Supporting Information

Solvent-Controlled Doublet Emission of an Organometallic Gold(I) Complex with a Polychlorinated Diphenyl(4-pyridyl)methyl Radical Ligand: Dual Fluorescence and Enhanced Emission Efficiency

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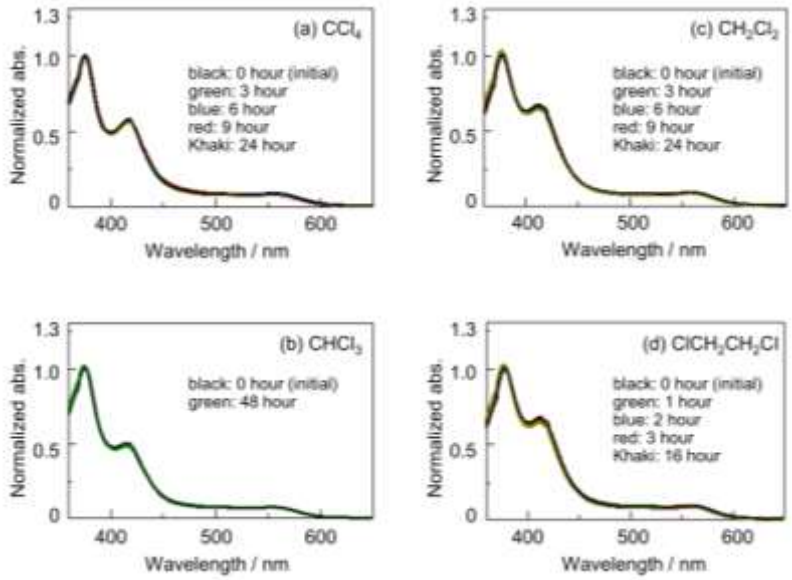


Figure S1. Time course of absorption spectra of $Au^{I}(C_6F_5)$(PyBTM) under stirring at ambient condition in CCl_4 (a), $CHCl_3$ (b), CH_2Cl_2 (c), and $ClCH_2CH_2Cl$ (d).

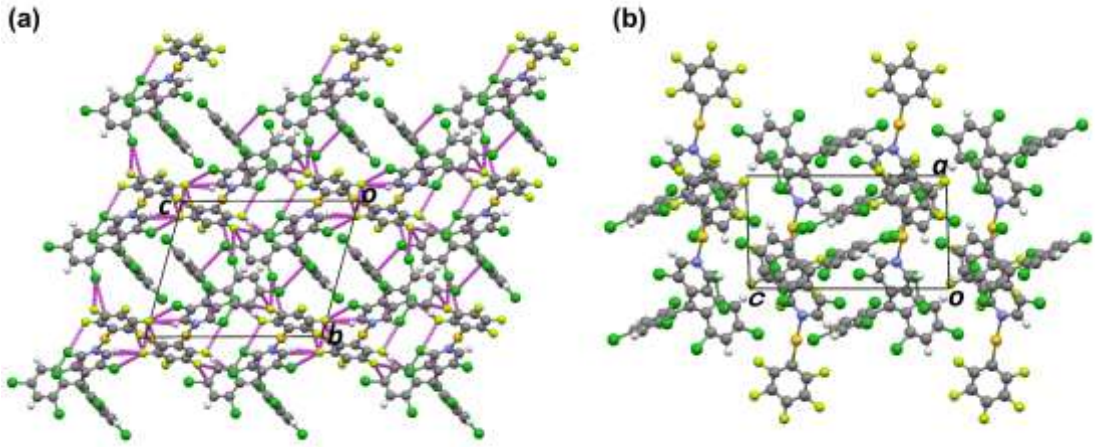
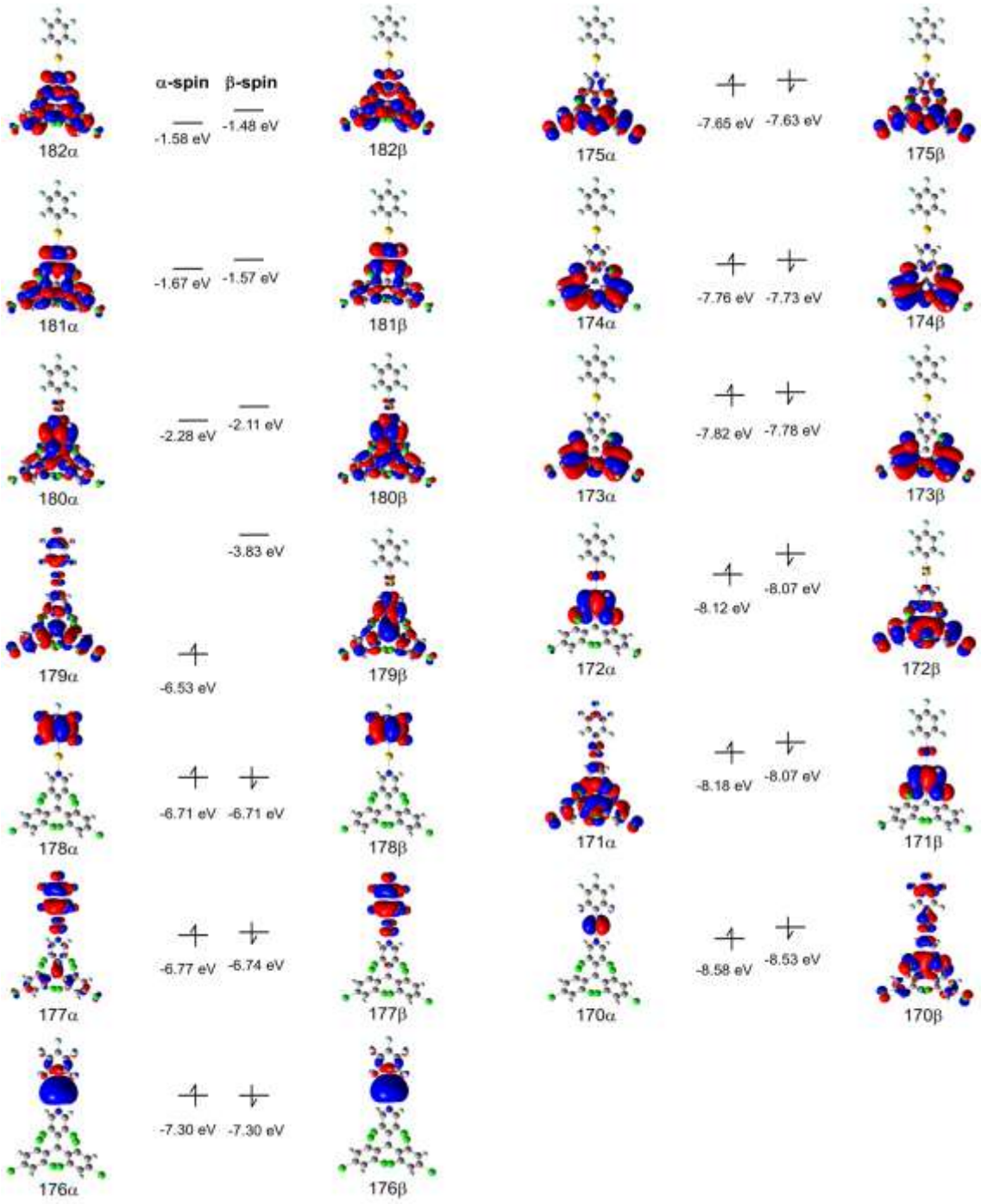
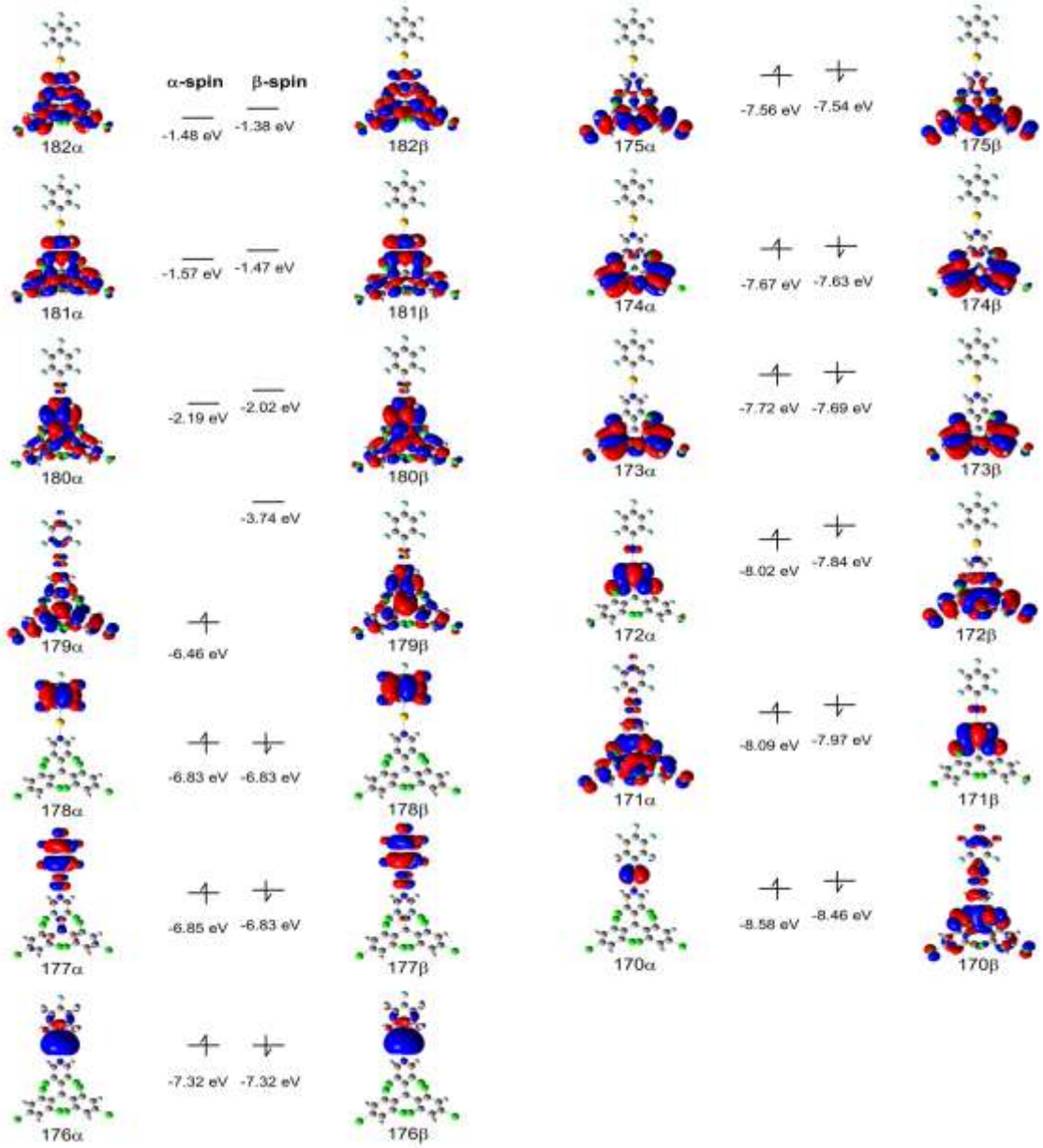


Figure S2. Crystal structure of $Au^{I}(C_6F_5)$(PyBTM) viewed along the *a*-axis (a) and the *b*-axis (b). Pinkish dashed lines in (a) indicate intermolecular short contacts.

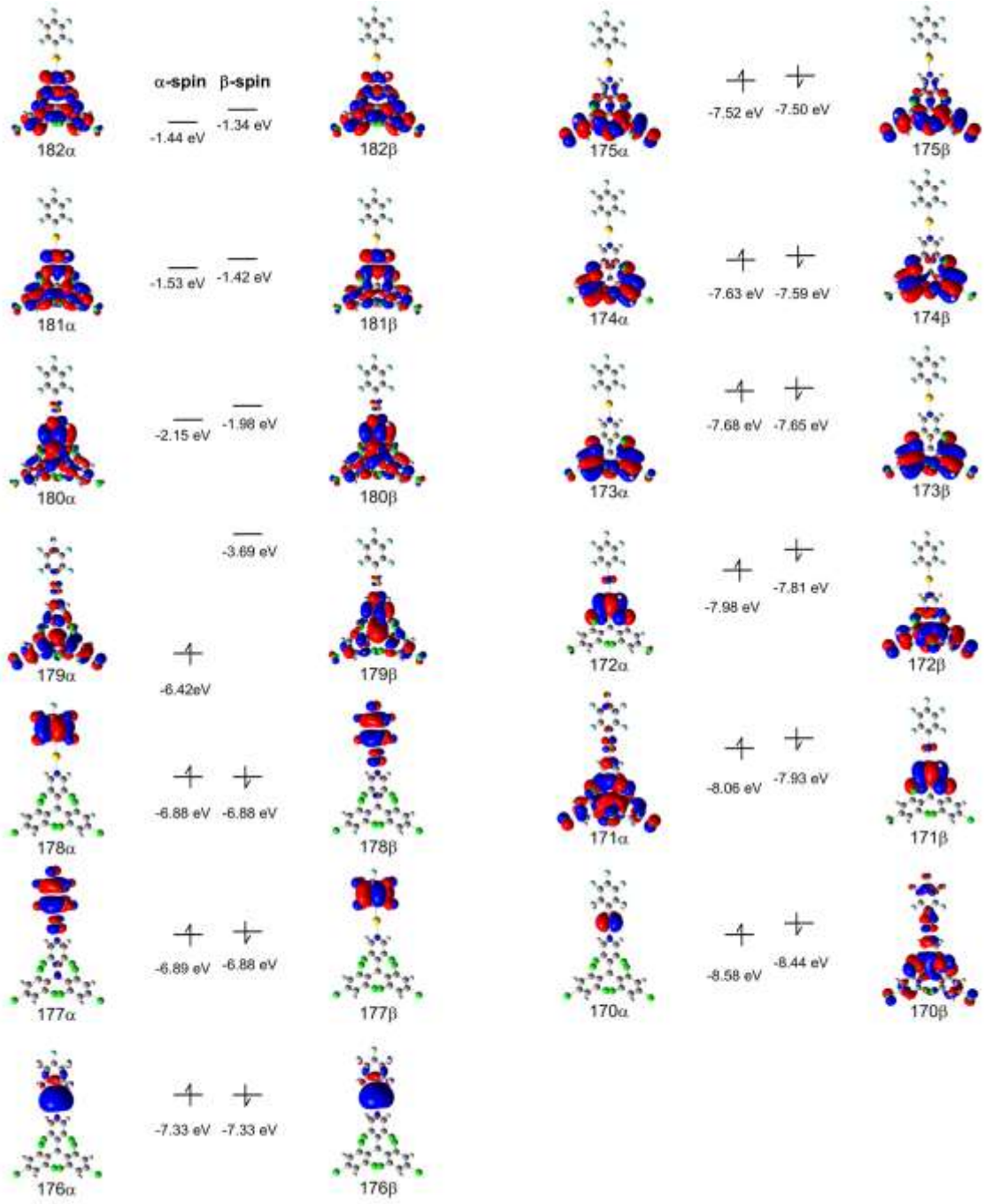
(a)


α-spin
β-spin
182α
-1.58 eV
-1.48 eV
182β
175α
-7.65 eV
-7.63 eV
175β
181α
-1.67 eV
-1.57 eV
181β
174α
-7.76 eV
-7.73 eV
174β
180α
-2.28 eV
-2.11 eV
180β
173α
-7.82 eV
-7.78 eV
173β
179α
-3.83 eV
-6.53 eV
179β
172α
-8.12 eV
-8.07 eV
172β
178α
-6.71 eV
-6.71 eV
178β
171α
-8.18 eV
-8.07 eV
171β
177α
-6.77 eV
-6.74 eV
177β
170α
-8.58 eV
-8.53 eV
170β
176α
-7.30 eV
-7.30 eV
176β

(b)


α-spin
β-spin
182α
-1.48 eV
-1.38 eV
182β
181α
-1.57 eV
-1.47 eV
181β
180α
-2.19 eV
-2.02 eV
180β
-3.74 eV
179α
-6.46 eV
179β
178α
-6.83 eV
-6.83 eV
178β
177α
-6.85 eV
-6.83 eV
177β
176α
-7.32 eV
-7.32 eV
176β
175α
-7.56 eV
-7.54 eV
175β
174α
-7.67 eV
-7.63 eV
174β
173α
-7.72 eV
-7.69 eV
173β
172α
-8.02 eV
-7.84 eV
172β
171α
-8.09 eV
-7.97 eV
171β
170α
-8.58 eV
-8.46 eV
170β

(c)


α-spin
β-spin
182α
-1.44 eV
-1.34 eV
182β
175α
-7.52 eV
-7.50 eV
175β
181α
-1.53 eV
-1.42 eV
181β
174α
-7.63 eV
-7.59 eV
174β
180α
-2.15 eV
-1.98 eV
180β
173α
-7.68 eV
-7.65 eV
173β
179α
-3.69 eV
-6.42eV
179β
172α
-7.98 eV
-7.81 eV
172β
178α
-6.88 eV
-6.88 eV
178β
171α
-8.06 eV
-7.93 eV
171β
177α
-6.89 eV
-6.88 eV
177β
170α
-8.58 eV
-8.44 eV
170β
176α
-7.33 eV
-7.33 eV
176β

(d)

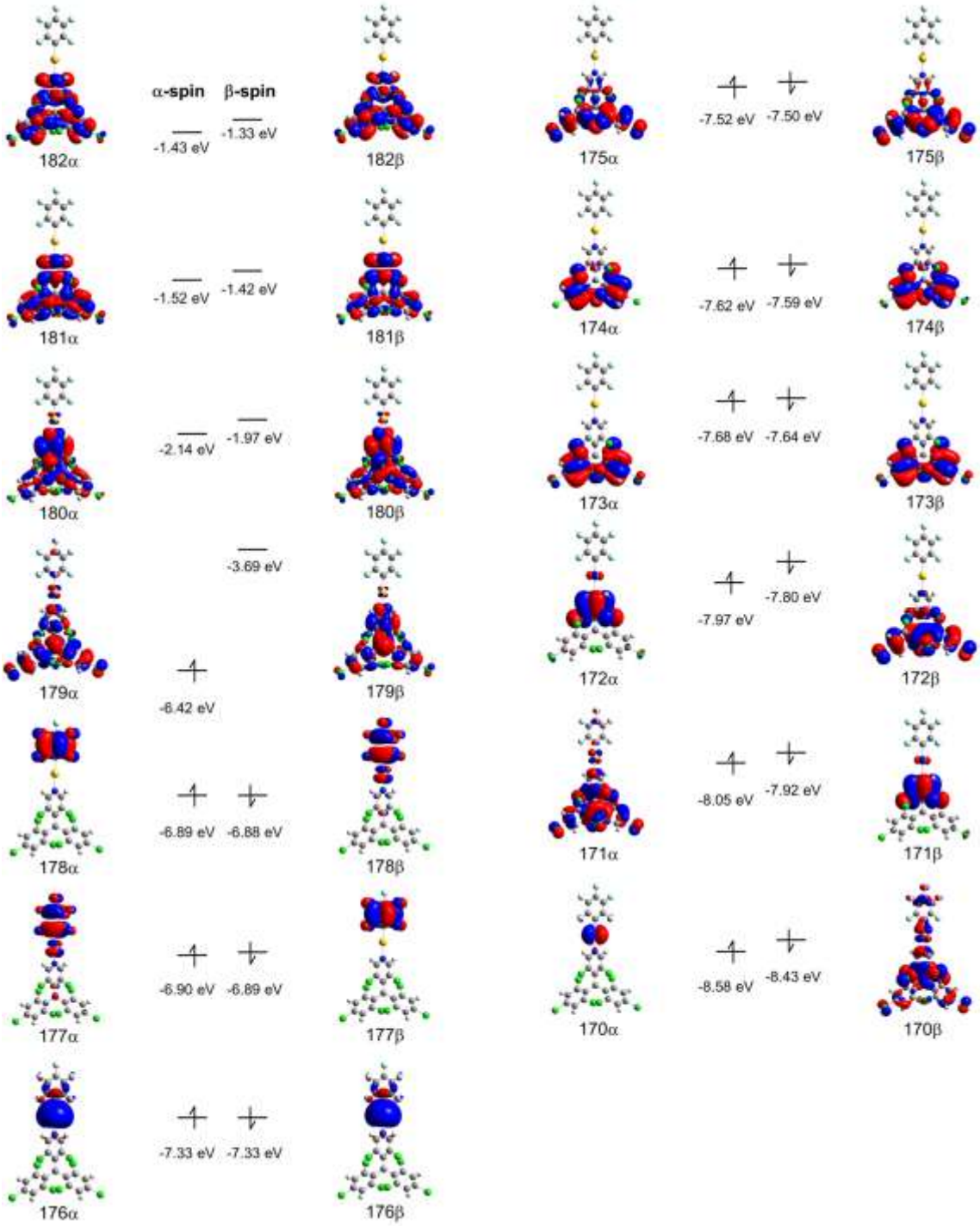


Figure S3. Unrestricted molecular orbitals of $Au^{I}(C_6F_5)$(PyBTM) calculated using DFT in (a) CCl_4, (b) $CHCl_3$, (c) CH_2Cl_2, and (d) $ClCH_2CH_2Cl$. Solvent effect was treated using PCM model.

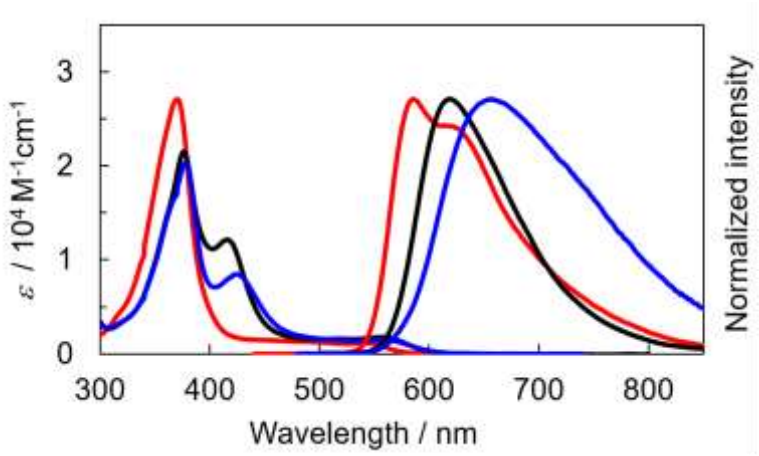


Figure S4. Absorption spectra and emission spectra of PyBTM (red), $[Au^{I}(PyBTM)PPh_3](BF_4)$ (blue), and $Au^{I}(C_6F_5)(PyBTM)$ (black) in $CHCl_3$.

(a) (b)

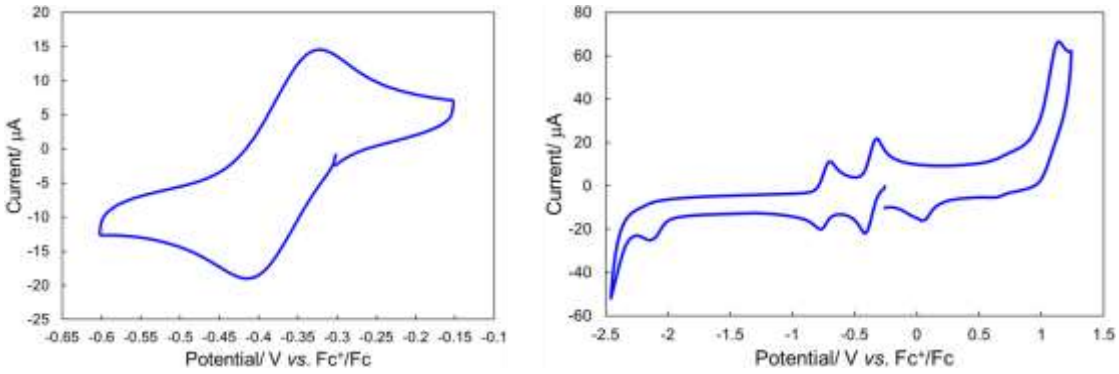


Figure S5. Cyclic voltammograms of $Au^{I}(C_6F_5)$(PyBTM) (0.5 mM) in a 0.1 M Bu_4NClO_4/CH_2Cl_2 solution at a scan rate of 0.1 V s^{-1}. (a) A redox wave at $E^{0'}$= −0.37 V attributed to the reduction of $Au^{I}(C_6F_5)$(PyBTM). (b) A sweep area from −2.4 V to 1.3 V. A redox wave at −0.74 V would be attributed to free PyBTM, suggesting that the presence of electrolyte promoted the partial dissociation of PyBTM from the Au^{I} complex.

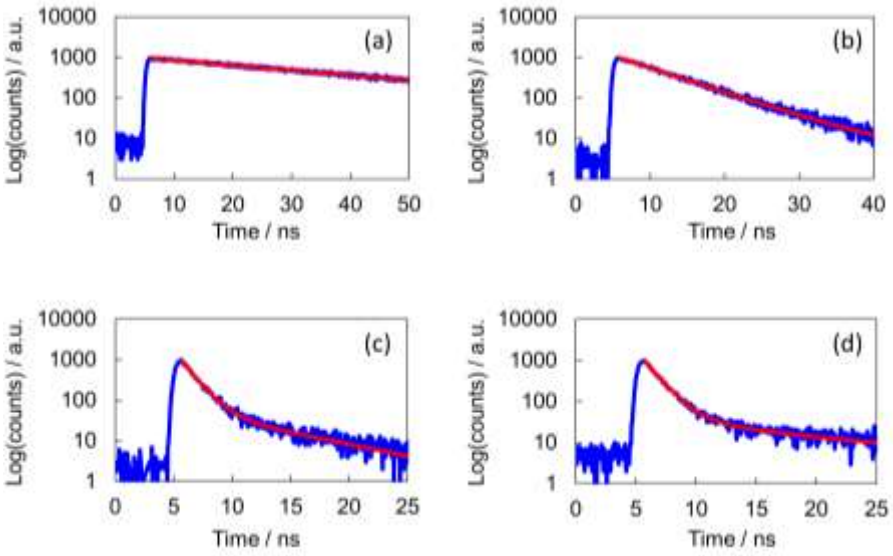


Figure S6. Fluorescence lifetime measurements of $Au^{I}(C_6F_5)$(PyBTM) at λ_{exc} = 405 nm with a LED light in halogenated solvents. Blue solid lines indicate experimental plots and red solid lines indicate calculated fitting lines. (a) In CCl_4, λ_{em} = 611 nm. (b) In $CHCl_3$, λ_{em} = 619 nm. (c) In CH_2Cl_2, λ_{em} = 625 nm. (d) In $ClCH_2CH_2Cl$, λ_{em} = 641 nm.

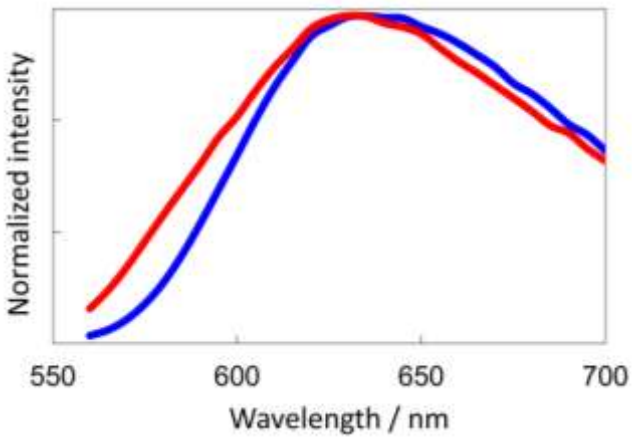


Figure S7. Time-resolved fluorescence spectra in CH_2Cl_2. Red: Component with τ_1 = 7.2 ns, Blue: Component with τ_2 = 1.2 ns.

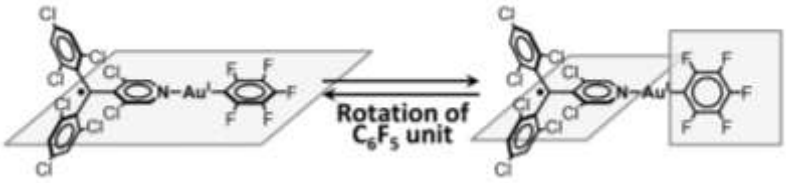


Figure S8. Possible conformational change of the complex in the excited state.

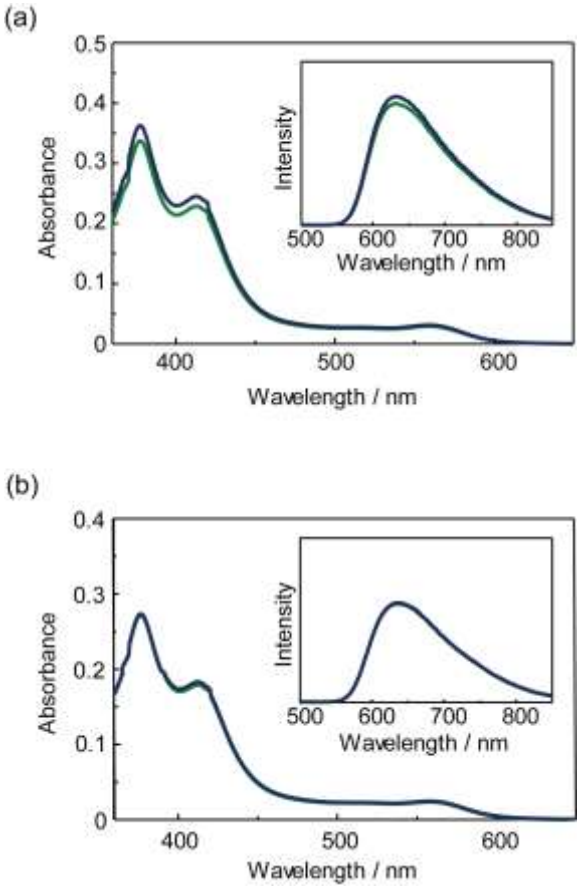


Figure S9. Absorption and emission spectra of $Au^{I}(C_6F_5)$(PyBTM) in CH_2Cl_2 (a) and $ClCH_2CH_2Cl$ (b) taken before (green) and after (blue) lifetime measurements. Slight increase in absorbance and emission intensity in (a) after the lifetime measurements would be due to increased concentration by evaporation of the solvent.

Table S1. Crystallographic data of $Au^{I}(C_6F_5)$(PyBTM).

Empirical formula	$C_{24}H_6AuCl_8F_5N$
Fw / g· mol^{-1}	883.90
Crystal system	*triclinic*
Space group	*P*-1
Crystal size / mm	0.075 × 0.050 × 0.013
Temperature / K	100
a / Å	7.962(2)
b / Å	11.660(3)
c / Å	14.579(4)
α / º	74.674(6)
β / º	87.725(7)
γ / º	87.251(6)
V / $Å^3$	1303.3(6)
Z	2
D_{calcd} / g· cm^{-3}	2.252
λ / Å	0.35400
μ / mm^{-1}	1.066
Reflections collected	22829
Independent reflections	5960
Parameters	353
R_{int}	0.0714
R_1 ($I > 2.00\sigma(I)$) [a]	0.0446
wR_2 (All reflections) [b]	0.1140
GoF [c]	1.048

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

[c] $GOF = [\Sigma(w(F_o^2 - F_c^2)^2/\Sigma(N_r - N_p)^2]$.

Table S2. Half-lives $t_{1/2}$ of compounds in CH_2Cl_2 upon continuous photoirradiation.

Compound	$t_{1/2}$ / s
TTM [1a]	177
PyBTM [7]	$(1.5\pm0.2)\times10^4$
$[Au^I(PyBTM)PPh_3]BF_4$ [7]	$(5.0\pm1.1)\times10^4$
$Au^I(C_6F_5)(PyBTM)$	$(1.2\pm0.4)\times10^5$

Table S3. Hyperfine coupling constants (hccs) for nitrogen and hydrogen atoms in $Au^{I}(C_6F_5)$(PyBTM) obtained by simulation (Sim.) and DFT calculation (Calc.)

hcc / mT	N	H
Sim.	0.120	0.165
		0.165
		0.145
		0.145
		0.094
		0.094
Calc.	0.207	0.162
		0.161
		0.147
		0.146
		0.117
		0.110

Table S4. Electronic transitions of $Au^{I}(C_6F_5)$(PyBTM) in solvents calculated by TDDFT. The transitions with the oscillator strengths over 0.01 are shown.

In CCl_4.	Electronic transition	coefficient	Excitation energy / eV	Oscillator strength
	170B ->179B	0.12675	2.3914	0.0464
	172B ->179B	-0.13823		
	174B ->179B	-0.11999		
	177B ->179B	0.96061		
	179A ->181A	0.13716	2.4981	0.0424
	179A ->182A	-0.14013		
	173B ->179B	-0.18479		
	175B ->179B	0.90370		
	175B ->180B	0.12576		
	176B ->179B	-0.10513		
	172A ->180A	-0.17695	2.9896	0.0132
	179A ->181A	-0.15202		
	171B ->179B	0.93278		
	171B ->180B	-0.16306		
	171A ->180A	0.19675	3.0065	0.1734
	177A ->180A	-0.13412		
	179A ->180A	0.73399		
	170B ->179B	-0.34775		
	171B ->181B	-0.10100		
	172B ->179B	-0.40266		
	171A ->180A	-0.19978	3.2110	0.0927
	172A ->181A	-0.15705		
	173A ->182A	0.12628		

	173A ->183A	0.11324		
	174A ->184A	0.14508		
	175A ->181A	-0.11502		
	175A ->182A	0.13546		
	177A ->180A	-0.21250		
	179A ->180A	0.33117		
	179A ->191A	0.11579		
	166B ->179B	0.17665		
	170B ->179B	0.54960		
	170B ->180B	-0.11371		
	171B ->181B	0.20525		
	172B ->179B	-0.23032		
	172B ->180B	0.15649		
	173B ->182B	0.11600		
	173B ->183B	-0.10387		
	174B ->184B	0.12898		
	175B ->182B	-0.14177		
	177B ->179B	-0.10388		
	173A ->184A	0.22541	3.3014	0.1296
	174A ->182A	0.10828		
	174A ->183A	0.22506		
	175A ->180A	-0.18460		
	175A ->191A	-0.12790		
	177A ->181A	-0.16254		
	177A ->182A	0.15481		
	179A ->181A	0.42123		
	179A ->182A	-0.40622		
	171B ->179B	0.16137		
	172B ->181B	-0.11171		
	172B ->182B	-0.15597		
	173B ->179B	0.16200		

	173B ->184B	-0.19853		
	174B ->182B	-0.12936		
	174B ->183B	0.17898		
	175B ->179B	-0.30392		
	175B ->180B	0.19792		
	175B ->191B	-0.12511		
In $CHCl_3$.	**Electronic transition**	**coefficient**	**Excitation energy / eV**	**Oscillator strength**
	179A ->181A	0.15131	2.4999	0.0422
	179A ->182A	-0.14175		
	173B ->179B	-0.18974		
	175B ->179B	0.90138		
	175B ->180B	0.12589		
	176B ->179B	-0.11303		
	179A ->180A	0.18284	2.5425	0.0445
	170B ->179B	-0.17107		
	172B ->179B	0.32153		
	174B ->179B	0.30872		
	177B ->179B	0.82997		
	172A ->180A	-0.17944	2.9842	0.0129
	179A ->181A	-0.14988		
	171B ->179B	0.93469		
	171B ->180B	-0.16340		
	171A ->180A	0.19067	3.0153	0.1828
	179A ->180A	0.76072		
	170B ->179B	-0.33620		
	172B ->179B	-0.39589		
	177B ->179B	-0.12020		

171A ->180A	-0.20264	3.2224	0.0788
172A ->181A	-0.15787		
173A ->182A	0.12508		
173A ->183A	0.11325		
174A ->184A	-0.14491		
175A ->181A	-0.11919		
175A ->182A	0.13009		
177A ->180A	-0.14304		
179A ->180A	0.33843		
179A ->191A	-0.12848		
166B ->179B	0.11981		
170B ->179B	0.57139		
170B ->180B	-0.11730		
171B ->181B	0.20783		
172B ->179B	-0.22623		
172B ->180B	0.15739		
173B ->182B	0.11684		
173B ->183B	-0.10424		
174B ->184B	0.12954		
175B ->182B	-0.13908		
177B ->179B	0.14216		
173A ->184A	0.22542	3.3047	0.1283
174A ->182A	-0.10837		
174A ->183A	-0.22611		
175A ->180A	-0.18395		
175A ->191A	0.13526		
179A ->181A	0.45960		
179A ->182A	-0.40632		
171B ->179B	0.15801		
172B ->181B	-0.11766		

	172B ->182B	-0.15381		
	173B ->179B	0.16266		
	173B ->184B	-0.19861		
	174B ->182B	-0.12858		
	174B ->183B	0.18074		
	175B ->179B	-0.30469		
	175B ->180B	0.19764		
	175B ->191B	-0.11170		
In CH_2Cl_2.	**Electronic transition**	**coefficient**	**Excitation energy / eV**	**Oscillator strength**
	179A ->181A	0.15865	2.5020	0.0418
	179A ->182A	0.13736		
	173B ->179B	-0.19116		
	175B ->179B	0.89855		
	175B ->180B	-0.12566		
	176B ->179B	0.12835		
	179A ->180A	-0.23660	2.5851	0.0364
	170B ->179B	0.17877		
	172B ->179B	-0.43933		
	174B ->179B	-0.44267		
	178B ->179B	0.66766		
	172A ->180A	-0.17962	2.9811	0.0126
	179A ->181A	0.14541		
	171B ->179B	0.93124		
	171B ->180B	0.16264		
	176B ->179B	0.10795		
	171A ->180A	0.18701	3.0218	0.1876
	179A ->180A	0.76695		

170B ->179B	-0.32796		
172B ->179B	-0.39004		
178B ->179B	0.14775		
171A ->180A	-0.20270	3.2292	0.0721
172A ->181A	0.15549		
172A ->182A	-0.10073		
173A ->182A	-0.12383		
173A ->183A	-0.11325		
174A ->184A	-0.14490		
175A ->181A	0.12314		
175A ->182A	0.12475		
177A ->180A	-0.12758		
179A ->180A	0.33320		
179A ->191A	0.12949		
165B ->179B	-0.10123		
170B ->179B	0.57457		
170B ->180B	0.11791		
171B ->181B	0.20690		
172B ->179B	-0.22767		
172B ->180B	-0.15723		
173B ->182B	0.11712		
173B ->183B	0.10421		
174B ->184B	0.12958		
175B ->182B	-0.13640		
178B ->179B	-0.16677		
173A ->184A	0.22562	3.3072	0.1273
174A ->182A	0.10933		
174A ->183A	0.22629		
175A ->180A	0.18302		
175A ->191A	0.13599		

	179A ->181A	0.47763		
	179A ->182A	0.39011		
	171B ->179B	-0.15637		
	172B ->181B	0.12307		
	172B ->182B	-0.15037		
	173B ->179B	0.16290		
	173B ->184B	-0.19862		
	174B ->182B	-0.12887		
	174B ->183B	-0.18106		
	175B ->179B	-0.30614		
	175B ->180B	-0.19715		
In $ClCH_2CH_2Cl$.	**Electronic transition**	**coefficient**	**Excitation energy / eV**	**Oscillator strength**
	179A ->181A	0.15937	2.5020	0.0422
	179A ->182A	-0.13616		
	173B ->179B	-0.19139		
	175B ->179B	0.89820		
	175B ->180B	0.12567		
	176B ->179B	-0.13116		
	179A ->180A	0.24149	2.5891	0.0353
	170B ->179B	-0.17844		
	172B ->179B	0.45269		
	174B ->179B	0.45842		
	178B ->179B	0.64350		
	179A ->180A	-0.10969	2.7306	0.0100
	172B ->179B	-0.34121		
	174B ->179B	-0.54036		
	178B ->179B	0.71200		

172A ->180A	-0.17919	2.9805	0.0127
179A ->181A	-0.14411		
171B ->179B	0.92966		
171B ->180B	-0.16245		
176B ->179B	0.12323		
171A ->180A	0.18609	3.0221	0.1901
179A ->180A	0.76903		
170B ->179B	-0.32500		
172B ->179B	-0.38887		
178B ->179B	-0.15157		
171A ->180A	-0.20294	3.2299	0.0711
172A ->181A	-0.15525		
172A ->182A	-0.10212		
173A ->182A	0.12346		
173A ->183A	0.11305		
174A ->184A	-0.14467		
175A ->181A	-0.12385		
175A ->182A	0.12398		
177A ->180A	0.12586		
179A ->180A	0.33054		
179A ->191A	-0.12967		
170B ->179B	0.57575		
170B ->180B	-0.11820		
171B ->181B	0.20668		
172B ->179B	-0.22676		
172B ->180B	0.15728		
173B ->182B	-0.11710		
173B ->183B	-0.10421		
174B ->184B	0.12957		
175B ->182B	0.13577		

	178B ->179B	0.17107		
	173A ->184A	0.22542	3.3069	0.1284
	174A ->182A	-0.10944		
	174A ->183A	-0.22601		
	175A ->180A	-0.18307		
	175A ->191A	0.13609		
	179A ->181A	0.48104		
	179A ->182A	-0.38752		
	171B ->179B	0.15593		
	172B ->181B	-0.12395		
	172B ->182B	0.14952		
	173B ->179B	0.16261		
	173B ->184B	-0.19864		
	174B ->182B	0.12889		
	174B ->183B	0.18111		
	175B ->179B	-0.30595		
	175B ->180B	0.19675		

Cartesian coordinates of the optimised geometries of radicals by DFT calculation for $Au^{I}(C_6F_5)$(PyBTM) in solvents

In CCl_4.

Tag	Elements	Coordinates / Å		
		X	Y	Z
1	Au	-3.463330	-0.065640	0.054997
2	Cl	1.486683	1.894199	2.008373
3	Cl	1.499701	-2.003503	-1.874741
4	Cl	5.230144	0.650996	2.041903
5	Cl	2.043124	1.875595	-2.258344
6	Cl	5.770612	5.307785	-0.539291
7	Cl	2.319130	-1.936589	2.329448
8	Cl	5.144562	-0.479399	-2.145830
9	Cl	6.164864	-5.096183	0.356413
10	F	-5.606621	-2.036971	-1.245745
11	F	-8.287350	-1.970867	-1.315410
12	F	-9.637016	0.051534	-0.111737
13	F	-8.278112	2.020084	1.168945
14	F	-5.597371	1.977214	1.254173
15	N	-1.313479	-0.085521	0.087841
16	C	2.978615	0.001381	0.017835
17	C	-0.635408	0.766429	0.867338
18	C	0.748995	0.807456	0.877661
19	C	1.516871	-0.044729	0.057479
20	C	0.757351	-0.931547	-0.733004
21	C	-0.627313	-0.926217	-0.696842
22	C	4.964279	3.778945	-0.376440
23	C	5.380687	2.889988	0.605198
24	C	4.727567	1.673025	0.723820
25	C	3.655645	1.293327	-0.112679

26	C	3.282946	2.243107	-1.087969
27	C	3.914506	3.468316	-1.229752
28	C	5.245742	-3.626668	0.258192
29	C	4.233006	-3.393726	1.178926
30	C	3.509462	-2.215528	1.086440
31	C	3.752488	-1.238408	0.097237
32	C	4.794309	-1.537816	-0.806810
33	C	5.536312	-2.706703	-0.739711
34	C	-5.491450	-0.032297	0.007671
35	C	-6.227663	-1.017256	-0.635738
36	C	-7.615892	-1.008801	-0.688033
37	C	-8.310243	0.024757	-0.073439
38	C	-7.611226	1.030110	0.581330
39	C	-6.223105	0.982183	0.609125
40	H	4.020942	-4.108826	1.968937
41	H	6.317060	-2.903564	-1.469180
42	H	6.189872	3.146733	1.283381
43	H	-1.200574	-1.602002	-1.327151
44	H	3.603916	4.160276	-2.007660
45	H	-1.214380	1.427311	1.508158

In $CHCl_3$.

Tag	Elements	Coordinates / Å		
		X	Y	Z
1	Au	-3.461242	-0.069581	0.057678
2	Cl	1.486454	1.888637	2.013314
3	Cl	1.500105	-2.004324	-1.874141
4	Cl	5.231282	0.653538	2.038938
5	Cl	2.035520	1.874430	-2.256147

6	Cl	5.759350	5.313460	-0.540547
7	Cl	2.325540	-1.938977	2.329018
8	Cl	5.140753	-0.473585	-2.150152
9	Cl	6.179196	-5.087417	0.351687
10	F	-5.610634	-2.045439	-1.235305
11	F	-8.289753	-1.975586	-1.308245
12	F	-9.638929	0.054635	-0.116100
13	F	-8.277942	2.027729	1.156469
14	F	-5.598783	1.982225	1.245005
15	N	-1.313772	-0.090943	0.092326
16	C	2.977850	0.001261	0.017774
17	C	-0.636130	0.760539	0.873089
18	C	0.748130	0.802605	0.881917
19	C	1.516071	-0.047383	0.059700
20	C	0.756860	-0.934147	-0.730926
21	C	-0.627681	-0.930343	-0.694181
22	C	4.955726	3.782340	-0.377314
23	C	5.375715	2.894160	0.603444
24	C	4.724783	1.676058	0.721943
25	C	3.652338	1.294644	-0.113038
26	C	3.276631	2.244357	-1.087213
27	C	3.905471	3.470848	-1.229630
28	C	5.254887	-3.620186	0.254330
29	C	4.242706	-3.391019	1.176544
30	C	3.515662	-2.214982	1.084534
31	C	3.754525	-1.236950	0.095244
32	C	4.795950	-1.533534	-0.810147
33	C	5.541855	-2.699945	-0.744326
34	C	-5.491245	-0.034177	0.008450
35	C	-6.229759	-1.020437	-0.630325
36	C	-7.617778	-1.010764	-0.684527
37	C	-8.311812	0.026266	-0.076145

38	C	-7.611802	1.033398	0.574172
39	C	-6.223912	0.983380	0.603465
40	H	4.033940	-4.106763	1.966805
41	H	6.322253	-2.894561	-1.474718
42	H	6.185398	3.152141	1.280513
43	H	-1.200300	-1.605754	-1.325121
44	H	3.592591	4.162594	-2.006761
45	H	-1.214659	1.419923	1.515499

In CH_2Cl_2.

Tag	Elements	Coordinates / Å		
		X	Y	Z
1	Au	3.460181	-0.070412	-0.057338
2	Cl	-1.486223	1.885811	-2.015727
3	Cl	-1.500762	-2.003486	1.875184
4	Cl	-5.231162	0.654124	-2.038973
5	Cl	-2.034109	1.873672	2.255679
6	Cl	-5.755148	5.315740	0.539013
7	Cl	-2.326473	-1.940358	-2.328411
8	Cl	-5.140528	-0.471395	2.150450
9	Cl	-6.183443	-5.085054	-0.350521
10	F	5.612370	-2.048047	1.232556
11	F	8.290825	-1.977772	1.304994
12	F	9.639892	0.054762	0.116069
13	F	8.278000	2.029718	-1.153098
14	F	5.599479	1.984333	-1.241107
15	N	1.313818	-0.092377	-0.092754
16	C	-2.977629	0.001096	-0.018031
17	C	0.636519	0.758348	-0.874783

18	C	-0.747674	0.800574	-0.883420
19	C	-1.515743	-0.048261	-0.060282
20	C	-0.756789	-0.934377	0.731148
21	C	0.627705	-0.930935	0.694767
22	C	-4.952671	3.783543	0.376250
23	C	-5.373734	2.895610	-0.604253
24	C	-4.723608	1.677054	-0.722242
25	C	-3.651330	1.294971	0.112611
26	C	-3.274973	2.244705	1.086504
27	C	-3.902709	3.471755	1.228774
28	C	-5.257538	-3.618375	-0.253477
29	C	-4.245178	-3.390694	-1.175833
30	C	-3.517156	-2.215268	-1.083922
31	C	-3.755119	-1.236662	-0.094972
32	C	-4.796810	-1.532238	0.810420
33	C	-5.543932	-2.697855	0.745072
34	C	5.491106	-0.034497	-0.007932
35	C	6.230685	-1.021275	0.628836
36	C	7.618639	-1.011675	0.682926
37	C	8.312582	0.026243	0.076301
38	C	7.612135	1.034106	-0.572093
39	C	6.224318	0.983791	-0.601063
40	H	-4.037109	-4.106844	-1.965889
41	H	-6.324538	-2.891570	1.475451
42	H	-6.183300	3.154065	-1.281249
43	H	1.199964	-1.605719	1.326534
44	H	-3.589260	4.163435	2.005706
45	H	1.214982	1.416854	-1.517984

In $ClCH_2CH_2Cl$.

Tag	Elements	Coordinates / Å		
		X	Y	Z
1	Au	-3.460023	-0.070395	0.057109
2	Cl	1.486221	1.885741	2.015603
3	Cl	1.500848	-2.003449	-1.875365
4	Cl	5.230797	0.653967	2.039227
5	Cl	2.034465	1.873701	-2.255935
6	Cl	5.755046	5.315863	-0.538324
7	Cl	2.326533	-1.940287	2.328424
8	Cl	5.140418	-0.471491	-2.150640
9	Cl	6.183627	-5.084970	0.350613
10	F	-5.612731	-2.048571	-1.231788
11	F	-8.291097	-1.978376	-1.303802
12	F	-9.640086	0.054653	-0.115548
13	F	-8.277993	2.030174	1.152579
14	F	-5.599552	1.984957	1.240163
15	N	-1.313834	-0.092386	0.092531
16	C	2.977589	0.001066	0.017923
17	C	-0.636581	0.758293	0.874668
18	C	0.747602	0.800503	0.883289
19	C	1.515673	-0.048279	0.060131
20	C	0.756749	-0.934331	-0.731364
21	C	-0.627738	-0.930909	-0.695060
22	C	4.952595	3.783563	-0.375826
23	C	5.373567	2.895604	0.604691
24	C	4.723434	1.677036	0.722455
25	C	3.651303	1.294960	-0.112584
26	C	3.275100	2.244758	-1.086477
27	C	3.902803	3.471841	-1.228579
28	C	5.257607	-3.618307	0.253500

29	C	4.245256	-3.390672	1.175873
30	C	3.517190	-2.215281	1.083882
31	C	3.755087	-1.236695	0.094889
32	C	4.796783	-1.532301	-0.810488
33	C	5.543981	-2.697859	-0.745118
34	C	-5.491109	-0.034456	0.007845
35	C	-6.230887	-1.021456	-0.628356
36	C	-7.618839	-1.011941	-0.682245
37	C	-8.312736	0.026181	-0.075978
38	C	-7.612189	1.034300	0.571852
39	C	4.037249	-4.106786	1.965976
40	H	4.037249	-4.106786	1.965976
41	H	6.324590	-2.891571	-1.475490
42	H	6.183011	3.154048	1.281833
43	H	-1.199949	-1.605657	-1.326881
44	H	3.589466	4.163558	-2.005517
45	H	-1.215027	1.416747	1.517911