Supporting Information for

Near-Unity Thermally Activated Delayed Fluorescence Efficiency in Three- and Four-Coordinate Gold(I) Complexes with Diphosphine Ligands

Masahisa Osawa,*[a] Masa-aki Aino,[a] Takaki Nagakura,[a] Mikio Hoshino,[a] Yuya Tanaka[b] and Munetaka Akita[b]

[a] Department of Applied Chemistry, Nippon Institute of Technology, Gakuendai 4-1, Miyashiro-Machi, Saitama, 345-8501, Japan

[b] Laboratory for Chemistry and Life Science Institute of Innovative Research, Tokyo Institute of Technology R1-27, 4259 Nagatsuta, Midori-ku, Yokohama 226-8503, Japan

Contents

1. General Information

^{1}H, ^{13}C, and ^{31}P NMR spectra were recorded on a JEOL ECA400. ^{1}H chemical shifts were referenced to residual solvent peaks. ^{31}P chemical shifts were referenced to an external standard, 85% phosphoric acid ($\delta = 0$ ppm). Elemental analyses (C and H) were carried out using an elemental analyser (Vario EL CHNOS) from Elementar. For the photo-physical studies, dissolved oxygen was removed by repeated freeze-pump-thaw cycles. Steady-state emission spectra were recorded at room temperature and at 77 K using a Hitachi F-7000 spectrofluorometer. The intensity distribution of the Xenon lamp incorporated in the spectrofluorometer was corrected using Rhodamine B in ethylene glycol. The output of the photomultiplier tube was calibrated between 300 and 850 nm with a secondary standard lamp.

Laser photolysis studies were performed using a Nd:YAG laser (Sure Light 400, Hoya Continuum Ltd.) equipped with second, third, and fourth harmonic generators. The laser pulses used for the emission lifetime measurements were of the third harmonic (355 nm). The duration and energy of the laser pulse were 10 ns and 30 mJ/pulse, respectively. The system used to monitor the emission decay was reported elsewhere.[1]

An Optistat DN-V2 cryostat from Oxford Instruments was used to measure the emission spectra and lifetimes in the temperature range 309–83 K. Crystalline powders of samples used for emission measurements were sealed in quartz tubes with a diameter of 3 mm. Solution sample was filled into the quartz cell (optical path is 10 mm) for measurement. Optical measurements at 77 K were carried out at the temperature of liquid nitrogen using a Dewar vessel with four optical windows. After filling the vessel with liquid nitrogen, the sample, which was placed in a quartz tube with a diameter of 5 mm, was immersed into the liquid nitrogen for rapid cooling, and luminescence spectra and lifetimes were measured.

Emission quantum yields were determined at room temperature and at 77 K using an absolute PL quantum yield measurement system (C-9920-02G, Hamamatsu).[2]

A suitable crystal for **1d**, **1, 3, 4** was selected and mounted using Paratone-N oil on a Cryo-Loop. Data collections were performed at 90(2) K on a Bruker APEX-II CCD. The crystallographic data are summarized in Table S1 and S2. Lorentz and polarization corrections and empirical absorption corrections were carried out for data reduction. The structures were solved by direct methods (Shelxs)[3] or charge flipping methods (olex2.solve)[4] and were refined with all non-hydrogen atoms refined anisotropically. Hydrogen atoms were inserted at idealized positions and treated as fixed-atoms. CCDC reference numbers are 1830024 for **1d**, 1830025 for **1**, 1830026 for **3**, and 1830027 for **4**, respectively.

The structure in the singlet ground (S_0) was optimized by using density functional theory (DFT) and the singlet excited (S_1) structure was optimized using time-dependent (TD)–DFT.[5] The lowest triplet excited (T_1) states was optimized by both methods (DFT and TD-DFT). The input coordinates were

extracted from the X-ray crystallographic data. The PBE0 level of theory[5] were used for all calculations. The def2–SVP basis set[6] for Au and I atoms, 6-31+G* basis set for P atoms, and 6–31G* basis set for C and H atoms, were used. Solvent (THF) effects were applied by the integral equation formalism[7] for the polarizable continuum model (PCM)[8] equipped in Gaussian16 A. 03.[9] Natural transition orbitals (NTOs) were generated by orbital transformation followed by a singular value decomposition of the transition density matrix. In the NTO representation, the electronic transitions can be expressed by one single "hole (approximately HOMO) - electron (approximately LUMO)" pair with an associated eigenvalue of essentially one, even for transitions that are highly mixed in the canonical MO basis. This procedure can be a helpful strategy for obtaining a simple orbital interpretation of "what got excited to where".[10]

2. NMR Experiments

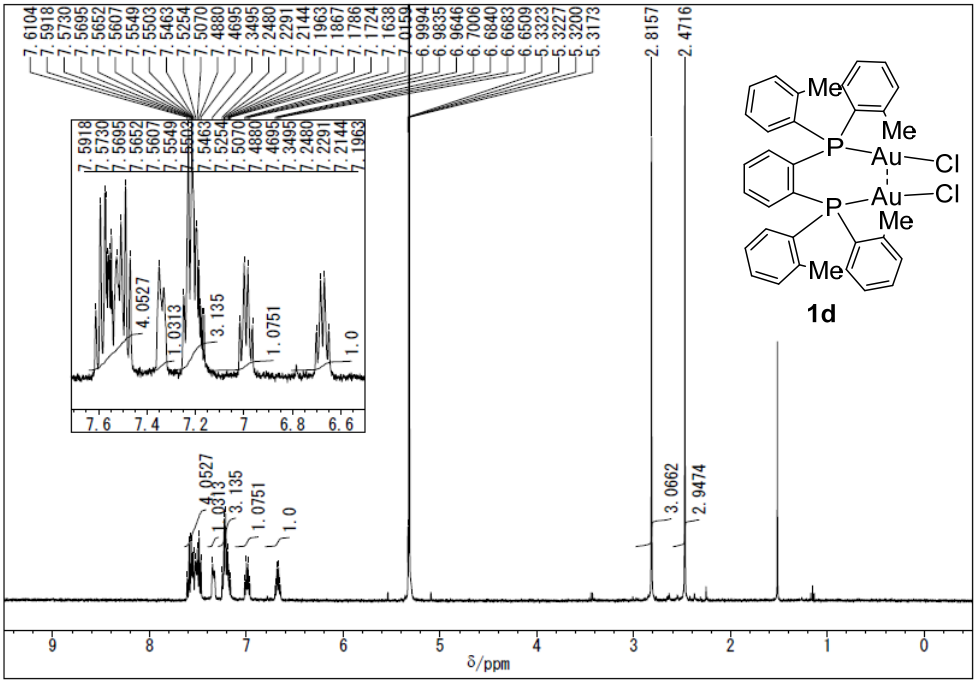


Fig. S1 ^{1}H NMR spectrum of **1d** in CD_2Cl_2 at 293 K.

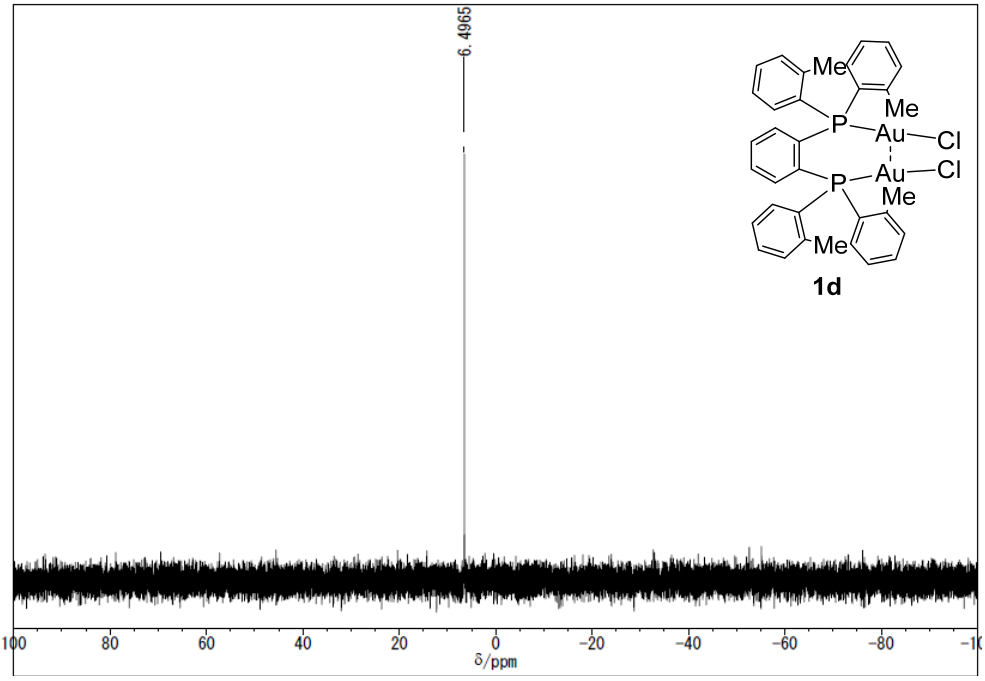


Fig. S2 ^{31}P $\{^{1}$H$\}$ NMR spectrum of **1d** in CD_2Cl_2 at 293 K.

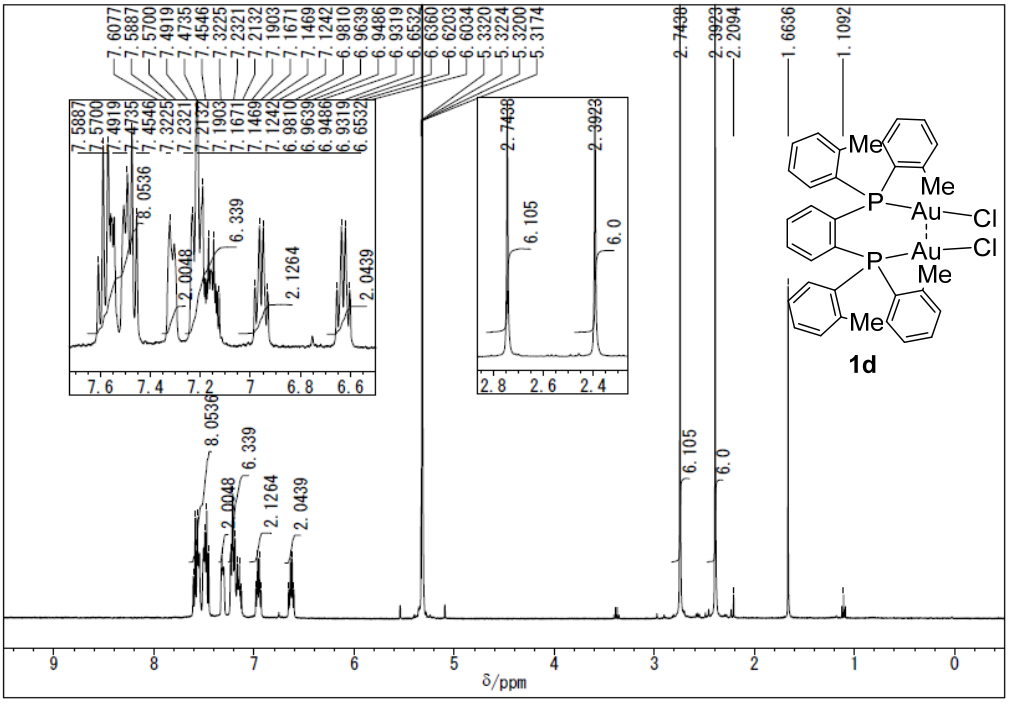


Fig. S3 ^{1}H NMR spectrum of **1d** in CD_2Cl_2 at 223 K.

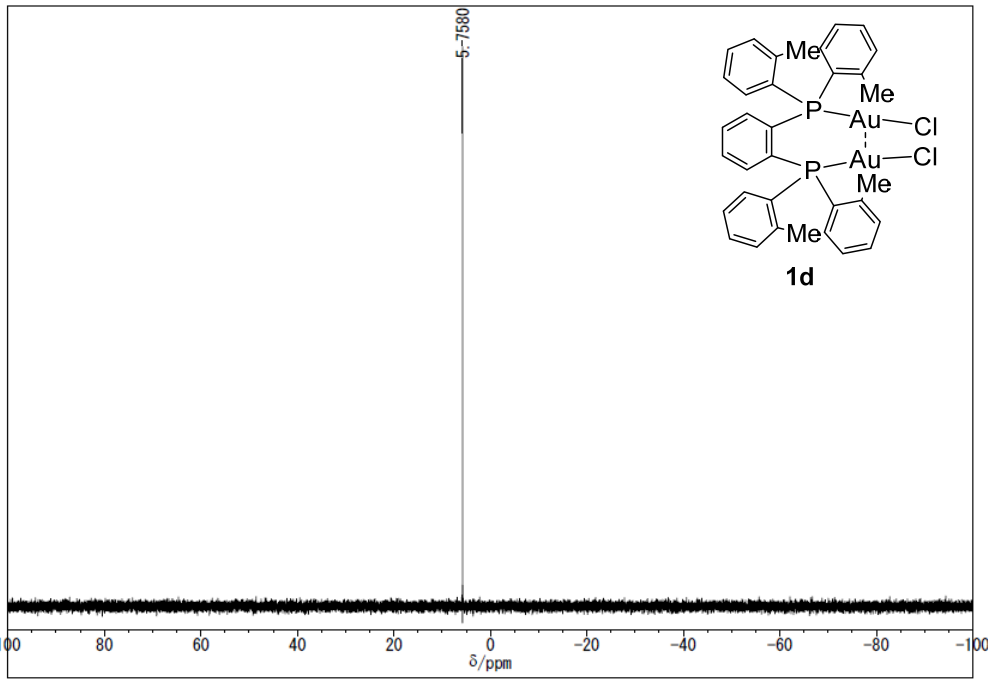


Fig. S4 ^{31}P {^{1}H} NMR spectrum of **1d** in CD_2Cl_2 at 223 K.

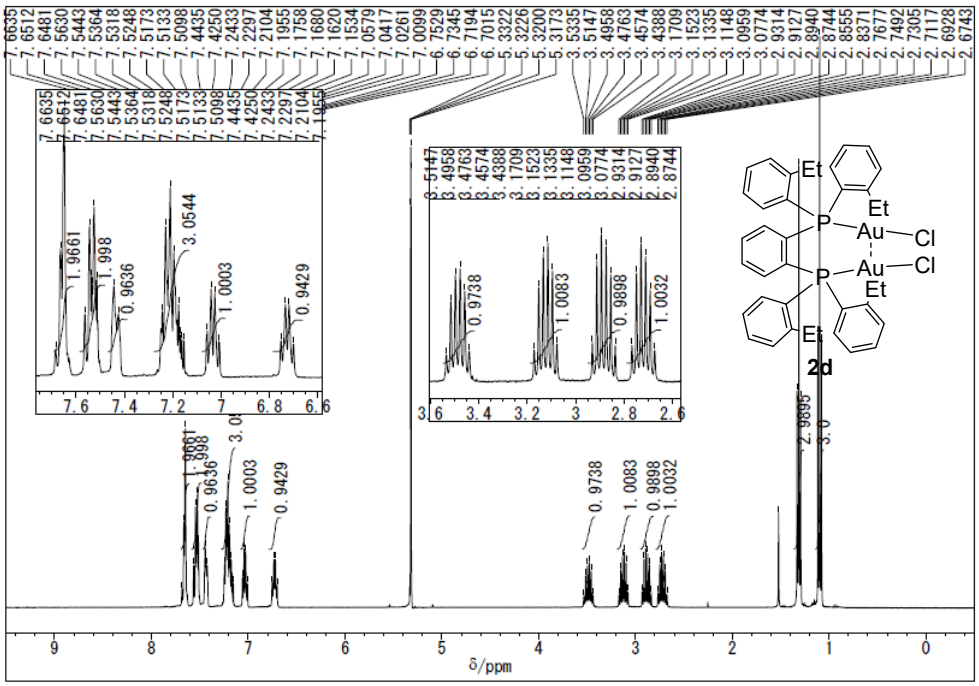


Fig. S5 ^{1}H NMR spectrum of **2d** in CD_2Cl_2 at 293 K.

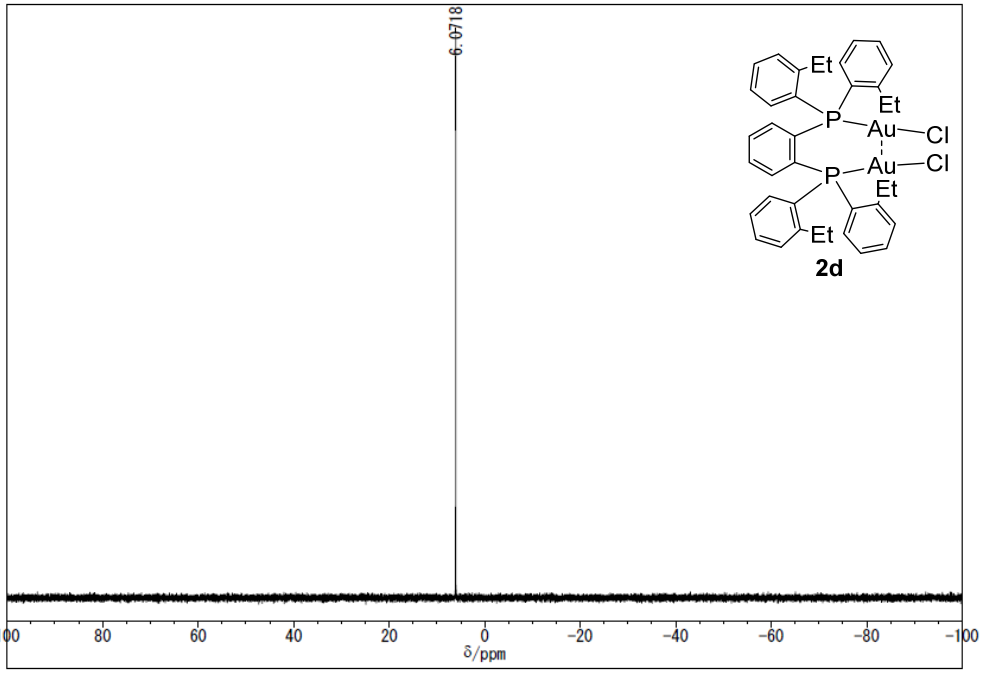


Fig. S6 ^{31}P {^{1}H} NMR spectrum of **2d** in CD_2Cl_2 at 293 K.

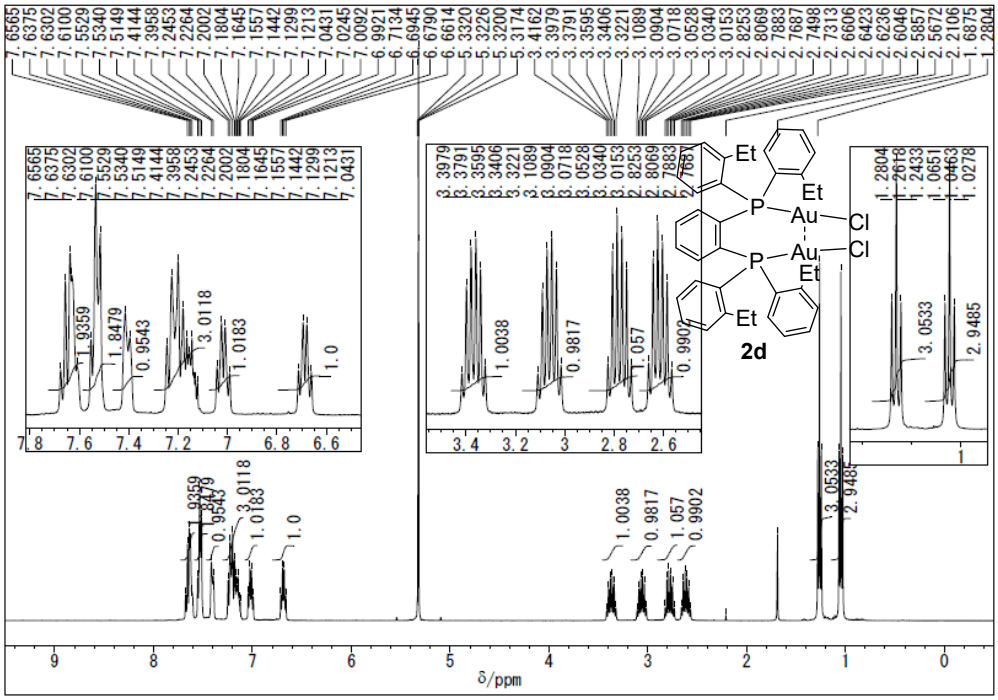


Fig. S7 ^{1}H NMR spectrum of **2d** in CD_2Cl_2 at 223 K.

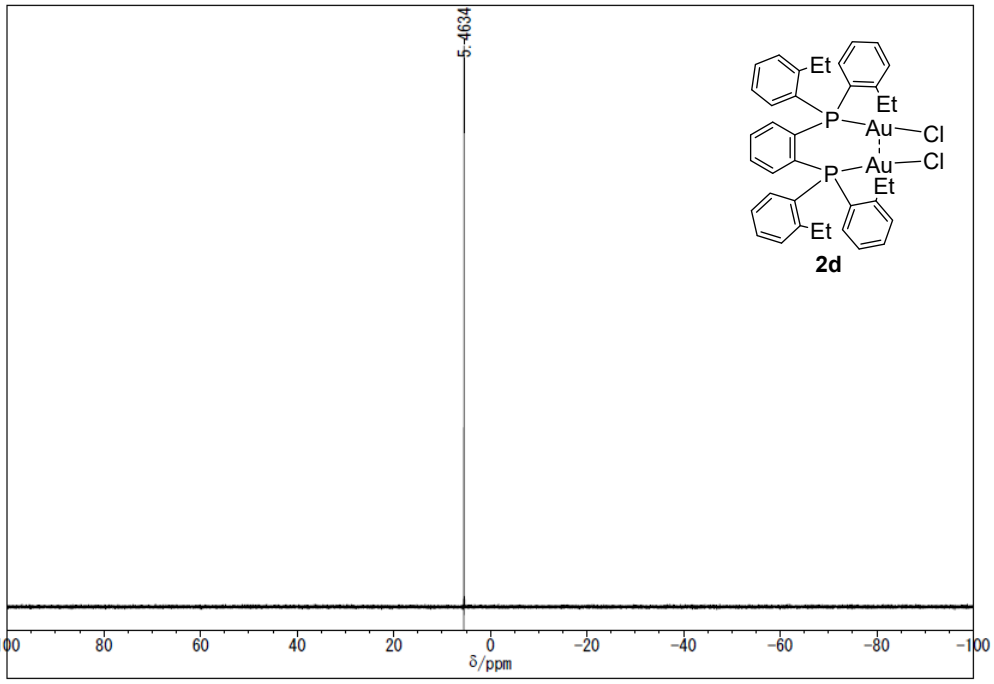


Fig. S8 ^{31}P {^{1}H} NMR spectrum of **2d** in CD_2Cl_2 at 223 K.

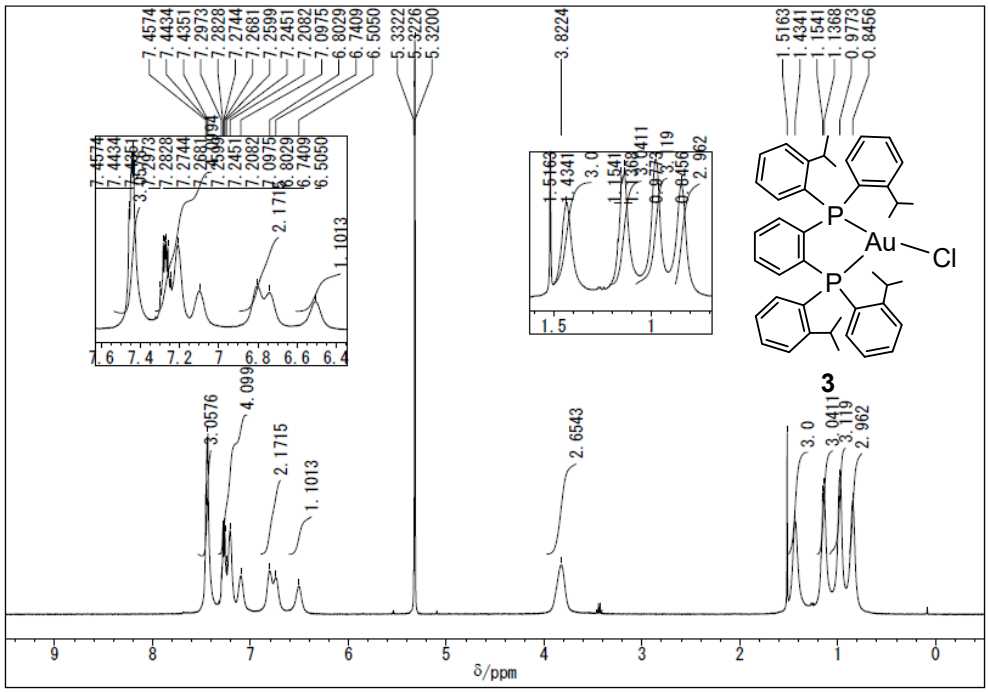


Fig. S9 ^{1}H NMR spectrum of **3** in CD_2Cl_2 at 293 K.

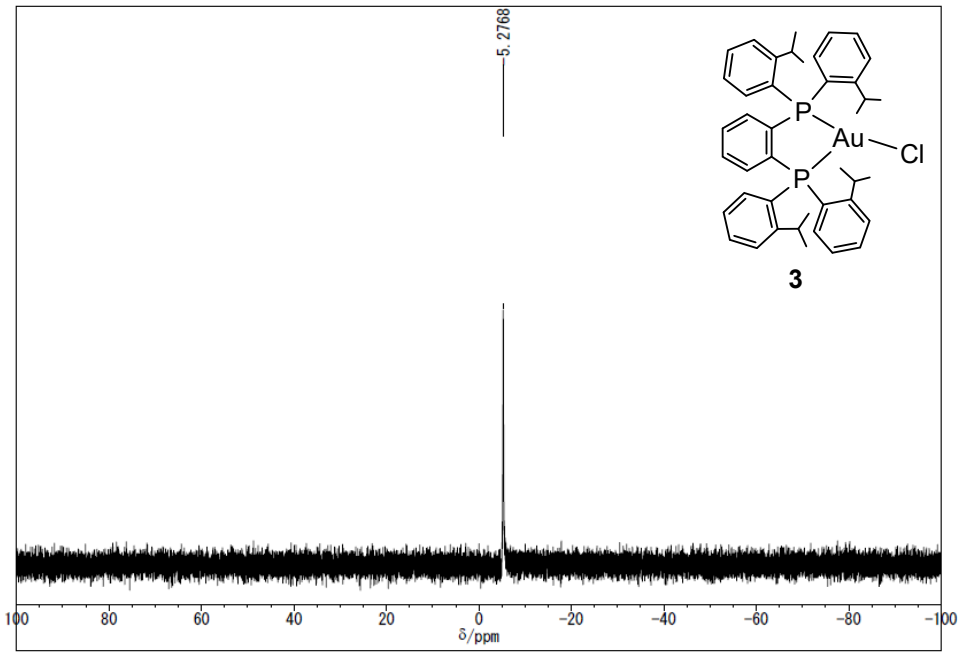


Fig. S10 ^{31}P $\{^{1}$H$\}$ NMR spectrum of **3** in CD_2Cl_2 at 293 K.

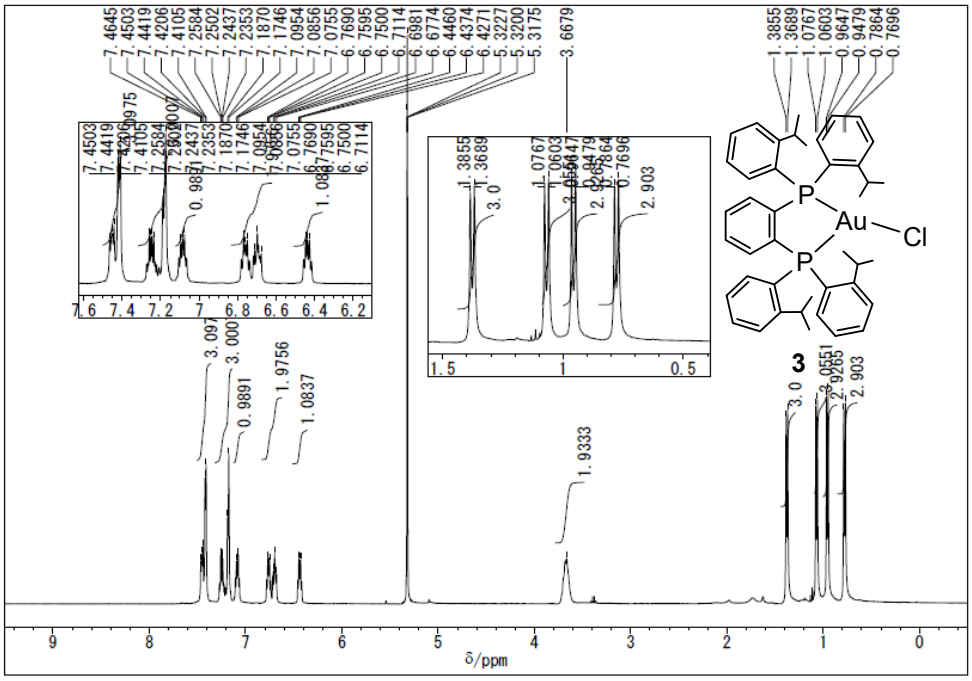


Fig. S11 ^{1}H NMR spectrum of **3** in CD_2Cl_2 at 223 K.

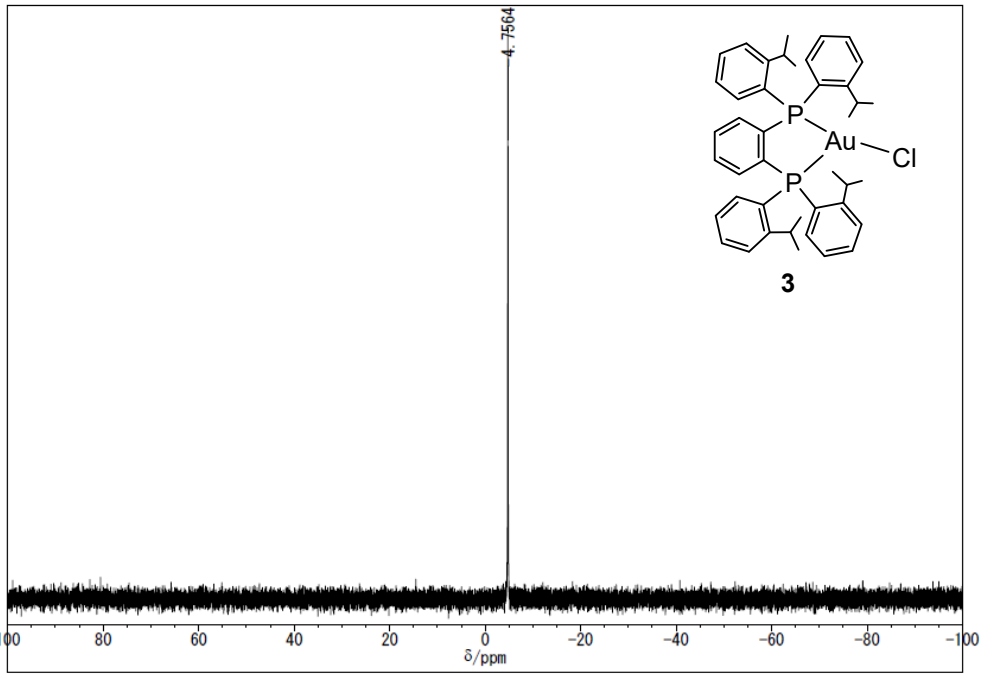


Fig. S12 ^{31}P $\{^{1}H\}$ NMR spectrum of **3** in CD_2Cl_2 at 223 K.

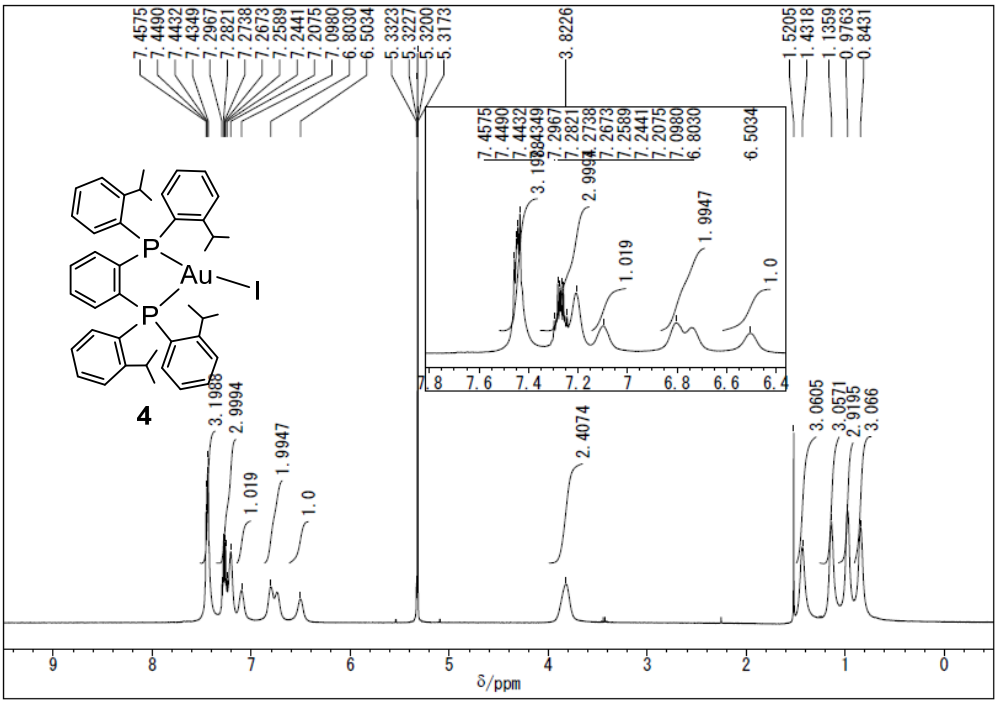


Fig. S13 ^{1}H NMR spectrum of **4** in CD_2Cl_2 at 293 K.

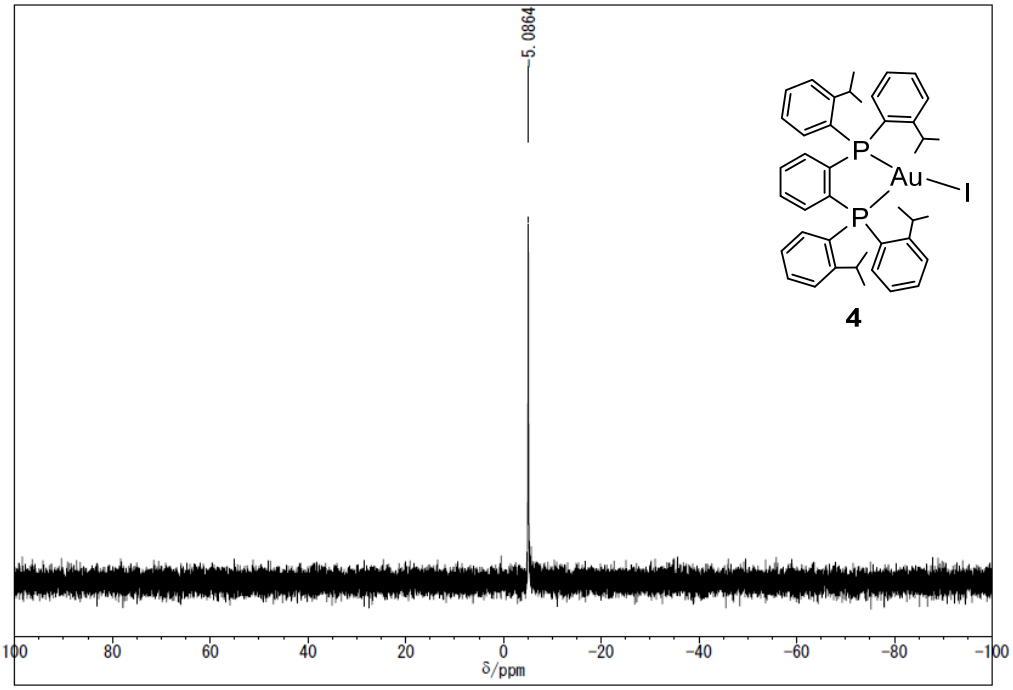


Fig. S14 ^{31}P {^{1}H} NMR spectrum of **4** in CD_2Cl_2 at 293 K.

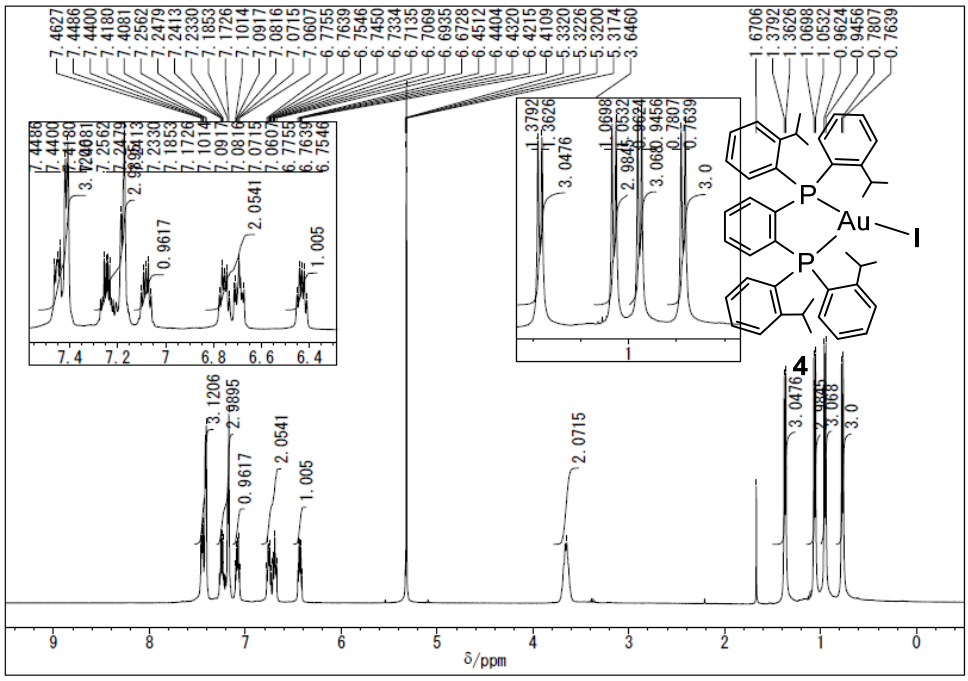


Fig. S15 ^{1}H NMR spectrum of **4** in CD_2Cl_2 at 223 K.

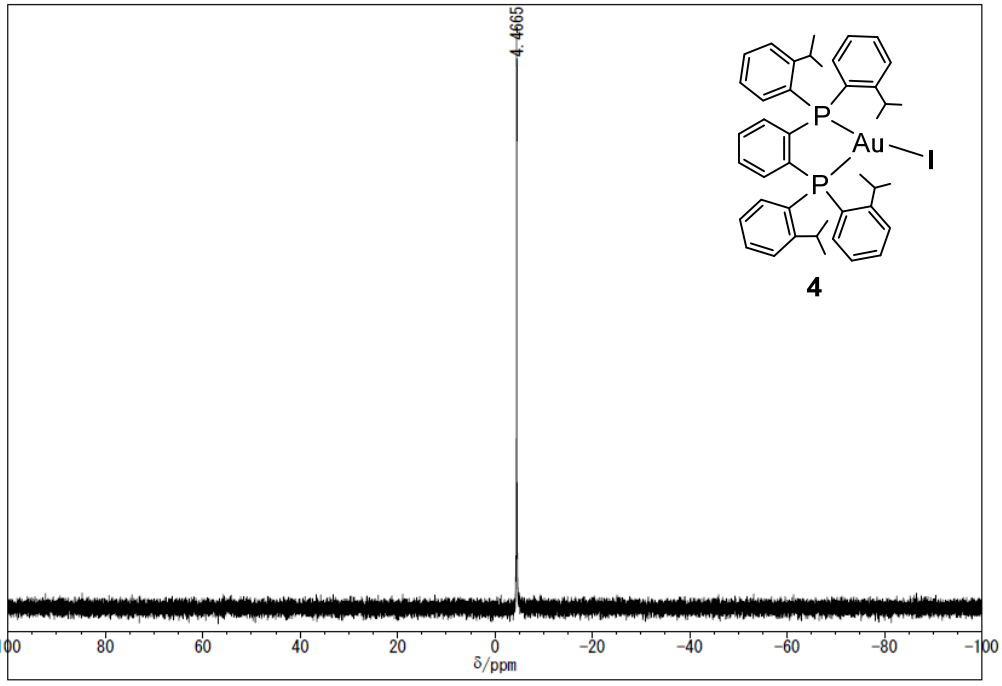


Fig. S16 ^{31}P {^{1}H} NMR spectrum of **4** in CD_2Cl_2 at 223 K.

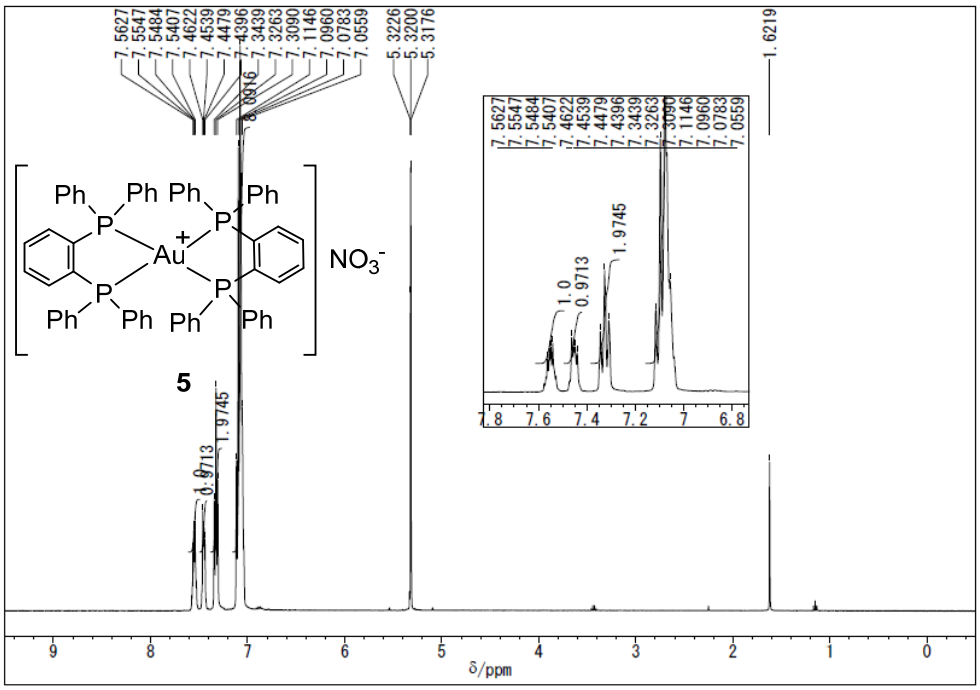


Fig. S17 ^{1}H NMR spectrum of **5** in CD_2Cl_2 at 293 K.

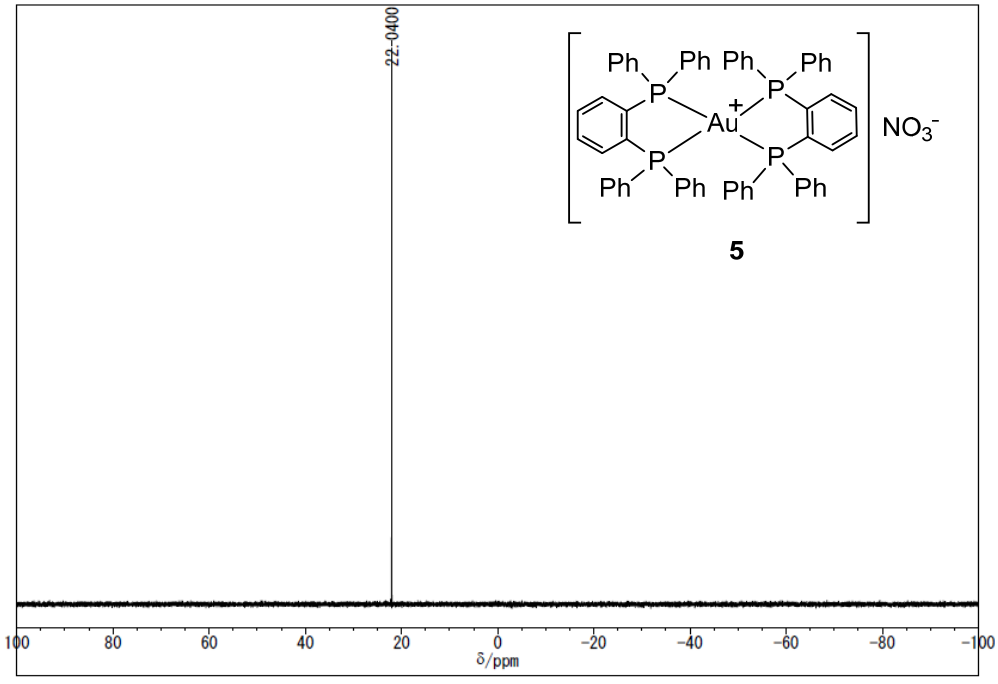


Fig. S18 ^{31}P $\{^{1}H\}$ NMR spectrum of **5** in CD_2Cl_2 at 293 K.

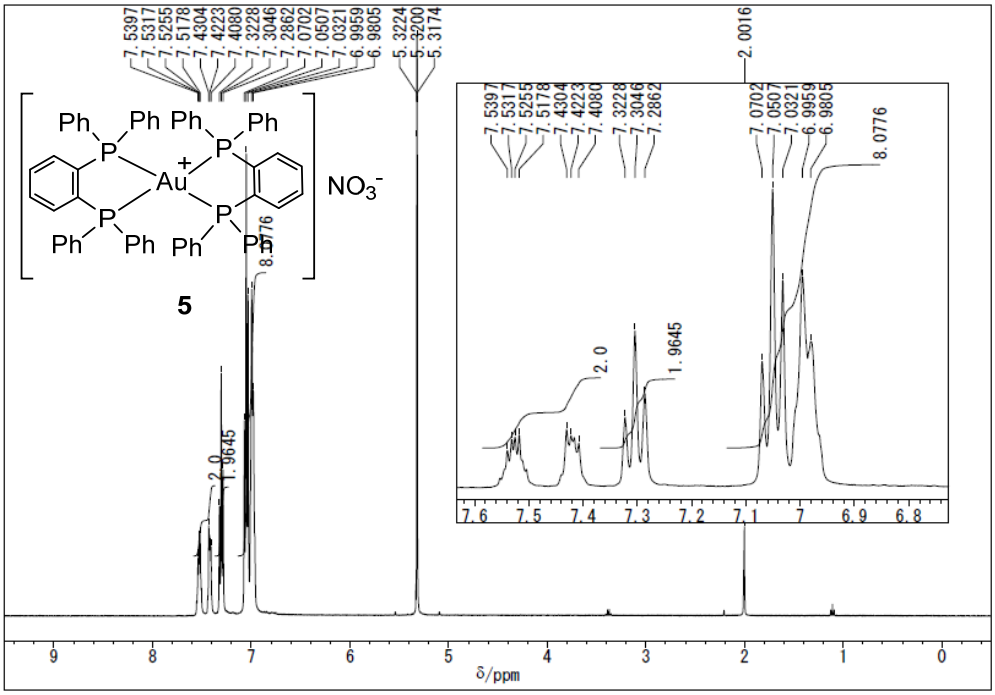


Fig. S19 ^{1}H NMR spectrum of **5** in CD_2Cl_2 at 223 K.

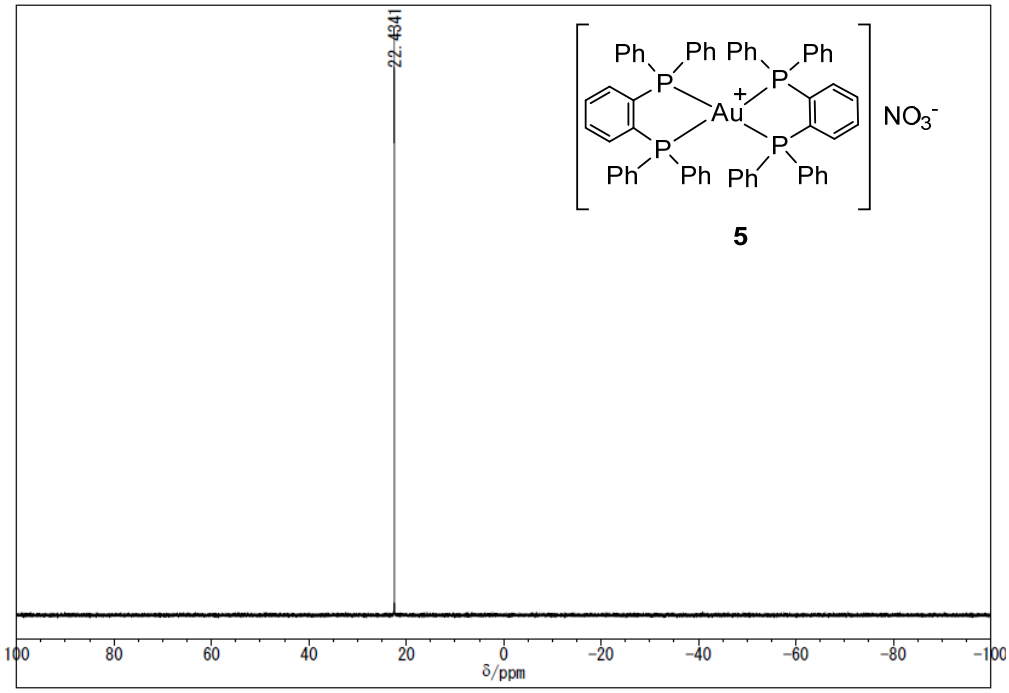


Fig. S20 ^{31}P $\{^{1}H\}$ NMR spectrum of **5** in CD_2Cl_2 at 223 K.

3. Crystal Structure determination

Table S1. Crystallographic data for **1** and **1d**.

	1d	**1**
formula	$C_{34}H_{32}Au_2Cl_2P_2$	$C_{34}H_{32}AuClP_2$
formula weight	967.38	734.96
cryst syst	triclinic	triclinic
space group	$P\bar{1}$	$P\bar{1}$
a / Å	11.0644(7)	8.9273(11)
b / Å	11.2837(7)	17.009(2)
c / Å	13.1885(9)	20.077(3)
α / deg	90.233(1)	17.720(2)
β / deg	93.362(2)	92.630(2)
γ / deg	103.812(1)	92.460(2)
V / Å^3	1595.91(18)	2895.7(7)
Z	2	4
d_{calcd} / g cm^{-3}	2.013	1.6858
T / K	90.0(2)	90(2)
radiation	Mo Kα	Mo Kα
	(λ = 0.71073 Å)	(λ = 0.71073 Å)
μ / cm^{-1}	9.473	5.306
diffractometer	Bruker APEX-II CCD	Bruker APEX-II CCD
max 2θ / deg	50	50
reflns collcd	7458	13785
indep reflns	5645	10254
	(*R*int = 0.0182)	(Rint = 0.0245)
no. of param refined	365	700
R1,[a] *wR2* ($I > 2\sigma I$)[b]	0.0532, 0.1341	0.0194, 0.0494
S	1.0296	1.1342

[a] $R1 = \Sigma||Fo| - |Fc||/\Sigma|Fo|$. [b] $wR2 = [\Sigma w(|Fo| - |Fc|)^2/\Sigma w|Fo|^2]^{1/2}$

Table S2. Crystallographic data for **3** and **4**.

	3	**4**
formula	$C_{42}H_{48}$ AuClP$_2$	$C_{42}H_{48}$AuIP$_2$
formula weight	847.16	938.61
cryst syst	orthorhmbic	orthorhmbic
space group	*P*na2$_1$	*P*na2$_1$
a / Å	20.5328(16)	20.304(2)
b / Å	19.5790(15)	9.7110(11)
c / Å	9.3602(7)	19.713(2)
α / deg	-	-
β / deg	-	-
γ / deg	-	-
V / Å^3	3762.9(5)	3886.9(7)
Z	4	4
d_{calcd} / g cm^{-3}	1.495	1.604
T / K	90(2)	90(2)
radiation	Mo Kα	Mo Kα
	(λ = 0.71073 Å)	(λ = 0.71073 Å)
μ / cm^{-1}	2.144	4.689
diffractometer	Bruker APEX-II CCD	Bruker APEX-II CCD
max 2θ / deg	50	50
reflns collcd	16584	16898
indep reflns	6640	6866
	(Rint = 0.0295)	(Rint = 0.0260)
no. of param refined	423	424
R1,[a] *wR2* ($I > 2\sigma I$)[b]	0.0119, 0.0293	0.0180, 0.0430
S	0.931	1.056

[a] $R1 = \Sigma||Fo| - |Fc||/\Sigma|Fo|$. [b] $wR2 = [\Sigma w(|Fo| - |Fc|)^2/\Sigma w|Fo|^2]^{1/2}$

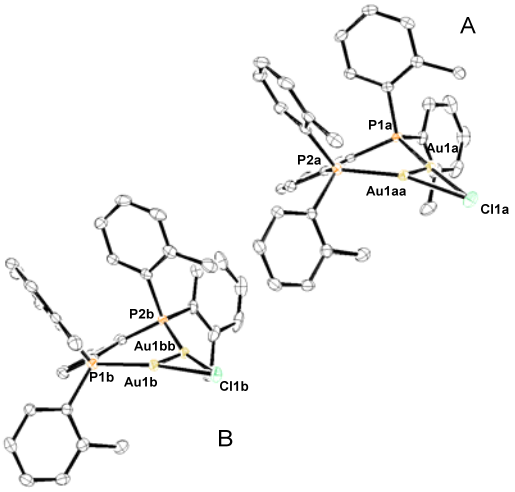


Fig. S21 Perspective views of the structures of **1** (A and B).

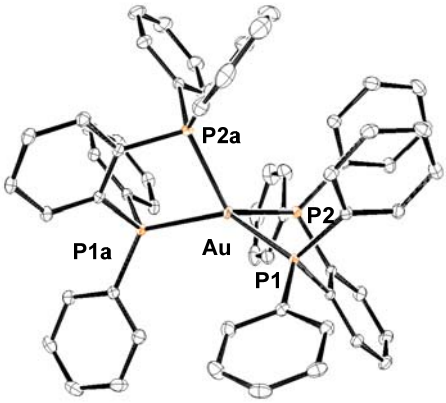


Fig. S22 Perspective views of the structures of **5**.

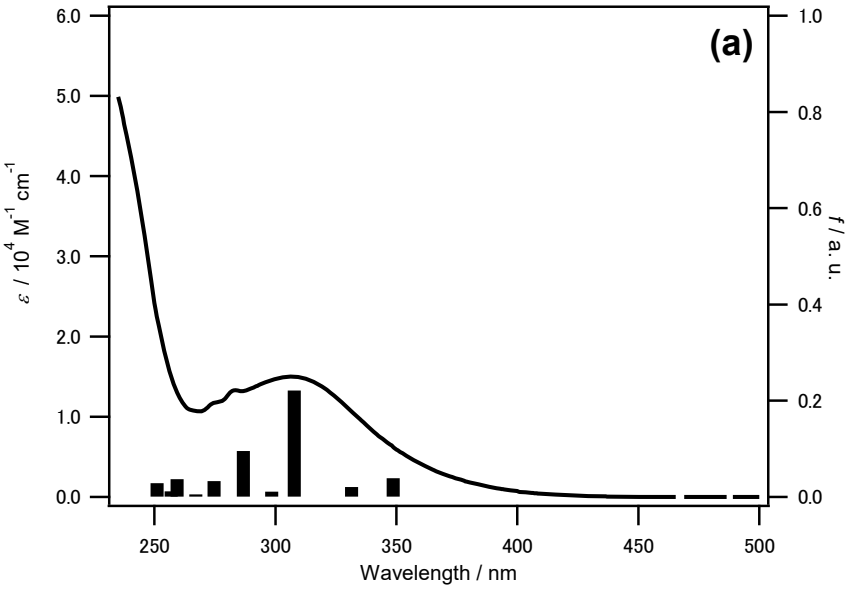
Table S3 Bond lengths and angles for **5**

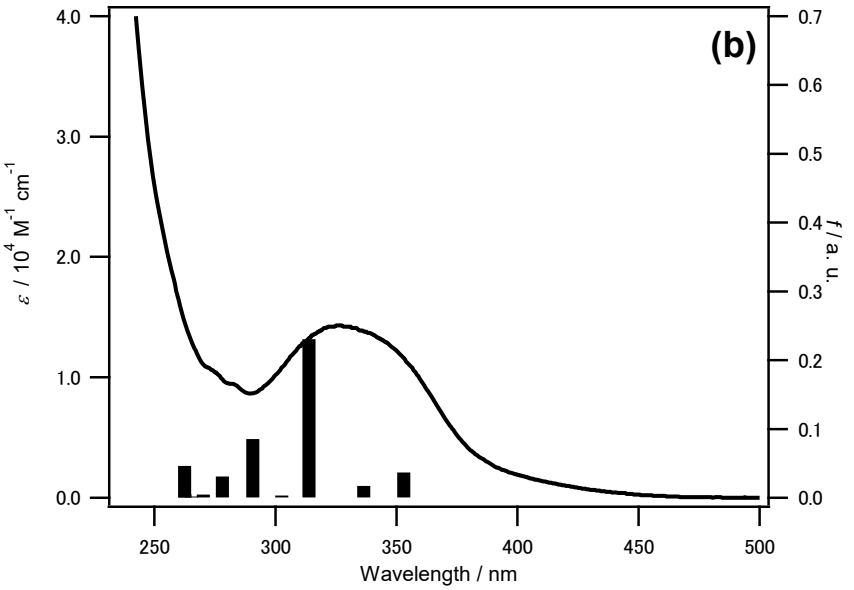
	Au-P1 (Å)	Au-P2 (Å)	P1-Au-P2 (º)	P1-Au-P2a (º)	P1-Au-P1a (º)	P2-Au-P2a (º)
5	2.3749(8)	2.4428(8)	81.55(3)	122.27(3)	133.24(3)	121.66(3)

Table S4 Dihedral angles for **5**

	(P1-Au-P1a) and (P2-Au-P2a) (º)
5	85.64(4)

4. Photophysical data and theoretical studies





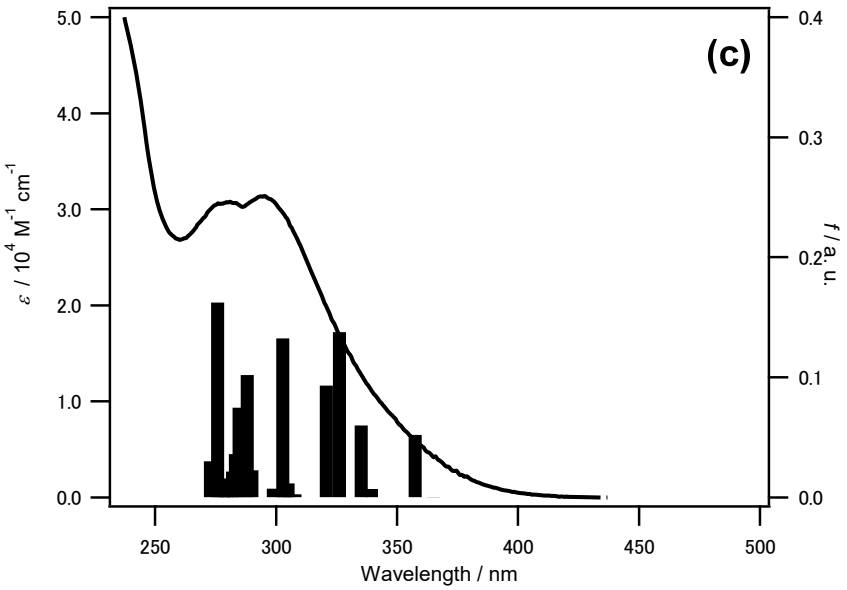


Fig. S23 Absorption spectra and calculated singlet transitions (bar graph) at the optimized ground state S_0 geometry in CH_2Cl_2. The oscillator strengths of $S_n \leftarrow S_0$ ($n \leq 10$ for **3** and **4**, $n \leq 20$ for **5**) transitions calculated are presented with bars; (a) complex **3**, (b) complex **4** and (c) complex **5**.

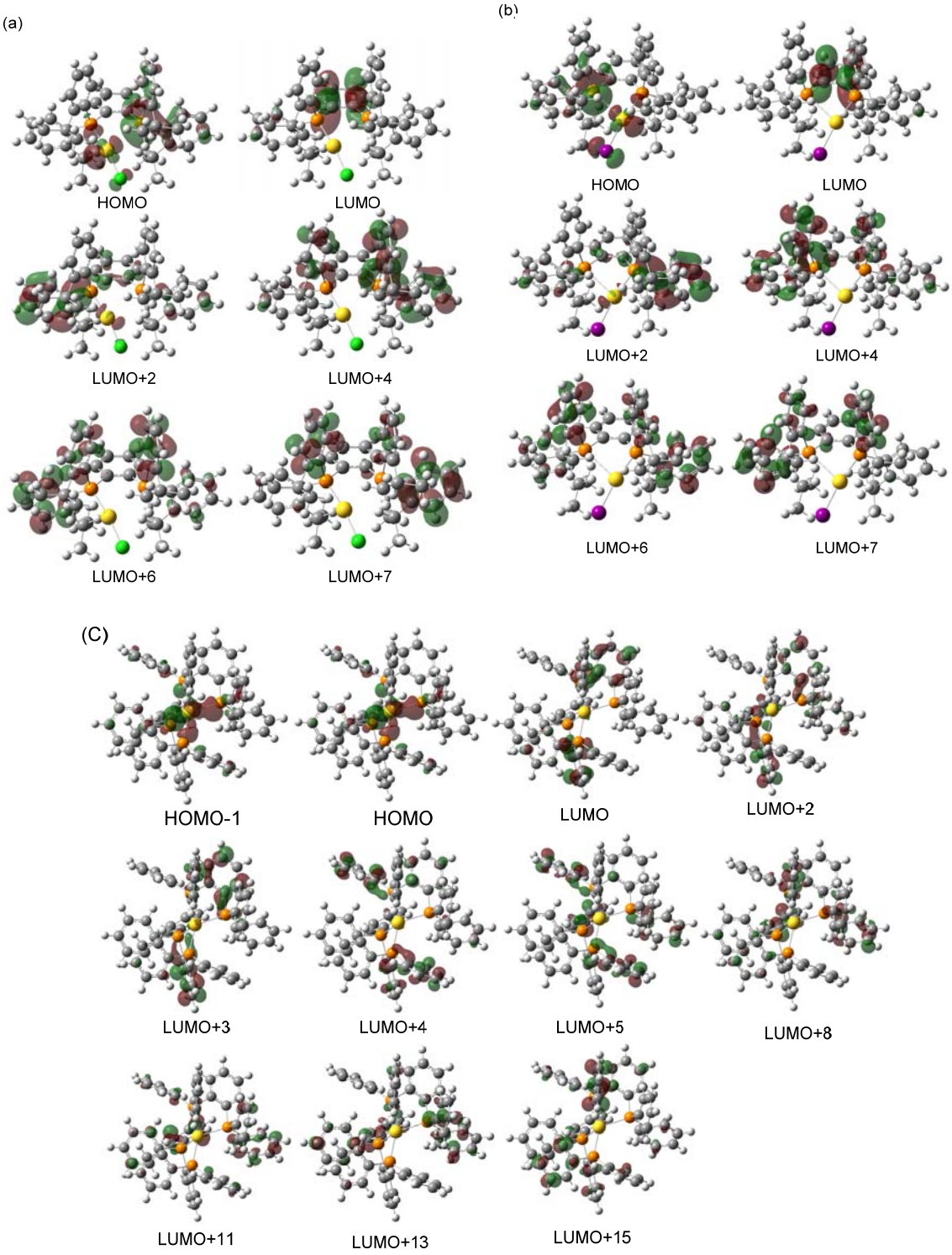


Figure S24 Selected frontier orbitals obtained with the calculation of **3**−**5** in the optimized S_0 structures.

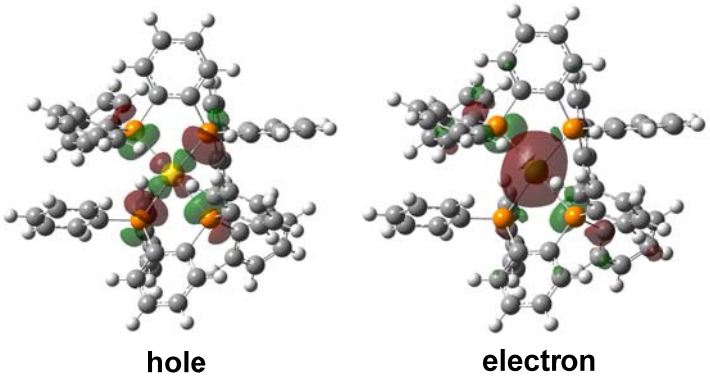


Fig. S25 NTO pairs of **5** for the optimized T_1 geometry in THF.

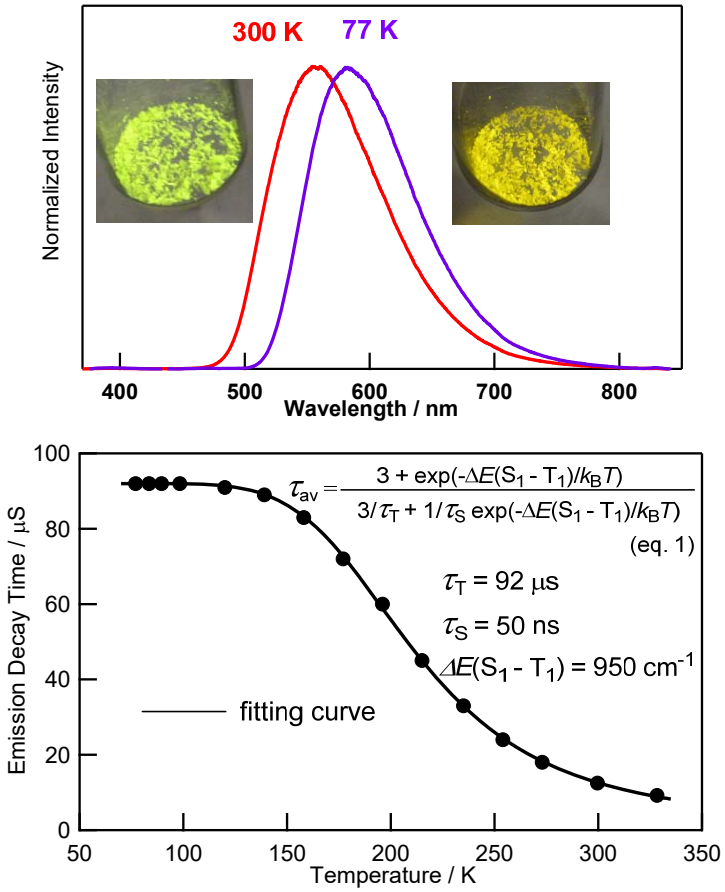


Fig. S26 Temperature-dependent change of (A) corrected emission spectra and (B) emission decay for **3**; λ_{exc} = 355 nm. The inset shows luminescence image of **3** at 309and 77 K; λ_{exc} = 365 nm.

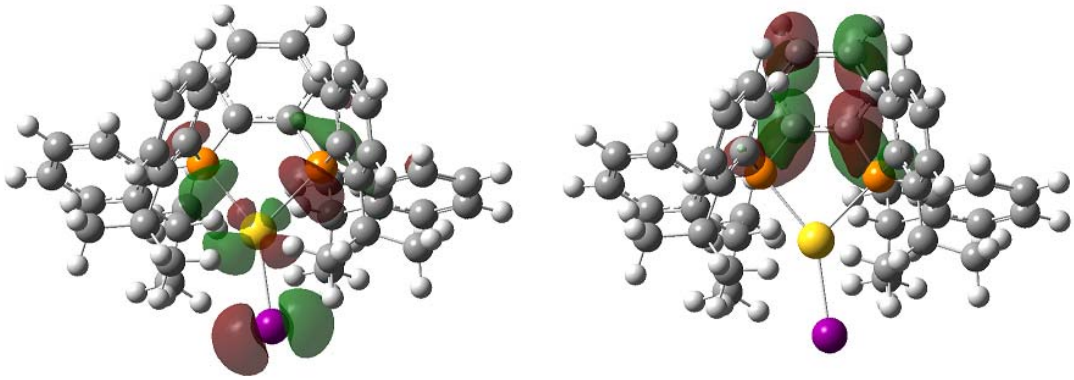


Fig. S27 NTO pairs for the T_1 state of **4** in the T_1. The generation probability is 99.8%.

Table S5 Calculated energy levels, oscillator strengths (*f*), and orbital transitions for selected lower-lying transitions of **3**−**5**

	states	λ_{cal} / nm (eV)	*f*	assignments
3	S1	349 (3.553)	0.0391	HOMO→LUMO (100%)
	S3	308 (4.026)	0.2211	HOMO→LUMO+2 (85%)
				HOMO→LUMO+4 (15%)
	S5	287 (4.320)	0.0951	HOMO→LUMO+2 (14%)
				HOMO→LUMO+4 (85%)
	S8	259 (4.787)	0.0370	HOMO→LUMO+6 (22%)
				HOMO→LUMO+7 (60%)
				HOMO→LUMO+9 (18%)
4	S1	353 (3.512)	0.0366	HOMO→LUMO (100%)
	S3	314 (3.949)	0.2306	HOMO→LUMO+2 (88%)
				HOMO→LUMO+4 (12%)
	S5	291 (4.261)	0.0851	HOMO→LUMO+2 (13%)
				HOMO→LUMO+4 (87%)
	S6	278 (4.460)	0.0308	HOMO→LUMO+5 (69%)
				HOMO→LUMO+6 (31%)
5	S1	365 (3.396)	7.32E-5	HOMO→LUMO (100%)
	S5	326 (3.801)	0.1380	HOMO-1→LUMO (14%)
				HOMO→LUMO+4 (86%)
	S10	303 (4.092)	0.1326	HOMO-1→LUMO (72%)
				HOMO→LUMO+4 (13%)
				HOMO→LUMO+8 (15%)
	S13	288 (4.303)	0.1024	HOMO-1→LUMO+2 (73%)
				HOMO→LUMO+3 (12%)
				HOMO→LUMO+11 (15%)
	S19	276 (4.494)	0.1629	HOMO-1→LUMO+5 (52%)
				HOMO→LUMO+11 (14%)
				HOMO→LUMO+13 (14%)
				HOMO→LUMO+15 (20%)

Table S6 k_r and k_{nr} values of **3**, **4**, $L_{iPr}CuBr$, and $L_{iPr}AgI$ in 2-MeTHF at 293 K

	k_r	k_{nr}
3	2.5×10^4	1.2×10^6
4	5.7×10^4	1.4×10^6
$L_{iPr}CuBr$	5.8×10^4	7.6×10^4
$L_{iPr}AgI$	3.3×10^4	1.3×10^5

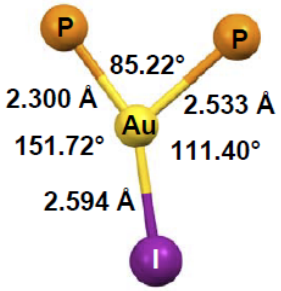
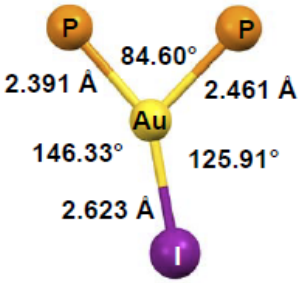
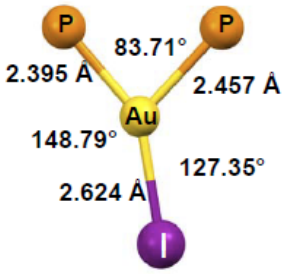
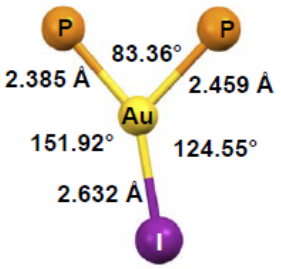
[a] Radiative rate constant. $k_r = \Phi / \tau$. [b] Non-radiative constant. $k_{nr} = (1 / \Phi - 1) \times k_r$.

Table S7 Composition of hole and electron for the optimized T_1 of **5** in THF.[a]

	percentage composition (%) [b]		
	hole	electron	Difference
Au	25	42	17
P	50	22	-28
phenylene unit (L) [c]	4	8	4
phenyl groups (L) [c]	20	28	8

[a] The optimized T_1 geometry was obtained by unrestricted (U)-DFT. [b] The atomic component was evaluated by the Mulliken analysis. [c] Two dppb ligands have same contributions to hole and electron.

Table S8 Calculation results of **4**

The X-ray and the optimized core atructures of **4**	 X-ray	 S_1: TD DFT	 T_1: TD DFT	 T_1: UDFT[a]
$E(S_1, S_1)$: total energy of S_1 state in the S_1 optimized geometry / Hartree	–	-2743.3131006	–	–
$E(S_0, S_1)$: total energy of S_0 state in the S_1 optimized geometry / Hartree	–	-2743.3848585	–	–
$E(T_1, T_1)$: total energy of T_1 state in the T_1 optimized geometry / Hartree	–	–	-2743.3205495	-2743.3134506
$E(S_0, T_1)$: total energy of S_0 state in the T_1 optimized geometry / Hartree	–	–	-2743.3843775	-2743.3830493[b]
TADF / eV(nm)	–	1.9510 (635)	–	–
Phosphorescence / eV(nm)	–	–	1.7368 (714)	1.8939 (655)
ΔE_{ST} [c] / cm^{-1}	–	–	1627	81

[a] T_1 optimized with the unrestricted (U)–DFT. [b] $E(S_0, T_1)$ is obtained by single point calculation. [c] The energy gap = $E(S_1, S_1) - E(T_1, T_1)$.

Table S9 k_r and k_{nr} values of **3**, **4**, and **5** in the crystal at 293 K and 77 K

	293 K		77 K	
	k_S^r	k_S^{nr}	k_T^r	k_T^{nr}
3	6.3×10^4	1.4×10^4	1.3×10^3	4.6×10^3
4	1.0×10^5	9.0×10^3	9.5×10^3	3.3×10^3
5	2.5×10^5	1.3×10^4	5.0×10^4	2.6×10^3

[a] Radiative rate constant. $k^r = \Phi / \tau$. [b] Non-radiative constant. $k^{nr} = (1 / \Phi - 1) \times k^r$.

Table S10 Composition of hole and electron for T_1 of **4** in the optimized T_1 geometry.[a]

	percentage composition (%) [b]		
	hole	electron	Difference
Au	23	3	20
P[c]	24	6	18
P	15	5	10
I	16	0	16
phenylene unit (L_{iPr})	6	72	-66
cumenyl groups (L_{iPr})	16	14	2

[a] The optimized T_1 geometry was obtained by TD-DFT. [b] The atomic component was evaluated by the Mulliken analysis. [c] The P atom have the large distance from the Au(I) atom.

Table S11 Geometry data of **3** for the optimized S_0 state in THF

Au	-0.078704	-0.126130	-0.110725
P	-0.075565	0.052358	2.967185
P	2.150280	-0.038701	0.400337
Cl	-2.298020	-0.199193	-0.907157
C	2.513045	-0.753231	2.058036
C	1.331383	2.051973	4.412936
C	3.924919	-2.867228	-2.027642
C	3.856816	3.447093	1.727810
C	3.406436	2.137195	1.608937
C	1.590956	-0.730820	3.131532
C	3.037254	-2.279109	-1.119054
C	3.760967	-1.368110	2.235150
C	0.194305	1.744399	3.650824
C	-0.755214	2.755364	3.383509
C	5.024226	-2.184901	-2.535853
C	2.768209	1.691337	0.443274
C	3.277152	-0.940724	-0.738419
C	-2.032759	2.499770	2.604549
C	1.930595	2.192986	-1.957645
C	4.398200	-0.263556	-1.240187
C	0.910505	-3.501062	-1.692518
C	1.956033	-1.357805	4.331469
C	0.601886	2.931553	-2.146057
C	1.892815	-3.119161	-0.581762
C	2.856723	2.431453	-3.154793
C	-0.516100	4.039085	3.889032
C	-2.137275	3.399363	1.370930
C	0.617434	4.335015	4.637101
C	4.105096	-1.971218	3.440083
C	-1.570310	-2.074875	4.080097
C	-1.049188	-0.780185	4.297375
C	3.671382	4.330190	0.670143
C	3.194057	-1.972104	4.491117
C	2.410583	-4.358994	0.154408
C	5.270324	-0.876496	-2.132711
C	3.047030	3.891892	-0.492231
C	1.548007	3.334540	4.903736
C	2.586214	2.579180	-0.642357
C	-3.267934	2.643615	3.499547
C	-1.295451	-2.873818	2.818753
C	-1.351692	-0.108704	5.491690
C	-2.152001	-0.693899	6.467646
C	-2.367430	-2.645416	5.078933
C	-2.661582	-1.972046	6.259503
C	-0.503964	-4.148455	3.126178
C	-2.588389	-3.193452	2.063827
H	2.057858	1.274351	4.630334
H	3.752033	-3.893710	-2.340780
H	4.342508	3.770811	2.643657
H	3.551813	1.453473	2.438307
H	4.471731	-1.383725	1.414210
H	5.690142	-2.678337	-3.238448
H	-2.008421	1.463508	2.244043
H	1.705268	1.119556	-1.935170
H	4.592597	0.757700	-0.927956
H	0.504736	-2.610595	-2.184928
H	0.071563	-4.070426	-1.276491
H	1.393470	-4.122946	-2.455258
H	1.251994	-1.360017	5.158821
H	0.756063	4.015616	-2.200414
H	-0.087569	2.725981	-1.320229
H	0.118988	2.611687	-3.076243
H	1.335344	-2.521820	0.150300
H	2.369611	2.088246	-4.074319
H	3.801250	1.888169	-3.049204
H	3.088279	3.495296	-3.280415
H	-1.240382	4.826200	3.693338
H	-2.222232	4.456837	1.648545
H	-3.024426	3.134779	0.784666
H	-1.258793	3.288742	0.726241
H	0.770793	5.342960	5.013595
H	5.077268	-2.443038	3.549581
H	4.013552	5.358703	0.745675
H	3.444535	-2.445176	5.436571
H	2.954799	-5.029868	-0.520138
H	1.571435	-4.922971	0.576482
H	3.082690	-4.083596	0.974337
H	6.131731	-0.332004	-2.508759
H	2.913958	4.591361	-1.313488
H	2.436489	3.548162	5.491950
H	-3.215448	1.968948	4.361067
H	-4.175527	2.403924	2.933757
H	-3.368509	3.668586	3.876653
H	-0.679568	-2.258233	2.149449
H	-0.953987	0.887732	5.659884
H	-2.371522	-0.153346	7.384474
H	-2.771681	-3.643346	4.925935
H	-3.287447	-2.444377	7.012035
H	0.446324	-3.918498	3.620379
H	-0.285030	-4.692089	2.199916
H	-1.071383	-4.821477	3.779856
H	-3.251049	-3.834318	2.657395
H	-2.361982	-3.720660	1.129906
H	-3.134355	-2.278332	1.811940

Table S12 Geometry data of **4** for the optimized S_0 state in THF

Au	0.270929	-0.126094	0.290424
I	-0.187192	-0.243471	2.889341
P	1.053110	-0.021096	-1.889437
P	-2.279445	0.077316	-1.308690
C	0.311613	-1.307082	-4.245061
C	-2.415237	-1.295810	-3.773840
C	-4.023744	-2.057193	-0.656738
C	3.613649	-0.262344	-2.976821
C	-5.103018	-0.037999	-1.471234

C -3.928575 -0.742246 -1.164342
C -1.917379 -1.892853 -4.927701
C -1.570743 -0.687077 -2.834632
C -2.820023 2.090186 -3.232773
C -0.176292 -0.708406 -3.074593
C 2.986952 2.154058 -0.447494
C 4.822913 -0.883038 -3.268403
C -2.715070 1.781295 -1.867738
C -0.547324 -1.892818 -5.168755
C -5.297326 -2.612238 -0.487778
C 5.035213 -2.192408 -2.849126
C 1.358114 1.713231 -2.413775
C -6.358333 -0.608949 -1.288392
C -2.942845 2.793029 -0.908790
C 2.204191 2.576224 -1.679596
C 0.693455 2.191061 -3.551801
C -2.809946 -2.896843 -0.301244
C 2.603821 -0.932381 -2.270351
C 2.800241 -2.271194 -1.867636
C 4.031699 -2.867357 -2.164047
C 4.494673 2.362137 -0.625062
C 2.484457 2.885157 0.801022
C -6.455272 -1.906045 -0.794222
C 1.748527 -3.104600 -1.158471
C 1.370579 -4.340119 -1.981641
C 0.838491 3.508777 -3.970721
C 2.200527 -3.491700 0.252187
C -2.806848 -3.283246 1.179997
C 2.329788 3.896915 -2.124780
C -3.137797 3.373095 -3.662884
C -3.266403 4.076809 -1.366636
C -3.362801 4.373206 -2.720833
C -1.909093 3.488427 1.288244
C 1.660467 4.367151 -3.249037
C -2.708935 -4.136344 -1.195603
C -4.283431 2.634886 1.215036
C -2.888292 2.543721 0.587634
H 1.381229 -1.322998 -4.432443
H -3.486773 -1.297962 -3.594599
H 3.451808 0.759985 -3.303984
H -5.033909 0.973458 -1.860030
H -2.600965 -2.352532 -5.636078
H -2.654029 1.312781 -3.972755
H 2.827305 1.081455 -0.281395
H 5.590409 -0.343893 -3.816346
H -0.143501 -2.351943 -6.066484
H -5.384056 -3.625468 -0.102488
H 5.976647 -2.691903 -3.060806
H -7.252252 -0.042050 -1.534254
H 0.048655 1.526690 -4.117271
H -1.910110 -2.291782 -0.475207
H 4.205650 -3.894409 -1.853335
H 4.877503 1.821263 -1.496384
H 5.026360 1.996927 0.260714
H 4.743349 3.422695 -0.746438
H 2.635964 3.967521 0.714142
H 3.027302 2.538027 1.687312
H 1.417736 2.701081 0.966949
H -7.427827 -2.367956 -0.646427
H 0.838817 -2.500747 -1.050760
H 1.007504 -4.060017 -2.976468
H 0.577782 -4.901148 -1.474507
H 2.224410 -5.015358 -2.109418
H 0.307549 3.857530 -4.851645
H 3.100767 -4.116690 0.224792
H 1.412417 -4.059241 0.759952
H 2.418747 -2.603141 0.854545
H -2.828923 -2.394962 1.819896
H -1.899772 -3.849274 1.421728
H -3.669846 -3.910807 1.431993
H 2.973585 4.577060 -1.573072
H -3.212433 3.586856 -4.725758
H -3.450466 4.864429 -0.640083
H -3.615184 5.381435 -3.038646
H -0.911216 3.426866 0.840613
H -1.821766 3.221786 2.347216
H -2.241628 4.531776 1.232234
H 1.784336 5.400977 -3.559669
H -3.571667 -4.798396 -1.055816
H -1.807671 -4.709501 -0.949825
H -2.660939 -3.861962 -2.255008
H -4.700659 3.643609 1.107586
H -4.233035 2.404137 2.285303
H -4.978224 1.929103 0.746882
H -2.519735 1.522741 0.750883

Table S13 Geometry data of **5** for the optimized S_0 state in THF

Au 0.224938 0.296326 -0.164393
P 0.016017 0.334832 2.319778
P 2.587221 -0.057784 0.438736
C -1.490244 -0.144295 3.237443
C -1.718520 0.245567 4.563999
C -2.887933 -0.139947 5.214207
C -3.838599 -0.911819 4.547588
C -3.624286 -1.291826 3.224325
C -2.458703 -0.902706 2.569014
C 0.524437 1.919388 3.086403
C 1.615434 2.024484 3.956149
C 1.969201 3.262322 4.491976
C 1.235964 4.401518 4.171246
C 0.145778 4.302634 3.307465
C -0.203807 3.071586 2.761767
C 1.334315 -0.827415 2.846850
C 2.480616 -0.974218 2.035229
C 3.507697 -1.826105 2.457053
C 3.403393 -2.536811 3.649379
C 2.263443 -2.406607 4.437302

C	1.238921	-1.552420	4.039336
C	3.597091	1.422315	0.807651
C	4.850097	1.330333	1.429030
C	5.578450	2.482185	1.707064
C	5.063808	3.734450	1.369264
C	3.819761	3.833253	0.752829
C	3.087776	2.680536	0.472783
C	3.647254	-1.120363	-0.601101
C	3.372717	-2.493279	-0.691625
C	4.106381	-3.301353	-1.555322
C	5.108757	-2.748059	-2.352081
C	5.374776	-1.382886	-2.278756
C	4.649937	-0.570724	-1.408015
P	-0.750471	-1.310405	-1.797609
P	-1.253061	1.835412	-1.401590
C	-0.949184	-3.098332	-1.476931
C	-1.126250	-4.032549	-2.506279
C	-1.265502	-5.385092	-2.205932
C	-1.225648	-5.816438	-0.880678
C	-1.036160	-4.894688	0.146891
C	-0.889732	-3.542074	-0.150390
C	-0.004899	-1.230387	-3.469329
C	-0.723132	-0.826975	-4.600404
C	-0.094938	-0.759408	-5.843560
C	1.249296	-1.098606	-5.970397
C	1.969497	-1.504637	-4.847434
C	1.349680	-1.562975	-3.603331
C	-2.437380	-0.639471	-2.062036
C	-2.649495	0.749734	-1.923275
C	-3.924110	1.270801	-2.173549
C	-4.978854	0.438051	-2.536174
C	-4.772407	-0.933731	-2.650808
C	-3.507206	-1.466394	-2.420409
C	-0.606978	2.556291	-2.953754
C	-1.437576	3.223060	-3.864744
C	-0.909572	3.739963	-5.043109
C	0.449755	3.595450	-5.323439
C	1.280337	2.933996	-4.423413
C	0.753910	2.415629	-3.241389
C	-2.076235	3.214756	-0.533247
C	-3.046261	2.938016	0.441991
C	-3.608333	3.970278	1.187483
C	-3.197606	5.287491	0.983062
C	-2.223536	5.566857	0.027531
C	-1.664356	4.538035	-0.728705
H	-0.986544	0.856942	5.085530
H	-3.057665	0.165911	6.242805
H	-4.751281	-1.207999	5.057070
H	-4.369606	-1.880323	2.696759
H	-2.302612	-1.176034	1.527776
H	2.196548	1.144522	4.215852
H	2.820967	3.331632	5.162946
H	1.513878	5.364411	4.590816
H	-0.432118	5.185570	3.048563
H	-1.048559	3.008709	2.081449
H	4.389985	-1.957088	1.837100
H	4.209549	-3.197438	3.955004
H	2.169787	-2.966795	5.363195
H	0.354392	-1.450446	4.661571
H	5.259051	0.360686	1.700024
H	6.548535	2.403174	2.189825
H	5.634389	4.632287	1.589969
H	3.413296	4.806467	0.492832
H	2.109546	2.754001	0.002667
H	2.584003	-2.934699	-0.086930
H	3.890125	-4.364656	-1.608721
H	5.679414	-3.379920	-3.026638
H	6.153347	-0.944288	-2.896669
H	4.871141	0.491666	-1.355196
H	-1.146851	-3.704057	-3.542215
H	-1.402694	-6.103371	-3.009444
H	-1.331594	-6.872873	-0.650558
H	-0.988946	-5.228744	1.179524
H	-0.713831	-2.825148	0.648639
H	-1.772317	-0.559263	-4.517451
H	-0.662534	-0.440505	-6.713404
H	1.735736	-1.045127	-6.940395
H	3.019619	-1.769745	-4.934350
H	1.924092	-1.870625	-2.733962
H	-4.104303	2.335987	-2.060400
H	-5.961725	0.862409	-2.719498
H	-5.593467	-1.591148	-2.921934
H	-3.350558	-2.536923	-2.517999
H	-2.497965	3.338931	-3.657347
H	-1.559655	4.255128	-5.744769
H	0.858639	3.998420	-6.245834
H	2.338187	2.815637	-4.639982
H	1.396709	1.887278	-2.540639
H	-3.364936	1.914086	0.622070
H	-4.365160	3.743042	1.932992
H	-3.635967	6.091748	1.566951
H	-1.897758	6.590154	-0.137129
H	-0.909740	4.769812	-1.475124

Table S14 Geometry data of **5** for the optimized T_1 state in THF

Au	-0.050209	-0.068892	0.037627
P	0.192152	0.870530	2.367088
P	2.299415	-0.653533	0.476827
C	-1.252801	0.494269	3.423753
C	-1.633096	1.306301	4.499228
C	-2.712740	0.944102	5.301442
C	-3.415328	-0.231716	5.044965
C	-3.033243	-1.050768	3.983539
C	-1.958676	-0.690257	3.176167
C	0.627937	2.604146	2.713323
C	1.956086	2.988137	2.960211
C	2.289845	4.334561	3.074133

C	1.311305	5.318924	2.941447
C	-0.009176	4.946563	2.688695
C	-0.350452	3.604031	2.566056
C	1.541738	-0.120974	3.109685
C	2.458749	-0.797451	2.288181
C	3.474950	-1.564462	2.867436
C	3.586147	-1.651152	4.254271
C	2.682037	-0.976234	5.068936
C	1.660903	-0.217576	4.499327
C	3.477763	0.643694	-0.038662
C	4.538289	1.069539	0.772055
C	5.394729	2.075364	0.329579
C	5.207333	2.657039	-0.922764
C	4.153658	2.237016	-1.733663
C	3.285716	1.243667	-1.291323
C	2.970460	-2.214525	-0.176740
C	2.222861	-3.384433	0.012084
C	2.691726	-4.599632	-0.476919
C	3.904997	-4.655519	-1.163134
C	4.651702	-3.494582	-1.353238
C	4.189687	-2.275106	-0.861665
P	-0.410060	-1.157981	-2.211656
P	-1.627817	1.539209	-0.958414
C	-0.622693	-2.969102	-2.075424
C	-0.278160	-3.851944	-3.105958
C	-0.508496	-5.218232	-2.961678
C	-1.091016	-5.713632	-1.796633
C	-1.449322	-4.837487	-0.773060
C	-1.216045	-3.472541	-0.910382
C	0.671437	-0.883767	-3.650327
C	0.355407	0.073210	-4.628404
C	1.264745	0.374548	-5.638098
C	2.501449	-0.267321	-5.689901
C	2.826258	-1.214304	-4.718368
C	1.926953	-1.516022	-3.701367
C	-2.063625	-0.568701	-2.734610
C	-2.604059	0.604982	-2.183809
C	-3.873040	1.038093	-2.582017
C	-4.597295	0.314806	-3.528297
C	-4.060705	-0.845569	-4.078099
C	-2.800489	-1.288474	-3.679996
C	-0.808319	2.886501	-1.880578
C	-1.229051	3.300558	-3.151352
C	-0.552937	4.324741	-3.810796
C	0.537960	4.948338	-3.208394
C	0.960873	4.540313	-1.943920
C	0.299724	3.507456	-1.286809
C	-2.865012	2.352177	0.101328
C	-3.610669	1.552633	0.977759
C	-4.560181	2.130663	1.814371
C	-4.768108	3.509842	1.787762
C	-4.029223	4.308710	0.917543
C	-3.079691	3.735059	0.073991
H	-1.091270	2.223150	4.711296
H	-3.002460	1.583458	6.130723
H	-4.255913	-0.511617	5.673839
H	-3.574261	-1.971098	3.781438
H	-1.664560	-1.322325	2.339046
H	2.730443	2.234555	3.070690
H	3.320772	4.613638	3.274128
H	1.575454	6.368441	3.033249
H	-0.780905	5.704445	2.584191
H	-1.382539	3.333582	2.358402
H	4.177347	-2.099116	2.233805
H	4.377449	-2.250855	4.694432
H	2.761966	-1.045999	6.149822
H	0.946736	0.292504	5.139886
H	4.698544	0.618569	1.747294
H	6.212708	2.401488	0.965968
H	5.878071	3.440455	-1.264083
H	3.996524	2.691406	-2.707710
H	2.452889	0.935573	-1.919998
H	1.269258	-3.340345	0.532731
H	2.101927	-5.500193	-0.332433
H	4.267087	-5.603834	-1.550107
H	5.598353	-3.535039	-1.884740
H	4.775434	-1.373355	-1.014351
H	0.172462	-3.477468	-4.020257
H	-0.233309	-5.895884	-3.765091
H	-1.270227	-6.779778	-1.688731
H	-1.909204	-5.217044	0.135229
H	-1.485065	-2.785115	-0.108984
H	-0.605109	0.579658	-4.605602
H	1.000506	1.111472	-6.391650
H	3.207579	-0.030973	-6.480615
H	3.786643	-1.721887	-4.748641
H	2.202470	-2.247972	-2.946432
H	-4.297975	1.939364	-2.148778
H	-5.582576	0.658510	-3.829403
H	-4.624512	-1.415110	-4.811133
H	-2.393668	-2.204552	-4.099447
H	-2.083042	2.827469	-3.627742
H	-0.884072	4.637299	-4.797248
H	1.061340	5.747267	-3.726000
H	1.815401	5.016198	-1.471387
H	0.647299	3.179173	-0.309560
H	-3.439437	0.479335	1.011378
H	-5.127904	1.503946	2.496011
H	-5.505345	3.960881	2.445907
H	-4.190684	5.382730	0.891986
H	-2.505635	4.363336	-0.600726

Table S15 Geometry data of **4** for the optimized S_0 state

Au	0.303309	-0.187593	0.30873
I	-0.199258	-0.302879	2.872182
P	1.035125	-0.042157	-1.881583
P	-2.294382	0.077364	-1.337607

C	0.309834	-1.3147	-4.255286
C	-2.418803	-1.314793	-3.798072
C	-4.04385	-2.03017	-0.642755
C	3.587296	-0.243099	-3.005243
C	-5.114102	-0.059251	-1.579881
C	-3.944951	-0.738377	-1.205093
C	-1.912597	-1.913852	-4.946662
C	-1.581986	-0.696402	-2.858082
C	-2.864686	2.076299	-3.27393
C	-0.185704	-0.716442	-3.087762
C	2.96835	2.1101	-0.407017
C	4.799488	-0.847698	-3.316538
C	-2.720548	1.777569	-1.910687
C	-0.54182	-1.905711	-5.181933
C	-5.316484	-2.593096	-0.498534
C	5.030044	-2.158568	-2.913631
C	1.326063	1.704963	-2.371332
C	-6.36842	-0.637112	-1.41776
C	-2.898551	2.799837	-0.952852
C	2.169641	2.55614	-1.6207
C	0.642656	2.208158	-3.486336
C	-2.834737	-2.833224	-0.198356
C	2.592158	-0.930852	-2.295744
C	2.807222	-2.271437	-1.909301
C	4.041553	-2.850707	-2.22515
C	4.472539	2.330177	-0.599252
C	2.476835	2.80629	0.865682
C	-6.468849	-1.914616	-0.876776
C	1.772114	-3.122803	-1.196592
C	1.402095	-4.357517	-2.024617
C	0.766299	3.538879	-3.867375
C	2.238159	-3.509559	0.209555
C	-2.89985	-3.173687	1.29241
C	2.275518	3.88968	-2.030066
C	-3.174905	3.360418	-3.704321
C	-3.213816	4.084963	-1.411504
C	-3.350058	4.371429	-2.763701
C	-1.830655	3.519613	1.224932
C	1.58734	4.384613	-3.131351
C	-2.660447	-4.093735	-1.050852
C	-4.185607	2.607295	1.197262
C	-2.801628	2.554748	0.54153
H	1.380853	-1.328274	-4.435051
H	-3.490741	-1.322457	-3.619639
H	3.409526	0.781799	-3.316786
H	-5.039743	0.937958	-2.003541
H	-2.590325	-2.381535	-5.656038
H	-2.735991	1.288017	-4.010571
H	2.817155	1.033086	-0.263487
H	5.555862	-0.294715	-3.866619
H	-0.131159	-2.365039	-6.076905
H	-5.405559	-3.589026	-0.071064
H	5.974827	-2.645567	-3.140104
H	-7.259475	-0.090412	-1.714918
H	-0.004358	1.553058	-4.06006
H	-1.9399	-2.212037	-0.339342
H	4.22899	-3.87858	-1.924966
H	4.848586	1.807742	-1.484704
H	5.017406	1.951558	0.272674
H	4.715018	3.394204	-0.703463
H	2.61538	3.892371	0.80292
H	3.034785	2.442792	1.735426
H	1.416687	2.603835	1.04751
H	-7.441486	-2.381528	-0.744815
H	0.856007	-2.530926	-1.078661
H	1.03418	-4.076633	-3.017398
H	0.613963	-4.926462	-1.519033
H	2.259755	-5.027282	-2.157495
H	0.215288	3.908067	-4.727349
H	3.151353	-4.115646	0.174926
H	1.464182	-4.095453	0.717707
H	2.436622	-2.621781	0.818898
H	-2.97209	-2.267171	1.90093
H	-1.99145	-3.703738	1.599503
H	-3.758607	-3.816359	1.521286
H	2.917144	4.560243	-1.46408
H	-3.284333	3.567117	-4.765918
H	-3.357572	4.880824	-0.684981
H	-3.595719	5.381436	-3.081903
H	-0.852076	3.509481	0.733428
H	-1.686071	3.223595	2.269332
H	-2.204289	4.550991	1.215484
H	1.694006	5.429164	-3.411755
H	-3.516941	-4.769886	-0.941517
H	-1.764191	-4.642443	-0.738493
H	-2.558049	-3.848537	-2.113732
H	-4.633256	3.604156	1.09826
H	-4.105655	2.377019	2.265573
H	-4.870357	1.882389	0.743652
H	-2.403828	1.543861	0.697371

Table S16 Geometry data of **4** for the optimized S_1 state

Au	-0.219015	0.022462	-0.093986
I	0.813034	-0.128482	2.312984
P	1.044115	0.071323	-2.205956
P	-2.146367	0.021985	-1.508992
C	0.282551	-1.020386	-4.649663
C	-2.436111	-1.164047	-4.013717
C	-3.741882	-2.077522	-0.375092
C	3.746897	-0.340387	-2.721569
C	-4.897834	-0.211088	-1.42386
C	-3.697501	-0.83637	-1.043539
C	-2.002149	-1.581289	-5.259
C	-1.54848	-0.681793	-3.036029
C	-2.524049	2.252183	-3.123555
C	-0.126733	-0.608101	-3.35387
C	2.807058	2.305461	-0.561471

C	4.939542	-1.048323	-2.806506
C	-2.650886	1.772362	-1.813582
C	-0.612237	-1.501013	-5.577883
C	-4.997732	-2.61881	-0.081668
C	4.976498	-2.376863	-2.400396
C	1.570638	1.754461	-2.761932
C	-6.131835	-0.783701	-1.138614
C	-3.066276	2.63949	-0.779934
C	2.320031	2.643008	-1.959391
C	1.115669	2.171831	-4.02157
C	-2.508724	-2.857561	0.032966
C	2.573784	-0.939253	-2.231911
C	2.600741	-2.295944	-1.839491
C	3.815477	-2.981372	-1.932326
C	4.328821	2.412594	-0.426811
C	2.110364	3.192534	0.4752
C	-6.181405	-1.990588	-0.451047
C	1.377605	-3.060761	-1.374769
C	0.97725	-4.108798	-2.418572
C	1.420473	3.433717	-4.515019
C	1.583754	-3.68717	0.006361
C	-2.378918	-2.937509	1.556225
C	2.601232	3.912937	-2.476219
C	-2.818096	3.575402	-3.432357
C	-3.355544	3.965059	-1.118881
C	-3.236425	4.434951	-2.422403
C	-2.250382	2.96847	1.580517
C	2.169238	4.310025	-3.735493
C	-2.500064	-4.25046	-0.603103
C	-4.658397	2.349155	1.159934
C	-3.214808	2.20486	0.668394
H	1.342758	-0.991295	-4.897085
H	-3.495591	-1.227046	-3.771036
H	3.72331	0.692372	-3.052112
H	-4.864139	0.738498	-1.948895
H	-2.708278	-1.988664	-5.975296
H	-2.195293	1.572665	-3.904671
H	2.5363	1.26655	-0.337506
H	5.830359	-0.560085	-3.192282
H	-0.254026	-1.846664	-6.543381
H	-5.047509	-3.566378	0.448629
H	5.900651	-2.945836	-2.455883
H	-7.044766	-0.283121	-1.449366
H	0.516639	1.492226	-4.620046
H	-1.627249	-2.32503	-0.347582
H	3.84946	-4.025789	-1.632984
H	4.844469	1.752069	-1.130946
H	4.633348	2.127479	0.586344
H	4.678047	3.43699	-0.602123
H	2.388146	4.24529	0.343766
H	2.389625	2.887288	1.489019
H	1.020905	3.119521	0.391887
H	-7.136845	-2.44753	-0.207557
H	0.541782	-2.354254	-1.294463
H	0.765871	-3.640159	-3.384859
H	0.077981	-4.644997	-2.096836
H	1.775299	-4.847379	-2.561219
H	1.06934	3.730147	-5.499669
H	2.381306	-4.439064	-0.005894
H	0.666563	-4.190242	0.333595
H	1.83845	-2.9298	0.754772
H	-2.348652	-1.940079	2.006502
H	-1.454614	-3.455325	1.835272
H	-3.220182	-3.486259	1.996358
H	3.174503	4.610553	-1.87053
H	-2.71559	3.930024	-4.454172
H	-3.682279	4.648778	-0.338979
H	-3.46741	5.473297	-2.645672
H	-1.2115	2.843876	1.258581
H	-2.325853	2.598407	2.608881
H	-2.47652	4.041267	1.590043
H	2.410426	5.304261	-4.102479
H	-3.347879	-4.854925	-0.260743
H	-1.585002	-4.786665	-0.328119
H	-2.547213	-4.18737	-1.6953
H	-4.983027	3.396327	1.144208
H	-4.741811	1.991492	2.192501
H	-5.351355	1.768447	0.542948
H	-2.954584	1.141227	0.740517

Table S17 Geometry data of **4** for the optimized T_1 state with TD-DFT

Au	-0.23146	0.011861	-0.103712
I	0.74688	-0.151252	2.32603
P	1.021579	0.031597	-2.216775
P	-2.145196	0.044614	-1.543413
C	0.283934	-1.192921	-4.601256
C	-2.449111	-1.245896	-3.994465
C	-3.76381	-2.031755	-0.415273
C	3.724464	-0.311252	-2.775825
C	-4.901656	-0.130817	-1.423126
C	-3.708247	-0.77904	-1.061518
C	-2.004197	-1.76196	-5.1918
C	-1.56596	-0.681496	-3.046984
C	-2.488882	2.300866	-3.113523
C	-0.137246	-0.655667	-3.358266
C	2.740228	2.299023	-0.537549
C	4.931524	-0.991883	-2.873893
C	-2.606135	1.813853	-1.80543
C	-0.606029	-1.730944	-5.501456
C	-5.025122	-2.564234	-0.128177
C	5.004542	-2.315899	-2.45624
C	1.495528	1.742105	-2.731772
C	-6.141224	-0.694375	-1.145064
C	-3.002348	2.677164	-0.761363
C	2.23558	2.636887	-1.928849
C	1.039367	2.150213	-3.993698
C	-2.538315	-2.833538	-0.025539

C	2.573131	-0.935282	-2.265846
C	2.635925	-2.288242	-1.861591
C	3.865942	-2.944472	-1.96509
C	4.264542	2.399206	-0.427137
C	2.065656	3.189565	0.510218
C	-6.201937	-1.914873	-0.481988
C	1.438862	-3.078238	-1.368929
C	1.062634	-4.164075	-2.382901
C	1.322987	3.418242	-4.484602
C	1.674274	-3.667294	0.024065
C	-2.425641	-2.979264	1.494203
C	2.498909	3.910864	-2.444841
C	-2.766013	3.630363	-3.409963
C	-3.275393	4.009503	-1.087982
C	-3.160731	4.487975	-2.388754
C	-2.194918	2.985288	1.607642
C	2.057446	4.303922	-3.702511
C	-2.524667	-4.196899	-0.722341
C	-4.600771	2.378451	1.170872
C	-3.155719	2.232154	0.683488
H	1.347215	-1.195202	-4.836241
H	-3.511407	-1.28288	-3.760104
H	3.67041	0.718957	-3.11144
H	-4.857118	0.827965	-1.93063
H	-2.708863	-2.205746	-5.887995
H	-2.180666	1.619172	-3.901635
H	2.467365	1.261487	-0.309113
H	5.805419	-0.487467	-3.276951
H	-0.244994	-2.147633	-6.436923
H	-5.084481	-3.521445	0.383598
H	5.941191	-2.8632	-2.520231
H	-7.049705	-0.177717	-1.442138
H	0.459991	1.454686	-4.594011
H	-1.650462	-2.288919	-0.371402
H	3.930498	-3.984515	-1.655904
H	4.766255	1.732848	-1.13572
H	4.583202	2.117879	0.582738
H	4.614941	3.421349	-0.613286
H	2.355527	4.239457	0.381945
H	2.351555	2.875048	1.519282
H	0.974881	3.130909	0.437681
H	-7.16201	-2.365666	-0.245185
H	0.582261	-2.396435	-1.298328
H	0.826093	-3.727927	-3.35835
H	0.183968	-4.719555	-2.037698
H	1.881438	-4.881616	-2.514937
H	0.969635	3.710717	-5.469608
H	2.49343	-4.395826	0.021476
H	0.773765	-4.189228	0.368426
H	1.911013	-2.887249	0.754682
H	-2.401572	-2.002369	1.987767
H	-1.502852	-3.507032	1.75941
H	-3.269235	-3.548483	1.902657
H	3.065919	4.614805	-1.840597
H	-2.670647	3.991085	-4.430337
H	-3.58662	4.691611	-0.300358
H	-3.379114	5.531246	-2.601602
H	-1.154471	2.859443	1.292637
H	-2.278544	2.606673	2.632191
H	-2.417796	4.058666	1.625022
H	2.284095	5.302236	-4.067787
H	-3.385199	-4.808464	-0.427103
H	-1.619686	-4.751095	-0.448884
H	-2.543867	-4.084861	-1.8114
H	-4.920234	3.427319	1.160969
H	-4.688893	2.01428	2.200769
H	-5.294647	1.805253	0.548152
H	-2.898897	1.167068	0.747963

Table S18 Geometry data of **4** for the optimized T_1 state with U-DFT

Au	-0.295586	0.008516	-0.101194
I	-0.441911	-0.114044	2.523473
P	0.929498	-0.064454	-2.145711
P	-2.247161	0.141312	-1.608513
C	0.229839	-1.371361	-4.507495
C	-2.527626	-1.139159	-4.058716
C	-3.757051	-2.066464	-0.634812
C	3.515474	-0.40833	-3.050755
C	-4.97445	-0.007299	-1.098323
C	-3.75992	-0.714377	-1.049523
C	-2.067784	-1.741924	-5.204528
C	-1.639863	-0.614266	-3.080057
C	-2.783495	2.267846	-3.2851
C	-0.203649	-0.73103	-3.32205
C	2.832585	2.010405	-0.453442
C	4.731205	-1.052251	-3.247405
C	-2.757262	1.887282	-1.934856
C	-0.660132	-1.865618	-5.433998
C	-4.977866	-2.637412	-0.263896
C	4.959494	-2.279804	-2.635666
C	1.364942	1.683124	-2.554779
C	-6.17271	-0.604782	-0.729841
C	-3.077133	2.828113	-0.932193
C	2.174217	2.49759	-1.733622
C	0.796227	2.206382	-3.722967
C	-2.518528	-2.941529	-0.612139
C	2.505872	-0.984156	-2.259727
C	2.720585	-2.243847	-1.661503
C	3.962496	-2.856798	-1.857281
C	4.360705	2.06782	-0.546518
C	2.335919	2.789851	0.767271
C	-6.172638	-1.927447	-0.30074
C	1.681447	-2.968986	-0.830273
C	1.32709	-4.324674	-1.447395
C	1.019473	3.525866	-4.098677
C	2.131279	-3.114381	0.625817
C	-2.261702	-3.535205	0.775177

C	2.383738	3.820469	-2.136914
C	-3.147026	3.554177	-3.661377
C	-3.430131	4.119624	-1.340031
C	-3.47143	4.48584	-2.6799
C	-1.965263	3.362721	1.249005
C	1.817976	4.335801	-3.298214
C	-2.616963	-4.035013	-1.68156
C	-4.398777	2.718853	1.22882
C	-3.038734	2.520335	0.553306
H	1.29895	-1.480878	-4.680566
H	-3.599999	-1.074813	-3.880196
H	3.343902	0.556589	-3.518172
H	-4.980781	1.021568	-1.442138
H	-2.774279	-2.14262	-5.925821
H	-2.521314	1.534889	-4.043143
H	2.55741	0.958928	-0.299958
H	5.49314	-0.592016	-3.870465
H	-0.294259	-2.362667	-6.327351
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H	5.908604	-2.792411	-2.767684
H	-7.098123	-0.037809	-0.782118
H	0.176785	1.559974	-4.339386
H	-1.652845	-2.318573	-0.870063
H	4.149827	-3.819932	-1.389363
H	4.734481	1.474214	-1.386567
H	4.808331	1.674175	0.373104
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H	2.60401	3.850807	0.699116
H	2.783616	2.386844	1.682291
H	1.249	2.719369	0.873411
H	-7.099688	-2.410449	-0.003756
H	0.76314	-2.367677	-0.832544
H	0.948918	-4.207319	-2.468468
H	0.554851	-4.821099	-0.848965
H	2.196071	-4.992165	-1.480243
H	0.570034	3.915994	-5.007612
H	3.029973	-3.737879	0.704291
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H	2.350889	-2.139978	1.074308
H	-2.15976	-2.752333	1.533582
H	-1.334016	-4.119446	0.767202
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H	-0.990977	3.242517	0.764391
H	-1.859784	3.056116	2.294782
H	-2.223029	4.428554	1.226253
H	2.001891	5.370637	-3.575127
H	-3.47365	-4.693801	-1.494607
H	-1.712797	-4.653423	-1.677544
H	-2.726824	-3.601954	-2.680844
H	-4.730768	3.76199	1.165339
H	-4.327421	2.456663	2.290232
H	-5.170891	2.087593	0.778023
H	-2.763096	1.466835	0.68548

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