Electronic Supplementary Information

Improving the Quantum Yield of Luminescence for Three-coordinated Gold(I) TADF Emitters by Exploiting Inversion Symmetry and Using Perhaloaryl Ligands

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I. Characterization of complexes 1-3

1. IR spectra

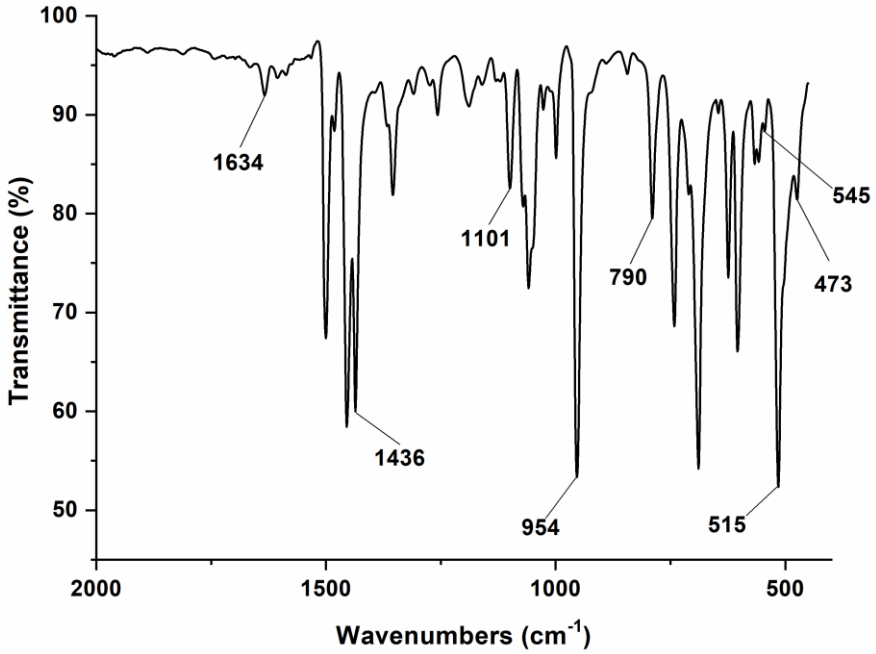


Figure S1. FT-IR spectrum of complex **1**.

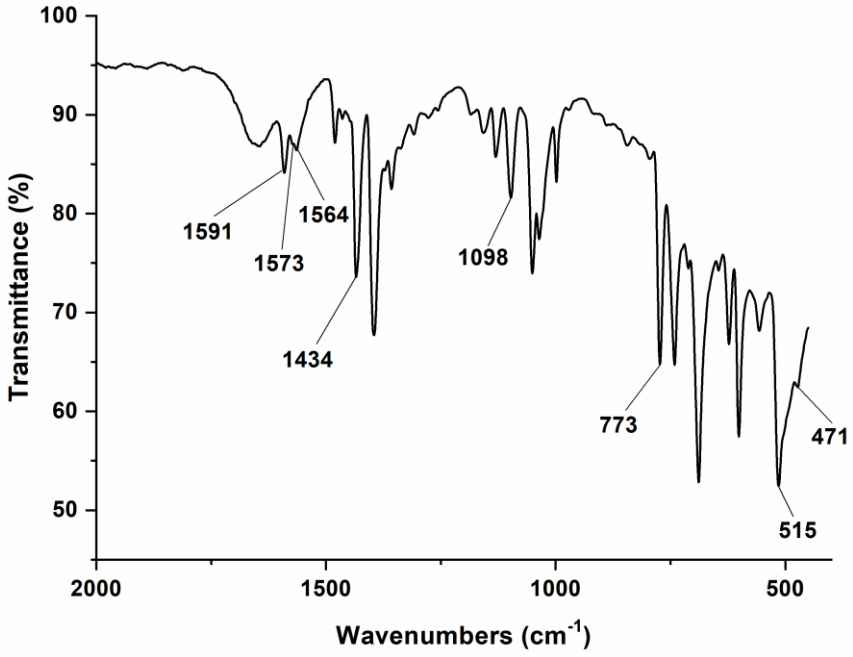


Figure S2. FT-IR spectrum of complex **2**.

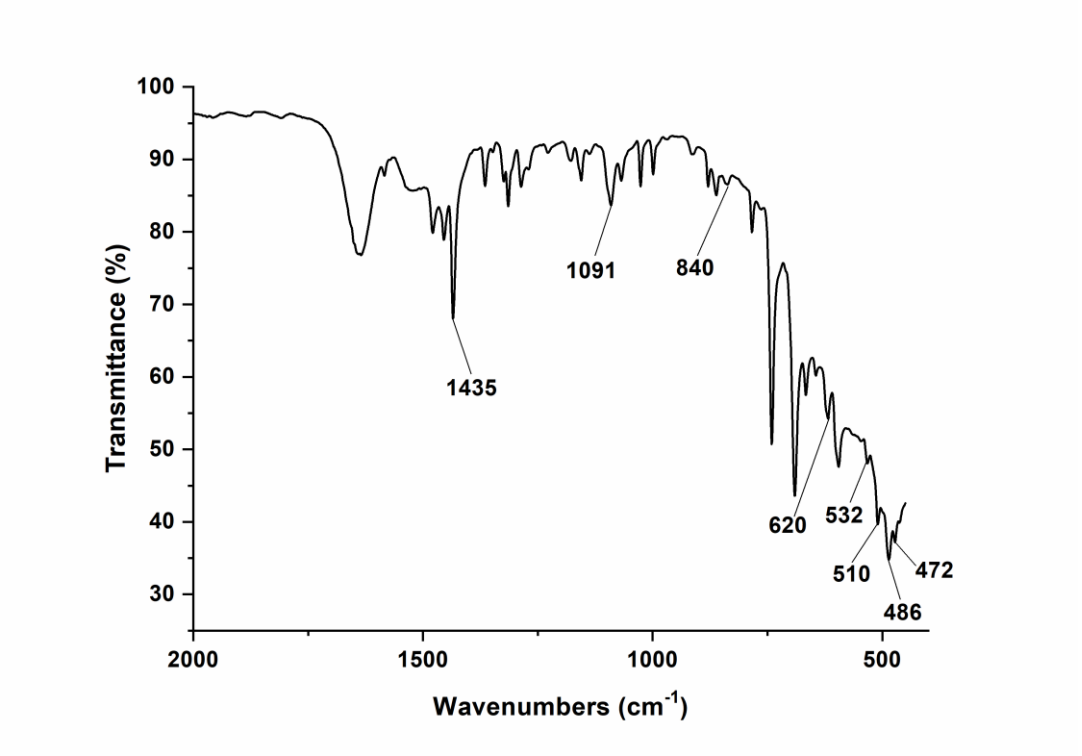


Figure S3. FT-IR spectrum of complex **3**.

2. ^{1}H NMR spectra (400 MHz, 298K)

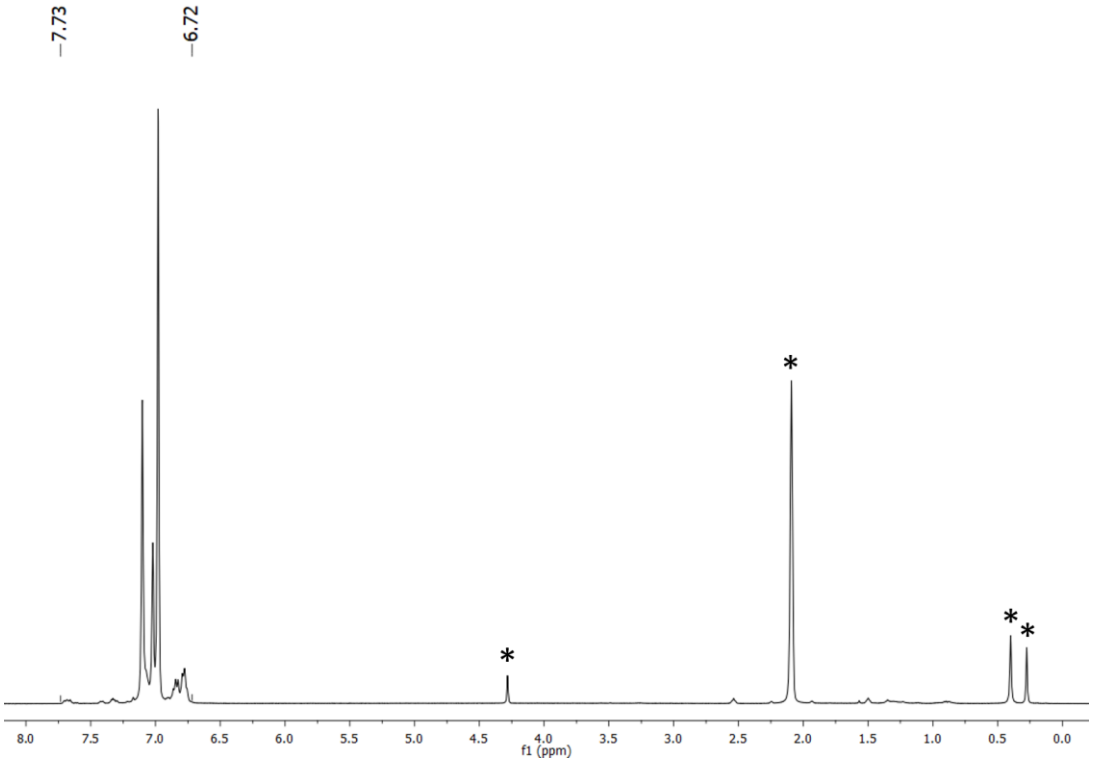


Figure S4. ^{1}H NMR spectrum of complex **1** in toluene-d_8.

(* Solvent residual peaks)

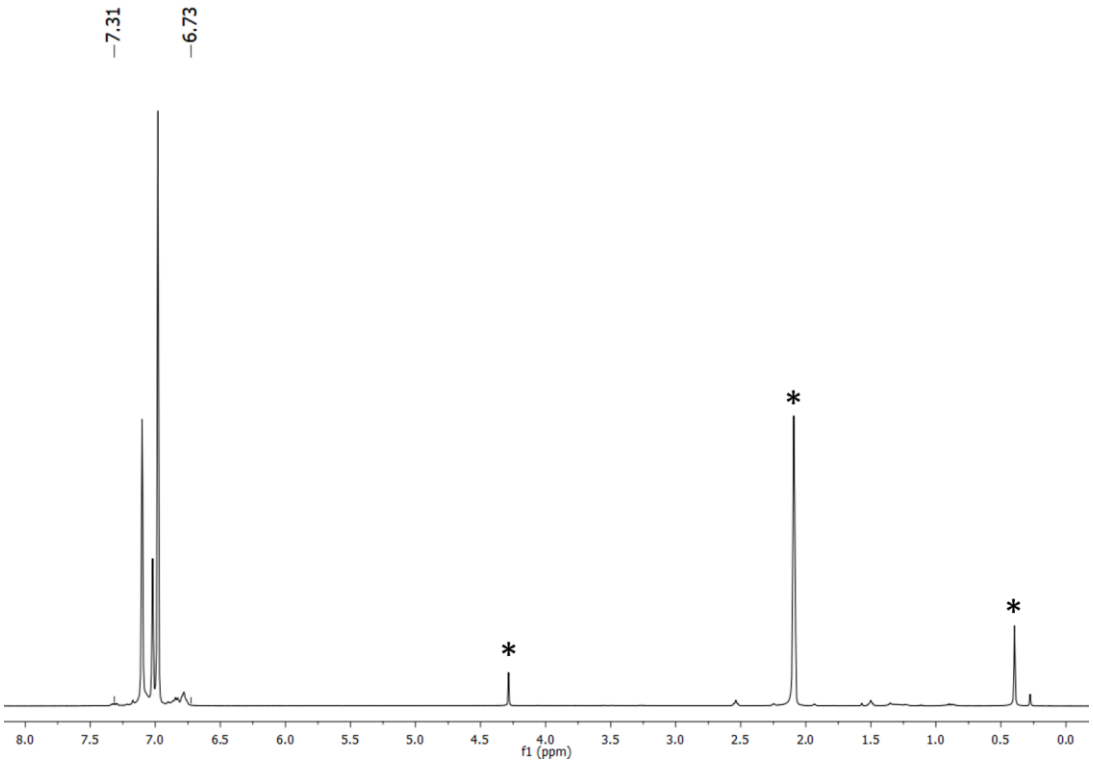


Figure S5. ^{1}H NMR spectrum of complex **2** in toluene-d_8.

(* Solvent residual peaks)

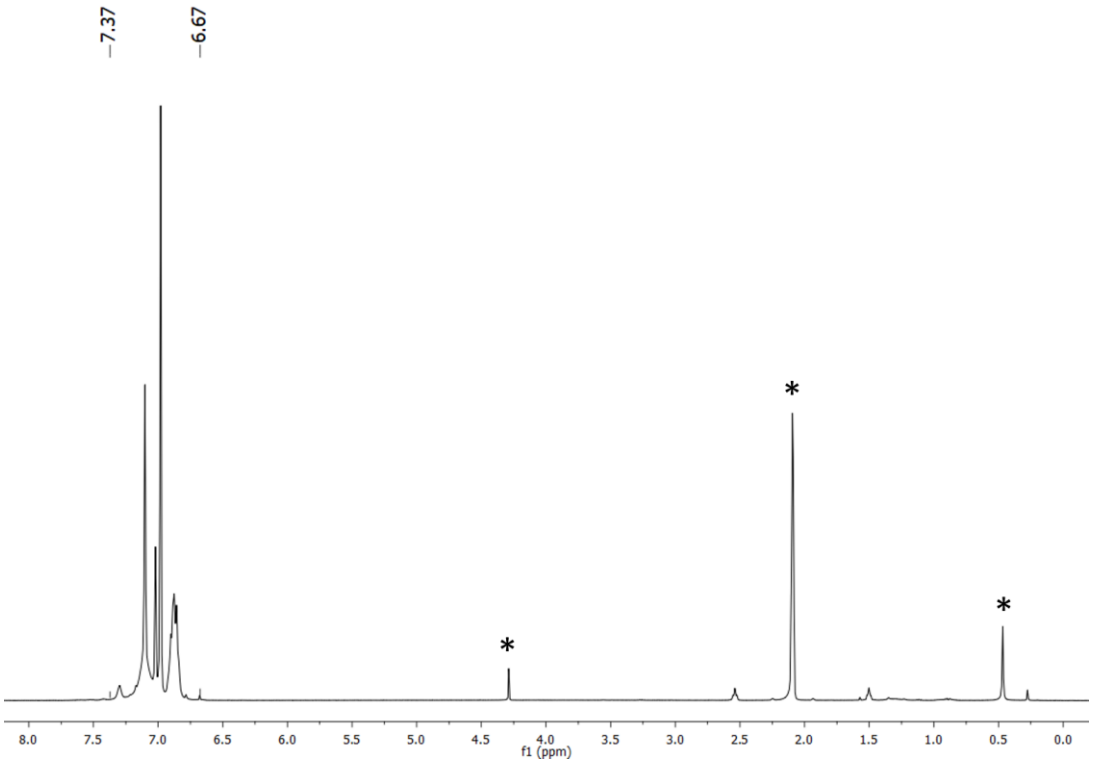


Figure S6. ^{1}H NMR spectrum of complex **3** in toluene-d_8.

(* Solvent residual peaks)

3. ^{19}F NMR spectra (282 MHz, 298K)

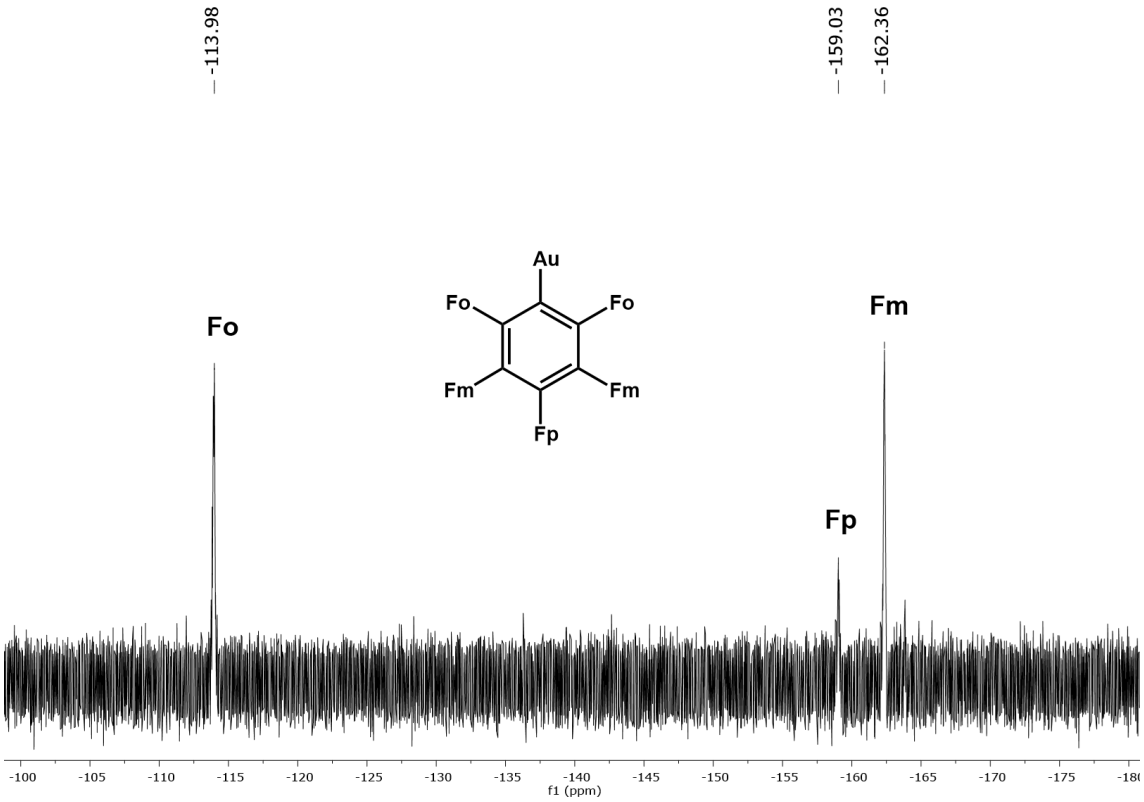


Figure S7. ^{19}F NMR spectrum of complex **1** in toluene-d_8.

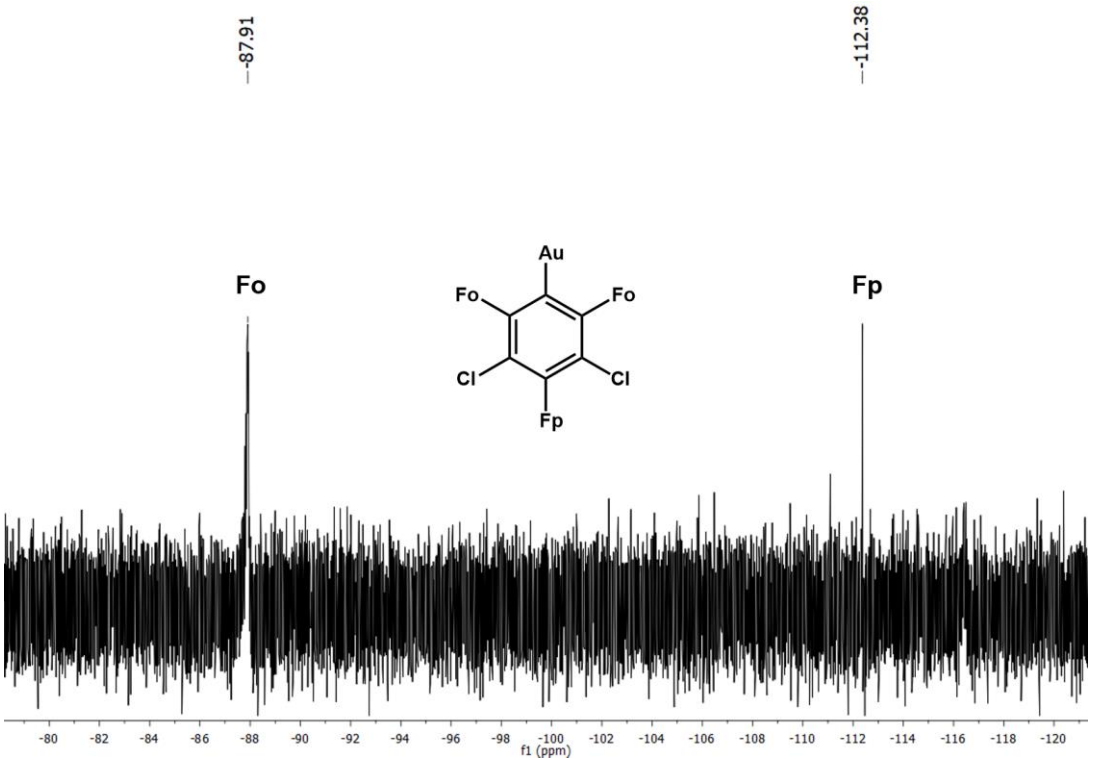


Figure S8. ^{19}F NMR spectrum of complex **2** in toluene-d_8.

4. $^{31}P\{^{1}H\}$ NMR spectra (122 MHz, 298K)

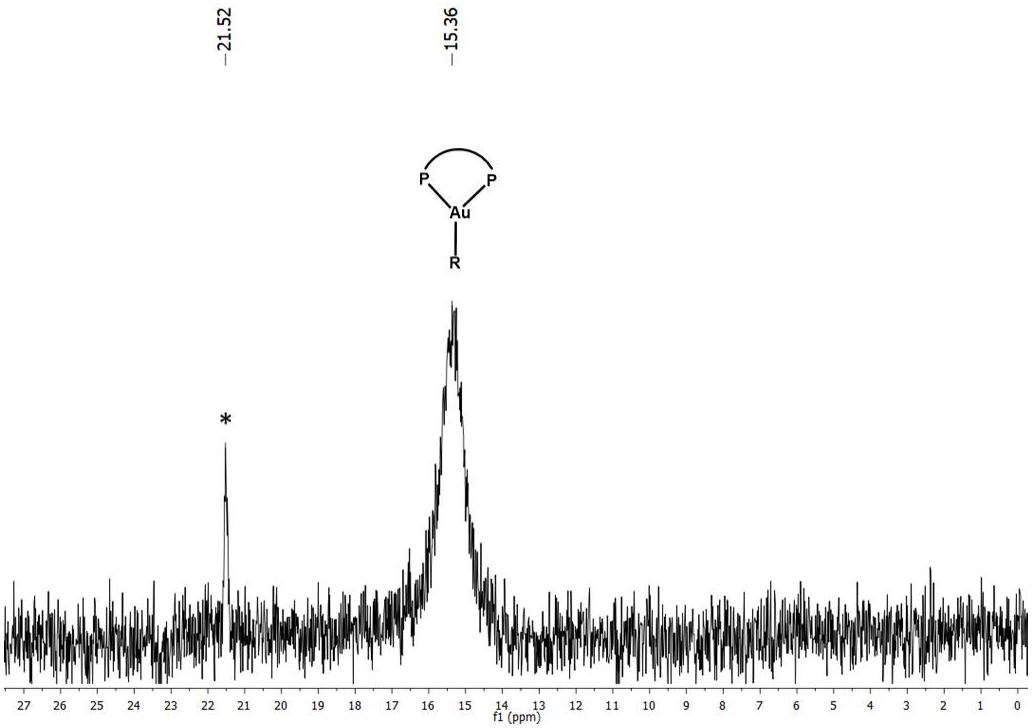


Figure S9. $^{31}P\{^{1}H\}$ NMR spectrum of complex **1** in toluene-d_8.

(* Tetracoordinated gold(I) complex)

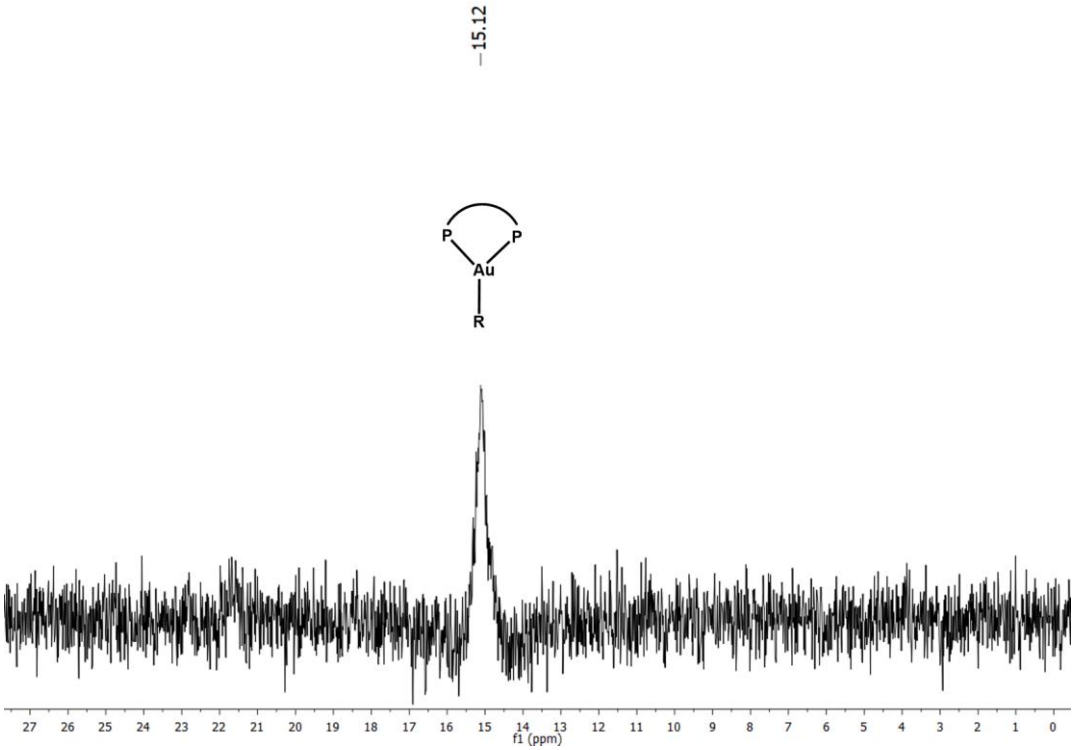


Figure S10. $^{31}P\{^{1}H\}$ NMR spectrum of complex **2** in toluene-d_8.

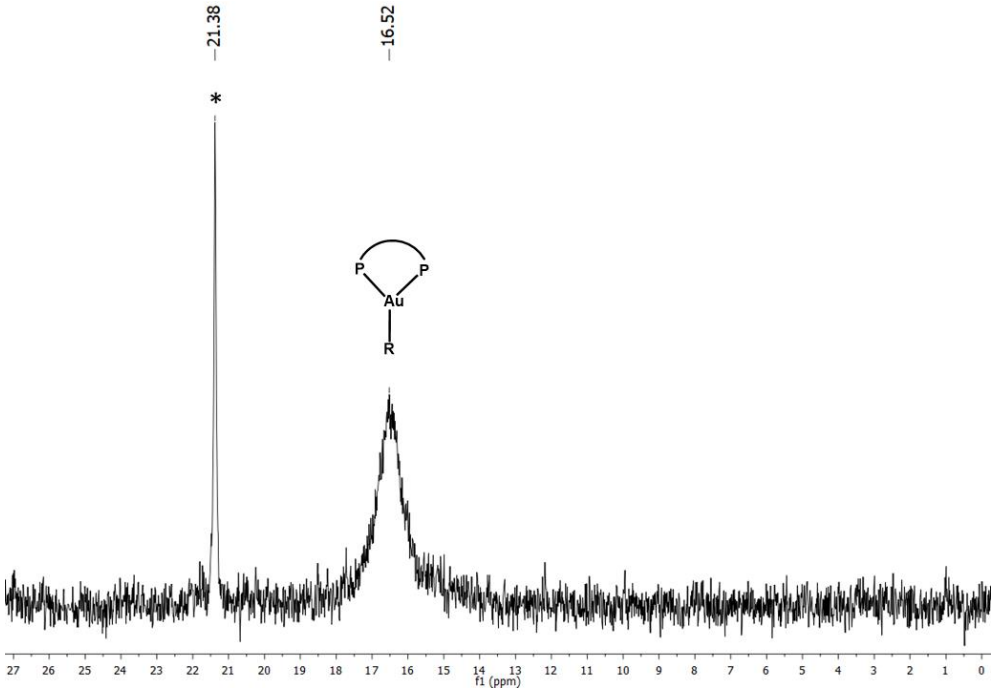


Figure S11. $^{31}P\{^{1}H\}$ NMR spectrum of complex **3** in toluene-d_8.

(* Tetracoordinated gold(I) complex)

5. Single crystals X-ray diffraction analyses

Table S1. Data collection and structure refinement details for **1** and **3.**

	1·C_6H_{12}	**3**
Chemical Formula	$C_{66}H_{42}Au_2F_{10}P_4$·$C_6H_{12}$	$C_{66}H_{42}Au_2Cl_{10}P_4$
Crystal habit	Orange prism	Orange prism
Crystal size/mm	0.043x0.034x0.028	0.155x0.096x0.030
Crystal system	Monoclinic	Triclinic
Space group	C*2/c*	P-*1*
a/Å	27.618(2)	11.8447(8)
b/Å	13.6224(10)	12.2786(8)
c/Å	22.572(2)	13.4926(11)
α/°	90	85.614(3)
β/°	125.596(5)	74.160(2)
γ/°	90	64.692(2)
V/Å^3	6905.4(11)	1704.8(2)
Z	4	1
D_c/g cm^{-3}	1.565	1.663
M	1626.96	1707.31
F(000)	3176	826
T/ºC	100(2)	100(2)
2θmax/°	53.464	55.872
μ(Mo-*K*α)/mm^{-1}	4.404	4.822
No. refl. Measured	7334	38924
No. unique refl.	7334	38924
R_{int}	0.1631	0.0708
$R[F>2\sigma(F)]$[a]	0.0684	0.0455
$wR[F^2$, all refl.][b]	0.1570	0.1101
No. of refl. Used [$F>2\sigma(F)$]	7334	8106
No. of parameters	382	370
No. of restrains	104	83
S [c]	1.092	1.031
Max. residual electron density/e·Å^{-3}	2.165	2.690

[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.

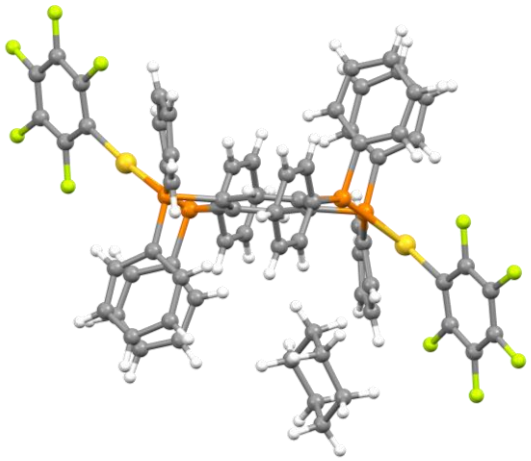
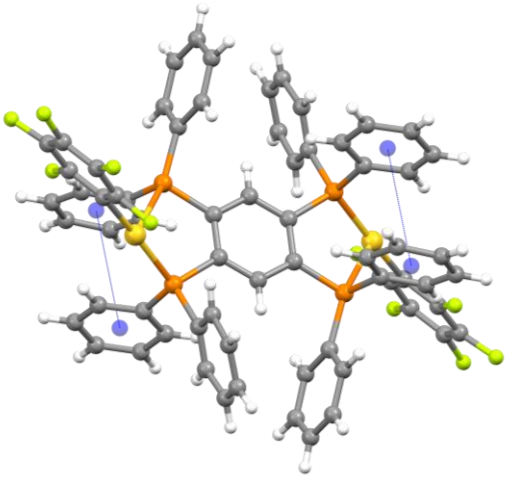
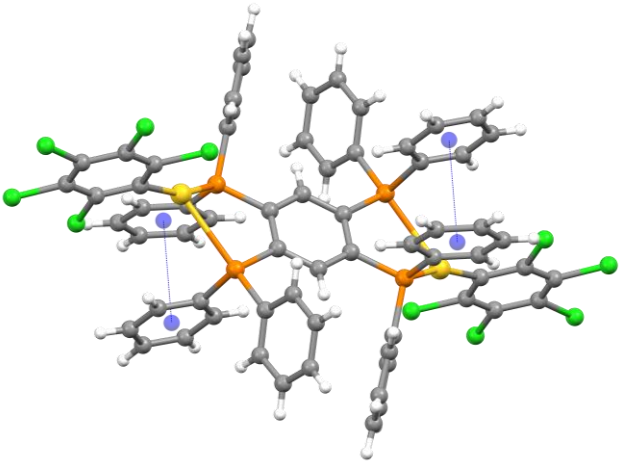


Figure S12. Molecular structure of complex **1**·C_6H_{12}.



$[Au_2(C_6F_5)_2(tpbz)]$ (**1**)



$[Au_2(C_6Cl_5)_2(tpbz)]$ (**3**)

Figure S13. Molecular structures of complexes **1** (top) and **3** (bottom) showing π···π stacking interaction between phenyl rings.

II. Optical properties

1. UV-Vis absorption spectra in solid state

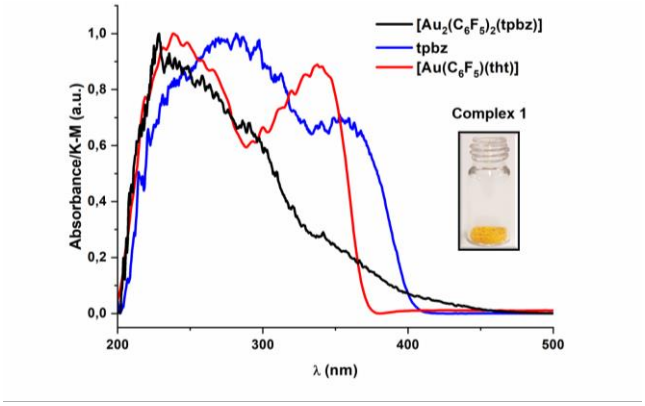


Figure S14. UV-Vis absorption spectra in solid state for complexes $[Au_2(C_6F_5)_2(tpbz)]$ (**1**) (black), tpbz (blue) and $[Au(C_6F_5)(tht)]$ (red).

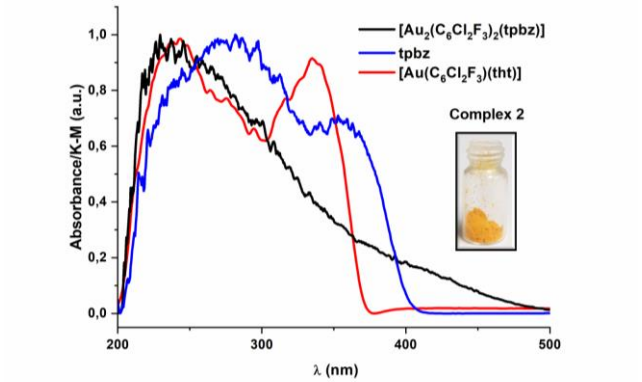


Figure S15. UV-Vis absorption spectra in solid state for complexes $[Au_2(C_6Cl_2F_3)_2(tpbz)]$ (**2**) (black), tpbz (blue) and $[Au(C_6Cl_2F_3)(tht)]$ (red).

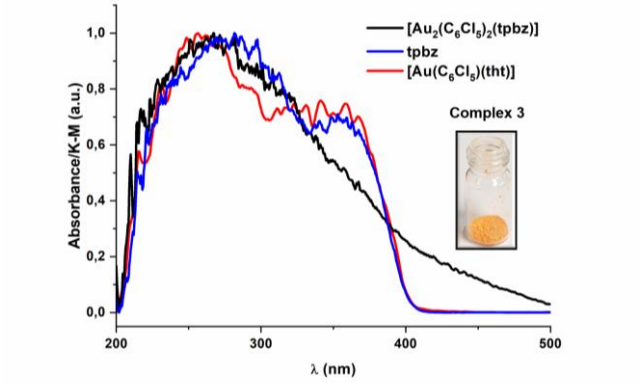


Figure S16. UV-Vis absorption spectra in solid state for complexes $[Au_2(C_6Cl_5)_2(tpbz)]$ (**3**) (black), tpbz (blue) and $[Au(C_6Cl_5)(tht)]$ (red).

2. Excitation and emission spectra

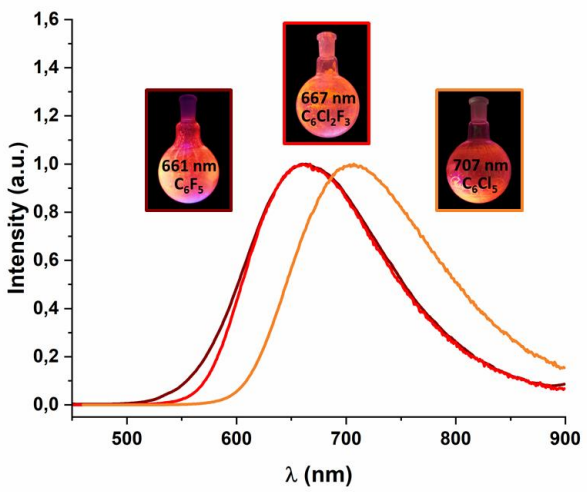


Figure S17. Emission spectra in the solid state of the complexes [$(Au_2(C_6F_5)_2(tpbz)$] (**1**) (maroon), [$(Au_2(C_6Cl_3F_2)_2(tpbz)$] (**2**) (red) and [$(Au_2(C_6Cl_5)_2(tpbz)$] (**3**) (orange) measured at 77 K

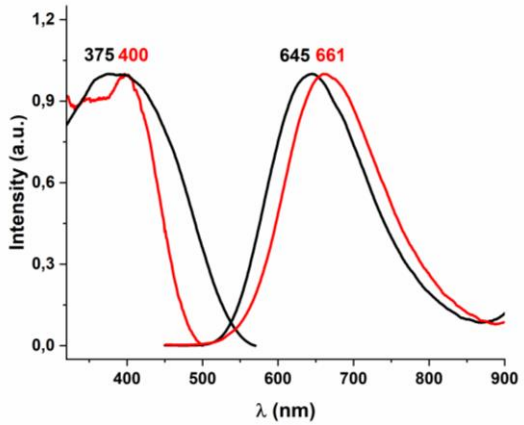


Figure S18. Excitation and emission spectra in solid state for complex **1** at room temperature (black) and 77K (red).

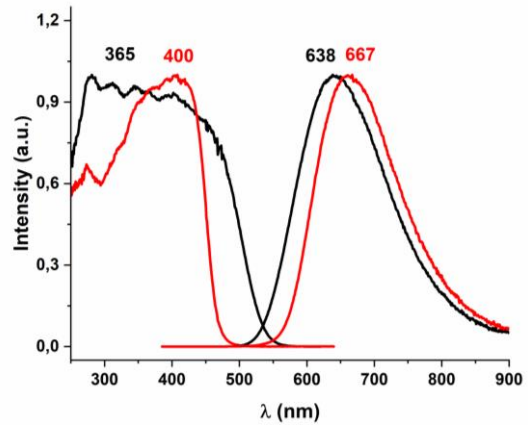


Figure S19. Excitation and emission spectra in solid state for complex **2** at room temperature (black) and 77K (red).

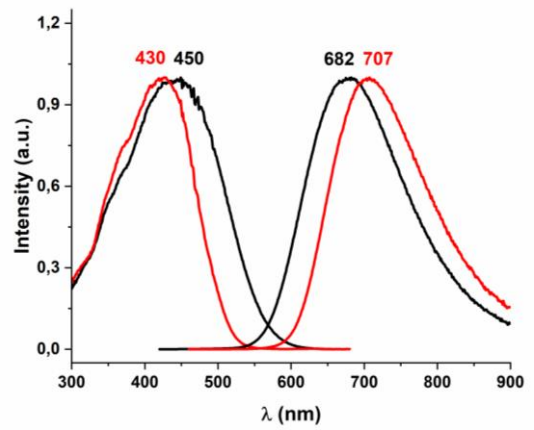


Figure S20. Excitation and emission spectra in solid state for complex **3** at room temperature (black) and 77K.

3. Lifetimes

Complex 1:

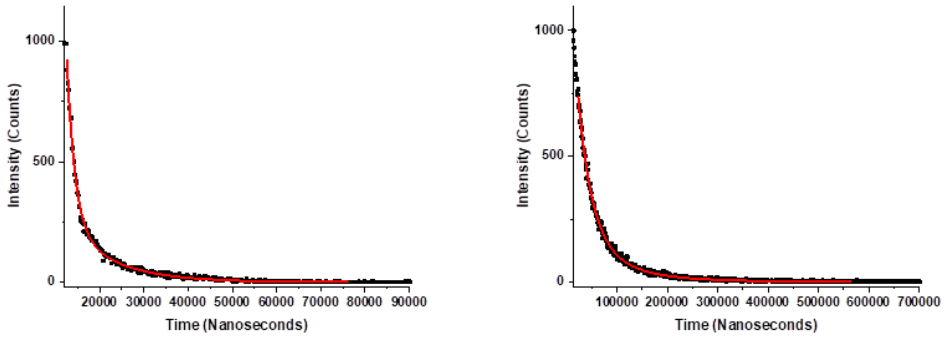


Figure S21. Lifetime decay for complex **1** at room temperature: τ_1 = 3.93 ± 0.10 µs (100%) (left) and at 77 K: τ_1 = 41.20 ± 1.34 µs (100%) (right).

Complex 2:

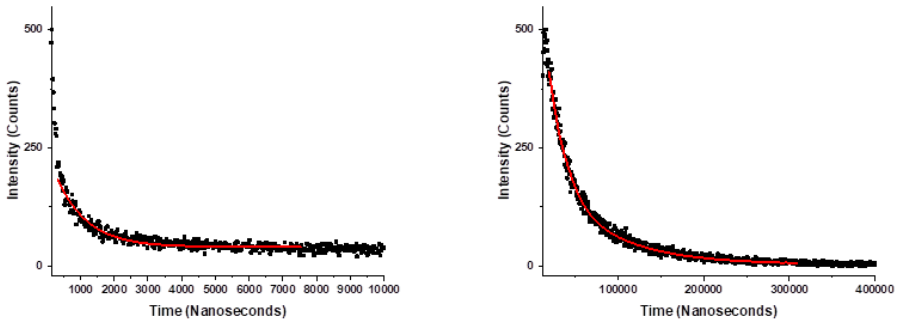


Figure S22. Lifetime decay for complex **2** at room temperature: τ_1 = 0.90 ± 0.03 µs (100%) (left) and at 77 K: τ_1 = 27.83 ± 1.34 µs (100%) (right).

Complex 3:

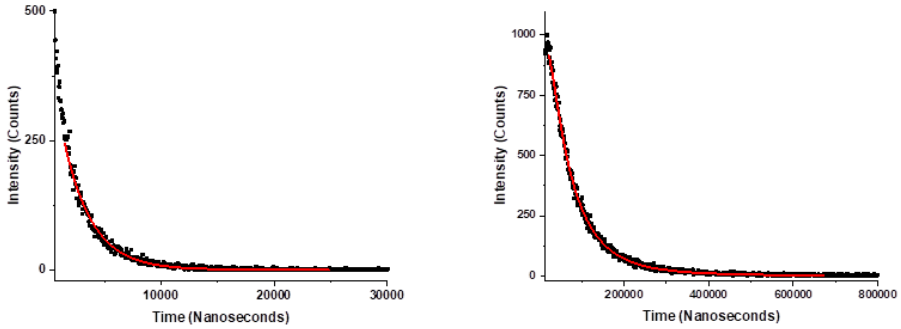


Figure S23. Lifetime decay for complex **3** at room temperature: τ_1 = 2.50 ± 0.03 µs (100%) (left) and at 77 K: τ_1 = 60.78 ± 2.90 µs (100%) (right).

4. TADF studies

Boltzmann-type equation:

$$\tau_{\mathrm{av}} = \frac{3+\exp(-\Delta E(\mathrm{S_1}-\mathrm{T_1})/k_{\mathrm{B}}T}{3/\tau_{\mathrm{T}}+1/\tau_{\mathrm{S}}\exp(\Delta E(\mathrm{S_1}-\mathrm{T_1})/k_{\mathrm{B}}T)} \qquad \text{(Eq. S1)}$$

where k_{B} is Boltzmann's constant. τ_{T} and τ_{S} are the phosphorescence ($\mathrm{T_1} \rightarrow \mathrm{S_0}$) decay time and the prompt fluorescence ($\mathrm{S_1} \rightarrow \mathrm{S_0}$) decay time without thermal activation, respectively.

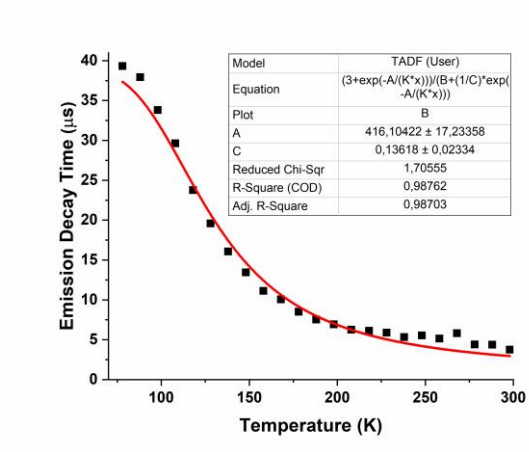


Figure S24. Temperature dependence of the emission decay time for complex **1**. The solid red line represents the fit of the experimental data according to Eq. S1. The fit parameters are showed in the attached tables.

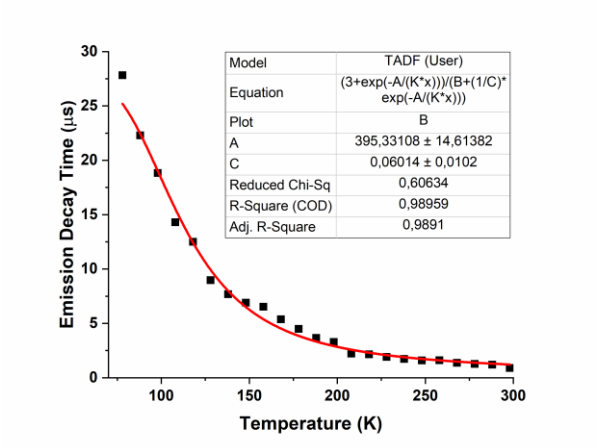


Figure S25. Temperature dependence of the emission decay time for complex **2**. The solid red line represents the fit of the experimental data according to Eq. S1. The fit parameters are showed in the attached tables.

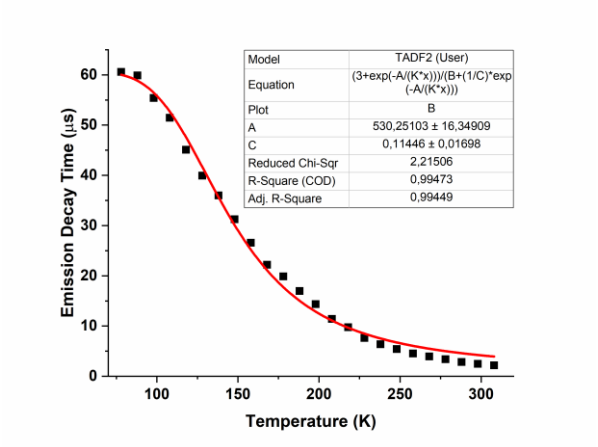


Figure S26. Temperature dependence of the emission decay time for complex **3**. The solid red line represents the fit of the experimental data according to Eq. S1. The fit parameters are showed in the attached tables.

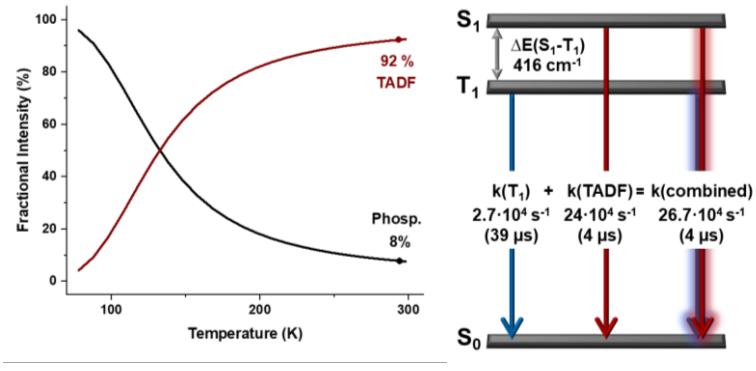


Figure S27. Left: Fractional emission intensities (simulation results) stemming from TADF (maroon) and direct phosphorescence (black) as a function of temperature calculated on the basis of the experimental data from figure **S23** and Equations. 2 and 3 (main text) for complex **1**; Right: Schematic energy level diagram and decay times of **1** in powder.

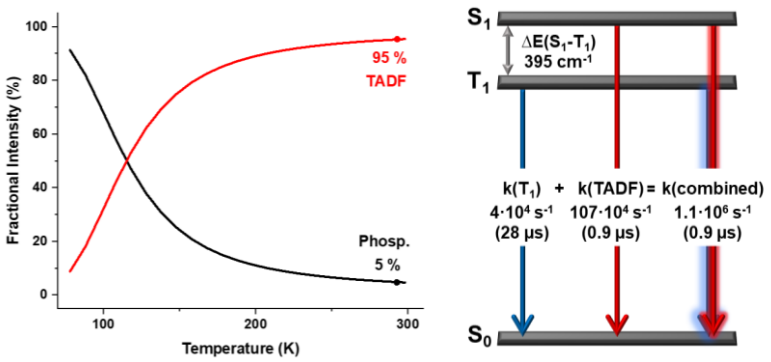


Figure S28. Left: Fractional emission intensities (simulation results) stemming from TADF (red) and direct phosphorescence (black) as a function of temperature calculated on the basis of the experimental data from figure **S24** and Equations. 2 and 3 (main text) for complex **2**; Right: Schematic energy level diagram and decay times of **2** in powder.

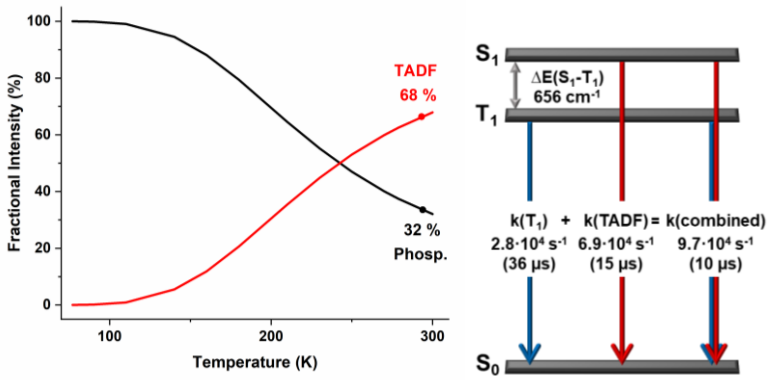


Figure S29. Left: Fractional emission intensities (simulation results) stemming from TADF (red) and direct phosphorescence (black) as a function of temperature calculated on the basis of the experimental data from ref. 30 main text and Equations. 2 and 3 (main text) for **monomer** [Au(C_6F_5)dppBz] (**1m**); Right: Schematic energy level diagram and decay times of monomer [Au(C_6F_5)dppBz] (**1m**) in powder.

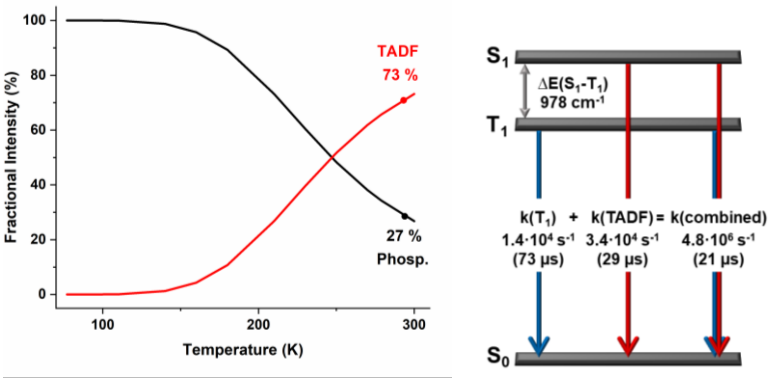


Figure S30. Left: Fractional emission intensities (simulation results) stemming from TADF (red) and direct phosphorescence (black) as a function of temperature calculated on the basis of the experimental data from ref. 30 main text and Equations. 2 and 3 (main text) for **monomer** [Au($C_6Cl_2F_3$)dppBz] (**2m**); Right: Schematic energy level diagram and decay times of monomer [Au($C_6Cl_2F_5$)dppBz] (**2m**) in powder.

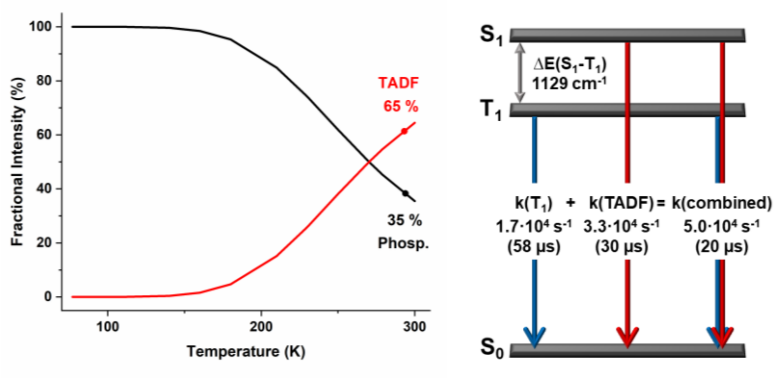


Figure S31. Left: Fractional emission intensities (simulation results) stemming from TADF (red) and direct phosphorescence (black) as a function of temperature calculated on the basis of the experimental data from ref. 30 main text and Equations. 2 and 3 (main text) for **monomer** [Au(C_6Cl_5)dppBz] (**3m**); Right: Schematic energy level diagram and decay times of monomer [Au(C_6Cl_5)dppBz] (**3m**) in powder.

Table S2. Photophysical parameters for monomers **1m-3m.**

		1 m	**2** m	**3** m
298 K	λ_{em} / nm	560	545	555
	τ / µs	10.3	20.8	19.9
	Φ / %	29	16	11
	k_r [a] / s^{-1}	$28.16 \cdot 10^3$	$7.69 \cdot 10^3$	$5.53 \cdot 10^3$
	k_{nr} [b] / s^{-1}	$68{,}93 \cdot 10^3$	$40.38 \cdot 10^3$	$44.72 \cdot 10^3$
77 K	λ_{em} / nm	575	570	585
	τ / µs	35.5	72.8	58.0
	k_{S1} / s^{-1}	$4.18 \cdot 10^6$	$12.27 \cdot 10^6$	$21.16 \cdot 10^6$
	k_{T1} / s^{-1}	$2.82 \cdot 10^4$	$1.37 \cdot 10^4$	$1.74 \cdot 10^4$
	ΔE_{ST} / cm^{-1}	656	978	1129
	k_{TADF} [c] / s^{-1}	$6.89 \cdot 10^4$	$3.43 \cdot 10^4$	$3.30 \cdot 10^4$
	τ_{TADF} / µs	14.52	29.11	30.29

III. Computational Methods

1. Coordination environment for the gold(I) centers for complexes **1**-**3** at the ground state S_0, the first singlet excited state S_1 and the first triplet excited state T_1

Table S3. Selected bond lengths (Å) and angles (°) for the coordination environment of the gold(I) centers for complexes **1-3.**

	1				**2**			**3**			
	X-Ray	S_0	S_1	T_1	S_0	S_1	T_1	X-Ray	S_0	S_1	T_1
P1-Au (Å)	2.275	2.306	2.335	2.331	2.306	2.334	2.333	2.276	2.990	2.335	2.333
P2-Au (Å)	2.897	3.069	2.517	2.542	3.065	2.520	2.541	2.844	2.300	2.500	2.521
Au-C_{ipso} (Å)	2.048	2.077	2.068	2.067	2.077	2.069	2.069	2.043	2.086	2.072	2.072
P1-C1 (Å)	1.839	1.832	1.797	1.781	1.832	1.772	1.773	1.821	1.842	1.772	1.774
P2-C2 (Å)	1.841	1.844	1.771	1.762	1.844	1.797	1.771	1.838	1.832	1.797	1.771
C1-C2 (Å)	1.394	1.408	1.425	1.453	1.408	1.425	1.449	1.417	1.409	1.426	1.450
C1-C3 (Å)	1.392	1.393	1.373	1.382	1.393	1.417	1.396	1.392	1.395	1.416	1.392
C2-C4 (Å)	1.400	1.395	1.417	1.393	1.395	1.373	1.381	1.401	1.393	1.372	1.383
P1-Au-P2 (º)	76.98	75.38	80.89	80.70	75.54	80.93	80.82	78.11	77.05	81.02	80.79
P1-Au-C1 (º)	170.23	175.37	169.01	171.67	175.48	169.87	172.17	162.55	178.56	167.50	168.77
P2-Au-C1 (º)	111.92	108.68	110.9	107.61	108.12	109.19	107.01	119.34	103.96	111.29	109.93

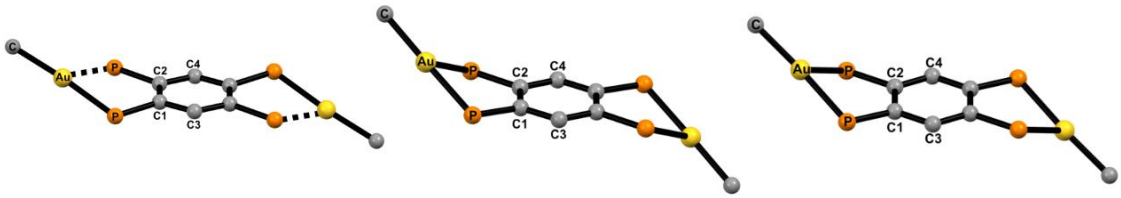


Figure S32. Computed coordination environment for the gold(I) center for complex **2** in the ground state S_0 (left), in the first singlet excited stated S_1 (middle) and in the first triplet excited state T_1 (right).

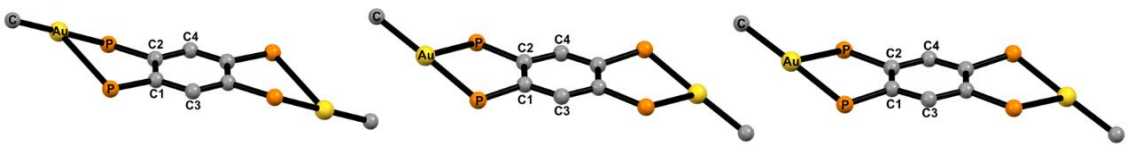
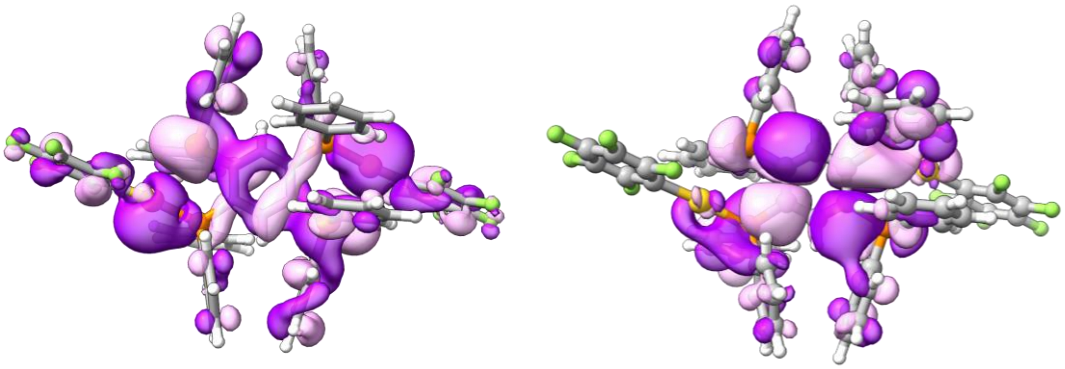


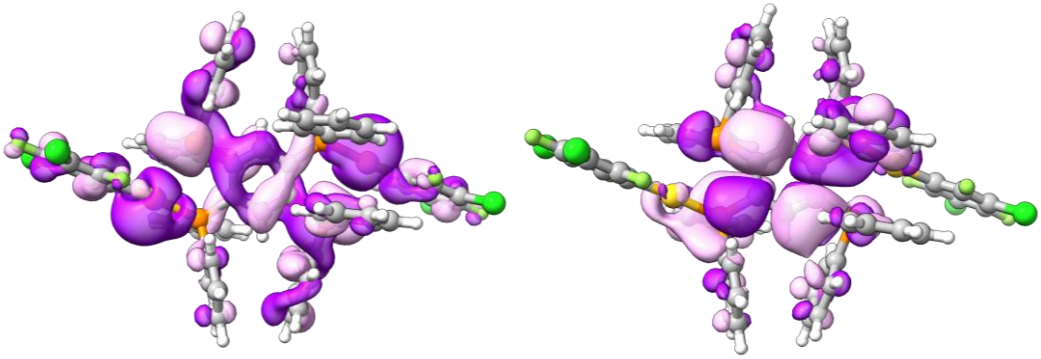
Figure S33. Computed coordination environment for the gold(I) center for complex **3** in the ground state S_0 (left), in the first singlet excited stated S_1 (middle) and in the first triplet excited state T_1 (right).

1. Frontier HOMO and LUMO for complexes **1**-**3**.



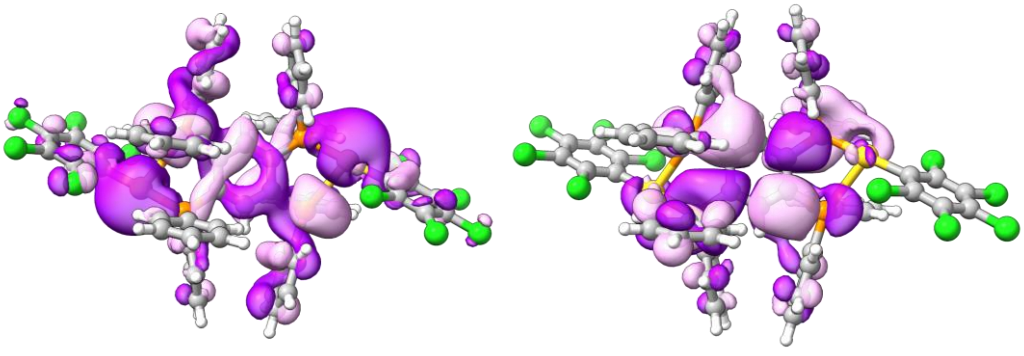
HOMO **LUMO**

$[Au_2(C_6F_5)_2(tpbz)]$ (**1**)



HOMO **LUMO**

$[Au_2(C_6Cl_2F_3)_2(tpbz)]$ (**2**)



HOMO **LUMO**

$[Au_2(C_6Cl_5)_2(tpbz)]$ (**3**)

Figure S34. The orbitals obtained in the DFT/B3LYP-D3(BJ) calculation that correspond to the HOMO (left) and the LUMO (right) of complexes **1**-**3**.

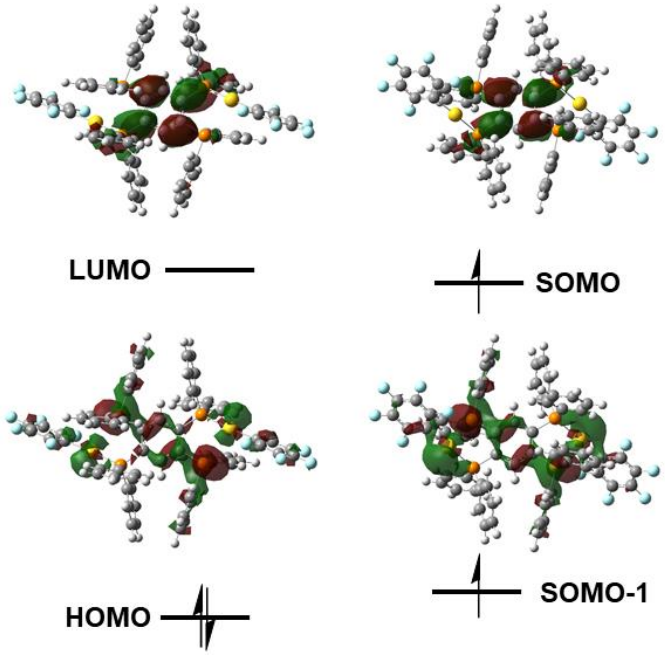


Figure S35. The frontier molecular orbitals obtained in the DFT/B3LYP-D3(BJ) calculation that correspond to the HOMO and LUMO of the S_0 state and the SOMO and SOMO-1 of the T_1 state of model **1a**.

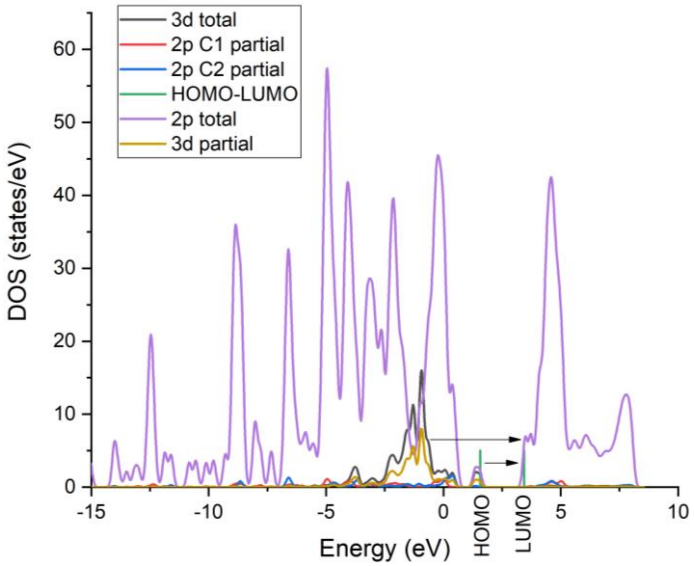
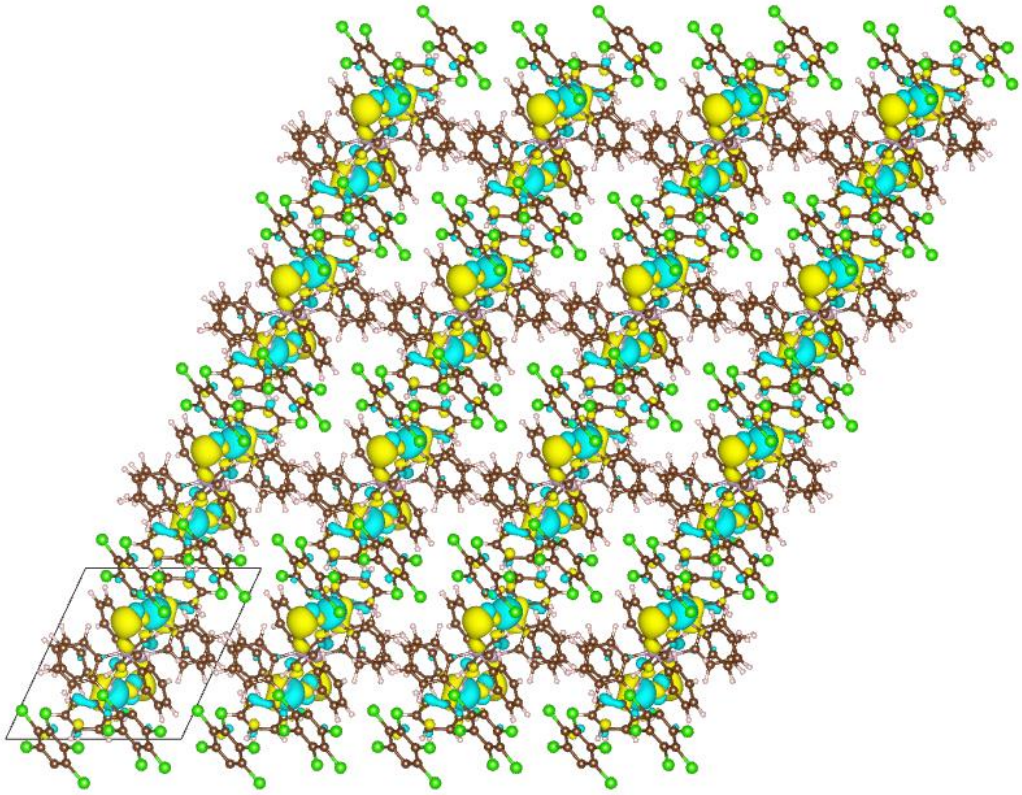
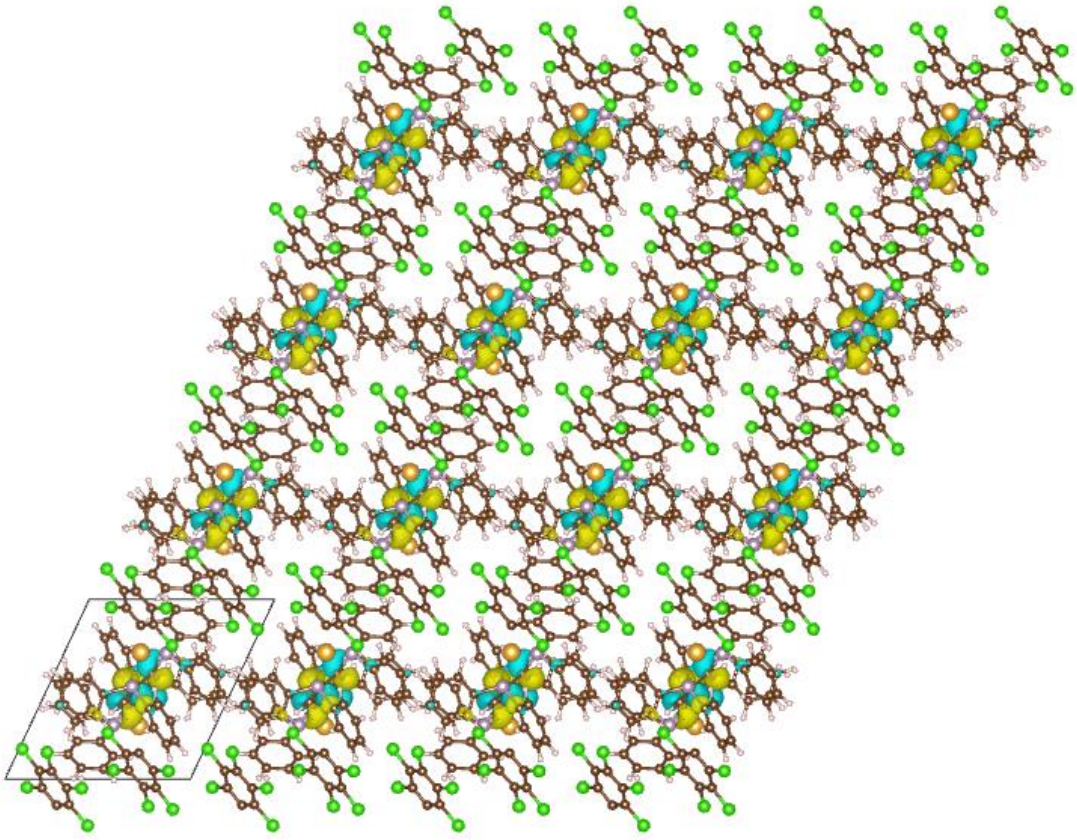


Figure S36. Calculated partial densities of states (DOS) of complex 1, by PBE-GGA method. The vertical lines correspond to the HOMO and LUMO eigenvalues in the DOS.



HOMO



LUMO

Figure S37. Frontier MOs for extended model system **1** through periodic-DFT calculations.

2. Transition density calculations for complexes **1**-**3**.

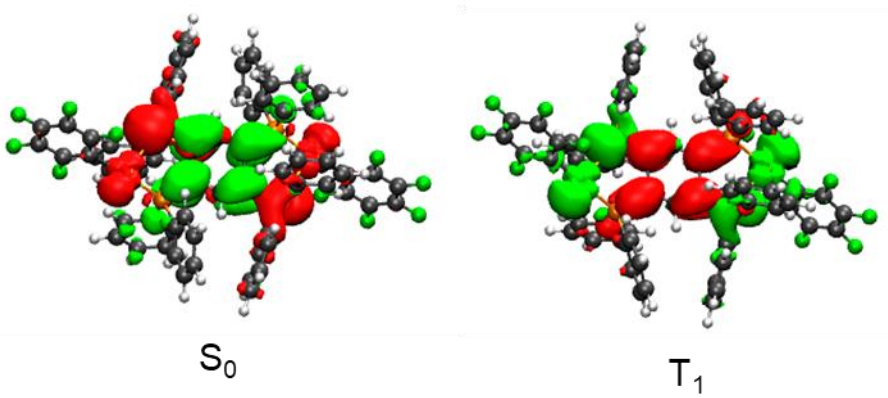


Figure S38. Transition densities for complex $[Au_2(C_6F_5)_2(tpbz)]$ **(1)**. (During the transition the electron density increases in the green areas and decreases in the red).

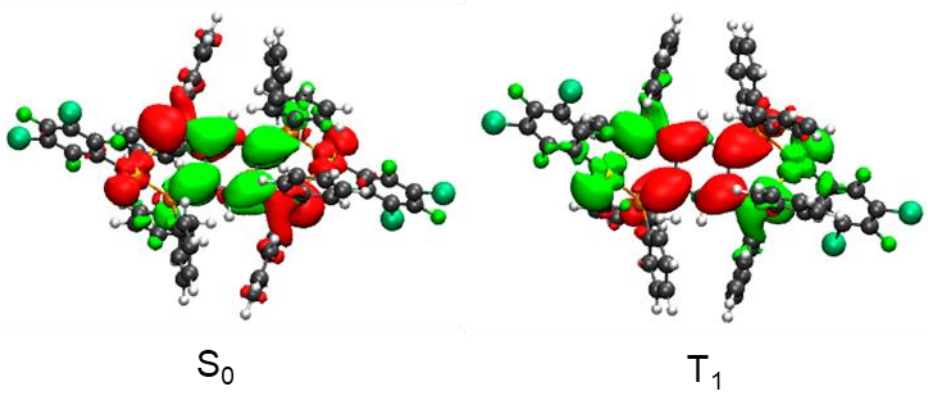


Figure S39. Transition densities for complex $[Au_2(C_6Cl_2F_3)_2(tpbz)]$ **(2)**. (During the transition the electron density increases in the green areas and decreases in the red).

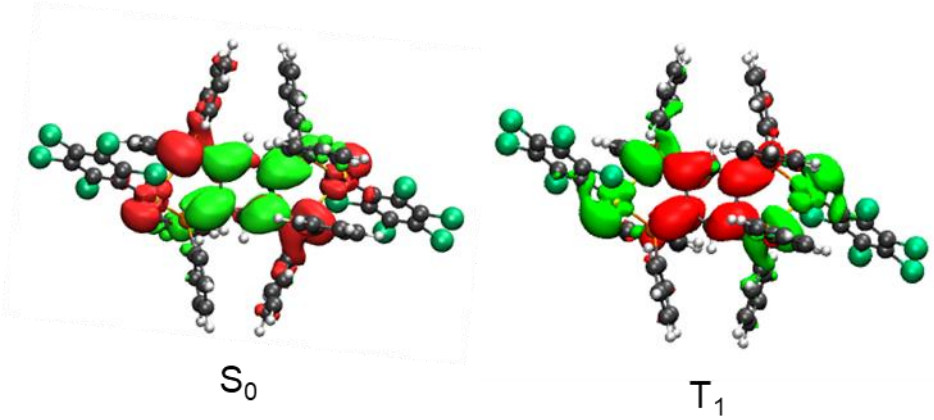
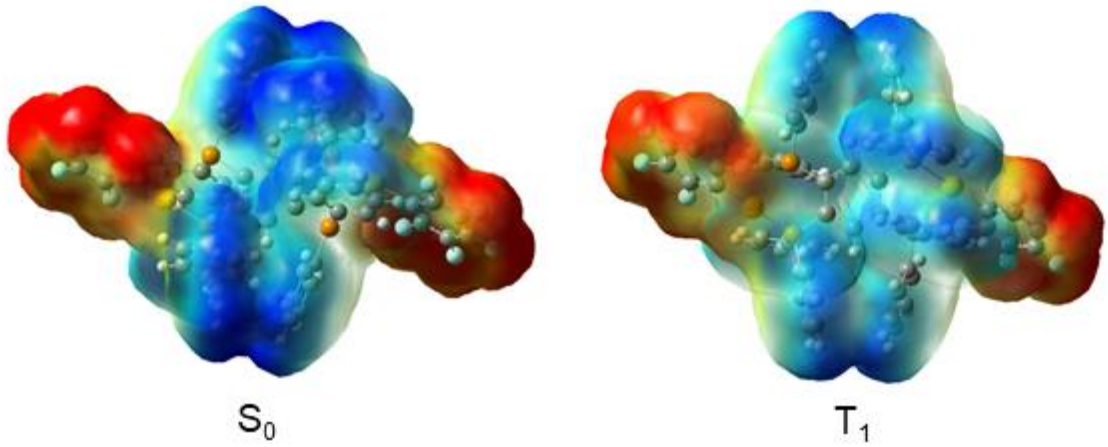
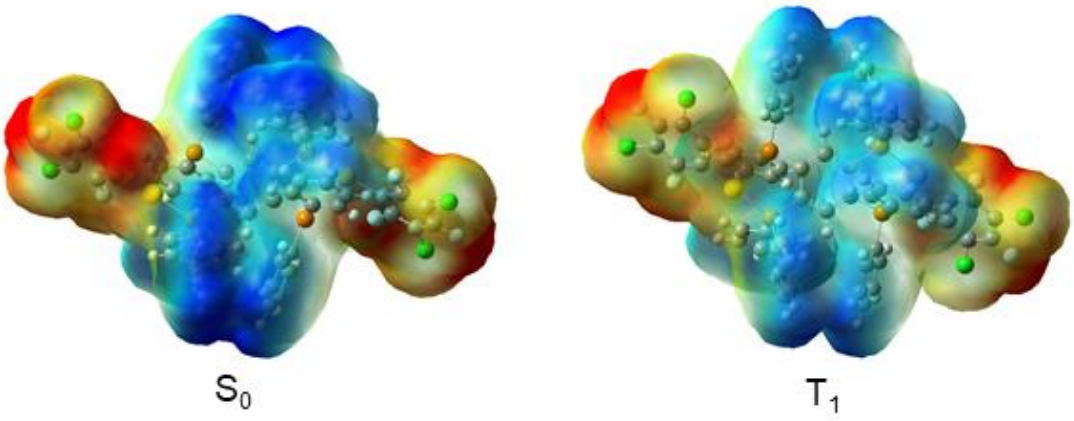


Figure S40. Transition densities for complex $[Au_2(C_6Cl_5)_2(tpbz)]$ **(3)**. (During the transition the electron density increases in the green areas and decreases in the red).

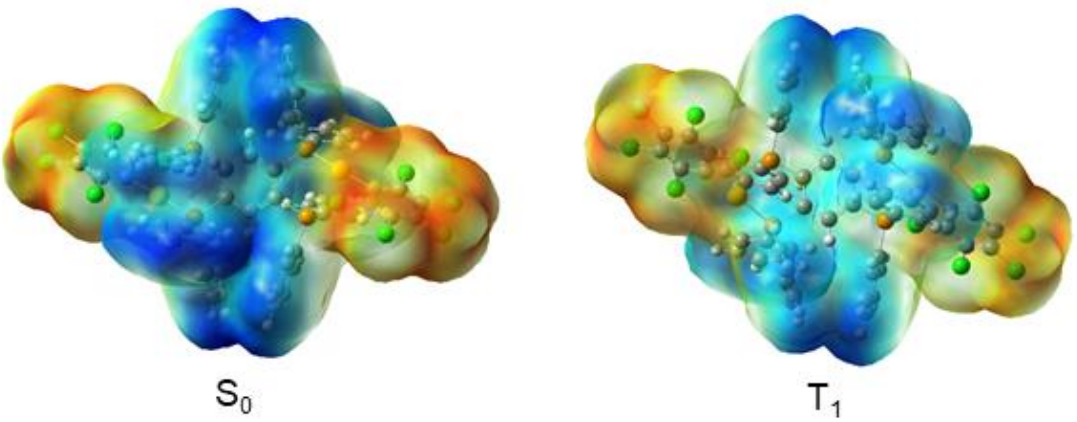
3. Electrostatic Potential Surface (ESP) calculations for complexes **2** and **3**.



$[Au_2(C_6F_5)_2(tpbz)]$ (**1**)



$[Au_2(C_6Cl_2F_3)_2(tpbz)]$ (**2**)



$[Au_2(C_6Cl_5)_2(tpbz)]$ (**3**)

Figure S41. Electrostatic Potential Surface (ESP) for model systems **1**-**3**.

4. TD-DFT Calculations for complexes **2** and **3**.

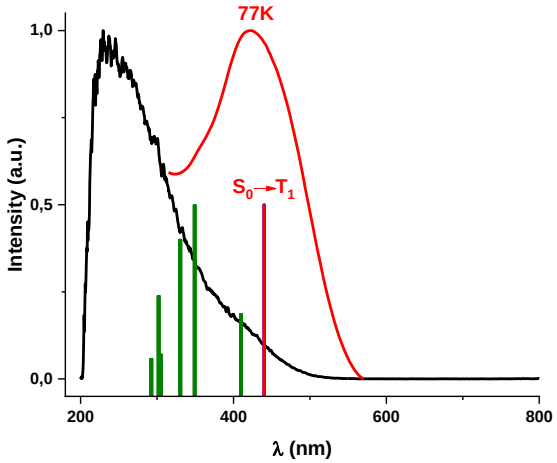


Figure S42. Absorption spectrum in solid state (black), excitation spectrum in solid state at 77 K (red), theorical singlet excitations (green) and first triplet excitation (red line) for complex **2**.

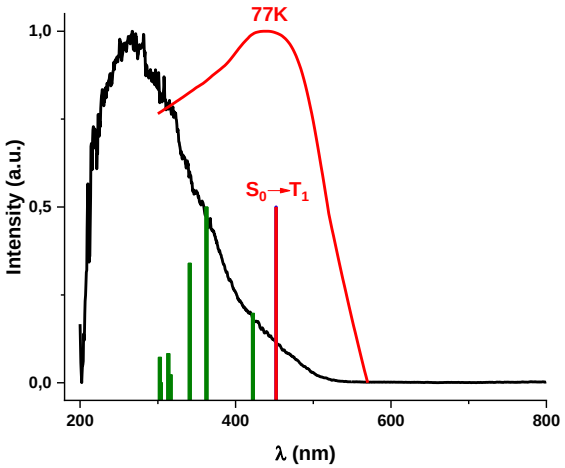


Figure S43. Absorption spectrum in solid state (black), excitation spectrum in solid state at 77 K (red), theorical singlet excitations (green) and first triplet excitation (red line) for complex **3**.

5. Population analyses

Model system **1a**

Table S4. Population analysis for model system **1a**. Contribution from each part of the molecule to the orbitals involved in the most important transitions (%).

Orbital	Au_1	Au_2	$R_1(C_6F_5)$	$R_2(C_6F_5)$	$P_1(Ph_2)_2$	$P_2(Ph_2)_2$	$P_3(Ph_2)_2$	$P_4(Ph_2)_2$	C_6H_2
LUMO+8	3	2	7	7	23	20	19	12	6
LUMO+6	1	1	2	3	27	15	30	17	4
LUMO+5	1	1	3	3	39	9	35	7	1
LUMO+4	2	2	2	2	21	25	21	25	2
LUMO+3	1	1	1	1	27	14	26	13	16
LUMO+2	1	1	2	2	37	8	38	8	3
LUMO+1	1	2	2	2	17	9	19	10	38
LUMO	1	1	0	0	14	5	13	5	60
HOMO	14	14	4	4	3	26	3	25	9
HOMO-1	18	18	7	7	1	22	1	22	5
HOMO-6	18	16	8	7	1	23	1	19	7

Model system **2a**

Table S5. Population analysis for model system **2a**. Contribution from each part of the molecule to the orbitals involved in the most important transitions (%).

Orbital	Au_1	Au_2	$R_1(C_6Cl_2F_3)$	$R_2(C_6Cl_2F_3)$	$P_1(Ph_2)_2$	$P_2(Ph_2)_2$	$P_3(Ph_2)_2$	$P_4(Ph_2)_2$	C_6H_2
LUMO+9	0	0	0	0	33	10	35	9	13
LUMO+6	1	1	0	0	27	19	28	19	4
LUMO+4	1	1	0	0	15	32	15	32	2
LUMO+3	1	1	1	1	31	13	31	13	9
LUMO+1	1	1	1	1	15	10	15	10	47
LUMO	1	1	0	0	14	5	14	5	61
HOMO	11	11	5	5	3	26	3	26	10
HOMO-1	13	13	11	11	1	22	1	22	5
HOMO-6	12	11	0	0	8	26	8	25	11
HOMO-8	7	7	10	10	15	12	15	12	12

Model system **3a**

Table S6. Population analysis for model system **3a**. Contribution from each part of the molecule to the orbitals involved in the most important transitions (%).

Orbital	Au_1	Au_2	$R_1(C_6Cl_5)$	$R_2(C_6F_5)$	$P_1(Ph_2)_2$	$P_2(Ph_2)_2$	$P_3(Ph_2)_2$	$P_4(Ph_2)_2$	C_6H_2
LUMO+9	0	0	0	0	34	9	34	9	12
LUMO+6	1	1	0	0	29	18	29	18	4
LUMO+3	1	1	1	1	31	13	31	13	9
LUMO+2	1	1	1	1	40	7	40	7	3
LUMO+1	1	1	1	1	14	10	14	10	47
LUMO	1	1	0	0	14	5	14	5	61
HOMO	11	11	4	4	3	26	3	26	10
HOMO-1	14	14	10	10	1	22	1	22	5
HOMO-6	12	12	0	0	7	26	7	26	10
HOMO-8	6	6	11	11	16	10	16	10	12

6. TD-DFT singlet excitation calculations for models **1a-3a.**

Table S7. TD-DFT singlet-singlet excitation calculations for model system **1a.**

$[Au_2(C_6F_5)_2(tpbz)]$ (**1a**)			
Transition	λ/nm	Oscillator strength	Contributions
S_0-S_1	409.57	0.0597	HOMO→LUMO (98%)
S_0-S_3	349.10	0.1429	HOMO→LUMO+1 (94%)
S_0-S_5	330.42	0.1225	HOMO→LUMO+3 (91%)
S_0-S_{12}	304.75	0.0274	HOMO→LUMO+4 (11%) HOMO→LUMO+6 (55%)
S_0-S_{16}	301.86	0.0771	HOMO-6→LUMO (88%)
S_0-S_{18}	291.88	0.0143	HOMO-8→LUMO (27%) HOMO-1→LUMO+4 (17%) HOMO→LUMO+9 (20%)

Table S8. TD-DFT singlet-singlet excitation calculations for model system **2a.**

$[Au_2(C_6Cl_2F_3)_2(tpbz)]$ (**2a**)			
Transition	λ/nm	Oscillator strength	Contributions
S_0-S_1	409.86	0.0606	HOMO→LUMO (98%)
S_0-S_3	349.19	0.1518	HOMO→LUMO+1 (94%)
S_0-S_5	330.37	0.1228	HOMO→LUMO+3 (91%)
S_0-S_{12}	304.92	0.0268	HOMO→LUMO+6 (68%)
S_0-S_{14}	304.33	0.0059	HOMO-1→LUMO+2 (83%)
S_0-S_{16}	302.09	0.0756	HOMO-6→LUMO (87%)
S_0-S_{18}	292.45	0.0231	HOMO-8→LUMO (54%) HOMO→LUMO+9 (14%)

Table S9. TD-DFT singlet-singlet excitation calculations for model system **3a.**

$[Au_2(C_6Cl_5)_2(tpbz)]$ (3**a**)			
Transition	λ/nm	Oscillator strength	Contributions
S_0-S_1	422.42	0.0662	HOMO→LUMO (99%)
S_0-S_3	362.57	0.1556	HOMO→LUMO+1 (92%)
S_0-S_5	314.13	0.1083	HOMO→LUMO+3 (89%)
S_0-S_8	316.47	0.0144	HOMO-1→LUMO+2 (86%)
S_0-S_{14}	313.45	0.0323	HOMO→LUMO+6 (60%) HOMO→LUMO+5 (43%)
S_0-S_{16}	304.03	0.0077	HOMO-1→LUMO+4 (36%) HOMO→LUMO+6 (26%) HOMO→LUMO+8 (11%)
S_0-S_{18}	302.69	0.0292	HOMO-6→LUMO (92%)

7. Excitation energies (eV)

Table S10. Excitation energies (eV) of the S_1, S_2, and T_1 states of **1a**-**3a** calculated at the TDDFT/PBE0/def2-TZVP level.

State/structure	1a	2a	3a
T_1/S_0	2.713	2.711	2.633
T_2/S_0	3.161	3.157	3.033
S_1/S_0	2.983	2.981	2.887
S_2/S_0	3.342	3.338	3.210
T_1/S_1	1.501	1.498	1.513
T_2/S_1	1.699	1.698	1.686
S_1/S_1	1.654	1.654	1.663
S_2/S_1	1.893	1.893	1.882
T_1/T_1	1.478	1.453	1.492
T_2/T_1	1.730	1.709	1.708
S_1/T_1	1.773	1.706	1.734
S_2/T_1	2.095	2.023	2.026

Table S11. Excitation energies (eV) of the S_1, S_2, and T_1 states of **1a**-**3a** calculated at the ADC(2)/def2-SVP level.

State/structure	1a	2a	3a
T_1/S_0	3.593	3.584	3.482
T_2/S_0	3.956	3.950	3.887
S_1/S_0	3.793	3.781	3.648
S_2/S_0	4.260	4.237	4.040
T_1/S_1	2.087	2.087	2.037
T_2/S_1	2.308	2.308	2.228
S_1/S_1	2.112	2.088	2.057
S_2/S_1	2.349	2.325	2.268
T_1/T_1	2.027	1.989	1.988
T_2/T_1	2.314	2.274	2.234
S_1/T_1	2.086	2.032	2.023
S_2/T_1	2.398	2.341	2.301

8. Representation of DFT optimized complexes **1-3** in the S_0 state (B3LYP functional)

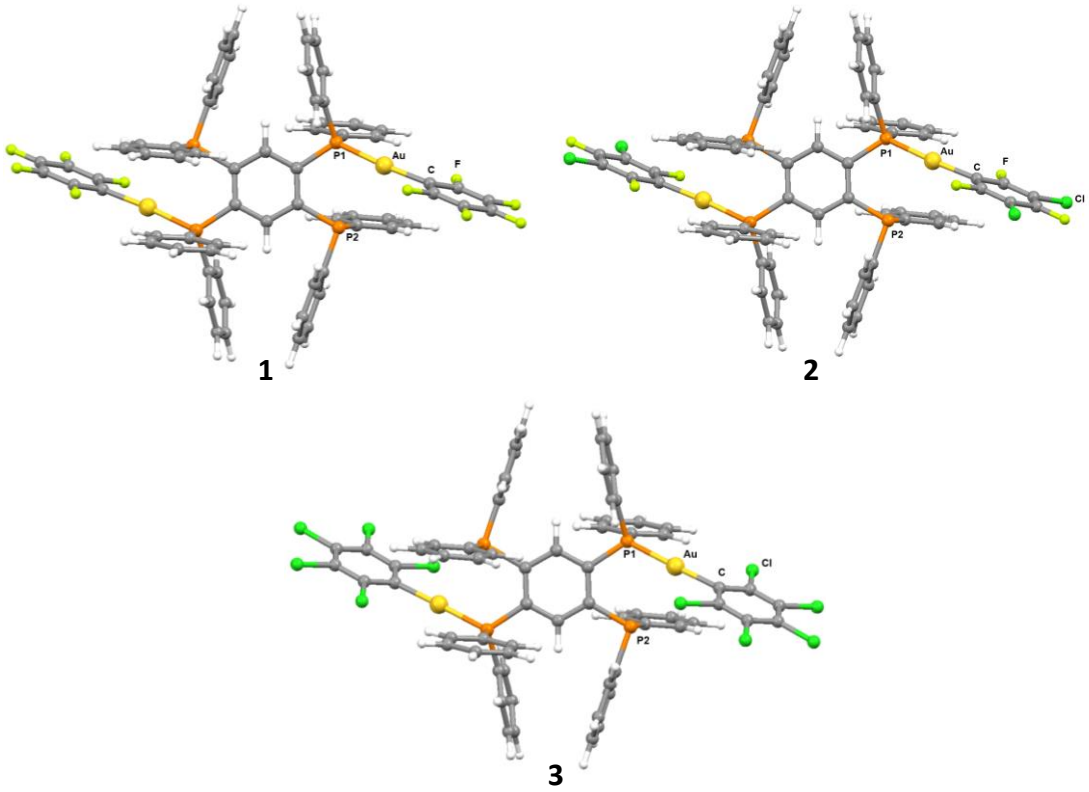


Figure S44. Model Systems of complexes **1**-**3** in the ground state S_0.

9. xyz coordinates for models **1a-3a** in the S_0 state (B3LYP functional)

124
Model_1 S0

Au	-4.73265000	0.78489900	0.39529900
P	-2.70703400	1.78863300	-0.18503700
P	2.87932400	1.57230400	0.31795600
F	-6.06694200	-0.59191000	3.00031200
F	-8.50239500	-1.65689200	3.42418000
F	-10.36780200	-1.64032200	1.44543100
F	-9.77501500	-0.54370900	-0.97444700
F	-7.34891300	0.52936800	-1.41770500
C	-6.61233700	0.02176800	0.77922200
C	-6.96064300	-0.55222800	1.99358000
C	-8.20827600	-1.11232500	2.24001300
C	-9.16506200	-1.10679900	1.23183500
C	-8.85863600	-0.54428500	-0.00118300
C	-7.59803000	0.00536800	-0.19743400
C	-1.19065200	0.73207000	-0.04401500
C	0.03869800	1.36701700	0.14390500
H	0.05491900	2.44803600	0.27249900

C	1.24756800	0.66637500	0.18655000
C	-2.69647700	2.35504600	-1.93513900
C	-3.91374400	2.41796100	-2.61946500
H	-4.83435100	2.11318900	-2.11763700
C	-3.94461700	2.84095900	-3.94607500
H	-4.89790400	2.87486800	-4.47755300
C	-2.76511400	3.19976100	-4.59328700
H	-2.79024800	3.52547800	-5.63601900
C	-1.54861400	3.13594500	-3.91276600
H	-0.62077600	3.41400300	-4.41854100
C	-1.51116900	2.71446900	-2.58733900
H	-0.55438300	2.66367600	-2.06585700
C	-2.30552400	3.26601600	0.83669800
C	-2.19771500	3.08415700	2.22163300
H	-2.31306500	2.08540600	2.65064900
C	-1.95907100	4.17379400	3.05111700
H	-1.87515700	4.02568100	4.13019400
C	-1.84474200	5.45365600	2.50665400
H	-1.66720800	6.31114500	3.15993200
C	-1.95799100	5.63619900	1.13196700
H	-1.86366400	6.63537300	0.70143600
C	-2.18365200	4.54542000	0.29332100
H	-2.26615000	4.69475400	-0.78385700
C	2.28380100	3.33180100	0.39728500
C	2.15093400	4.00001500	-0.82736500
H	2.40406700	3.47888100	-1.75528100
C	1.70546000	5.31888700	-0.87020800
H	1.60048500	5.82746700	-1.83178500
C	1.41208500	5.99138300	0.31482500
H	1.07057600	7.02873500	0.28554000
C	1.55860900	5.33915300	1.53729700
H	1.32491600	5.86209600	2.46721600
C	1.98816200	4.01477200	1.58133900
H	2.09116300	3.50871600	2.54254700
C	3.32676800	1.20531400	2.08055300
C	2.39706600	0.83186400	3.05791000
H	1.33716900	0.76562200	2.80569600
C	2.81964500	0.52311100	4.34792600
H	2.08772600	0.21636200	5.09859400
C	4.17385200	0.58201500	4.67357400
H	4.50413000	0.32476500	5.68281800
C	5.10704100	0.95101800	3.70655700
H	6.17189300	0.98283700	3.94760500
C	4.68532600	1.25781900	2.41543500
H	5.41977500	1.52396700	1.65338800
P	2.70753900	-1.78945700	0.18945900
P	-2.87905100	-1.57311800	-0.32318800

C	1.19090900	-0.73405200	0.04388300
C	-0.03836300	-1.36909500	-0.14464500
H	-0.05463300	-2.45022400	-0.27278300
C	-1.24716600	-0.66820800	-0.18820000
C	2.69604100	-2.34766400	1.94219800
C	3.91336900	-2.41030400	2.62648600
H	4.83458300	-2.11018300	2.12296400
C	3.94359400	-2.82699000	3.95508500
H	4.89694800	-2.86066300	4.48645800
C	2.76339800	-3.17977000	4.60437800
H	2.78806000	-3.50051800	5.64865900
C	1.54685000	-3.11607800	3.92398700
H	0.61847200	-3.38922900	4.43143800
C	1.51005700	-2.70079800	2.59656200
H	0.55321800	-2.64954700	2.07517500
C	2.30809900	-3.27136000	-0.82633300
C	2.21289600	-3.09692300	-2.21314000
H	2.33775700	-2.10134900	-2.64686700
C	1.97532700	-4.19006000	-3.03833700
H	1.90142700	-4.04777300	-4.11892800
C	1.84961100	-5.46609200	-2.48749800
H	1.67299400	-6.32641500	-3.13728800
C	1.95034600	-5.64129800	-1.11087200
H	1.84712700	-6.63744500	-0.67545200
C	2.17475600	-4.54692400	-0.27662000
H	2.24762600	-4.69051700	0.80202700
C	-2.28555000	-3.33293800	-0.41013200
C	-2.15808500	-4.00823800	0.81117900
H	-2.41227400	-3.49145000	1.74123300
C	-1.71735200	-5.32890200	0.84797800
H	-1.61699400	-5.84316500	1.80702400
C	-1.42312600	-5.99589500	-0.33991200
H	-1.08564400	-7.03468800	-0.31542400
C	-1.56355100	-5.33632100	-1.55916800
H	-1.32896100	-5.85493800	-2.49129900
C	-1.98853900	-4.01030900	-1.59709700
H	-2.08739600	-3.49874100	-2.55581700
C	-3.32596500	-1.19852700	-2.08439900
C	-2.39598200	-0.82121900	-3.06001200
H	-1.33615500	-0.75591700	-2.80725900
C	-2.81816200	-0.50747200	-4.34896100
H	-2.08600300	-0.19780800	-5.09819800
C	-4.17225500	-0.56515100	-4.67526400
H	-4.50222400	-0.30400300	-5.68360500
C	-5.10573600	-0.93790900	-3.70996100
H	-6.17051400	-0.96881000	-3.95145700
C	-4.68442100	-1.24974600	-2.41991900

H	-5.41910200	-1.51895100	-1.65916800
Au	4.73301700	-0.78677800	-0.39347200
F	6.06818300	0.58048000	-3.00315200
F	8.50391800	1.64353400	-3.43021800
F	10.36874600	1.63397300	-1.45086500
F	9.77508500	0.54633000	0.97284500
F	7.34871200	-0.52477900	1.41931600
C	6.61281700	-0.02507400	-0.77965500
C	6.96157800	0.54439800	-1.99600400
C	8.20937400	1.10338600	-2.24413700
C	9.16586400	1.10142000	-1.23566700
C	8.85898900	0.54347900	-0.00068200
C	7.59824500	-0.00526000	0.19721800

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Model_2 S0

Au	-0.89843700	-1.90181200	-4.32752600
P	-0.32151300	0.07661100	-3.23398900
P	1.83431800	2.33731200	1.42815900
C	-1.52891300	-3.53672900	-5.42213100
C	-0.13014600	-0.02549800	-1.39294400
C	0.68157200	0.91995600	-0.76282100
H	1.22826600	1.63272900	-1.37795400
C	0.82984600	0.97781400	0.62603200
C	3.34620100	1.38601400	1.93020100
C	-0.87437800	-4.76001300	-5.40608900
C	1.27451300	0.79796000	-3.79951900
C	2.42897500	0.01988600	-3.64292500
H	2.36551000	-0.95825800	-3.15918000
C	-2.69523900	-3.49464800	-6.17236000
C	-1.59290100	1.38382400	-3.47805400
C	-1.32912100	-5.88828800	-6.08577900
C	3.65160000	0.48417200	-4.11390700
H	4.54850800	-0.12663200	-3.98798600
C	1.35366900	2.03573100	-4.43885500
H	0.45930500	2.64721900	-4.56407500
C	-1.61495900	2.54520000	-2.69682700
H	-0.86902900	2.70265800	-1.91661900
C	2.40832700	3.26471400	-0.07749600
C	-2.55979500	1.19396900	-4.46964600
H	-2.55712800	0.27676700	-5.06202600
C	-2.50676800	-5.78653900	-6.82101400
C	-3.20741100	-4.58517500	-6.87145400
C	3.72713100	0.16875700	1.35379400
H	3.13482800	-0.26059500	0.54376700
C	2.58062900	2.49003200	-4.92081500
H	2.63681300	3.45949900	-5.42049200

C	3.59618000	2.99805600	-0.76564400
H	4.25101500	2.19232700	-0.43005600
C	-3.56028700	3.31622200	-3.90230200
H	-4.33362300	4.07110900	-4.06390900
C	-2.59701100	3.50721400	-2.91093700
H	-2.61141700	4.41142200	-2.29757600
C	3.72755300	1.71896100	-4.75969600
H	4.68695300	2.07906100	-5.13842800
C	1.58218100	4.30668500	-0.51976200
H	0.66409700	4.53587000	0.02913000
C	3.10819900	4.77772900	-2.32687500
H	3.38293600	5.36527400	-3.20600300
C	1.92321000	5.05159600	-1.64607300
H	1.26789000	5.85783700	-1.98492800
C	3.94374200	3.75534000	-1.88194900
H	4.87060300	3.53560700	-2.41617100
C	4.84855800	-0.51010800	1.82251300
H	5.12721100	-1.46770300	1.37677400
C	-3.53993600	2.16103500	-4.67942300
H	-4.29916700	1.99902800	-5.44732400
C	4.10367200	1.90765000	2.98604900
H	3.80077200	2.84449400	3.45673800
C	5.59848500	0.01822700	2.87217600
H	6.46932900	-0.52423400	3.24796100
C	5.22620600	1.22903200	3.45324200
H	5.79730600	1.64219400	4.28763700
P	0.32151300	-0.07661100	3.23398900
P	-1.83431800	-2.33731200	-1.42815900
C	0.13014600	0.02549800	1.39294400
C	-0.68157200	-0.91995600	0.76282100
H	-1.22826600	-1.63272900	1.37795400
C	-0.82984600	-0.97781400	-0.62603200
C	-3.34620100	-1.38601400	-1.93020100
C	-1.27451300	-0.79796000	3.79951900
C	-2.42897500	-0.01988600	3.64292500
H	-2.36551000	0.95825800	3.15918000
C	1.59290100	-1.38382400	3.47805400
C	-3.65160000	-0.48417200	4.11390700
H	-4.54850800	0.12663200	3.98798600
C	-1.35366900	-2.03573100	4.43885500
H	-0.45930500	-2.64721900	4.56407500
C	1.61495900	-2.54520000	2.69682700
H	0.86902900	-2.70265800	1.91661900
C	-2.40832700	-3.26471400	0.07749600
C	2.55979500	-1.19396900	4.46964600
H	2.55712800	-0.27676700	5.06202600
C	-3.72713100	-0.16875700	-1.35379400

H	-3.13482800	0.26059500	-0.54376700
C	-2.58062900	-2.49003200	4.92081500
H	-2.63681300	-3.45949900	5.42049200
C	-3.59618000	-2.99805600	0.76564400
H	-4.25101500	-2.19232700	0.43005600
C	3.56028700	-3.31622200	3.90230200
H	4.33362300	-4.07110900	4.06390900
C	2.59701100	-3.50721400	2.91093700
H	2.61141700	-4.41142200	2.29757600
C	-3.72755300	-1.71896100	4.75969600
H	-4.68695300	-2.07906100	5.13842800
C	-1.58218100	-4.30668500	0.51976200
H	-0.66409700	-4.53587000	-0.02913000
C	-3.10819900	-4.77772900	2.32687500
H	-3.38293600	-5.36527400	3.20600300
C	-1.92321000	-5.05159600	1.64607300
H	-1.26789000	-5.85783700	1.98492800
C	-3.94374200	-3.75534000	1.88194900
H	-4.87060300	-3.53560700	2.41617100
C	-4.84855800	0.51010800	-1.82251300
H	-5.12721100	1.46770300	-1.37677400
C	3.53993600	-2.16103500	4.67942300
H	4.29916700	-1.99902800	5.44732400
C	-4.10367200	-1.90765000	-2.98604900
H	-3.80077200	-2.84449400	-3.45673800
C	-5.59848500	-0.01822700	-2.87217600
H	-6.46932900	0.52423400	-3.24796100
C	-5.22620600	-1.22903200	-3.45324200
H	-5.79730600	-1.64219400	-4.28763700
Au	0.89843700	1.90181200	4.32752600
C	1.52891300	3.53672900	5.42213100
C	0.87437800	4.76001300	5.40608900
C	2.69523900	3.49464800	6.17236000
C	1.32912100	5.88828800	6.08577900
C	2.50676800	5.78653900	6.82101400
C	3.20741100	4.58517500	6.87145400
F	-3.39540300	-2.34509300	-6.22600900
F	-2.96805400	-6.84625000	-7.47752500
F	0.25667000	-4.88230600	-4.69310200
F	3.39540300	2.34509300	6.22600900
F	-0.25667000	4.88230600	4.69310200
F	2.96805400	6.84625000	7.47752500
Cl	0.46144000	7.40479900	6.02551500
Cl	4.69274200	4.47006300	7.78765500
Cl	-4.69274200	-4.47006300	-7.78765500
Cl	-0.46144000	-7.40479900	-6.02551500

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Model_3 S0

Au	4.61759400	-1.01122700	-0.44836100
Cl	7.36028600	-1.86575900	1.30732700
Cl	10.15400200	-0.43922000	1.11234200
Cl	10.56857000	1.94180900	-0.89898000
Cl	8.18879200	2.89254400	-2.72117500
Cl	5.39505500	1.45805900	-2.53360900
P	2.53524200	-2.02665900	-0.21203400
P	-2.96243300	-1.10895400	-0.92081900
C	6.50057400	-0.15545000	-0.63645800
C	7.58262300	-0.53949400	0.15600300
C	8.83273700	0.08269300	0.09436800
C	9.01993700	1.14348000	-0.79903800
C	7.95925000	1.56324800	-1.61023300
C	6.72940300	0.90764800	-1.51139900
C	1.11922800	-0.83513100	-0.11088600
C	-0.13977900	-1.26235000	-0.53744800
H	-0.23613800	-2.25410200	-0.97701000
C	-1.27914800	-0.45870400	-0.43471200
C	2.37419900	-3.03971000	1.31336300
C	3.53988100	-3.40545100	1.99198500
H	4.51000000	-3.07209300	1.61893200
C	3.45664900	-4.16918000	3.15365400
H	4.37051400	-4.43979600	3.68684200
C	2.21477400	-4.56898000	3.64064500
H	2.15125000	-5.16310400	4.55549000
C	1.04983700	-4.20343300	2.96541500
H	0.07356400	-4.51284300	3.34659700
C	1.12608900	-3.43914100	1.80518400
H	0.20940600	-3.15139500	1.28825100
C	2.08893100	-3.12623400	-1.61794800
C	2.15663100	-2.57983500	-2.90626600
H	2.44084000	-1.53271400	-3.03876500
C	1.88121900	-3.37279200	-4.01439200
H	1.93537800	-2.94149500	-5.01665600
C	1.55608600	-4.71935000	-3.84563600
H	1.35054300	-5.34490600	-4.71743200
C	1.49560200	-5.26458500	-2.56687500
H	1.23600100	-6.31642700	-2.43047300
C	1.75626700	-4.47108200	-1.45052700
H	1.70235400	-4.90367700	-0.45088700
C	-2.52857300	-2.82588200	-1.48212000
C	-2.60311700	-3.83176700	-0.50917000
H	-2.90697600	-3.57344000	0.50948700
C	-2.30683800	-5.15345900	-0.83432000
H	-2.36545900	-5.92925500	-0.06682500

C	-1.95755500	-5.48534600	-2.14223200
H	-1.73542200	-6.52287100	-2.40296000
C	-1.89665100	-4.49241300	-3.11805100
H	-1.61846500	-4.74907100	-4.14254900
C	-2.17624500	-3.16749400	-2.79176000
H	-2.11987700	-2.39488700	-3.56031700
C	-3.22668100	-0.19968100	-2.51562600
C	-2.19143400	0.34198900	-3.28608100
H	-1.15415100	0.22090900	-2.96842000
C	-2.47826600	1.05499500	-4.44698000
H	-1.66357200	1.48810600	-5.03187900
C	-3.80082900	1.23330100	-4.84978500
H	-4.02371100	1.80384300	-5.75462700
C	-4.83820400	0.69995600	-4.08718900
H	-5.87832100	0.85018800	-4.38537500
C	-4.55255000	-0.00821500	-2.92281400
H	-5.36788400	-0.40016000	-2.31200000
P	-2.53568400	2.01826200	0.23991300
P	2.96417900	1.11531300	0.90479600
C	-1.12009300	0.82706400	0.11979100
C	0.13923700	1.25438200	0.54442800
H	0.23503500	2.24512300	0.98587900
C	1.27955600	0.45339000	0.43717200
C	-2.37107200	3.06599900	-1.26145300
C	-3.53427000	3.43593300	-1.94189800
H	-4.50433700	3.08563100	-1.58461000
C	-3.44838500	4.22610300	-3.08564700
H	-4.36022900	4.50009100	-3.62057100
C	-2.20628500	4.64815800	-3.55270700
H	-2.14052700	5.26314700	-4.45350500
C	-1.04374600	4.27901600	-2.87507700
H	-0.06722300	4.60658900	-3.24008800
C	-1.12257100	3.48864200	-1.73274500
H	-0.20744200	3.20043100	-1.21349900
C	-2.08652600	3.08581300	1.66973400
C	-2.11638400	2.50152100	2.94281300
H	-2.37218400	1.44426000	3.05034500
C	-1.83769900	3.26875100	4.06800900
H	-1.86152700	2.80772400	5.05815000
C	-1.54726100	4.62706700	3.93235500
H	-1.33891400	5.23203600	4.81791800
C	-1.52511000	5.20982200	2.66904800
H	-1.29281900	6.27107300	2.55818900
C	-1.78915400	4.44245600	1.53523600
H	-1.76403500	4.90430900	0.54761000
C	2.52294200	2.84075200	1.43369200
C	2.56306200	3.82284700	0.43458600

H	2.85173500	3.54354100	-0.58295300
C	2.24897300	5.14696600	0.73152200
H	2.27907300	5.90365000	-0.05642700
C	1.91729600	5.50619000	2.03696000
H	1.68058400	6.54591400	2.27517400
C	1.89314300	4.53785800	3.03865100
H	1.62931400	4.81570400	4.06138400
C	2.18968900	3.20978700	2.74068500
H	2.15941400	2.45589600	3.52901300
C	3.23993500	0.23800300	2.51505700
C	2.20985300	-0.28727300	3.30355100
H	1.17039100	-0.17076100	2.99130800
C	2.50465900	-0.97783100	4.47591200
H	1.69399600	-1.39865200	5.07519800
C	3.83008200	-1.14963200	4.87230600
H	4.05914200	-1.70260000	5.78647600
C	4.86227100	-0.63231900	4.09191100
H	5.90441800	-0.77772300	4.38534600
C	4.56859900	0.05324500	2.91601900
H	5.37966400	0.43230300	2.29156100
Au	-4.61941100	1.00131400	0.45406000
Cl	-7.35694600	1.88269800	-1.29581300
Cl	-10.15104100	0.45303300	-1.13135900
Cl	-10.57110000	-1.95935300	0.84108200
Cl	-8.19652900	-2.93831000	2.65505900
Cl	-5.40271500	-1.50044700	2.49871800
C	-6.50281000	0.14256400	0.62379200
C	-7.58254000	0.53869800	-0.16588300
C	-8.83271100	-0.08455700	-0.11775100
C	-9.02234900	-1.15927300	0.75832300
C	-7.96399000	-1.59154000	1.56597000
C	-6.73401300	-0.93420000	1.48121800

10. Representation of DFT optimized complexes **1-3** in the T_1 state (B3LYP functional)

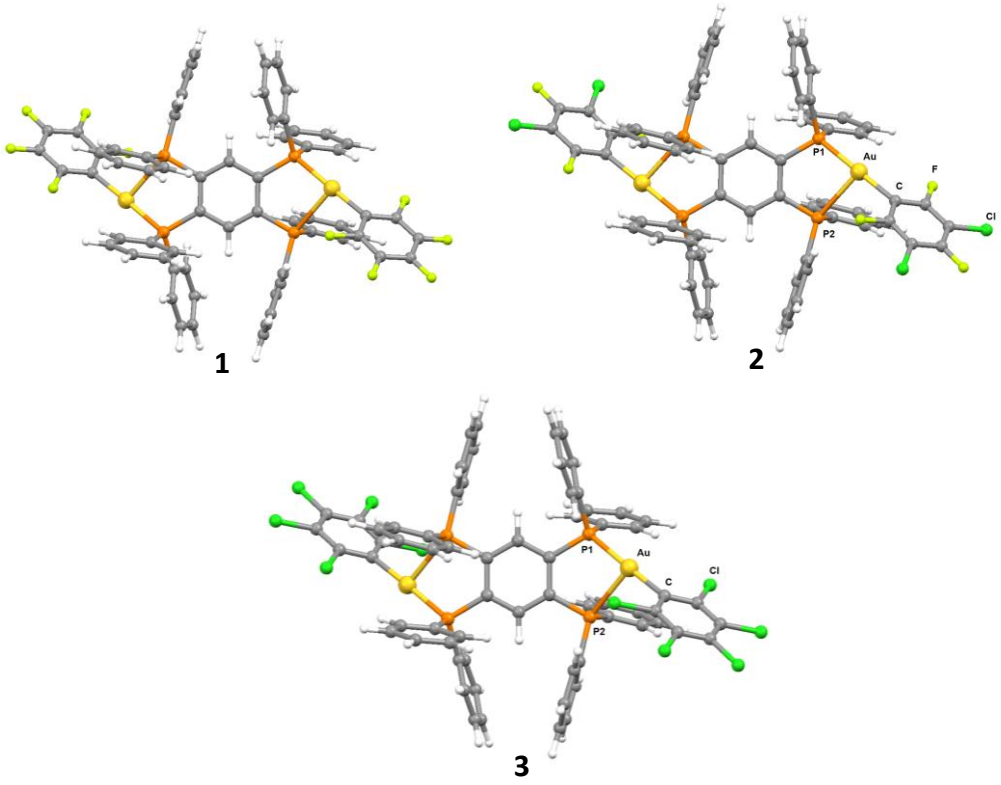

Figure S45. Model Systems of complexes **1**-**3** in the ground state T_1.

11. xyz coordinates for models **1a-3a** in the T_1 state (B3LYP functional)

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Model_1 T1

Au	-1.03006500	-1.78378400	-4.01712900
P	-0.40627600	0.33698100	-3.18824300
P	2.08055700	1.91050300	1.54906400
C	-1.47211500	-3.66086600	-4.80349700
C	-0.19892200	0.18090200	-1.40080800
C	0.70357500	0.98776900	-0.70180700
H	1.27060500	1.74077900	-1.25059500
C	0.93827400	0.83602800	0.66015400
C	3.61007500	0.93328200	1.85355900
C	-0.75691700	-4.79217900	-4.41156600
C	1.19758900	1.01315900	-3.77745400
C	2.28393400	0.13027800	-3.83441700
H	2.13432100	-0.92607400	-3.59702800
C	-2.55479800	-3.88313800	-5.65389900
C	-1.67084400	1.64372400	-3.49462700

C	-1.08436000	-6.08418600	-4.82775300
C	3.54417600	0.59736300	-4.18994000
H	4.38706600	-0.09643200	-4.23434400
C	1.38255200	2.36115800	-4.09193700
H	0.54214900	3.05488200	-4.05266900
C	-1.73703100	2.78366900	-2.68587900
H	-1.01931400	2.92033100	-1.87417000
C	2.53990200	3.22597300	0.35655500
C	-2.61803500	1.45126100	-4.50321100
H	-2.58293000	0.54503200	-5.11255400
C	-2.17860400	-6.26441300	-5.68250500
C	-2.92116200	-5.15439100	-6.10311400
C	3.81634000	-0.31290100	1.25433200
H	3.08242900	-0.69838800	0.54455200
C	2.64887000	2.82385400	-4.44980800
H	2.78912300	3.88114200	-4.68515300
C	3.68103700	3.13758100	-0.44831300
H	4.34830000	2.27904900	-0.35614900
C	-3.67453600	3.53981100	-3.91210200
H	-4.46362500	4.27897800	-4.07048000
C	-2.73163800	3.73269700	-2.90145700
H	-2.77804100	4.62391000	-2.27037500
C	3.72876900	1.94713400	-4.49679000
H	4.71950600	2.31323800	-4.77682200
C	1.68329300	4.32822300	0.23594200
H	0.80560800	4.40535800	0.88147200
C	3.08966100	5.22647700	-1.50923400
H	3.30502600	6.00866600	-2.24125300
C	1.95648500	5.32156300	-0.70030100
H	1.28626900	6.17970700	-0.79137300
C	3.95001100	4.13751300	-1.38012300
H	4.83308800	4.05777700	-2.01792900
C	4.94404500	-1.06158700	1.58123600
H	5.09276300	-2.04248300	1.12452800
C	-3.61940100	2.39796400	-4.70807000
H	-4.36768500	2.23426600	-5.48692400
C	4.53498600	1.42034300	2.78479500
H	4.35854900	2.37775500	3.27882400
C	5.86867100	-0.56978900	2.50051800
H	6.74746600	-1.16437400	2.76155200
C	5.66592200	0.67409000	3.09923100
H	6.38252100	1.05862700	3.82886700
P	0.40627600	-0.33698100	3.18824300
P	-2.08055700	-1.91050300	-1.54906400
C	0.19892200	-0.18090200	1.40080800
C	-0.70357500	-0.98776900	0.70180700
H	-1.27060500	-1.74077900	1.25059500

C	-0.93827400	-0.83602800	-0.66015400
C	-3.61007500	-0.93328200	-1.85355900
C	-1.19758900	-1.01315900	3.77745400
C	-2.28393400	-0.13027800	3.83441700
H	-2.13432100	0.92607400	3.59702800
C	1.67084400	-1.64372400	3.49462700
C	-3.54417600	-0.59736300	4.18994000
H	-4.38706600	0.09643200	4.23434400
C	-1.38255200	-2.36115800	4.09193700
H	-0.54214900	-3.05488200	4.05266900
C	1.73703100	-2.78366900	2.68587900
H	1.01931400	-2.92033100	1.87417000
C	-2.53990200	-3.22597300	-0.35655500
C	2.61803500	-1.45126100	4.50321100
H	2.58293000	-0.54503200	5.11255400
C	-3.81634000	0.31290100	-1.25433200
H	-3.08242900	0.69838800	-0.54455200
C	-2.64887000	-2.82385400	4.44980800
H	-2.78912300	-3.88114200	4.68515300
C	-3.68103700	-3.13758100	0.44831300
H	-4.34830000	-2.27904900	0.35614900
C	3.67453600	-3.53981100	3.91210200
H	4.46362500	-4.27897800	4.07048000
C	2.73163800	-3.73269700	2.90145700
H	2.77804100	-4.62391000	2.27037500
C	-3.72876900	-1.94713400	4.49679000
H	-4.71950600	-2.31323800	4.77682200
C	-1.68329300	-4.32822300	-0.23594200
H	-0.80560800	-4.40535800	-0.88147200
C	-3.08966100	-5.22647700	1.50923400
H	-3.30502600	-6.00866600	2.24125300
C	-1.95648500	-5.32156300	0.70030100
H	-1.28626900	-6.17970700	0.79137300
C	-3.95001100	-4.13751300	1.38012300
H	-4.83308800	-4.05777700	2.01792900
C	-4.94404500	1.06158700	-1.58123600
H	-5.09276300	2.04248300	-1.12452800
C	3.61940100	-2.39796400	4.70807000
H	4.36768500	-2.23426600	5.48692400
C	-4.53498600	-1.42034300	-2.78479500
H	-4.35854900	-2.37775500	-3.27882400
C	-5.86867100	0.56978900	-2.50051800
H	-6.74746600	1.16437400	-2.76155200
C	-5.66592200	-0.67409000	-3.09923100
H	-6.38252100	-1.05862700	-3.82886700
Au	1.03006500	1.78378400	4.01712900
C	1.47211500	3.66086600	4.80349700

C	0.75691700	4.79217900	4.41156600
C	2.55479800	3.88313800	5.65389900
C	1.08436000	6.08418600	4.82775300
C	2.17860400	6.26441300	5.68250500
C	2.92116200	5.15439100	6.10311400
F	-0.29755144	4.62675912	3.58498717
F	0.36930713	7.15268948	4.41604957
F	2.51733661	7.50364431	6.09731336
F	3.97632224	5.32540363	6.92766937
F	3.28583854	2.82007493	6.05136173
F	0.29755144	-4.62675912	-3.58498717
F	-0.36930713	-7.15268948	-4.41604957
F	-2.51733661	-7.50364431	-6.09731336
F	-3.97632224	-5.32540363	-6.92766937
F	-3.28583854	-2.82007493	-6.05136173

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Model_2 T1

Au	-0.95320600	-1.79853700	-4.07285600
P	-0.33919800	0.30987800	-3.20125300
P	1.96208000	2.01001000	1.57621800
C	-1.55090500	-3.62356200	-4.85977200
C	-0.17950500	0.16480700	-1.40866600
C	0.66067000	1.02459400	-0.68867900
H	1.19925300	1.80542000	-1.22678300
C	0.87858300	0.88498500	0.67535100
C	3.50018600	1.06790900	1.94802500
C	-1.08144300	-4.82444200	-4.34865800
C	1.26411200	1.03152400	-3.74539300
C	2.41750100	0.25795700	-3.55917600
H	2.33282900	-0.74433600	-3.13196500
C	-2.55896200	-3.73126500	-5.80672000
C	-1.61574200	1.59356600	-3.55790800
C	-1.55733000	-6.07254400	-4.74059200
C	3.66344500	0.76588600	-3.90817600
H	4.55843100	0.15687900	-3.76026300
C	1.37125500	2.31167300	-4.29219500
H	0.47893400	2.92122900	-4.43935900
C	-1.69892000	2.75630800	-2.78343100
H	-0.98439800	2.92884600	-1.97591400
C	2.42594200	3.31632700	0.37522600
C	-2.55223400	1.36386800	-4.56864600
H	-2.50274700	0.44242600	-5.15420600
C	-2.56362800	-6.12039600	-5.70165300
C	-3.07873300	-4.94720400	-6.24619200
C	3.76443300	-0.17132600	1.35700400
H	3.07510600	-0.57168600	0.61155800

C	2.62376400	2.81609900	-4.64270900
H	2.70126000	3.82147000	-5.06312600
C	3.51609400	3.17849400	-0.49151100
H	4.14435300	2.28753300	-0.44124000
C	-3.63653900	3.45543700	-4.04349900
H	-4.43184100	4.18172600	-4.22843900
C	-2.70340800	3.68648000	-3.03124500
H	-2.76370100	4.59452000	-2.42601400
C	3.76848300	2.04810500	-4.45104300
H	4.74806300	2.44657000	-4.72610900
C	1.61961100	4.45986000	0.31105500
H	0.78561700	4.57512700	1.00723700
C	2.96977600	5.30246000	-1.50479300
H	3.18235800	6.07884500	-2.24373400
C	1.89084700	5.44773500	-0.63246700
H	1.26186200	6.33985100	-0.67947400
C	3.78169900	4.17133400	-1.43123500
H	4.62198300	4.05383800	-2.11853300
C	4.89110400	-0.89592900	1.73770900
H	5.08422800	-1.87180100	1.28691400
C	-3.56157800	2.29402700	-4.80842100
H	-4.29963200	2.10106100	-5.59014600
C	4.36604700	1.57109700	2.92739800
H	4.14355300	2.52397600	3.41310000
C	5.75635100	-0.38782500	2.70437400
H	6.63307200	-0.96443900	3.00874200
C	5.49596300	0.84857800	3.29632600
H	6.16633200	1.24494400	4.06249800
P	0.33919800	-0.30987800	3.20125300
P	-1.96208000	-2.01001000	-1.57621800
C	0.17950500	-0.16480700	1.40866600
C	-0.66067000	-1.02459400	0.68867900
H	-1.19925300	-1.80542000	1.22678300
C	-0.87858300	-0.88498500	-0.67535100
C	-3.50018600	-1.06790900	-1.94802500
C	-1.26411200	-1.03152400	3.74539300
C	-2.41750100	-0.25795700	3.55917600
H	-2.33282900	0.74433600	3.13196500
C	1.61574200	-1.59356600	3.55790800
C	-3.66344500	-0.76588600	3.90817600
H	-4.55843100	-0.15687900	3.76026300
C	-1.37125500	-2.31167300	4.29219500
H	-0.47893400	-2.92122900	4.43935900
C	1.69892000	-2.75630800	2.78343100
H	0.98439800	-2.92884600	1.97591400
C	-2.42594200	-3.31632700	-0.37522600
C	2.55223400	-1.36386800	4.56864600

H	2.50274700	-0.44242600	5.15420600
C	-3.76443300	0.17132600	-1.35700400
H	-3.07510600	0.57168600	-0.61155800
C	-2.62376400	-2.81609900	4.64270900
H	-2.70126000	-3.82147000	5.06312600
C	-3.51609400	-3.17849400	0.49151100
H	-4.14435300	-2.28753300	0.44124000
C	3.63653900	-3.45543700	4.04349900
H	4.43184100	-4.18172600	4.22843900
C	2.70340800	-3.68648000	3.03124500
H	2.76370100	-4.59452000	2.42601400
C	-3.76848300	-2.04810500	4.45104300
H	-4.74806300	-2.44657000	4.72610900
C	-1.61961100	-4.45986000	-0.31105500
H	-0.78561700	-4.57512700	-1.00723700
C	-2.96977600	-5.30246000	1.50479300
H	-3.18235800	-6.07884500	2.24373400
C	-1.89084700	-5.44773500	0.63246700
H	-1.26186200	-6.33985100	0.67947400
C	-3.78169900	-4.17133400	1.43123500
H	-4.62198300	-4.05383800	2.11853300
C	-4.89110400	0.89592900	-1.73770900
H	-5.08422800	1.87180100	-1.28691400
C	3.56157800	-2.29402700	4.80842100
H	4.29963200	-2.10106100	5.59014600
C	-4.36604700	-1.57109700	-2.92739800
H	-4.14355300	-2.52397600	-3.41310000
C	-5.75635100	0.38782500	-2.70437400
H	-6.63307200	0.96443900	-3.00874200
C	-5.49596300	-0.84857800	-3.29632600
H	-6.16633200	-1.24494400	-4.06249800
Au	0.95320600	1.79853700	4.07285600
C	1.55090500	3.62356200	4.85977200
C	1.08144300	4.82444200	4.34865800
C	2.55896200	3.73126500	5.80672000
C	1.55733000	6.07254400	4.74059200
C	2.56362800	6.12039600	5.70165300
C	3.07873300	4.94720400	6.24619200
F	-3.08970200	-2.60886100	-6.32188300
F	-3.04090200	-7.29576700	-6.09715200
F	-0.12561200	-4.79736800	-3.40061700
F	3.08970200	2.60886100	6.32188300
F	0.12561200	4.79736800	3.40061700
F	3.04090200	7.29576700	6.09715200
Cl	0.93288300	7.55007800	4.04498400
Cl	4.35350600	5.02005600	7.44023600
Cl	-4.35350600	-5.02005600	-7.44023600

Cl	-0.93288300	-7.55007800	-4.04498400

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Model_3 T1

Au	-1.03006500	-1.78378400	-4.01712900
P	-0.40627600	0.33698100	-3.18824300
P	2.08055700	1.91050300	1.54906400
C	-1.47211500	-3.66086600	-4.80349700
C	-0.19892200	0.18090200	-1.40080800
C	0.70357500	0.98776900	-0.70180700
H	1.27060500	1.74077900	-1.25059500
C	0.93827400	0.83602800	0.66015400
C	3.61007500	0.93328200	1.85355900
C	-0.75691700	-4.79217900	-4.41156600
C	1.19758900	1.01315900	-3.77745400
C	2.28393400	0.13027800	-3.83441700
H	2.13432100	-0.92607400	-3.59702800
C	-2.55479800	-3.88313800	-5.65389900
C	-1.67084400	1.64372400	-3.49462700
C	-1.08436000	-6.08418600	-4.82775300
C	3.54417600	0.59736300	-4.18994000
H	4.38706600	-0.09643200	-4.23434400
C	1.38255200	2.36115800	-4.09193700
H	0.54214900	3.05488200	-4.05266900
C	-1.73703100	2.78366900	-2.68587900
H	-1.01931400	2.92033100	-1.87417000
C	2.53990200	3.22597300	0.35655500
C	-2.61803500	1.45126100	-4.50321100
H	-2.58293000	0.54503200	-5.11255400
C	-2.17860400	-6.26441300	-5.68250500
C	-2.92116200	-5.15439100	-6.10311400
C	3.81634000	-0.31290100	1.25433200
H	3.08242900	-0.69838800	0.54455200
C	2.64887000	2.82385400	-4.44980800
H	2.78912300	3.88114200	-4.68515300
C	3.68103700	3.13758100	-0.44831300
H	4.34830000	2.27904900	-0.35614900
C	-3.67453600	3.53981100	-3.91210200
H	-4.46362500	4.27897800	-4.07048000
C	-2.73163800	3.73269700	-2.90145700
H	-2.77804100	4.62391000	-2.27037500
C	3.72876900	1.94713400	-4.49679000
H	4.71950600	2.31323800	-4.77682200
C	1.68329300	4.32822300	0.23594200
H	0.80560800	4.40535800	0.88147200
C	3.08966100	5.22647700	-1.50923400
H	3.30502600	6.00866600	-2.24125300

C	1.95648500	5.32156300	-0.70030100
H	1.28626900	6.17970700	-0.79137300
C	3.95001100	4.13751300	-1.38012300
H	4.83308800	4.05777700	-2.01792900
C	4.94404500	-1.06158700	1.58123600
H	5.09276300	-2.04248300	1.12452800
C	-3.61940100	2.39796400	-4.70807000
H	-4.36768500	2.23426600	-5.48692400
C	4.53498600	1.42034300	2.78479500
H	4.35854900	2.37775500	3.27882400
C	5.86867100	-0.56978900	2.50051800
H	6.74746600	-1.16437400	2.76155200
C	5.66592200	0.67409000	3.09923100
H	6.38252100	1.05862700	3.82886700
P	0.40627600	-0.33698100	3.18824300
P	-2.08055700	-1.91050300	-1.54906400
C	0.19892200	-0.18090200	1.40080800
C	-0.70357500	-0.98776900	0.70180700
H	-1.27060500	-1.74077900	1.25059500
C	-0.93827400	-0.83602800	-0.66015400
C	-3.61007500	-0.93328200	-1.85355900
C	-1.19758900	-1.01315900	3.77745400
C	-2.28393400	-0.13027800	3.83441700
H	-2.13432100	0.92607400	3.59702800
C	1.67084400	-1.64372400	3.49462700
C	-3.54417600	-0.59736300	4.18994000
H	-4.38706600	0.09643200	4.23434400
C	-1.38255200	-2.36115800	4.09193700
H	-0.54214900	-3.05488200	4.05266900
C	1.73703100	-2.78366900	2.68587900
H	1.01931400	-2.92033100	1.87417000
C	-2.53990200	-3.22597300	-0.35655500
C	2.61803500	-1.45126100	4.50321100
H	2.58293000	-0.54503200	5.11255400
C	-3.81634000	0.31290100	-1.25433200
H	-3.08242900	0.69838800	-0.54455200
C	-2.64887000	-2.82385400	4.44980800
H	-2.78912300	-3.88114200	4.68515300
C	-3.68103700	-3.13758100	0.44831300
H	-4.34830000	-2.27904900	0.35614900
C	3.67453600	-3.53981100	3.91210200
H	4.46362500	-4.27897800	4.07048000
C	2.73163800	-3.73269700	2.90145700
H	2.77804100	-4.62391000	2.27037500
C	-3.72876900	-1.94713400	4.49679000
H	-4.71950600	-2.31323800	4.77682200
C	-1.68329300	-4.32822300	-0.23594200

H	-0.80560800	-4.40535800	-0.88147200
C	-3.08966100	-5.22647700	1.50923400
H	-3.30502600	-6.00866600	2.24125300
C	-1.95648500	-5.32156300	0.70030100
H	-1.28626900	-6.17970700	0.79137300
C	-3.95001100	-4.13751300	1.38012300
H	-4.83308800	-4.05777700	2.01792900
C	-4.94404500	1.06158700	-1.58123600
H	-5.09276300	2.04248300	-1.12452800
C	3.61940100	-2.39796400	4.70807000
H	4.36768500	-2.23426600	5.48692400
C	-4.53498600	-1.42034300	-2.78479500
H	-4.35854900	-2.37775500	-3.27882400
C	-5.86867100	0.56978900	-2.50051800
H	-6.74746600	1.16437400	-2.76155200
C	-5.66592200	-0.67409000	-3.09923100
H	-6.38252100	-1.05862700	-3.82886700
Au	1.03006500	1.78378400	4.01712900
C	1.47211500	3.66086600	4.80349700
C	0.75691700	4.79217900	4.41156600
C	2.55479800	3.88313800	5.65389900
C	1.08436000	6.08418600	4.82775300
C	2.17860400	6.26441300	5.68250500
C	2.92116200	5.15439100	6.10311400
Cl	0.15875200	7.46732200	4.29481900
Cl	4.28671000	5.37570900	7.17022200
Cl	-4.28671000	-5.37570900	-7.17022200
Cl	-0.15875200	-7.46732200	-4.29481900
Cl	-0.62664200	4.57513300	3.32701900
Cl	3.51273300	2.49013000	6.17472300
Cl	2.61635400	7.86589300	6.21856900
Cl	0.62664200	-4.57513300	-3.32701900
Cl	-3.51273300	-2.49013000	-6.17472300
Cl	-2.61635400	-7.86589300	-6.21856900

13. Representation of DFT optimized complexes **1-3** in the S_0 state (PBE0 functional)

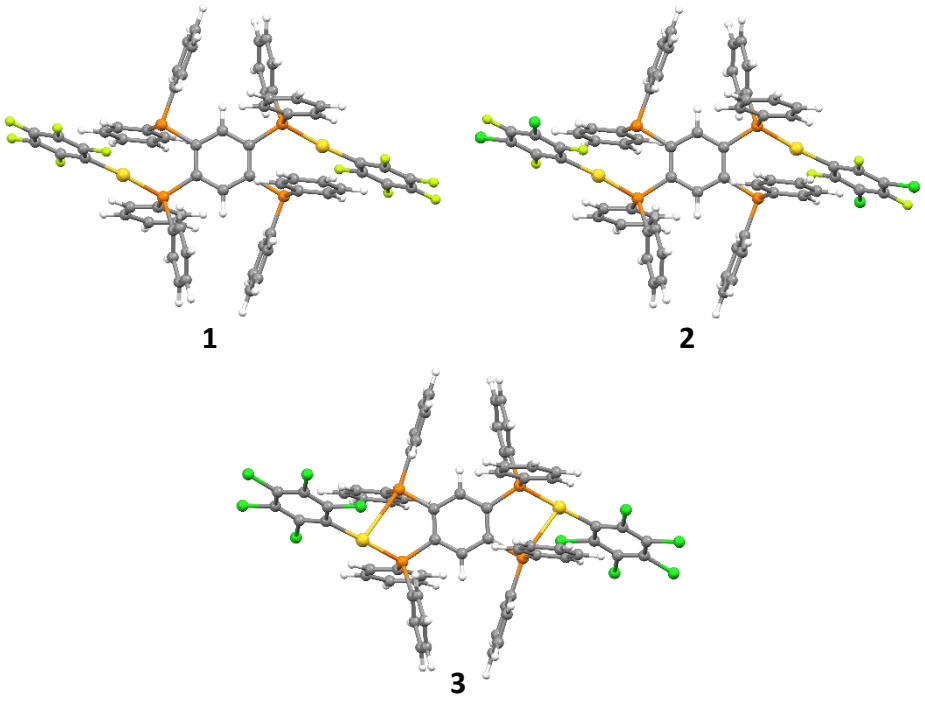

Figure S46. Model Systems of complexes **1**-**3** in the ground state S_0.

14. xyz coordinates for models **1a-3a** in the S_0 state (PBE0 functional)

124
Model_1 S0
Au -4.672695 0.773207 0.371925
P -2.685180 1.781379 -0.221231
P 2.841102 1.548530 0.448300
F -5.905387 -0.430307 3.102081
F -8.311989 -1.487289 3.690179
F -10.248791 -1.632618 1.783866
F -9.756136 -0.712527 -0.731486
F -7.359139 0.349486 -1.342544
C -6.540296 0.006719 0.859682
C -6.836298 -0.477168 2.122575
C -8.065538 -1.027732 2.454983
C -9.056213 -1.105254 1.486376
C -8.801110 -0.633690 0.206864
C -7.556325 -0.090582 -0.075004
C -1.188731 0.736387 -0.064440
C 0.033834 1.359523 0.176089
H 0.047920 2.427972 0.328276
C 1.238949 0.659916 0.241123
C -2.649914 2.345336 -1.949876

C -3.850258 2.421908 -2.656480
H -4.773754 2.124711 -2.177335
C -3.855947 2.853157 -3.976841
H -4.790587 2.897073 -4.520087
C -2.666594 3.208621 -4.599442
H -2.671718 3.538522 -5.630483
C -1.465851 3.131908 -3.899920
H -0.536187 3.403380 -4.383538
C -1.455381 2.701725 -2.581274
H -0.516502 2.640942 -2.048319
C -2.311935 3.241101 0.797789
C -2.208482 3.058689 2.180634
H -2.314596 2.066930 2.603142
C -1.984690 4.143413 3.013220
H -1.903910 3.992957 4.081969
C -1.882132 5.424019 2.476819
H -1.717681 6.272314 3.128685
C -1.991691 5.610406 1.106412
H -1.907814 6.603254 0.684376
C -2.201974 4.523227 0.265235
H -2.281775 4.676547 -0.801665
C 2.283063 3.294763 0.491210
C 2.166058 3.944911 -0.741931
H 2.415953 3.410539 -1.651461
C 1.741432 5.264866 -0.809418
H 1.649708 5.753732 -1.771034
C 1.453126 5.961098 0.359231
H 1.129563 6.992792 0.310319
C 1.585451 5.329999 1.589779
H 1.359173 5.867476 2.501381
C 1.993385 4.003462 1.657788
H 2.083379 3.517960 2.619817
C 3.236975 1.182457 2.197303
C 2.281626 0.816297 3.147868
H 1.239368 0.747140 2.866157
C 2.662033 0.521780 4.449981
H 1.914619 0.223757 5.173840
C 4.001296 0.591313 4.817522
H 4.297630 0.350442 5.830475
C 4.960626 0.951929 3.878445
H 6.006932 0.991169 4.152118
C 4.581112 1.240448 2.574226
H 5.333756 1.492097 1.838861
P 2.685180 -1.781379 0.221231
P -2.841102 -1.548530 -0.448300
C 1.188731 -0.736387 0.064440
C -0.033834 -1.359523 -0.176089

H -0.047920 -2.427972 -0.328276
C -1.238949 -0.659916 -0.241123
C 2.649914 -2.345336 1.949876
C 3.850258 -2.421908 2.656480
H 4.773754 -2.124711 2.177335
C 3.855947 -2.853157 3.976841
H 4.790587 -2.897073 4.520087
C 2.666594 -3.208621 4.599442
H 2.671718 -3.538522 5.630483
C 1.465851 -3.131908 3.899920
H 0.536187 -3.403380 4.383538
C 1.455381 -2.701725 2.581274
H 0.516502 -2.640942 2.048319
C 2.311935 -3.241101 -0.797789
C 2.208482 -3.058689 -2.180634
H 2.314596 -2.066930 -2.603142
C 1.984690 -4.143413 -3.013220
H 1.903910 -3.992957 -4.081969
C 1.882132 -5.424019 -2.476819
H 1.717681 -6.272314 -3.128685
C 1.991691 -5.610406 -1.106412
H 1.907814 -6.603254 -0.684376
C 2.201974 -4.523227 -0.265235
H 2.281775 -4.676547 0.801665
C -2.283063 -3.294763 -0.491210
C -2.166058 -3.944911 0.741931
H -2.415953 -3.410539 1.651461
C -1.741432 -5.264866 0.809418
H -1.649708 -5.753732 1.771034
C -1.453126 -5.961098 -0.359231
H -1.129563 -6.992792 -0.310319
C -1.585451 -5.329999 -1.589779
H -1.359173 -5.867476 -2.501381
C -1.993385 -4.003462 -1.657788
H -2.083379 -3.517960 -2.619817
C -3.236975 -1.182457 -2.197303
C -2.281626 -0.816297 -3.147868
H -1.239368 -0.747140 -2.866157
C -2.662033 -0.521780 -4.449981
H -1.914619 -0.223757 -5.173840
C -4.001296 -0.591313 -4.817522
H -4.297630 -0.350442 -5.830475
C -4.960626 -0.951929 -3.878445
H -6.006932 -0.991169 -4.152118
C -4.581112 -1.240448 -2.574226
H -5.333756 -1.492097 -1.838861
Au 4.672695 -0.773207 -0.371925

F 5.905387 0.430307 -3.102081
F 8.311989 1.487289 -3.690179
F 10.248791 1.632618 -1.783866
F 9.756136 0.712527 0.731486
F 7.359139 -0.349486 1.342544
C 6.540296 -0.006719 -0.859682
C 6.836298 0.477168 -2.122575
C 8.065538 1.027732 -2.454983
C 9.056213 1.105254 -1.486376
C 8.801110 0.633690 -0.206864
C 7.556325 0.090582 0.075004

124
Model_2 S0
Au -0.915256 -1.871830 -4.268667
P -0.357407 0.098176 -3.208692
P 1.931672 2.231769 1.399730
C -1.446473 -3.558548 -5.358682
C -0.150216 -0.011706 -1.391755
C 0.705316 0.892240 -0.765857
H 1.267165 1.580608 -1.378573
C 0.876155 0.937832 0.617907
C 3.415139 1.264188 1.861171
C -0.689436 -4.717317 -5.357561
C 1.220955 0.788843 -3.791719
C 2.365360 -0.004385 -3.660052
H 2.295666 -0.977576 -3.189500
C -2.616481 -3.613251 -6.094995
C -1.599714 1.407771 -3.431460
C -1.048202 -5.877073 -6.038800
C 3.584973 0.444163 -4.140959
H 4.465869 -0.175402 -4.033429
C 1.313934 2.027324 -4.421850
H 0.436042 2.648348 -4.530474
C -1.604854 2.557261 -2.636944
H -0.863891 2.687976 -1.860351
C 2.481396 3.185128 -0.067041
C -2.569486 1.252815 -4.422246
H -2.582352 0.353125 -5.023199
C -2.236468 -5.869688 -6.760116
C -3.040637 -4.736901 -6.798157
C 3.769311 0.054035 1.260910
H 3.157486 -0.353904 0.467379
C 2.537437 2.466746 -4.915501
H 2.600738 3.430063 -5.404291
C 3.666854 2.948960 -0.764217
H 4.326132 2.150852 -0.451610

C -3.529546 3.378808 -3.827621
H -4.282632 4.142016 -3.976937
C -2.565708 3.537600 -2.836249
H -2.565041 4.424193 -2.215098
C 3.671624 1.680007 -4.776098
H 4.622709 2.025631 -5.160240
C 1.647210 4.227619 -0.484490
H 0.738485 4.436409 0.068571
C 3.158724 4.752600 -2.280473
H 3.422025 5.357077 -3.138825
C 1.976124 4.998114 -1.591456
H 1.318217 5.797917 -1.907015
C 4.003337 3.732208 -1.861466
H 4.922822 3.535701 -2.397214
C 4.892724 -0.640576 1.688163
H 5.148105 -1.585493 1.226282
C -3.529740 2.237108 -4.618253
H -4.284796 2.101849 -5.381273
C 4.203784 1.761278 2.901946
H 3.922323 2.682596 3.394422
C 5.675825 -0.133164 2.719093
H 6.545216 -0.681675 3.058525
C 5.330767 1.069307 3.325232
H 5.924724 1.462109 4.140162
P 0.357407 -0.098176 3.208692
P -1.931672 -2.231769 -1.399730
C 0.150216 0.011706 1.391755
C -0.705316 -0.892240 0.765857
H -1.267165 -1.580608 1.378573
C -0.876155 -0.937832 -0.617907
C -3.415139 -1.264188 -1.861171
C -1.220955 -0.788843 3.791719
C -2.365360 0.004385 3.660052
H -2.295666 0.977576 3.189500
C 1.599714 -1.407771 3.431460
C -3.584973 -0.444163 4.140959
H -4.465869 0.175402 4.033429
C -1.313934 -2.027324 4.421850
H -0.436042 -2.648348 4.530474
C 1.604854 -2.557261 2.636944
H 0.863891 -2.687976 1.860351
C -2.481396 -3.185128 0.067041
C 2.569486 -1.252815 4.422246
H 2.582352 -0.353125 5.023199
C -3.769311 -0.054035 -1.260910
H -3.157486 0.353904 -0.467379
C -2.537437 -2.466746 4.915501

H -2.600738 -3.430063 5.404291
C -3.666854 -2.948960 0.764217
H -4.326132 -2.150852 0.451610
C 3.529546 -3.378808 3.827621
H 4.282632 -4.142016 3.976937
C 2.565708 -3.537600 2.836249
H 2.565041 -4.424193 2.215098
C -3.671624 -1.680007 4.776098
H -4.622709 -2.025631 5.160240
C -1.647210 -4.227619 0.484490
H -0.738485 -4.436409 -0.068571
C -3.158724 -4.752600 2.280473
H -3.422025 -5.357077 3.138825
C -1.976124 -4.998114 1.591456
H -1.318217 -5.797917 1.907015
C -4.003337 -3.732208 1.861466
H -4.922822 -3.535701 2.397214
C -4.892724 0.640576 -1.688163
H -5.148105 1.585493 -1.226282
C 3.529740 -2.237108 4.618253
H 4.284796 -2.101849 5.381273
C -4.203784 -1.761278 -2.901946
H -3.922323 -2.682596 -3.394422
C -5.675825 0.133164 -2.719093
H -6.545216 0.681675 -3.058525
C -5.330767 -1.069307 -3.325232
H -5.924724 -1.462109 -4.140162
Au 0.915256 1.871830 4.268667
C 1.446473 3.558548 5.358682
C 0.689436 4.717317 5.357561
C 2.616481 3.613251 6.094995
C 1.048202 5.877073 6.038800
C 2.236468 5.869688 6.760116
C 3.040637 4.736901 6.798157
F -3.415975 -2.523064 -6.138940
F -2.611602 -6.965966 -7.423032
F 0.462744 -4.745286 -4.657317
F 3.415975 2.523064 6.138940
F -0.462744 4.745286 4.657317
F 2.611602 6.965966 7.423032
Cl 0.061593 7.297024 5.998693
Cl 4.520653 4.744593 7.693841
Cl -4.520653 -4.744593 -7.693841
Cl -0.061593 -7.297024 -5.998693

124
Model_3 S0
Au 4.555873 -1.010374 -0.449006
Cl 7.324321 -1.850351 1.262891
Cl 10.083203 -0.397129 1.079829
Cl 10.461204 2.001484 -0.888292
Cl 8.075138 2.950605 -2.671204
Cl 5.314648 1.494546 -2.491710
P 2.505217 -2.027806 -0.222018
P -2.931971 -1.063446 -0.965530
C 6.438445 -0.131958 -0.639051
C 7.523802 -0.518470 0.143313
C 8.765415 0.119280 0.084929
C 8.936785 1.194251 -0.792939
C 7.868229 1.615165 -1.591157
C 6.646075 0.945891 -1.497333
C 1.112732 -0.842414 -0.109490
C -0.142382 -1.243963 -0.560621
H -0.241767 -2.218805 -1.013200
C -1.274551 -0.434570 -0.463973
C 2.343605 -3.044247 1.276298
C 3.501313 -3.430624 1.951812
H 4.466567 -3.103906 1.588409
C 3.411575 -4.208211 3.099166
H 4.314113 -4.492750 3.623754
C 2.169372 -4.603016 3.578800
H 2.100807 -5.203490 4.476947
C 1.011279 -4.218088 2.910000
H 0.041199 -4.519873 3.283798
C 1.095790 -3.440759 1.764152
H 0.189853 -3.139926 1.255839
C 2.064781 -3.101597 -1.621627
C 2.107337 -2.541566 -2.902640
H 2.371803 -1.498340 -3.025569
C 1.828664 -3.320333 -4.014399
H 1.862801 -2.878954 -5.002060
C 1.525220 -4.670418 -3.861104
H 1.317901 -5.280637 -4.730677
C 1.490191 -5.231728 -2.592874
H 1.249864 -6.279343 -2.468459
C 1.754300 -4.451123 -1.472848
H 1.720408 -4.895293 -0.488143
C -2.543168 -2.781821 -1.469011
C -2.605379 -3.753407 -0.464497
H -2.885849 -3.461451 0.541130
C -2.328338 -5.083723 -0.749623
H -2.376792 -5.825517 0.037481

C -2.011650 -5.463191 -2.049376
H -1.805656 -6.501349 -2.276317
C -1.966412 -4.507575 -3.057306
H -1.717097 -4.798762 -4.069296
C -2.225982 -3.173240 -2.770454
H -2.180725 -2.434995 -3.559470
C -3.196001 -0.196766 -2.555149
C -2.164997 0.335868 -3.331597
H -1.137784 0.232465 -3.008082
C -2.449974 1.016152 -4.507855
H -1.643619 1.439334 -5.092766
C -3.768147 1.168985 -4.923013
H -3.989152 1.708756 -5.835062
C -4.802190 0.644463 -4.156025
H -5.831854 0.774971 -4.462790
C -4.517861 -0.028997 -2.975773
H -5.326221 -0.409283 -2.364983
P -2.505217 2.027806 0.222018
P 2.931971 1.063446 0.965530
C -1.112732 0.842414 0.109490
C 0.142382 1.243963 0.560621
H 0.241767 2.218805 1.013200
C 1.274551 0.434570 0.463973
C -2.343605 3.044247 -1.276298
C -3.501313 3.430624 -1.951812
H -4.466567 3.103906 -1.588409
C -3.411575 4.208211 -3.099166
H -4.314113 4.492750 -3.623754
C -2.169372 4.603016 -3.578800
H -2.100807 5.203490 -4.476947
C -1.011279 4.218088 -2.910000
H -0.041199 4.519873 -3.283798
C -1.095790 3.440759 -1.764152
H -0.189853 3.139926 -1.255839
C -2.064781 3.101597 1.621627
C -2.107337 2.541566 2.902640
H -2.371803 1.498340 3.025569
C -1.828664 3.320333 4.014399
H -1.862801 2.878954 5.002060
C -1.525220 4.670418 3.861104
H -1.317901 5.280637 4.730677
C -1.490191 5.231728 2.592874
H -1.249864 6.279343 2.468459
C -1.754300 4.451123 1.472848
H -1.720408 4.895293 0.488143
C 2.543168 2.781821 1.469011
C 2.605379 3.753407 0.464497

H 2.885849 3.461451 -0.541130
C 2.328338 5.083723 0.749623
H 2.376792 5.825517 -0.037481
C 2.011650 5.463191 2.049376
H 1.805656 6.501349 2.276317
C 1.966412 4.507575 3.057306
H 1.717097 4.798762 4.069296
C 2.225982 3.173240 2.770454
H 2.180725 2.434995 3.559470
C 3.196001 0.196766 2.555149
C 2.164997 -0.335868 3.331597
H 1.137784 -0.232465 3.008082
C 2.449974 -1.016152 4.507855
H 1.643619 -1.439334 5.092766
C 3.768147 -1.168985 4.923013
H 3.989152 -1.708756 5.835062
C 4.802190 -0.644463 4.156025
H 5.831854 -0.774971 4.462790
C 4.517861 0.028997 2.975773
H 5.326221 0.409283 2.364983
Au -4.555873 1.010374 0.449006
Cl -7.324321 1.850351 -1.262891
Cl -10.083203 0.397129 -1.079829
Cl -10.461204 -2.001484 0.888292
Cl -8.075138 -2.950605 2.671204
Cl -5.314648 -1.494546 2.491710
C -6.438445 0.131958 0.639051
C -7.523802 0.518470 -0.143313
C -8.765415 -0.119280 -0.084929
C -8.936785 -1.194251 0.792939
C -7.868229 -1.615165 1.591157
C -6.646075 -0.945891 1.497333

15. Representation of DFT optimized complexes **1-3** in the S_1 state (PBE0 functional)

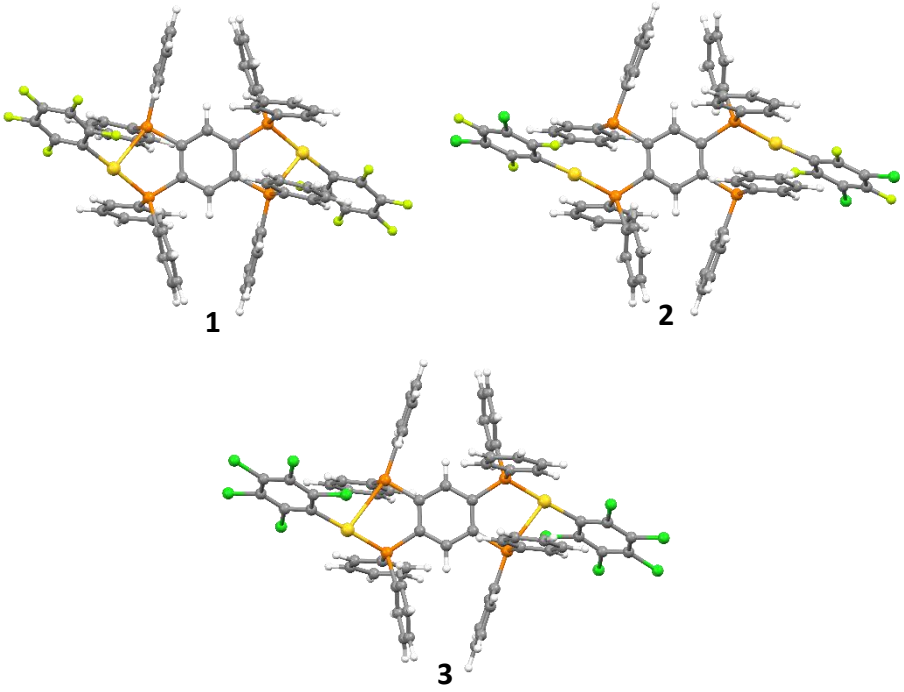

Figure S47. Model Systems of complexes **1**-**3** in the ground state S_0.

16. xyz coordinates for models **1a-3a** in the S_1 state (PBE0 functional)

124
Model_1 S1
Au -1.048646 -1.906952 -3.906608
P -0.308379 0.182619 -3.173314
P 1.976342 1.954016 1.566743
C -1.534387 -3.655485 -4.898831
C -0.128105 0.090113 -1.413615
C 0.709955 0.980362 -0.697259
H 1.288104 1.717867 -1.239886
C 0.843529 0.889068 0.666089
C 3.505712 1.003169 1.717522
C -0.889761 -4.849991 -4.638261
C 1.302629 0.758920 -3.766997
C 2.450546 0.117437 -3.299920
H 2.356491 -0.705807 -2.600184
C -2.577476 -3.718920 -5.804203
C -1.470119 1.524165 -3.555890
C -1.233807 -6.045638 -5.243801
C 3.702024 0.538304 -3.713351
H 4.588015 0.037139 -3.341067
C 1.426858 1.818843 -4.660058

H 0.540861 2.325173 -5.023837
C -1.374164 2.761498 -2.916831
H -0.555224 2.961698 -2.234878
C 2.324212 3.328632 0.452768
C -2.536561 1.277697 -4.415950
H -2.622576 0.310046 -4.899866
C -2.278777 -6.062171 -6.153377
C -2.959593 -4.889256 -6.437055
C 3.653968 -0.252929 1.134795
H 2.857696 -0.658792 0.522588
C 2.683224 2.235570 -5.074142
H 2.771298 3.063998 -5.767369
C 3.320539 3.252432 -0.519739
H 3.949476 2.371877 -0.581635
C -3.395533 3.481750 -4.000509
H -4.148334 4.243275 -4.168212
C -2.332295 3.734055 -3.140871
H -2.252386 4.692456 -2.640730
C 3.821114 1.600041 -4.600968
H 4.801744 1.929863 -4.923957
C 1.518394 4.463465 0.535346
H 0.761136 4.531275 1.309408
C 2.673212 5.414436 -1.345406
H 2.807120 6.227244 -2.049674
C 1.692671 5.501213 -0.365573
H 1.066545 6.383083 -0.297959
C 3.487526 4.293377 -1.419561
H 4.250138 4.222882 -2.186103
C 4.809756 -0.986013 1.353560
H 4.912589 -1.969516 0.910456
C -3.495267 2.254988 -4.637426
H -4.326176 2.050139 -5.301995
C 4.521949 1.513804 2.525947
H 4.396743 2.478398 3.006615
C 5.823139 -0.468978 2.146415
H 6.723606 -1.046649 2.319798
C 5.679997 0.783516 2.729260
H 6.465970 1.185953 3.357311
P 0.308379 -0.182619 3.173314
P -1.976342 -1.954016 -1.566743
C 0.128105 -0.090113 1.413615
C -0.709955 -0.980362 0.697259
H -1.288104 -1.717867 1.239886
C -0.843529 -0.889068 -0.666089
C -3.505712 -1.003169 -1.717522
C -1.302629 -0.758920 3.766997
C -2.450546 -0.117437 3.299920

H -2.356491 0.705807 2.600184
C 1.470119 -1.524165 3.555890
C -3.702024 -0.538304 3.713351
H -4.588015 -0.037139 3.341067
C -1.426858 -1.818843 4.660058
H -0.540861 -2.325173 5.023837
C 1.374164 -2.761498 2.916831
H 0.555224 -2.961698 2.234878
C -2.324212 -3.328632 -0.452768
C 2.536561 -1.277697 4.415950
H 2.622576 -0.310046 4.899866
C -3.653968 0.252929 -1.134795
H -2.857696 0.658792 -0.522588
C -2.683224 -2.235570 5.074142
H -2.771298 -3.063998 5.767369
C -3.320539 -3.252432 0.519739
H -3.949476 -2.371877 0.581635
C 3.395533 -3.481750 4.000509
H 4.148334 -4.243275 4.168212
C 2.332295 -3.734055 3.140871
H 2.252386 -4.692456 2.640730
C -3.821114 -1.600041 4.600968
H -4.801744 -1.929863 4.923957
C -1.518394 -4.463465 -0.535346
H -0.761136 -4.531275 -1.309408
C -2.673212 -5.414436 1.345406
H -2.807120 -6.227244 2.049674
C -1.692671 -5.501213 0.365573
H -1.066545 -6.383083 0.297959
C -3.487526 -4.293377 1.419561
H -4.250138 -4.222882 2.186103
C -4.809756 0.986013 -1.353560
H -4.912589 1.969516 -0.910456
C 3.495267 -2.254988 4.637426
H 4.326176 -2.050139 5.301995
C -4.521949 -1.513804 -2.525947
H -4.396743 -2.478398 -3.006615
C -5.823139 0.468978 -2.146415
H -6.723606 1.046649 -2.319798
C -5.679997 -0.783516 -2.729260
H -6.465970 -1.185953 -3.357311
Au 1.048646 1.906952 3.906608
C 1.534387 3.655485 4.898831
C 0.889761 4.849991 4.638261
C 2.577476 3.718920 5.804203
C 1.233807 6.045638 5.243801
C 2.278777 6.062171 6.153377

C 2.959593 4.889256 6.437055
F -0.120833 4.888108 3.752370
F 0.585290 7.173937 4.967074
F 2.628910 7.196540 6.746122
F 3.965843 4.908993 7.307006
F 3.277023 2.612373 6.102433
F 0.120833 -4.888108 -3.752370
F -0.585290 -7.173937 -4.967074
F -2.628910 -7.196540 -6.746122
F -3.965843 -4.908993 -7.307006
F -3.277023 -2.612373 -6.102433

124
Model_2 S1
Au -1.015250 -1.907185 -3.915129
P -0.283451 0.181980 -3.176175
P 1.962203 1.957685 1.579839
C -1.510873 -3.664357 -4.888095
C -0.119066 0.090638 -1.414623
C 0.713438 0.981130 -0.692358
H 1.294503 1.719424 -1.230896
C 0.838575 0.889751 0.671837
C 3.490512 1.008732 1.750725
C -0.882455 -4.862707 -4.608413
C 1.331707 0.761690 -3.755205
C 2.476136 0.117734 -3.282968
H 2.376894 -0.709640 -2.588811
C -2.556766 -3.738777 -5.788904
C -1.445027 1.520394 -3.570517
C -1.236957 -6.076402 -5.181692
C 3.730654 0.541415 -3.684061
H 4.613917 0.038266 -3.307983
C 1.462544 1.827123 -4.640638
H 0.579322 2.335532 -5.008204
C -1.363660 2.755517 -2.925333
H -0.556522 2.955662 -2.229440
C 2.323503 3.331460 0.469124
C -2.496921 1.273447 -4.448151
H -2.572131 0.307144 -4.936527
C -2.288592 -6.085120 -6.086994
C -2.965451 -4.915653 -6.403115
C 3.646055 -0.249899 1.175492
H 2.857146 -0.658970 0.555913
C 2.722023 2.246785 -5.042256
H 2.815219 3.079688 -5.729412
C 3.328688 3.252750 -0.494154
H 3.952929 2.368669 -0.553394

C -3.369987 3.472987 -4.038414
H -4.122738 4.232521 -4.215137
C -2.321464 3.725673 -3.161021
H -2.253016 4.682405 -2.656027
C 3.856338 1.608627 -4.564223
H 4.839365 1.940686 -4.877481
C 1.524430 4.471271 0.548567
H 0.760020 4.541007 1.315215
C 2.704688 5.423244 -1.315646
H 2.851906 6.238791 -2.014089
C 1.715077 5.512268 -0.345265
H 1.095146 6.398554 -0.278546
C 3.511446 4.296519 -1.387525
H 4.281076 4.224295 -2.146861
C 4.799589 -0.981368 1.411050
H 4.907953 -1.966883 0.973789
C -3.455409 2.248248 -4.681247
H -4.275103 2.042953 -5.359472
C 4.497331 1.523825 2.568147
H 4.366540 2.490802 3.042492
C 5.803419 -0.460183 2.213262
H 6.701980 -1.036696 2.399887
C 5.653183 0.795088 2.788351
H 6.431612 1.201012 3.423506
P 0.283451 -0.181980 3.176175
P -1.962203 -1.957685 -1.579839
C 0.119066 -0.090638 1.414623
C -0.713438 -0.981130 0.692358
H -1.294503 -1.719424 1.230896
C -0.838575 -0.889751 -0.671837
C -3.490512 -1.008732 -1.750725
C -1.331707 -0.761690 3.755205
C -2.476136 -0.117734 3.282968
H -2.376894 0.709640 2.588811
C 1.445027 -1.520394 3.570517
C -3.730654 -0.541415 3.684061
H -4.613917 -0.038266 3.307983
C -1.462544 -1.827123 4.640638
H -0.579322 -2.335532 5.008204
C 1.363660 -2.755517 2.925333
H 0.556522 -2.955662 2.229440
C -2.323503 -3.331460 -0.469124
C 2.496921 -1.273447 4.448151
H 2.572131 -0.307144 4.936527
C -3.646055 0.249899 -1.175492
H -2.857146 0.658970 -0.555913
C -2.722023 -2.246785 5.042256

H -2.815219 -3.079688 5.729412
C -3.328688 -3.252750 0.494154
H -3.952929 -2.368669 0.553394
C 3.369987 -3.472987 4.038414
H 4.122738 -4.232521 4.215137
C 2.321464 -3.725673 3.161021
H 2.253016 -4.682405 2.656027
C -3.856338 -1.608627 4.564223
H -4.839365 -1.940686 4.877481
C -1.524430 -4.471271 -0.548567
H -0.760020 -4.541007 -1.315215
C -2.704688 -5.423244 1.315646
H -2.851906 -6.238791 2.014089
C -1.715077 -5.512268 0.345265
H -1.095146 -6.398554 0.278546
C -3.511446 -4.296519 1.387525
H -4.281076 -4.224295 2.146861
C -4.799589 0.981368 -1.411050
H -4.907953 1.966883 -0.973789
C 3.455409 -2.248248 4.681247
H 4.275103 -2.042953 5.359472
C -4.497331 -1.523825 -2.568147
H -4.366540 -2.490802 -3.042492
C -5.803419 0.460183 -2.213262
H -6.701980 1.036696 -2.399887
C -5.653183 -0.795088 -2.788351
H -6.431612 -1.201012 -3.423506
Au 1.015250 1.907185 3.915129
C 1.510873 3.664357 4.888095
C 0.882455 4.862707 4.608413
C 2.556766 3.738777 5.788904
C 1.236957 6.076402 5.181692
C 2.288592 6.085120 6.086994
C 2.965451 4.915653 6.403115
F -3.231961 -2.623339 -6.093231
F -2.654471 -7.225033 -6.651986
F 0.126425 -4.874664 -3.725386
F 3.231961 2.623339 6.093231
F -0.126425 4.874664 3.725386
F 2.654471 7.225033 6.651986
Cl 0.419432 7.530478 4.790924
Cl 4.267404 4.945605 7.516280
Cl -4.267404 -4.945605 -7.516280
Cl -0.419432 -7.530478 -4.790924

124
Model_3 S1
Au 4.371567 -0.701614 -0.290961
Cl 7.083199 -1.089493 1.595187
Cl 9.813341 0.332350 1.173672
Cl 10.190607 2.291883 -1.207017
Cl 7.842423 2.815381 -3.172763
Cl 5.121594 1.372412 -2.758465
P 2.449948 -2.028822 -0.279689
P -2.896272 -0.759818 -1.100472
C 6.218500 0.181084 -0.611517
C 7.290882 -0.016455 0.252168
C 8.520814 0.616394 0.087237
C 8.693575 1.497161 -0.982277
C 7.637283 1.729321 -1.864768
C 6.427369 1.069824 -1.660834
C 1.078864 -0.917549 -0.125649
C -0.223479 -1.259048 -0.564142
H -0.391234 -2.221183 -1.032474
C -1.265116 -0.372430 -0.452971
C 2.381802 -3.211534 1.094841
C 3.521162 -3.423675 1.865826
H 4.450188 -2.933244 1.593574
C 3.463617 -4.238084 2.986887
H 4.353350 -4.390034 3.586446
C 2.269136 -4.843093 3.344295
H 2.222393 -5.474352 4.224150
C 1.127772 -4.634977 2.577930
H 0.192012 -5.105964 2.856487
C 1.180727 -3.821900 1.459793
H 0.282912 -3.651633 0.875760
C 2.088132 -2.990776 -1.769775
C 1.757692 -2.299665 -2.936559
H 1.733060 -1.215417 -2.927707
C 1.448965 -2.992121 -4.093471
H 1.188584 -2.446733 -4.993158
C 1.472662 -4.381229 -4.100641
H 1.230482 -4.923284 -5.007427
C 1.809196 -5.072037 -2.946735
H 1.829961 -6.155659 -2.947917
C 2.115955 -4.381853 -1.783187
H 2.368034 -4.925975 -0.880973
C -2.928934 -2.554170 -1.268566
C -3.387261 -3.309897 -0.190367
H -3.778737 -2.810794 0.689894
C -3.341643 -4.692990 -0.246891
H -3.701716 -5.277133 0.591855

C -2.845013 -5.326984 -1.378583
H -2.810528 -6.409429 -1.420873
C -2.399918 -4.577661 -2.458230
H -2.006237 -5.070607 -3.339220
C -2.445635 -3.193158 -2.409839
H -2.090528 -2.606401 -3.249047
C -2.916020 -0.080222 -2.773762
C -1.820944 0.597987 -3.303886
H -0.905338 0.673604 -2.730248
C -1.910241 1.186601 -4.555555
H -1.059953 1.726407 -4.955280
C -3.084733 1.094537 -5.286823
H -3.152703 1.558705 -6.263856
C -4.177758 0.415446 -4.763859
H -5.099443 0.347022 -5.329668
C -4.099582 -0.161073 -3.508172
H -4.964076 -0.663150 -3.087943
P -2.449948 2.028822 0.279689
P 2.896272 0.759818 1.100472
C -1.078864 0.917549 0.125649
C 0.223479 1.259048 0.564142
H 0.391234 2.221183 1.032474
C 1.265116 0.372430 0.452971
C -2.381802 3.211534 -1.094841
C -3.521162 3.423675 -1.865826
H -4.450188 2.933244 -1.593574
C -3.463617 4.238084 -2.986887
H -4.353350 4.390034 -3.586446
C -2.269136 4.843093 -3.344295
H -2.222393 5.474352 -4.224150
C -1.127772 4.634977 -2.577930
H -0.192012 5.105964 -2.856487
C -1.180727 3.821900 -1.459793
H -0.282912 3.651633 -0.875760
C -2.088132 2.990776 1.769775
C -1.757692 2.299665 2.936559
H -1.733060 1.215417 2.927707
C -1.448965 2.992121 4.093471
H -1.188584 2.446733 4.993158
C -1.472662 4.381229 4.100641
H -1.230482 4.923284 5.007427
C -1.809196 5.072037 2.946735
H -1.829961 6.155659 2.947917
C -2.115955 4.381853 1.783187
H -2.368034 4.925975 0.880973
C 2.928934 2.554170 1.268566
C 3.387261 3.309897 0.190367

H 3.778737 2.810794 -0.689894
C 3.341643 4.692990 0.246891
H 3.701716 5.277133 -0.591855
C 2.845013 5.326984 1.378583
H 2.810528 6.409429 1.420873
C 2.399918 4.577661 2.458230
H 2.006237 5.070607 3.339220
C 2.445635 3.193158 2.409839
H 2.090528 2.606401 3.249047
C 2.916020 0.080222 2.773762
C 1.820944 -0.597987 3.303886
H 0.905338 -0.673604 2.730248
C 1.910241 -1.186601 4.555555
H 1.059953 -1.726407 4.955280
C 3.084733 -1.094537 5.286823
H 3.152703 -1.558705 6.263856
C 4.177758 -0.415446 4.763859
H 5.099443 -0.347022 5.329668
C 4.099582 0.161073 3.508172
H 4.964076 0.663150 3.087943
Au -4.371567 0.701614 0.290961
Cl -7.083199 1.089493 -1.595187
Cl -9.813341 -0.332350 -1.173672
Cl -10.190607 -2.291883 1.207017
Cl -7.842423 -2.815381 3.172763
Cl -5.121594 -1.372412 2.758465
C -6.218500 -0.181084 0.611517
C -7.290882 0.016455 -0.252168
C -8.520814 -0.616394 -0.087237
C -8.693575 -1.497161 0.982277
C -7.637283 -1.729321 1.864768
C -6.427369 -1.069824 1.660834

17. Representation of DFT optimized complexes **1-3** in the T_1 state (PBE0 functional)

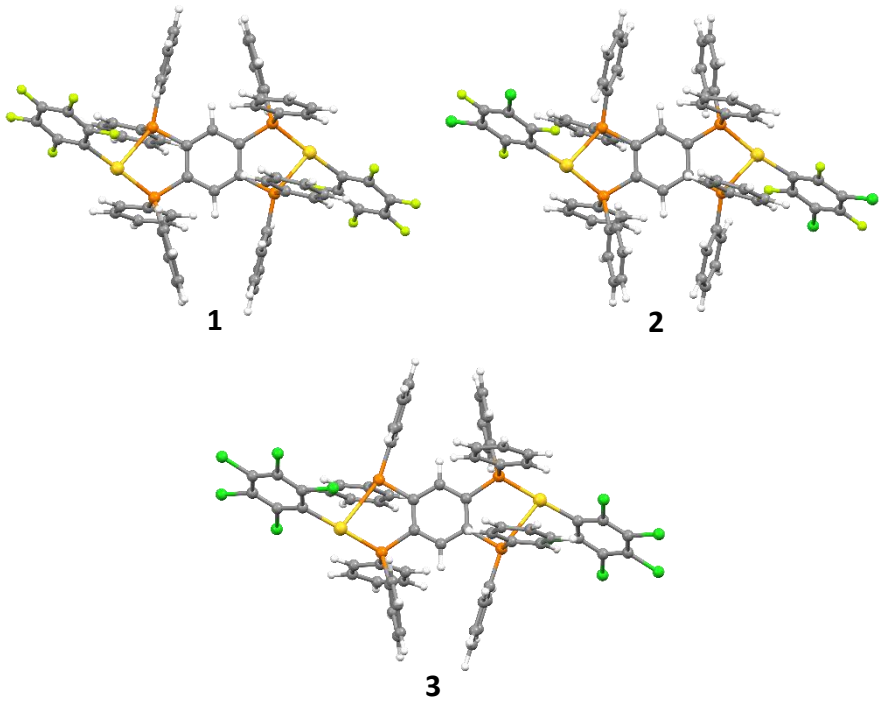

Figure S48. Model Systems of complexes **1**-**3** in the ground state S_0.

18. xyz coordinates for models **1a-3a** in the T_1 state (PBE0 functional)

124
Model_1 T1
Au -1.069808 -1.856937 -3.863328
P -0.351862 0.247798 -3.163951
P 2.099267 1.822914 1.539479
C -1.542930 -3.673182 -4.730390
C -0.149759 0.147089 -1.397699
C 0.782050 0.908243 -0.718313
H 1.401331 1.603789 -1.274768
C 0.972362 0.794387 0.657187
C 3.648655 0.931548 1.816979
C -0.885383 -4.838864 -4.385820
C 1.229420 0.882770 -3.769513
C 2.324313 0.018336 -3.748375
H 2.188404 -1.011620 -3.435500
C -2.588206 -3.813316 -5.624022
C -1.585589 1.538359 -3.491524
C -1.221654 -6.079458 -4.898240
C 3.576528 0.472477 -4.119806

H 4.422665 -0.204198 -4.099180
C 1.401405 2.198651 -4.184933
H 0.555824 2.874836 -4.209678
C -1.642825 2.683621 -2.699659
H -0.934555 2.813989 -1.888454
C 2.480597 3.203802 0.450214
C -2.520459 1.354662 -4.505645
H -2.491664 0.450700 -5.105131
C -2.270880 -6.173659 -5.797987
C -2.962819 -5.031120 -6.165511
C 3.888699 -0.304111 1.223201
H 3.158008 -0.715789 0.536520
C 2.659724 2.648957 -4.560739
H 2.787551 3.677838 -4.875850
C 3.602510 3.208532 -0.376549
H 4.304091 2.383489 -0.338275
C -3.544443 3.454532 -3.948290
H -4.313298 4.198658 -4.121589
C -2.614732 3.641642 -2.933712
H -2.654082 4.531524 -2.316070
C 3.746453 1.791326 -4.525167
H 4.728061 2.145638 -4.817806
C 1.581355 4.270085 0.403653
H 0.723080 4.278168 1.067081
C 2.903757 5.309567 -1.312416
H 3.068166 6.130421 -2.000820
C 1.792412 5.315935 -0.478265
H 1.094323 6.144324 -0.507536
C 3.807366 4.259012 -1.257931
H 4.672923 4.250889 -1.909853
C 5.046873 -1.003863 1.523967
H 5.223823 -1.971223 1.068786
C -3.498726 2.310836 -4.730738
H -4.232759 2.154830 -5.512227
C 4.572974 1.456670 2.720494
H 4.372421 2.404183 3.209432
C 5.970164 -0.472118 2.411608
H 6.872676 -1.023356 2.649046
C 5.734211 0.760592 3.007012
H 6.449319 1.172840 3.709161
P 0.351862 -0.247798 3.163951
P -2.099267 -1.822914 -1.539479
C 0.149759 -0.147089 1.397699
C -0.782050 -0.908243 0.718313
H -1.401331 -1.603789 1.274768
C -0.972362 -0.794387 -0.657187
C -3.648655 -0.931548 -1.816979

C -1.229420 -0.882770 3.769513
C -2.324313 -0.018336 3.748375
H -2.188404 1.011620 3.435500
C 1.585589 -1.538359 3.491524
C -3.576528 -0.472477 4.119806
H -4.422665 0.204198 4.099180
C -1.401405 -2.198651 4.184933
H -0.555824 -2.874836 4.209678
C 1.642825 -2.683621 2.699659
H 0.934555 -2.813989 1.888454
C -2.480597 -3.203802 -0.450214
C 2.520459 -1.354662 4.505645
H 2.491664 -0.450700 5.105131
C -3.888699 0.304111 -1.223201
H -3.158008 0.715789 -0.536520
C -2.659724 -2.648957 4.560739
H -2.787551 -3.677838 4.875850
C -3.602510 -3.208532 0.376549
H -4.304091 -2.383489 0.338275
C 3.544443 -3.454532 3.948290
H 4.313298 -4.198658 4.121589
C 2.614732 -3.641642 2.933712
H 2.654082 -4.531524 2.316070
C -3.746453 -1.791326 4.525167
H -4.728061 -2.145638 4.817806
C -1.581355 -4.270085 -0.403653
H -0.723080 -4.278168 -1.067081
C -2.903757 -5.309567 1.312416
H -3.068166 -6.130421 2.000820
C -1.792412 -5.315935 0.478265
H -1.094323 -6.144324 0.507536
C -3.807366 -4.259012 1.257931
H -4.672923 -4.250889 1.909853
C -5.046873 1.003863 -1.523967
H -5.223823 1.971223 -1.068786
C 3.498726 -2.310836 4.730738
H 4.232759 -2.154830 5.512227
C -4.572974 -1.456670 -2.720494
H -4.372421 -2.404183 -3.209432
C -5.970164 0.472118 -2.411608
H -6.872676 1.023356 -2.649046
C -5.734211 -0.760592 -3.007012
H -6.449319 -1.172840 -3.709161
Au 1.069808 1.856937 3.863328
C 1.542930 3.673182 4.730390
C 0.885383 4.838864 4.385820
C 2.588206 3.813316 5.624022

C 1.221654 6.079458 4.898240
C 2.270880 6.173659 5.797987
C 2.962819 5.031120 6.165511
F -0.132586 4.801490 3.508002
F 0.560782 7.177982 4.541811
F 2.613653 7.352602 6.301956
F 3.972936 5.123971 7.026340
F 3.299274 2.738020 6.000734
F 0.132586 -4.801490 -3.508002
F -0.560782 -7.177982 -4.541811
F -2.613653 -7.352602 -6.301956
F -3.972936 -5.123971 -7.026340
F -3.299274 -2.738020 -6.000734

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Model_2 T1
Au -1.031112 -1.849228 -3.895467
P -0.340587 0.255401 -3.164319
P 2.029419 1.884043 1.559100
C -1.513131 -3.653124 -4.786633
C -0.168236 0.158492 -1.402455
C 0.710015 0.981007 -0.695566
H 1.284539 1.725781 -1.235151
C 0.911096 0.843249 0.663988
C 3.556398 0.953974 1.829738
C -0.879804 -4.832376 -4.444803
C 1.253345 0.886894 -3.748255
C 2.396728 0.143841 -3.450961
H 2.302591 -0.789075 -2.905549
C -2.558058 -3.779138 -5.682313
C -1.552730 1.549752 -3.556201
C -1.231413 -6.076460 -4.950915
C 3.644011 0.599544 -3.836381
H 4.526760 0.017513 -3.598678
C 1.376777 2.082028 -4.448198
H 0.494861 2.664906 -4.683820
C -1.571429 2.743378 -2.836049
H -0.837690 2.917026 -2.056353
C 2.432922 3.253009 0.460701
C -2.516133 1.321171 -4.533371
H -2.515157 0.383001 -5.078657
C -2.283849 -6.137555 -5.853115
C -2.963782 -4.988806 -6.231760
C 3.763845 -0.291400 1.243326
H 3.018680 -0.694021 0.567208
C 2.630587 2.534283 -4.835958
H 2.718631 3.469627 -5.376274

C 3.491965 3.183655 -0.443076
H 4.130249 2.307898 -0.460755
C -3.496085 3.466445 -4.079026
H -4.257975 4.211415 -4.277560
C -2.536091 3.699582 -3.101664
H -2.545114 4.626344 -2.539568
C 3.763387 1.798415 -4.529410
H 4.741356 2.154805 -4.831648
C 1.615092 4.382413 0.487038
H 0.806469 4.444520 1.207341
C 2.888696 5.342497 -1.310044
H 3.065563 6.157125 -2.002685
C 1.843283 5.422152 -0.399028
H 1.209248 6.300551 -0.372139
C 3.712224 4.226200 -1.329580
H 4.525121 4.161395 -2.043037
C 4.908871 -1.014290 1.539640
H 5.058461 -1.990174 1.093036
C -3.486418 2.277906 -4.791877
H -4.241429 2.087036 -5.545221
C 4.501965 1.466674 2.718151
H 4.328347 2.423209 3.199684
C 5.852865 -0.495220 2.412770
H 6.745133 -1.064454 2.646284
C 5.650981 0.748011 2.998386
H 6.382784 1.151439 3.688284
P 0.340587 -0.255401 3.164319
P -2.029419 -1.884043 -1.559100
C 0.168236 -0.158492 1.402455
C -0.710015 -0.981007 0.695566
H -1.284539 -1.725781 1.235151
C -0.911096 -0.843249 -0.663988
C -3.556398 -0.953974 -1.829738
C -1.253345 -0.886894 3.748255
C -2.396728 -0.143841 3.450961
H -2.302591 0.789075 2.905549
C 1.552730 -1.549752 3.556201
C -3.644011 -0.599544 3.836381
H -4.526760 -0.017513 3.598678
C -1.376777 -2.082028 4.448198
H -0.494861 -2.664906 4.683820
C 1.571429 -2.743378 2.836049
H 0.837690 -2.917026 2.056353
C -2.432922 -3.253009 -0.460701
C 2.516133 -1.321171 4.533371
H 2.515157 -0.383001 5.078657
C -3.763845 0.291400 -1.243326

H -3.018680 0.694021 -0.567208
C -2.630587 -2.534283 4.835958
H -2.718631 -3.469627 5.376274
C -3.491965 -3.183655 0.443076
H -4.130249 -2.307898 0.460755
C 3.496085 -3.466445 4.079026
H 4.257975 -4.211415 4.277560
C 2.536091 -3.699582 3.101664
H 2.545114 -4.626344 2.539568
C -3.763387 -1.798415 4.529410
H -4.741356 -2.154805 4.831648
C -1.615092 -4.382413 -0.487038
H -0.806469 -4.444520 -1.207341
C -2.888696 -5.342497 1.310044
H -3.065563 -6.157125 2.002685
C -1.843283 -5.422152 0.399028
H -1.209248 -6.300551 0.372139
C -3.712224 -4.226200 1.329580
H -4.525121 -4.161395 2.043037
C -4.908871 1.014290 -1.539640
H -5.058461 1.990174 -1.093036
C 3.486418 -2.277906 4.791877
H 4.241429 -2.087036 5.545221
C -4.501965 -1.466674 -2.718151
H -4.328347 -2.423209 -3.199684
C -5.852865 0.495220 -2.412770
H -6.745133 1.064454 -2.646284
C -5.650981 -0.748011 -2.998386
H -6.382784 -1.151439 -3.688284
Au 1.031112 1.849228 3.895467
C 1.513131 3.653124 4.786633
C 0.879804 4.832376 4.444803
C 2.558058 3.779138 5.682313
C 1.231413 6.076460 4.950915
C 2.283849 6.137555 5.853115
C 2.963782 4.988806 6.231760
F -3.237443 -2.683786 -6.045690
F -2.647264 -7.307686 -6.354671
F 0.130927 -4.793841 -3.564378
F 3.237443 2.683786 6.045690
F -0.130927 4.793841 3.564378
F 2.647264 7.307686 6.354671
Cl 0.409690 7.504824 4.481526
Cl 4.266987 5.082264 7.339961
Cl -4.266987 -5.082264 -7.339961
Cl -0.409690 -7.504824 -4.481526

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Model_3 T1
Au 4.324836 -0.725547 -0.235908
Cl 7.137144 -1.076811 1.516058
Cl 9.780202 0.486021 1.042484
Cl 9.970413 2.547208 -1.273751
Cl 7.523265 3.029478 -3.125994
Cl 4.890450 1.447348 -2.662287
P 2.419222 -2.071335 -0.190019
P -2.849577 -0.713721 -1.215342
C 6.121317 0.241890 -0.595751
C 7.237942 0.058812 0.212917
C 8.431444 0.751560 0.021787
C 8.520388 1.677537 -1.019283
C 7.419603 1.891672 -1.850242
C 6.249122 1.171662 -1.622012
C 1.046419 -0.955221 -0.063026
C -0.208419 -1.250543 -0.588238
H -0.367447 -2.211087 -1.066343
C -1.249076 -0.339975 -0.556950
C 2.372411 -3.200927 1.229728
C 3.550572 -3.509681 1.902009
H 4.491271 -3.098780 1.550269
C 3.517233 -4.316518 3.029421
H 4.436547 -4.541461 3.556995
C 2.309582 -4.821012 3.486004
H 2.283684 -5.446970 4.370525
C 1.130097 -4.515334 2.818182
H 0.184248 -4.903844 3.177895
C 1.159083 -3.702283 1.698352
H 0.235098 -3.440902 1.193627
C 2.055587 -3.081181 -1.646908
C 1.997929 -2.434478 -2.882486
H 2.208520 -1.371820 -2.941324
C 1.667033 -3.141553 -4.023520
H 1.622803 -2.631660 -4.978739
C 1.398628 -4.503374 -3.945311
H 1.140599 -5.057070 -4.840641
C 1.467414 -5.151818 -2.723447
H 1.259843 -6.213502 -2.657881
C 1.795797 -4.445193 -1.574363
H 1.841886 -4.955550 -0.620234
C -2.895299 -2.501352 -1.427227
C -3.256894 -3.286876 -0.332906
H -3.567354 -2.811445 0.591373
C -3.219602 -4.667554 -0.429548
H -3.505801 -5.273740 0.421966

C -2.827746 -5.271616 -1.617651
H -2.799191 -6.352561 -1.691401
C -2.479282 -4.493326 -2.711579
H -2.168263 -4.962916 -3.637264
C -2.516479 -3.110304 -2.622466
H -2.237113 -2.501098 -3.474032
C -2.960145 0.008298 -2.869125
C -1.871263 0.649887 -3.452803
H -0.922250 0.673575 -2.930273
C -2.009386 1.263633 -4.687998
H -1.162681 1.774488 -5.131059
C -3.227806 1.230807 -5.349112
H -3.333982 1.713759 -6.313601
C -4.315351 0.587237 -4.772266
H -5.270459 0.565191 -5.283888
C -4.187186 -0.012618 -3.531835
H -5.044813 -0.486639 -3.067469
P -2.419222 2.071335 0.190019
P 2.849577 0.713721 1.215342
C -1.046419 0.955221 0.063026
C 0.208419 1.250543 0.588238
H 0.367447 2.211087 1.066343
C 1.249076 0.339975 0.556950
C -2.372411 3.200927 -1.229728
C -3.550572 3.509681 -1.902009
H -4.491271 3.098780 -1.550269
C -3.517233 4.316518 -3.029421
H -4.436547 4.541461 -3.556995
C -2.309582 4.821012 -3.486004
H -2.283684 5.446970 -4.370525
C -1.130097 4.515334 -2.818182
H -0.184248 4.903844 -3.177895
C -1.159083 3.702283 -1.698352
H -0.235098 3.440902 -1.193627
C -2.055587 3.081181 1.646908
C -1.997929 2.434478 2.882486
H -2.208520 1.371820 2.941324
C -1.667033 3.141553 4.023520
H -1.622803 2.631660 4.978739
C -1.398628 4.503374 3.945311
H -1.140599 5.057070 4.840641
C -1.467414 5.151818 2.723447
H -1.259843 6.213502 2.657881
C -1.795797 4.445193 1.574363
H -1.841886 4.955550 0.620234
C 2.895299 2.501352 1.427227
C 3.256894 3.286876 0.332906

H 3.567354 2.811445 -0.591373
C 3.219602 4.667554 0.429548
H 3.505801 5.273740 -0.421966
C 2.827746 5.271616 1.617651
H 2.799191 6.352561 1.691401
C 2.479282 4.493326 2.711579
H 2.168263 4.962916 3.637264
C 2.516479 3.110304 2.622466
H 2.237113 2.501098 3.474032
C 2.960145 -0.008298 2.869125
C 1.871263 -0.649887 3.452803
H 0.922250 -0.673575 2.930273
C 2.009386 -1.263633 4.687998
H 1.162681 -1.774488 5.131059
C 3.227806 -1.230807 5.349112
H 3.333982 -1.713759 6.313601
C 4.315351 -0.587237 4.772266
H 5.270459 -0.565191 5.283888
C 4.187186 0.012618 3.531835
H 5.044813 0.486639 3.067469
Au -4.324836 0.725547 0.235908
Cl -7.137144 1.076811 -1.516058
Cl -9.780202 -0.486021 -1.042484
Cl -9.970413 -2.547208 1.273751
Cl -7.523265 -3.029478 3.125994
Cl -4.890450 -1.447348 2.662287
C -6.121317 -0.241890 0.595751
C -7.237942 -0.058812 -0.212917
C -8.431444 -0.751560 -0.021787
C -8.520388 -1.677537 1.019283
C -7.419603 -1.891672 1.850242
C -6.249122 -1.171662 1.622012