

Electronic Supplementary Information

**The Role of the Electron Density of
the Acceptor in Efficient
Diphenylphosphino-Gold(I) TADF
Emitters**

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1. Characterization

1.1. Infrared spectra

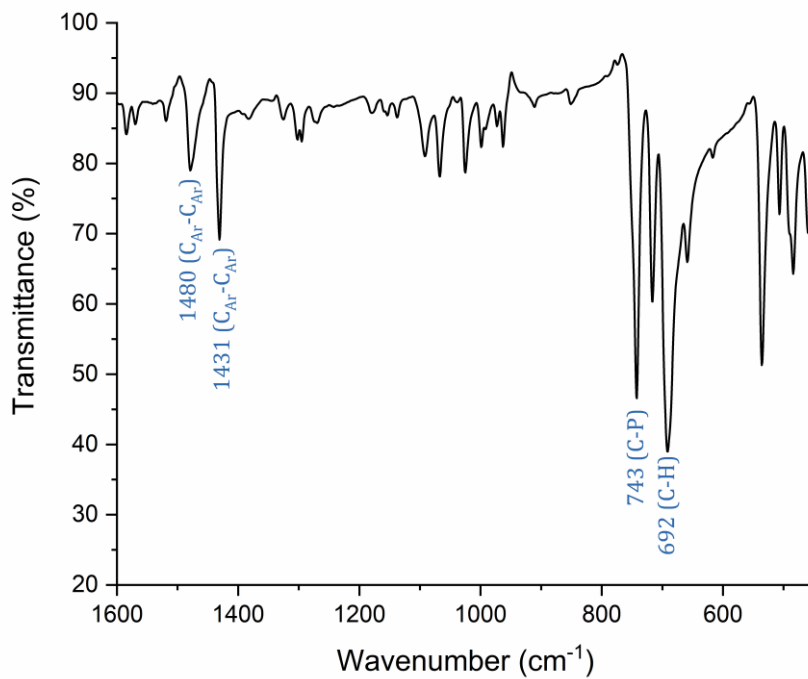


Figure S1. FT-IR spectrum of dppe.

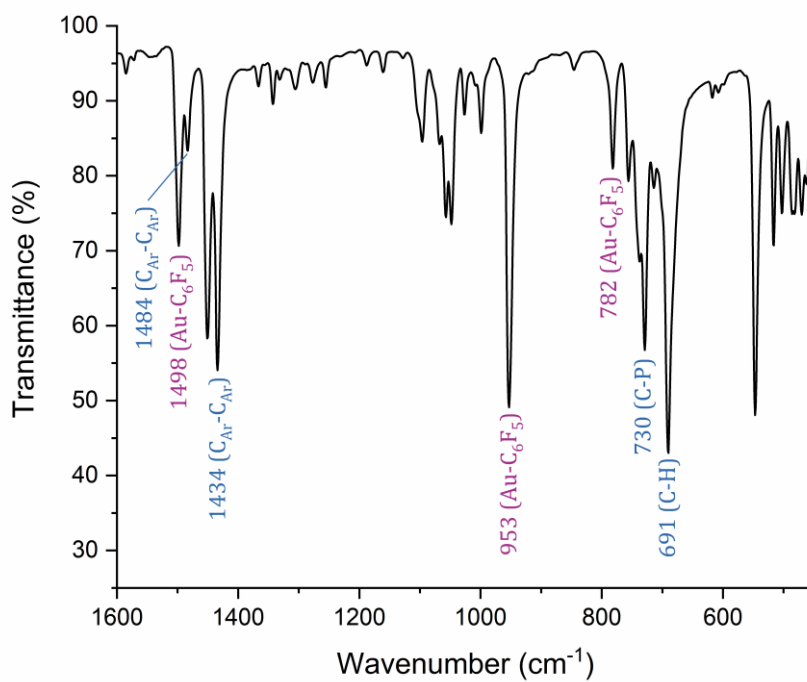


Figure S2. FT-IR spectrum of **1**. Signals related to the [Au(C₆F₅)₂]⁻ fragment and the dppe ligand are shown in magenta and blue, respectively.

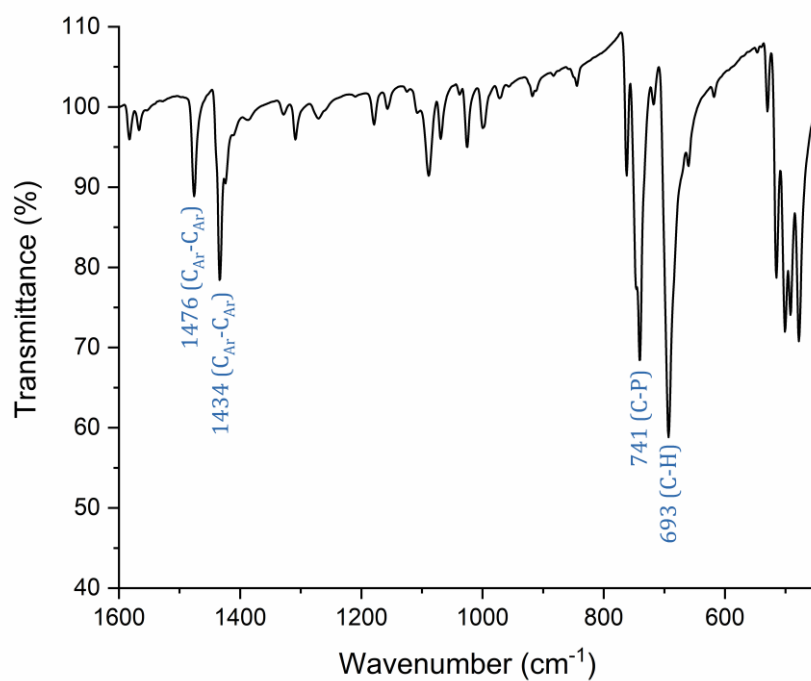


Figure S3. FT-IR spectrum of dppBz.

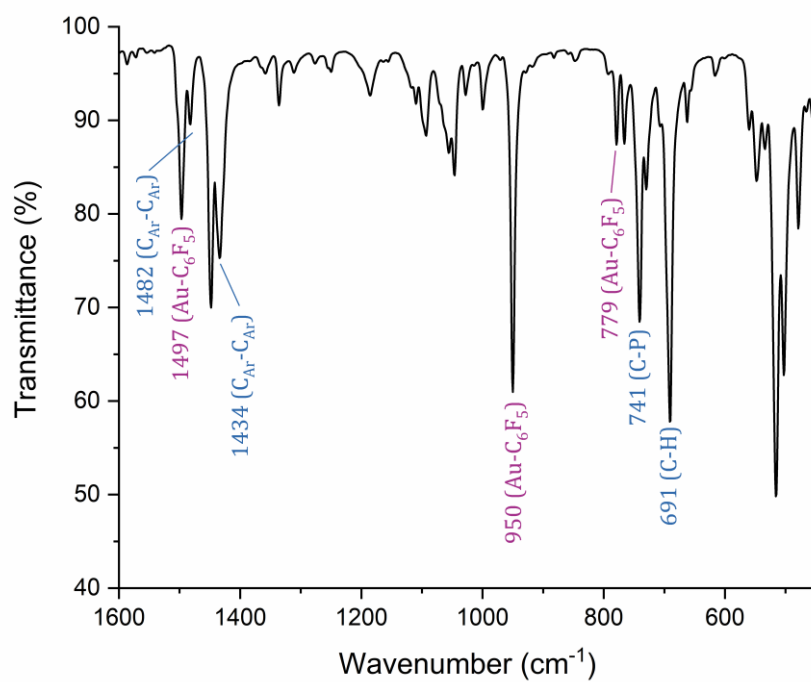


Figure S4. FT-IR spectrum of **2**. Signals related to the $[\text{Au}(\text{C}_6\text{F}_5)_2]^-$ fragment and the dppBz ligand are shown in magenta and blue, respectively.

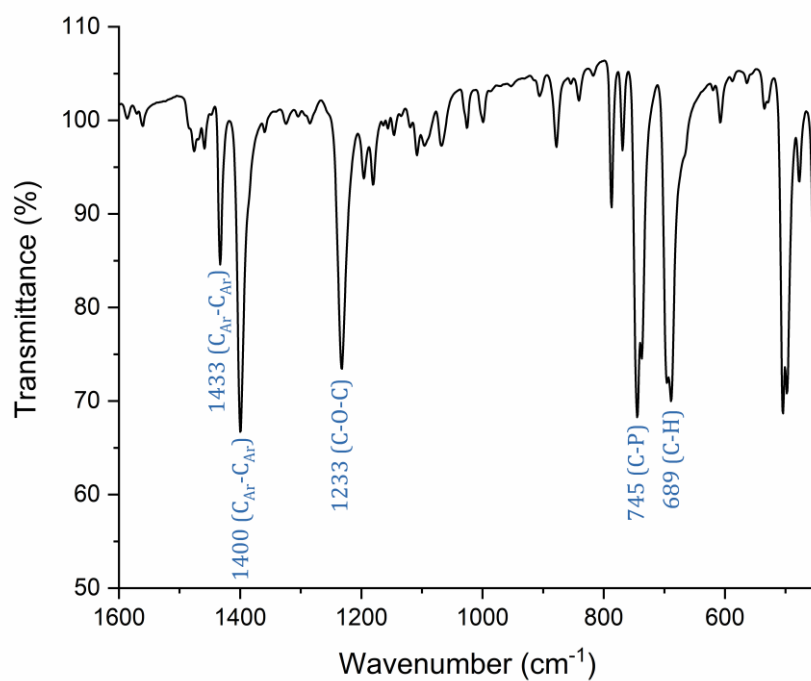


Figure S5. FT-IR spectrum of Xantphos.

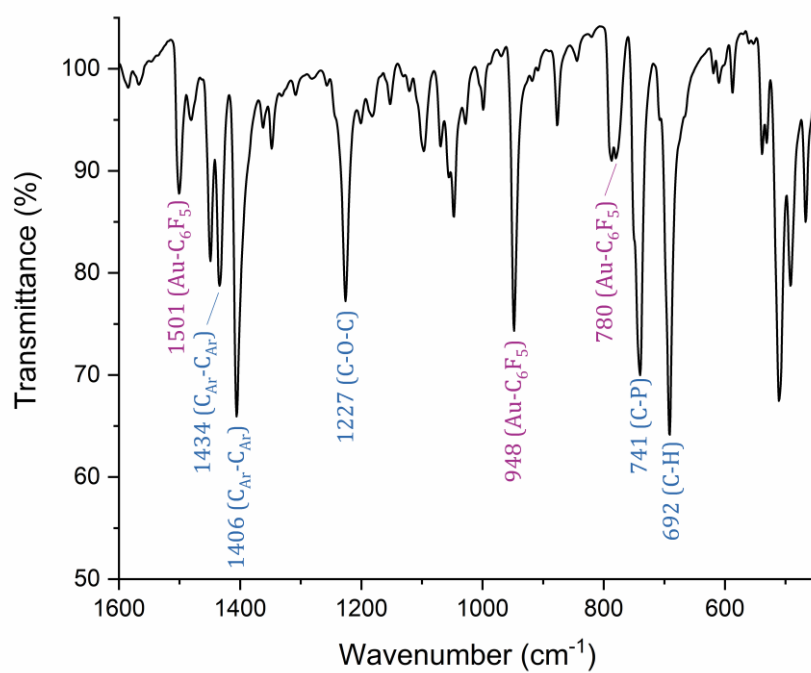


Figure S6. FT-IR spectrum of **3**. Signals related to the $[\text{Au}(\text{C}_6\text{F}_5)_2]^-$ fragment and the Xantphos ligand are shown in magenta and blue, respectively.

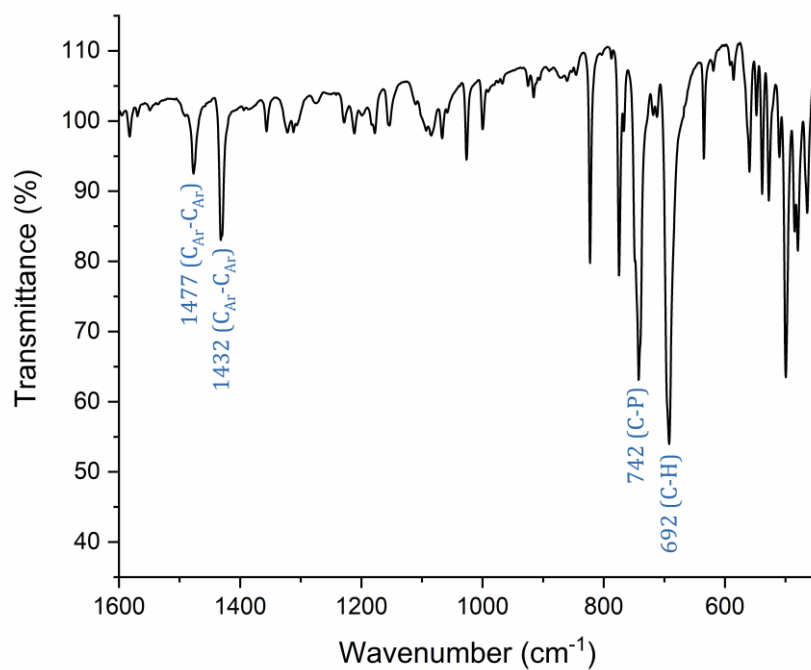


Figure S7. FT-IR spectrum of dpnp.

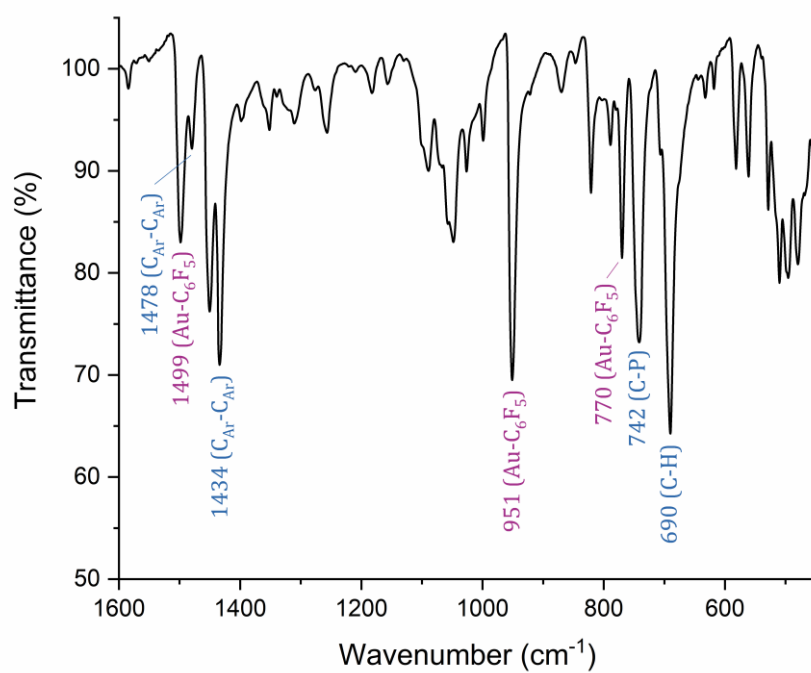


Figure S8. FT-IR spectrum of **4**. Signals related to the $[\text{Au}(\text{C}_6\text{F}_5)_2]^-$ fragment and the dpnp ligand are shown in magenta and blue, respectively.

1.2. ^1H NMR spectra

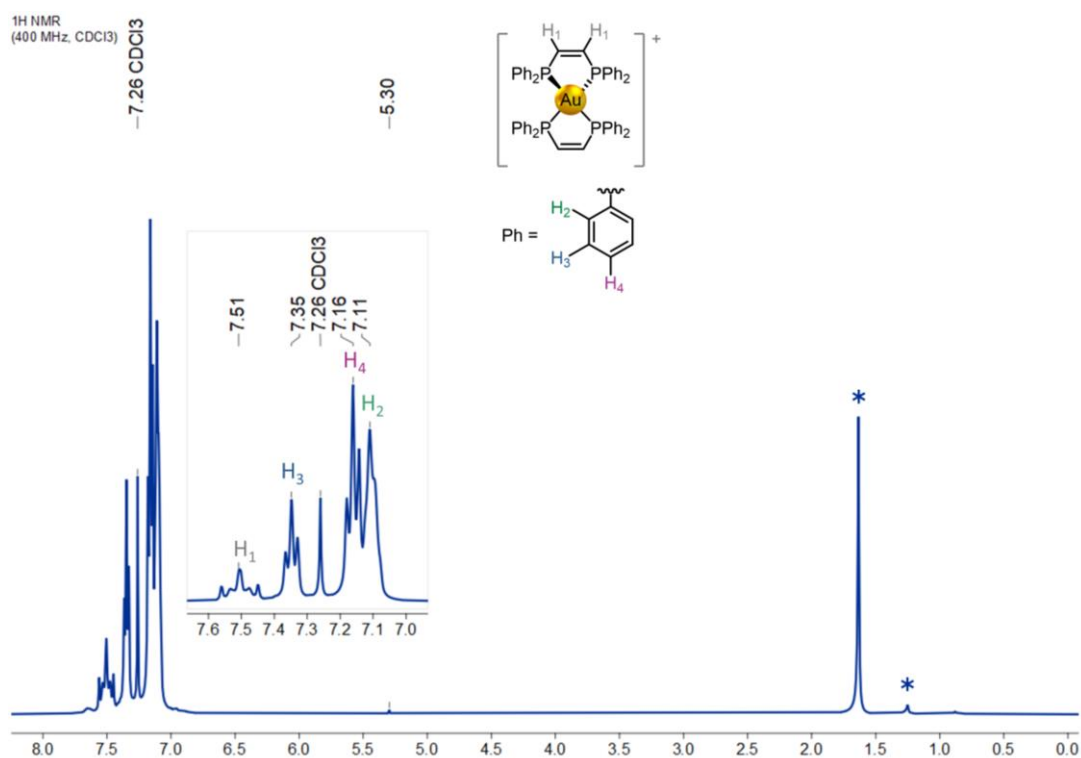


Figure S9. ^1H NMR (400 MHz, 298 K) spectrum of **1** in CDCl_3 .
(* Solvent residual peaks: Et_2O and H_2O)

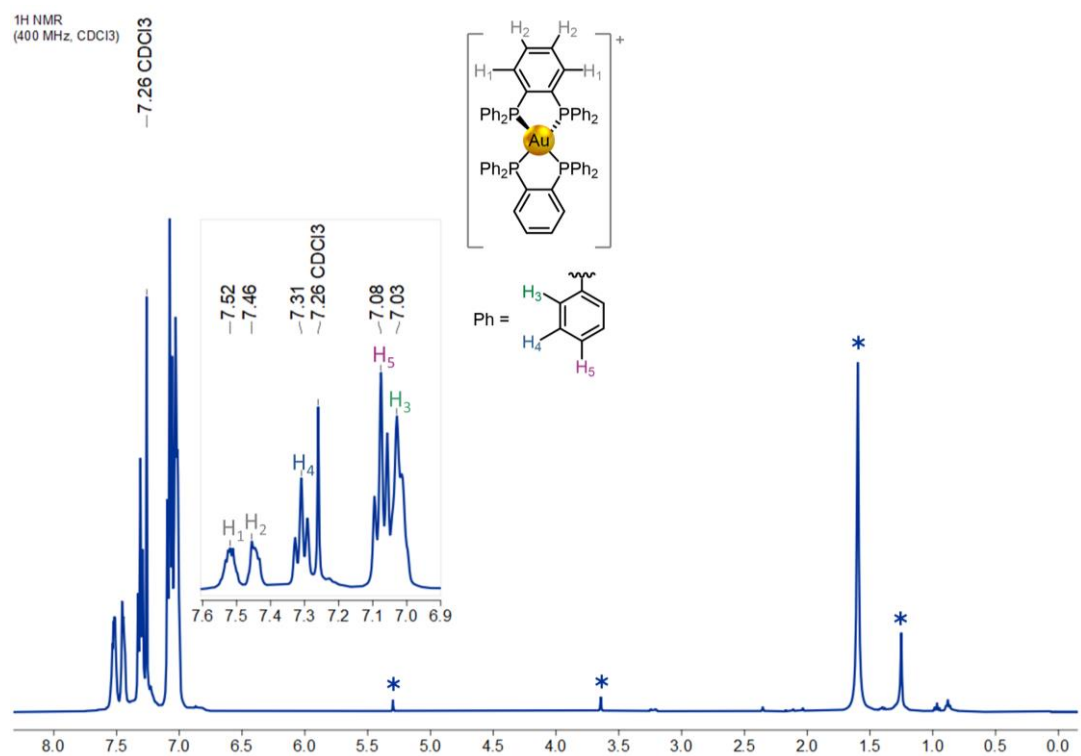


Figure S10. ^1H NMR (400 MHz, 298 K) spectrum of **2** in CDCl_3 .
(* Solvent residual peaks: CH_2Cl_2 , Et_2O and H_2O)

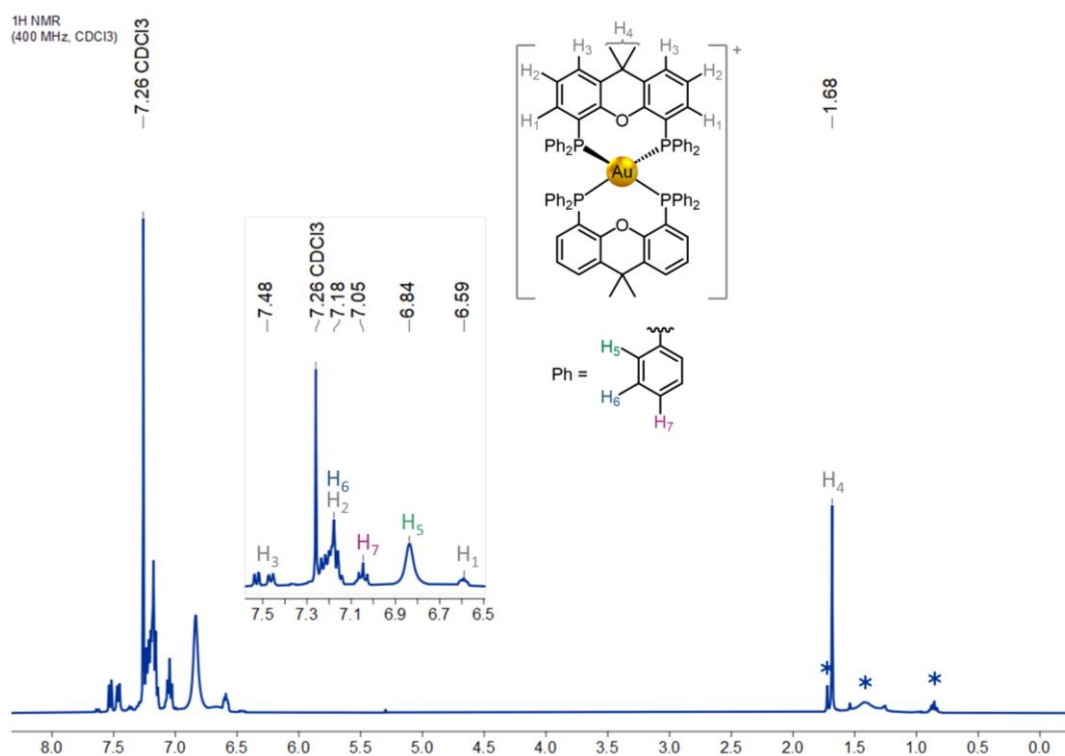


Figure S11. ¹H NMR (400 MHz, 298 K) spectrum of **3** in CDCl₃.
(* Solvent residual peaks: H₂O and *n*-hexane)

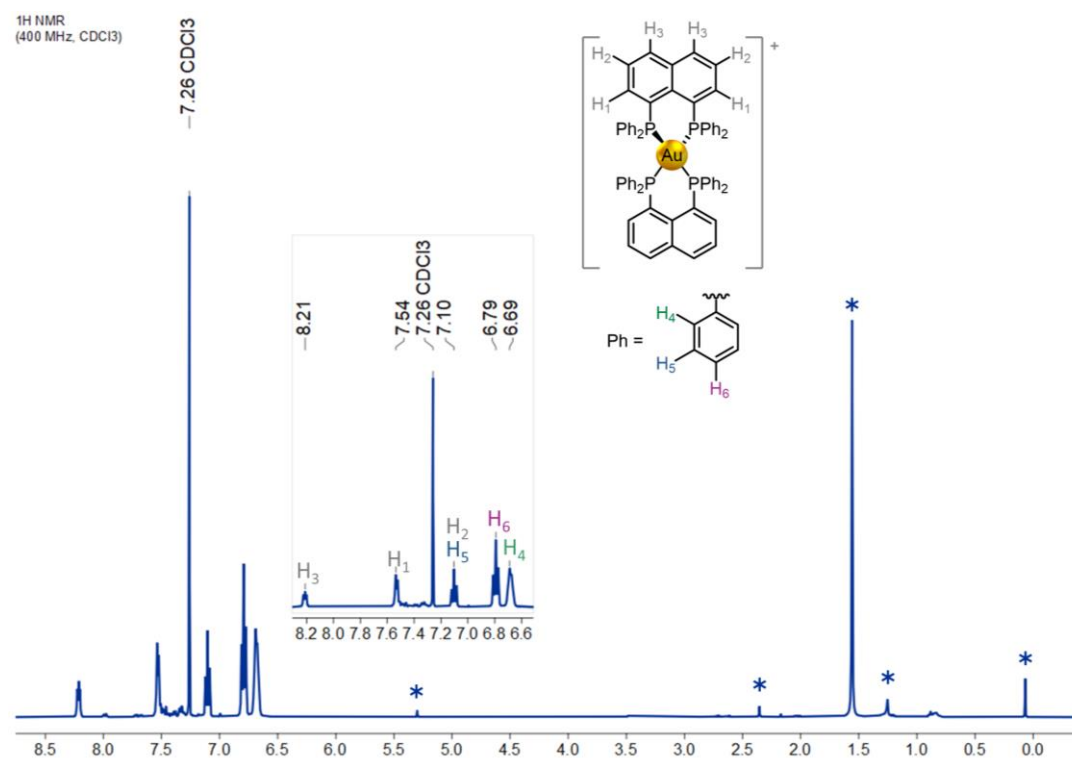


Figure S12. ¹H NMR (400 MHz, 298 K) spectrum of **4** in CDCl₃.
(* Solvent residual peaks: CH₂Cl₂, Et₂O, acetone, H₂O and silicon grease)

1.3. ^{13}C NMR spectra

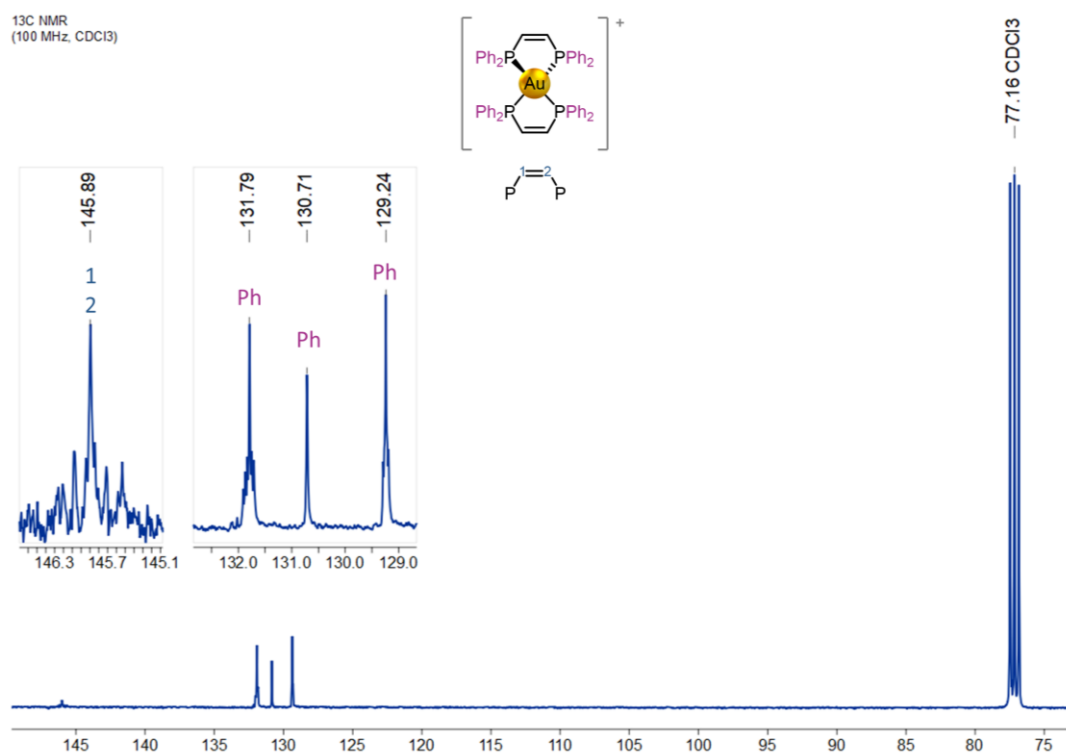


Figure S13. ^{13}C NMR (300 MHz, 298 K) spectrum of **1** in CDCl_3 .

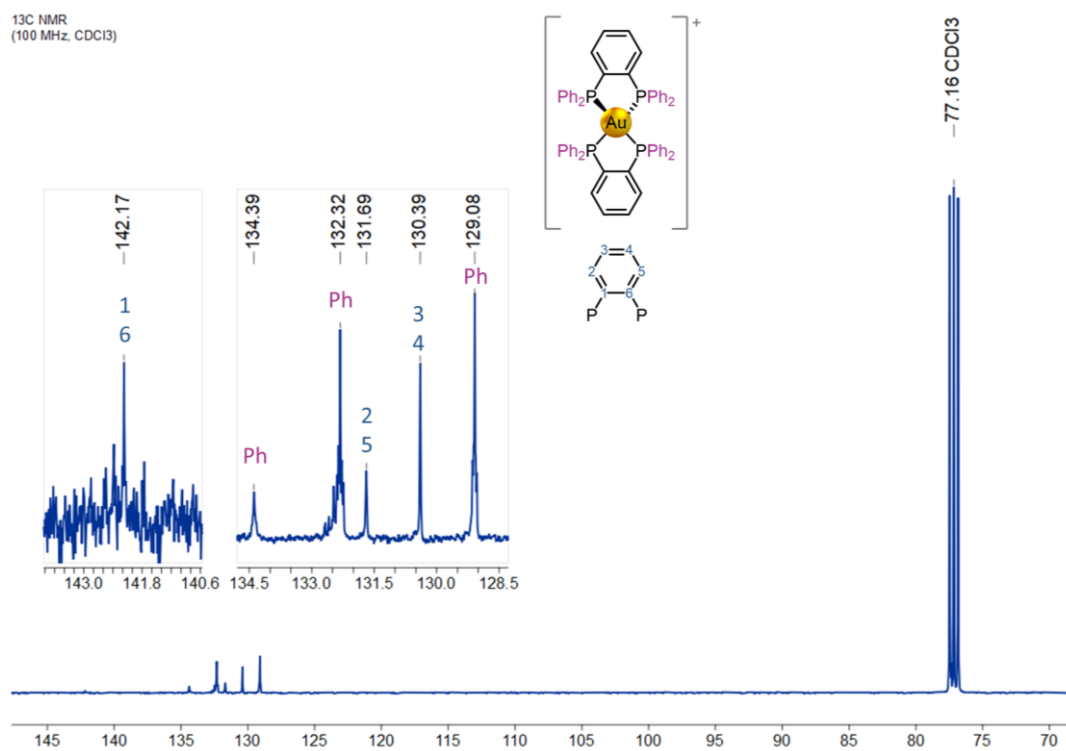


Figure S14. ^{13}C NMR (100 MHz, 298 K) spectrum of **2** in CDCl_3 .

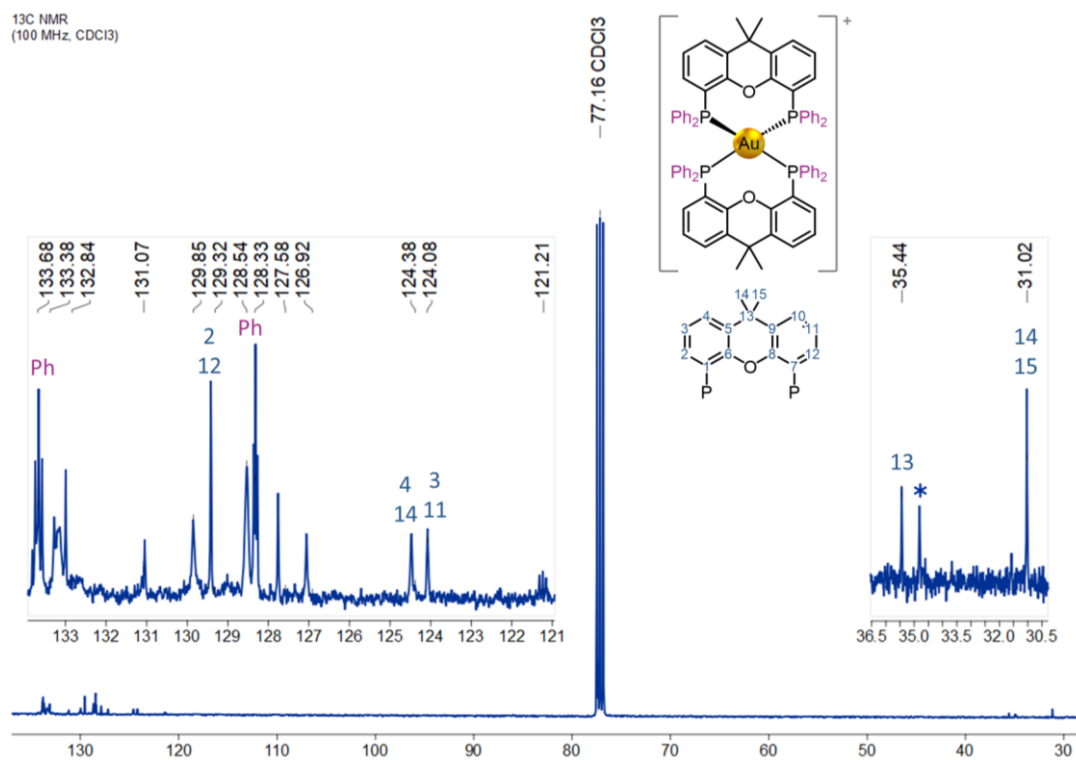


Figure S15. ¹³C NMR (100 MHz, 298 K) spectrum of **3** in CDCl₃.
(* Solvent residual peaks: acetone)

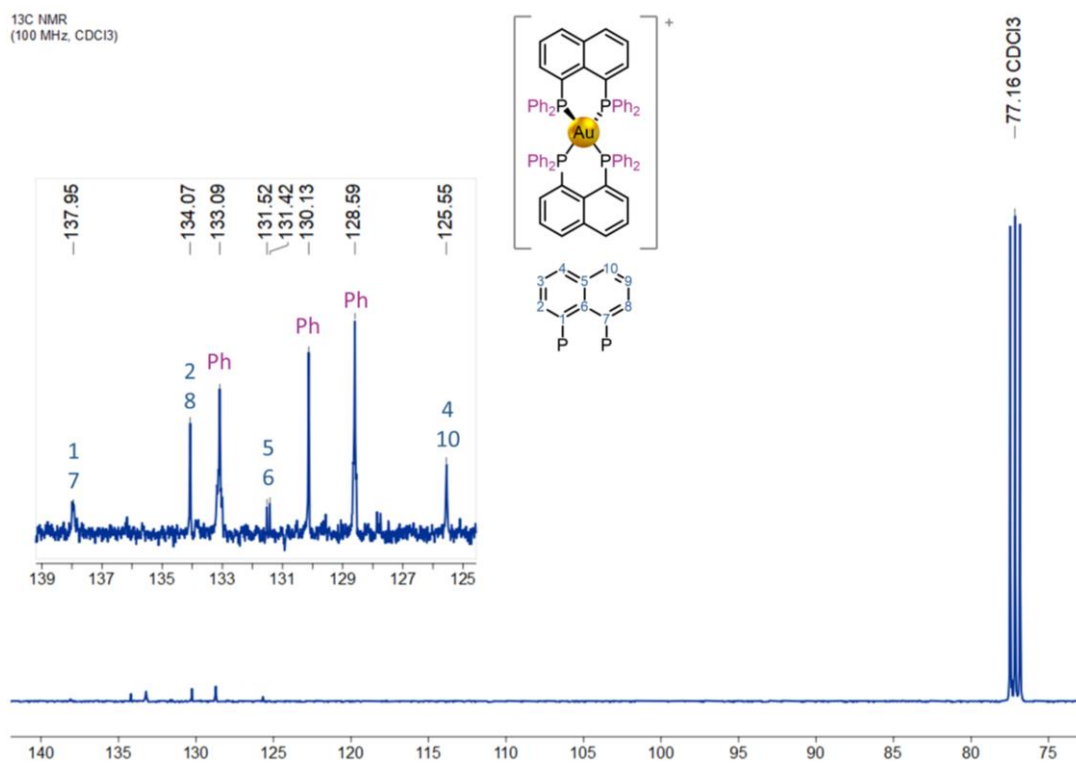


Figure S16. ¹³C NMR (100 MHz, 298 K) spectrum of **4** in CDCl₃.

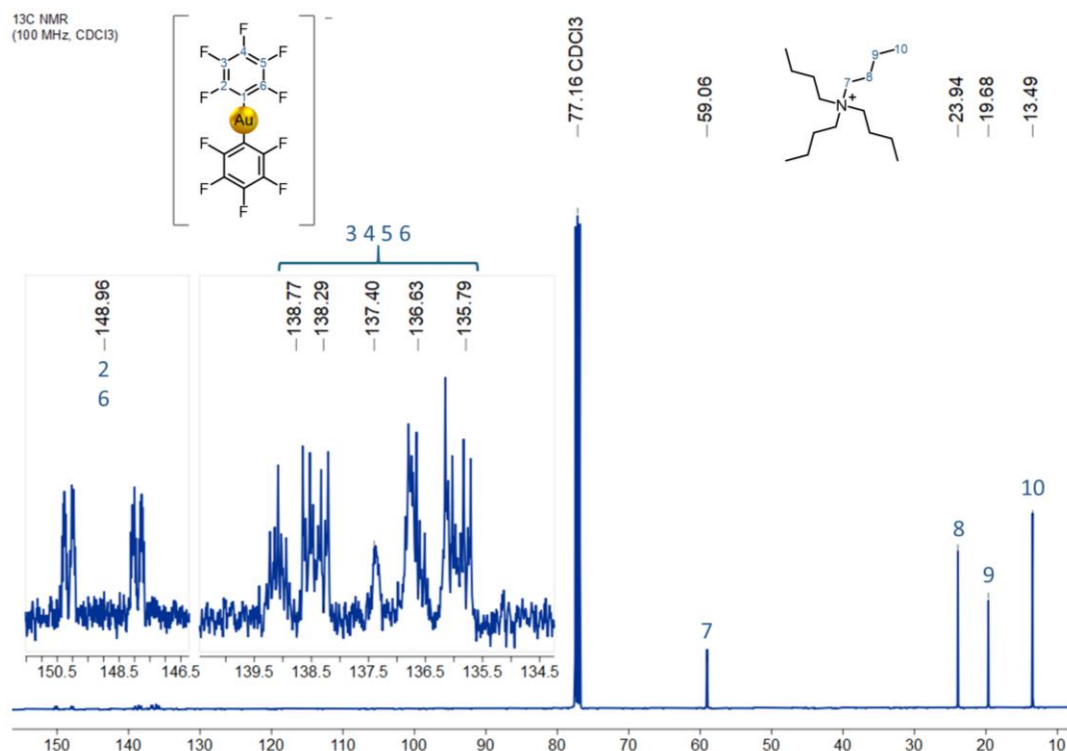


Figure S18. ¹³C NMR (100 MHz, 298 K) spectrum of NBu₄[Au(C₆F₅)₂] in CDCl₃.

None of the carbon atoms located on the perhaloaryl groups of the counterions were observed in the ¹³C{¹H} NMR spectra of complexes **1-4** (Figures S13-S16); nevertheless, the presence of those moieties was already confirmed by IR and ¹⁹F NMR spectroscopy. For comparison, the ¹³C{¹H} NMR spectrum of NBu₄[Au(C₆F₅)₂] (Figure S18) was also registered to indicate where the corresponding signals are expected to appear. In this case, the spectrum required an acquisition time twice as long as that of the complex samples, and even then, the perhaloaryl carbon signals are barely visible compared to those of the tetrabutylammonium cations. This can be attributed to the different ¹³C-¹⁹F couplings experienced by each carbon, which significantly reduces the signal intensity.

1.4. ^{19}F NMR spectra

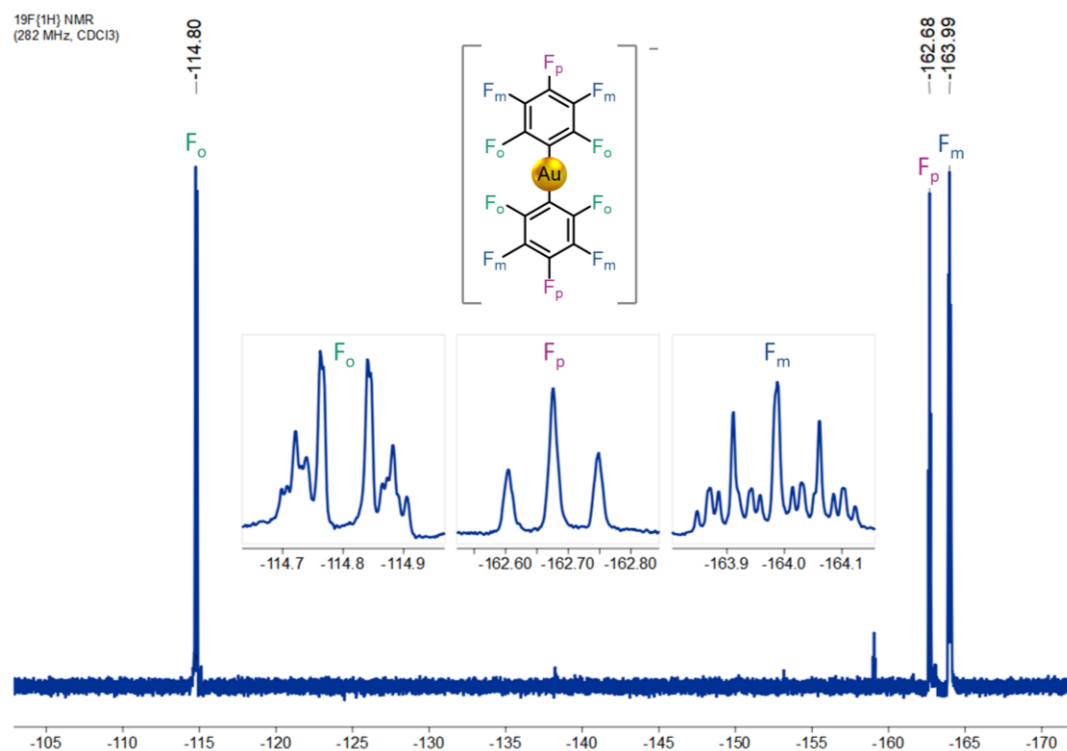


Figure S19. $^{19}\text{F}\{^1\text{H}\}$ NMR (282 MHz, 298 K) spectrum of **1** in CDCl_3 .

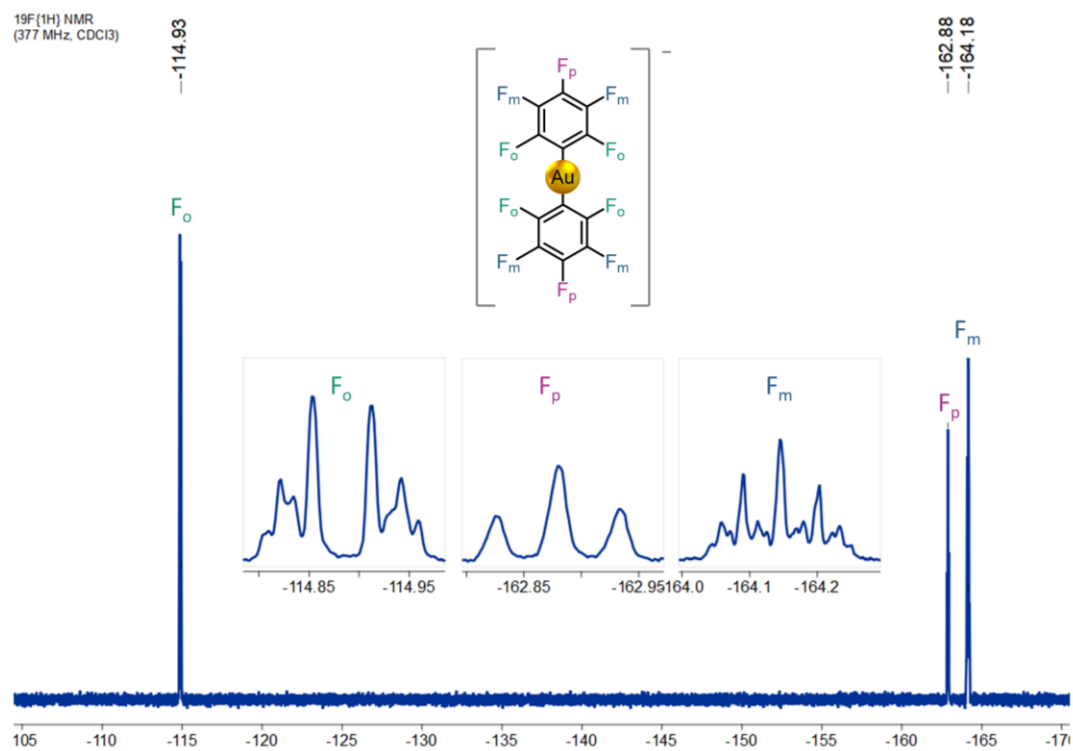


Figure S20. $^{19}\text{F}\{^1\text{H}\}$ NMR (377 MHz, 298 K) spectrum of **2** in CDCl_3 .

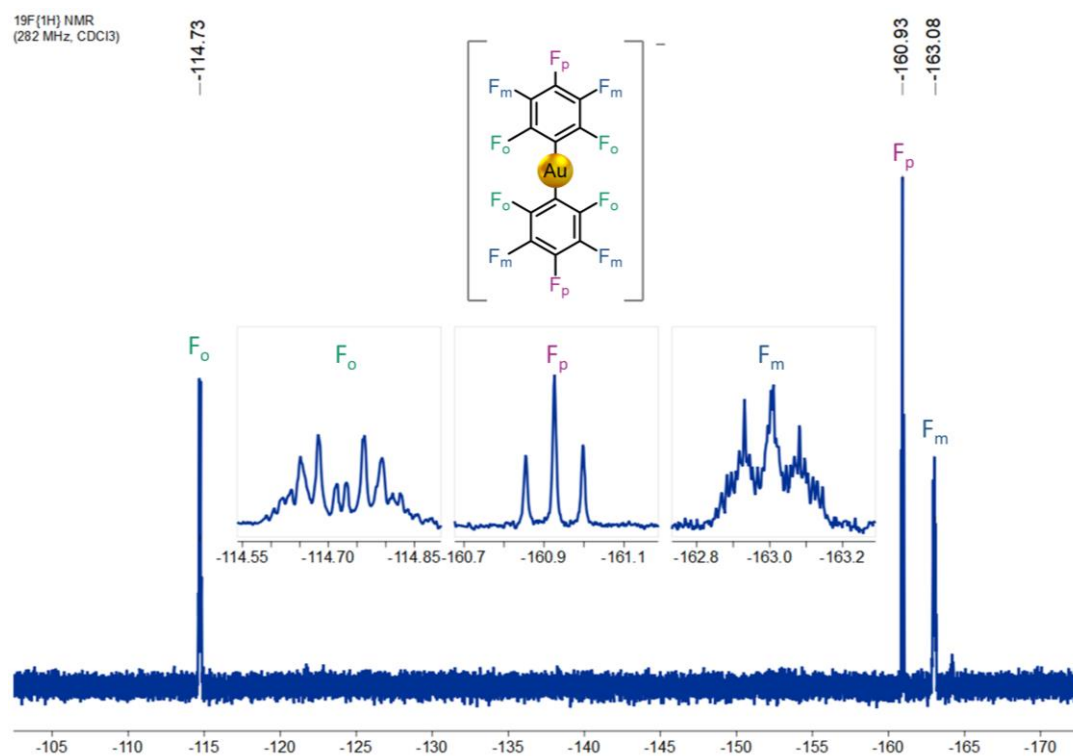


Figure S21. ¹⁹F{¹H} NMR (282 MHz, 298 K) spectrum of **3** in CDCl₃.

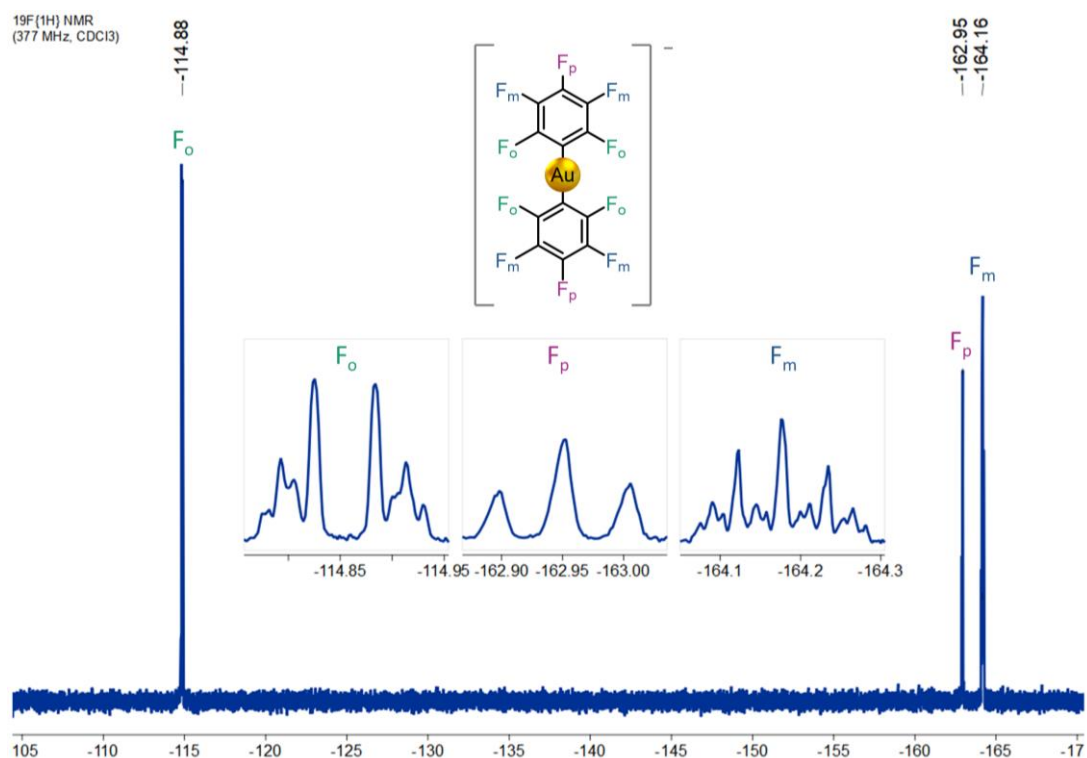


Figure S22. ¹⁹F{¹H} NMR (377 MHz, 298 K) spectrum of **4** in CDCl₃.

1.5. $^{31}\text{P}\{^1\text{H}\}$ NMR spectra

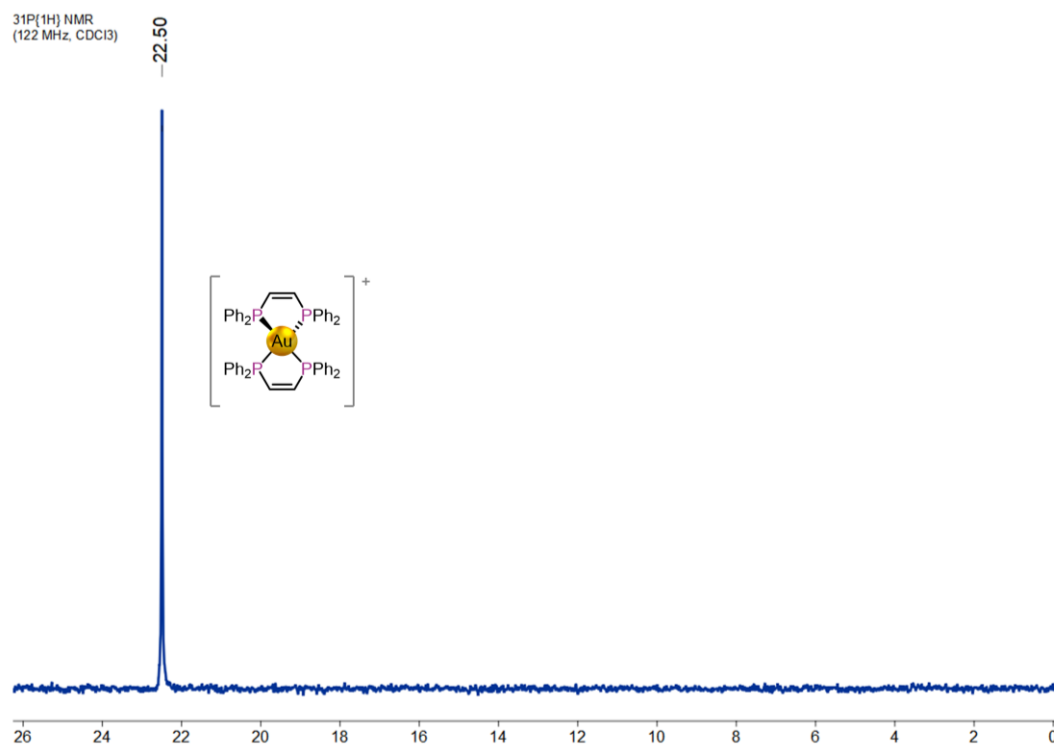


Figure S23. $^{31}\text{P}\{^1\text{H}\}$ (122 MHz, 298 K) NMR spectrum of **1** in CDCl_3 .

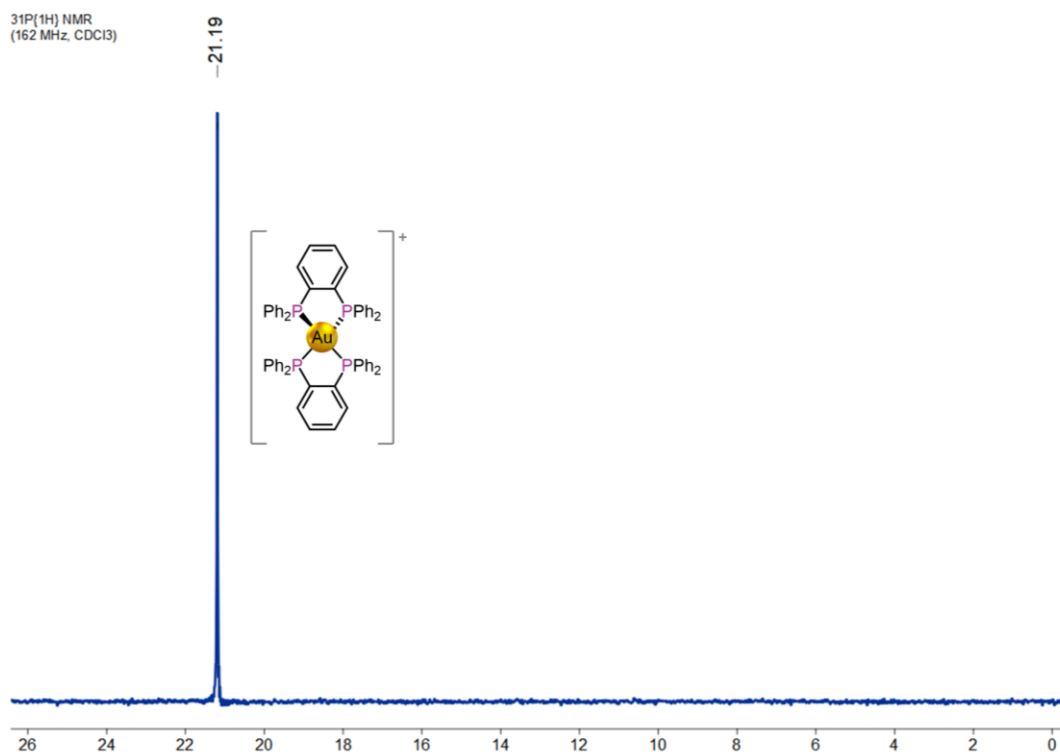


Figure S24. $^{31}\text{P}\{^1\text{H}\}$ (162 MHz, 298 K) NMR spectrum of **2** in CDCl_3 .

$^{31}\text{P}\{^1\text{H}\}$ NMR
(122 MHz, CDCl_3)

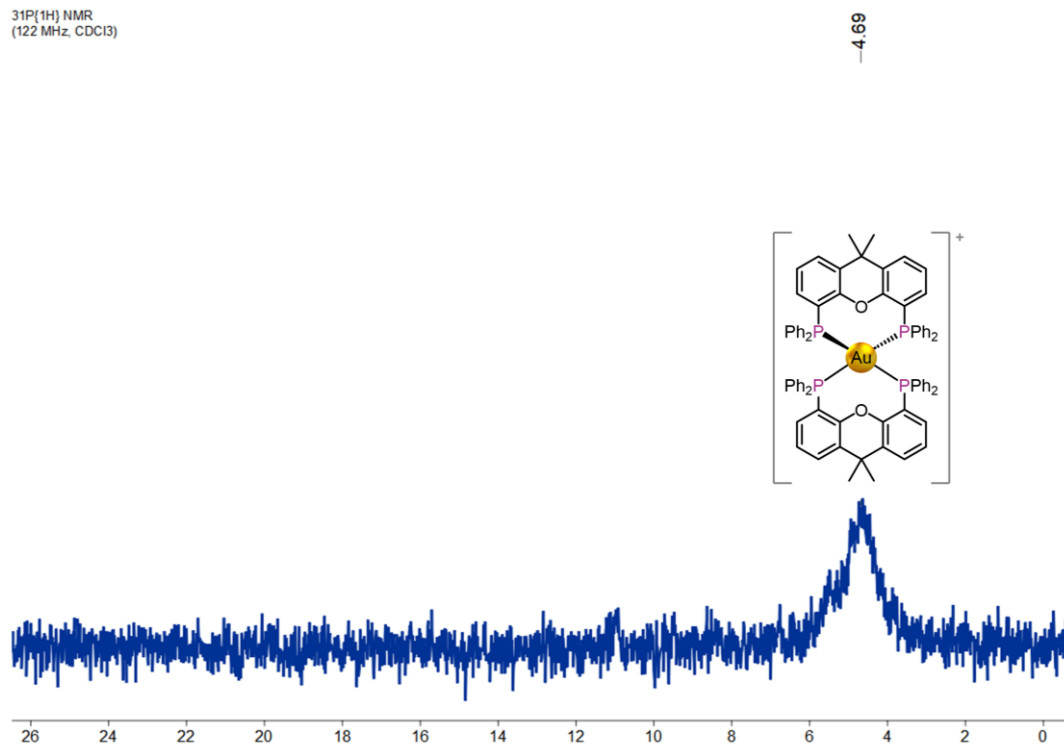


Figure S25. $^{31}\text{P}\{^1\text{H}\}$ (122 MHz, 298 K) NMR spectrum of **3** in CDCl_3 .

$^{31}\text{P}\{^1\text{H}\}$ NMR
(162 MHz, CDCl_3)

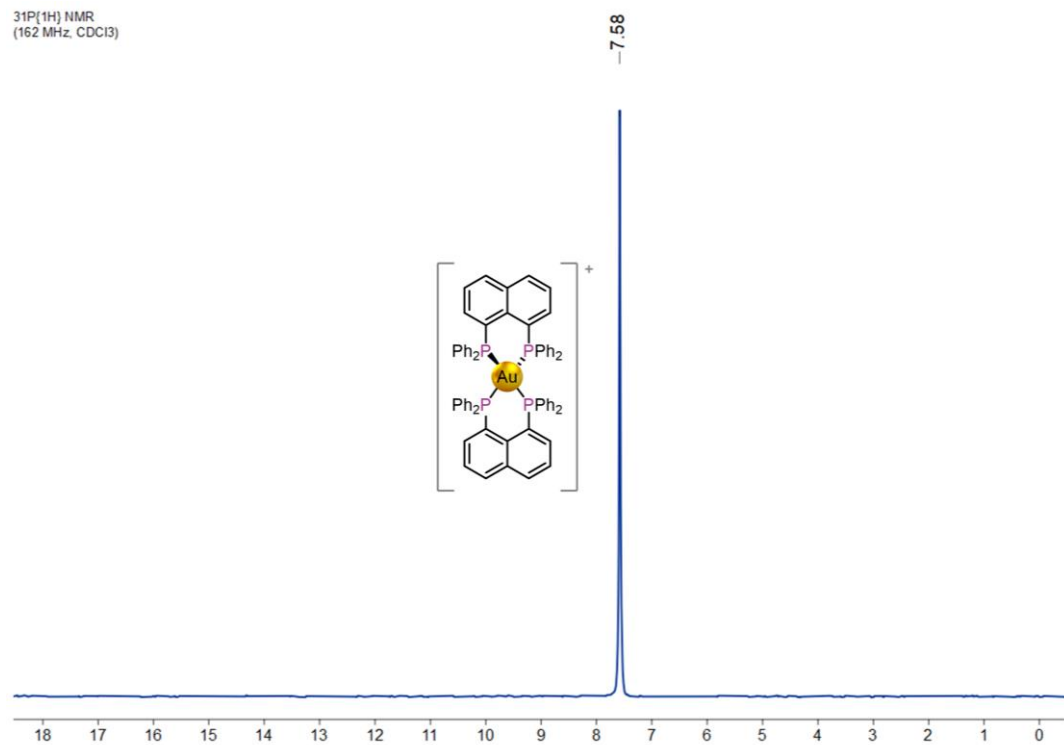


Figure S26. $^{31}\text{P}\{^1\text{H}\}$ (162 MHz, 298 K) NMR spectrum of **4** in CDCl_3 .

Table S1. $^{31}\text{P}\{^1\text{H}\}$ NMR chemical shift data for compounds **1-4** and their respective free diphosphine ligands.

Complex	Coordinated ligand (ppm)	Free ligand (ppm)
[Au(<i>dppe</i>) ₂][Au(C ₆ F ₅) ₂] (1)	22.50	-23.27
[Au(<i>dppBz</i>) ₂][Au(C ₆ F ₅) ₂] (2)	21.19	-13.90
[Au(<i>Xantphos</i>) ₂][Au(C ₆ F ₅) ₂] (3)	4.69	-18.10
[Au(<i>dppn</i>) ₂][Au(C ₆ F ₅) ₂] (4)	7.58	-14.26

1.6. Single crystal X-ray diffraction analyses

Table S2. Data collection and structure refinement details for complexes **1**·CH₂Cl₂, **2** and **4**.

Complex	1 ·CH ₂ Cl ₂	2	4
Chemical Formula	C ₆₄ H ₄₄ Au ₂ F ₁₀ P ₄ ·CH ₂ Cl ₂	C ₇₂ H ₄₈ Au ₂ F ₁₀ P ₄	C ₈₀ H ₅₂ Au ₂ F ₁₀ P ₄
Crystal habit	Colourless prism	Colourless prism	Orange prism
Crystal size/mm	0.081 x 0.063 x 0.035	0.448 x 0.255 x 0.222	0.230 x 0.065 x 0.019
Crystal system	Triclinic	Monoclinic	Monoclinic
Space group	P-1	C2/c	C2/c
a/Å	11.4807(7)	19.3527(10)	40.936(2)
b/Å	12.1800(8)	13.7248(7)	13.3646(6)
c/Å	22.4139(15)	22.9401(9)	29.6644(15)
α/°	76.001(3)	90	90
β/°	88.386(2)	95.829(2)	114.579(2)
γ/°	74.952(2)	90	90
V/Å³	2934.9(3)	6061.7(5)	14758.6(13)
Z	2	4	8
D_c/g cm⁻³	1.817	1.776	1.549
M	1605.73	1620.91	1721.03
F(000)	1556	3152	6720
T/K	100(2)	125.55	300.00
2θ_{max}/°	55.832	53.472	55.828
μ(Mo-Kα)/mm⁻¹	5.267	5.016	4.125
No. refl. measured	78031	15203	240733
No. unique refl.	13960	4818	17609
R_{int}	0.0521	0.0558	0.0764
R[F > 2σ(F)]^[a]	0.0280	0.0303	0.0395
wR[F², all refl.]^[b]	0.0620	0.0542	0.1052
No. of refl. Used [F > 2σ(F)]	13960	4817	17609
No. of parameters	760	399	835
No. of restraints	0	0	0
S^[c]	1.023	1.021	1.026
Max. residual electron density/e·Å⁻³	0.75	0.54	0.99

^[a] $R: (F) = \sum ||F_o| - |F_c|| / \sum |F_o|$.

^[b] $wR: (F^2) = [\sum \{w(F_o^2 - F_c^2)^2\} / \sum \{w(F_o^2)^2\}]^{0.5}$; $w^{-1} = \sigma^2(F_o^2) + (aP)^2 + bP$, where $P = [F_o^2 + 2F_c^2]/3$ and a and b are constants adjusted by the program.

^[c] $S = [\sum \{w(F_o^2 - F_c^2)^2\} / (n-p)]^{0.5}$, where n is the number of data and p the number of parameters.

2. Optical properties

2.1. UV-Vis absorption spectra in the solid state

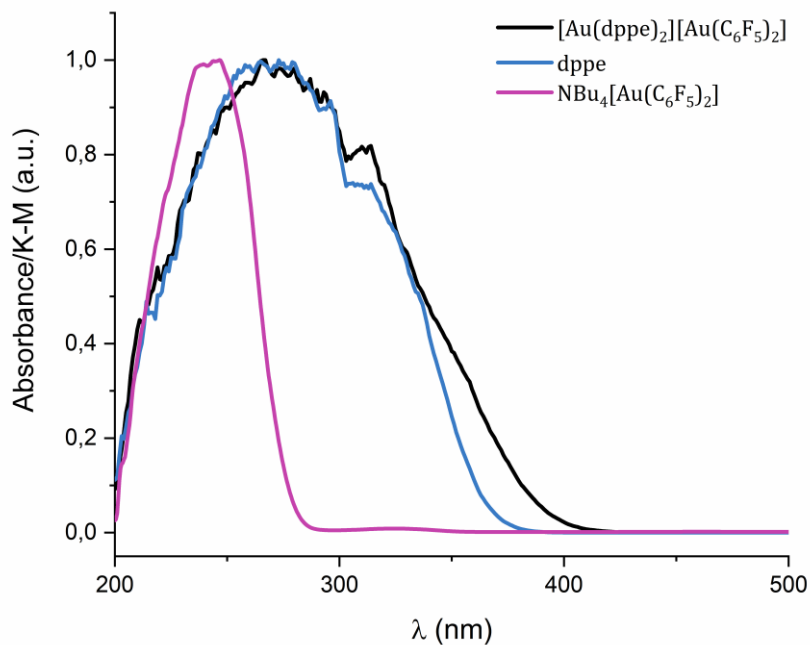


Figure S27. UV-Vis absorption spectra in the solid state for $[\text{Au}(\text{dppe})_2][\text{Au}(\text{C}_6\text{F}_5)_2]$ (**1**) (black), dppe (blue) and $\text{NBu}_4[\text{Au}(\text{C}_6\text{F}_5)_2]$ (magenta).

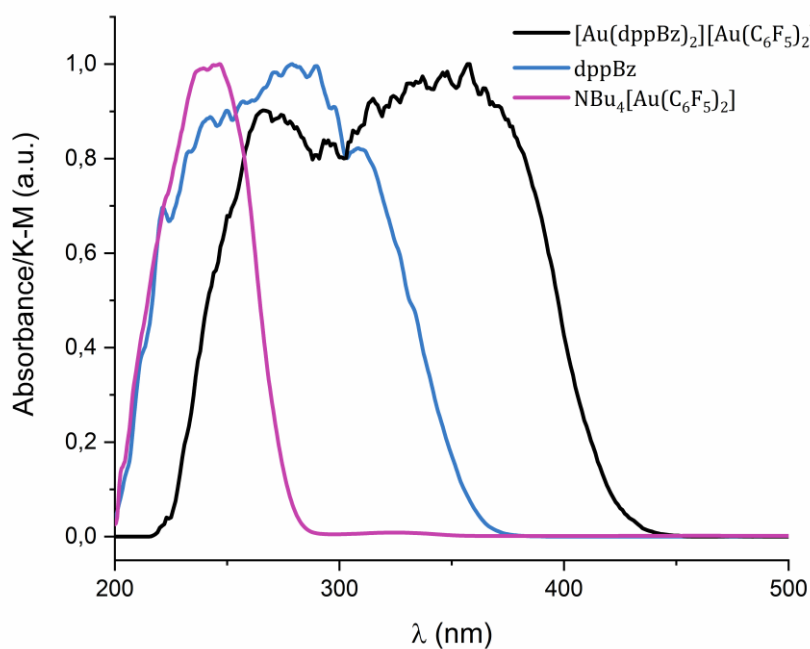


Figure S28. UV-Vis absorption spectra in the solid state for $[\text{Au}(\text{dppBz})_2][\text{Au}(\text{C}_6\text{F}_5)_2]$ (**2**) (black), dppBz (blue) and $\text{NBu}_4[\text{Au}(\text{C}_6\text{F}_5)_2]$ (magenta).

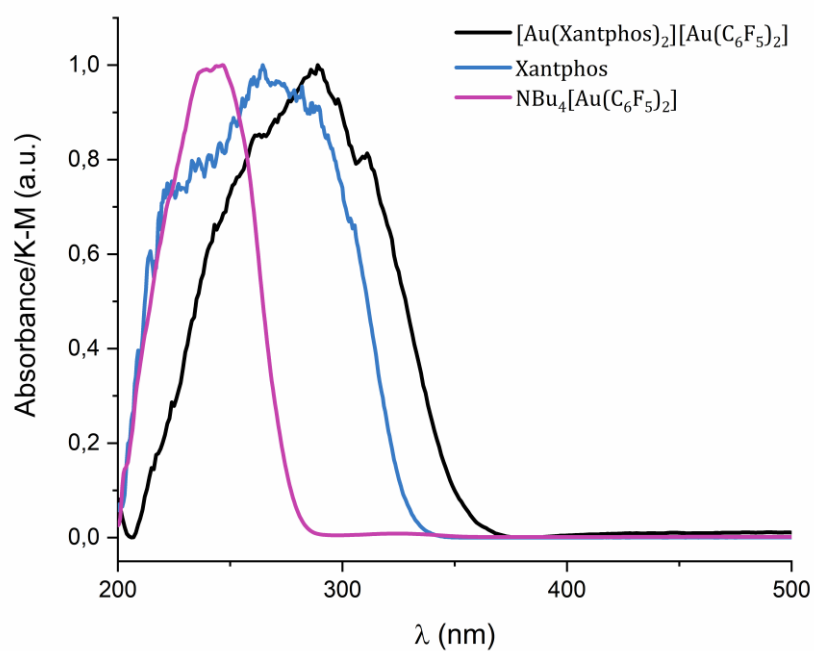


Figure S29. UV-Vis absorption spectra in the solid state for [Au(Xantphos)₂][Au(C₆F₅)₂] (**3**) (black), Xantphos (blue) and NBu₄[Au(C₆F₅)₂] (magenta).

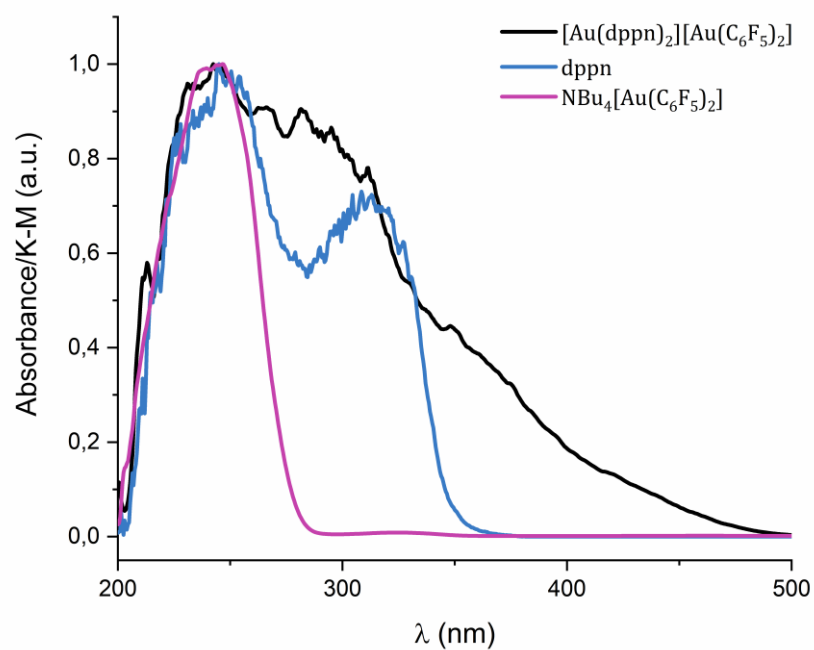


Figure S30. UV-Vis absorption spectra in the solid state for [Au(dppn)₂][Au(C₆F₅)₂] (**4**) (black), dppn (blue) and NBu₄[Au(C₆F₅)₂] (magenta).

2.2. UV-Vis absorption spectra in CH₂Cl₂ solution

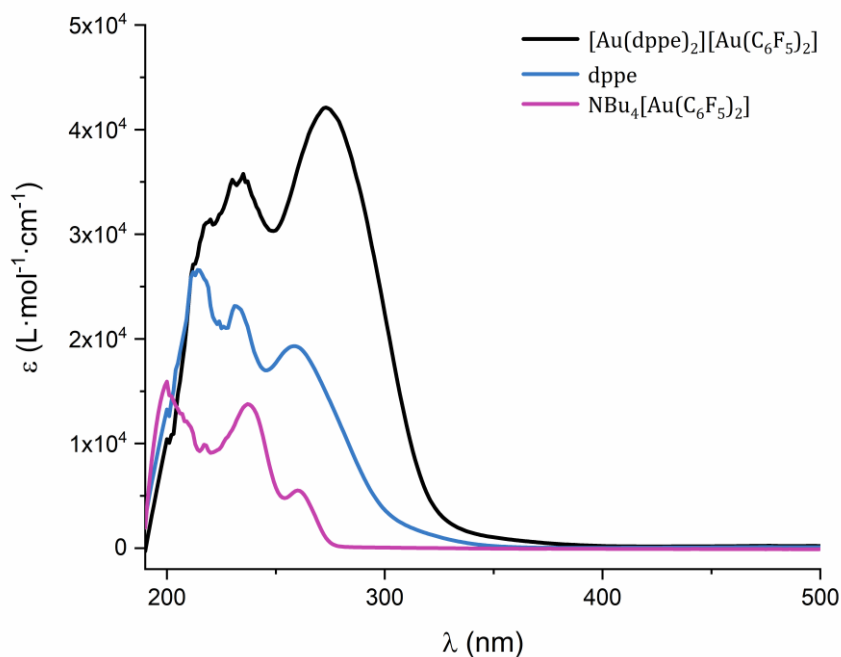


Figure S31. UV-Vis absorption spectra in CH₂Cl₂ solution ($5 \cdot 10^{-5}$ M) of complex [Au(dppe)₂][Au(C₆F₅)₂] (**1**) (black), dppe (blue) and NBu₄[Au(C₆F₅)₂] (magenta).

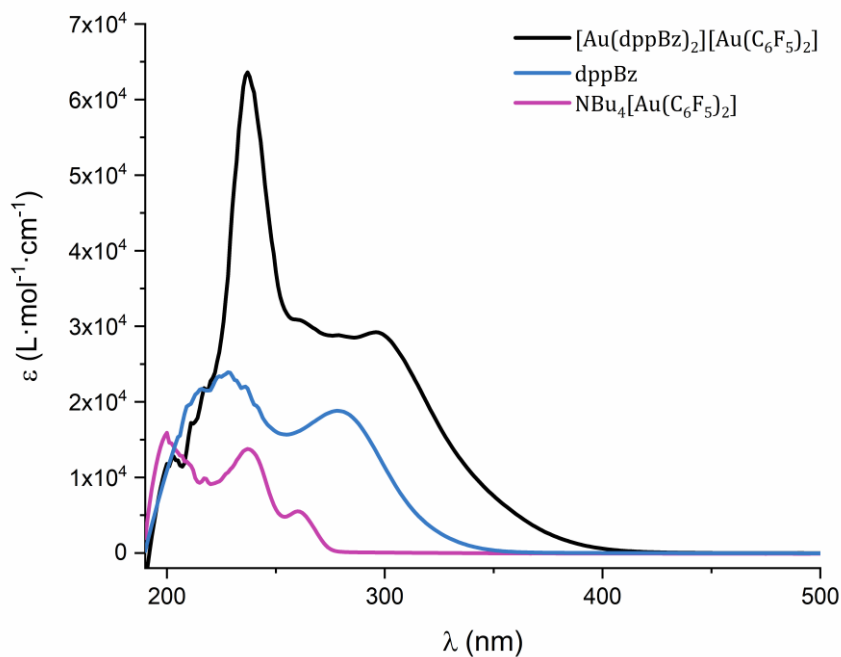


Figure S32. UV-Vis absorption spectra in CH₂Cl₂ solution ($5 \cdot 10^{-5}$ M) of complex [Au(dppBz)₂][Au(C₆F₅)₂] (**2**) (black), dppBz (blue) and NBu₄[Au(C₆F₅)₂] (magenta).

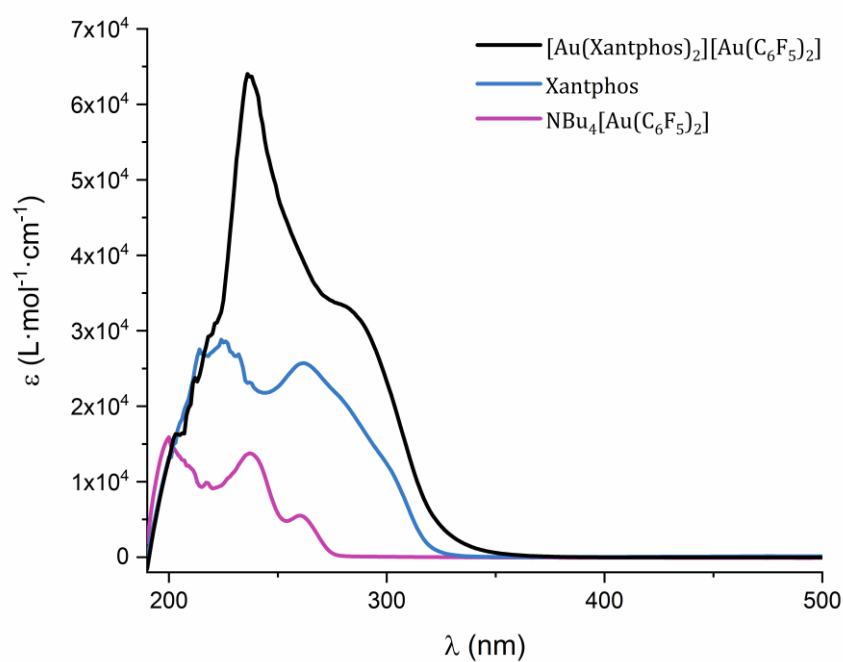


Figure S33. UV-Vis absorption spectra in CH_2Cl_2 solution ($5 \cdot 10^{-5} \text{ M}$) of complex $[\text{Au}(\text{Xantphos})_2][\text{Au}(\text{C}_6\text{F}_5)_2]$ (**3**) (black), Xantphos (blue) and $\text{NBu}_4[\text{Au}(\text{C}_6\text{F}_5)_2]$ (magenta).

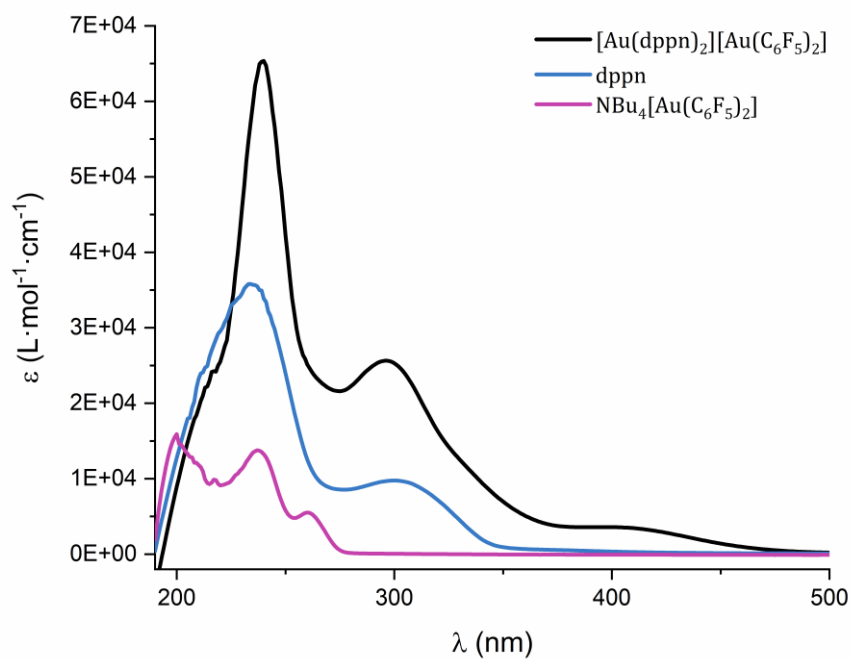


Figure S34. UV-Vis absorption spectra in CH_2Cl_2 solution ($5 \cdot 10^{-5} \text{ M}$) of complex $[\text{Au}(\text{dppn})_2][\text{Au}(\text{C}_6\text{F}_5)_2]$ (**4**) (black), dppn (blue) and $\text{NBu}_4[\text{Au}(\text{C}_6\text{F}_5)_2]$ (magenta).

2.3. Excitation and emission spectra

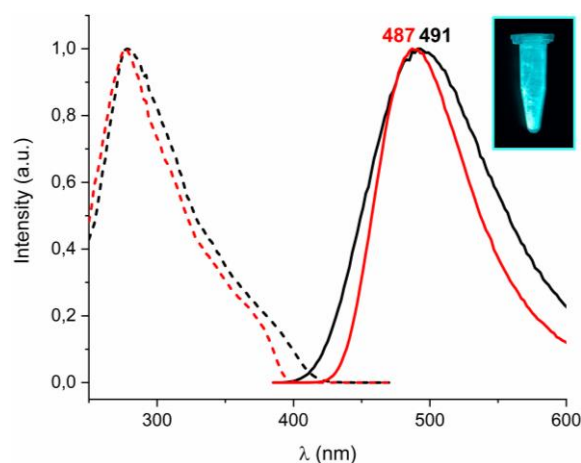


Figure S35. Excitation (dashed) and emission (solid) spectra in the solid state of **2** at room temperature (black) and 77 K (red).

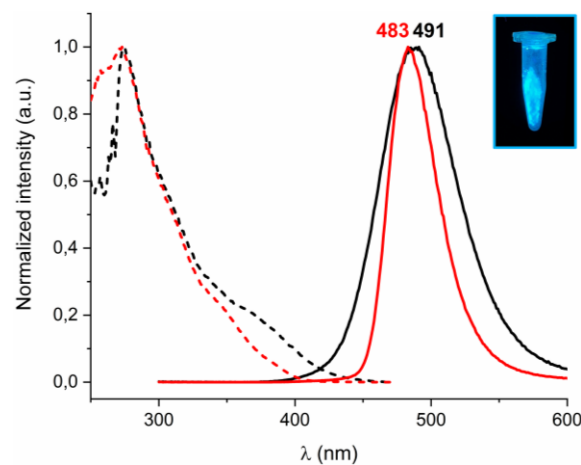


Figure S36. Excitation (dashed) and emission (solid) spectra in the solid state of **3** at room temperature (black) and 77 K (red).

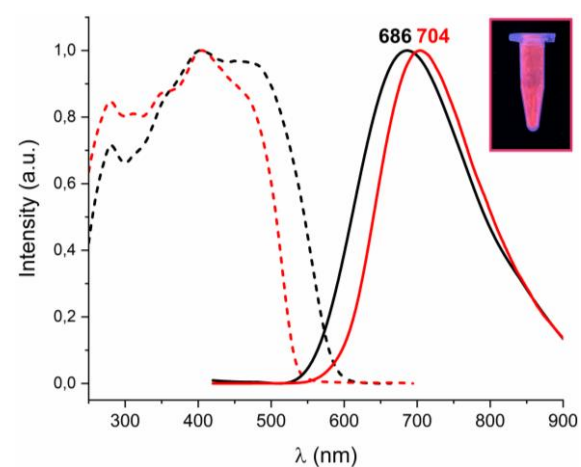


Figure S37. Excitation (dashed) and emission (solid) spectra in the solid state of **4** at room temperature (black) and 77 K (red).

2.4. Lifetimes at room temperature and at 77 K

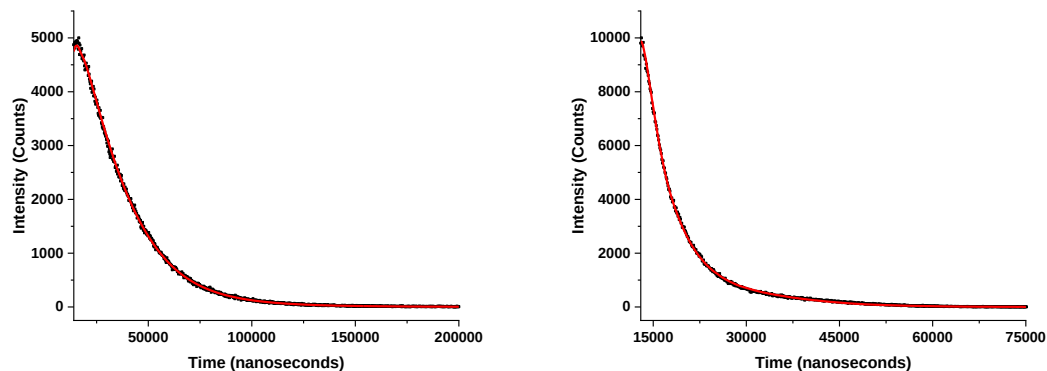


Figure S38. Lifetime decay of **2** at room temperature: $\tau_1 = 3.12 \pm 0.02 \mu\text{s}$ (97 %), $\tau_2 = 9.59 \pm 0.26 \mu\text{s}$ (3 %) ($\chi^2 = 1.34$) (left); and at 77 K: $\tau_1 = 18.37 \pm 0.13 \mu\text{s}$ (95 %), $\tau_2 = 37.42 \pm 1.74 \mu\text{s}$ (5 %) ($\chi^2 = 1.13$) (right).

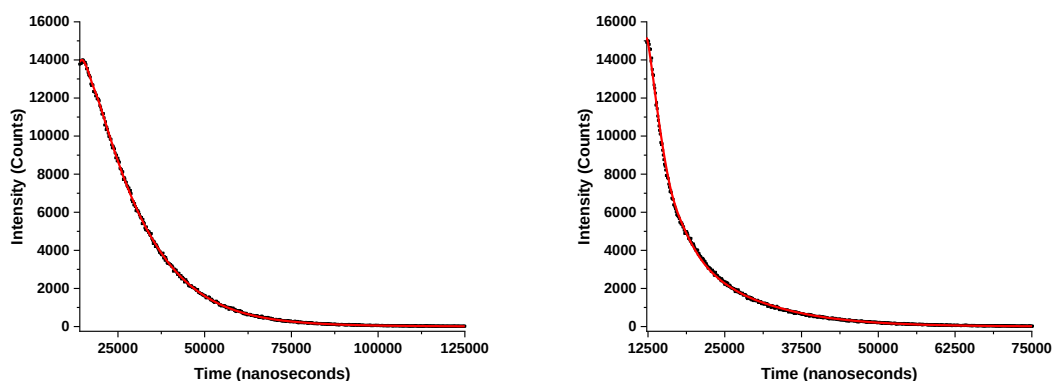


Figure S39. Lifetime decay of **3** at room temperature: $\tau_1 = 2.26 \pm 0.02 \mu\text{s}$ (88 %), $\tau_2 = 8.78 \pm 0.06 \mu\text{s}$ (12 %) ($\chi^2 = 1.28$) (left); and at 77 K: $\tau_1 = 10.96 \pm 0.07 \mu\text{s}$ (93 %), $\tau_2 = 20.92 \pm 0.57 \mu\text{s}$ (7 %) ($\chi^2 = 1.13$) (right).

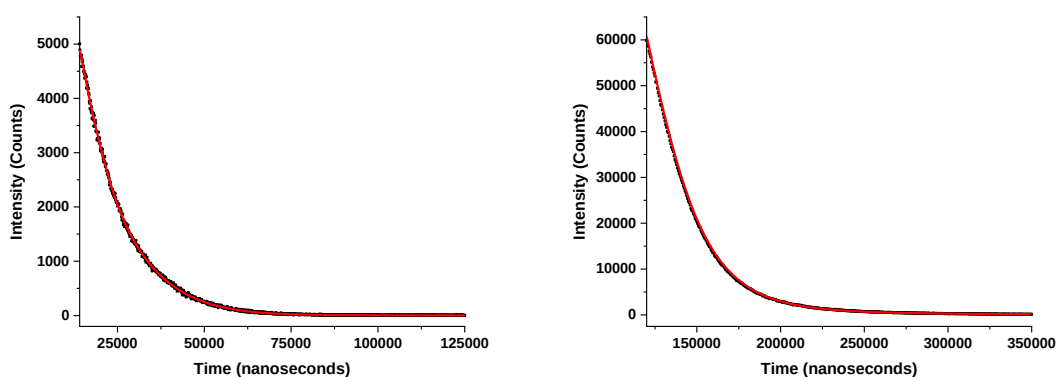


Figure S40. Lifetime decay of **4** at room temperature: $\tau_1 = 5.18 \pm 0.35 \mu\text{s}$ (40 %), $\tau_2 = 9.47 \pm 0.14 \mu\text{s}$ (60 %) ($\chi^2 = 1.16$) (left); and at 77 K: $\tau_1 = 22.37 \pm 0.03 \mu\text{s}$ (98 %), $\tau_2 = 85.79 \pm 0.37 \mu\text{s}$ (2 %) ($\chi^2 = 2.09$) (right).

2.5. Thermally activated delayed fluorescence studies

The Boltzmann-type equation:

$$\tau_{av} = \frac{3 + \exp(-\Delta E(S_1-T_1)/k_B T)}{3/\tau_T + 1/\tau_S \exp(\Delta E(S_1-T_1)/k_B T)} \quad (\text{Eq. S1})$$

where k_B is Boltzmann's constant. τ_T and τ_S are the phosphorescence ($T_1 \rightarrow S_0$) decay time and the prompt fluorescence ($S_1 \rightarrow S_0$) decay time without thermal activation, respectively.

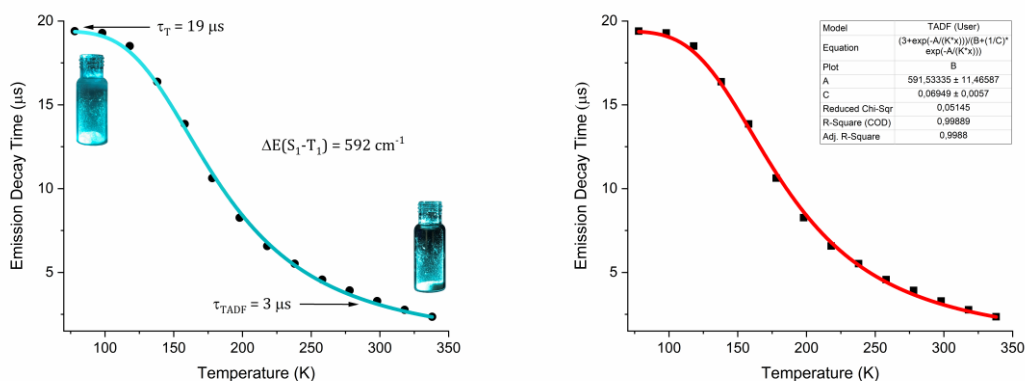


Figure S41. Temperature dependence of the emission decay time of **2**. The solid red line represents the fit of the experimental data according to Eq. S1. The fit parameters are showed in the accompanying tables.

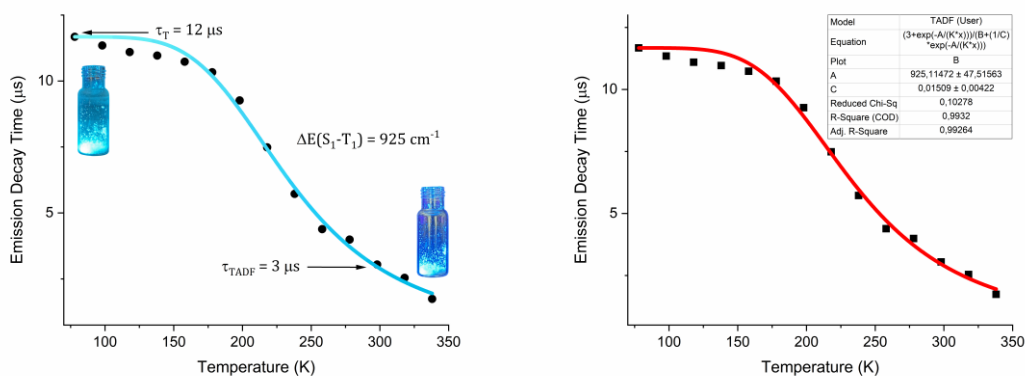


Figure S42. The temperature dependence of the emission decay time of **3**. The solid red line represents the fit of the experimental data according to Eq. S1. The fit parameters are shown in the accompanying tables.

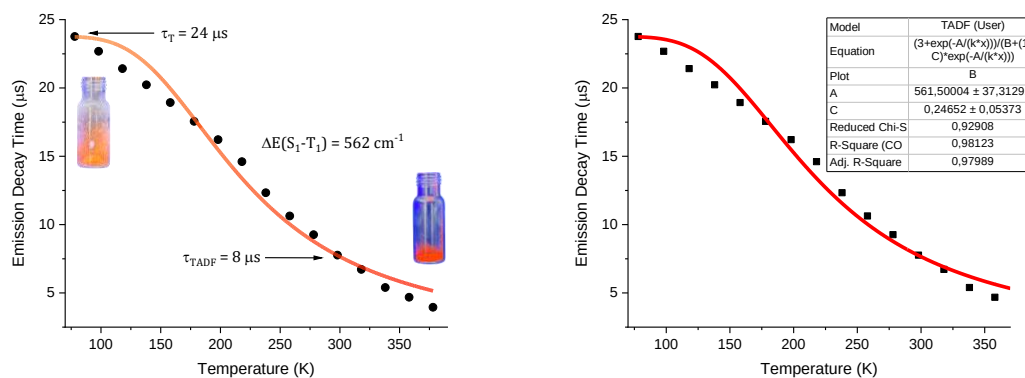


Figure S43. The temperature dependence of the emission decay time of **4**. The solid red line represents the fit of the experimental data according to Eq. S1. The fit parameters are shown in the accompanying tables.

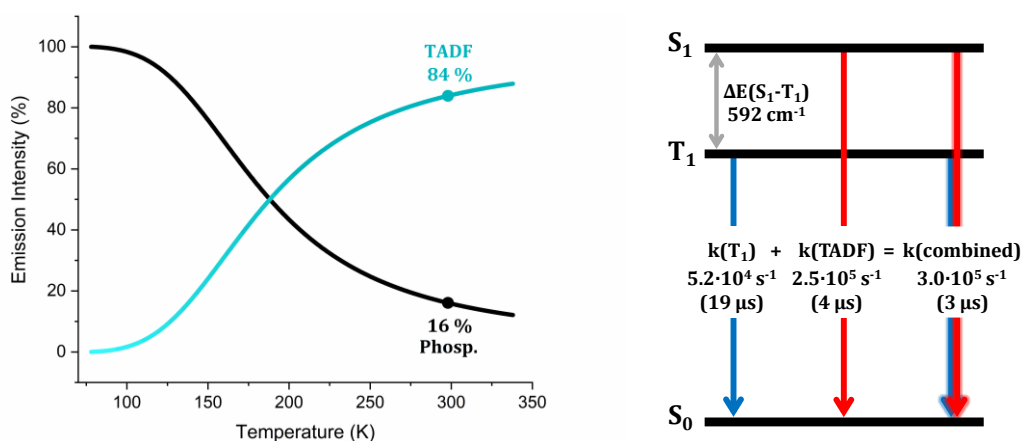


Figure S44. Left: Fractional emission intensities from TADF (turquoise) and direct phosphorescence (black) as a function of temperature calculated from the experimental data in Figure S31 using equations 4 and 5 (main text) for **2**; Right: Schematic energy-level diagram and decay times of **2** in the solid-state.

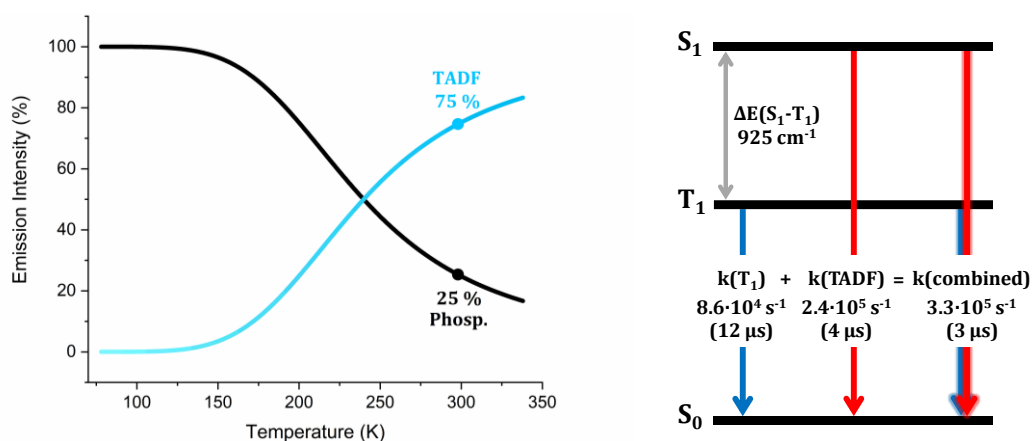


Figure S45. Left: Fractional emission intensities from TADF (blue) and direct phosphorescence (black) as a function of temperature calculated from the experimental data in Figure S32 using equations 4 and 5 (main text) for **3**; Right: Schematic energy-level diagram and decay times of **3** in the solid-state.

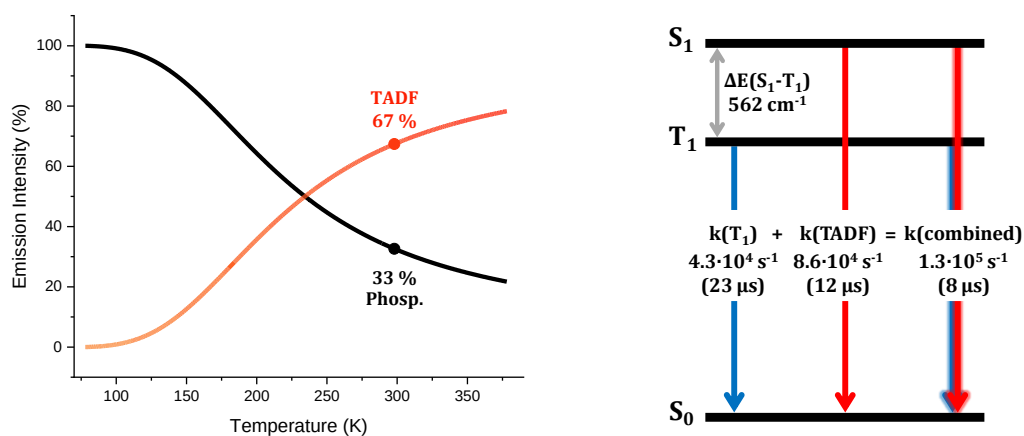


Figure S46. Left: Fractional emission intensities from TADF (orange) and direct phosphorescence (black) as a function of temperature calculated from the experimental data in Figure S33 using equations 4 and 5 (main text) for **4**; Right: Schematic energy-level diagram and decay times of **4** in the solid-state.

Table S3. Photophysical experimental parameters for **2**, **3** and **4**.

		2	3	4
298 K	λ_{em} / nm	491	491	686
	$\tau / \mu\text{s}$	3.29	3.05	7.76
	Φ	0.60	0.21	0.59
	k_r^a / s^{-1}	$1.81 \cdot 10^5$	$6.96 \cdot 10^4$	$7.65 \cdot 10^4$
	k_{nr}^b / s^{-1}	$1.22 \cdot 10^5$	$2.95 \cdot 10^5$	$5.23 \cdot 10^4$
77 K	λ_{em} / nm	487	483	704
	$\tau / \mu\text{s}$	19.40	11.67	23.76
	k_{S1} / s^{-1}	$1.44 \cdot 10^7$	$6.66 \cdot 10^7$	$4.06 \cdot 10^6$
	k_{T1} / s^{-1}	$5.16 \cdot 10^4$	$8.57 \cdot 10^4$	$4.26 \cdot 10^4$
	$\Delta E_{ST} / \text{cm}^{-1}$	592	925	562
	$\tau_s / \mu\text{s}$	0.07	0.02	0.25
	$k_{TADF}^c / \text{s}^{-1}$	$2.52 \cdot 10^5$	$2.43 \cdot 10^5$	$8.62 \cdot 10^4$
	$\tau_{TADF} / \mu\text{s}$	3.97	4.12	11.60

3. Computational methods

3.1. Data extracted from the gas phase and crystal phase optimizations

Table S4. Excitation energies, oscillator strengths (f), spin-orbit coupling (SOC) matrix elements and rate constants for models **2a**, **3a** and **4a** calculated in the gas phase using TDDFT at the CAM-B3LYP/def2-TZVP/D3(BJ) level. Geometry optimizations were performed in the S_0 and S_1 states.

	Model 2a		Model 3a		Model 4a	
	S_0	S_1	S_0	S_1	S_0	S_1
$E(S_1) / \text{cm}^{-1}$	32653.3	9505.2	38045.2	26955.8	27629.3	17089.3
$E(T_1) / \text{cm}^{-1}$	26821.9	7606.6	27755.9	22457.7	19804.9	13253.3
$E(T_2) / \text{cm}^{-1}$	27027.6	17868.4	27939.0	25946.8	20030.8	18454.8
$\Delta E(S_1-T_1) / \text{cm}^{-1}$	5831.4	1898.6	10289.2	4498.2	7824.4	3836.0
$f(S_1)$	0.0710	0.0008	0.0029	0.0104	0.0468	0.0514
$\text{SOC}(S_1-T_1) / \text{cm}^{-1}$	103.31	26.08	18.53	108.91	107.48	113.02
$\tau_s / \mu\text{s}$	0.02	20.75	0.36	0.20	0.04	0.09
$k_r(S_1-S_0) / \text{s}^{-1}$	$5.1 \cdot 10^7$	$4.8 \cdot 10^4$	$2.8 \cdot 10^6$	$5.0 \cdot 10^6$	$2.4 \cdot 10^7$	$1.0 \cdot 10^7$
$k_{ic}(S_1-S_0) / \text{s}^{-1}$	$2.1 \cdot 10^4$	$1.2 \cdot 10^{10}$	$2.6 \cdot 10^3$	$6.8 \cdot 10^5$	$2.9 \cdot 10^5$	$6.4 \cdot 10^7$
$k_{isc}(S_1-T_1) / \text{s}^{-1}$	$3.5 \cdot 10^9$	$1.6 \cdot 10^{11}$	$1.2 \cdot 10^4$	$4.9 \cdot 10^{10}$	$1.4 \cdot 10^8$	$2.8 \cdot 10^{11}$
$k_{RISC}(T_1-S_1) / \text{s}^{-1}$	$2.5 \cdot 10^{-3}$	$1.8 \cdot 10^7$	$4.3 \cdot 10^{-18}$	$2.1 \cdot 10^1$	$6.9 \cdot 10^{-9}$	$2.9 \cdot 10^3$
Φ	0.99	0.0	0.999	0.88	0.99	0.14

Table S5. Excitation energies, oscillator strengths (f), SOC matrix elements and rate constants for **2** calculated at the CAM-B3LYP/def2-TZVP/D3(BJ) level for geometries optimized in the S_0 , S_1 , and T_1 states (model **2a**). Calculations were performed in the gas phase, as well as in supercells constructed from the unit cell with dimensions $1 \times 1 \times 1$, $1 \times 1 \times 2$, and $2 \times 2 \times 2$. Additionally, calculations were carried out for the geometry optimized in the $1 \times 1 \times 2$ supercell but then used in the gas phase calculations, without including the environment (" S_1 $1 \times 1 \times 2$ gas phase").

	S_0 <i>gas phase</i>	S_1 <i>gas phase</i>	T_1 <i>gas phase</i>	S_1 $1 \times 1 \times 1$ <i>crystal</i>	S_1 $1 \times 1 \times 2$ <i>crystal</i>	S_1 $1 \times 1 \times 2$ <i>gas phase</i>	S_1 $2 \times 2 \times 2$ <i>crystal</i>
$E(S_1) / \text{cm}^{-1}$	32502.8	9505.3	8086.8	20357.3	21472.9	22369.78	22868
$E(T_1) / \text{cm}^{-1}$	30192.1	7606.6	6782.7	19272.7	20259.0	21092.19	21611.2
$E(T_2) / \text{cm}^{-1}$	30286.5	17868.4	16587.3	24363.4	24954.6	24174.04	26433.1
$\Delta E(S_1-T_1) / \text{cm}^{-1}$	2310.7	1898.6	1304.1	1084.6	1213.9	1277.59	1256.8
$f(S_1)$	0.02996	0.0003	0.00221	0.01944	0.028143	0.0208	0.02869
$\text{SOC}(S_1-T_1) / \text{cm}^{-1}$	103.31	24.8	-	-	-	63.73	-
$\tau_s / \mu\text{s}$	0.047	55.34	10.38	0.186	0.12	0.14	0.099
$k_r(S_1-S_0) / \text{s}^{-1}$	-	$8.30 \cdot 10^4$	-	-	-	$6.94 \cdot 10^6$	-
$k_{ic}(S_1-S_0) / \text{s}^{-1}$	-	$4.86 \cdot 10^7$	-	-	-	$2.85 \cdot 10^6$	-
$k_{isc}(S_1-T_1) / \text{s}^{-1}$	-	$4.36 \cdot 10^{11}$	-	-	-	$1.60 \cdot 10^{12}$	-
$k_{RISC}(T_1-S_1) / \text{s}^{-1}$	-	$2.55 \cdot 10^{10}$	-	-	-	$3.50 \cdot 10^9$	-
Φ	-	0.0	-	-	-	0.71	-

Table S6. Excitation energies, oscillator strengths (f), and fluorescence lifetimes for models **2b**, **3b** and **4b** computed using the two-layer ONIOM approach with the molecule treated at the TDDFT level in the S_1 state and the environment at the xTB level.

	Model 2b	Model 3b	Model 4b
$E(S_1) / \text{cm}^{-1}$	21472.9	26512.9	17094.3
$E(T_1) / \text{cm}^{-1}$	20259.0	24400.6	14910.4
$E(T_2) / \text{cm}^{-1}$	24954.6	28678.3	21296.9
$\Delta E(S_1-T_1) / \text{cm}^{-1}$	1213.9	2112.3	2183.9
$f(S_1)$	0.0281	0.0102	0.0561
$\tau_s / \mu\text{s}$	0.12	0.21	0.09
$k_r(S_1-S_0) / \text{s}^{-1}$	$8.6 \cdot 10^6$	$4.8 \cdot 10^6$	$1.1 \cdot 10^7$

3.2. Coordination environment for the gold(I) centres on the X-ray structures and computational models

Table S7. Selected bond lengths and angles describing the coordination environment of the gold(I) centre in **2**, obtained from the X-ray structure and from the optimized geometries in the S_0 , S_1 and T_1 gas-phase and the S_1 crystal-phase states. The dihedral angle between the P-Au-P planes of each ligand is denoted as " θ_{P-Au-P} ".

Complex 2	Experimental	Model 2a			Model 2b
	X-Ray structure ^[a]	S_0 gas phase	S_1 gas phase	T_1 gas phase	S_1 crystal phase
Au-P1 / Å	2.4053(12)	2.421	2.507	2.430	2.546
Au-P2 / Å	2.3942(12)	2.421	2.441	2.428	2.499
Au-P3 / Å	2.4053(12)	2.421	2.507	2.428	2.430
Au-P4 / Å	2.3942(12)	2.421	2.441	2.430	2.444
P1-Au-P2 / °	84.62(4)	86.23	79.58	79.18	80.81
P1-Au-P3 / °	124.17(6)	124.75	173.25	177.22	117.28
P1-Au-P4 / °	118.83(4)	119.73	99.05	102.91	130.02
P2-Au-P3 / °	118.83(4)	119.75	99.05	98.81	139.26
P2-Au-P4 / °	130.98(6)	124.71	156.83	177.21	115.95
P3-Au-P4 / °	84.62(2)	86.23	79.57	79.16	81.48
θ_{P-Au-P} / °	82.12	85.48	23.32	2.97	72.92

^[a] P2, P3 and P4 correspond to P2#1, P1#1 and P2 in the X-ray structure, respectively.

Table S8. Selected bond lengths and angles describing the coordination environment of the gold(I) centre in **3**, obtained from the X-ray structure and from the optimized geometries in the S_0 , S_1 and T_1 gas-phase and the S_1 crystal-phase states. The dihedral angle between the P-Au-P planes of each ligand is denoted as " θ_{P-Au-P} ".

Complex 3	Experimental	Model 3a			Model 3b
	X-Ray structure ^[a]	S_0 gas phase	S_1 gas phase	T_1 gas phase	S_1 crystal phase
Au-P1 / Å	2.459(4)	2.502	2.468	2.534	2.497
Au-P2 / Å	2.452(3)	2.495	2.621	2.498	2.476
Au-P3 / Å	2.455(4)	2.507	2.513	2.482	2.529
Au-P4 / Å	2.497(4)	2.528	2.581	2.513	2.505
P1-Au-P2 / °	108.1(1)	107.30	108.36	105.71	118.52
P1-Au-P3 / °	109.4(1)	107.48	92.51	112.05	109.20
P1-Au-P4 / °	106.4(1)	109.37	117.27	107.22	98.72
P2-Au-P3 / °	114.8(1)	114.60	120.71	114.76	113.56
P2-Au-P4 / °	108.9(1)	112.84	115.56	106.73	99.78
P3-Au-P4 / °	108.9(1)	105.08	105.66	109.94	116.11
θ_{P-Au-P} / °	89.30	88.67	76.20	88.99	89.66

^[a] Data extracted for comparison from the crystal structure of $[\text{Au}(\text{C}_6\text{F}_5)_2][\text{Au}(\text{C}_6\text{Cl}_2\text{F}_3)_2]$ (**3***), reported by J.M. López-de-Luzuriaga *et al.* in *J. Organomet. Chem.* 2020, **913**, 121198 (DOI: 10.5517/ccdc.csd.cc24dbd9).

Table S9. Selected bond lengths and angles describing the coordination environment of the gold(I) centre in **4**, obtained from the X-ray structure and from the optimized geometries in the S_0 , S_1 and T_1 gas-phase and the S_1 crystal-phase states. The dihedral angle between the P-Au-P planes of each ligand is denoted as " θ_{P-Au-P} ".

Complex 4	Experimental	Model 4a			Model 4b
	X-Ray structure	S_0 <i>gas phase</i>	S_1 <i>gas phase</i>	T_1 <i>gas phase</i>	S_1 <i>crystal phase</i>
Au-P1 / Å	2.3932(11)	2.401	2.431	2.437	2.420
Au-P2 / Å	2.3718(11)	2.401	2.401	2.398	2.400
Au-P3 / Å	2.3846(12)	2.407	2.411	2.412	2.398
Au-P4 / Å	2.3855(13)	2.392	2.389	2.390	2.375
P1-Au-P2 / °	86.47(4)	85.73	85.46	85.43	85.13
P1-Au-P3 / °	121.60(4)	123.00	130.23	130.08	126.68
P1-Au-P4 / °	115.39(4)	118.29	110.75	110.59	112.10
P2-Au-P3 / °	117.12(4)	117.13	110.18	110.13	111.56
P2-Au-P4 / °	134.89(4)	134.23	145.31	145.86	142.75
P3-Au-P4 / °	85.71(4)	85.38	83.17	83.04	85.08
θ_{P-Au-P} / °	79.90	79.58	65.60	65.40	70.15

3.3. Representation of the cluster crystal-phase models

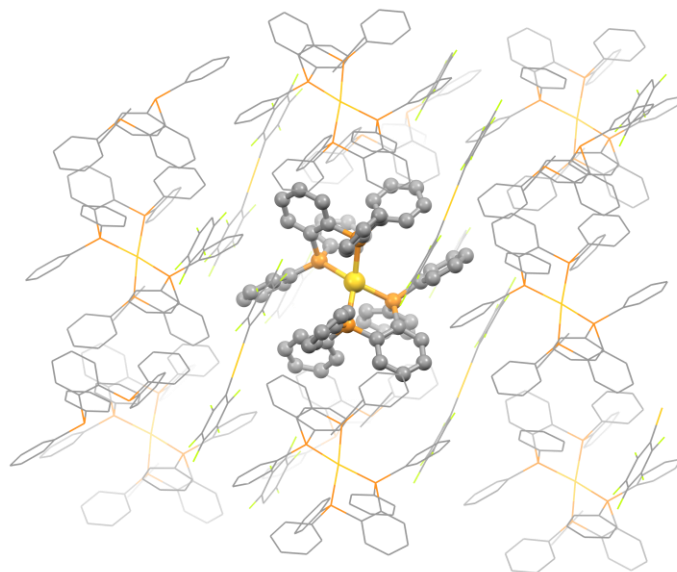


Figure S47. Cluster constructed from the unit cell, consisting on the central emitter and 16 surrounding molecules, illustrating the position of **2** within the crystal environment in **model 2b**. The region treated at the TDDFT level is shown in the ball and stick representation, while the region treated with xTB is depicted as a wireframe to highlight spatial arrangement and packing effects. Hydrogen atoms have been omitted for clarity.

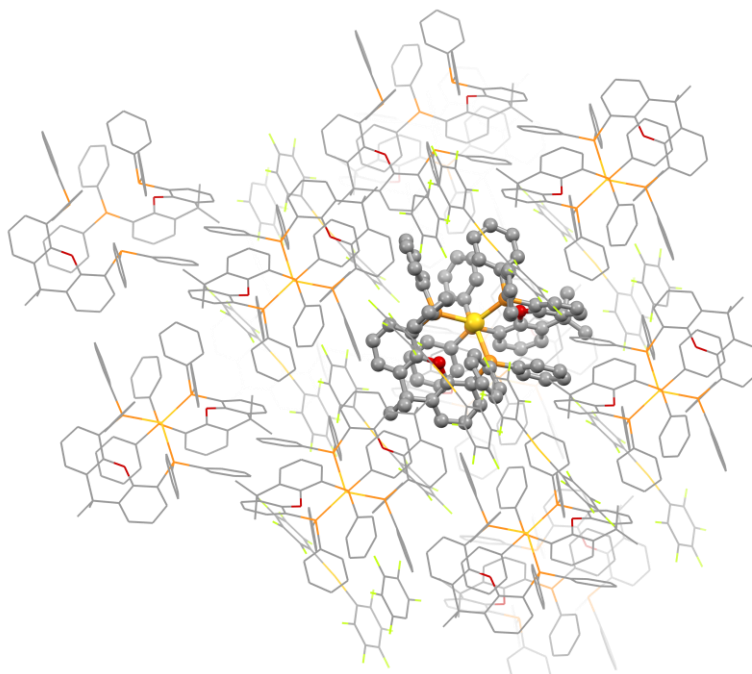


Figure S48. Cluster constructed from the unit cell, consisting on the central emitter and 23 surrounding molecules, illustrating the position of **3** within the crystal environment in **model 3b**. The region treated at the TDDFT level is shown in the ball and stick representation, while the region treated with xTB is depicted as a wireframe to highlight spatial arrangement and packing effects. Hydrogen atoms have been omitted for clarity.

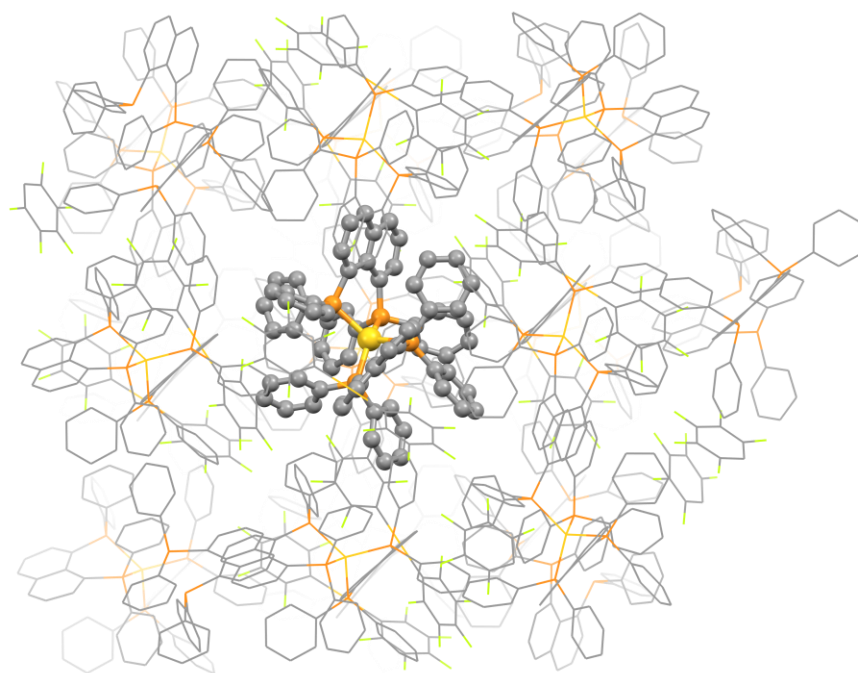


Figure S49. Cluster constructed from the unit cell, consisting on the central emitter and 30 surrounding molecules, illustrating the position of **4** within the crystal environment **in model 4b**. The region treated at the TDDFT level is shown in the ball and stick representation, while the region treated with xTB is depicted as a wireframe to highlight spatial arrangement and packing effects. Hydrogen atoms have been omitted for clarity.

3.4. Frontier HOMO and LUMO representations for the gas-phase and crystal-phase states

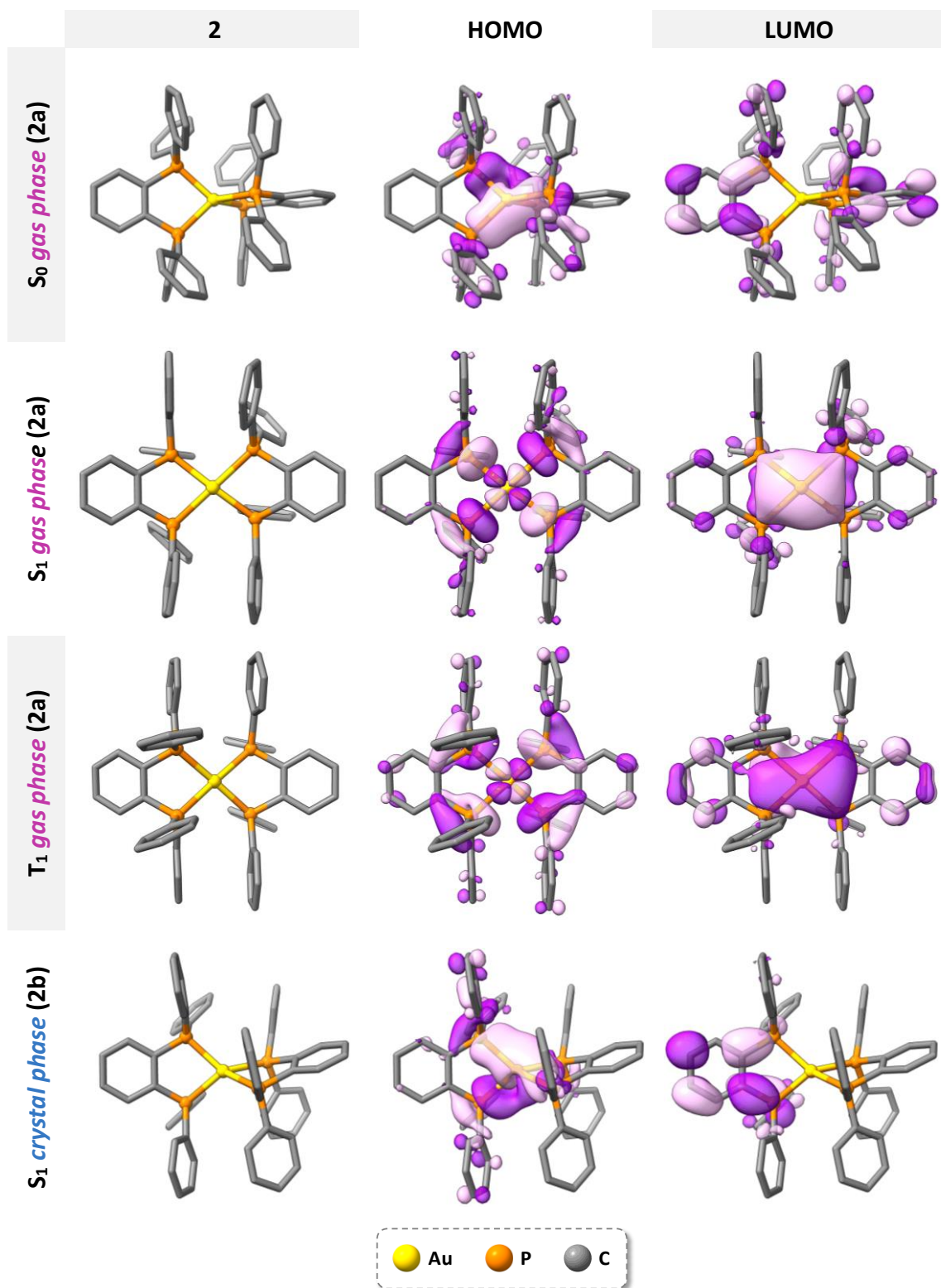


Figure S50. Representation of the optimized molecular structures of **2** in the S_0 , S_1 and T_1 gas-phase (model **2a**) and S_1 crystal-phase (model **2b**) states along with their corresponding frontier molecular orbitals (HOMO and LUMO, Isovalue = 0.03). Hydrogen atoms have been omitted for clarity.

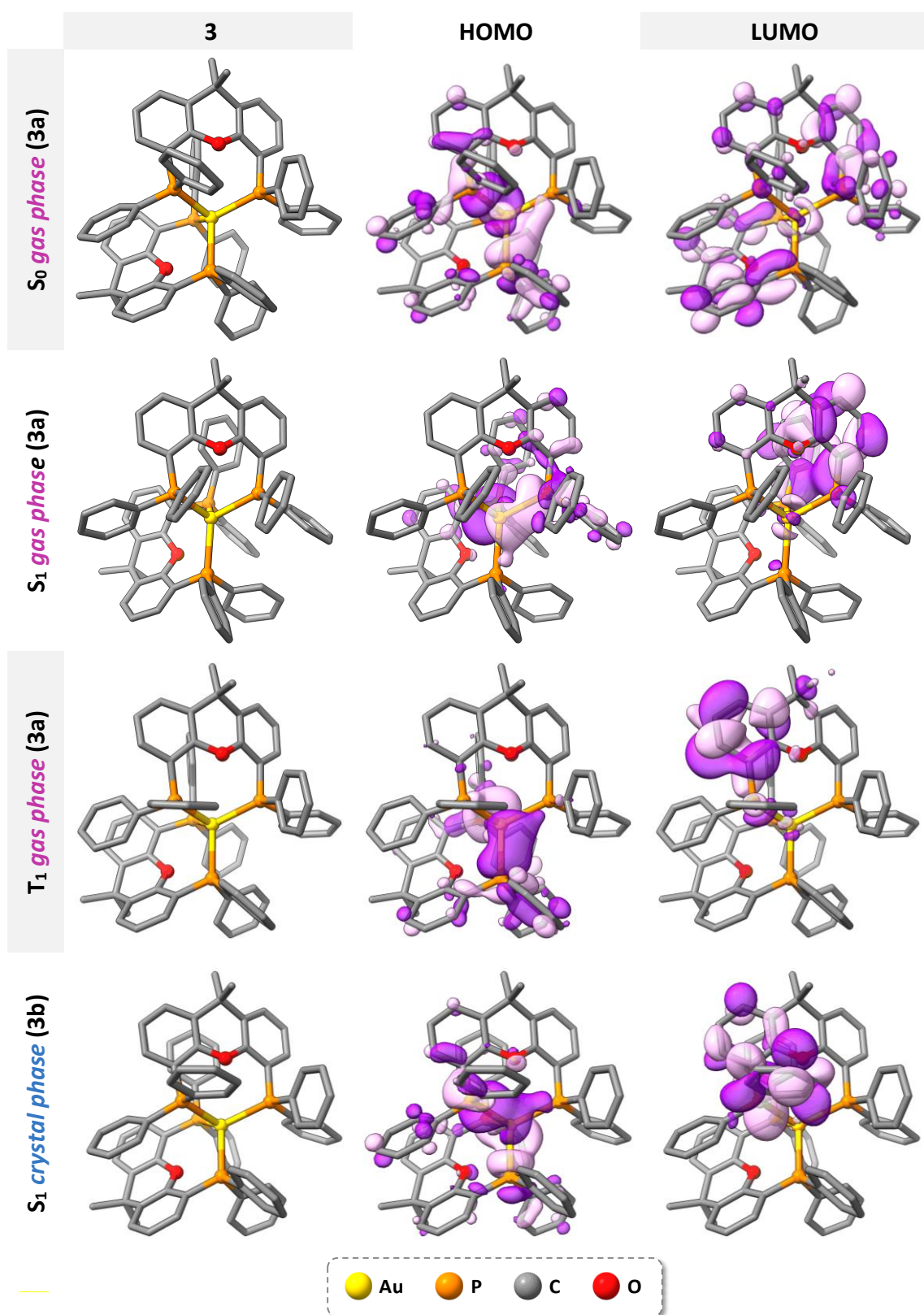


Figure S51. Representation of the optimized molecular structures of **3** in the *S*₀, *S*₁ and *T*₁ gas-phase (model **3a**) and *S*₁ crystal-phase (model **3b**) states along with their corresponding frontier molecular orbitals (HOMO and LUMO, Isovalue = 0.03). Hydrogen atoms have been omitted for clarity.

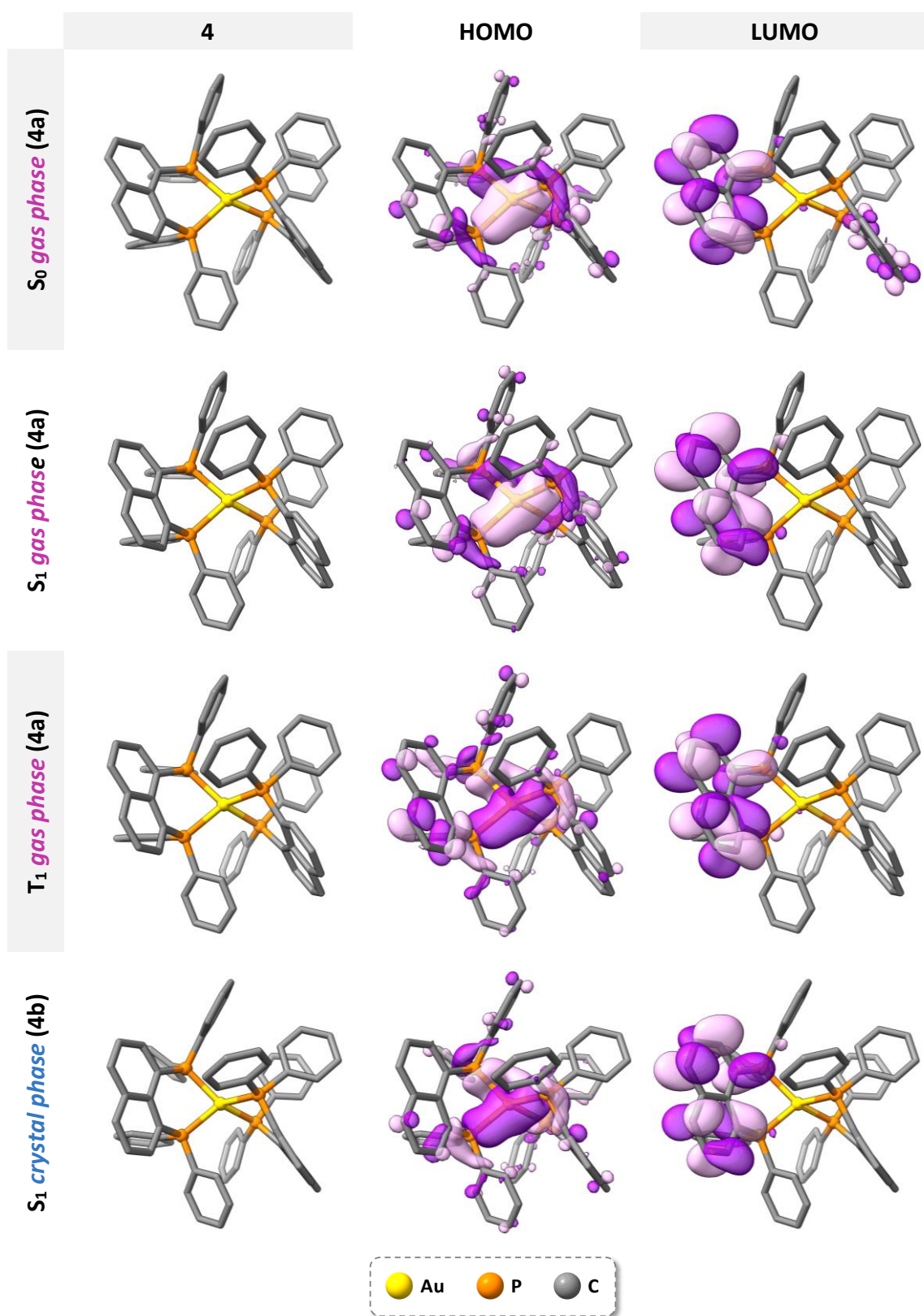


Figure S52. Representation of the optimized molecular structures of **4** in the S_0 , S_1 and T_1 gas-phase (model **4a**) and S_1 crystal-phase (model **4b**) states along with their corresponding frontier molecular orbitals (HOMO and LUMO, Isovalue = 0.03). Hydrogen atoms have been omitted for clarity.

3.5. Electron density calculations

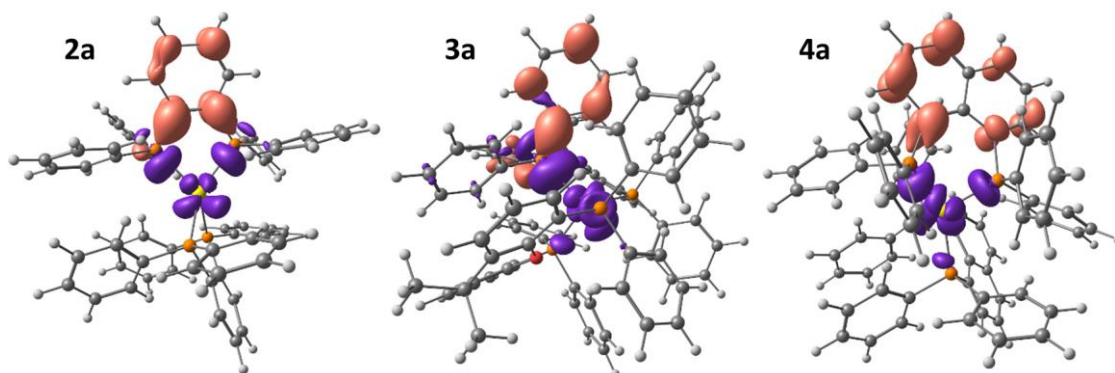


Figure S53. Difference between electron density of S_1 and S_0 states for models **2a**, **3a** and **4a** with geometries optimized in S_1 at the ONIOM level. The orange isosurface represents areas of electron density loss, while the purple isosurface represents areas of electron density increase for the $S_1 \rightarrow S_0$ transition.

3.6. xyz coordinates of the optimized gas-phase and crystal-phase models

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S_0 of model 2a

Au	0.000014000000	-0.000172000000	-0.000092000000
P	1.203768000000	-1.112137000000	-1.781993000000
P	-1.224332000000	1.135820000000	-1.752285000000
C	-0.545530000000	0.489109000000	-3.334098000000
C	0.506253000000	-0.444226000000	-3.346700000000
C	-0.565865000000	0.490085000000	-5.759140000000
H	-0.992187000000	0.850470000000	-6.697286000000
C	1.027598000000	-0.873748000000	-4.573493000000
H	1.855754000000	-1.585523000000	-4.591271000000
C	-1.080886000000	0.935815000000	-4.548654000000
H	-1.909055000000	1.647804000000	-4.546908000000
C	0.498597000000	-0.411257000000	-5.771598000000
H	0.914059000000	-0.758364000000	-6.719575000000
P	1.226220000000	1.108638000000	1.767971000000
P	-1.206280000000	-1.134761000000	1.765967000000
C	-0.507898000000	-0.489930000000	3.339949000000
C	0.545383000000	0.441773000000	3.340531000000
C	-0.500521000000	-0.490908000000	5.765073000000
H	-0.916581000000	-0.850720000000	6.708035000000
C	1.081124000000	0.870785000000	4.561278000000
H	1.910168000000	1.581694000000	4.569576000000
C	-1.029962000000	-0.935910000000	4.560559000000
C	0.565182000000	0.409060000000	5.765352000000

H	0.991799000000	0.755752000000	6.708516000000
H	-1.859052000000	-1.646793000000	4.568286000000
C	1.024653000000	-2.920993000000	-1.888518000000
C	1.680667000000	-3.699276000000	-0.924050000000
C	0.169194000000	-3.544983000000	-2.799967000000
C	1.516240000000	-5.077599000000	-0.900890000000
C	-0.003946000000	-4.928280000000	-2.764847000000
C	0.674336000000	-5.696755000000	-1.824552000000
H	2.327819000000	-3.224506000000	-0.183176000000
H	-0.368589000000	-2.958015000000	-3.545462000000
H	2.036126000000	-5.671023000000	-0.146916000000
H	-0.674589000000	-5.404660000000	-3.482993000000
H	0.538238000000	-6.779887000000	-1.800626000000
C	2.988597000000	-0.750457000000	-1.922008000000
C	3.390948000000	0.557560000000	-1.624600000000
C	3.951576000000	-1.698761000000	-2.273590000000
C	4.732728000000	0.912344000000	-1.675203000000
C	5.299303000000	-1.343610000000	-2.313114000000
C	5.691762000000	-0.042221000000	-2.012562000000
H	2.642831000000	1.300276000000	-1.337265000000
H	3.658672000000	-2.722732000000	-2.510032000000
H	5.034398000000	1.933177000000	-1.432870000000
H	6.046490000000	-2.093723000000	-2.580575000000
H	6.749002000000	0.229962000000	-2.037130000000
C	3.012154000000	0.745525000000	1.887815000000
C	3.979216000000	1.692017000000	2.233105000000
C	3.410675000000	-0.561681000000	1.581929000000
C	5.327028000000	1.335934000000	2.257849000000
C	4.752675000000	-0.917434000000	1.617770000000
C	5.715639000000	0.035394000000	1.948704000000
H	3.689337000000	2.715265000000	2.476336000000
H	2.659135000000	-1.302862000000	1.299762000000
H	6.077335000000	2.084593000000	2.520624000000
H	5.051311000000	-1.937590000000	1.368921000000
H	6.772923000000	-0.237438000000	1.961401000000
C	1.049731000000	2.917605000000	1.876971000000
C	0.201232000000	3.541194000000	2.795193000000
C	1.698992000000	3.696398000000	0.908366000000
C	0.028481000000	4.924587000000	2.762574000000
C	1.534917000000	5.074817000000	0.887556000000
C	0.700166000000	5.693562000000	1.817956000000
H	-0.331266000000	2.953766000000	3.544140000000
H	2.340626000000	3.221950000000	0.162495000000
H	-0.636655000000	5.400653000000	3.486028000000
H	2.049475000000	5.668671000000	0.130265000000
H	0.564447000000	6.776782000000	1.795988000000
C	-3.011124000000	0.778345000000	-1.876473000000
C	-3.412146000000	-0.532540000000	-1.590052000000
C	-3.976519000000	1.731978000000	-2.206455000000
C	-4.754899000000	-0.884963000000	-1.630256000000
C	-5.325101000000	1.379081000000	-2.235521000000
C	-5.716144000000	0.074764000000	-1.945977000000

H	-2.661952000000	-1.279437000000	-1.319555000000
H	-3.684725000000	2.758234000000	-2.434191000000
H	-5.055404000000	-1.908146000000	-1.396563000000
H	-6.074072000000	2.133248000000	-2.486043000000
H	-6.773986000000	-0.195694000000	-1.962115000000
C	-1.043831000000	2.945723000000	-1.836371000000
C	-1.689896000000	3.712258000000	-0.855912000000
C	-0.195378000000	3.580266000000	-2.747097000000
C	-1.522691000000	5.089875000000	-0.816017000000
C	-0.019332000000	4.962657000000	-2.695196000000
C	-0.687813000000	5.719756000000	-1.738795000000
H	-2.331424000000	3.228824000000	-0.115736000000
H	0.334510000000	3.002271000000	-3.505174000000
H	-2.034843000000	5.674192000000	-0.049736000000
H	0.645806000000	5.447358000000	-3.412888000000
H	-0.549422000000	6.802223000000	-1.701672000000
C	-1.030005000000	-2.945176000000	1.847285000000
C	-0.174347000000	-3.582794000000	2.749078000000
C	-1.688003000000	-3.709210000000	0.872829000000
C	-0.002981000000	-4.965675000000	2.694635000000
C	-1.525283000000	-5.087283000000	0.830394000000
C	-0.683192000000	-5.720212000000	1.744492000000
H	0.364949000000	-3.006844000000	3.502045000000
H	-2.335301000000	-3.223403000000	0.139264000000
H	0.667775000000	-5.452798000000	3.405428000000
H	-2.046688000000	-5.669580000000	0.068827000000
H	-0.548524000000	-6.803083000000	1.705446000000
C	-2.990528000000	-0.772103000000	1.910807000000
C	-3.955221000000	-1.723543000000	2.249064000000
C	-3.390578000000	0.540717000000	1.631781000000
C	-5.302339000000	-1.366594000000	2.293496000000
C	-4.731735000000	0.897098000000	1.687292000000
C	-5.692494000000	-0.060450000000	2.011099000000
H	-3.664114000000	-2.751174000000	2.471430000000
H	-2.641012000000	1.286029000000	1.355139000000
H	-6.050854000000	-2.119001000000	2.550581000000
H	-5.031658000000	1.921761000000	1.459392000000
H	-6.749276000000	0.213144000000	2.039189000000

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Au	0.000046400000	0.696464300000	-0.000162000000
P	1.416239300000	0.205413800000	-1.926947700000
P	-1.729630100000	0.547858100000	-1.808533600000
C	-0.832093000000	1.014824500000	-3.334055000000
C	0.569688900000	0.911863800000	-3.376590600000
C	-0.822321600000	1.906687400000	-5.582852700000
H	-1.368792600000	2.295683100000	-6.443890800000
C	1.261693300000	1.319316400000	-4.518339000000
H	2.351046800000	1.254331500000	-4.546786700000
C	-1.518608700000	1.511638800000	-4.442921800000

H	-2.605943500000	1.602238200000	-4.412012600000
C	0.565604700000	1.816730500000	-5.617876900000
H	1.113558900000	2.137105700000	-6.505983800000
P	1.729866300000	0.550136500000	1.808355200000
P	-1.416362600000	0.207023200000	1.927324000000
C	-0.569404000000	0.913184400000	3.376920100000
C	0.832407000000	1.015581600000	3.334396200000
C	-0.564733300000	1.815282300000	5.619347900000
H	-1.112455500000	2.134548100000	6.507996300000
C	1.519180700000	1.511202100000	4.443657700000
H	2.606489600000	1.602031700000	4.412522700000
C	-1.261084300000	1.319208400000	4.519391200000
C	0.823196300000	1.905167600000	5.584125000000
H	1.369859000000	2.293613100000	6.445288600000
H	-2.350388700000	1.253585900000	4.548295100000
C	1.461106300000	-1.591512000000	-2.274333500000
C	1.311562900000	-2.488222900000	-1.213418500000
C	1.599037500000	-2.088546300000	-3.576037300000
C	1.309163300000	-3.860060700000	-1.444231900000
C	1.581950400000	-3.460524200000	-3.806632800000
C	1.436885900000	-4.348172400000	-2.741807900000
H	1.188311800000	-2.111975400000	-0.197749900000
H	1.710332000000	-1.403471000000	-4.418194000000
H	1.203095200000	-4.545856200000	-0.601607600000
H	1.683660500000	-3.839206700000	-4.825569900000
H	1.423636300000	-5.424179400000	-2.926429500000
C	3.140443600000	0.765290200000	-1.982702500000
C	3.398546900000	2.129075700000	-1.800201400000
C	4.207489200000	-0.127371800000	-2.125297900000
C	4.707118300000	2.593597800000	-1.775500100000
C	5.517880600000	0.342600800000	-2.084691500000
C	5.768515700000	1.700617700000	-1.911850200000
H	2.567201500000	2.824539600000	-1.664759700000
H	4.016519300000	-1.191917600000	-2.268217500000
H	4.900867500000	3.657484900000	-1.632420000000
H	6.347454200000	-0.358414100000	-2.194626300000
H	6.796585200000	2.066515100000	-1.881395500000
C	2.485686000000	-1.069282200000	2.138552600000
C	3.441968000000	-1.573427200000	1.244314600000
C	1.998975200000	-1.901456800000	3.153859400000
C	3.908992500000	-2.875448600000	1.374935300000
C	2.456663800000	-3.210106100000	3.267950000000
C	3.413112000000	-3.700991000000	2.382666800000
H	3.814719700000	-0.949508500000	0.429726900000
H	1.252367500000	-1.531256700000	3.856444700000
H	4.657420200000	-3.252695800000	0.675278700000
H	2.062000500000	-3.849304400000	4.059972700000
H	3.773910400000	-4.726806100000	2.478080000000
C	3.069669600000	1.778549000000	1.703840800000
C	2.693088500000	3.090868700000	1.390686100000
C	4.412750000000	1.490089400000	1.958468800000
C	3.646706400000	4.099808800000	1.341347300000

C	5.367186900000	2.502402800000	1.891154200000
C	4.986942500000	3.806100500000	1.586838900000
H	1.642845400000	3.312310900000	1.181769500000
H	4.720843500000	0.477261200000	2.218569900000
H	3.343055500000	5.122101800000	1.107106200000
H	6.415094600000	2.268779500000	2.088563200000
H	5.737389100000	4.598120200000	1.544420600000
C	-2.483676300000	-1.072194600000	-2.139923300000
C	-2.000490100000	-1.901028300000	-3.159590700000
C	-3.435688600000	-1.579713000000	-1.243053600000
C	-2.457457600000	-3.209804200000	-3.275354700000
C	-3.902025400000	-2.881805300000	-1.375229800000
C	-3.409608800000	-3.704054500000	-2.387358200000
H	-1.257147500000	-1.528195200000	-3.864235100000
H	-3.805855000000	-0.958153600000	-0.425458000000
H	-2.065607700000	-3.846463300000	-4.070811600000
H	-4.647005600000	-3.261746100000	-0.673357100000
H	-3.769795000000	-4.729960800000	-2.484093200000
C	-3.071080300000	1.774462700000	-1.704260400000
C	-4.414154100000	1.483251300000	-1.955681200000
C	-2.696047300000	3.088026700000	-1.394454700000
C	-5.370081300000	2.494198500000	-1.888863300000
C	-3.651157600000	4.095569200000	-1.345755100000
C	-4.991340700000	3.799209900000	-1.588353800000
H	-4.721052700000	0.469315700000	-2.212882100000
H	-1.645850300000	3.311539900000	-1.187595200000
H	-6.418013400000	2.258423500000	-2.083561900000
H	-3.348741600000	5.118827300000	-1.114149400000
H	-5.742920000000	4.590195700000	-1.546716000000
C	-1.462224300000	-1.589786700000	2.275728900000
C	-1.604489200000	-2.085967600000	3.577311000000
C	-1.308360600000	-2.487161900000	1.216053700000
C	-1.587053900000	-3.457736100000	3.809016000000
C	-1.305931600000	-3.858857300000	1.447854800000
C	-1.437713900000	-4.346089600000	2.745321800000
H	-1.719489100000	-1.400388100000	4.418552900000
H	-1.181311300000	-2.111610500000	0.200598700000
H	-1.691726900000	-3.835752700000	4.827898600000
H	-1.196691800000	-4.545157900000	0.606050500000
H	-1.424249200000	-5.421943200000	2.930819500000
C	-3.140194200000	0.767986600000	1.983065200000
C	-4.207851500000	-0.123915800000	2.125836500000
C	-3.397352600000	2.131953400000	1.800547700000
C	-5.517927600000	0.346952300000	2.085294400000
C	-4.705601700000	2.597382300000	1.776168900000
C	-5.767616500000	1.705147200000	1.912608500000
H	-4.017646900000	-1.188551500000	2.269108000000
H	-2.565523200000	2.826833400000	1.664951500000
H	-6.347972700000	-0.353541600000	2.194976100000
H	-4.898656200000	3.661422300000	1.633286800000
H	-6.795430300000	2.071759900000	1.882150100000

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Au	-0.000182036974	-0.063858464523	-0.000093664373
P	1.642037003647	-1.643744129452	0.837306048370
P	1.729097244652	1.449907561498	0.788823357994
C	2.442968995453	0.602847188897	2.227886490129
C	2.377885485598	-0.796039748139	2.265888825088
C	2.848804552902	1.926159677117	-1.697741375940
H	1.822528779736	2.037910270206	-2.016280150153
C	3.122747972809	1.637475495761	-0.365192098839
C	3.074315025095	-1.960077822068	-0.240886246340
C	1.320147479094	3.122438404119	1.338818969147
C	3.533647227354	0.599785898511	4.372478893733
H	3.980953876629	1.145793100739	5.191703484682
C	3.013060641814	-1.597708354676	-1.578106041841
H	2.111943225696	-1.133620965657	-1.957500728866
C	2.887281559854	-1.476776536316	3.360699931304
H	2.827759173709	-2.555761538546	3.401510609924
C	4.442069935394	1.447360631399	0.027687612022
H	4.677157986617	1.206561170127	1.054149126402
C	4.251347046373	-2.509257441903	0.261920512811
H	4.323323089896	-2.784869886855	1.305098736486
C	3.034670653131	1.289238765157	3.277644503719
H	3.097588240506	2.368213183841	3.250145807974
C	1.757878666048	4.252557274742	0.660463478591
H	2.406523499960	4.155272800108	-0.197709087062
C	0.110625562258	-3.293587026699	2.416655127569
H	-0.265579244310	-2.367428413981	2.830734208203
C	3.873332982791	2.048791212800	-2.615752246556
H	3.647065257955	2.282041431437	-3.647594964381
C	1.093358514667	-3.258177660260	1.429450098229
C	3.455319469311	-0.779524655375	4.416240264694
H	3.837563775822	-1.319130400421	5.271916172086
C	0.485918596426	3.271297022617	2.444803652975
H	0.151071108576	2.394476779886	2.984379764095
C	4.104479721863	-1.787997318352	-2.407569154204
H	4.048741482226	-1.490928323486	-3.445873655416
C	1.367323630842	5.511569964613	1.084304291936
H	1.712430278018	6.385081262005	0.548590116380
C	-0.381131975934	-4.501475902544	2.869327634150
H	-1.142030650498	-4.518446087743	3.637638494441
C	5.466551268509	1.545695522871	-0.898695371850
H	6.488147527261	1.381124044319	-0.584579461084
C	5.268199231089	-2.338856546776	-1.903084373997
H	6.124788498413	-2.481362392400	-2.547992158176
C	1.562113247022	-4.449771581076	0.891355683406
H	2.308011863286	-4.438349290157	0.110367852938
C	0.542382867249	5.653012163966	2.185034774859
H	0.242560033979	6.638178273366	2.515572114016
C	5.340980153207	-2.698957431302	-0.565904795967
H	6.251935503562	-3.123844957247	-0.166728934197
C	0.103718211627	4.528595178201	2.868189373887

H	-0.535461228832	4.634168685263	3.734328703024
C	0.099607562757	-5.688455397750	2.336738250248
H	-0.284526964888	-6.635232872798	2.691566941843
C	5.186400599470	1.852018769468	-2.218194079636
H	5.989135498163	1.930055480024	-2.938774210422
C	1.067607162199	-5.659177078917	1.349370234315
H	1.438592164383	-6.581977003636	0.925044165432
P	-1.643515524881	-1.643697032677	-0.836518103447
P	-1.728241565041	1.450618246543	-0.789957384839
C	-2.444149060718	0.602850363960	-2.227615551377
C	-2.380366797719	-0.796108541181	-2.264711934887
C	-2.846152845707	1.933087136483	1.696255975402
H	-1.819675456009	2.046432669801	2.013630559667
C	-3.121037671941	1.640833125406	0.364656042286
C	-3.074978084188	-1.960023845989	0.242772234055
C	-1.318574764310	3.122262188095	-1.342313655700
C	-3.537250395242	0.599400128297	-4.370971796928
H	-3.984898363843	1.145235877095	-5.190121773885
C	-3.015961062316	-1.590279764454	1.578048361521
H	-2.116719579545	-1.121054064348	1.955598865833
C	-2.891953136608	-1.477089809247	-3.358356205268
H	-2.833585415220	-2.556157363128	-3.398491124541
C	-4.440627398214	1.449170417590	-0.026612323852
H	-4.676496515056	1.205705490516	-1.052262080332
C	-4.249676433798	-2.516197072347	-0.257871248501
H	-4.319877087651	-2.797922572878	-1.299543962904
C	-3.036234371902	1.289105941667	-3.277237566414
H	-3.097908392741	2.368176670611	-3.250391346218
C	-1.758508916152	4.253850583938	-0.667885189508
H	-2.408891568149	4.158398650118	0.189170282973
C	-0.117487403646	-3.293617718980	-2.421234098305
H	0.253671168676	-2.367659664439	-2.840342479513
C	-3.869952598524	2.057472365570	2.614816661179
H	-3.642930266931	2.293473247547	3.645869846549
C	-1.094869315713	-3.258008852717	-1.428738884006
C	-3.460558853253	-0.780034253066	-4.413713443330
H	-3.844479064112	-1.319861723379	-5.268498216234
C	-0.482222822519	3.268743213213	-2.447010851281
H	-0.145989948631	2.390678345593	-2.983685483545
C	-4.107278011156	-1.780017854615	2.407818396688
H	-4.053291877390	-1.477155427226	3.444535895331
C	-1.367854924800	5.512001773248	-1.094232186305
H	-1.714582971067	6.386712186287	-0.561521091636
C	0.375358652147	-4.501460556404	-2.872823379056
H	1.132006975048	-4.518625478830	-3.645309977020
C	-5.464387462738	1.549403467855	0.900365455248
H	-6.486176342009	1.383692141508	0.587467181332
C	-5.268610930989	-2.337812480063	1.905528643710
H	-6.125105475585	-2.480037861745	2.550624814990
C	-1.557082888093	-4.449315959465	-0.884353080870
H	-2.298610500280	-4.437637546757	-0.099224438428
C	-0.540716488092	5.651070083463	-2.193614325597

H	-0.240784115131	6.635557787629	-2.526075224054
C	-5.339154491698	-2.705403339372	0.570229761623
H	-6.248239729655	-3.135865747635	0.172766317431
C	-0.099947294550	4.525152880196	-2.872937681342
H	0.540902229306	4.628850983088	-3.738068927820
C	-0.098857718595	-5.688187104885	-2.333857938482
H	0.286157889169	-6.634924362462	-2.687829892110
C	-5.183298562436	1.859091223401	2.218868780628
H	-5.985461420524	1.938579996328	2.939923054230
C	-1.061509981936	-5.658670656290	-1.341293401964
H	-1.427364081513	-6.581212342511	-0.912002592130

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Au	8.093227000000	5.857546000000	17.082088000000
P	9.127556000000	4.837293000000	15.117051000000
P	7.002219000000	4.769610000000	19.108484000000
P	5.758833000000	6.696807000000	16.777491000000
P	10.342143000000	6.732838000000	17.363771000000
C	4.967642000000	6.577905000000	18.430083000000
C	11.102296000000	6.649409000000	15.776431000000
C	5.512720000000	5.782827000000	19.448698000000
C	10.464631000000	5.894755000000	14.722541000000
C	4.787898000000	5.891473000000	14.306223000000
C	11.024874000000	5.933395000000	19.953207000000
H	5.492696000000	6.606697000000	13.884063000000
H	10.300961000000	6.664947000000	20.309445000000
C	4.678222000000	5.729479000000	15.691259000000
C	11.277340000000	5.783434000000	18.585880000000
C	9.704605000000	3.141899000000	15.488981000000
C	6.259334000000	3.147428000000	18.706774000000
C	5.506994000000	8.456609000000	16.369565000000
C	10.361262000000	8.480216000000	17.845603000000
C	3.157500000000	7.220035000000	19.905994000000
C	12.934531000000	7.228468000000	14.292577000000
H	2.242646000000	7.788108000000	20.087810000000
H	13.861549000000	7.770115000000	14.099606000000
C	9.742765000000	2.667200000000	16.803608000000
C	6.319846000000	2.657898000000	17.400853000000
H	9.316333000000	3.260909000000	17.614489000000
H	6.840013000000	3.222800000000	16.625626000000
C	4.865477000000	5.714981000000	20.687090000000
C	11.160181000000	5.776056000000	13.482765000000
H	5.279129000000	5.097675000000	21.485639000000
H	10.734013000000	5.171916000000	12.679494000000
C	3.781892000000	4.792399000000	16.212131000000
C	12.197154000000	4.828974000000	18.142780000000
H	3.698693000000	4.643019000000	17.288499000000
H	12.377987000000	4.702468000000	17.074701000000
C	10.298093000000	2.376152000000	14.470427000000
C	5.575202000000	2.409490000000	19.683749000000

H	10.304899000000	2.734565000000	13.438815000000
H	5.507720000000	2.773662000000	20.710607000000
C	3.786345000000	7.289787000000	18.670213000000
C	12.322633000000	7.302196000000	15.526247000000
H	3.363415000000	7.908522000000	17.876150000000
H	12.774825000000	7.896570000000	16.325314000000
C	4.569248000000	8.917091000000	15.442406000000
C	11.227784000000	8.980880000000	18.822405000000
H	3.975991000000	8.216508000000	14.856790000000
H	11.818441000000	8.307074000000	19.441077000000
C	7.848945000000	5.824406000000	12.887518000000
C	8.057487000000	5.737741000000	21.464354000000
H	8.238220000000	6.786433000000	13.225703000000
H	7.753726000000	6.716108000000	21.083707000000
C	3.980574000000	5.149603000000	13.454616000000
C	11.708795000000	5.148359000000	20.870572000000
H	4.060441000000	5.299737000000	12.378333000000
H	11.511947000000	5.273608000000	21.934437000000
C	8.065262000000	4.680297000000	13.664537000000
C	7.819492000000	4.581043000000	20.714020000000
C	3.699275000000	6.431295000000	20.919020000000
C	12.335416000000	6.440733000000	13.260816000000
H	3.214465000000	6.363160000000	21.894674000000
H	12.804593000000	6.364547000000	12.279958000000
C	6.251460000000	9.380184000000	17.114088000000
C	9.626994000000	9.373065000000	17.049664000000
H	6.969812000000	9.034171000000	17.861290000000
H	8.986838000000	8.992577000000	16.250638000000
C	10.319519000000	1.433311000000	17.090507000000
C	5.722861000000	1.441619000000	17.077438000000
H	10.315365000000	1.066913000000	18.119035000000
H	5.792697000000	1.066495000000	16.054521000000
C	4.384594000000	10.286294000000	15.261530000000
C	11.355989000000	10.358243000000	18.996351000000
H	3.648674000000	10.634202000000	14.533419000000
H	12.045944000000	10.736776000000	19.753624000000
C	7.157564000000	5.726292000000	11.689667000000
C	8.687337000000	5.647362000000	22.696291000000
H	6.998724000000	6.619525000000	11.087983000000
H	8.864757000000	6.552586000000	23.274363000000
C	2.983867000000	4.045067000000	15.353144000000
C	12.878511000000	4.044882000000	19.067621000000
H	2.268916000000	3.332067000000	15.764582000000
H	13.613461000000	3.316562000000	18.721627000000
C	10.880467000000	0.669290000000	16.071641000000
C	5.067792000000	0.704384000000	18.057968000000
C	7.534174000000	3.451657000000	13.252977000000
C	8.266663000000	3.344601000000	21.189191000000
H	7.691273000000	2.549121000000	13.844890000000
H	8.104336000000	2.430022000000	20.617496000000
C	5.127717000000	11.199160000000	16.002676000000
C	10.619560000000	11.238025000000	18.211977000000

H	4.975828000000	12.274454000000	15.886022000000
H	10.731507000000	12.319377000000	18.316134000000
C	10.875024000000	1.147606000000	14.760702000000
C	4.992409000000	1.190423000000	19.363472000000
H	11.308492000000	0.550659000000	13.955413000000
H	4.495278000000	0.608427000000	20.142747000000
C	6.058482000000	10.744098000000	16.935297000000
C	9.754010000000	10.741221000000	17.235445000000
H	6.616598000000	11.459757000000	17.541305000000
H	9.213160000000	11.436625000000	16.592086000000
C	6.674403000000	4.493891000000	11.257952000000
C	9.099688000000	4.410281000000	23.184560000000
H	6.175919000000	4.425387000000	10.289833000000
H	9.557579000000	4.345838000000	24.172860000000
C	3.079242000000	4.229228000000	13.978995000000
C	12.629515000000	4.203890000000	20.427012000000
H	2.440831000000	3.654763000000	13.312562000000
H	13.151253000000	3.585857000000	21.154897000000
C	6.846911000000	3.359022000000	12.046186000000
C	8.904199000000	3.260589000000	22.425349000000
H	6.475172000000	2.385383000000	11.718060000000
H	9.227464000000	2.285316000000	22.798578000000
H	11.321576000000	-0.305763000000	16.287305000000
H	4.621608000000	-0.262787000000	17.817720000000

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Au	0.041979100000	0.265404300000	0.001407700000
P	-0.892043900000	-0.604627300000	2.183934900000
P	0.653691000000	-1.665261100000	-1.467457700000
P	-1.867063300000	1.468111100000	-1.091819300000
P	2.098879800000	1.644305800000	0.309207700000
O	3.216480600000	-0.996909300000	-0.378439000000
O	-3.243402900000	-0.494698200000	0.459246800000
C	3.505709300000	0.804724200000	1.116069000000
C	1.693040000000	-4.251884500000	-0.777689800000
H	0.785085100000	-4.697150000000	-1.153440900000
C	-1.391793900000	-3.531969100000	-1.067444200000
H	-1.011857900000	-3.630393700000	-0.060056600000
C	-1.690905200000	0.599873100000	3.310974000000
C	1.855764900000	-2.872983000000	-0.806624600000
C	-0.779691500000	-2.667386000000	-1.969953500000
C	4.189609700000	1.349621100000	2.197088400000
H	3.900924300000	2.314401300000	2.584992200000
C	-2.699440100000	2.641821700000	0.020834400000
C	-3.242814200000	0.428194000000	-1.689455600000
C	-0.997932600000	1.850742300000	-3.696856200000
H	-0.885087000000	0.776069000000	-3.710051400000
C	0.320556000000	-1.417594500000	3.269243400000
C	-1.330465700000	-2.525673300000	-3.239544200000

H	-0.878331400000	-1.854074600000	-3.955032000000
C	3.917055900000	-0.442656900000	0.664222600000
C	2.827504400000	2.304849000000	-1.224003900000
C	2.689531600000	4.309522700000	1.055200100000
H	3.358982300000	4.348497200000	0.208295800000
C	3.061444800000	-2.362461100000	-0.341119400000
C	-2.171782000000	-1.903610200000	1.997403100000
C	-4.255713400000	-2.600271800000	0.920335900000
C	-5.410416900000	-2.184782900000	0.019405500000
C	1.951080000000	3.158480400000	1.313226600000
C	-5.350475700000	-1.259599700000	-2.388559400000
H	-6.165861100000	-1.904322900000	-2.681432000000
C	-1.483912000000	2.483333100000	-2.555966000000
C	-2.446298400000	-3.254786800000	-3.608788300000
H	-2.862982400000	-3.129398700000	-4.598669200000
C	4.118176700000	2.016977800000	-1.642329100000
H	4.745024900000	1.355010000000	-1.063380400000
C	-1.910207400000	3.403994500000	0.872173300000
H	-0.841836500000	3.251960600000	0.889656300000
C	4.979992100000	-1.141605200000	1.216273200000
C	1.532197100000	-1.813438200000	2.725619400000
H	1.737711500000	-1.591170900000	1.691456200000
C	3.871452800000	-4.521220500000	0.199227700000
H	4.636908500000	-5.176098400000	0.588334800000
C	1.471232800000	-1.296770600000	-3.055008400000
C	-4.838924700000	-1.329358900000	-1.102270600000
C	1.728775900000	5.379098700000	2.979132600000
H	1.641942900000	6.243799700000	3.623105100000
C	-3.036315500000	0.933767700000	3.195450800000
H	-3.652103100000	0.471997800000	2.442312200000
C	2.573546600000	5.413344000000	1.881490600000
H	3.149443100000	6.303594500000	1.668122600000
C	0.994945800000	4.236039100000	3.245510800000
H	0.325918000000	4.197827700000	4.094136000000
C	-0.666782800000	2.578267800000	-4.822826700000
H	-0.295346100000	2.066666800000	-5.700344300000
C	2.687999100000	-5.065810900000	-0.267358400000
H	2.542372000000	-6.136715900000	-0.241643300000
C	-0.932455400000	1.240180600000	4.287877800000
H	0.111282900000	0.991636700000	4.416076900000
C	-4.075103900000	2.837391100000	0.018284000000
H	-4.706566100000	2.257213600000	-0.639962700000
C	1.672832000000	0.010571800000	-3.457193000000
H	1.345251700000	0.819041600000	-2.825786900000
C	-3.233720000000	-1.688314300000	1.129860600000
C	-3.848989500000	4.543862500000	1.692747000000
H	-4.298381500000	5.281505000000	2.343823900000
C	-3.784973200000	-0.485848700000	-0.797286500000
C	4.085651500000	-3.152310100000	0.154750200000
C	-4.172775500000	-3.808963300000	1.591667000000
H	-4.940297300000	-4.556597800000	1.456213900000
C	1.919220800000	-2.334889500000	-3.871463900000

H	1.778864200000	-3.363471600000	-3.567695300000
C	2.553691700000	3.747639200000	-3.133405500000
H	1.935244000000	4.422596200000	-3.707835600000
C	-4.843876000000	-0.353832800000	-3.304330500000
H	-5.268714300000	-0.299587900000	-4.296974900000
C	6.170923600000	-2.133420100000	-0.724418300000
H	5.586132700000	-1.522925900000	-1.411084400000
H	6.443118300000	-3.055427100000	-1.238071300000
H	7.083499600000	-1.592264900000	-0.473977400000
C	-2.121537200000	-3.133005600000	2.644637100000
H	-1.302528400000	-3.362506100000	3.307844400000
C	2.199661400000	-2.764035700000	4.819885300000
H	2.929664900000	-3.284754800000	5.424839700000
C	2.046226400000	3.169004500000	-1.986730200000
H	1.034959100000	3.400769100000	-1.680870000000
C	1.104431000000	3.137868300000	2.412057800000
H	0.512327800000	2.258300900000	2.608725800000
C	5.625575700000	-0.571102500000	2.301619200000
H	6.449201800000	-1.086862900000	2.772636300000
C	-3.014771000000	-4.151273700000	-2.722362400000
H	-3.871784400000	-4.739833600000	-3.020800600000
C	2.467454900000	-2.487559200000	3.493103500000
H	3.404954000000	-2.788846500000	3.049857100000
C	-4.645787100000	3.780068800000	0.856311600000
H	-5.718028700000	3.922994200000	0.849354800000
C	5.230774800000	0.661520100000	2.790942200000
H	5.745256000000	1.094688800000	3.637189400000
C	5.376291400000	-2.455029900000	0.557374000000
C	-2.485355100000	-4.286092400000	-1.450801800000
H	-2.928104000000	-4.974163600000	-0.745267800000
C	2.543859500000	-2.059769300000	-5.070455700000
H	2.886074000000	-2.871893700000	-5.697463800000
C	2.298964400000	0.289801900000	-4.662413200000
H	2.450555600000	1.318305700000	-4.956446400000
C	-3.605834900000	1.872398200000	4.036020800000
H	-4.653638200000	2.115443900000	3.926616500000
C	2.733984000000	-0.743183500000	-5.469250800000
H	3.226923600000	-0.529194200000	-6.408123500000
C	-3.807957200000	0.493875300000	-2.956661800000
H	-3.439418200000	1.206714300000	-3.677772500000
C	-2.844461700000	2.498754900000	5.006047900000
H	-3.293813200000	3.227644800000	5.666691600000
C	0.991322200000	-2.370463200000	5.377535000000
H	0.776813000000	-2.585824600000	6.415503200000
C	0.057008200000	-1.705558200000	4.608565900000
H	-0.883051400000	-1.408513600000	5.052244100000
C	4.622336600000	2.587190400000	-2.800458100000
H	5.630084600000	2.353468400000	-3.115841800000
C	3.846345100000	3.457581800000	-3.543272300000
H	4.245419300000	3.909449600000	-4.441410200000
C	-1.503978900000	2.178689300000	5.128503000000
H	-0.899074400000	2.648380100000	5.892809300000

C	6.239880200000	-3.319435600000	1.466512300000
H	7.164704500000	-2.804395000000	1.719186100000
H	6.523877600000	-4.240506800000	0.961304100000
H	5.727565700000	-3.580214200000	2.392856700000
C	-2.477579800000	4.355883800000	1.697695900000
H	-1.845928200000	4.940139200000	2.352459700000
C	-0.804470300000	3.957327600000	-4.821992700000
H	-0.545319100000	4.529841000000	-5.702388400000
C	-6.366163700000	-1.301230600000	0.847050000000
H	-6.767245300000	-1.865348000000	1.689089200000
H	-7.195915800000	-0.962112100000	0.226778200000
H	-5.853993800000	-0.422758800000	1.238204500000
C	-6.186191100000	-3.384030300000	-0.511121400000
H	-5.554169500000	-4.041742700000	-1.105977300000
H	-7.021183900000	-3.057727300000	-1.127802200000
H	-6.612909300000	-3.959243400000	0.308180300000
C	-3.109460000000	-4.077818500000	2.436085300000
H	-3.055227400000	-5.029120900000	2.946883300000
C	-1.621076000000	3.865907200000	-2.564400200000
H	-2.000873100000	4.380384200000	-1.693849300000
C	-1.277550600000	4.597446200000	-3.690626400000
H	-1.391747600000	5.673012900000	-3.682680400000

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Au	0.042800700000	0.279013100000	0.045587400000
P	-0.927153000000	-0.523014400000	2.299283700000
P	0.503938500000	-1.440987400000	-1.663315100000
P	-1.908718000000	1.196015400000	-1.245081400000
P	2.213681700000	1.708431400000	0.385230000000
O	3.116031500000	-0.928117500000	-0.412333500000
O	-3.238904300000	-0.607884900000	0.515801900000
C	3.629687400000	0.812149000000	1.086258900000
C	1.277177000000	-4.027060700000	-0.781086700000
H	0.333103200000	-4.381960100000	-1.162030300000
C	-1.691879200000	-3.074966000000	-1.387863200000
H	-1.468763700000	-3.079879200000	-0.330548500000
C	-1.797728900000	0.686346600000	3.360363400000
C	1.584291400000	-2.671839600000	-0.847779000000
C	-0.893021500000	-2.331147600000	-2.281642100000
C	4.411365100000	1.296879700000	2.128209000000
H	4.212385000000	2.275164400000	2.539719300000
C	-2.564669300000	2.434429600000	-0.079092800000
C	-3.254258400000	0.159673500000	-1.710612700000
C	-1.144498700000	1.491659100000	-3.892589200000
H	-1.156799200000	0.412168500000	-3.920080400000
C	0.330761000000	-1.224468400000	3.406722400000
C	-1.228002400000	-2.348838100000	-3.648780200000
H	-0.629782400000	-1.796285900000	-4.358999000000
C	3.917881500000	-0.454866600000	0.598178100000
C	2.873941400000	2.451001700000	-1.134255500000
C	2.805076700000	4.326749000000	1.270074000000

H	3.470595200000	4.410913000000	0.422995300000
C	2.830196300000	-2.271553500000	-0.377023300000
C	-2.122172000000	-1.893152600000	2.131335800000
C	-4.173996200000	-2.720872700000	1.089540100000
C	-5.362500000000	-2.370324400000	0.205695300000
C	2.072940200000	3.159986600000	1.472543900000
C	-5.340841000000	-1.638375500000	-2.273444900000
H	-6.141001300000	-2.320844400000	-2.512837400000
C	-1.471504700000	2.157834900000	-2.714332200000
C	-2.293782300000	-3.088127100000	-4.097964400000
H	-2.533564300000	-3.086076900000	-5.152504500000
C	4.161624900000	2.221050300000	-1.596375600000
H	4.818784800000	1.547575800000	-1.065410800000
C	-1.702597700000	3.193124700000	0.702820600000
H	-0.637407400000	3.017867800000	0.659575000000
C	4.938349600000	-1.248093200000	1.096831900000
C	1.562709000000	-1.575370100000	2.876418400000
H	1.760673400000	-1.390260700000	1.832756600000
C	3.422771200000	-4.494182300000	0.189949500000
H	4.123635600000	-5.216294800000	0.581704200000
C	1.521076400000	-1.001598800000	-3.094784800000
C	-4.826119400000	-1.579568500000	-0.978769700000
C	1.839585100000	5.292944000000	3.244890100000
H	1.748645000000	6.123725900000	3.931471600000
C	-3.150734200000	0.960517700000	3.187320900000
H	-3.717298000000	0.454257900000	2.424198200000
C	2.686435700000	5.385945300000	2.151804300000
H	3.259568800000	6.287863300000	1.985105400000
C	1.106934100000	4.136980900000	3.451599600000
H	0.433368300000	4.058731900000	4.293482100000
C	-0.816604000000	2.200308900000	-5.032248000000
H	-0.566105300000	1.667185200000	-5.939004300000
C	2.181395100000	-4.924271400000	-0.244952900000
H	1.924389500000	-5.972653300000	-0.188106400000
C	-1.101592700000	1.382372000000	4.345861800000
H	-0.055449100000	1.179194000000	4.521613600000
C	-3.933267900000	2.667515300000	-0.003889700000
H	-4.612943600000	2.082465400000	-0.607494400000
C	1.708369800000	0.311633500000	-3.482715500000
H	1.263080000000	1.108737600000	-2.912970000000
C	-3.188863900000	-1.757803000000	1.253192600000
C	-3.555915300000	4.411377900000	1.602561100000
H	-3.943613900000	5.179446900000	2.257931000000
C	-3.789680800000	-0.710311200000	-0.744494000000
C	3.779740000000	-3.156897900000	0.107779800000
C	-4.019924800000	-3.909359800000	1.784765300000
H	-4.750036800000	-4.697498000000	1.674252500000
C	2.119843300000	-2.026179200000	-3.828339600000
H	1.985189500000	-3.057231200000	-3.531545200000
C	2.507464600000	3.970831200000	-2.966156700000
H	1.853842400000	4.647636200000	-3.498276600000
C	-4.861791000000	-0.770933600000	-3.253978600000

H	-5.301424600000	-0.792718900000	-4.241785200000
C	5.919230600000	-2.385421600000	-0.882062800000
H	5.374681800000	-1.718619100000	-1.549344800000
H	6.059901100000	-3.337493600000	-1.393710000000
H	6.898436000000	-1.949280700000	-0.683918500000
C	-2.002538900000	-3.102270600000	2.810917900000
H	-1.172317000000	-3.269520100000	3.478568100000
C	2.279800700000	-2.404401700000	5.005394800000
H	3.037559500000	-2.858888600000	5.629225000000
C	2.046945500000	3.324222100000	-1.836405900000
H	1.036469700000	3.507271800000	-1.495959700000
C	1.222211000000	3.080911600000	2.565986700000
H	0.633455000000	2.189732000000	2.716939200000
C	5.692224200000	-0.734359900000	2.141101700000
H	6.492985400000	-1.320445700000	2.567304600000
C	-3.055245100000	-3.853182900000	-3.209651800000
H	-3.875038800000	-4.456475400000	-3.571756500000
C	2.533616100000	-2.164487100000	3.668560300000
H	3.488836600000	-2.424995800000	3.237798500000
C	-4.423539500000	3.654096100000	0.833043000000
H	-5.489183800000	3.833463500000	0.881558400000
C	5.432069200000	0.526017000000	2.651847700000
H	6.031040800000	0.910279700000	3.465489700000
C	5.157674700000	-2.602046000000	0.441165400000
C	-2.729034700000	-3.846330500000	-1.863447900000
H	-3.302151800000	-4.437552300000	-1.163718900000
C	2.880111900000	-1.729082200000	-4.941339500000
H	3.337688300000	-2.528544900000	-5.507940400000
C	2.464760200000	0.608628400000	-4.604541600000
H	2.595017900000	1.639268400000	-4.899306200000
C	-3.788555500000	1.892803400000	3.984369900000
H	-4.841595500000	2.086461400000	3.833749000000
C	3.051228900000	-0.408673200000	-5.332773000000
H	3.645662400000	-0.177523200000	-6.206527400000
C	-3.850205800000	0.117430900000	-2.992403300000
H	-3.531110900000	0.800407100000	-3.762387900000
C	-3.090214500000	2.572847600000	4.965655200000
H	-3.593854500000	3.294922500000	5.593760200000
C	1.049704800000	-2.061322000000	5.547887600000
H	0.844789400000	-2.252076400000	6.592524800000
C	0.080696600000	-1.478858500000	4.755241900000
H	-0.876640500000	-1.222202900000	5.186726000000
C	4.621285000000	2.866217700000	-2.733129900000
H	5.628251400000	2.681907200000	-3.081822300000
C	3.800671300000	3.746741600000	-3.414381800000
H	4.164753600000	4.255953000000	-4.296529900000
C	-1.742621700000	2.314372200000	5.142036300000
H	-1.187339900000	2.826346700000	5.916794600000
C	5.963173700000	-3.546344700000	1.323771500000
H	6.948289800000	-3.131726000000	1.528646000000
H	6.124323900000	-4.497061000000	0.819358300000
H	5.467238200000	-3.742613400000	2.274620200000

C	-2.192643200000	4.178785300000	1.537878900000
H	-1.507335300000	4.757967600000	2.140906700000
C	-0.806272400000	3.584933300000	-5.010598900000
H	-0.553449000000	4.139401900000	-5.904270900000
C	-6.303421000000	-1.452850300000	1.013297400000
H	-6.680350500000	-1.974544900000	1.893409600000
H	-7.149748500000	-1.152124800000	0.395928500000
H	-5.789370400000	-0.551229200000	1.344080900000
C	-6.148528700000	-3.601923600000	-0.226847400000
H	-5.542882300000	-4.292065900000	-0.811875800000
H	-7.006860100000	-3.309777700000	-0.828278400000
H	-6.539401300000	-4.132038500000	0.639996600000
C	-2.935048800000	-4.104605700000	2.623702500000
H	-2.824115300000	-5.042317300000	3.150022200000
C	-1.462556700000	3.550556400000	-2.702044800000
H	-1.729955300000	4.088943300000	-1.805107100000
C	-1.130877500000	4.257088000000	-3.844308800000
H	-1.137799400000	5.338565400000	-3.823503800000

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Au	0.069940827823	0.322672706882	-0.032927525142
P	-0.885459590498	-0.645202535907	2.105091967853
P	0.654547806124	-1.610146136736	-1.528476095189
P	-1.818908148998	1.535013021746	-1.129775434589
P	2.086550126225	1.705713431196	0.390427503489
O	3.292266729463	-0.828867258781	-0.354268822065
O	-3.226213766888	-0.453265185099	0.365211149220
C	3.431701759511	0.851164671345	1.278541447068
C	2.124082551788	-4.106819214481	-1.434822834838
H	2.143704444180	-4.355803989440	-2.494269025503
C	-0.773692592914	-3.844755823813	-0.703469713617
H	-0.030795470006	-3.923351874721	0.079162799741
C	-1.635357728410	0.564247942000	3.255808533716
C	2.037962658754	-2.673054734141	-1.072266567876
C	-0.703703609961	-2.809915846050	-1.631735510141
C	4.008421350916	1.327513626400	2.449721826327
H	3.676357335396	2.264118198013	2.871640138728
C	-2.690534517030	2.692789341288	-0.029426488462
C	-3.172493280102	0.494354740130	-1.771068938157
C	-0.775213448327	1.939207600545	-3.655374928296
H	-0.543701576953	0.884973276606	-3.613460385934
C	0.307997034235	-1.527682858493	3.158966451263
C	-1.703154330020	-2.696637518243	-2.590399893733
H	-1.687288537741	-1.884153057914	-3.303302191814
C	3.895185886466	-0.359914614135	0.785264640995
C	2.889178660291	2.325843019868	-1.123211519992
C	2.734552538956	4.348589186827	1.142424887549
H	3.462116751075	4.341994050773	0.343619659106
C	3.162321435021	-2.187180588604	-0.478992195414
C	-2.206344742676	-1.900679263400	1.904695189543

C	-4.285612331601	-2.544772114616	0.787047439147
C	-5.414182829593	-2.099092156204	-0.132952608748
C	1.923940836912	3.238269482975	1.361516439711
C	-5.274789075371	-1.168862053731	-2.536469852756
H	-6.091529179136	-1.800494368265	-2.853544922698
C	-1.405122761738	2.556730991266	-2.578995065663
C	-2.718140635756	-3.634231122135	-2.657453530486
H	-3.479767458215	-3.540242363408	-3.418787188749
C	4.206604051616	2.053010872183	-1.463740783964
H	4.821027522012	1.440022530487	-0.821177254998
C	-1.921287542185	3.524195063332	0.774631353353
H	-0.845082308045	3.443778642688	0.752558311943
C	4.918921079659	-1.085321899786	1.371841217017
C	1.458325183998	-2.029423854664	2.569538139046
H	1.638002027123	-1.840519218670	1.522989585471
C	3.887627647818	-4.435549413332	0.170524193427
H	4.497928827444	-5.052563206362	0.813555515081
C	1.124363009686	-1.285558866567	-3.267205953305
C	-4.804843694206	-1.244772000923	-1.234650956859
C	1.693958816964	5.491692479609	2.980200851360
H	1.605116306984	6.369075237755	3.606544039290
C	-2.973106171983	0.932217163042	3.157094751333
H	-3.609607975561	0.484787744645	2.411711024532
C	2.615037857270	5.468950028978	1.944825346221
H	3.247089280184	6.327424225663	1.762534896662
C	0.886932819959	4.390415885765	3.206188641432
H	0.159446396896	4.396337908359	4.006340625973
C	-0.437949737159	2.659071225336	-4.784120054780
H	0.048858935400	2.158796050145	-5.610093243186
C	2.873395419663	-4.973428453015	-0.521621127062
H	2.646270956860	-6.029936122416	-0.457203851364
C	-0.846622213839	1.183992818812	4.221655969286
H	0.195032508537	0.915417902095	4.326857993919
C	-4.074494422226	2.805496157666	0.013465973455
H	-4.692698334889	2.175196840623	-0.609833916115
C	1.833162596555	-0.122859611078	-3.539566604061
H	1.993802288147	0.602354524878	-2.757500310359
C	-3.245820842318	-1.658027681757	1.017690401478
C	-3.897476694777	4.560037831982	1.643590138873
H	-4.368479372085	5.283659144418	2.295109992778
C	-3.746646891026	-0.418748011501	-0.898610703490
C	4.156422702270	-3.016686035147	0.090770302698
C	-4.257087031993	-3.746612494505	1.474645539534
H	-5.041681205414	-4.473456496387	1.325445601711
C	0.931174154684	-2.212578979847	-4.288819145730
H	0.392918869978	-3.129953779409	-4.098967811638
C	2.675719141590	3.664803279341	-3.114298599675
H	2.070044558651	4.293431983809	-3.751215807394
C	-4.719632398508	-0.279054213779	-3.440806254080
H	-5.107941076293	-0.225062259063	-4.448325868832
C	6.287451234628	-1.921729405188	-0.530514479908
H	5.756664228437	-1.261928985690	-1.215029593643

H	6.613678954269	-2.800052511306	-1.087304197761
H	7.168478436489	-1.397788365067	-0.159222025743
C	-2.216849969424	-3.118611923431	2.575104554528
H	-1.422648583048	-3.364684106811	3.262131143487
C	2.134454425868	-3.012233008596	4.647613491628
H	2.843994331708	-3.586815782270	5.227638324130
C	2.127563479731	3.133531546789	-1.962962367253
H	1.096956919960	3.351657879650	-1.718844964630
C	0.999634873742	3.275336761736	2.395010190553
H	0.350901138053	2.429836403665	2.559638820249
C	5.457454182421	-0.587441251647	2.547984220517
H	6.245437206944	-1.126382879245	3.052992886201
C	-2.755611147580	-4.684780255712	-1.757422515260
H	-3.541014962191	-5.425948556547	-1.818675311009
C	2.364326376947	-2.773598411451	3.306204729024
H	3.250486598123	-3.162618832635	2.827156440822
C	-4.673248425102	3.730901221982	0.851689615176
H	-5.751897928955	3.808332024587	0.878859162671
C	5.001376949421	0.604296076205	3.085069494326
H	5.433684069573	0.979987580841	4.001836269229
C	5.389323669967	-2.344246746234	0.654181086291
C	-1.790373853378	-4.778888608497	-0.770290512380
H	-1.827843306848	-5.581682245865	-0.047630185828
C	1.420956803383	-1.965533110328	-5.558287848864
H	1.257878663026	-2.689672487291	-6.345105095907
C	2.333236155214	0.118345199966	-4.807453067220
H	2.882138486171	1.030265769623	-4.996441842397
C	-3.506691467467	1.885412499766	4.004935660377
H	-4.548676396446	2.157130729342	3.908898985696
C	2.124029634063	-0.800071549599	-5.820705259111
H	2.509722588705	-0.612537482680	-6.813783626738
C	-3.687526150413	0.559861062606	-3.059263636601
H	-3.282557385298	1.265435843319	-3.768517786727
C	-2.716633538951	2.488794686862	4.966928568865
H	-3.138611119203	3.227821936548	5.634374012079
C	0.989233365736	-2.512557920405	5.249952670366
H	0.801927903389	-2.698876467183	6.298756577376
C	0.079752832374	-1.781316455584	4.511014322458
H	-0.814731876105	-1.407839028557	4.989175709591
C	4.751174537612	2.572742836466	-2.626935878536
H	5.778151999810	2.349521055875	-2.882491447396
C	3.990012861955	3.381791878094	-3.451456475393
H	4.419747122323	3.793730436756	-4.354666258354
C	-1.383256099455	2.133994570839	5.072372956678
H	-0.755689453725	2.588927722627	5.827199322311
C	6.192745440729	-3.262285663244	1.567056291704
H	7.092759522284	-2.758466588016	1.914002358998
H	6.515231877220	-4.150265724978	1.026447226594
H	5.623321086879	-3.578355825590	2.441214772873
C	-2.517385075271	4.457222925920	1.600906172791
H	-1.900651217006	5.096213979278	2.217691361249
C	-0.709523501345	4.016975501146	-4.846077714625

H	-0.443115565463	4.584992243513	-5.727308649726
C	-6.368621203675	-1.204323808719	0.684300796949
H	-6.798159668461	-1.768880790232	1.511826062226
H	-7.178672507013	-0.841747962199	0.051251345743
H	-5.846421685881	-0.341029865650	1.095678956904
C	-6.202334661659	-3.277896392089	-0.690097933712
H	-5.570175286585	-3.942920320212	-1.276387166487
H	-7.018664123879	-2.930002039165	-1.320043231175
H	-6.656103623499	-3.852040477823	0.115195007803
C	-3.232127851823	-4.030853703678	2.359610878481
H	-3.224919399337	-4.973522646565	2.889115688199
C	-1.675258222162	3.917456310990	-2.648209333123
H	-2.165001711744	4.418405657996	-1.826057333632
C	-1.321184137324	4.643593861245	-3.774962107265
H	-1.535859705344	5.702888707216	-3.815807711584

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Au	9.628750000000	6.134898000000	14.736909000000
P	7.143561000000	5.861154000000	14.886424000000
P	10.571296000000	8.280157000000	15.687400000000
C	6.367904000000	7.092678000000	13.812906000000
C	5.189472000000	6.858733000000	13.089199000000
H	4.831876000000	5.853328000000	12.941538000000
C	4.482954000000	7.905288000000	12.530864000000
H	3.606773000000	7.687296000000	11.933771000000
C	4.885170000000	9.214529000000	12.715291000000
H	4.322252000000	10.019969000000	12.268302000000
C	6.006326000000	9.497676000000	13.494473000000
C	6.719457000000	8.437109000000	14.006567000000
C	9.895433000000	9.761861000000	14.890888000000
C	10.666415000000	10.881736000000	14.604084000000
H	11.722705000000	10.884961000000	14.828653000000
C	10.092849000000	11.990722000000	14.013612000000
H	10.706997000000	12.844578000000	13.760218000000
C	8.733130000000	12.012833000000	13.753833000000
H	8.296070000000	12.898736000000	13.318416000000
C	7.928701000000	10.923105000000	14.040059000000
C	8.544784000000	9.797717000000	14.565711000000
C	6.419466000000	10.905459000000	13.885847000000
C	5.798625000000	11.210697000000	15.263202000000
H	4.711589000000	11.168143000000	15.195254000000
H	6.078685000000	12.213472000000	15.589056000000
H	6.131248000000	10.488825000000	16.008042000000
C	5.935577000000	11.949618000000	12.890920000000
H	6.342787000000	11.788071000000	11.893125000000
H	6.216916000000	12.948766000000	13.212511000000
H	4.851897000000	11.953302000000	12.810756000000
O	7.823497000000	8.665904000000	14.794626000000
C	6.558097000000	6.035485000000	16.526545000000
C	5.174062000000	5.786492000000	16.782716000000

H	4.577649000000	5.265246000000	16.051342000000
C	4.603533000000	6.169419000000	17.972182000000
H	3.555509000000	5.957479000000	18.148562000000
C	5.344389000000	6.814803000000	18.960391000000
H	4.903006000000	7.056945000000	19.915424000000
C	6.684046000000	7.113939000000	18.699826000000
H	7.276415000000	7.621767000000	19.448813000000
C	7.272352000000	6.760326000000	17.512899000000
H	8.304714000000	7.008811000000	17.345526000000
C	6.572450000000	4.264316000000	14.274649000000
C	6.398178000000	4.014597000000	12.915536000000
H	6.667366000000	4.763692000000	12.188137000000
C	5.857529000000	2.819975000000	12.482047000000
H	5.707343000000	2.645159000000	11.425649000000
C	5.510998000000	1.845146000000	13.401775000000
H	5.076914000000	0.919430000000	13.050800000000
C	5.729569000000	2.058759000000	14.752040000000
H	5.473922000000	1.294810000000	15.472941000000
C	6.258141000000	3.258807000000	15.186992000000
H	6.395724000000	3.441264000000	16.241863000000
C	12.364607000000	8.519301000000	15.533097000000
C	12.933592000000	8.376251000000	14.273158000000
H	12.318116000000	8.127813000000	13.420916000000
C	14.288882000000	8.549475000000	14.091014000000
H	14.703371000000	8.452490000000	13.099967000000
C	15.106587000000	8.835430000000	15.173701000000
H	16.173437000000	8.944288000000	15.029568000000
C	14.549562000000	8.969972000000	16.432405000000
H	15.172786000000	9.193552000000	17.287831000000
C	13.183014000000	8.825813000000	16.611421000000
H	12.763878000000	8.951631000000	17.597797000000
C	10.262234000000	8.539982000000	17.457439000000
C	9.637051000000	9.678466000000	17.945109000000
H	9.299948000000	10.448390000000	17.266876000000
C	9.438118000000	9.834533000000	19.307050000000
H	8.940808000000	10.719255000000	19.679584000000
C	9.872961000000	8.867292000000	20.194844000000
H	9.716745000000	8.993712000000	21.257261000000
C	10.498277000000	7.726723000000	19.715141000000
H	10.838214000000	6.966402000000	20.404528000000
C	10.678303000000	7.561173000000	18.355414000000
H	11.145153000000	6.653712000000	18.000157000000
P	10.349673000000	4.108693000000	15.962905000000
P	9.857175000000	6.168224000000	12.250173000000
C	9.683874000000	2.535149000000	15.376224000000
C	9.351223000000	1.501328000000	16.240758000000
H	9.457737000000	1.638630000000	17.306321000000
C	8.897280000000	0.298382000000	15.738787000000
H	8.639576000000	-0.503394000000	16.416202000000
C	8.795316000000	0.106915000000	14.372367000000
H	8.464452000000	-0.850208000000	13.997924000000
C	9.137025000000	1.107873000000	13.474864000000

C	9.555928000000	2.315157000000	14.007513000000
C	9.305875000000	4.676281000000	11.352042000000
C	8.853308000000	4.743065000000	10.040387000000
H	8.796312000000	5.694856000000	9.539321000000
C	8.456367000000	3.604169000000	9.373049000000
H	8.094793000000	3.669436000000	8.358052000000
C	8.518725000000	2.373049000000	9.996378000000
H	8.192940000000	1.495994000000	9.457785000000
C	9.004317000000	2.251796000000	11.286778000000
C	9.400106000000	3.413783000000	11.934023000000
C	9.180842000000	0.904951000000	11.969614000000
C	8.127418000000	-0.100539000000	11.509670000000
H	8.277653000000	-1.066408000000	11.985570000000
H	8.204280000000	-0.288595000000	10.443214000000
H	7.118810000000	0.244500000000	11.727112000000
C	10.572758000000	0.361981000000	11.596440000000
H	11.368464000000	1.033304000000	11.920556000000
H	10.651104000000	0.235266000000	10.517768000000
H	10.725148000000	-0.617211000000	12.049041000000
O	9.924348000000	3.350024000000	13.196198000000
C	10.233653000000	4.022278000000	17.762631000000
C	8.988631000000	4.229218000000	18.344541000000
H	8.126485000000	4.420078000000	17.723151000000
C	8.851884000000	4.240422000000	19.719209000000
H	7.887410000000	4.454375000000	20.159171000000
C	9.958712000000	4.041807000000	20.526097000000
H	9.865228000000	4.069660000000	21.601297000000
C	11.201770000000	3.828264000000	19.953364000000
H	12.064265000000	3.690250000000	20.590304000000
C	11.343134000000	3.815202000000	18.576761000000
H	12.320453000000	3.656511000000	18.144343000000
C	12.130271000000	3.981633000000	15.615506000000
C	12.935838000000	5.081316000000	15.888986000000
H	12.506428000000	5.979192000000	16.304978000000
C	14.289408000000	5.051960000000	15.621546000000
H	14.883846000000	5.930949000000	15.824114000000
C	14.860408000000	3.918270000000	15.066607000000
H	15.918564000000	3.892091000000	14.836936000000
C	14.067619000000	2.817147000000	14.790424000000
H	14.500926000000	1.931955000000	14.343209000000
C	12.710706000000	2.844672000000	15.067616000000
H	12.108815000000	1.975976000000	14.846108000000
C	9.071456000000	7.593327000000	11.451226000000
C	7.814530000000	7.528309000000	10.858811000000
H	7.258697000000	6.604921000000	10.851715000000
C	7.257347000000	8.644397000000	10.264919000000
H	6.284149000000	8.573629000000	9.800528000000
C	7.936043000000	9.848960000000	10.265796000000
H	7.502051000000	10.715396000000	9.783057000000
C	9.160674000000	9.940905000000	10.902565000000
H	9.697468000000	10.878795000000	10.931832000000
C	9.716798000000	8.826991000000	11.501844000000

H	10.673422000000	8.932967000000	11.991992000000
C	11.605552000000	6.200046000000	11.710309000000
C	12.079074000000	6.995268000000	10.672737000000
H	11.447532000000	7.727340000000	10.195793000000
C	13.385962000000	6.871392000000	10.234711000000
H	13.726981000000	7.501422000000	9.424836000000
C	14.232787000000	5.944964000000	10.815732000000
H	15.249503000000	5.837943000000	10.460351000000
C	13.769713000000	5.148901000000	11.848757000000
H	14.418382000000	4.416907000000	12.307148000000
C	12.469197000000	5.280901000000	12.297185000000
H	12.122085000000	4.646805000000	13.097458000000

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P	-1.880992900000	-1.202785100000	0.921658100000
P	1.623427900000	-1.288298400000	-1.115493500000
P	-1.654418200000	1.378283200000	-1.067797800000
P	1.866142600000	1.130231600000	1.048315000000
C	2.816432600000	-2.157969200000	-0.058573900000
C	-2.714559200000	0.309128100000	-2.099278000000
C	-1.359330400000	-2.849452200000	1.496449400000
C	2.363920100000	-2.747085200000	1.116524900000
H	1.328576300000	-2.646168100000	1.405140800000
C	-3.128108400000	-1.591755200000	-0.377886700000
C	-3.866841700000	-2.719139900000	-0.100047800000
H	-3.712115700000	-3.228741200000	0.839155200000
C	-2.798347900000	-0.492993200000	2.326893800000
C	-3.307430800000	-0.929018600000	-1.647807700000
C	1.012476300000	-2.550895800000	-2.267010100000
C	-1.173031700000	-3.105462600000	2.848474300000
H	-1.468249400000	-2.371824000000	3.585886300000
C	-1.037885100000	2.704024800000	-2.143982200000
C	-4.774782300000	-3.288309000000	-0.996277200000
H	-5.327976000000	-4.173713700000	-0.716478800000
C	2.683871000000	-0.164132600000	-2.076959600000
C	3.234713700000	-3.449465000000	1.927488400000
H	2.868123200000	-3.899916400000	2.839108400000
C	-4.187962000000	-1.570217000000	-2.575012900000
C	3.370003100000	0.956897000000	-1.482697900000
C	3.233369300000	1.461408900000	-0.140260700000
C	-2.938062800000	0.748275100000	-3.380444800000
H	-2.486585600000	1.672723300000	-3.705722800000
C	-2.823532000000	2.210206400000	0.043822300000
C	1.617796400000	-3.792630900000	-2.415777800000
H	2.527742400000	-4.020739900000	-1.878984300000
C	2.849210500000	-0.443330800000	-3.409223000000
H	2.330164000000	-1.286863600000	-3.839060200000
C	4.309978100000	1.629929200000	-2.321673700000
C	-0.169343000000	-2.284113800000	-2.952917400000

H	-0.661622500000	-1.330275900000	-2.822035100000
C	4.160906600000	-2.267482600000	-0.398882900000
H	4.531295700000	-1.808655600000	-1.305111300000
C	-0.973471500000	-3.812107800000	0.564755700000
H	-1.098218900000	-3.625798400000	-0.493257400000
C	0.181074000000	2.504191400000	-2.784527800000
H	0.708342000000	1.569521400000	-2.652879800000
C	2.245168500000	-0.929084200000	4.524318000000
H	1.559145000000	-1.354280400000	5.244440800000
C	4.570976600000	-3.555950600000	1.581924300000
H	5.254962400000	-4.096386300000	2.222362900000
C	-4.374334100000	-1.068234000000	-3.882966400000
H	-5.038130300000	-1.607559100000	-4.545833100000
C	-0.612099900000	-4.304305300000	3.262339600000
H	-0.476640600000	-4.493570000000	4.318723500000
C	-1.692793400000	3.920682400000	-2.294589300000
H	-2.635658800000	4.094414900000	-1.794973900000
C	2.617679300000	0.287205300000	2.475732400000
C	-4.076445300000	-0.903387100000	2.693708700000
H	-4.609546600000	-1.631843200000	2.101533100000
C	1.753136100000	-0.275335200000	3.411646900000
H	0.684762500000	-0.220309200000	3.254943100000
C	-2.159107600000	0.472686500000	3.093737400000
H	-1.188075100000	0.835146200000	2.786648400000
C	-4.907161900000	-2.731650000000	-2.224926200000
H	-5.568409500000	-3.165545000000	-2.963401300000
C	1.240269400000	3.096651200000	2.966143500000
H	1.420503900000	2.343650800000	3.720284100000
C	4.434186600000	1.300696300000	-3.691246400000
H	5.141794500000	1.860692300000	-4.288457100000
C	-0.422731900000	-5.007221300000	0.981014500000
H	-0.127908800000	-5.743257000000	0.245551500000
C	1.462063500000	2.812177700000	1.625925700000
C	1.047176800000	-4.750573000000	-3.237944000000
H	1.521045100000	-5.717221400000	-3.342478600000
C	-0.731256200000	-3.236010600000	-3.781840300000
H	-1.651038000000	-3.014089400000	-4.305748700000
C	3.986696700000	0.142753700000	2.656170800000
H	4.678380200000	0.533484000000	1.925403700000
C	3.695244400000	0.305734700000	-4.239025200000
H	3.783241900000	0.054298800000	-5.286648400000
C	-3.744688500000	0.057917300000	-4.293574700000
H	-3.879572900000	0.444596100000	-5.293894100000
C	4.098910500000	2.436146600000	0.300717700000
H	3.990269500000	2.817845900000	1.306200500000
C	1.235156900000	3.806967100000	0.675695700000
H	1.391583700000	3.601741800000	-0.374762500000
C	5.034129400000	-2.960737700000	0.420442900000
H	6.078451200000	-3.036889500000	0.149508200000
C	-2.304390900000	3.076865000000	1.001989900000
H	-1.238085000000	3.238247700000	1.062716200000
C	-0.124921100000	-4.474966400000	-3.921405100000

H	-0.569235700000	-5.227253100000	-4.558949300000
C	4.479142000000	-0.530020500000	3.761777000000
H	5.547547200000	-0.645493100000	3.883124100000
C	-0.237469300000	-5.256993500000	2.332700100000
H	0.196679000000	-6.192657900000	2.657458400000
C	5.150755500000	2.640461000000	-1.811556400000
H	5.858107300000	3.106634300000	-2.484878900000
C	-1.132857600000	4.920326100000	-3.072346400000
H	-1.645483300000	5.866752400000	-3.178780100000
C	-3.142103900000	3.730807600000	1.881514000000
H	-2.723233500000	4.405339400000	2.615870000000
C	-4.686971500000	-0.373530900000	3.814567800000
H	-5.681670200000	-0.699151300000	4.087083500000
C	3.613095300000	-1.056969600000	4.702623300000
H	4.002074900000	-1.579092300000	5.566265000000
C	-4.194405000000	1.998506600000	-0.005047600000
H	-4.618446300000	1.332088000000	-0.742040400000
C	0.733654200000	3.497933800000	-3.570358100000
H	1.682706800000	3.327483800000	-4.060504400000
C	0.078345000000	4.711226000000	-3.710855800000
H	0.513631700000	5.495745600000	-4.314980300000
C	5.081462000000	3.012564600000	-0.508398800000
H	5.735814500000	3.772679000000	-0.105620600000
C	-4.509356700000	3.505108900000	1.836500700000
H	-5.165313600000	4.004011600000	2.536887000000
C	0.797546700000	4.353852400000	3.350178600000
H	0.634678200000	4.564377800000	4.398674800000
C	-2.765758900000	0.996969400000	4.221594100000
H	-2.254503500000	1.751764400000	4.803512500000
C	0.803647600000	5.060072500000	1.062347200000
H	0.633243400000	5.820510400000	0.312391300000
C	-4.029541200000	0.571622600000	4.586315100000
H	-4.509909800000	0.983551200000	5.463482400000
C	-5.031744000000	2.636522200000	0.896388900000
H	-6.097098800000	2.454702500000	0.857318700000
C	0.578920300000	5.337270800000	2.402938700000
H	0.239638000000	6.318537100000	2.705417600000
Au	-0.013522800000	0.032465100000	0.055467900000

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P	-1.826936000000	-1.389231000000	0.749539000000
P	1.722261000000	-1.349502000000	-0.975162000000
P	-1.645384000000	1.467909000000	-0.850263000000
P	1.916966000000	1.233733000000	0.879599000000
C	2.942154000000	-2.143268000000	0.085883000000
C	-2.680840000000	0.474574000000	-1.992479000000
C	-1.299643000000	-3.008058000000	1.376854000000
C	2.516041000000	-2.816152000000	1.226478000000
H	1.470853000000	-2.812900000000	1.501048000000
C	-3.007917000000	-1.696653000000	-0.603347000000

C	-3.682796000000	-2.890718000000	-0.503929000000
H	-3.506052000000	-3.524455000000	0.351877000000
C	-2.801932000000	-0.675310000000	2.107783000000
C	-3.226939000000	-0.839748000000	-1.742249000000
C	0.968539000000	-2.670297000000	-1.955911000000
C	-1.087844000000	-3.163544000000	2.743705000000
H	-1.366835000000	-2.377116000000	3.430621000000
C	-0.897707000000	2.775253000000	-1.854635000000
C	-4.566483000000	-3.353154000000	-1.482011000000
H	-5.070714000000	-4.300172000000	-1.352276000000
C	2.598306000000	-0.261014000000	-2.094812000000
C	3.429510000000	-3.483666000000	2.017317000000
H	3.091988000000	-4.001391000000	2.904299000000
C	-4.097921000000	-1.359640000000	-2.751342000000
C	3.254980000000	0.911246000000	-1.633126000000
C	3.177592000000	1.487566000000	-0.311437000000
C	-2.960480000000	1.108764000000	-3.180958000000
H	-2.546367000000	2.087352000000	-3.364996000000
C	-2.811707000000	2.296364000000	0.253224000000
C	1.476039000000	-3.963335000000	-1.961522000000
H	2.373732000000	-4.196110000000	-1.407183000000
C	2.643421000000	-0.646324000000	-3.441907000000
H	2.117905000000	-1.527582000000	-3.770974000000
C	4.112711000000	1.574318000000	-2.579809000000
C	-0.189093000000	-2.388950000000	-2.677691000000
H	-0.591820000000	-1.385262000000	-2.682125000000
C	4.291236000000	-2.130422000000	-0.245786000000
H	4.625644000000	-1.597784000000	-1.124911000000
C	-0.931606000000	-4.035950000000	0.512287000000
H	-1.080716000000	-3.934653000000	-0.552292000000
C	0.253507000000	2.464680000000	-2.572584000000
H	0.672384000000	1.469007000000	-2.533707000000
C	2.170793000000	-0.806610000000	4.415967000000
H	1.477857000000	-1.224881000000	5.133795000000
C	4.774339000000	-3.473961000000	1.682003000000
H	5.490380000000	-3.991214000000	2.306334000000
C	-4.343742000000	-0.653785000000	-3.949000000000
H	-5.000724000000	-1.103784000000	-4.681442000000
C	-0.521105000000	-4.326706000000	3.235246000000
H	-0.366015000000	-4.436450000000	4.299859000000
C	-1.404739000000	4.068647000000	-1.902021000000
H	-2.297005000000	4.326177000000	-1.350080000000
C	2.565401000000	0.395370000000	2.362943000000
C	-4.062234000000	-1.172525000000	2.425840000000
H	-4.506406000000	-1.958537000000	1.832462000000
C	1.690695000000	-0.153688000000	3.296509000000
H	0.622600000000	-0.086972000000	3.141870000000
C	-2.265550000000	0.348953000000	2.876036000000
H	-1.304199000000	0.769291000000	2.615992000000
C	-4.748471000000	-2.602363000000	-2.595530000000
H	-5.401671000000	-2.938181000000	-3.390075000000
C	1.018143000000	3.107931000000	2.787062000000

H	1.094114000000	2.321422000000	3.523304000000
C	4.124582000000	1.151010000000	-3.923958000000
H	4.746575000000	1.698677000000	-4.620247000000
C	-0.372038000000	-5.197236000000	1.009359000000
H	-0.092837000000	-5.986764000000	0.325624000000
C	1.388387000000	2.871825000000	1.465703000000
C	0.826124000000	-4.960979000000	-2.669103000000
H	1.228307000000	-5.965032000000	-2.669260000000
C	-0.834291000000	-3.384271000000	-3.383945000000
H	-1.735397000000	-3.153280000000	-3.935291000000
C	3.933752000000	0.241845000000	2.552041000000
H	4.624335000000	0.625354000000	1.815383000000
C	3.387653000000	0.076039000000	-4.355492000000
H	3.411976000000	-0.227271000000	-5.393064000000
C	-3.773672000000	0.553984000000	-4.173792000000
H	-3.952783000000	1.099494000000	-5.089354000000
C	4.101753000000	2.512551000000	0.050904000000
H	4.087343000000	2.905044000000	1.057651000000
C	1.319953000000	3.916902000000	0.546333000000
H	1.626845000000	3.753972000000	-0.475940000000
C	5.204074000000	-2.794052000000	0.555417000000
H	6.253908000000	-2.779127000000	0.296550000000
C	-2.310832000000	3.237730000000	1.149283000000
H	-1.257082000000	3.474047000000	1.157451000000
C	-0.330461000000	-4.676712000000	-3.374905000000
H	-0.837733000000	-5.459758000000	-3.921816000000
C	4.413172000000	-0.415937000000	3.670668000000
H	5.480177000000	-0.528797000000	3.805848000000
C	-0.162161000000	-5.345962000000	2.370565000000
H	0.277758000000	-6.255593000000	2.755760000000
C	4.945999000000	2.635787000000	-2.177675000000
H	5.594724000000	3.089135000000	-2.913797000000
C	-0.757888000000	5.038376000000	-2.648640000000
H	-1.153218000000	6.044744000000	-2.674865000000
C	-3.158794000000	3.881210000000	2.027312000000
H	-2.758789000000	4.618925000000	2.709367000000
C	-4.762650000000	-0.660493000000	3.500879000000
H	-5.741568000000	-1.053188000000	3.739566000000
C	3.536133000000	-0.934025000000	4.608385000000
H	3.916037000000	-1.447877000000	5.480989000000
C	-4.167154000000	1.996215000000	0.264866000000
H	-4.572626000000	1.269046000000	-0.423781000000
C	0.891972000000	3.431831000000	-3.324083000000
H	1.793266000000	3.176149000000	-3.863058000000
C	0.389895000000	4.723337000000	-3.356685000000
H	0.896673000000	5.485784000000	-3.932486000000
C	4.968775000000	3.057410000000	-0.860361000000
H	5.649294000000	3.838893000000	-0.550236000000
C	-4.510634000000	3.574111000000	2.039740000000
H	-5.173465000000	4.071987000000	2.734349000000
C	0.576417000000	4.359812000000	3.176807000000
H	0.302016000000	4.532641000000	4.208818000000

C	-2.966315000000	0.860191000000	3.953723000000
H	-2.540272000000	1.665240000000	4.536003000000
C	0.876823000000	5.166343000000	0.940812000000
H	0.833588000000	5.968120000000	0.216658000000
C	-4.213615000000	0.353925000000	4.269430000000
H	-4.764780000000	0.754785000000	5.109170000000
C	-5.010729000000	2.628623000000	1.162958000000
H	-6.063940000000	2.383878000000	1.170206000000
C	0.501236000000	5.391556000000	2.254688000000
H	0.162997000000	6.371702000000	2.562615000000
Au	0.031408000000	-0.012014000000	0.103589000000

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P	-1.819097747915	-1.401770794290	0.738983454977
P	1.729010819424	-1.343538203604	-0.978663372985
P	-1.653693646003	1.460968260312	-0.852425859482
P	1.914872209976	1.241321347210	0.869403648957
C	2.936406798413	-2.139483281934	0.097687765907
C	-2.699835780867	0.474603971909	-1.990465635089
C	-1.293537949297	-3.020225468927	1.369601479602
C	2.503347622137	-2.814369703408	1.233701268909
H	1.456240252096	-2.813260950069	1.500521227489
C	-3.002567205136	-1.707696332433	-0.613007455579
C	-3.670283650603	-2.905857480496	-0.516679601117
H	-3.485169368366	-3.544013169357	0.333950929296
C	-2.794902912867	-0.684592532366	2.094725549590
C	-3.236126934254	-0.843970517228	-1.744392541523
C	0.970248608042	-2.667700513444	-1.950938079003
C	-1.086163339238	-3.172601316929	2.737408418609
H	-1.368568456819	-2.385275895681	3.421882351770
C	-0.895636939021	2.761568995473	-1.858259780107
C	-4.558869228696	-3.366859512148	-1.491268356911
H	-5.056470423622	-4.317689040270	-1.363830351901
C	2.589026874568	-0.256985998465	-2.086470511508
C	3.412390594707	-3.482060467903	2.029672504469
H	3.069547873638	-4.002969502308	2.912785241494
C	-4.113431749883	-1.361205357574	-2.749352801094
C	3.261241226107	0.908242136888	-1.622720901619
C	3.185763426224	1.495826790278	-0.314643796822
C	-2.995844992457	1.117714474355	-3.169657059384
H	-2.586817332007	2.099344203327	-3.350012656999
C	-2.811739798316	2.300543785858	0.252031438885
C	1.487832837667	-3.956100553828	-1.966507764861
H	2.390698015111	-4.184605184981	-1.418733518089
C	2.617140976994	-0.626362121892	-3.455513111142
H	2.066981183308	-1.491373261009	-3.788172879701
C	4.125450672276	1.565478332774	-2.577031765151
C	-0.193669871829	-2.391292312913	-2.663462750907
H	-0.602021741181	-1.389896432538	-2.662660899205
C	4.287518237548	-2.122428243164	-0.224072549438

H	4.624838597141	-1.587150495959	-1.100711554252
C	-0.921743051917	-4.049368562558	0.508342609355
H	-1.067417335736	-3.950482443020	-0.556848885161
C	0.262897569808	2.446131840244	-2.561769139684
H	0.680777190860	1.450211288072	-2.513287460036
C	2.152796085034	-0.809350741453	4.403709786654
H	1.458985147404	-1.229145492012	5.119735939746
C	4.759637902193	-3.468554679152	1.704258754690
H	5.472095791928	-3.985999909788	2.332570677781
C	-4.375976633638	-0.646654841700	-3.938248589996
H	-5.037193353709	-1.094982284472	-4.667922536554
C	-0.518779297065	-4.333743447196	3.233116550720
H	-0.366961783979	-4.441126417651	4.298452939258
C	-1.400621516557	4.055502160799	-1.917760909202
H	-2.298288443007	4.317072733987	-1.376384759335
C	2.550885958670	0.383882263558	2.347516738835
C	-4.053124705005	-1.185747840450	2.414841758848
H	-4.493431794514	-1.976782386747	1.825170972324
C	1.674395980752	-0.166474484609	3.278074693071
H	0.607033023271	-0.107877311966	3.116558519909
C	-2.263342318331	0.345755360274	2.858161004634
H	-1.303660586185	0.769064853203	2.597283870605
C	-4.754619862511	-2.609404252152	-2.597732554703
H	-5.412019616501	-2.943611700119	-3.389491026060
C	1.046733913782	3.114062327325	2.789863505007
H	1.129441656039	2.325544331062	3.523442118191
C	4.131456056161	1.147819881353	-3.919371414038
H	4.760762271553	1.687966821263	-4.614689549016
C	-0.361700280427	-5.208671182747	1.009509929762
H	-0.079287008225	-5.999196909244	0.328251780284
C	1.407387248773	2.882832158167	1.466201717469
C	0.840915000166	-4.955352250324	-2.674868335700
H	1.250652742400	-5.956294001367	-2.682850694038
C	-0.836450897936	-3.387903631899	-3.370316214357
H	-1.742703550622	-3.160988633327	-3.914864506660
C	3.918810856578	0.247632388414	2.547591518081
H	4.610245714275	0.637715402806	1.814868875555
C	3.365854287046	0.081608524692	-4.359177224522
H	3.381829005170	-0.212711431408	-5.399487767892
C	-3.816804358723	0.567025572213	-4.158466866357
H	-4.009052363034	1.119107448795	-5.067397679809
C	4.102741030635	2.539067075861	0.045087526189
H	4.080760230111	2.934309504930	1.051130963963
C	1.324105693165	3.927728842625	0.548568102606
H	1.619416581290	3.766046798855	-0.477626748775
C	5.196348105147	-2.785192870189	0.582502683803
H	6.248137990037	-2.766824212399	0.331866849369
C	-2.302637491519	3.243430231178	1.141873728277
H	-1.247875355608	3.476116140489	1.143444172890
C	-0.322578571541	-4.676353425528	-3.371095554859
H	-0.827432177707	-5.460519843811	-3.918678969732
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H	5.463967105498	-0.505388032853	3.814717923957
C	-0.155143127507	-5.353905953110	2.371559208629
H	0.286087402760	-6.261597803869	2.759812031755
C	4.961217100607	2.624264602367	-2.175410458895
H	5.616143956395	3.068177442149	-2.912608983136
C	-0.744295775420	5.020546056592	-2.661930179509
H	-1.137804852659	6.027352059949	-2.697380573060
C	-3.143702735690	3.893585903178	2.021696099376
H	-2.737397432889	4.632478445504	2.698723894799
C	-4.756287972077	-0.671364439960	3.486918209214
H	-5.733316515453	-1.067538247446	3.727512217418
C	3.518235633199	-0.924806739476	4.604783763673
H	3.896696978559	-1.432037901979	5.481898557044
C	-4.167995755788	2.005105805233	0.272290899903
H	-4.579548829991	1.276606558083	-0.411382139368
C	0.910974183773	3.408772027761	-3.311501105356
H	1.817620777170	3.148342678228	-3.839477291338
C	0.411004677236	4.700518251686	-3.355903246464
H	0.925098152095	5.459644346511	-3.929636404897
C	4.974895168304	3.070992522236	-0.858806377119
H	5.657465449814	3.853295157080	-0.555548511448
C	-4.496670618575	3.591876039713	2.042107000339
H	-5.154187341904	4.095605345313	2.737565684796
C	0.604221673883	4.364530593243	3.186165606225
H	0.338124063415	4.534459107716	4.220799802832
C	-2.966916512704	0.859623299789	3.932720269984
H	-2.544511928746	1.669318456255	4.511164206622
C	0.882755902222	5.175210305148	0.948909794773
H	0.828562066386	5.977567826378	0.226141277933
C	-4.212300300736	0.349729036905	4.250208389228
H	-4.765975117256	0.753049647727	5.087115141613
C	-5.004618900919	2.644278260552	1.172182847348
H	-6.058589895676	2.403110470749	1.186174013348
C	0.519158203850	5.397265371616	2.267379972491
H	0.181407363857	6.376103426011	2.579998570939
Au	0.031837049585	-0.016179493844	0.104746455939

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Au	20.359980000000	13.230335000000	15.418644000000
P	20.582390000000	12.209414000000	17.551190000000
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P	18.798135000000	13.611005000000	13.636143000000
C	22.630468000000	12.170740000000	13.074736000000
C	22.858650000000	13.512530000000	12.782277000000
H	22.760653000000	14.257307000000	13.558730000000
C	19.699953000000	13.221228000000	18.763335000000
C	21.737667000000	16.305001000000	16.677346000000
C	20.321753000000	14.304185000000	19.380250000000
H	21.359725000000	14.516026000000	19.169732000000

C	22.756954000000	11.228255000000	12.065009000000
H	22.584067000000	10.184130000000	12.271671000000
C	22.382901000000	11.895006000000	19.491083000000
H	21.494700000000	11.869287000000	20.102541000000
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C	23.606848000000	11.838752000000	20.108363000000
H	23.662674000000	11.719633000000	21.183195000000
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C	19.695230000000	10.618236000000	17.637289000000
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C	18.365047000000	12.952351000000	19.051385000000
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C	17.175925000000	14.045514000000	14.314206000000
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H	24.783010000000	12.056433000000	14.086641000000
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H	20.099387000000	15.927028000000	20.756490000000
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C	18.284130000000	14.822839000000	20.548198000000
H	17.729464000000	15.443665000000	21.240310000000
C	24.759024000000	11.950001000000	19.356928000000
H	25.737195000000	11.932022000000	19.822426000000
C	20.288175000000	15.915610000000	12.669498000000
C	21.789459000000	9.966004000000	14.732345000000
C	22.041956000000	17.113195000000	13.855398000000
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C	23.435098000000	12.047604000000	17.254204000000
C	20.726842000000	9.471843000000	13.981706000000
H	20.074748000000	10.147136000000	13.447168000000
C	23.183181000000	13.905244000000	11.500461000000
H	23.327373000000	14.954516000000	11.279816000000
C	18.617193000000	17.697809000000	15.193530000000
H	19.225213000000	18.042063000000	14.369051000000
C	16.708494000000	13.360900000000	15.432862000000
H	17.327209000000	12.618306000000	15.918325000000
C	17.661636000000	13.746744000000	19.938026000000
H	16.631392000000	13.503241000000	20.158531000000
C	17.467584000000	18.390103000000	15.527917000000
H	17.184094000000	19.270007000000	14.966543000000
C	19.810307000000	9.796161000000	18.758453000000
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H	26.824359000000	12.165744000000	17.811593000000
C	23.072907000000	11.623165000000	10.776747000000
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C	21.637390000000	17.581474000000	17.221195000000
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C	22.446427000000	17.769973000000	12.685906000000
H	23.281840000000	18.455713000000	12.718158000000
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H	22.932866000000	14.524617000000	16.560644000000
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C	16.669352000000	17.950418000000	16.570143000000
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H	18.422420000000	15.219121000000	17.492396000000
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H	26.876808000000	12.213805000000	15.332111000000
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C	18.528058000000	12.155986000000	12.594011000000
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H	24.719037000000	15.390605000000	17.996147000000
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H	23.423656000000	9.466531000000	16.025254000000
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C	17.482320000000	11.278856000000	12.860394000000
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H	20.250933000000	12.519036000000	11.352367000000
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C	14.653076000000	14.587901000000	15.355519000000
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C	17.347230000000	10.115014000000	12.123141000000

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H	15.105165000000	13.074194000000	16.809704000000
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