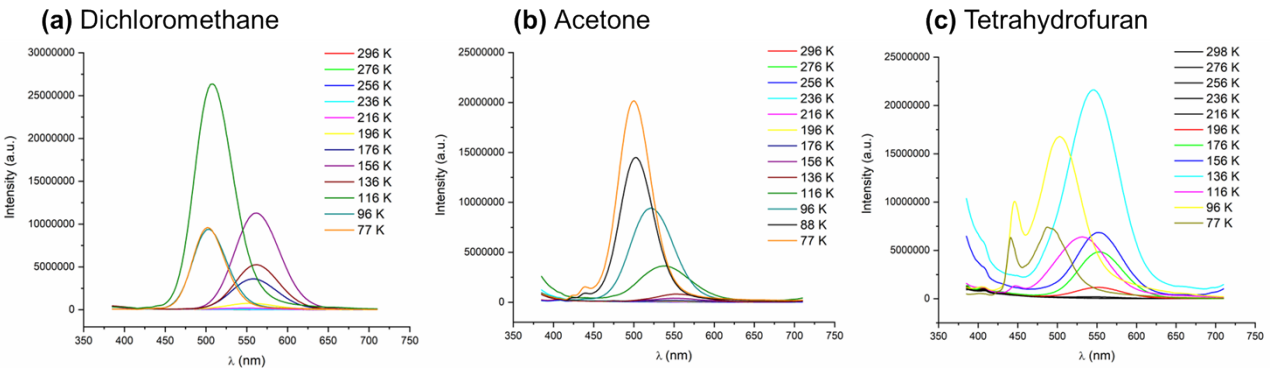


Figure S40. Emission (λ_{ex} = 365 nm) spectra of complex **6**, in CH_2Cl_2 (**a**); acetone (**b**) and THF (**c**), at $5 \cdot 10^{-4}$ M, at different temperatures.

Table S1. Photophysical data of complex **6**, in CH_2Cl_2 ($5 \cdot 10^{-4}$ M), at different temperatures.

Temperature (K)	λ_{ex}^{max} (nm)	λ_{em}^{max} (nm)
298	334 325	381 433, 456
268	331 323	383 431, 455
238	330 323 359	385 430, 455 551
208[a]	328 333 358	385 423, 450 550
178[a]	280 359	422, 450 556
148	280 375	426, 441, 466 561
118	285, 343 370	426, 443 508
88	278, 318, 340 369	425, 441 504

[a]At these temperatures the intensity of the structured band is totally negligible compared to that shown by the band at 550 nm.

Table S2. Emission maxima (λ_{ex} = 365 nm) of complex **6** in different solvents.

Temperature (K)	CH_2Cl_2 λ_{max} (nm)	THF λ_{max} (nm)	Acetone λ_{max} (nm)
216	550	545	542
196	554	548	550
176	558	547	553
156	562	552	552
136	562	555	545
116	507	537	530
96	502	521	503
77	502	500	490

Complex 9

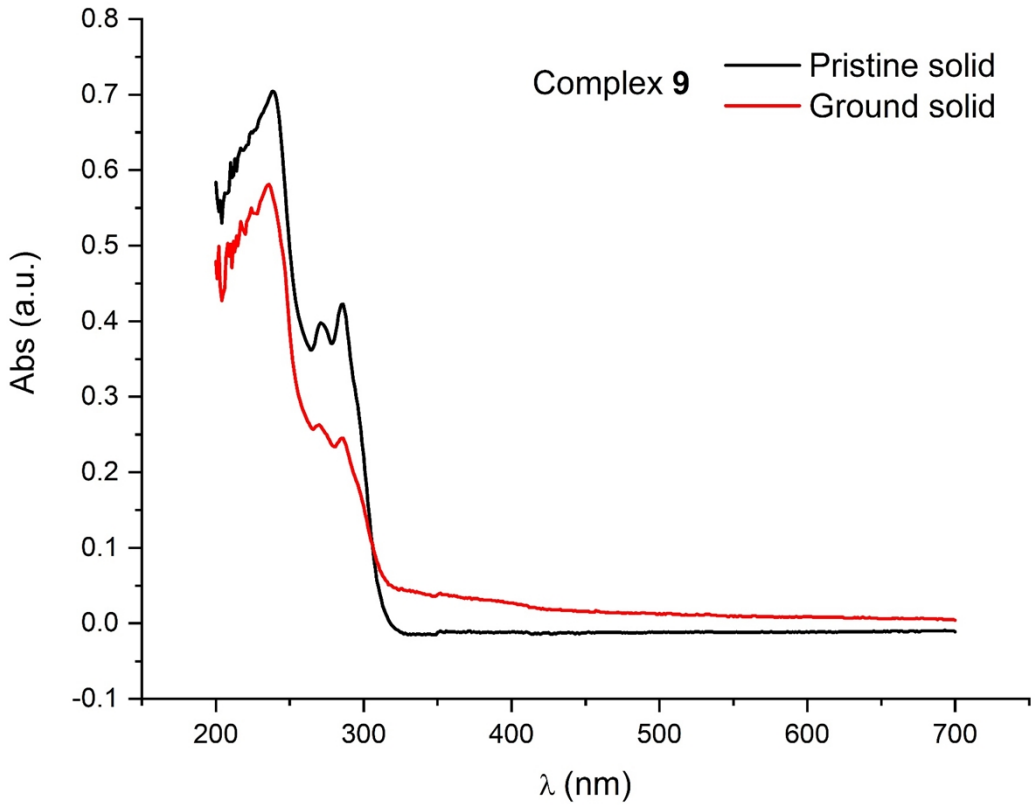


Figure S41. Absorption spectra of complex **9** as a pristine solid (black) and after being ground (red), in CH_2Cl_2 ($5 \cdot 10^{-4}$ M)

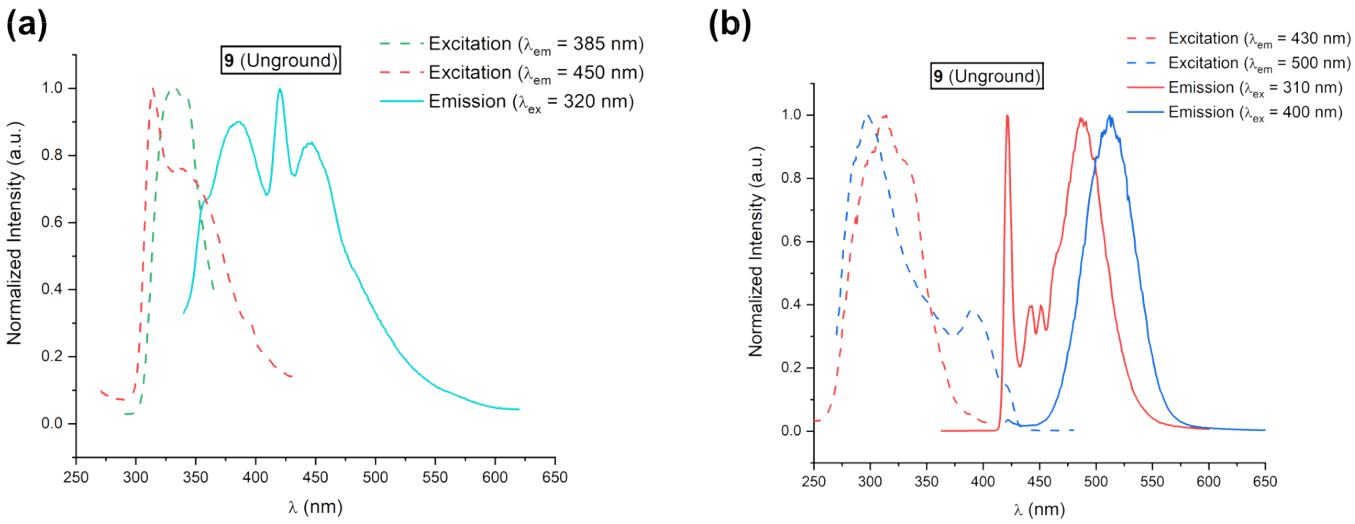


Figure S42. **a**) Excitation and emission spectra of complex **9**, in CH_2Cl_2 ($5 \cdot 10^{-4}$ M), at room temperature. (**b**) Excitation and emission spectra of complex **9**, in CH_2Cl_2 ($5 \cdot 10^{-4}$ M), vitrificated solution (77 K).

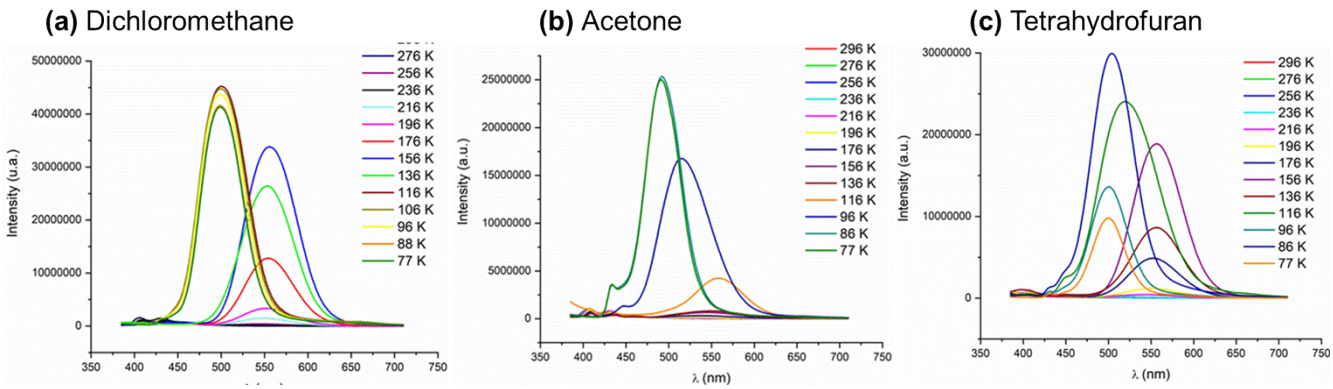


Figure S43. Emission (λ_{ex} = 365 nm) spectra of complex **9**, in CH_2Cl_2 (**a**); acetone (**b**) and THF (**c**), at $5 \cdot 10^{-4}$ M, at different temperatures.

Table S3. Photophysical data of complex **9**, in CH_2Cl_2 ($5 \cdot 10^{-4}$ M), at different temperatures.

Temperature (K)	λ_{ex}^{max} (nm)	λ_{em}^{max} (nm)
298	332 340	378 419, 439
268	328 341	380 418, 442
238	329 340 357	379 418, 440 549
208	333 342 365	379 418, 440 549
178[a]	280, 330 360	418, 442, 457 553
148[a]	284 341, 374	418, 442, 457 557
118	250, 345 366	424, 448 500
88	250, 345 366	425, 445 500

[a]At these temperatures the intensity of the structured band is totally negligible compared to that shown by the band at 550 nm.

Table S4. Emission maxima (λ_{ex} = 365 nm) of complex **9** in different solvents.

Temperature (K)	CH_2Cl_2 λ_{max} (nm)	THF λ_{max} (nm)	Acetone λ_{max} (nm)
236	545	546	545
216	549	549	545
196	552	551	550
176	555	538	553
156	557	545	556
136	553	555	556
116	499	555	520
106	499	514	505
96	499	492	500
77	499	492	503

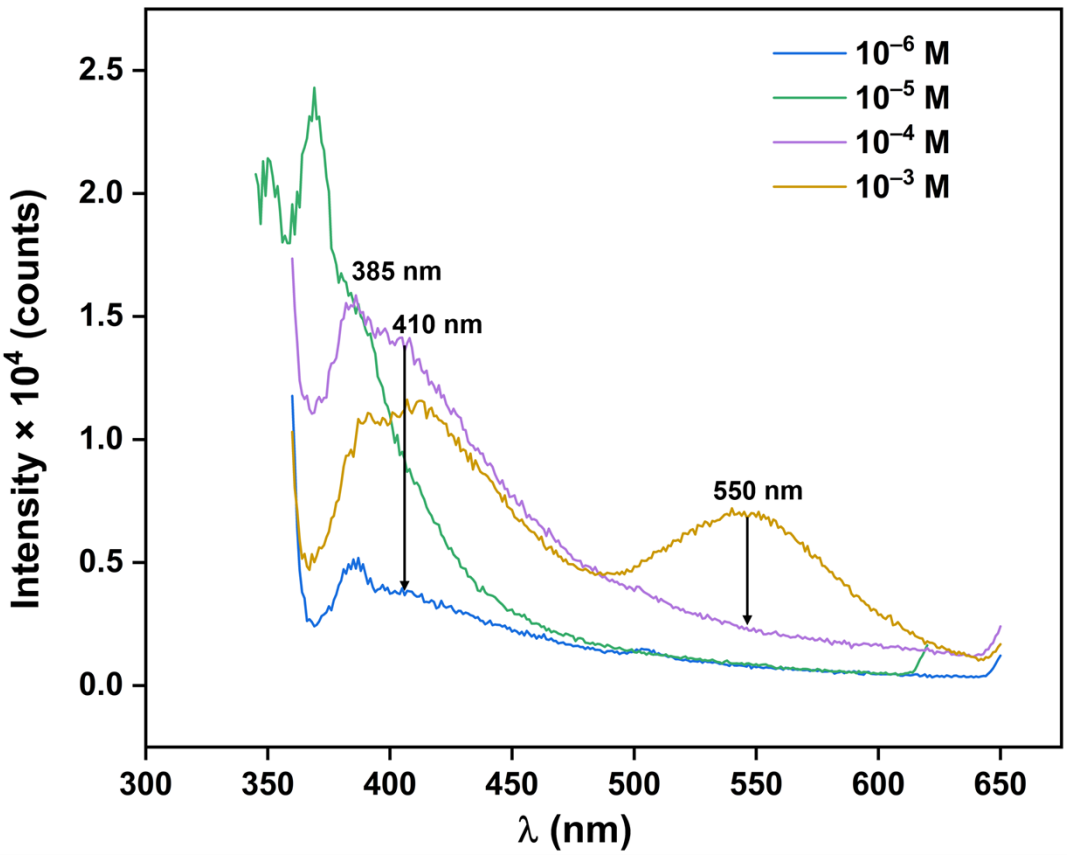


Figure S44. Emission (λ_{ex} = 300 nm) spectra of complex **7** at room temperature, in CH_2Cl_2 at different concentrations.

5. LIFETIME DECAY CURVES AND FITTING DATA

Components corresponding to the adjustment of radiative decay to a double or triple exponential (for selected cases). The lifetime values have been calculated according to the equation:[6]

$$\tau_{av} = \frac{\sum_i A_i \tau_i}{\sum_i A_i}$$

where:

- A_i is the amplitude (or relative contribution) of the i-th component,
- τ_i is the lifetime of the i-th component.

Average Lifetime for a Two-Exponential System

$$\tau_{av} = \frac{A_1\tau_1^2 + A_2\tau_2^2}{A_1\tau_1 + A_2\tau_2}$$

Average Lifetime for a Three-Exponential System

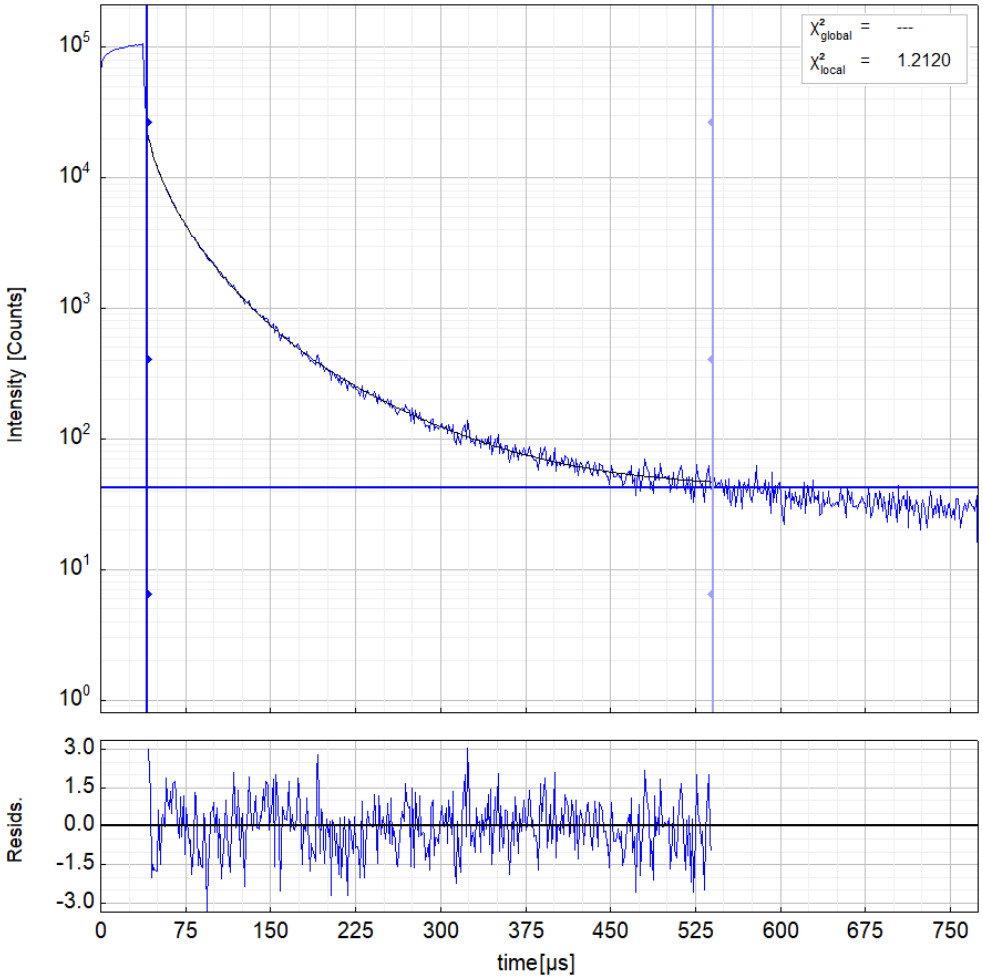
$$\tau_{av} = \frac{A_1\tau_1^2 + A_2\tau_2^2 + A_3\tau_3^2}{A_1\tau_1 + A_2\tau_2 + A_3\tau_3}$$

The emission decay profiles of the gold(I) complexes were best fitted to a triple-exponential model, suggesting the presence of multiple emissive states. The short-lived component (τ_1) may be attributed to prompt fluorescence or phosphorescence from the monomeric species, while the intermediate (τ_2) and long-lived (τ_3) components could be associated with emissive states influenced by aurophilic interactions and aggregation.

COMPLEX 6 PRISTINE ROOM TEMPERATURE

Excitation: V pol 372±2nm with LDH-P-C-375

Detection: U pol 520±14nm 200000 peak counts grating 1200/500+detector UV-red [PMT]



Parameter	Value	Δ	δ
A_1[kCnts/Chnl]	9.40	±0.49	5.2%
τ_1[ns]	28 800	±2 700	9.1%
I_1[kCnts]	211.0	±8.5	4.0%
A_2[kCnts/Chnl]	8.58	±0.83	9.6%
τ_2[ns]	8 140	±690	8.4%
I_2[kCnts]	55	±11	18%
A_3[kCnts/Chnl]	1.69	±0.45	26%
τ_3[ns]	84 600	±9 200	11%
I_3[kCnts]	112	±19	16%
$Bkgr_{Dec}$[kCnts]	0.0423	±0.0024	5.5%
τ_{AvInt}[ns]	42 280	±720	1.7%

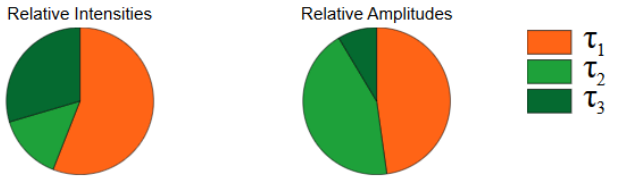
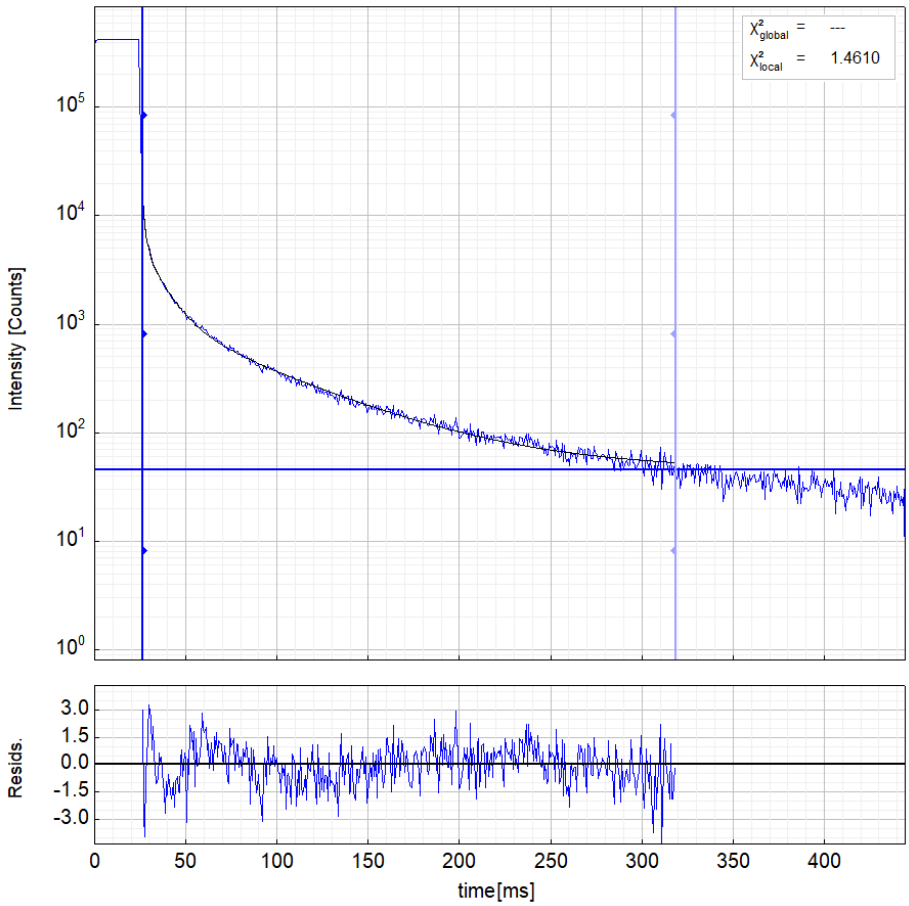


Figure S45. Decay curve and fitted parameters of lifetimes of complex **6** at room temperature.

COMPLEX 6 PRISTINE 77 K

Excitation: V pol 372±2nm with LDH-P-C-375

Detection: U pol 520±6nm 500000 peak counts grating 1200/500+ detector UV-red [PMT]



Parameter	Value	Δ	δ
A_1[kCnts/Chnl]	9.22	±0.38	4.1%
τ_1[ns]	1 360 000	±150 000	10%
I_1[kCnts]	19.1	±1.8	9.2%
A_2[kCnts/Chnl]	1.142	±0.081	7.0%
τ_2[ns]	57 600 000	±2 600 000	4.4%
I_2[kCnts]	100.3	±2.1	2.0%
A_3[kCnts/Chnl]	4.22	±0.23	5.4%
τ_3[ns]	10 420 000	±710 000	6.8%
I_3[kCnts]	67.1	±1.8	2.6%
$Bkgr_{Dec}$[kCnts]	0.0457	±0.0022	4.6%
τ_{AvInt}[ns]	34 850 000	±670 000	1.9%

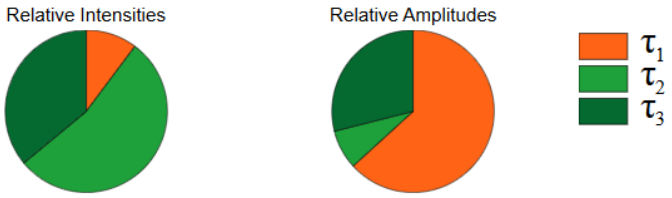
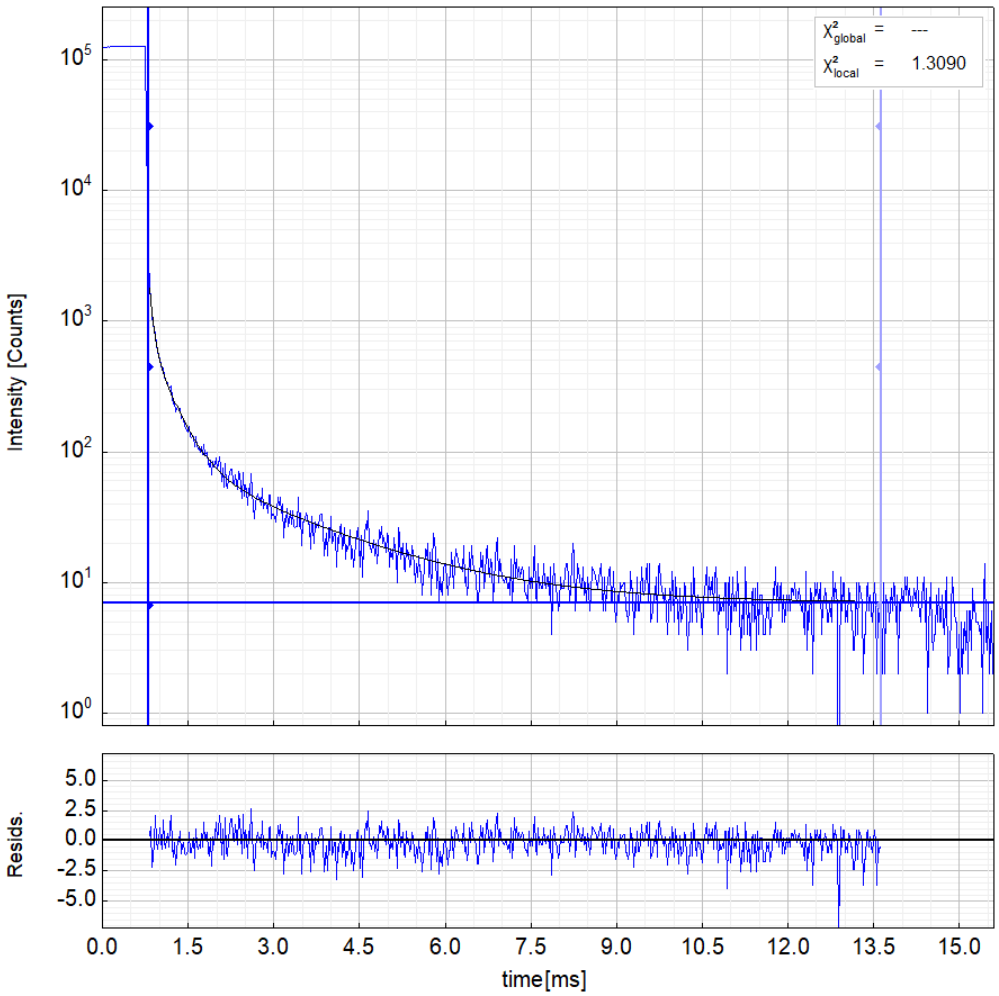


Figure S46. Decay curve and fitted parameters of lifetimes of complex **6** at 77 K.

COMPLEX 6 GROUND ROOM TEMPERATURE

Excitation: V pol 372±2nm with LDH-P-C-375

Detection: U pol 559±14nm 500000 peak counts grating 1200/500+, detector UV-red [PMT]



Parameter	Value	Δ	δ
A_1[kCnts/Chnl]	1.06	±0.12	11%
τ_1[ns]	60 000	±15 000	25%
I_1[kCnts]	3.10	±0.99	32%
A_2[kCnts/Chnl]	0.088	±0.021	24%
τ_2[ns]	2 040 000	±310 000	15%
I_2[kCnts]	8.68	±0.63	7.2%
A_3[kCnts/Chnl]	0.64	±0.11	16%
τ_3[ns]	333 000	±45 000	14%
I_3[kCnts]	10.38	±0.56	5.4%
$Bkgr_{Dec}$[kCnts]	0.0070	±0.0006	7.6%
τ_{AvInt}[ns]	960 000	±84 000	8.7%

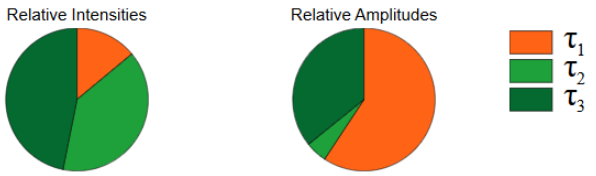
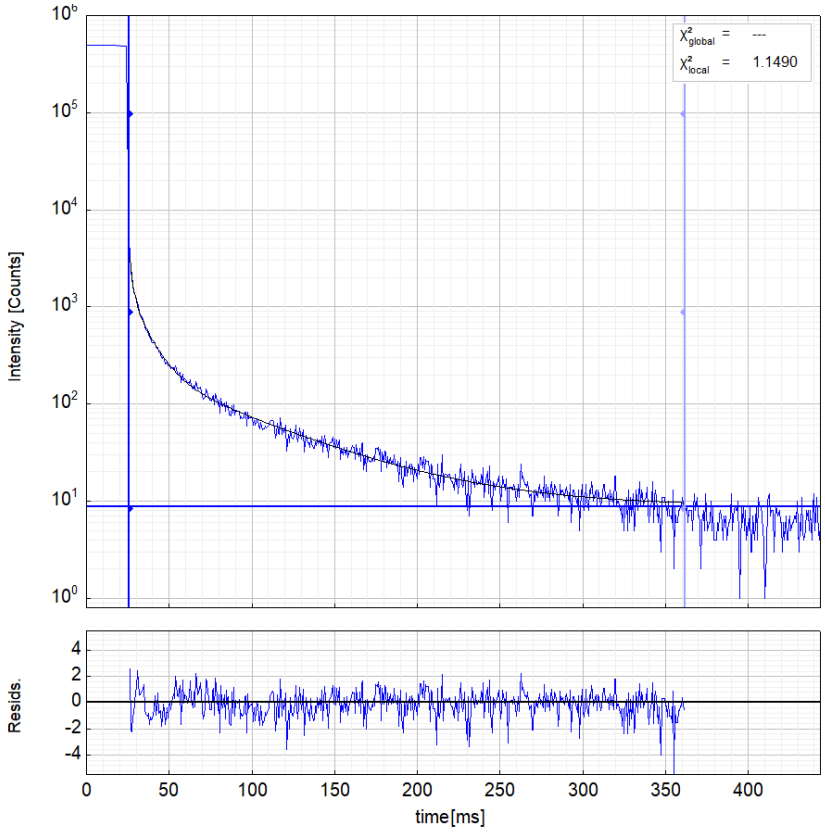


Figure S47. Decay curve and fitted parameters of lifetimes of complex **6**$_{\textbf{ground}}$ at room temperature.

COMPLEX 6 GROUND 77 K

Excitation: V pol 372±2nm with LDH-P-C-375

Detection: U pol 559±5nm 500000 peak counts, grating 1200/500+, detector UV-red [PMT]



Parameter	Value	Δ	δ
A_1[kCnts/Chnl]	1.87	±0.12	6.3%
τ_1[ns]	1 800 000	±1 500 000	86%
I_1[kCnts]	5.0	±3.7	73%
A_2[kCnts/Chnl]	1.11	±0.42	37%
τ_2[ns]	9 900 000	±4 500 000	45%
I_2[kCnts]	16.8	±1.5	8.6%
A_3[kCnts/Chnl]	0.220	±0.051	23%
τ_3[ns]	60 000 000	±11 000 000	18%
I_3[kCnts]	20.0	±1.9	9.2%
$Bkgr_{Dec}$[kCnts]	0.0089	±0.0013	14%
τ_{AvInt}[ns]	32 900 000	±3 400 000	10%

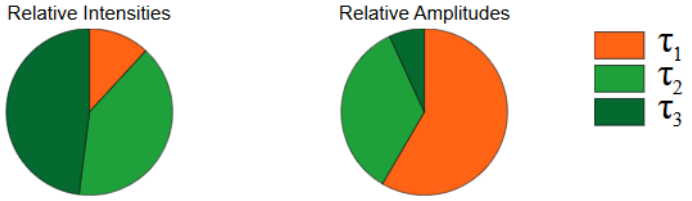
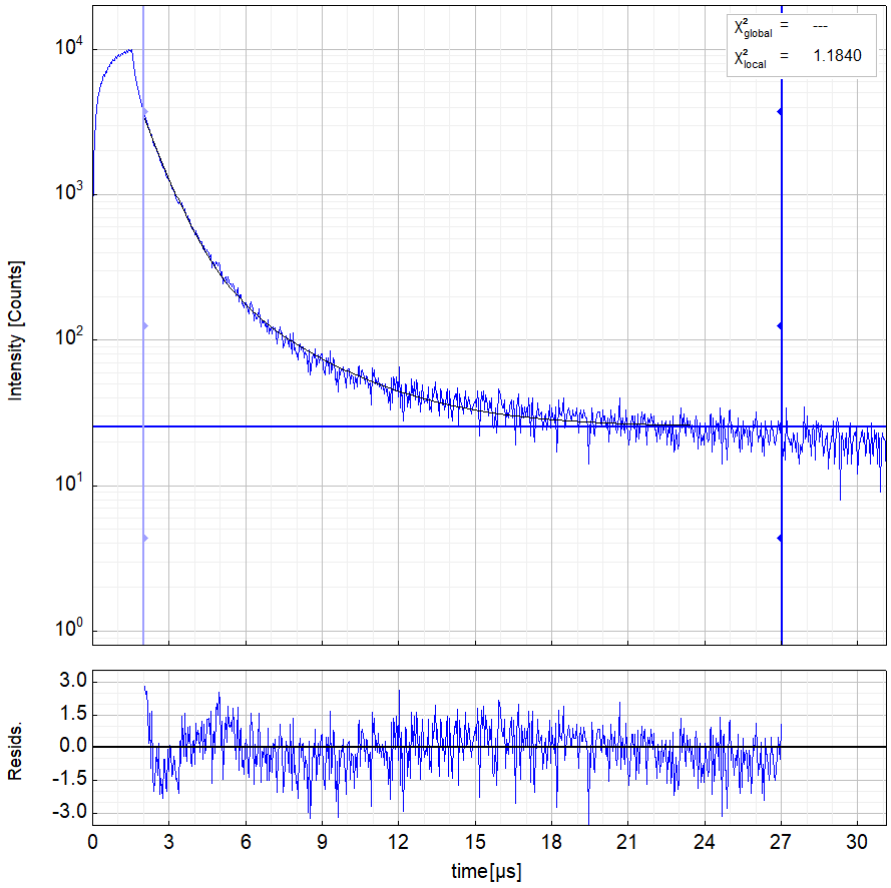


Figure S48. Decay curve and fitted parameters of lifetimes of complex $\mathbf{6}_{\mathbf{ground}}$ at 77 K.

COMPLEX 6 FILM ROOM TEMPERATURE

Excitation: V pol 372±2nm with LDH-P-C-375

Detection: U pol 503±5nm 10000 peak counts, grating 1200/500+, detector UV-red [PMT]



Parameter	Value	Δ	δ
A_1[kCnts/Chnl]	0.401	±0.051	13%
τ_1[ns]	3 290	±250	7.3%
I_1[kCnts]	32.9	±2.1	6.1%
A_2[kCnts/Chnl]	2.915	±0.033	1.1%
τ_2[ns]	870	±26	2.9%
I_2[kCnts]	63.4	±2.4	3.7%
$Bkgr_{Dec}$[kCnts]	0.0254	±0.0005	1.9%
τ_{AvInt}[ns]	1 694	±39	2.3%

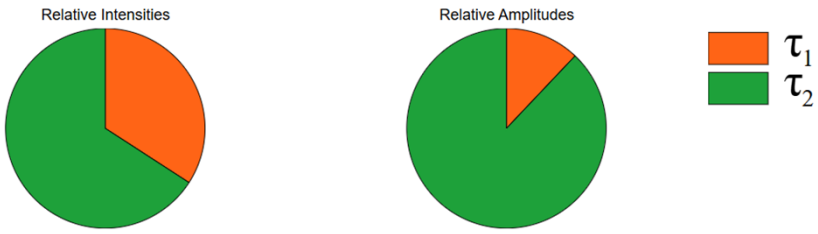
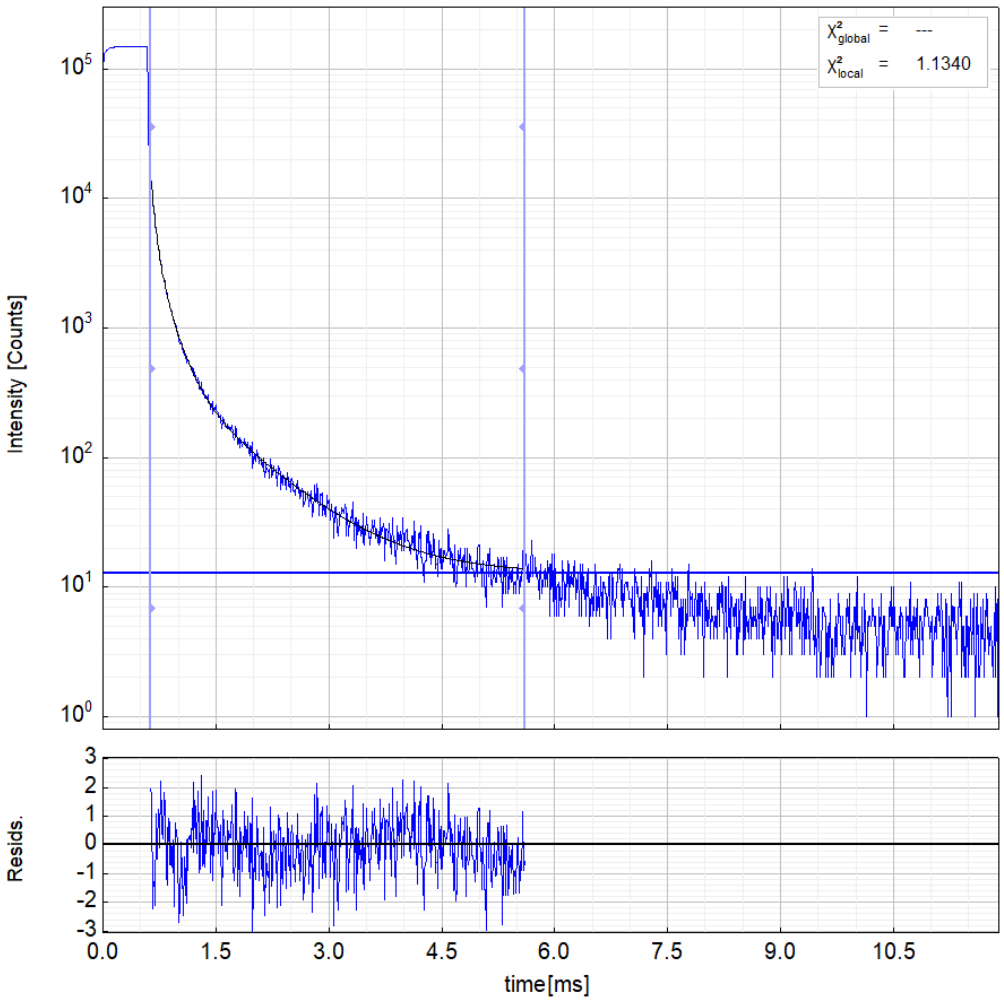


Figure S49. Decay curve and fitted parameters of lifetimes of complex $\mathbf{6}_{\mathbf{film}}$ (PMMA, 5% w/w) at room temperature.

COMPLEX 7 PRISTINE ROOM TEMPERATURE

Excitation: V pol 372±2nm with LDH-P-C-375

Detection: U pol 528±14nm 500000 peak counts grating 1200/500+, detector UV-red [PMT]



Parameter	Value	Δ	δ
A_1[kCnts/Chnl]	0.508	±0.053	10%
τ_1[ns]	810 000	±36 000	4.4%
I_1[kCnts]	40.2	±2.1	5.0%
A_2[kCnts/Chnl]	9.81	±0.41	4.1%
τ_2[ns]	51 000	±3 400	6.6%
I_2[kCnts]	48.8	±5.4	11%
A_3[kCnts/Chnl]	4.24	±0.43	9.9%
τ_3[ns]	180 000	±12 000	6.4%
I_3[kCnts]	74.4	±2.7	3.5%
$Bkgr_{Dec}$[kCnts]	0.0128	±0.0007	5.3%
τ_{AvInt}[ns]	296 400	±2 400	0.8%

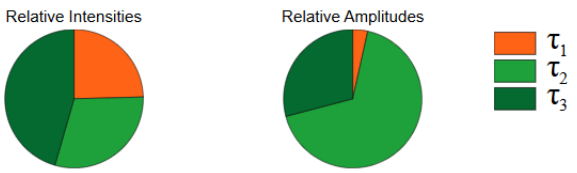
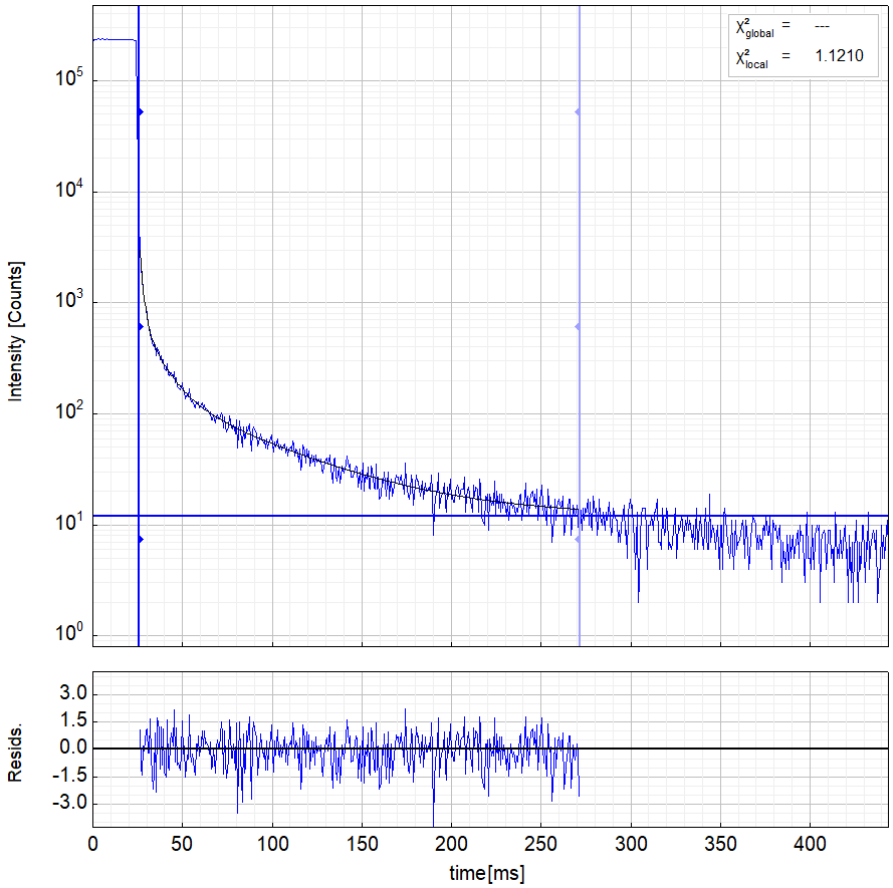


Figure S50. Decay curve and fitted parameters of lifetimes of complex **7** at room temperature.

COMPLEX 7 PRISTINE 77 K

Excitation: V pol 372±2nm with LDH-P-C-375

Detection: U pol 528±5nm 500000 peak counts grating 1200/500+, detector UV-red [PMT]



Parameter	Value	Δ	δ
A_1[kCnts/Chnl]	0.161	±0.014	8.2%
τ_1[ns]	54 700 000	±3 300 000	6.0%
I_1[kCnts]	13.38	±0.34	2.5%
A_2[kCnts/Chnl]	0.564	±0.064	11%
τ_2[ns]	9 900 000	±1 200 000	12%
I_2[kCnts]	8.49	±0.56	6.5%
A_3[kCnts/Chnl]	2.24	±0.12	5.0%
τ_3[ns]	1 670 000	±130 000	7.7%
I_3[kCnts]	5.70	±0.48	8.4%
$Bkgr_{Dec}$[kCnts]	0.0121	±0.0008	6.1%
τ_{AvInt}[ns]	30 000 000	±1 200 000	3.8%

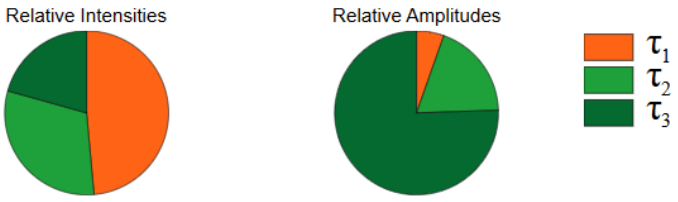
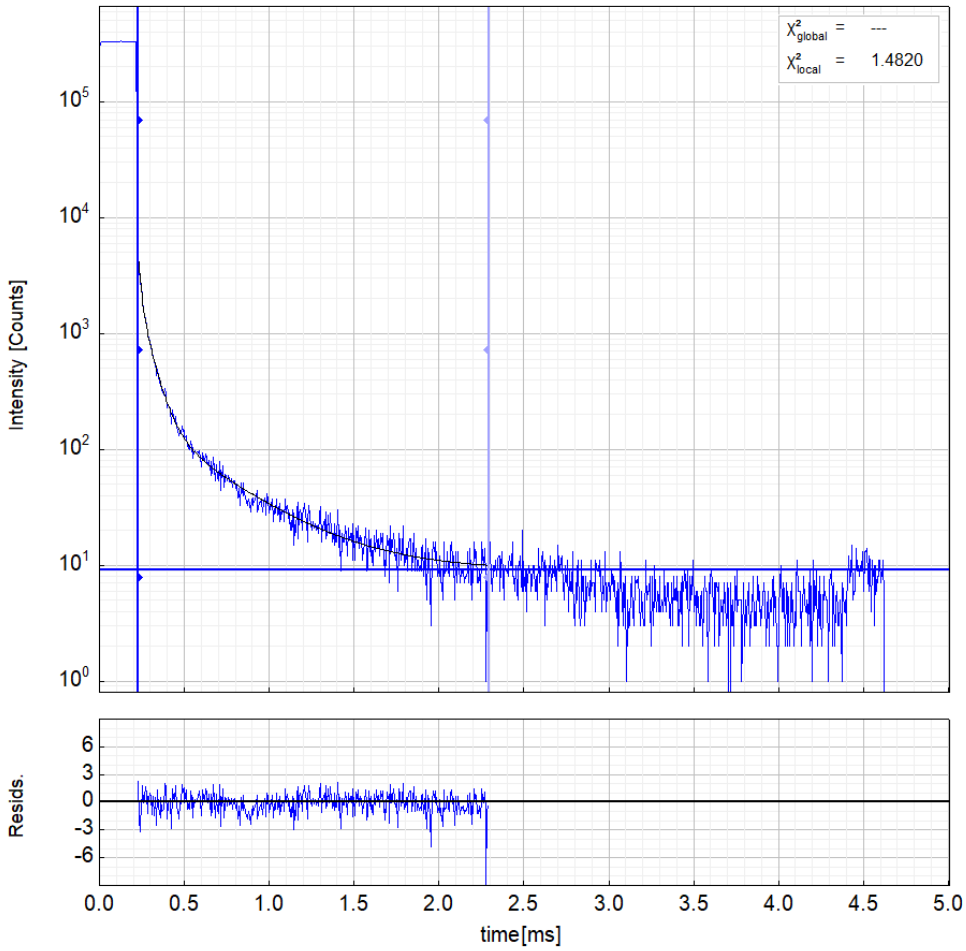


Figure S51. Decay curve and fitted parameters of lifetimes of complex **7** at 77 K.

COMPLEX 7 GROUND ROOM TEMPERATURE

Excitation: V pol 372±2nm with LDH-P-C-375

Detection: U pol 523±9nm 500000 peak counts grating 1200/500+ detector UV-red [PMT]



Parameter	Value	Δ	δ
A_1[kCnts/Chnl]	2.64	±0.14	5.2%
τ_1[ns]	13 900	±5 800	42%
I_1[kCnts]	7.2	±3.4	47%
A_2[kCnts/Chnl]	0.175	±0.036	20%
τ_2[ns]	395 000	±66 000	17%
I_2[kCnts]	13.46	±0.92	6.8%
A_3[kCnts/Chnl]	1.86	±0.43	23%
τ_3[ns]	64 000	±14 000	21%
I_3[kCnts]	23.1	±1.6	6.6%
$Bkgr_{Dec}$[kCnts]	0.0091	±0.0015	16%
τ_{AvInt}[ns]	158 000	±17 000	11%

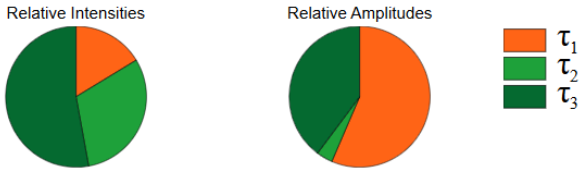
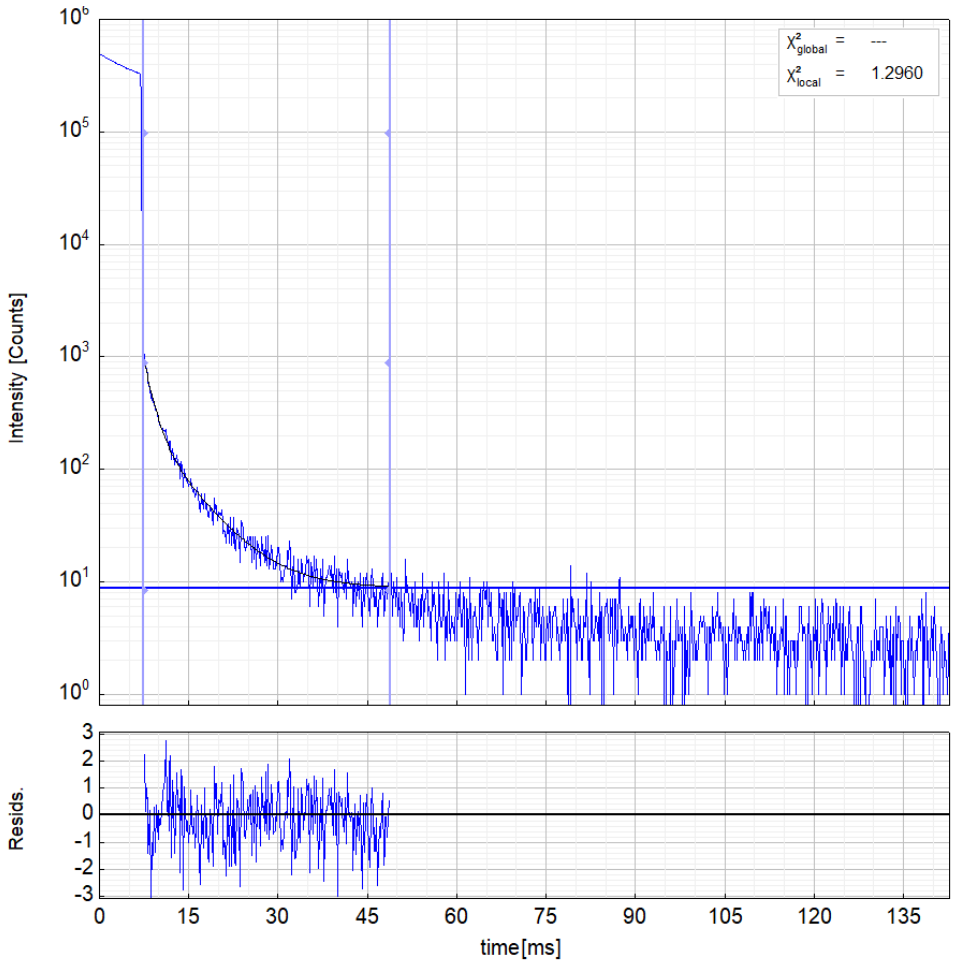


Figure S52. Decay curve and fitted parameters of lifetimes of complex **7**$_{\mathbf{ground}}$ at room temperature.

COMPLEX 7 GROUND 77 K

Excitation: V pol 405±15nm with PLS-400

Detection: U pol 540±5nm 500000 peak counts grating 1200/500+ detector UV-red [PMT]



Parameter	Value	Δ	δ
A_1[kCnts/Chnl]	0.223	±0.043	19%
τ_1[ns]	6 150 000	±770 000	13%
I_1[kCnts]	8.36	±0.58	6.9%
A_2[kCnts/Chnl]	0.671	±0.025	3.6%
τ_2[ns]	1 420 000	±120 000	7.8%
I_2[kCnts]	5.79	±0.67	11%
$Bkgr_{Dec}$[kCnts]	0.0089	±0.0009	10%
τ_{AvInt}[ns]	4 210 000	±220 000	5.0%

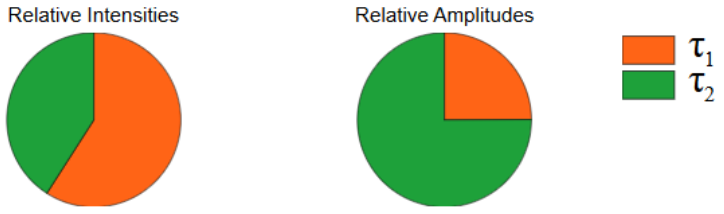
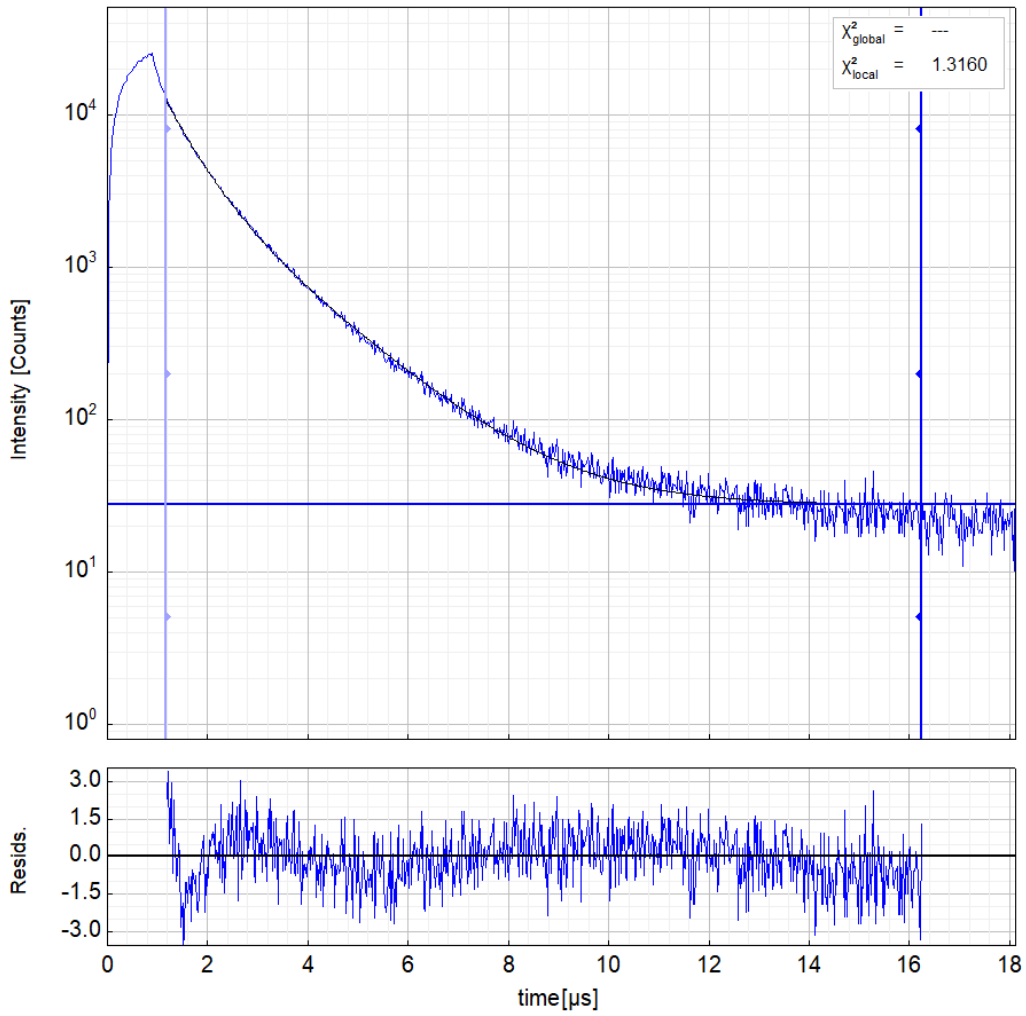


Figure S53. Decay curve and fitted parameters of lifetimes of complex **7**$_{ground}$ at 77K.

COMPLEX 7 FILM ROOM TEMPERATURE

Excitation: V pol 372±2nm with LDH-P-C-375

Detection: U pol 538±5nm 100000 peak counts, grating 1200/500+, detector UV-red [PMT]



Parameter	Value	Δ	δ
A_1[kCnts/Chnl]	4.11	±0.17	4.1%
τ_1[ns]	1 543	±25	1.6%
I_1[kCnts]	316.9	±8.1	2.5%
A_2[kCnts/Chnl]	8.16	±0.13	1.5%
τ_2[ns]	559	±11	1.8%
I_2[kCnts]	227.9	±7.4	3.2%
$Bkgr_{Dec}$[kCnts]	0.0276	±0.0006	1.9%
τ_{AvInt}[ns]	1 131.0	±3.4	0.3%

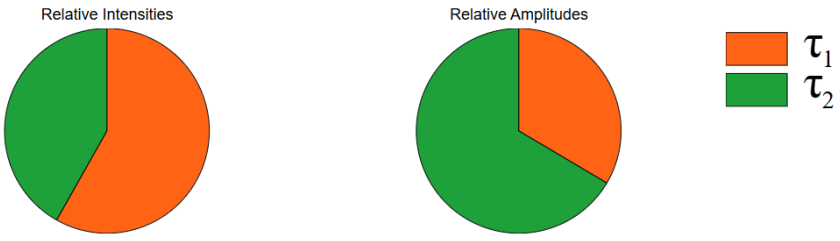
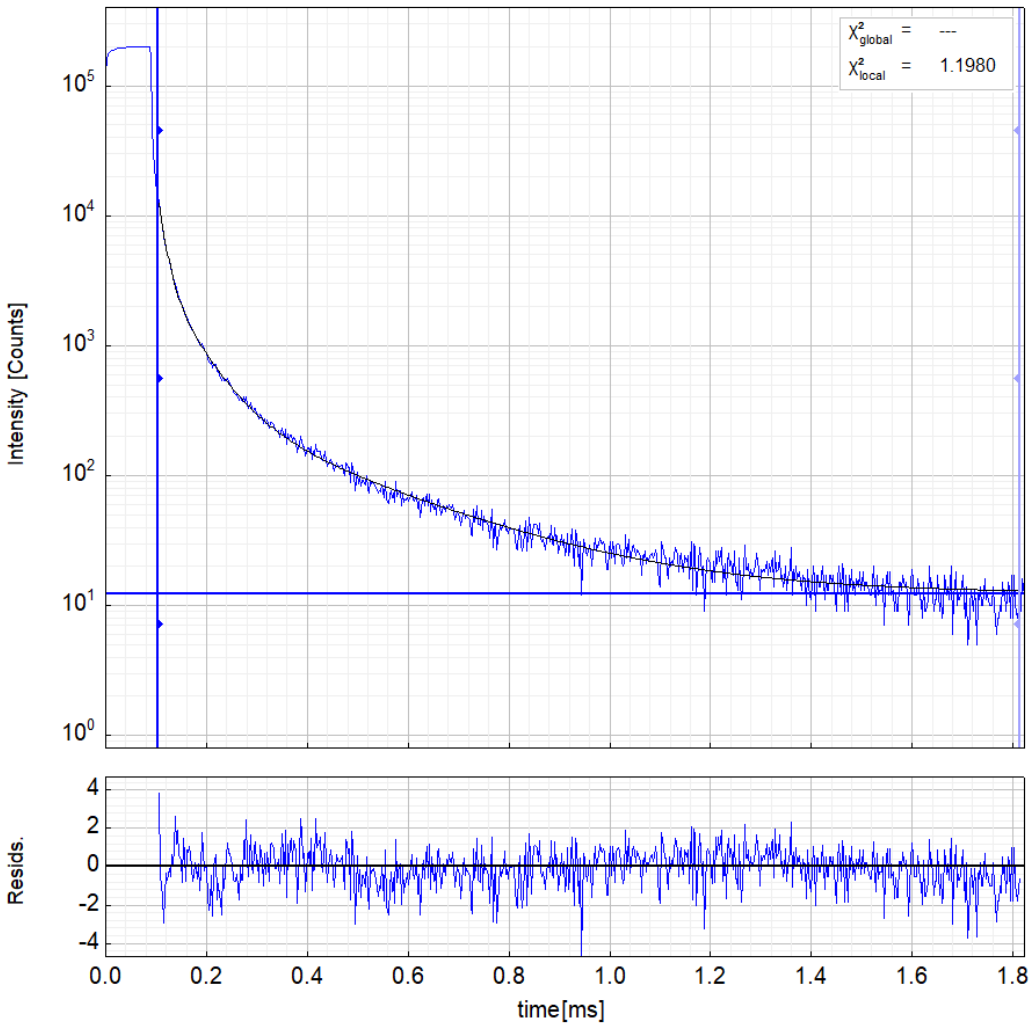


Figure S54. Decay curve and fitted parameters of lifetimes of complex **7**$_{\mathbf{film}}$ (PMMA, 5% w/w) at room temperature.

COMPLEX 8 PRISTINE ROOM TEMPERATURE

Excitation: V pol 372±2nm with LDH-P-C-375

Detection: U pol 520±14nm 200000 peak counts grating 1200/500+ detector UV-red [PMT]



Parameter	Value	Δ	δ
A_1[kCnts/Chnl]	0.371	±0.059	16%
τ_1[ns]	267 000	±24 000	8.9%
I_1[kCnts]	38.6	±3.0	7.7%
A_2[kCnts/Chnl]	3.04	±0.46	15%
τ_2[ns]	58 100	±6 800	12%
I_2[kCnts]	68.9	±3.0	4.3%
A_3[kCnts/Chnl]	9.06	±0.24	2.6%
τ_3[ns]	13 800	±1 800	12%
I_3[kCnts]	48.6	±6.5	13%
$Bkgr_{Dec}$[kCnts]	0.0124	±0.0009	6.9%
τ_{AvInt}[ns]	95 800	±3 800	3.9%

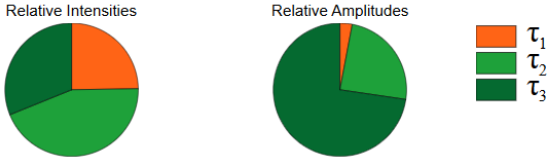
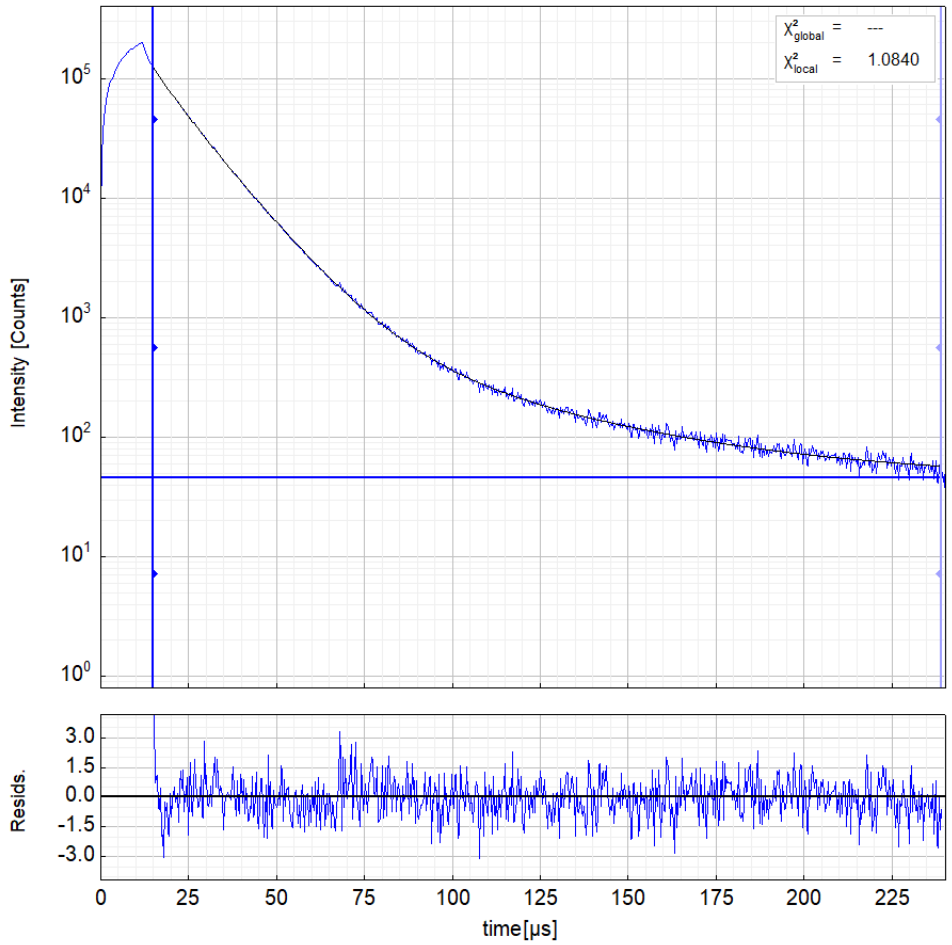


Figure S55. Decay curve and fitted parameters of lifetimes of complex **8** at room temperature.

COMPLEX 8 PRISTINE 77 K

Excitation: V pol 372±2nm with LDH-P-C-375

Detection: U pol 528±5nm 200000 peak counts grating 1200/500+ detector UV-red [PMT]



Parameter	Value	Δ	δ
A_1[kCnts/Chnl]	1.29	±0.29	22%
τ_1[ns]	47 500	±5 000	10%
I_1[kCnts]	191	±23	12%
A_2[kCnts/Chnl]	88.6	±8.5	9.6%
τ_2[ns]	12 560	±410	3.3%
I_2[kCnts]	3 480	±210	6.0%
A_3[kCnts/Chnl]	31.3	±8.6	27%
τ_3[ns]	6 590	±820	12%
I_3[kCnts]	650	±250	38%
$Bkgr_{Dec}$[kCnts]	0.0457	±0.0043	9.4%
τ_{AvInt}[ns]	13 210	±110	0.8%

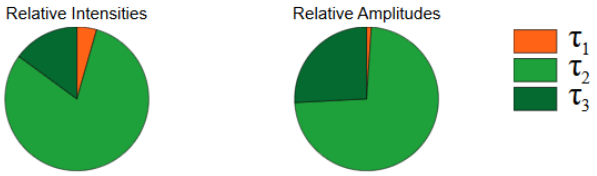
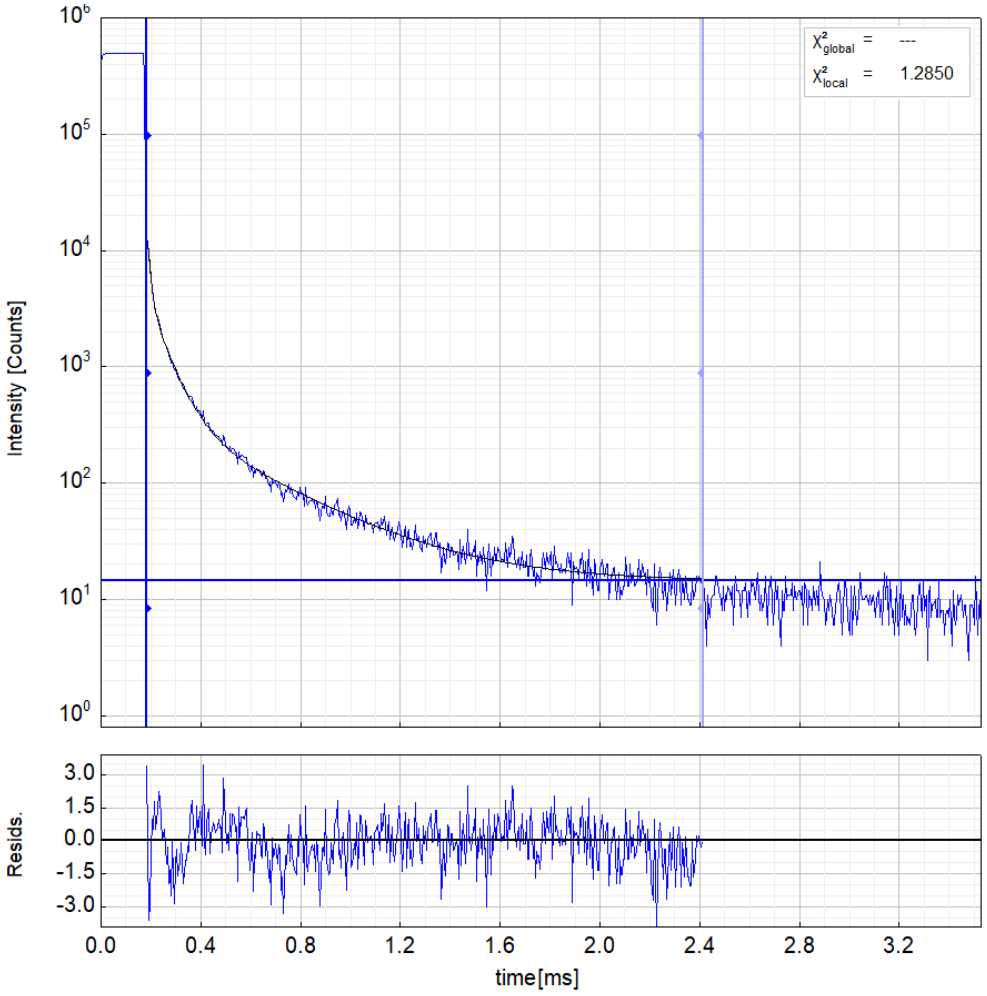


Figure S56. Decay curve and fitted parameters of lifetimes of complex **8** at 77K.

COMPLEX 8 GROUND ROOM TEMPERATURE

Excitation: V pol 372±2nm with LDH-P-C-375

Detection: U pol 520±12nm 500000 peak counts grating 1200/500+ detector UV-red [PMT]



Parameter	Value	Δ	δ
A_1[kCnts/Chnl]	0.385	±0.063	16%
τ_1[ns]	352 000	±37 000	10%
I_1[kCnts]	26.4	±1.8	6.5%
A_2[kCnts/Chnl]	9.18	±0.56	6.0%
τ_2[ns]	12 100	±2 900	24%
I_2[kCnts]	21.7	±2.8	13%
A_3[kCnts/Chnl]	3.57	±0.47	13%
τ_3[ns]	68 200	±7 400	11%
I_3[kCnts]	47.5	±1.1	2.3%
$Bkgr_{Dec}$[kCnts]	0.0144	±0.0012	8.0%
τ_{AvInt}[ns]	133 800	±4 900	3.6%

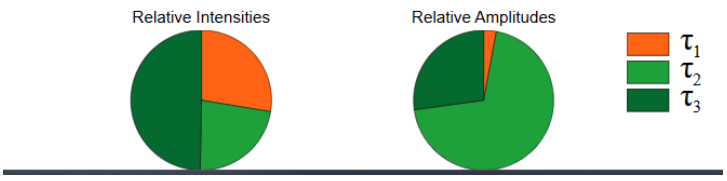
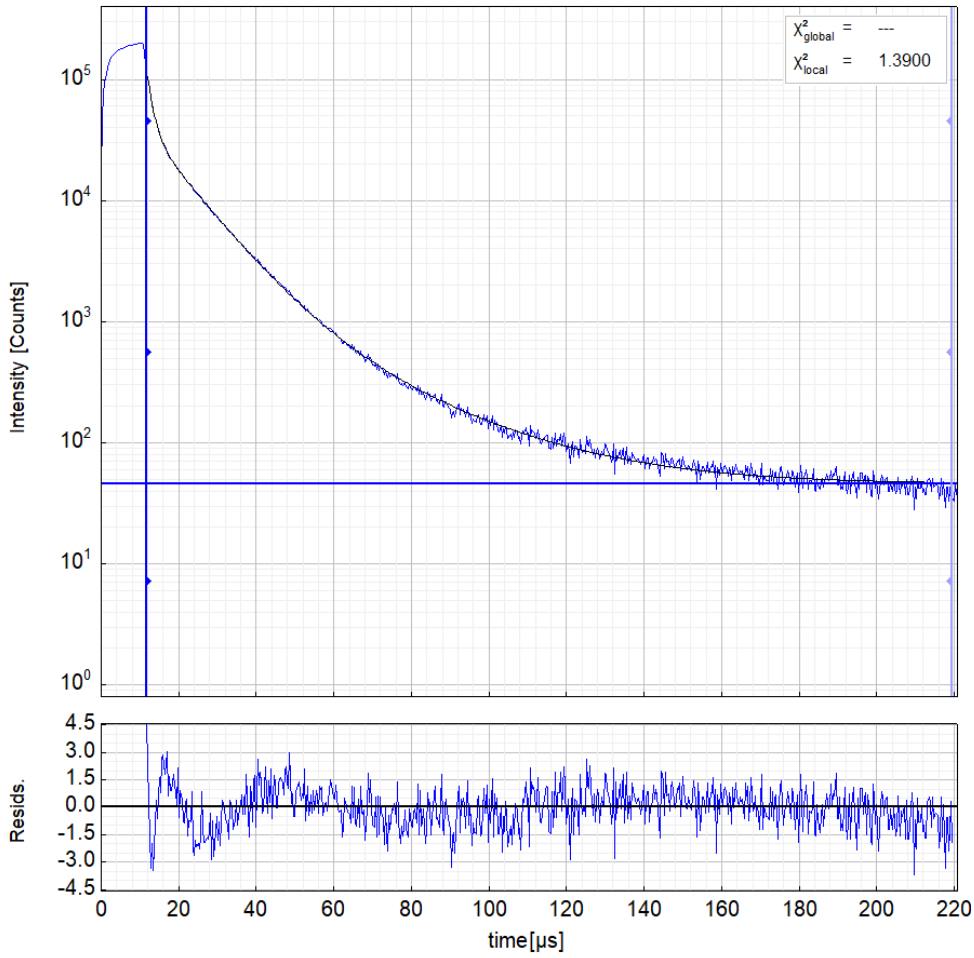


Figure S57. Decay curve and fitted parameters of lifetimes of complex $\mathbf{8_{ground}}$ at room temperature.

COMPLEX 8 GROUND 77 K

Excitation: V pol 372±2nm with LDH-P-C-375

Detection: U pol 520±14nm 200000 peak counts, grating 1200/500+, detector UV-red [PMT]



Parameter	Value	Δ	δ
A_1[kCnts/ChnI]	2.45	±0.55	22%
τ_1[ns]	27 400	±2 000	7.3%
I_1[kCnts]	209	±31	15%
A_2[kCnts/ChnI]	73.93	±0.70	0.9%
τ_2[ns]	1 443	±28	1.9%
I_2[kCnts]	333.4	±6.8	2.0%
A_3[kCnts/ChnI]	34.50	±0.30	0.9%
τ_3[ns]	10 360	±180	1.7%
I_3[kCnts]	1 117	±25	2.2%
$Bkgr_{Dec}$[kCnts]	0.0456	±0.0019	4.0%
τ_{AvInt}[ns]	10 711	±78	0.7%

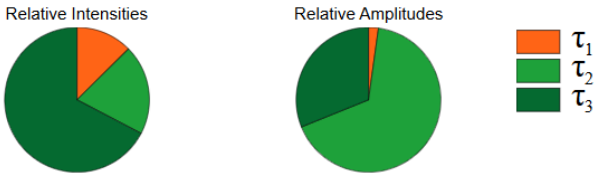
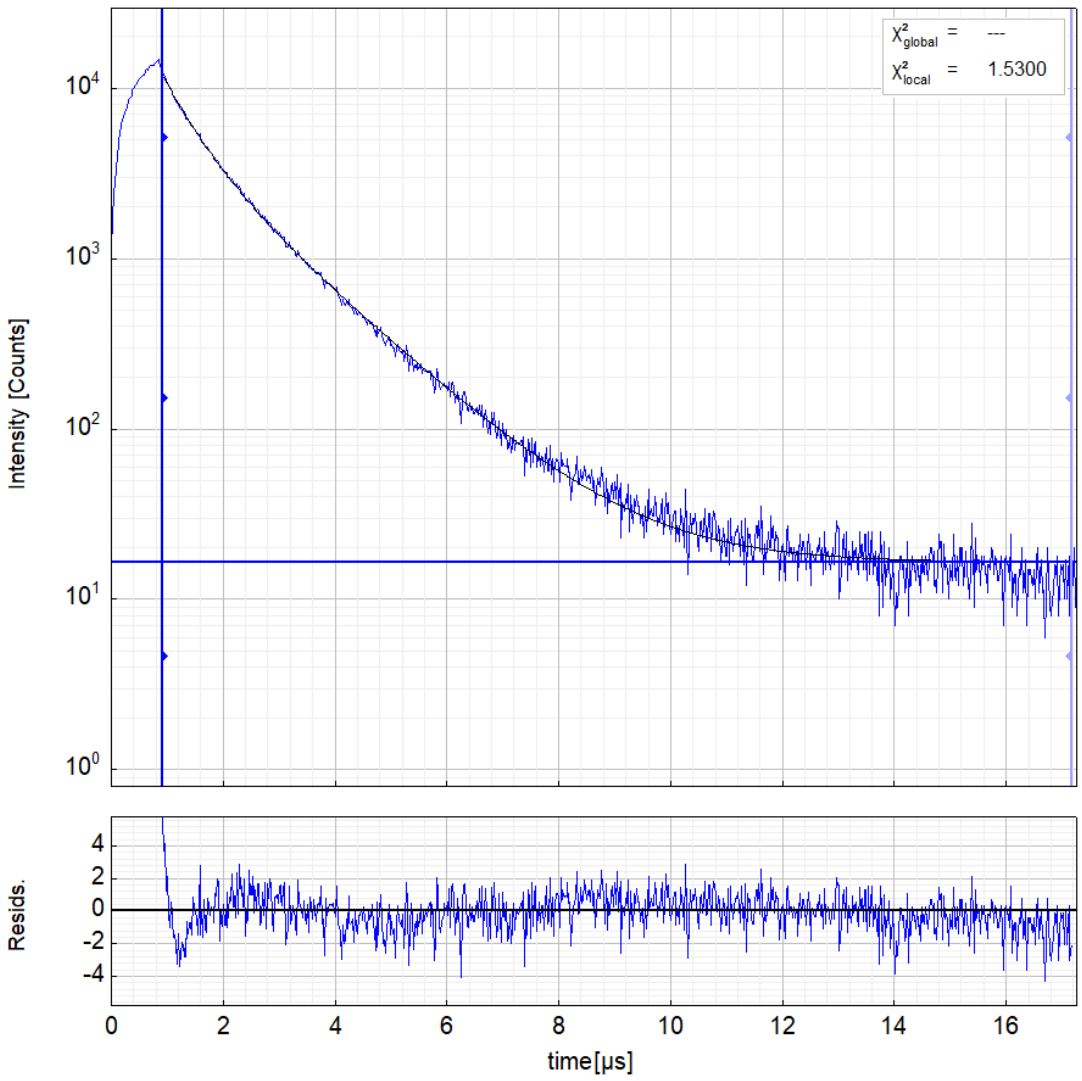


Figure S58. Decay curve and fitted parameters of lifetimes of complex $\mathbf{8_{ground}}$ at 77K.

COMPLEX 8 FILM ROOM TEMPERATURE

Excitation: V pol 400±2nm with LDH-405

Detection: U pol 526±14nm 100000 peak counts, grating 1200/500+, detector UV-red [PMT]



Parameter	Value	Δ	δ
A_1[kCnts/Chnl]	5.07	±0.16	3.1%
τ_1[ns]	1 465	±15	1.0%
I_1[kCnts]	370.8	±8.4	2.3%
A_2[kCnts/Chnl]	6.81	±0.15	2.1%
τ_2[ns]	523	±18	3.4%
I_2[kCnts]	177.9	±9.3	5.2%
$Bkgr_{Dec}$[kCnts]	0.0165	±0.0003	1.4%
τ_{AvInt}[ns]	1 159.4	±2.0	0.2%

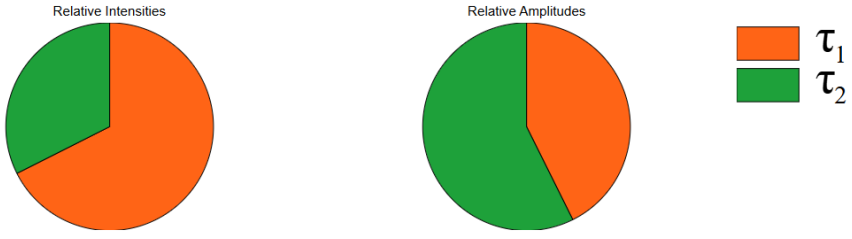
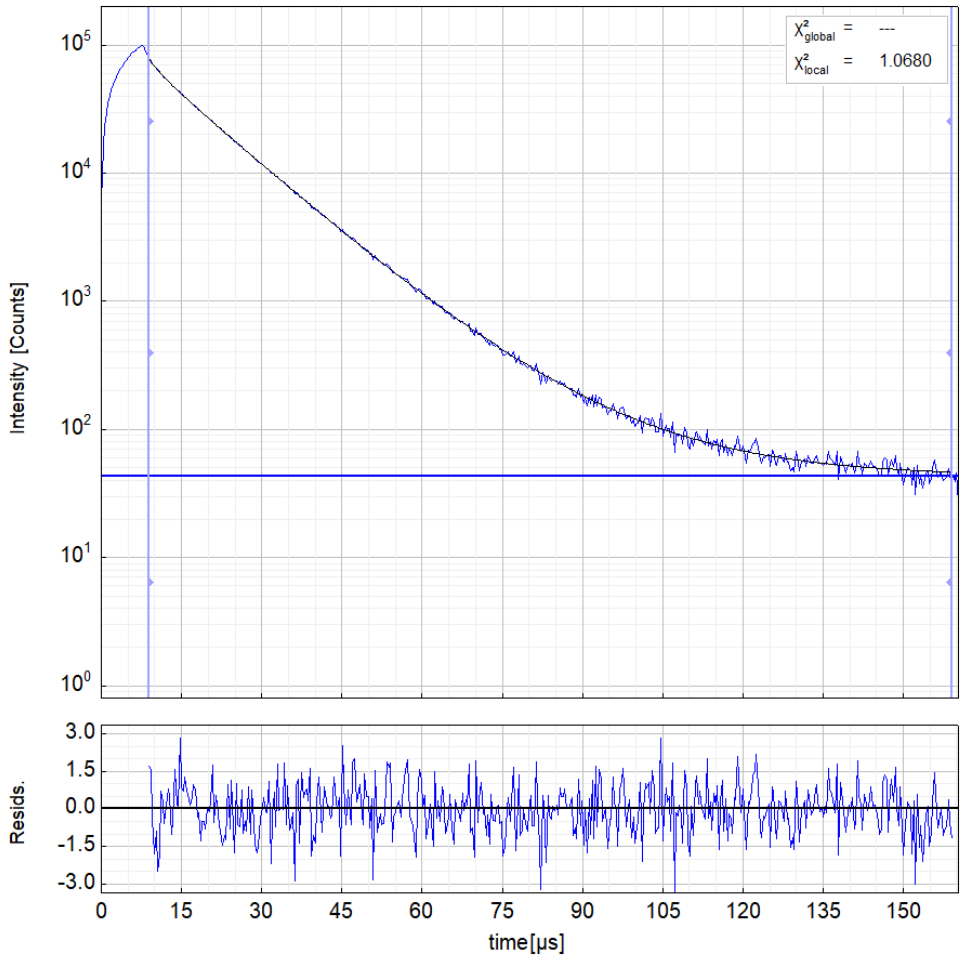


Figure S59. Decay curve and fitted parameters of lifetimes of complex $\mathbf{8_{film}}$ (PMMA, 5% w/w) at room temperature.

COMPLEX 9 PRISTINE ROOM TEMPERATURE

Excitation: V pol 372±2nm with LDH-P-C-375

Detection: U pol 523±5nm 100000 peak counts, grating 1200/500+, detector UV-red [PMT]



Parameter	Value	Δ	δ
A_1[kCnts/Chnl]	3.4	±1.9	55%
τ_1[ns]	21 900	±3 300	15%
I_1[kCnts]	230	±110	45%
A_2[kCnts/Chnl]	10.28	±0.55	5.3%
τ_2[ns]	2 290	±260	11%
I_2[kCnts]	74	±11	15%
A_3[kCnts/Chnl]	64.3	±1.1	1.7%
τ_3[ns]	11 590	±240	2.0%
I_3[kCnts]	2 325	±86	3.7%
$Bkgr_{Dec}$[kCnts]	0.0428	±0.0024	5.5%
τ_{AvInt}[ns]	12 218	±26	0.2%

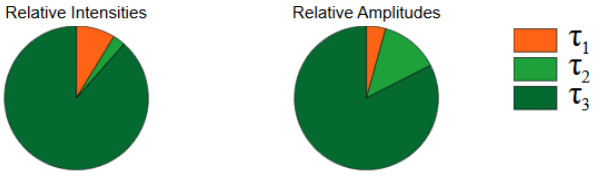
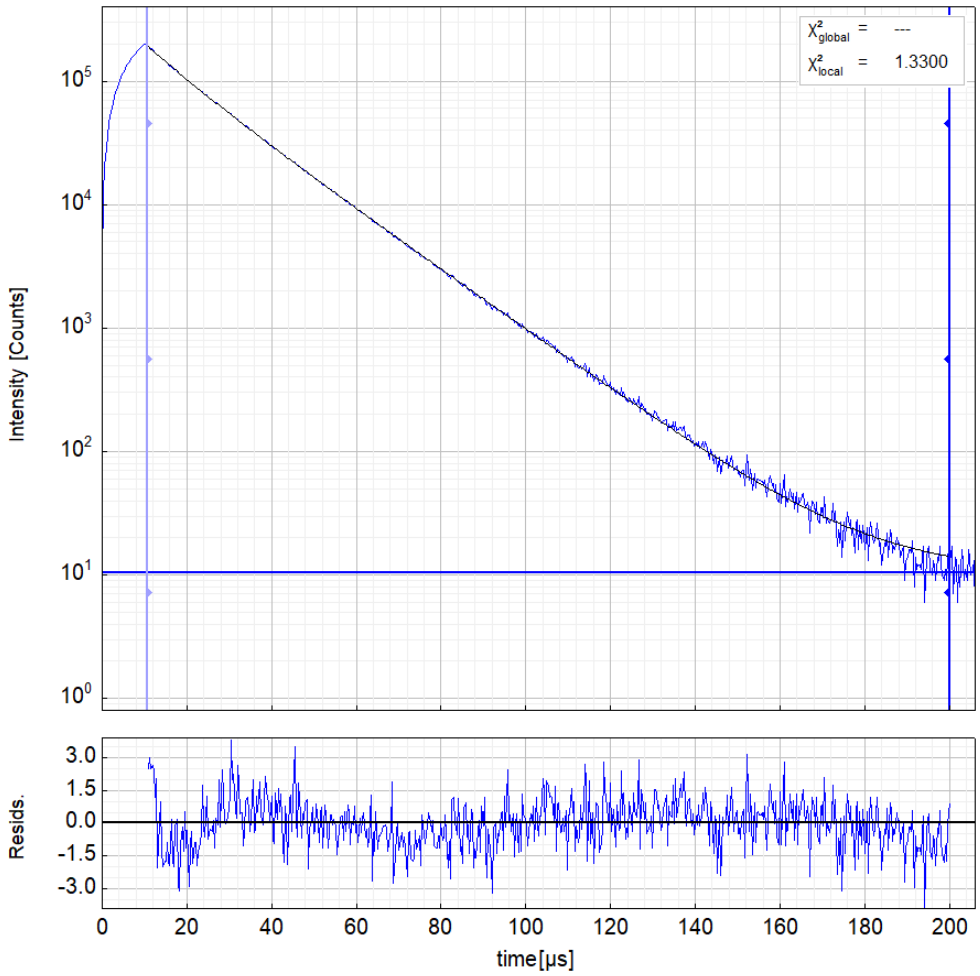


Figure S60. Decay curve and fitted parameters of lifetimes of complex **9** at room temperature.

COMPLEX 9 PRISTINE 77 K

Excitation: V pol 372±2nm with LDH-P-C-375

Detection: U pol 423±5nm 200000 peak counts grating 1200/500+ detector UV-red [PMT]



Parameter	Value	Δ	δ
A_1[kCnts/Chnl]	139.8	±4.1	2.9%
τ_1[ns]	17 930	±120	0.6%
I_1[kCnts]	7 830	±180	2.3%
A_2[kCnts/Chnl]	49.9	±3.2	6.4%
τ_2[ns]	9 400	±400	4.2%
I_2[kCnts]	1 470	±180	12%
$Bkgr_{Dec}$[kCnts]	0.0105	±0.0009	8.1%
τ_{AvInt}[ns]	16 581	±15	0.1%

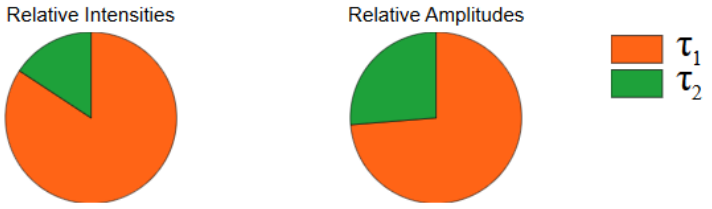
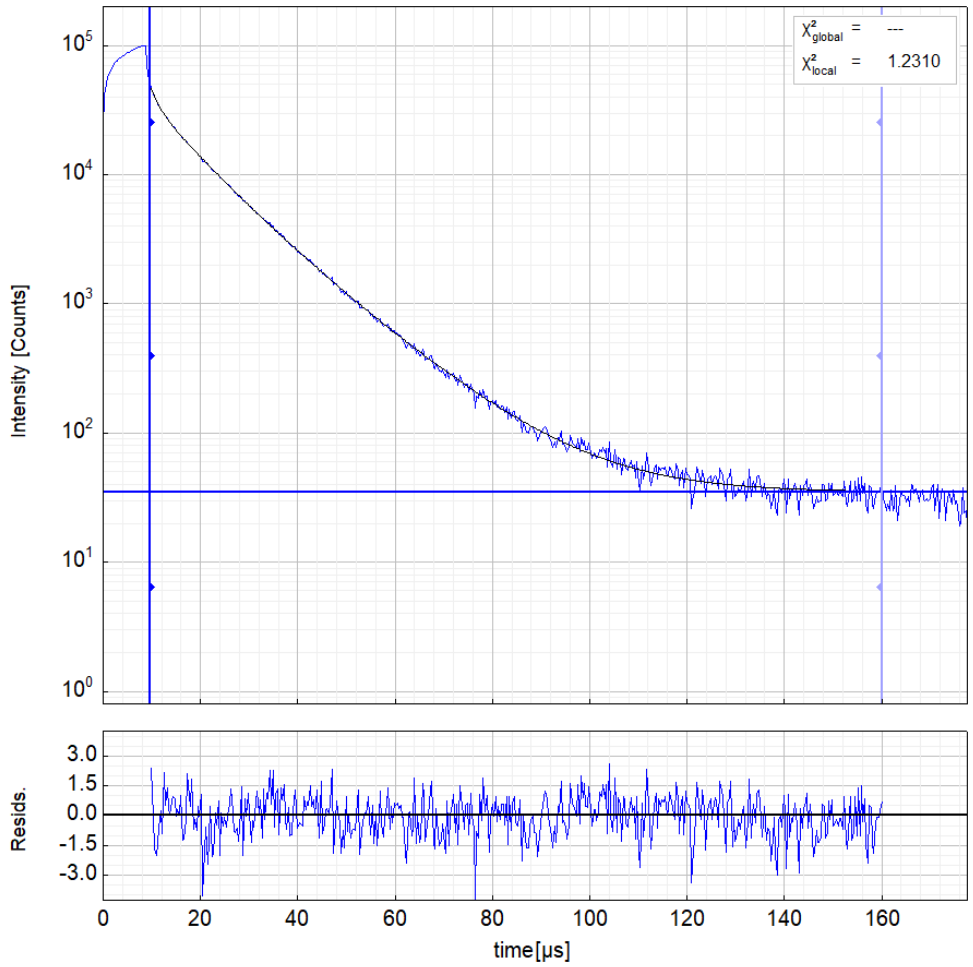


Figure S61. Decay curve and fitted parameters of lifetimes of complex **9** at 77 K.

COMPLEX 9 GROUND ROOM TEMPERATURE

Excitation: V pol 372±2nm with LDH-P-C-375

Detection: U pol 520±14nm 100000 peak counts, grating 1200/500+, detector UV-red [PMT]



Parameter	Value	Δ	δ
A_1[kCnts/Chnl]	20.5	±2.2	11%
τ_1[ns]	8 570	±590	6.8%
I_1[kCnts]	547	±94	17%
A_2[kCnts/Chnl]	11.09	±0.43	3.9%
τ_2[ns]	1 540	±120	7.8%
I_2[kCnts]	53.1	±6.3	12%
A_3[kCnts/Chnl]	14.6	±2.7	18%
τ_3[ns]	14 850	±600	4.0%
I_3[kCnts]	680	±110	15%
$Bkgr_{Dec}$[kCnts]	0.0349	±0.0012	3.3%
τ_{AvInt}[ns]	11 599	±44	0.4%

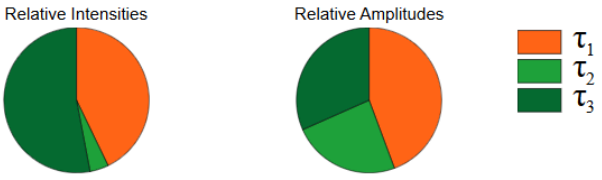
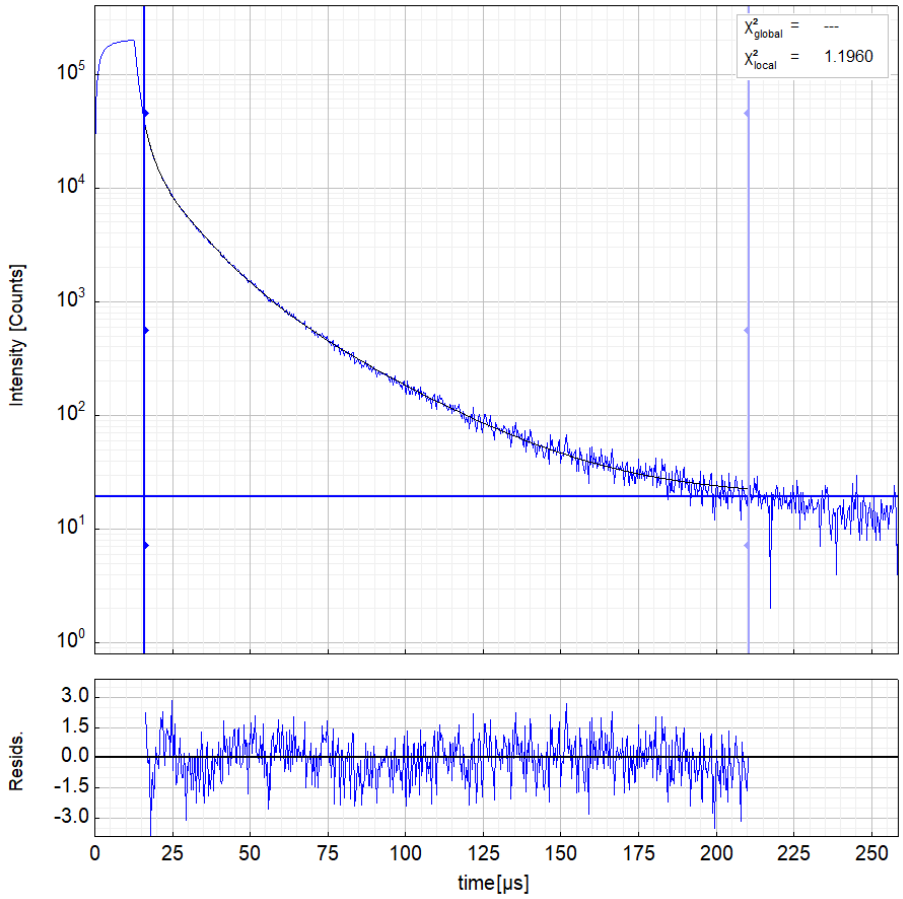


Figure S62. Decay curve and fitted parameters of lifetimes of complex $\mathbf{9_{ground}}$ at room temperature.

COMPLEX 9 GROUND 77 K

Excitation: V pol 372±2nm with LDH-P-C-375

Detection: U pol 508±5nm 200000 peak counts, grating 1200/500+, detector UV-red [PMT]



Parameter	Value	Δ	δ
A_1[kCnts/Chnl]	17.29	±0.30	1.7%
τ_1[ns]	2 217	±77	3.5%
I_1[kCnts]	119.8	±6.2	5.1%
A_2[kCnts/Chnl]	13.47	±0.20	1.5%
τ_2[ns]	10 330	±350	3.3%
I_2[kCnts]	435	±12	2.7%
A_3[kCnts/Chnl]	3.13	±0.29	9.3%
τ_3[ns]	28 180	±810	2.9%
I_3[kCnts]	275	±17	6.0%
$Bkgr_{Decl}$[kCnts]	0.0195	±0.0011	5.2%
τ_{AvInt}[ns]	15 071	±78	0.5%

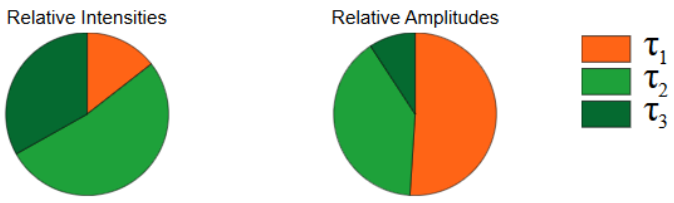
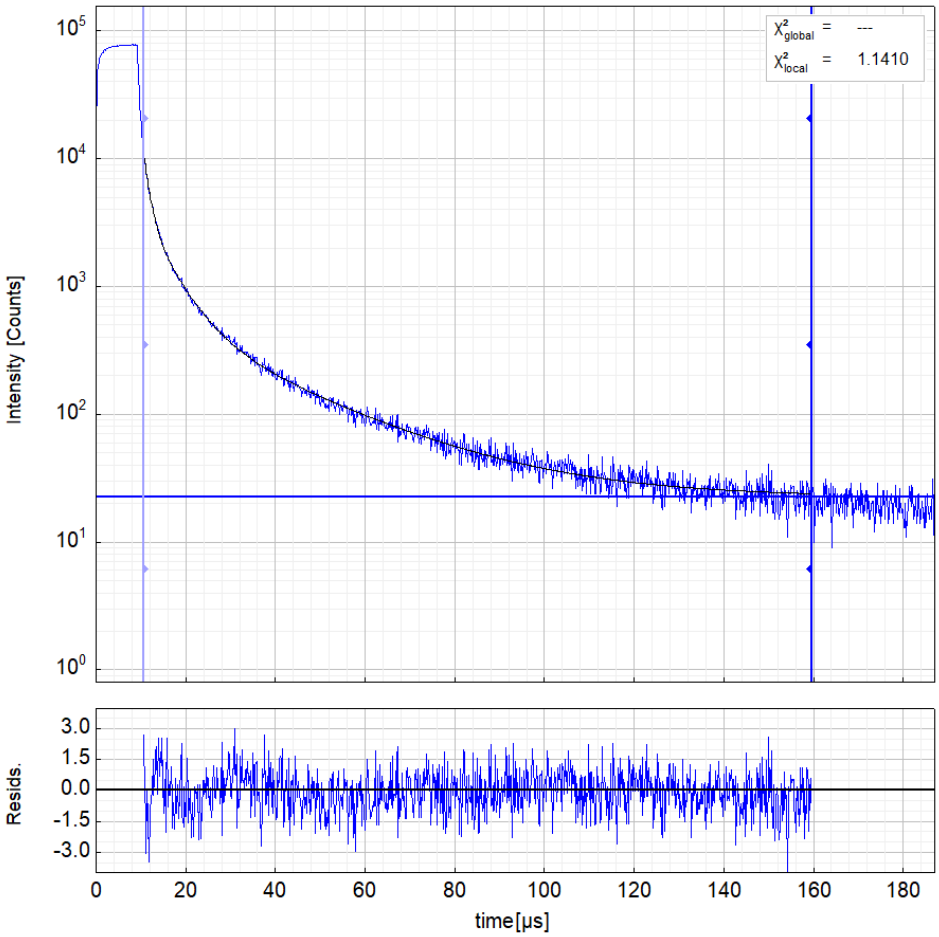


Figure S63. Decay curve and fitted parameters of lifetimes of complex $\mathbf{9}_{ground}$ at 77 K.

COMPLEX 9 FILM ROOM TEMPERATURE

Excitation: V pol 372±2nm with LDH-P-C-375

Detection: U pol 525±14nm 100000 peak counts, grating 1200/500+, detector UV-red [PMT]



Parameter	Value	Δ	δ
A_1[kCnts/Chnl]	0.552	±0.018	3.1%
τ_1[ns]	24 820	±560	2.2%
I_1[kCnts]	85.6	±1.7	2.0%
A_2[kCnts/Chnl]	8.06	±0.19	2.4%
τ_2[ns]	1 194	±35	2.9%
I_2[kCnts]	60.2	±2.1	3.4%
A_3[kCnts/Chnl]	3.07	±0.14	4.3%
τ_3[ns]	5 500	±160	2.8%
I_3[kCnts]	105.3	±1.1	1.0%
$Bkgr_{Dec}$[kCnts]	0.0226	±0.0007	2.7%
τ_{AvInt}[ns]	11 060	±180	1.6%

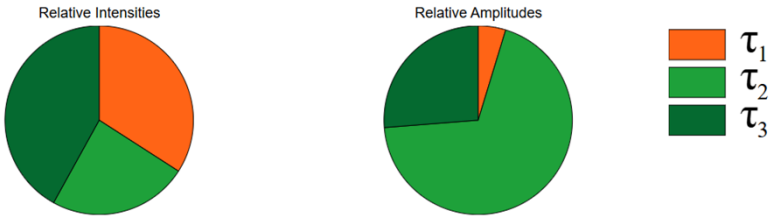


Figure S64. Decay curve and fitted parameters of lifetimes of complex $\mathbf{9_{film}}$ (PMMA, 5% w/w) at room temperature.

6. CRYSTAL DATA AND STRUCTURE REFINEMENT

Table S5. Crystal data and structure refinement for complex **6**.

Empirical Formula	$C_{166}H_{124}Au_8N_8Cl_{12}P_8$
M_t [g·mol^{-1}]	4479.62

Crystal system	Monoclinic
Space group	C2/c
a [Å]	13.869(6)
b [Å]	23.310(5)
c [Å]	22.682(4)
α [°]	90.00(2)
β [°]	103.47(4)
γ [°]	90.00(2)
V [$Å^3$]	7131(4)
Z	2
Density [$g \cdot cm^{-3}$]	2.086
T [K]	100(2)
μ [mm^{-1}]	8.570
F(000)	4264.0
2θ range [°]	3.488 to 50.996
no. of collected reflections	28152
no. of unique reflections	6652
R_{int}	0.0336
R_1, wR_2 [$I > 2\sigma(I)$][a]	$R_1 = 0.0306$, $wR_2 = 0.0788$
R_1, wR_2 (all data)[a]	$R_1 = 0.0383$, $wR_2 = 0.0826$
GOF (F^2)[b]	1.032

[a] $R_1 = \Sigma(|F_o| - |F_c|) / \Sigma |F_o|$. $wR_2 = [\Sigma w (F_o^2 - F_c^2)^2 / \Sigma w(F_o^2)^2]^{1/2}$

[b] Goodness-of-fit = $[\Sigma w (F_o^2 - F_c^2)^2 / (n_{obs} - n_{param})]^{1/2}$

Table S6. Crystal data and structure refinement for complex **7**.

Empirical Formula	$C_{40} H_{28} Au_2 N_2 P_2$
M_t [$g \cdot mol^{-1}$]	992.52

Crystal system	Triclinic
Space group	P-1
a [Å]	11.2933(6)
b [Å]	13.0846(7)
c [Å]	13.7251(7)
α [°]	61.589(2)
β [°]	71.999(2)
γ [°]	75.332(2)
V [Å^3]	1682.82(16)
Z	2
Density [g·cm^{-3}]	1.959
T [K]	100(2)
μ [mm^{-1}]	8.835
F(000)	940.0
2θ range [°]	4.396 to 56.594
no. of collected reflections	83996
no. of unique reflections	8284
R_{int}	0.0565
R_1, wR_2 [I > 2σ(I)][a]	R_1 = 0.0222, wR_2 = 0.0502
R_1, wR_2 (all data)[a]	R_1 = 0.0228, wR_2 = 0.0505
GOF (F^2)[b]	1.146

[a] $R_1 = \Sigma(|F_o| - |F_c|) / \Sigma |F_o|$. $wR_2 = [\Sigma w (F_o^2 - F_c^2)^2 / \Sigma w(F_o^2)^2]^{1/2}$

[b] Goodness-of-fit = $[\Sigma w (F_o^2 - F_c^2)^2 / (n_{obs} - n_{param})]^{1/2}$

Table S7. Crystal data and structure refinement for complex **8**.

Empirical Formula	$C_{80}H_{56}Au_4N_4P_4$
M_t [g·mol^{-1}]	1985.03

Crystal system	Monoclinic
Space group	$P2_1/c$
a [Å]	11.3636(4)
b [Å]	16.2629(6)
c [Å]	24.9957(6)
α [°]	90
β [°]	90.8470(10)
γ [°]	90
V [Å^3]	3403.1(2)
Z	2
Density [g·cm^{-3}]	1.937
T [K]	100(2)
μ [mm^{-1}]	8.738
F(000)	1880.0
2θ range [°]	4.374 to 56.632
no. of collected reflections	141471
no. of unique reflections	8447
R_{int}	0.0356
R_1, wR_2 [I > 2σ(I)][a]	R_1 = 0.0326, wR_2 = 0.0746
R_1, wR_2 (all data)[a]	R_1 = 0.0339, wR_2 = 0.0752
GOF (F^2)[b]	1.161

[a] $R_1 = \Sigma(|F_o| - |F_c|) / \Sigma |F_o|$. $wR_2 = [\Sigma w (F_o^2 - F_c^2)^2 / \Sigma w(F_o^2)^2]^{1/2}$

[b] Goodness-of-fit = $[\Sigma w (F_o^2 - F_c^2)^2 / (n_{obs} - n_{param})]^{1/2}$

Table S8. Crystal data and structure refinement for complex **9**.

Empirical Formula	$C_{42.5} H_{30} P_2 Cl Au_2$
M_t [g·mol^{-1}]	1031.99

Crystal system	Monoclinic
Space group	C2/c
a [Å]	13.974(3)
b [Å]	22.779(5)
c [Å]	23.033(5)
α [°]	90
β [°]	104.97(3)
γ [°]	90
V [Å^3]	7083(3)
Z	8
Density [g·cm^{-3}]	1.936
T [K]	100(2)
μ [mm^{-1}]	8.472
F(000)	3920.0
2θ range [°]	3.576 to 50.992
no. of collected reflections	27318
no. of unique reflections	6585
R_{int}	0.0411
R_1, wR_2 [I > 2σ(I)][a]	R_1 = 0.0388, wR_2 = 0.1041
R_1, wR_2 (all data)[a]	R_1 = 0.0520, wR_2 = 0.1093
GOF (F^2)[b]	1.108

[a] $R_1 = \Sigma(|F_o| - |F_c|) / \Sigma |F_o|$. $wR_2 = [\Sigma w (F_o^2 - F_c^2)^2 / \Sigma w(F_o^2)^2]^{1/2}$

[b] Goodness-of-fit = $[\Sigma w (F_o^2 - F_c^2)^2 / (n_{obs} - n_{param})]^{1/2}$

Table S9. Selected bond distances and angles for complexes **6**–**9**.

		Bond distances (Å)			Angles (°)
Complex	**Au–Au**	**Au–C**	**Au–P**	**C≡C**	**P–Au–C**
6	3.011(2)	2.023(6) 2.032(7)	2.282(2) 2.290(2)	1.204(9) 1.196(9)	175.8(2)
7	3.0735(3)	2.001(3) 1.998(2)	2.2715(6) 2.2664(8)	1.202(4) 1.206(5)	178.58(8)
8	2.9963(4)	2.101(6) 2066(3)	2.259(1) 2.270(1)	1.084(9) 1.201(8)	175.2(1)
9	3.006(1)	2.097(7) 2.100(5)	2.251(2) 2.252(2)	1.05(1) 1.20(1)	173.8(1)

7. THEORETICAL METHODS

All calculations were performed using the ORCA 6.0 software package[7] (ORCA-ESD module). All singlet and triplet structures of dimers were optimized using the B3LYP functional[8-10] and the def2-TZVP basis set[11] combined with the D4 dispersion correction.[12] In one case (dimer of compound **6**), full optimization using the Zero Order Regular Approximation (ZORA) in both the functional and basis set was performed (ZORA-B3LYP-D4/ZORA-def2-TZVP level of theory) providing comparable results.[13-16] For the computation of two-electron integrals, the resolution of identity approximation was used for the Coulomb part (RIJCOSX)[17] with the corresponding auxiliary basis. For the excited states, TDDFT with the Tamm-Dancoff approximation was employed.[18] It has been demonstrated that this approximation to TDDFT reduces the computational cost for the B3LYP functional and yields excited state transition energies, which are typically of the same quality as those which are obtained from TDDFT itself.[19] We searched for the first 10 roots and used the one that represents the first excited state. This is reasonable since, in all cases, the lowest lying transition corresponds to $S_0 \rightarrow S_1$ transitions. The convergence criteria for both the SCF and geometry optimizations were set to TIGHT. The other parameters were chosen as default. The theoretical prediction of absorption and emission spectra from first principles was made using the path integral approach.[20] Both singlet and triplet optimizations were performed without symmetry constrains. For computational efficiency, the hypochromic shifts were computed at the RI-BP86-D4/def2-TZVP level of theory using the Turbomole 7.7 program.[21]

Cartesian coordinates

6mon

Au	6.38784351691550	8.40696201353983	2.21288639157470
P	5.36041760498325	10.20394963761370	3.16687135803217
C	8.37912042646147	4.74720934694623	0.19544313313741
C	9.45278188428730	4.94283102641602	-0.70075713787560
H	9.79532610174442	5.95582139589753	-0.91045287089772
C	10.04870858510334	3.83583889427814	-1.29423010139966
H	10.88004239027625	3.96381462132662	-1.98937777125762
C	9.56531252439014	2.56272495316609	-0.98440318151894
H	10.00208601885793	1.66526991069987	-1.42438352642348
C	8.49738085693329	2.46469073333961	-0.08779507938195
H	8.09168492763658	1.48346077617134	0.17823451894667
N	7.90525697022693	3.51158770283506	0.49685070477052
C	7.75863941614679	5.86884245156217	0.81681534780701
C	7.25447766788727	6.85902862773220	1.34084095712339
C	3.54931665515173	10.26969513967838	2.97270988677412
C	2.86739913226443	9.10107465165781	2.61177660740558
H	3.42870653256189	8.18377765778786	2.42449119907964
C	1.47675723567571	9.12138605222277	2.49164759293786
H	0.94590750203875	8.21102447765194	2.21133892409679
C	0.77221523007290	10.30402110617296	2.72557445855569
H	-0.31408850101601	10.31846207227695	2.62835081838823
C	1.45551040433790	11.47209223977842	3.08039502509178
H	0.90429912859507	12.39633760624987	3.25892341102369
C	2.84328975941443	11.45808165703024	3.20600303656304
H	3.37809054643205	12.37026076828145	3.47469448385715
C	5.95012246096388	11.82918686146600	2.59525035436954
C	5.97195168834249	12.04536098226946	1.20915081349977
H	5.66938938771481	11.24768057732158	0.52791771427841
C	6.38809997574320	13.27599041711320	0.70517710160813
H	6.40467523033973	13.44037097604933	-0.37282177907848
C	6.79538742947449	14.28994491457469	1.57814088626551
H	7.12759738103133	15.24967439569646	1.18062068967301
C	6.78692767684809	14.07012503752793	2.95675674494110
H	7.11389312421584	14.85552027045443	3.63960331812149

C	6.36337826270039	12.84150284059801	3.46830305430814
H	6.36568049966711	12.66334215304667	4.54418691614622
C	5.55385114533855	10.28538083808050	4.90615848649211
P	5.86668728322599	10.20410999226596	7.86229399430987
C	7.67781774835956	10.26982528732275	8.05621314736151
C	8.35984307870800	9.10088853049787	8.41593275803550
H	7.79859780438242	8.18341808750602	8.60254469027754
C	9.75051232643442	9.12110554458848	8.53573398634758
H	10.28144008591396	8.21049506984827	8.81508264723609
C	10.45497966176498	10.30396725394564	8.30272781705461
H	11.54130916371204	10.31833808553246	8.39970396944181
C	9.77158261104675	11.47235381625214	7.94915436021466
H	10.32273517860050	12.39677533334062	7.77136459634995
C	8.38377069969749	11.45843633794700	7.82384146438188
H	7.84889950807900	12.37085452575917	7.55610779731939
C	5.27705245002434	11.82936858897323	8.43388577016033
C	5.25530311978854	12.04557652240670	9.81998082013565
H	5.55789256365693	11.24790129191100	10.50120781414844
C	4.83921472660382	13.27622720498578	10.32394903119168
H	4.82270520114226	13.44063490960910	11.40194406799974
C	4.43189987850665	14.29016646675345	9.45098197615392
H	4.09973174487570	15.24991555085268	9.84849393219757
C	4.44028094324823	14.07031812135444	8.07236901236683
H	4.11329755294296	14.85570528335933	7.38952144425665
C	4.86378006139652	12.84167515455425	7.56082701105963
H	4.86143693460187	12.66349435731913	6.48494609906226
C	5.67309742990653	10.28543484687459	6.12301179134426
Au	4.83933993876520	8.40718817815114	8.81648246075616
C	2.84829097073531	4.74741872186470	10.83397205209519
C	1.77458486035487	4.94291241822665	11.73013339549375
H	1.43193990662071	5.95587859004838	11.93988249891947
C	1.17872408829584	3.83581200350011	12.32351075419662
H	0.34730392582416	3.96371893779733	13.01865607270292
C	1.66217991084723	2.56274068394108	12.01368563081291
H	1.22550266378405	1.66530458624535	12.45354218532769
C	2.73019203357515	2.46490830948952	11.11711116198391
H	3.13601950726550	1.48366758325331	10.85104198300503
N	3.32227143187296	3.51186219918589	10.53253416130093
C	3.46866578072010	5.86907877849623	10.21267835926736
C	3.97278339150086	6.85929636304719	9.68864142115294

6

Au	5.93143300391168	8.34266552014863	2.56737860966066
Au	8.58753149312195	8.35509901436915	4.35604740130539
P	5.25719356403967	10.45241658442146	3.19484720461328
P	7.95706945627976	6.44708804165414	5.49659305082998
C	6.59209390589000	3.81356978984406	2.08136740443136
C	7.53773470211774	3.13526699294430	1.29946115730000
H	8.25238584720868	3.70550661433678	0.72316917939673
C	7.53417428130834	1.75320002927658	1.28372812007184
H	8.25662791826430	1.21190510060044	0.68547239245021
C	6.59480248744608	1.07216548429082	2.04828615281570
H	6.55329775342825	-0.00880373859510	2.06332403396158
C	5.69828610860570	1.82213299075395	2.79838124383429
H	4.94891930467281	1.32666611319304	3.40890604677672
N	5.68436570142227	3.15010599653638	2.82765629088361
C	6.54202597162456	5.23239987244826	2.10762599191589
C	6.39882660433217	6.43880416942110	2.15940799085565
C	3.48264717385835	10.79708757000297	3.00784887007396
C	2.96876359592483	10.85234743398197	1.71146255501547
H	3.61762833585581	10.69011925696107	0.85949076182676
C	1.62339448248987	11.11785964151861	1.51342014244608
H	1.22874014709878	11.16570388200023	0.50635707950605
C	0.78000832106578	11.30821267258351	2.60548184699467
H	-0.27276202131052	11.50590615282930	2.44717168633254
C	1.28893068319553	11.23958200019738	3.89507206188858
H	0.64498364184441	11.37031064739443	4.75499052848048
C	2.64200310887462	10.99309232335689	4.09731481790422
H	3.02067964455107	10.93963034404461	5.10644102743472
C	6.05344088666856	11.86770129109613	2.39418515247358
C	6.90942330141729	11.64822513647038	1.31992773729972
H	7.16406563001684	10.63724776809598	1.03239255477636
C	7.45626424783543	12.72920790885514	0.63957301795141
H	8.13923126489731	12.55441777983554	-0.18024260667329
C	7.15320458011477	14.02381140316242	1.03553109530638
H	7.59044911102606	14.86457494871212	0.51320165082989

C	6.30749200702464	14.24427210775559	2.11873619279911
H	6.08255819924213	15.25490547215346	2.43486074462628
C	5.75466010799699	13.17001901955309	2.79647667857473
H	5.08701950146663	13.34083944408606	3.63181470464259
C	5.52075089285912	10.65868367199166	4.91509517903472
C	9.78644334378812	12.61795045959481	3.03286690295372
C	9.35095606902982	13.61870485911190	3.91651154927984
H	8.79475052056837	13.34094956736308	4.80056838015024
C	9.63591519614965	14.94052541247365	3.63154431270497
H	9.30560509279983	15.72773303614531	4.29822943678062
C	10.34781363138744	15.24038416131099	2.47658120660139
H	10.59614154927812	16.26008946815613	2.21324415410130
C	10.74452435971875	14.18567190710891	1.66271487909629
H	11.30645924523803	14.38069607327604	0.75396086554680
N	10.47883669724954	12.90886358332561	1.91640425202217
C	9.48200703247751	11.25813084993574	3.31454710353185
C	9.17017967513949	10.12370723622331	3.62395793005528
C	8.42973908007501	6.51660923084746	7.24826917811975
C	9.31143808451050	7.51061281002664	7.67148203447169
H	9.68232770514085	8.24155090047782	6.96599821582850
C	9.70856411140574	7.56427195046891	9.00065017066188
H	10.39240626069416	8.33705955351388	9.32256741076705
C	9.21841844009173	6.63462489130196	9.90888760717277
H	9.51992115851158	6.68303729355047	10.94809760767892
C	8.33654526181096	5.64597246197290	9.48722574645169
H	7.93603727485628	4.93114070504093	10.19406342440618
C	7.94463085261757	5.57962598066258	8.15990651475577
H	7.24335058928081	4.81492255214748	7.85883708382559
C	8.55159556525456	4.84352624504680	4.89908356881332
C	7.93273817982963	3.65370345275611	5.28137224975114
H	7.03509245454897	3.67001927518989	5.88545972163469
C	8.47033808312703	2.44079118896134	4.87817123284930
H	7.98552096674736	1.51740914251339	5.16683752290024
C	9.61588581642801	2.40860579229101	4.09202165916036
H	10.02607336961578	1.45862526651331	3.77359398233298
C	10.22416330611628	3.59412656514062	3.69918446768416
H	11.10796196509670	3.57301032983218	3.07443102123480
C	9.69193999013238	4.81196659747062	4.10011866948668
H	10.15496391021446	5.73918060341116	3.78687361976487
C	6.22037306072564	6.28089190073307	5.52080218720789
P	5.95870280438545	10.45333895411073	7.83138807255377
C	7.73279649299185	10.80025685027011	8.01826514491181
C	8.24751104367671	10.85237107923519	9.31445046726690
H	7.59972577541718	10.68533242454722	10.16631685071457
C	9.59227688200440	11.12083381703629	9.51235506605979
H	9.98757524885792	11.16632172274149	10.51927125257476
C	10.43438532581519	11.31693612061176	8.42031858715378
H	11.48674766850503	11.51688769836800	8.57855479500456
C	9.92480068557623	11.25096251622123	7.13087662535663
H	10.56783912061839	11.38570892549351	6.27089946239538
C	8.57218399884310	11.00180604335334	6.92884326450424
H	8.19278467632350	10.95051927962879	5.91989094295589
C	5.16057967693494	11.86814521471726	8.63095951820398
C	4.30365374563172	11.64828704813121	9.70440962162209
H	4.04960489740671	10.63719227994848	9.99205398645163
C	3.75535272828144	12.72902632039805	10.38396296174051
H	3.07180231956965	12.55385582391377	11.20321360957044
C	4.05772089988345	14.02377826025856	9.98796912527913
H	3.61936133135807	14.86433734837648	10.50967550954658
C	4.90426608221776	14.24460674805409	8.90546304199898
H	5.12877602577601	15.25533614690257	8.58932917591823
C	5.45859300341255	13.17061170120544	8.22856574526369
H	6.12693098116859	13.34173550724763	7.39384125437969
C	5.69470691170155	10.65868249135752	6.11111261547226
P	3.27636215463769	6.43400180140218	5.53071317931937
C	2.80449745067343	6.50069169752788	3.77857594310558
C	1.92917636568617	7.49902490224177	3.35237073358877
H	1.56171001587602	8.23329528320718	4.05611092000382
C	1.53375719526033	7.55266891451690	2.02268369535665
H	0.85508861172175	8.32912103812589	1.69868892809506
C	2.01897668478348	6.61820805146078	1.11681978823746
H	1.71884035145178	6.66638668646290	0.07720723435527
C	2.89414984202745	5.62485661400604	1.54146295715056
H	3.29078480020778	4.90611738078844	0.83638747020293
C	3.28457433236218	5.55887371919011	2.86920784546799
H	3.98125474425011	4.79077941508609	3.17235637864776
C	2.69052924104611	4.82764698505127	6.12901353211675

C	3.31823265079430	3.64119917475656	5.75062472197255
H	4.21705045058773	3.66234717265920	5.14840020060037
C	2.78756568459233	2.42555933632302	6.15480905432482
H	3.27897008403805	1.50478692855252	5.86891941382816
C	1.64034874115395	2.38736259903600	6.93823827869708
H	1.23576283000960	1.43534151883481	7.25771848959167
C	1.02337267804901	3.56962838475615	7.32733541618682
H	0.13827587478527	3.54384479476937	7.95007183272797
C	1.54847043033631	4.79017106583493	6.92529003172738
H	1.07856928628511	5.71490647120525	7.23561213406361
C	5.01408113194298	6.27737996339815	5.50844213066706
Au	5.28816285835597	8.34315104925245	8.46089496580923
Au	2.63641150643032	8.34005887426356	6.66962976051058
C	4.64518314416275	3.81296716652701	8.95829178335757
C	3.70092636077162	3.13181100896275	9.73936555573128
H	2.98154336898447	3.69983453758927	10.31194819130290
C	3.71193269362026	1.74983010646369	9.75905950510579
H	2.99066003218335	1.20627440155329	10.35669050627249
C	4.65726267402755	1.07180474776362	8.99918034966330
H	4.70463901263168	-0.00896378300581	8.98728135208662
C	5.55201942528913	1.82452559589679	8.24971006761189
H	6.30567662131193	1.33130115871369	7.64267681819464
N	5.55886214846156	3.15245052114783	8.21669004445690
C	4.68770548574430	5.23196322431818	8.92777096019351
C	4.82550086308458	6.43882525247110	8.87225283007131
C	1.42573389661638	12.59960567377767	7.99305219800847
C	1.86059904984842	13.60189478840128	7.11087005041985
H	2.41909216724404	13.32597225714102	6.22769246204063
C	1.57208742047303	14.92287554611723	7.39613280957062
H	1.90192108413459	15.71124211847695	6.73058505178270
C	0.85723994456872	15.22039111703517	8.54986233163628
H	0.60608782958855	16.23936177582060	8.81336473018977
C	0.46144625461987	14.16427241984342	9.36235239413935
H	-0.10264806888506	14.35744838757727	10.27016644805140
N	0.73060158620528	12.88824066210200	9.10842238400182
C	1.73352771357752	11.24061316799134	7.71095935953074
C	2.04737223935234	10.10688667540506	7.40097394566706

9mon

Au	4.56892239064211	7.34512038596461	2.15688081118224
P	4.33123797397826	9.21573248762413	3.46885474297635
C	5.12102991459388	3.57326648473873	-0.47318491847479
C	5.72112468660159	3.65937875986335	-1.73882141259751
H	6.05269933795887	4.62555824795174	-2.09543147195538
C	5.88643267480825	2.52619440313880	-2.52068820126030
H	6.35133969183411	2.61129537640511	-3.49520757852032
C	5.45876307442326	1.28515595564581	-2.05989141207663
H	5.58898373892381	0.40198339903509	-2.67248604631221
C	4.86234355079975	1.18653193211169	-0.80686195812142
H	4.52652206608060	0.22399535144603	-0.44102192971667
C	4.94925136486498	4.73261344105178	0.33238308236191
C	4.80013306634675	5.72160517009243	1.02582530740755
C	2.66464565777811	9.55532387919475	4.10220646689290
C	1.57716696316231	8.91892561905322	3.50731675498112
H	1.74094108191158	8.20702543508543	2.70823174053173
C	0.28811574855465	9.19137068348248	3.94970976174566
H	-0.55451607154142	8.69369214444623	3.48751118888516
C	0.08605845081223	10.09032365350507	4.98868438788510
H	-0.91764127782303	10.29607872808577	5.33833947372290
C	1.17226218685108	10.72193113149742	5.58849074951443
H	1.01543697507397	11.41512048303542	6.40478805066066
C	2.45906522650959	10.45929377327899	5.14563765663297
H	3.30101514692717	10.94731545729489	5.61931462278310
C	4.89867616253276	10.76940579714422	2.70637778279952
C	4.56941905451962	10.98561313530342	1.36737447444054
H	4.02961540567361	10.22760972765175	0.81320584604810
C	4.94543503344418	12.16540803539215	0.74125725557234
H	4.68725457335628	12.32760418828543	-0.29727017131983
C	5.66458464861288	13.12747851951151	1.44239352726291
H	5.96555448639224	14.04315927100041	0.94942408466142
C	6.00476823716568	12.90869198809601	2.77184400597605
H	6.57462450815985	13.64753306897316	3.32012141172176
C	5.62023807665810	11.73507253137661	3.40647826832380
H	5.89815947496319	11.57094255901358	4.43742311416179
C	5.32056771572945	9.14166724991598	4.91093018947446
P	7.30398827798508	9.43182651281866	7.07922425177468

C	8.45811612199124	8.04759180528640	6.89284052229234
C	9.41634179865207	7.87035126927183	7.89255636664708
H	9.42510481939157	8.52307611261231	8.75695621878772
C	10.34858683878473	6.84915118800510	7.78478222470418
H	11.08920850994299	6.71388790401697	8.56228503504576
C	10.31975620916650	5.99277063918007	6.68877618718334
H	11.04187058299418	5.19002006147108	6.61130789577843
C	9.35799858272488	6.15874177890725	5.69980612118070
H	9.32583759587444	5.48716989155024	4.85165751863687
C	8.42788896698414	7.18609317526956	5.79727840856284
H	7.67642360679071	7.30580866877333	5.02836129746534
C	8.13159754139298	10.88884092433010	6.36113122575202
C	8.90382749935474	10.77722557550057	5.20437101550448
H	9.07744689833663	9.80756539183963	4.75649157465281
C	9.44695544490340	11.91244184105865	4.62278622468251
H	10.04368936759750	11.82299457543869	3.72427740421623
C	9.22195135762698	13.16309685429106	5.19085596040723
H	9.64855432975275	14.04768448550781	4.73502990317322
C	8.45691688928102	13.27658828038878	6.34469196053182
H	8.28735552013056	14.24675337279519	6.79369887963302
C	7.91244260795006	12.14068503356730	6.93278016759429
H	7.31941886345927	12.22367365220241	7.83492377771264
C	6.10643703010333	9.15479779982967	5.82891124434056
Au	6.39862970969596	9.75130751531758	9.16373497134717
C	4.59836861017318	10.47401695015082	13.36914472493080
C	4.98470910324505	11.58600989494165	14.13300678426796
H	5.71355738767449	12.27336121937741	13.72431997951344
C	4.44310034782493	11.80138786483913	15.39117052048979
H	4.75344611192689	12.66467667629521	15.96695983565228
C	3.50673083990805	10.91575397272615	15.91481778187419
H	3.08574431684010	11.08606164726324	16.89767168820653
C	3.11555824721213	9.80945088535629	15.16743315529297
H	2.38753315585811	9.11494926174390	15.56832369262310
C	5.15135825159138	10.24932027079679	12.07832815887146
C	5.62186087045790	10.05086569264376	10.97356636377039
C	4.69382876930644	2.31562156645646	-0.01989089614076
H	4.22989123180488	2.24126759022078	0.95473633430066
C	3.65317257076131	9.58798387018752	13.90864606169025
H	3.35055392847572	8.72796582240239	13.32606688392091

9

Au	6.21143985213874	8.28848074571170	2.34458886975298
Au	8.63987449387920	8.52260420555998	4.38743072045742
P	5.30823573579646	10.22968844789912	3.18332880995776
P	7.96335938838938	6.59734474216125	5.44934899772020
C	7.40525564444131	3.97974828096990	1.16950193190335
C	8.46058361889821	3.62720337768552	0.31492395269487
H	9.03896556199920	4.41364089710339	-0.15159540187040
C	8.76294654566954	2.29550853400675	0.07750986319716
H	9.58167525243190	2.04159739248812	-0.58456307138805
C	8.02090902537569	1.28694035714004	0.68434352047134
H	8.25880538450060	0.24736159908957	0.49743820810055
C	6.96697454384240	1.62363961817682	1.52719303922034
H	6.38388201529163	0.84448255087492	2.00268234255133
C	7.10563149268527	5.33957241317417	1.44594419397265
C	6.82455913455930	6.49461807149383	1.70576408478339
C	3.50762207886985	10.34627232210415	2.98710960014568
C	2.96610435779213	9.98763553582614	1.75253386788642
H	3.60423440903128	9.58376812471225	0.97650154972680
C	1.60690718649757	10.13733296582996	1.52598532688194
H	1.19021067670909	9.86098844665897	0.56611497809093
C	0.77933146930908	10.61535902729651	2.53686790315262
H	-0.28451726238233	10.71671756055353	2.36160220518542
C	1.31337235771812	10.94697221553111	3.77524411364276
H	0.67781913599881	11.29035036879226	4.58077480723510
C	2.67860041778020	10.82551797207169	3.99767477509281
H	3.07919374641575	11.08163088966156	4.96679946225633
C	5.93977033585600	11.81014601071553	2.56208419113586
C	6.69926429622414	11.82061206780088	1.39656057871602
H	6.97601427776975	10.88559754423879	0.92738103165732
C	7.11747096295577	13.02916569524037	0.85431287773404
H	7.71737376187636	13.03506275719191	-0.04561451124376
C	6.78782054430710	14.22331954087749	1.47919631805840
H	7.13225141057503	15.16201717571484	1.06638670501596
C	6.04163206474250	14.21246426025741	2.65319812627850
H	5.79833187489217	15.14317969572205	3.14954205386615

C	5.61380715141418	13.01033414333791	3.19372095511116
H	5.02860709633972	13.00510394176588	4.10469831425588
C	5.52966109092112	10.32542624495172	4.91634523524764
C	9.74122818310521	12.80595305581291	3.04007889151627
C	9.35823418472987	13.84290694313751	3.90354643291908
H	8.87197771310459	13.59420031654766	4.83736936047184
C	9.58404085268755	15.16691377959849	3.56274893998618
H	9.27723120178390	15.95463149893613	4.23996219794011
C	10.19851255191402	15.48746383459865	2.35657928886320
H	10.37450544580490	16.52254729397861	2.09227687675943
C	10.59328987090520	14.46793385031171	1.49597504901340
H	11.07890290223767	14.70873617366242	0.55824517066964
C	9.47446426184421	11.45353967418696	3.37904824519999
C	9.21029831702999	10.30528335583243	3.68280072277115
C	8.43790303025666	6.54720434477499	7.20037664388775
C	9.70940661524943	7.00748820320241	7.54329877240443
H	10.34822945412342	7.44789195803631	6.78812875969645
C	10.14731642944317	6.91181710416561	8.85496163082176
H	11.13455907150414	7.26878569309374	9.11715993774033
C	9.31059876220507	6.38519699467822	9.83339893366544
H	9.65010148117619	6.32591700952136	10.86002938576123
C	8.03434931335292	5.95212096906007	9.49831271211951
H	7.36054870197347	5.57077309206356	10.25405137103138
C	7.60107453330353	6.02120776894562	8.18103135001874
H	6.60265971063377	5.69005476788532	7.93795135747629
C	8.51391730597551	5.00636378102990	4.77899394116822
C	7.99971297536608	3.80642590530256	5.27117675971153
H	7.21900069491367	3.81682766974643	6.02114685210877
C	8.49299776941917	2.59990566840903	4.80133265926270
H	8.08696374508214	1.66911626075687	5.17632918525467
C	9.50296980318487	2.58464128325262	3.84465159131368
H	9.87785219816622	1.64175195398361	3.46957327244497
C	10.01132522847700	3.77764790226203	3.35163630805193
H	10.78258956669834	3.76708072852712	2.59347431887694
C	9.51560693164364	4.99036533413868	3.81378966549936
H	9.89217213056947	5.92255967830922	3.41391118925562
C	6.21872310144747	6.47331760463651	5.50342503216238
P	5.90883086979064	10.23178354172387	7.84644521474491
C	7.70922311105995	10.35405583050286	8.04144993100783
C	8.25181118834327	10.00238768821603	9.27754679668750
H	7.61507093138803	9.59925632777268	10.05512968787192
C	9.61034284772573	10.15832093439036	9.50376820679492
H	10.02784466235779	9.88746852441693	10.46485999259535
C	10.43633685372108	10.63558258637712	8.49120285016165
H	11.49969957862471	10.74191587251577	8.66648666677951
C	9.90139196128189	10.95989871105038	7.25133734432831
H	10.53553824019902	11.30251601310044	6.44434331164002
C	8.53664865692787	10.83232773131020	7.02906931031977
H	8.13530526099143	11.08306580541881	6.05877614758351
C	5.27464067933312	11.81105909116914	8.46817404289778
C	4.51275064687454	11.81992215510452	9.63208295754966
H	4.23616211178017	10.88420263904808	10.09999348784091
C	4.09207352799211	13.02763936286924	10.17436819292982
H	3.49039894435108	13.03202646262062	11.07310307791520
C	4.42163973394979	14.22258257666414	9.55101375647313
H	4.07543927878700	15.16060501677094	9.96385207098717
C	5.17043183012971	14.21334509111585	8.37859795987683
H	5.41393749877468	15.14474512876488	7.88361702494630
C	5.60075325216580	13.01213902677882	7.83816243514471
H	6.18836440803242	13.00802013561637	6.92873033481778
C	5.68614770386544	10.32652234517985	6.11364224163693
P	3.26595652563669	6.58637364846732	5.57869653397333
C	2.79641745373518	6.52919166840266	3.82672106987611
C	1.52466867833551	6.98497717061821	3.47900372628248
H	0.88292375580712	7.42680858471983	4.23078848811882
C	1.09042036083175	6.88306715827472	2.16651575055584
H	0.10299900310532	7.23673406081612	1.90054643926188
C	1.93086561255463	6.35444017196003	1.19241867693671
H	1.59425695162156	6.29017797524016	0.16512862571143
C	3.20730454527471	5.92558515024954	1.53241612380040
H	3.88388322876483	5.54316567425071	0.77973969453823
C	3.63701951321800	6.00126926880400	2.85040009393340
H	4.63558253509708	5.67465538365633	3.09844614040456
C	2.72033801606364	4.99460679527264	6.25126751880987
C	3.24218097860836	3.79586946206445	5.76423683857285
H	4.02557647208427	3.80780607922402	5.01703382690158
C	2.75339500320560	2.58833905941407	6.23609084531573

H	3.16513374100376	1.65831950022006	5.86542357688285
C	1.74077831749750	2.57082672124729	7.18995024931642
H	1.36973142679762	1.62714561911238	7.56684953400934
C	1.22503568948865	3.76268109442876	7.67799498381170
H	0.45177093583437	3.75052855323707	8.43411935454431
C	1.71594731187745	4.97647145707074	7.21355565048867
H	1.33359886114226	5.90797929231258	7.60951624586652
C	5.01138201420648	6.46962869487635	5.53103847965251
Au	5.00948710357914	8.28794251887609	8.68316148779158
Au	2.58234868009728	8.51112888931160	6.63649951695094
C	3.83834947589961	3.97213394437219	9.85743234593167
C	2.78332231366084	3.61771179860661	10.71162588278702
H	2.20084918228058	4.40324485111720	11.17455845887819
C	2.48619368924928	2.28551976653902	10.95278770244282
H	1.66755410465080	2.03036006217416	11.61447919145911
C	3.23317036032392	1.27820719045432	10.34995950283678
H	2.99906539087497	0.23827603564899	10.53965732461776
C	4.28698438548666	1.61680650891974	9.50772096550051
H	4.87413917196537	0.83861976778969	9.03564209163834
C	4.13091973268742	5.33260541501427	9.57675049679552
C	4.40498062044267	6.48940237888098	9.31721719556340
C	1.47255087286007	12.79214439265639	7.98479794019917
C	1.85553362866098	13.83029978209160	7.12274770898364
H	2.34377213138874	13.58303194923219	6.18954903659556
C	1.62733309659605	15.15372565720997	7.46409896342632
H	1.93428495736952	15.94225556774003	6.78791135660215
C	1.01035501409116	15.47260838057372	8.66942790717550
H	0.83243360225089	16.50727226208374	8.93404714718244
C	0.61566251411996	14.45193537063904	9.52870103274986
H	0.12819767636398	14.69139683031121	10.46580919472781
C	1.74144642692143	11.44034436350830	7.64516766259874
C	2.00863101943222	10.29265402349040	7.34181341235241
C	10.36950241955753	13.14180734305518	1.83165404220793
H	10.67145405395933	12.34726540737093	1.16215494750157
C	6.66028232040086	2.95327750821677	1.76823313389909
H	5.84794491462694	3.21466636924064	2.43305805843311
C	4.58873273574296	2.94693810729103	9.26328616947506
H	5.40127369898303	3.20915195402119	8.59900159232387
C	0.84188617734103	13.12636883980923	9.19247813996899
H	0.54000912961615	12.33094677128867	9.86099851029867

6 triplet

Au	5.80264108108961	8.26874124720498	2.56235967416436
Au	8.44264062474218	8.49899603741303	4.30686531291809
P	5.19554364208151	10.39584152098743	3.19663368356416
P	7.90467396052057	6.56213421887128	5.44912242911500
C	6.45722449816763	3.73755034641572	2.11222721905522
C	7.34926256560984	3.05334189656179	1.27367952359039
H	8.00097989394767	3.61914527512761	0.62305316396624
C	7.37695643250301	1.67187342793084	1.30021574193544
H	8.05959558257704	1.12686572526683	0.65995161040261
C	6.52117760431002	0.99609644599773	2.16164870301772
H	6.50697474040856	-0.08443213508372	2.21379438601229
C	5.66956079436828	1.75122907885867	2.95768890109165
H	4.98261221813188	1.25997236612298	3.64074414387124
N	5.62620828305769	3.07893410432286	2.94741378297456
C	6.38725551580313	5.15500192278447	2.10794844538805
C	6.23940768643673	6.36149675196903	2.14449380712102
C	3.44272526679086	10.83315445608661	2.99300419989344
C	2.95176082645180	10.95378554661054	1.69217670286666
H	3.61115861239081	10.81248320700201	0.84448692183840
C	1.61519886716797	11.25534292944519	1.48382508836581
H	1.23851001745143	11.35402668260668	0.47355036434489
C	0.75766432299429	11.41810952094872	2.56932702270573
H	-0.28829878136062	11.64316259907345	2.40281520513992
C	1.24436156212269	11.28866033528251	3.86319703149790
H	0.58901527879219	11.40001919187120	4.71728536980947
C	2.58815975008520	11.00449889833764	4.07650345749191
H	2.94852929741301	10.90104367889882	5.08873671636298
C	6.09019284431243	11.76161664902933	2.41734000815514
C	6.86849344330757	11.50562726380319	1.29152604230532
H	6.98942404850314	10.48917662143810	0.94111937036889
C	7.51055808871282	12.55217335608232	0.64235780295423
H	8.14026604056660	12.34817503275563	-0.21264417355407
C	7.38379663106105	13.84727113739000	1.12195322769424

H	7.90682188610130	14.65801180555144	0.63221292115184
C	6.61374087986146	14.10346460842945	2.25335721838529
H	6.52974652579100	15.11298661715850	2.63394451368076
C	5.96192134769871	13.06440116909362	2.89808548665608
H	5.35783075050681	13.26246045263222	3.77465730429215
C	5.45021905729245	10.59152882151594	4.91944713846259
C	9.83207871396780	12.67740597001044	3.05252980961267
C	9.49966596511542	13.75904420887029	3.97935311531626
H	8.89899462966623	13.52390718649819	4.84725600998111
C	9.94918080294079	15.01915661721130	3.74104099212445
H	9.71534483355292	15.82757697478555	4.42246382657387
C	10.73022025823220	15.25764041207768	2.58363541293459
H	11.11885655997640	16.23921068811908	2.35216608167129
C	10.99241680496711	14.15931085589671	1.70703052393410
H	11.57627161936811	14.34472787009534	0.80686867879384
N	10.58893027898069	12.94094752708834	1.88375823923189
C	9.41586604371427	11.41692354400356	3.29949072780388
C	9.00801147496310	10.26116824738793	3.59060995017740
C	8.43068447481794	6.62128141209518	7.18483684791370
C	9.38574322811422	7.56071484437973	7.57218149673676
H	9.77007032992060	8.27112860784416	6.85242629106922
C	9.83718469841719	7.58673592734606	8.88436040672176
H	10.57866928110882	8.31598117948776	9.17935376512672
C	9.32560537569872	6.68882929661856	9.81298505425545
H	9.67017688523519	6.71783488784729	10.83948284382488
C	8.36736275526352	5.75809901022212	9.42812634905355
H	7.95045639438141	5.06840510034345	10.15022443182004
C	7.92319764979879	5.71577736357300	8.11600570564685
H	7.17090136782059	4.99076497201512	7.84100426461758
C	8.53693664883962	4.99234888892066	4.80137502056344
C	8.01229280668669	3.77526649340484	5.23598149603966
H	7.17019820934764	3.75001118826520	5.91522707489934
C	8.57030958763644	2.58821137218942	4.78627310702002
H	8.15806778747729	1.64340046726504	5.11524871977093
C	9.64106936955381	2.60903997956749	3.90051174084335
H	10.06653124131520	1.67897807105938	3.54550775801514
C	10.15392543447134	3.82115221633092	3.45631590300479
H	10.97876986260975	3.84053133091846	2.75550703157783
C	9.60195403899557	5.01343849244005	3.90477937144832
H	9.99050696109327	5.96061577941707	3.55283502771021
C	6.17822338996995	6.32947210688260	5.52820631289018
P	5.86937544413455	10.42726102923018	7.84064944294915
C	7.64462956301882	10.76883131160823	8.02943194298301
C	8.16967352815227	10.73646085749297	9.32198451456223
H	7.53387065883252	10.48579031583141	10.16230225580714
C	9.50868519817247	11.02419803999115	9.53127057639647
H	9.91084797229942	11.00350914274417	10.53618241509710
C	10.33662745077239	11.32129382148673	8.45176597611154
H	11.38501497739395	11.53585838690933	8.61710472036228
C	9.81871971732144	11.33531588076518	7.16392479306370
H	10.45479050626943	11.54906053289641	6.31489590662077
C	8.47083214881907	11.06934586019990	6.95230398997031
H	8.08118825843226	11.08459786538079	5.94613735566435
C	5.07727051740349	11.86062231152138	8.61338615355699
C	4.21669913194741	11.66387236396395	9.68845237904512
H	3.95582042310845	10.65924684065747	9.99226900263762
C	3.67370117110823	12.75907225264384	10.34888083475947
H	2.98802380828271	12.60182278635635	11.16998658066002
C	3.98490349483799	14.04525689263398	9.93218743184173
H	3.55112288635158	14.89696548236819	10.43946078498611
C	4.83529374904012	14.24298257115068	8.84815038820775
H	5.06755375726803	15.24695853197468	8.51638117270701
C	5.38452950429598	13.15451922964072	8.19050325601983
H	6.05677716118988	13.30811813599058	7.35541505207347
C	5.61041685205789	10.60502605981360	6.11734414922586
P	3.23085331225197	6.39357450899306	5.55252835510230
C	2.75543175961801	6.44377485905748	3.79962782557163
C	1.97580439284909	7.50657389385868	3.34456242702811
H	1.66466684191648	8.28088713264590	4.03181441781702
C	1.60267239829207	7.57337946435733	2.00910804931968
H	1.00199376449343	8.40354847671121	1.66434357080993
C	2.00884750976874	6.58072121609965	1.12683859596397
H	1.72543914346434	6.63554616469285	0.08291161750557
C	2.78454012167521	5.51954443979566	1.58036839576436
H	3.12035073993431	4.75516234079322	0.89184693293365
C	3.15819993676766	5.44577081935034	2.91239818144028
H	3.78810693178100	4.63016098435544	3.23704270359995

C	2.68583798076868	4.78063444793365	6.16879492363044
C	3.34884736298690	3.60580746115274	5.81462755928998
H	4.25196004560593	3.64124860164664	5.21951523937640
C	2.84629833431369	2.38269182847897	6.23266693646083
H	3.36426993390897	1.47103165257187	5.96527253665518
C	1.69456106172580	2.32584122403797	7.00803005516039
H	1.31298170347277	1.36838479399586	7.33941588979590
C	1.04382898055578	3.49714371603104	7.37515921425999
H	0.15524813238367	3.45716026405112	7.99216952026545
C	1.53898951320536	4.72476126363997	6.95757498845378
H	1.04172417928493	5.64109085999247	7.24985555017559
C	4.97227996078883	6.28349787809847	5.52385055784809
Au	5.20115462168443	8.32738993701322	8.50094744728721
Au	2.57007877831232	8.30413496275929	6.67427791472405
C	4.67793417577272	3.78996050745771	9.01227123194087
C	3.75794222227777	3.06891378939201	9.78622160849304
H	3.01905576764801	3.60578119605241	10.36406981076883
C	3.81719907151391	1.68786277646744	9.79199135726603
H	3.11521269625683	1.11345717318732	10.38374740966279
C	4.78594488230739	1.05107362430447	9.02618890017919
H	4.87131890616619	-0.02722246030965	9.00363356332843
C	5.65485501327314	1.84211273303383	8.28531791528100
H	6.42608989373172	1.38122604061750	7.67496351167345
N	5.61550871579388	3.16967485548932	8.26550270184858
C	4.67268709487375	5.20977270891650	8.99255403738342
C	4.77156562906896	6.42015299118894	8.93064561628858
C	1.33632604497677	12.56523363644915	7.97665911979829
C	1.76820453493235	13.57014809386244	7.09609675845265
H	2.32985863029467	13.29814857940287	6.21373760384689
C	1.47303178125881	14.88960713531406	7.38213920483854
H	1.80068916449105	15.67995524153048	6.71785888178426
C	0.75469243152368	15.18290705199538	8.53471635712295
H	0.49834725628996	16.20052174591300	8.79859567243077
C	0.36254797400854	14.12425244483093	9.34585842698971
H	-0.20393007289782	14.31399084919655	10.25292475683730
N	0.63812401579997	12.84976526247081	9.09123410027257
C	1.65097409947715	11.20750692763118	7.69501780908085
C	1.97392719704920	10.07508509796417	7.38931370509783

9 triplet

Au	6.21896122887189	8.23335057764587	2.30938768073241
Au	8.69751380627782	8.49651872008555	4.30894333517077
P	5.35662996621802	10.18339934885602	3.16886262463887
P	7.99038747274726	6.59500492532632	5.39569669531151
C	7.46669124924153	3.96321691534612	1.03073993188188
C	8.60849422177616	3.67888353078786	0.26668105563199
H	9.21320912922600	4.50089857574043	-0.09286427984876
C	8.96165800148317	2.36884576010221	-0.01678752634057
H	9.84704144249827	2.16838621736472	-0.60762852934268
C	8.18516653096929	1.31402317815266	0.45275426400523
H	8.46229948319395	0.29144831745851	0.22947990797681
C	7.04571658823498	1.58312234855466	1.20400347233513
H	6.43383868916551	0.76778796946729	1.57026859630966
C	7.11635389992564	5.30124564157311	1.35164129561175
C	6.81897960174381	6.44270347097894	1.65068398751312
C	3.55709793227004	10.35003159730264	2.99003530498566
C	2.99590942267852	10.02705939718093	1.75478208338533
H	3.61507755468168	9.61124230465193	0.96971216508345
C	1.64175759257929	10.22919355132531	1.53800817275926
H	1.20998417375677	9.98023839430179	0.57728739521176
C	0.83784143733156	10.72583630673304	2.55869645531442
H	-0.22207475155336	10.87018407156767	2.39020092637903
C	1.39056957085937	11.02254836350793	3.79787588218421
H	0.77071086838685	11.38494644259784	4.60741322690013
C	2.75135428634580	10.84736408881414	4.01090249897898
H	3.17145864544830	11.08186918251830	4.97744308552619
C	6.01282435017809	11.75658455679375	2.55423388774569
C	6.76251046350448	11.76201354857999	1.38225262125279
H	7.02052807265147	10.82572285525041	0.90505765866093
C	7.19494290032428	12.96709461002810	0.84327985790546
H	7.78655221881015	12.96859981065461	-0.06213474019758
C	6.89047462022945	14.16254548095292	1.47827906944965
H	7.24671104741908	15.09807730144649	1.06826769637434
C	6.15486159602777	14.15654219413808	2.65902241563353
H	5.93150370474733	15.08811605808256	3.16310612446066

C	5.71191945587217	12.95817631932548	3.19574608828792
H	5.13295268910869	12.95700362649185	4.11077348834641
C	5.59465844930703	10.25322964812248	4.90000641128257
C	9.85594559572469	12.76706992342335	2.97330210819417
C	9.49328994590328	13.80476527798857	3.84469710356866
H	9.01389836791857	13.55758893142172	4.78250348425582
C	9.72801086943445	15.12761312955193	3.50550068997851
H	9.43669197300222	15.91590838191115	4.18888727921209
C	10.33108253493085	15.44636073259246	2.29297324249585
H	10.51371933601483	16.48062289555624	2.02985871570458
C	10.70618370466172	14.42588924916141	1.42465295676775
H	11.18304751036540	14.66509299973045	0.48201290131252
C	9.57548239385402	11.41643331413046	3.30861760461508
C	9.29646036008642	10.27021248959033	3.60699895542093
C	8.50381018904733	6.55653862401993	7.13665560318289
C	9.73450547029311	7.12076551996275	7.47212126267383
H	10.32392256512372	7.62385587458052	6.71627540542692
C	10.19264228571746	7.05083041888469	8.77905534168717
H	11.14733230415806	7.49014769405500	9.03579684990930
C	9.41477861602951	6.44444684685794	9.75900467653312
H	9.76769886770851	6.40608675230425	10.78211392173290
C	8.17752988333415	5.90398489694745	9.43160605294463
H	7.54763520557756	5.46111445539578	10.19155474867729
C	7.72582518448431	5.94938614865409	8.12011573507969
H	6.75586273319832	5.53817416241646	7.88272606466653
C	8.46779932097813	4.98135674853425	4.72342828988282
C	7.83081143111483	3.81023270050472	5.13393723163464
H	6.99168375218718	3.85729261106259	5.81613449804027
C	8.27169395266560	2.58354645845401	4.66307434033072
H	7.77014630226598	1.67584360641362	4.97367187066612
C	9.35020407348235	2.51844425449500	3.78722898682520
H	9.68300219725052	1.56103530375596	3.40947461806817
C	9.97931459827285	3.68364299405551	3.37267003654324
H	10.80303136917400	3.63656980897714	2.67338056989904
C	9.53703607738586	4.91632121772251	3.83526608839965
H	10.00968587704395	5.82867070597710	3.49521088670784
C	6.24603285968245	6.52195028204048	5.49178374492998
P	5.98432971948176	10.11296031609021	7.82817086742254
C	7.77525239394713	10.34516547081635	8.02637481416470
C	8.32366248292426	10.08264444749230	9.28184907207422
H	7.69834875103478	9.69611927419197	10.07727798042828
C	9.67342021398752	10.30429955892727	9.50585023602920
H	10.09482817333012	10.10292940244916	10.48236859747856
C	10.48709358517726	10.75790902044984	8.47221634342038
H	11.54424579730164	10.91593669768207	8.64618130140335
C	9.94748085658086	10.99405409319800	7.21443805917135
H	10.57227788231109	11.31975062596689	6.39310654359093
C	8.58991662509194	10.80135904479085	6.99360012332214
H	8.18521470486046	10.98766597290638	6.01032329195138
C	5.24021087332733	11.64071914767933	8.45681323330747
C	4.48945069541413	11.59158854792857	9.62768417407158
H	4.30361424789125	10.63901868880510	10.10655590672635
C	3.95672472279414	12.75945346404101	10.15749912158402
H	3.35671901400286	12.71662589799629	11.05668627862476
C	4.16241665211390	13.97233067856618	9.51598815992899
H	3.71934529568693	14.87592936881365	9.91282033951407
C	4.90883133541998	14.02189073473841	8.34222738231840
H	5.05791549458994	14.96675527245200	7.83590490615862
C	5.45259743038528	12.86162729872026	7.81478175812575
H	6.03486931135477	12.90160709862568	6.90278417678238
C	5.76062977380723	10.22071064315281	6.09597587810851
P	3.29878070480070	6.68861189488254	5.63866415066091
C	2.78381591655542	6.63867452387568	3.89773905220175
C	1.51663772402715	7.12464131314509	3.57658912032325
H	0.90493000721757	7.58699685987693	4.34115096713542
C	1.04856443085766	7.02494487900893	2.27555146934977
H	0.06424144508942	7.40146417318473	2.03026910630570
C	1.85168320068944	6.46824595887683	1.28585802464601
H	1.48924210115596	6.40555667803162	0.26726607615789
C	3.12429473737480	6.00824904165739	1.59874635541959
H	3.77188226871026	5.60267133108562	0.83265737688090
C	3.58712104658454	6.08103112579575	2.90578985187762
H	4.58067505681466	5.72443029699764	3.13346293803167
C	2.75461000668957	5.10696450524889	6.33460012533021
C	3.29800139807391	3.90423659313154	5.88284524280884
H	4.09458373290580	3.90812048633129	5.14962405540847
C	2.81720227260921	2.70151056629095	6.37596124677861

H	3.24664913839298	1.76864378365128	6.03357106319605
C	1.79073758424957	2.69265374445704	7.31446377842558
H	1.42846580143820	1.75350608258554	7.71061462022934
C	1.25265784644668	3.88908651190172	7.76661350181241
H	0.46914839196885	3.88413884365527	8.51218028819696
C	1.73575457815361	5.09769877043904	7.28190527718751
H	1.33470886094288	6.03300167940959	7.64984827217722
C	5.03892047812782	6.53884776198952	5.53772734637836
Au	5.14175957054766	8.14785716353370	8.67343892769163
Au	2.66398193823323	8.61306862113895	6.73118272080297
C	3.84413313784802	3.91001701865819	10.00468591343022
C	2.73490644957105	3.65266615515429	10.82452588447377
H	2.17998964582861	4.48902503770342	11.22859610042547
C	2.34899794994651	2.35118465701346	11.10477694509620
H	1.48888748184577	2.17182102487839	11.73821469098615
C	3.06020796496442	1.27769066729557	10.57747640032031
H	2.75712932489845	0.26186600350822	10.79767473904306
C	4.16904191133137	1.51956870799334	9.77273125037856
H	4.73078110211371	0.68963122092176	9.36170005638965
C	4.21899552962490	5.23941082707565	9.67730340349770
C	4.52961589347520	6.37251612859950	9.36003847099633
C	1.36080002563970	12.80301794500054	8.03851828290490
C	1.69382426690187	13.92478241477750	7.15276587448771
H	2.22575699756757	13.70794197066512	6.23662845731204
C	1.34359661653362	15.19620179582838	7.48167858377143
H	1.59601916347109	16.01157354335089	6.81431018417934
C	0.65150461331453	15.47727604395038	8.68887145363096
H	0.37577661152459	16.49296426396597	8.93578155224723
C	0.31357265736375	14.40840001849626	9.56952130743013
H	-0.21937576526424	14.62862476240962	10.48661562216248
C	1.71987208435242	11.54127517780666	7.73119985672632
C	2.06521013918060	10.36855683333796	7.42815101749688
C	10.47383557184592	13.10077227095772	1.75893917131079
H	10.76047500802085	12.30559061300373	1.08343845662874
C	6.68813889563885	2.89104940810846	1.49022924759549
H	5.80668143139099	3.10002518290417	2.08160986643537
C	4.55903126046426	2.81873384540282	9.48954849073137
H	5.41506287806668	3.00646506759880	8.85518213179027
C	0.64095731970446	13.12541675661090	9.27351092582169
H	0.38310844074769	12.31124396141676	9.93728690770870

6 triplet BP86

Au	5.8120708	8.2009649	2.6559943
Au	8.2434154	8.5265741	4.2037814
P	5.1806018	10.3250165	3.2347275
P	7.8470434	6.6003082	5.3991836
C	6.3928023	3.6722333	2.3406521
C	7.2480199	2.9243638	1.5015525
H	7.8794875	3.4493419	0.7863683
C	7.2690688	1.5415319	1.6125346
H	7.9246235	0.9479677	0.9737533
C	6.4436545	0.9245626	2.5574763
H	6.4266218	-0.1584428	2.6791831
C	5.6242145	1.7386381	3.3434751
H	4.9611070	1.2900785	4.0897187
N	5.5802100	3.0702252	3.2564207
C	6.3411046	5.0825120	2.2640541
C	6.1993557	6.3062698	2.2460362
C	3.4316174	10.8016552	3.0168203
C	2.9526409	10.9694113	1.7100722
H	3.6256170	10.8488377	0.8589942
C	1.6141602	11.2935157	1.5019164
H	1.2431939	11.4329148	0.4856019
C	0.7458784	11.4301240	2.5919557
H	-0.3038246	11.6751440	2.4241738
C	1.2232166	11.2503117	3.8912251
H	0.5589463	11.3435575	4.7512178
C	2.5673670	10.9417162	4.1054938
H	2.9244992	10.7947498	5.1241914
C	6.0853185	11.6739448	2.4274911
C	6.9247602	11.3871219	1.3433197
H	7.0853258	10.3496244	1.0482144
C	7.5614775	12.4274754	0.6648467
H	8.2299679	12.2023984	-0.1652797
C	7.3724368	13.7476370	1.0757446

H	7.8868469	14.5574991	0.5582430
C	6.5497931	14.0321349	2.1708643
H	6.4175652	15.0633442	2.4996825
C	5.8965436	12.9990520	2.8424729
H	5.2414915	13.2179604	3.6868370
C	5.4169661	10.5355519	4.9551820
C	9.7279095	12.7281751	3.1469242
C	9.2874796	13.7641844	4.0488423
H	8.6166951	13.4968267	4.8645139
C	9.7265889	15.0573812	3.8649678
H	9.4098402	15.8513244	4.5425694
C	10.5913358	15.3326082	2.7866527
H	10.9694397	16.3368593	2.5991760
C	10.9566917	14.2616401	1.9312177
H	11.6166949	14.4621878	1.0795219
N	10.5654761	13.0096969	2.0684169
C	9.3071623	11.4325855	3.3429931
C	8.9207902	10.2613491	3.6162226
C	8.4308325	6.7370689	7.1164663
C	9.4390245	7.6609114	7.4179046
H	9.8302343	8.3113720	6.6341054
C	9.9284363	7.7471874	8.7202395
H	10.7131176	8.4654919	8.9533966
C	9.3983975	6.9293621	9.7208595
H	9.7709177	7.0103789	10.7432153
C	8.3899464	6.0115917	9.4172351
H	7.9626786	5.3812388	10.1973184
C	7.9090357	5.9039394	8.1138798
H	7.1211509	5.1859718	7.8864676
C	8.5447393	5.0497429	4.7664302
C	8.1084537	3.8211658	5.2799573
H	7.2947934	3.7839097	6.0083711
C	8.7169089	2.6455651	4.8437363
H	8.3791795	1.6845332	5.2327945
C	9.7441630	2.6917127	3.8983825
H	10.2107701	1.7668789	3.5569310
C	10.1640309	3.9175546	3.3776743
H	10.9566356	3.9545104	2.6293768
C	9.5646014	5.0999417	3.8108139
H	9.8790461	6.0633869	3.4060769
C	6.1450251	6.2775887	5.5579325
P	5.8362340	10.3689593	7.8840465
C	7.6160068	10.7213631	8.0691873
C	8.1424953	10.7307346	9.3679040
H	7.5056786	10.4856436	10.2196748
C	9.4801146	11.0615530	9.5680549
H	9.8874402	11.0762204	10.5797178
C	10.3011193	11.3622816	8.4754777
H	11.3499681	11.6157446	8.6364161
C	9.7801144	11.3303645	7.1815984
H	10.4136301	11.5472797	6.3207788
C	8.4346018	11.0188784	6.9773082
H	8.0343246	10.9984880	5.9649013
C	5.0625516	11.7981632	8.6952832
C	4.1621050	11.5821613	9.7429645
H	3.8711855	10.5642118	10.0029462
C	3.6242738	12.6726555	10.4279709
H	2.9059627	12.5043528	11.2295201
C	3.9832529	13.9711952	10.0654228
H	3.5549065	14.8220857	10.5956182
C	4.8762870	14.1859191	9.0114316
H	5.1461161	15.2021312	8.7218111
C	5.4197238	13.1021207	8.3263008
H	6.1272884	13.2655529	7.5120178
C	5.5708687	10.5612136	6.1692964
P	3.1943599	6.3408674	5.6309381
C	2.7204575	6.4349604	3.8754187
C	1.9517131	7.5255692	3.4485877
H	1.6398818	8.2819338	4.1697464
C	1.5947944	7.6419453	2.1055495
H	1.0014503	8.4953213	1.7793546
C	2.0089047	6.6723824	1.1905615
H	1.7409003	6.7680196	0.1372656
C	2.7677967	5.5799553	1.6197169
H	3.1049805	4.8302034	0.9035434
C	3.1247299	5.4542158	2.9597924
H	3.7459188	4.6150807	3.2743182

C	2.5931821	4.7332545	6.2168308
C	3.1983603	3.5400031	5.7992131
H	4.1028552	3.5622491	5.1870496
C	2.6333342	2.3219774	6.1730845
H	3.0973335	1.3892205	5.8515948
C	1.4871610	2.2897458	6.9705751
H	1.0556289	1.3320423	7.2645704
C	0.9032604	3.4804181	7.4069918
H	0.0172833	3.4575363	8.0426422
C	1.4545324	4.7049865	7.0294389
H	1.0082882	5.6421071	7.3669811
C	4.9279116	6.1942505	5.5849322
Au	5.1491511	8.2809388	8.5043575
Au	2.6116162	8.2564219	6.7552567
C	4.7328620	3.7360420	8.7655046
C	3.8615958	2.9066926	9.4998907
H	3.1159086	3.3630940	10.1491397
C	3.9725271	1.5283302	9.3743728
H	3.3062747	0.8694716	9.9330266
C	4.9429850	1.0017220	8.5193332
H	5.0662783	-0.0737393	8.3913557
C	5.7635054	1.8954811	7.8283833
H	6.5355921	1.5195323	7.1500097
N	5.6799528	3.2249884	7.9319444
C	4.6716246	5.1495087	8.8672792
C	4.7380594	6.3766480	8.8892396
C	1.5298980	12.6028197	7.8378657
C	2.1123412	13.5303144	6.9455065
H	2.7334279	13.1665006	6.1282445
C	1.8840511	14.8864089	7.1355924
H	2.3271136	15.6202584	6.4606151
C	1.0847210	15.2919800	8.2064090
H	0.8769844	16.3454694	8.3952390
C	0.5451654	14.3043989	9.0349308
H	-0.0896776	14.5855004	9.8812482
N	0.7484559	12.9927699	8.8760702
C	1.7745932	11.2165076	7.6496159
C	2.0589240	10.0451139	7.4076907

9 triplet BP86

Au	6.2805234	8.1711236	2.3650519
Au	8.6192377	8.6345043	4.3024760
P	5.3655342	10.1144293	3.1498971
P	7.9920471	6.7106445	5.3707202
C	7.3635412	3.8544260	1.1487687
C	8.4384910	3.4854879	0.3101841
H	9.0432993	4.2714254	-0.1418901
C	8.7242524	2.1442657	0.0737131
H	9.5593927	1.8763526	-0.5753009
C	7.9475524	1.1411403	0.6631913
H	8.1743368	0.0908967	0.4758846
C	6.8726446	1.4928429	1.4863177
H	6.2599061	0.7148867	1.9443374
C	7.0877539	5.2132708	1.4312140
C	6.8470361	6.3865483	1.7161221
C	3.5681826	10.2624866	2.8808908
C	3.0558009	9.9059320	1.6277450
H	3.7149768	9.4721349	0.8735196
C	1.7020417	10.0947950	1.3570979
H	1.3023300	9.8162319	0.3816702
C	0.8555528	10.6134898	2.3414970
H	-0.2063422	10.7473783	2.1299932
C	1.3632396	10.9431281	3.5993931
H	0.7076211	11.3213640	4.3844989
C	2.7222573	10.7797558	3.8671884
H	3.1129125	11.0386295	4.8506259
C	6.0298582	11.6776264	2.5058489
C	6.7970365	11.6544481	1.3363677
H	7.0584085	10.6971345	0.8831368
C	7.2370446	12.8521656	0.7729808
H	7.8411683	12.8334895	-0.1341321
C	6.9228958	14.0688042	1.3798581
H	7.2854562	15.0019742	0.9488468
C	6.1723151	14.0893855	2.5584118
H	5.9432484	15.0393727	3.0423943
C	5.7205579	12.8977742	3.1212901

H	5.1298896	12.9122759	4.0384575
C	5.5398294	10.2171005	4.8754094
C	9.7675708	12.9268995	3.0663848
C	9.3585048	13.9549174	3.9447147
H	8.8487317	13.6821373	4.8683963
C	9.5877613	15.2898987	3.6281953
H	9.2619239	16.0719021	4.3158356
C	10.2303015	15.6329814	2.4338821
H	10.4086681	16.6805507	2.1881023
C	10.6513737	14.6244506	1.5604991
H	11.1593490	14.8859158	0.6309747
C	9.4919387	11.5735018	3.3722467
C	9.2111967	10.4059882	3.6445934
C	8.5357275	6.6379958	7.1078690
C	9.8179926	7.1064444	7.4191206
H	10.4287279	7.5751037	6.6451816
C	10.2988200	6.9854269	8.7212413
H	11.2966201	7.3510153	8.9648803
C	9.4937471	6.4239787	9.7166027
H	9.8682608	6.3447541	10.7382084
C	8.2055081	5.9826175	9.4105192
H	7.5573780	5.5712073	10.1846990
C	7.7285346	6.0778002	8.1034427
H	6.7209797	5.7343013	7.8714573
C	8.5452267	5.1317460	4.6631779
C	8.0029847	3.9171623	5.1027302
H	7.1878201	3.9132903	5.8278091
C	8.5062460	2.7162557	4.6074966
H	8.0780855	1.7700742	4.9402969
C	9.5525083	2.7225269	3.6812154
H	9.9360925	1.7817000	3.2865861
C	10.0838964	3.9335617	3.2361838
H	10.8849077	3.9406223	2.4968430
C	9.5798144	5.1400784	3.7217503
H	9.9737593	6.0923968	3.3633363
C	6.2611967	6.5854418	5.4722996
P	5.8667930	9.9919893	7.8162470
C	7.6670124	10.2006006	8.0668772
C	8.1926487	9.8729462	9.3221275
H	7.5428958	9.4413548	10.0867183
C	9.5433672	10.0925593	9.5834253
H	9.9528033	9.8410894	10.5623846
C	10.3751645	10.6114393	8.5863208
H	11.4348776	10.7713058	8.7911097
C	9.8557426	10.9085781	7.3247298
H	10.4990436	11.2867206	6.5293856
C	8.4989782	10.7125739	7.0660146
H	8.1003154	10.9460339	6.0792941
C	5.1573928	11.5049178	8.5222975
C	4.3135530	11.4204532	9.6358083
H	4.0288866	10.4401052	10.0204117
C	3.8347049	12.5854537	10.2336027
H	3.1746684	12.5171657	11.0985077
C	4.1818992	13.8350546	9.7141836
H	3.7890868	14.7437498	10.1706445
C	5.0123672	13.9186504	8.5933033
H	5.2741329	14.8935464	8.1801865
C	5.5091677	12.7589241	8.0010580
H	6.1684201	12.8243369	7.1343207
C	5.6975674	10.1700167	6.0902968
P	3.3079044	6.8216153	5.6242783
C	2.7726924	6.6956883	3.8820078
C	1.4843693	7.1396462	3.5613644
H	0.8658878	7.6094745	4.3293014
C	1.0064069	6.9880394	2.2615080
H	0.0021925	7.3308368	2.0106781
C	1.8210654	6.4209677	1.2768962
H	1.4479477	6.3155535	0.2570610
C	3.1166416	6.0064514	1.5911783
H	3.7720245	5.5902747	0.8256173
C	3.5915926	6.1343833	2.8965677
H	4.6055839	5.8138705	3.1341144
C	2.7134607	5.2878715	6.3891598
C	3.1685847	4.0441427	5.9277468
H	3.9265514	3.9961093	5.1445548
C	2.6515571	2.8714862	6.4753693
H	3.0140100	1.9039311	6.1261484

C	1.6725420	2.9333330	7.4705511
H	1.2762976	2.0144554	7.9032162
C	1.2210803	4.1728302	7.9294806
H	0.4696274	4.2233840	8.7175367
C	1.7437107	5.3502491	7.3961561
H	1.4118167	6.3227957	7.7626957
C	5.0372611	6.6254953	5.5081539
Au	4.9231598	8.0251079	8.5274066
Au	2.7605328	8.7618045	6.7180948
C	3.9263856	3.7608293	9.9259499
C	2.9086016	3.4258800	10.8578858
H	2.3588000	4.2325910	11.3422060
C	2.6140622	2.0982840	11.1340081
H	1.8257952	1.8574248	11.8487594
C	3.3238566	1.0662316	10.5022495
H	3.0894096	0.0247890	10.7242185
C	4.3392526	1.3806501	9.5887657
H	4.8963558	0.5808408	9.0987414
C	4.2002452	5.0957203	9.5977467
C	4.4535087	6.2687123	9.2799638
C	1.4109016	12.9875894	7.9099105
C	1.8881099	14.0534682	7.0984249
H	2.4877466	13.8121920	6.2215188
C	1.6035513	15.3711755	7.4257645
H	1.9770869	16.1775206	6.7930290
C	0.8426896	15.6721282	8.5643916
H	0.6239166	16.7093975	8.8192381
C	0.3605268	14.6310904	9.3734892
H	-0.2341831	14.8621081	10.2583951
C	1.7363485	11.6624389	7.6010318
C	2.0493038	10.4957958	7.3066782
C	10.4263353	13.2864979	1.8697692
H	10.7469106	12.4966326	1.1908422
C	6.5804626	2.8313088	1.7278680
H	5.7503763	3.1104952	2.3762955
C	4.6402738	2.7044266	9.2999505
H	5.4208737	2.9556644	8.5827484
C	0.6323112	13.3089580	9.0550284
H	0.2640551	12.4960921	9.6802951

6 mon triplet BP86

Au	6.4420739	8.3867573	2.3661532
P	5.3307598	10.1983652	3.2224388
C	8.3696154	4.8035265	0.2671489
C	9.5317517	5.0113973	-0.5834834
H	9.9426988	6.0174544	-0.6637721
C	10.0850807	3.9451690	-1.2478744
H	10.9577698	4.0797374	-1.8877250
C	9.4997290	2.6673988	-1.0854667
H	9.8993145	1.7892049	-1.5909652
C	8.3485875	2.5489438	-0.2488472
H	7.8797882	1.5651414	-0.1318839
N	7.7782694	3.5349283	0.4021356
C	7.8413769	5.8488090	0.9740800
C	7.3877994	6.8418450	1.6182442
C	3.5330920	10.1948178	2.9230838
C	2.9160247	9.0339612	2.4452933
H	3.5217901	8.1511810	2.2308258
C	1.5339355	9.0164603	2.2463442
H	1.0506833	8.1095123	1.8819435
C	0.7761873	10.1583272	2.5140914
H	-0.3027511	10.1446036	2.3551404
C	1.3955950	11.3213885	2.9840731
H	0.8019113	12.2131339	3.1883991
C	2.7732027	11.3411347	3.1934108
H	3.2612719	12.2451068	3.5610982
C	5.9340708	11.7910884	2.5811113
C	5.8040904	12.0238776	1.2036575
H	5.3396590	11.2703316	0.5650891
C	6.2701746	13.2179283	0.6550337
H	6.1661727	13.3983425	-0.4154652
C	6.8729304	14.1774619	1.4735151
H	7.2405744	15.1088256	1.0411512
C	7.0067592	13.9424426	2.8440786
H	7.4808427	14.6874932	3.4841551

C	6.5358490	12.7515448	3.4006251
H	6.6388247	12.5613795	4.4692539
C	5.4377924	10.3911822	4.9541847
P	5.8326081	10.2796907	7.8951343
C	7.6456382	10.3068858	8.0676235
C	8.3141854	9.1255944	8.4151392
H	7.7387233	8.2195380	8.6139190
C	9.7061015	9.1184666	8.5104476
H	10.2239152	8.1991951	8.7855338
C	10.4306456	10.2862778	8.2595256
H	11.5185081	10.2793803	8.3363667
C	9.7630610	11.4663527	7.9153097
H	10.3293021	12.3789163	7.7245955
C	8.3730605	11.4805264	7.8191674
H	7.8508286	12.4039467	7.5645594
C	5.2883406	11.8949582	8.5455405
C	5.3523961	12.0873008	9.9333391
H	5.7095170	11.2826178	10.5790537
C	4.9541098	13.3028107	10.4854169
H	5.0045496	13.4496477	11.5648875
C	4.4802856	14.3263238	9.6584194
H	4.1621264	15.2744781	10.0934722
C	4.4062815	14.1312205	8.2781038
H	4.0307579	14.9259626	7.6322984
C	4.8104979	12.9167571	7.7188153
H	4.7483738	12.7544604	6.6421338
C	5.5777180	10.3973433	6.1759069
Au	4.8049285	8.4689378	8.8375455
C	2.8470588	4.7847005	10.8442517
C	1.7502753	4.9751134	11.7148519
H	1.3874006	5.9853888	11.9013432
C	1.1594265	3.8679163	12.3116115
H	0.3111208	3.9922259	12.9864278
C	1.6701917	2.5987929	12.0313903
H	1.2387390	1.7009735	12.4745389
C	2.7597588	2.5055524	11.1595759
H	3.1865853	1.5270044	10.9180476
N	3.3474210	3.5523125	10.5722436
C	3.4594235	5.9072697	10.2216661
C	3.9519431	6.9040550	9.6961055

9 mon triplet BP86

Au	4.5555752	7.3544301	2.1555461
P	4.3322675	9.2085373	3.4747666
C	5.1157778	3.5814234	-0.4681833
C	5.7227900	3.6672523	-1.7417376
H	6.0566766	4.6414455	-2.0991772
C	5.8904323	2.5286207	-2.5248945
H	6.3605525	2.6127826	-3.5059950
C	5.4597072	1.2813333	-2.0610894
H	5.5920092	0.3913680	-2.6776191
C	4.8584028	1.1813946	-0.8022574
H	4.5207477	0.2110920	-0.4346167
C	4.9414843	4.7392983	0.3329774
C	4.7939696	5.7434072	1.0296854
C	2.6531813	9.5551387	4.0940443
C	1.5609907	8.9163998	3.4955376
H	1.7304371	8.1988636	2.6905539
C	0.2672148	9.1911603	3.9430825
H	-0.5840070	8.6903306	3.4806509
C	0.0673478	10.0951700	4.9878231
H	-0.9430878	10.3028253	5.3420959
C	1.1599890	10.7285079	5.5894944
H	1.0032628	11.4268393	6.4122763
C	2.4526667	10.4622954	5.1438412
H	3.3068344	10.9460547	5.6194732
C	4.9031758	10.7637776	2.7039875
C	4.5688101	10.9828751	1.3602141
H	4.0251966	10.2172411	0.8032463
C	4.9457421	12.1709760	0.7359932
H	4.6854651	12.3391854	-0.3096617
C	5.6693005	13.1344132	1.4442769
H	5.9701627	14.0595828	0.9510271

C	6.0161638	12.9090063	2.7781777
H	6.5943340	13.6497900	3.3312459
C	5.6319329	11.7274746	3.4124227
H	5.9151404	11.5499004	4.4497637
C	5.3040106	9.1446236	4.9171437
P	7.2964093	9.4323068	7.0863555
C	8.4763782	8.0482779	6.9097740
C	9.4430375	7.8693554	7.9082298
H	9.4546478	8.5306568	8.7774138
C	10.3760401	6.8401267	7.7938845
H	11.1266391	6.6989695	8.5724566
C	10.3398338	5.9815581	6.6908389
H	11.0653756	5.1714965	6.6071892
C	9.3682432	6.1513543	5.7021969
H	9.3303185	5.4764556	4.8464023
C	8.4345788	7.1831316	5.8094520
H	7.6655351	7.3107655	5.0467532
C	8.1315926	10.8888005	6.3863879
C	8.9021714	10.7694001	5.2177742
H	9.0800304	9.7876598	4.7779184
C	9.4372583	11.9101863	4.6210605
H	10.0295960	11.8156969	3.7101885
C	9.2158781	13.1690274	5.1857240
H	9.6398179	14.0584224	4.7178232
C	8.4544178	13.2878190	6.3548353
H	8.2873146	14.2679557	6.8028323
C	7.9087948	12.1525718	6.9518923
H	7.3049532	12.2363271	7.8578047
C	6.1186820	9.1031802	5.8344135
Au	6.3774887	9.7727590	9.1503336
C	4.6125183	10.4692016	13.3289169
C	5.0088611	11.6194470	14.1329558
H	5.7439180	12.3081183	13.7178571
C	4.4653348	11.8199295	15.3753649
H	4.7699134	12.6848797	15.9662100
C	3.5086628	10.9135146	15.9077467
H	3.0821548	11.0861708	16.8949995
C	3.1121663	9.7800078	15.1474329
H	2.3807143	9.0855068	15.5629705
C	5.1295822	10.2656595	12.0824114
C	5.6011311	10.0824410	10.9214528
C	4.6865487	2.3144870	-0.0119926
H	4.2184421	2.2418002	0.9696808
C	3.6369169	9.5497984	13.9020333
H	3.3394350	8.6838161	13.3118662

REFERENCES

1 R. Uson, A. Laguna, M. Laguna, D. A. Briggs, H. H. Murray and J. P. Fackler, in *Inorganic Synthesis*, 1989, vol. 26, pp. 85–91.

2 J. Vicente, J. Gil-Rubio, N. Barquero, P. G. Jones and D. Bautista, *Organometallics*, 2008, **27**, 646–659.

3 C. Würth, M. Grabolle, J. Pauli, M. Spieles and U. Resch-Genger, *Anal. Chem.*, 2011, **83**, 3431–3439.

4 G. M. Sheldrick, *Acta Cryst. A* 2015, **71**, 3–8.

5 M. Ferrer, A. Gutiérrez, L. Rodríguez, O. Rossell, J. C. Lima, M. Font-Bardia and X. Solans, *Eur. J. Inorg. Chem.*, 2008, **2008**, 2899–2909.

6 B. Valeur and M. N. Berberan-Santos, *Molecular Fluorescence: Principles and Applications*, Wiley, 2013.

7 F. Neese, *WIREs Comput. Mol. Sci*., 2025, **15**, e70019.

8 A. D. Becke, *Phys. Rev. A*, 1988, **38**, 3098.

9 C. Lee, W. Yang and R. G. Parr, *Phys. Rev. B*, 1988, **37**, 785.

10 A. D. Becke, *J. Chem. Phys*., 1993, **98**, 5648.

11 F. Weigend and R. Ahlrichs, *Phys. Chem. Chem. Phys*., 2005, **7**, 3297.

12 S. Grimme, A. Hansen, S. Ehlert and J.-M. Mewes, *J. Chem. Phys*., 2019, **150**, 194301

13 E. van Lenthe, E. J. Baerends and J. G. Snijders, *J. Chem. Phys*., 1993, **99**, 4597.

14 E. van Lenthe, E. J. Baerends and J. G. Snijders, *J. Chem. Phys*., 1994, **101**, 9783.

15 E. van Lenthe, J. G. Snijders and E. J. Baerends, *J. Chem. Phys*., 1996, **105**, 6505.

16 E. van Lenthe, R. van Leeuwen, E. J. Baerends and J. G. Snijders, *Int. J. Quantum Chem*., 1996, **57**, 281.

17 F. Neese, F. Wennmohs, A. Hansen and U. Becker, *Chem. Phys*., 2009, **356**, 98–109.

18 T. Petrenko, S. Kossmann and F. Neese, *J. Chem. Phys*., 2011, **134**, 134101.

19 S. Hirata and M. Head-Gordon, *Chem. Phys. Lett*., 1999, **314**, 291.

20 B. de Souza, F. Neese and R. Izsák, *J. Chem. Phys*., 2018, **148**, 034104.

21. F. Furche, R. Ahlrichs, C. Hättig, W. Klopper, M. Sierka and F. Weigend, *Wiley Interdiscip. Rev.: Comput. Mol. Sci.,* 2014, **4**, 91-100.