Supplementary Information

Amplification of luminescence of stable radical by coordination to NHC−gold(I) complex

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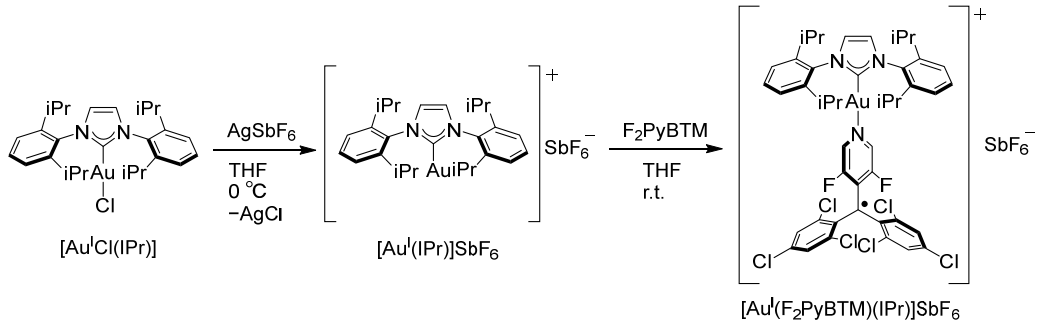
EXPERIMENTAL SECTION

Chloro(1,3-dicyclohexylimidazol-2-ylidene)gold(I), chloro[1,3-bis(2,6-diisopropylphenyl)-4,5-dihydroimidazol-2-ylidene]gold(I), chloro(*N*,*N*-dimethylbenzimidazol-2-ylidene)gold(I) were prepared according to literature procedures.[1,2,3] F_2PyBTM was synthesized according to previous report.[4] Commercially available compounds were used as received without further purification. ESR spectra were recorded with a JEOL JES-FR30EX spectrometer with X-band microwave. Sample solutions were charged in a 2.5mmϕ sample tube. Magnetic field was calibrated with the Mn^{2+}/MgO standard. Mass spectrometry was performed with a JEOL-JMS-S3000 (MALDI-Spiral-TOF MS) mass spectrometer with DCTB (20 mg/mL in $CHCl_3$) as a matrix and TFANa (1 mg/mL in THF) as a cationization agent. Absorption and emission spectra were monitored on Hitachi U-4150 spectrophotometer and Hitachi F-7100 fluorescence spectrophotometer, respectively. Photostability under 370 nm light were recorded with a JASCO FP-8600KS spectrofluorometer. Absolute luminescence quantum yields and fluorescence lifetimes were measured using Hamamatsu Photonics Quantaurus QY C11347 and Quantaurus Tau C11367, respectively. Elemental analysis was conducted at Center for Organic Elemental Microanalysis, Graduate School of Pharmaceutical Sciences, Kyoto University (**1**SbF_6, **2**SbF_6, **3**SbF_6, and **4**SbF_6) and NAIST (**5**SbF_6).

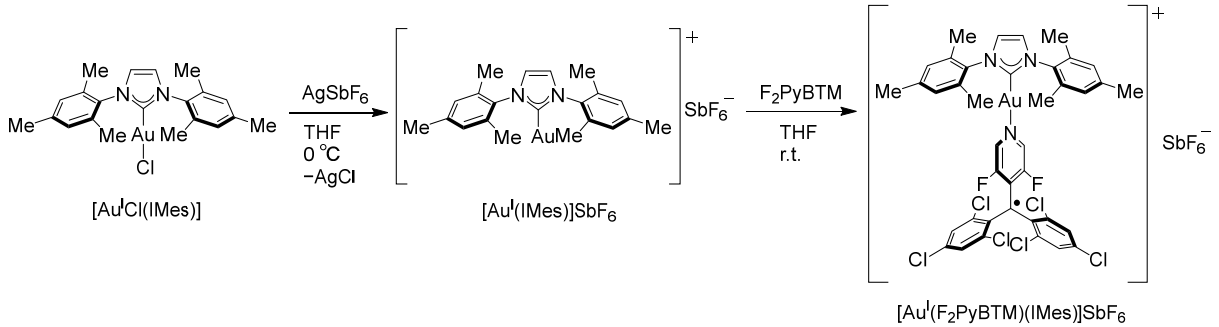
Synthesis of $[Au^I(F_2PyBTM)(IPr)]SbF_6$ (**1**SbF_6)



[Au^{I}Cl(IPr)] [Au^I(IPr)]SbF_6 [Au^I(F_2PyBTM)(IPr)]SbF_6

Under a nitrogen atmosphere, chloro[1,3-bis(2,6-diisopropylphenyl)imidazol-2-ylidene]gold(I) (31.1 mg, 0.0504 mmol) was dissolved in dry THF (2 mL) and silver hexafluoroantimonate (17.2 mg, 0.0501 mmol) was added at 0°C, stirred for 15 min, and filtered. The filtrate was added to a solution of F_2PyBTM (24.7 mg, 0.0507 mmol) in THF (2 mL), and stirred at room temperature for 30 min, and then evaporated. Red powder was precipitated from dichloromethane-hexane, washed with hexane, and dried in vacuo to afford $[Au^I(F_2PyBTM)(IPr)]SbF_6$ (45.9 mg, 0.0351 mmol, 70% yield). **ESI-TOF-MS** m/z: $[Au^I(F_2PyBTM)(IPr)]^+$ Calcd for $C_{45}H_{42}N_3AuCl_6F_2$ 1069.1144; Found 1069.1106. **Elemental Analysis** Found: C, 41.21; H, 3.39; N, 3.01. Calc. for $C_{45}H_{42}N_3F_8Cl_6SbAu$: C, 41.31; H, 3.24; N, 3.21%.

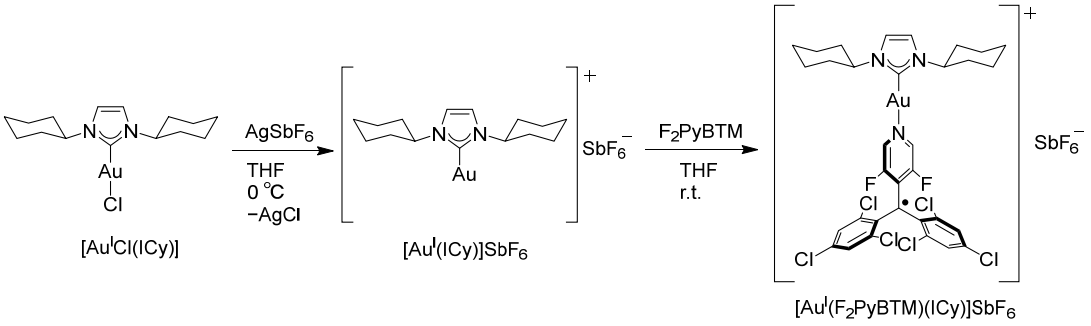
Synthesis of $[Au^I(F_2PyBTM)(IMes)]SbF_6$ (**2**SbF_6)



[Au^{I}Cl(IMes)] [Au^I(IMes)]SbF_6 [Au^I(F_2PyBTM)(IMes)]SbF_6

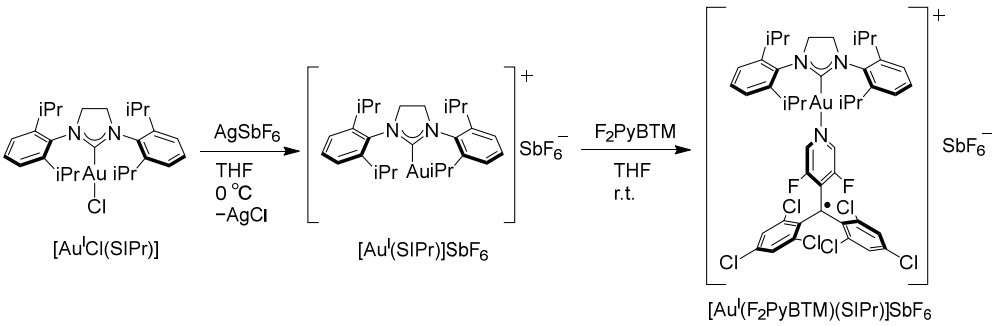
Under a nitrogen atmosphere, chloro[1,3-bis(2,4,6-trimethylphenyl)imidazol-2-ylidene]gold(I) (26.8 mg, 0.0499 mmol) was dissolved in dry THF (2 mL) and silver hexafluoroantimonate (17.4 mg, 0.0506 mmol) was added at 0°C, stirred for 15 min, and filtered. The filtrate was added to a solution of F_2PyBTM (24.4 mg, 0.0501 mmol) in THF (2 mL), and stirred at room temperature for 30 min, and then evaporated. Red powder was precipitated from dichloromethane-hexane, washed with hexane, and dried in vacuo to afford $[Au^I(F_2PyBTM)(IMes)]SbF_6$ (47.6 mg, 0.0389 mmol, 78% yield). **ESI-TOF-MS** m/z: $[Au^I(F_2PyBTM)(IMes)]^+$ Calcd for $C_{39}H_{30}N_3AuCl_6F_2$ 985.0204; Found 985.0182. **Elemental Analysis** Found: C, 38.34; H, 2.59; N, 3.56. Calc. for $C_{39}H_{30}N_3F_8Cl_6SbAu$: C, 38.27; H, 2.47; N, 3.43%.

Synthesis of $[Au^I(F_2PyBTM)(ICy)]SbF_6$ ($3SbF_6$)



Under an argon atmosphere, chloro(1,3-dicyclohexylimidazol-2-ylidene)gold(I) (42.9 mg, 0.0923 mmol) was dissolved in dry THF (3 mL) and silver hexafluoroantimonate (36.8 mg, 0.107 mmol) was added at 0°C, stirred for 15 min, and filtered. The filtrate was added to a solution of F_2PyBTM (45.5 mg, 0.0934 mmol) in THF (2 mL), and stirred at room temperature for 30 min, and then evaporated. Red sticky solid was precipitated from dichloromethane-hexane. The solid was reprecipitated from THF-hexane twice and dried in vacuo to afford $[Au^I(F_2PyBTM)(ICy)]SbF_6$ (90.8 mg, 0.0788 mmol, 85% yield). **HRMS** (MALDI-TOF MS) m/z calcd for $C_{33}H_{30}N_3F_2Cl_6Au^+$: 913.01990 $[M]^+$; found: 913.01982. **Elemental Analysis** Found: C, 35.02; H, 2.99; N, 3.57. Calc. for $C_{33}H_{30}N_3F_8Cl_6SbAu$: C, 34.41; H, 2.62; N, 3.65%. This product probably contains solvent molecules such as THF in crystals like Fig. S3. Calc. for **3**SbF_6·0.3THF, $C_{34.2}H_{32.1}N_3O_{0.3}F_8Cl_6SbAu$: C, 35.01; H, 2.76; N, 3.58%.

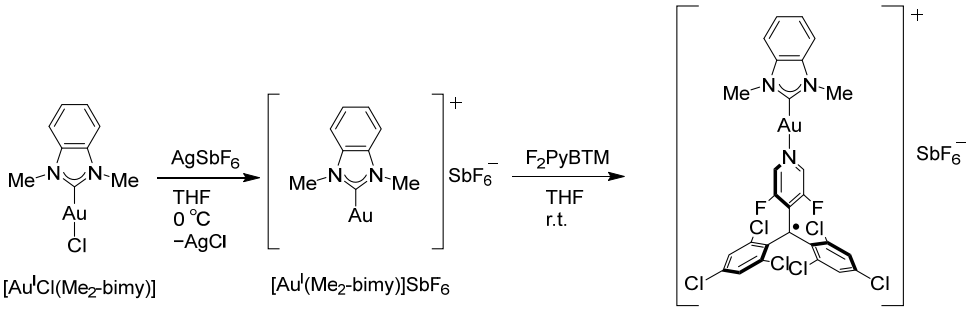
Synthesis of $[Au^I(F_2PyBTM)(SIPr)]SbF_6$ ($4SbF_6$)



Under an argon atmosphere, chloro[1,3-bis(2,6-diisopropylphenyl)-4,5-dihydroimidazol-2-ylidene]gold(I) (62.3 mg, 0.100 mmol) was dissolved in dry THF (2 mL) and silver hexafluoroantimonate (34.4 mg, 0.100 mmol) in dry THF (2 mL) was added at 0°C, stirred for 15 min, and filtered. The filtrate was added to a solution of F_2PyBTM (48.8 mg, 0.100 mmol) in THF (2 mL), and stirred at room temperature for 30 min, and then evaporated. Red powder was precipitated from dichloromethane-hexane, washed with hexane. The solid was recrystallized from acetone-water and dried in vacuo to afford $[Au^I(F_2PyBTM)(SIPr)]SbF_6$ (41.8 mg, 0.0313 mmol, 31% yield). **HRMS**

(MALDI-TOF MS) m/z calcd for $C_{45}H_{44}N_3F_2Cl_6Au^+$: 1071.12945 $[M]^+$; found: 1071.12950. **Elemental Analysis** Found: C, 41.52; H, 3.25; N, 3.01. Calc. for $C_{45}H_{44}N_3F_8Cl_6SbAu$: C, 41.25; H, 3.38; N, 3.21%.

Synthesis of $[Au^I(F_2PyBTM)(Me_2\text{-bimy})]SbF_6$ (5SbF_6)



Under an argon atmosphere, chloro(*N*,*N*-dimethylbenzimidazol-2-ylidene)gold(I) (37.8 mg, 0.0989 mmol) was dissolved in dry THF (2 mL) and silver hexafluoroantimonate (37.6 mg, 0.109 mmol) in dry THF (2 mL) was added at 0°C, stirred for 15 min, and filtered. The filtrate was added to a solution of F_2PyBTM (44.8 mg, 0.0920 mmol) in THF (2 mL), and stirred at room temperature for 30 min, and then evaporated. Red powder was precipitated from dichloromethane-hexane, washed with hexane, and dried in vacuo to afford $[Au^I(F_2PyBTM)(IMe_2\text{-bimy})]SbF_6$ (66.0 mg, 0.0619 mmol, 67% yield). **HRMS** (MALDI-TOF MS) m/z calcd for $C_{27}H_{16}N_3F_2Cl_6Au^+$: 826.91035 $[M]^+$; found: 826.90949. **Elemental Analysis** Found: C, 30.50; H, 1.28; N, 3.88. Calc. for $C_{27}H_{16}N_3F_8Cl_6SbAu$: C, 30.43; H, 1.51; N, 3.94%.

X-ray structural analysis

Red single crystals of **4**SbF_6·THF·cyclohexane were obtained by diffusing cyclohexane into a THF solution. Red single crystals of **5**SbF_6 were obtained by diffusing cyclohexane into a dichloromethane solution. Diffraction data for X-ray analysis were collected with a Rigaku VariMax RAPID II diffractometer. The crystal was kept at 103.15 K during data collection. Using Olex2,[5] the structure was solved with the SHELXT[6] structure solution program using Intrinsic Phasing and refined with the SHELXL[7] refinement package using Least Squares minimisation.

The crystallographic data are listed in Table S2. Crystal structure data (CIF, CCDC 2122598 and 2122599) can be obtained free of charge via the Internet at http://pubs.acs.org and from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

Computational details

DFT calculations of cations $\mathbf{1}^+$, $\mathbf{2}^+$, $\mathbf{3}^+$, $\mathbf{4}^+$, $\mathbf{5}^+$, and $[Au^I(F_2PyBTM)PPh_3]^+$ were executed using the Gaussian16 program package.[8] The geometries of the compounds were optimized without symmetry constraints. Calculations were performed using M06 functional[9] with the SDD basis set (Au) and the 6-31G(d) basis set (H, C, N, F, (P), Cl), and the solvent effect (dichloromethane) was treated using the polarizable continuum model.[10,11] *Surface=SAS* option was used to converge the structural optimization calculation of $\mathbf{1}^+$. Cartesian coordinates of all the optimized geometries are listed in the supporting information. Frequency calculations were carried out to ensure that the optimized geometries were minima on the potential energy surface, in which no imaginary frequencies were observed

in any of the compounds. TD-DFT calculations were performed using B3LYP to calculate the first 15 doublet transitions.

References

1. M. V. Baker, P. J. Barnard, S. J. Berners-Price, S. K. Brayshaw, J. L. Hickey, B. W. Skelton and A. H. White, *J. Organomet. Chem.*, 2005, **690**, 5625−5635.
2. P. de Frémont, N. M. Scott, E. D. Stevens and S. P. Nolan, *Organometallics*, 2005, **24**, 2411−2418.
3. H. M. J. Wang, C. Y. L. Chen and I. J. B. Lin, *Organometallics*, 1999, **18**, 1216−1223.
4. Y. Hattori, T. Kusamoto, H. Nishihara, *RSC Adv.*, 2015, **5**, 64802−64805.
5. O. V. Dolomanov, L. J. Bourhis, R. J. Gildea, J. A. K. Howard and H. Puschmann, *J. Appl. Cryst.*, 2009, **42**, 339−341.
6. G.M. Sheldrick, *Acta Cryst.*, 2015, **A71**, 3−8.
7. G. M. Sheldrick, *Acta Cryst.*, 2015, **C71**, 3−8.
8. Gaussian 16, Revision A03, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A. V. Marenich, J. Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H. P. Hratchian, J. V. Ortiz, A. F. Izmaylov, J. L. Sonnenberg, D. Williams-Young, F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone, T. Henderson, D. Ranasinghe, V. G. Zakrzewski, J. Gao, N. Rega, G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, K. Throssell, J. A. Montgomery Jr., J. E. Peralta, F. Ogliaro, M. J. Bearpark, J. J. Heyd, E. N. Brothers, K. N. Kudin, V. N. Staroverov, T. A. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. P. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi, J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas, J. B. Foresman and D. J. Fox, Gaussian, Inc., Wallingford CT, 2016.
9. Y. Zhao and D. G. Truhlar, *Theor. Chem. Acc.*, 2008, **120**, 215−241.
10. G. Scalmani and M. J. Frisch, *J. Chem. Phys.*, 2010, **132**, 114110.
11. R. Improta, V. Barone, G. Scalmani and M. J. Frisch, *J. Chem. Phys.*, 2006, **125**, 054103.

Table S1. Photostability of the new radical complexes in dichloromethane under 370 nm UV irradiation

Exp. no.	$t_{1/2}$ [s] (PyBTM)	$t_{1/2}$ [s] (**1**SbF_6)	$t_{1/2}$ [s] (**2**SbF_6)	$t_{1/2}$ [s] (**3**SbF_6)	$t_{1/2}$ [s] (**4**SbF_6)	$t_{1/2}$ [s] (**5**SbF_6)
1	314	2418	998	2096	434	2602
2	242	2308	1162	1824	488	1824
3	290	3136	1314	2174	548	2174
Ave.	282	2621	1158	2031	490	2512
σ	37	450	158	184	57	124
Relative Photostability	1.00 ± 0.13	9.29 ± 1.59	4.11 ± 0.56	7.20 ± 0.65	1.74 ± 0.20	8.91 ± 0.44

Table S2. Crystallographic data of **4**SbF_6·THF·cyclohexane and **5**SbF_6

	4SbF_6·THF·cyclohexane	**5**SbF_6
Empirical formula	$C_{55}H_{64}AuCl_6F_8N_3OSb$	$C_{27}H_{16}AuCl_6F_8N_3Sb$
Formula weight	1466.50	1065.84
Temperature/K	103.15	103.15
Crystal system	triclinic	monoclinic
Space group	*P*-1	$P2_1/c$
a / Å	12.4979(2)	15.9293(5)
b / Å	21.0791(4)	11.4765(4)
c / Å	22.2535(4)	17.8993(5)
α / °	90.337(6)	90
β / °	95.247(7)	95.454(7)
γ / °	91.396(6)	90
V / Å^3	5836.07(19)	3257.42(18)
Z	4	4
ρ_{calcd} / g cm^{-3}	1.669	2.173
μ /mm^{-1}	3.315	5.892
F(000)	2908.0	2012.0
Crystal size / mm^3	0.13 × 0.08 × 0.02	0.3 × 0.13 × 0.02
Radiation	MoKα (λ = 0.71075)	MoKα (λ = 0.71075)
2θ range for data collection/°	3.604 to 50.702	4.828 to 54.946
Index ranges	-15 ≤ h ≤ 15, -25 ≤ k ≤ 25, -26 ≤ l ≤ 26	-20 ≤ h ≤ 20, -14 ≤ k ≤ 14, -22 ≤ l ≤ 23
Reflections collected	67463	52270
Independent reflections	21345 [R_{int} = 0.0534, R_{sigma} = 0.0497]	7456 [R_{int} = 0.0634, R_{sigma} = 0.0352]
Data/restraints/parameters	21345/0/1333	7456/0/417
Goodness-of-fit on F^2	1.034	1.075
Final R indexes [I>=2σ (I)]	R_1 = 0.0490, wR_2 = 0.1167	R_1 = 0.0314, wR_2 = 0.0781
Final R indexes [all data]	R_1 = 0.0616, wR_2 = 0.1237	R_1 = 0.0344, wR_2 = 0.0797
Largest diff. peak/hole / e Å^{-3}	1.98/-1.19	2.07/-0.62
CCDC No.	2122599	2122598

Table S3. Summary of absorption and emission in dichloromethane

	λ_{abs} [nm] (ε [10^3 M^{-1} cm^{-1}])	λ_{em} [nm]
1SbF_6	372 (17), 415 (11), 557 (2.0)	629
2SbF_6	371 (21), 412 (12), 555 (2.3)	626
3SbF_6	371 (9.1), 410 (6.3), 554 (1.1)	631
4SbF_6	368 (13), 417 (6.3), 555 (1.2)	630
5SbF_6	280 (21), 287 (20), 371 (14), 413 (8.7), 555 (1.6)	629
$[Au^{I}(F_2PyBTM)PPh_3]BF_4$	367 (12), 419 (6.1), 552 (1.1)	630

Table S4. The dihedral angles between NHC ring and pyridine ring and the lengths of coordination bonds of DFT optimized structure

	Dihedral angle / °	*Coordination bond length* / Å
1SbF_6	26	2.118 (Au−N), 2.020 (Au−C)
2SbF_6	75	2.125 (Au−N), 2.021 (Au−C)
3SbF_6	88	2.129 (Au−N), 2.013 (Au−C)
4SbF_6	25	2.123 (Au−N), 2.026 (Au−C)
5SbF_6	88	2.127 (Au−N), 2.028 (Au−C)
$[Au^{I}(F_2PyBTM)PPh_3]BF_4$		2.144 (Au−N), 2.311 (Au−P)

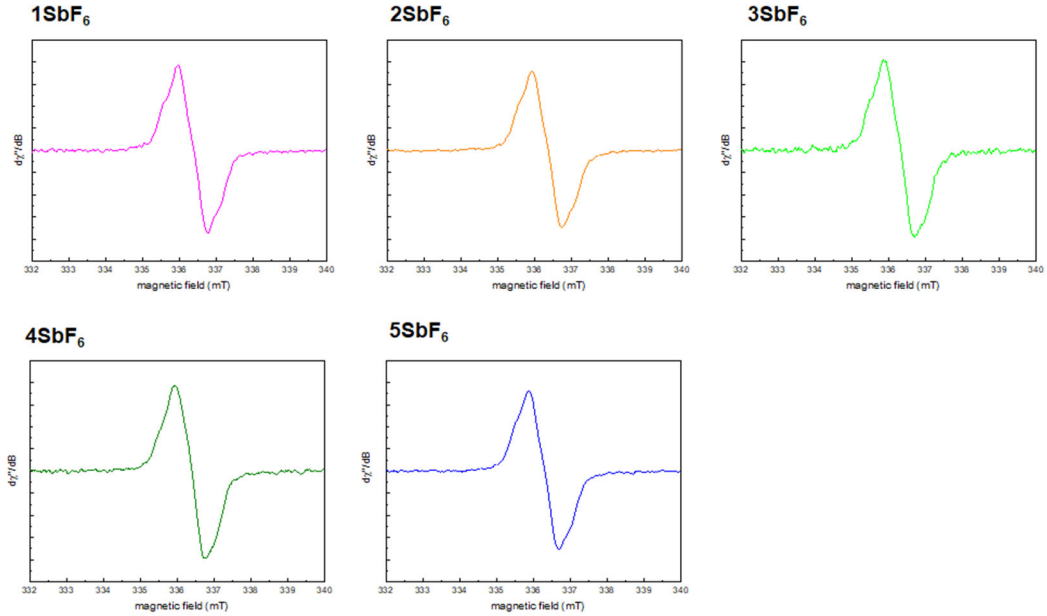


Fig. S1 ESR spectra of **1**SbF_6–**5**SbF_6 in dichloromethane. The *g* factors of **1**SbF_6–**5**SbF_6 were 2.005, 2.005, 2.005, 2.004, and 2.005, respectively.

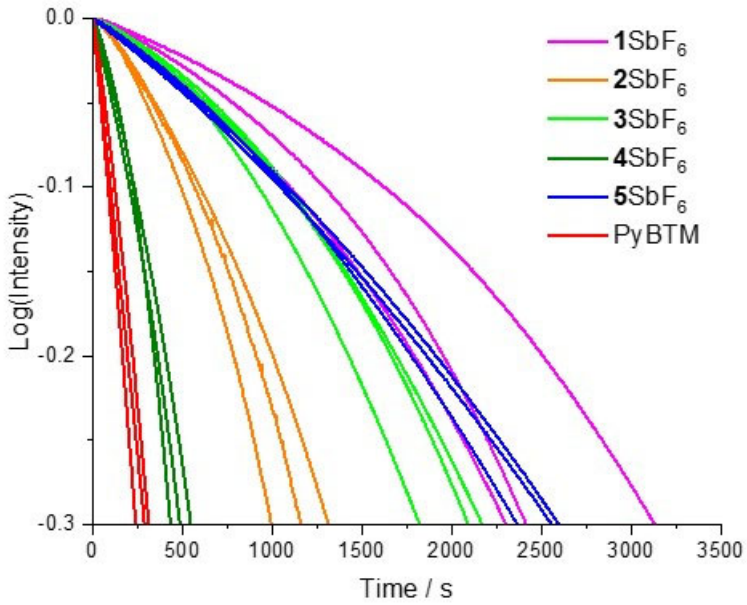


Fig. S2 Plots showing the emission decay of the radicals in dichloromethane under continuous excitation with light at λ_{ex} = 370 nm ± 10 nm. The emission was monitored at the peak emission.

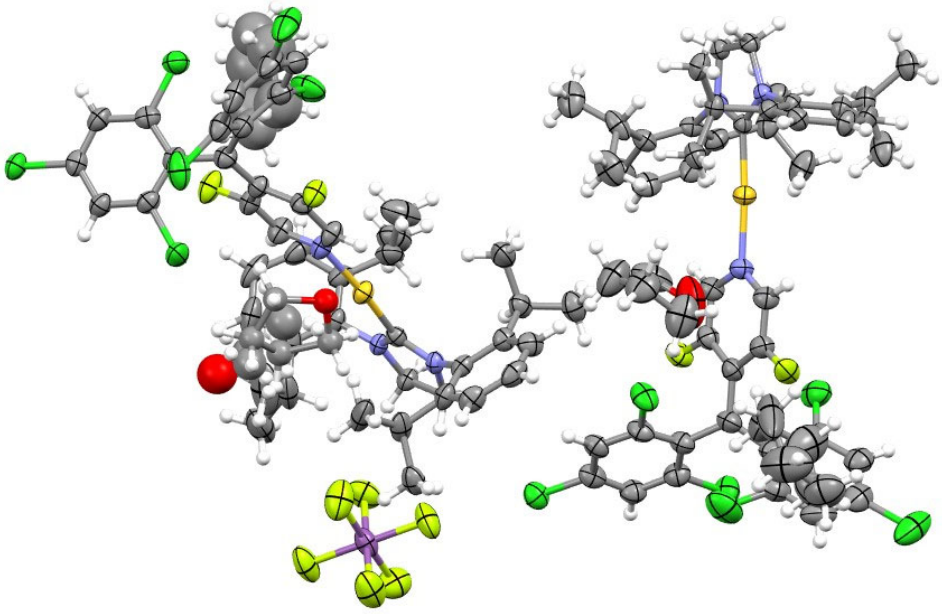


Fig. S3 Crystal structure of **4**SbF_6·THF·cyclohexane with thermal ellipsoids at the 50% probability level.

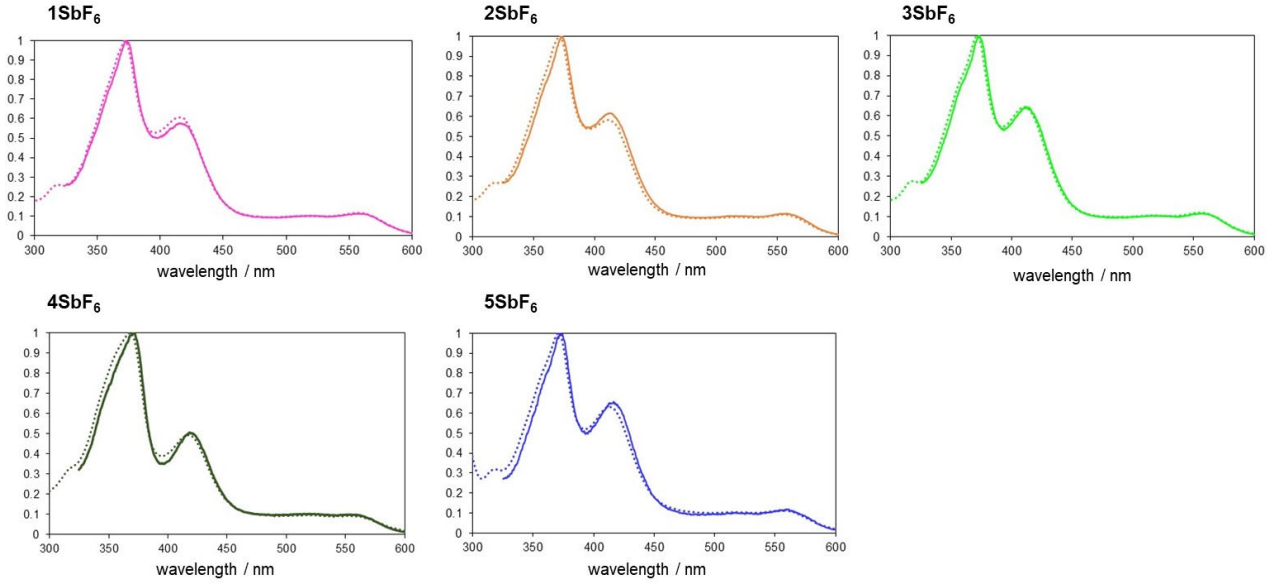


Fig. S4 Excitation spectra of **1**SbF_6–**5**SbF_6 in dichloromethane. Normalized absorption spectra are shown as dotted lines for comparison.

Cartesian coordinates of all the optimized geometries by DFT calculation

1^{+} (UM06/ SDD(Au), 6-31G(d)(H, C, N, F, Cl)) in dichloromethane

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	79	0	-2.231903	-0.013239	0.010182
2	17	0	6.294403	-0.377746	2.213468
3	17	0	7.323103	-5.153648	0.032930
4	17	0	6.294520	0.336574	-2.212831
5	17	0	7.283443	5.117817	-0.025180
6	17	0	3.445493	2.085426	2.142141
7	17	0	3.467963	-2.152698	-2.146252
8	7	0	-0.114143	-0.039588	-0.005346
9	6	0	6.685223	-2.702828	0.971735
10	6	0	2.721683	-0.035080	-0.005412
11	6	0	1.949048	-1.027143	0.629477
12	6	0	0.569788	-1.012039	0.621064
13	6	0	0.566982	0.934264	-0.633409
14	6	0	1.945991	0.953309	-0.642419
15	6	0	4.163249	-0.030074	-0.002058
16	6	0	4.897071	1.240198	-0.031484
17	6	0	4.641799	2.280982	0.886850
18	6	0	5.931158	1.486570	-0.958040
19	6	0	6.665775	2.663411	-0.967992
20	6	0	6.373346	3.643674	-0.030362
21	6	0	5.360000	3.464483	0.903528
22	6	0	4.907140	-1.294154	0.030620
23	6	0	5.941658	-1.531643	0.959262
24	6	0	6.402014	-3.686374	0.034677
25	6	0	5.389289	-3.515769	-0.901437
26	6	0	4.662177	-2.337742	-0.887495
27	1	0	7.464479	-2.848882	1.714726
28	1	0	0.011063	-1.791549	1.133404
29	1	0	0.005492	1.712660	-1.145205
30	1	0	7.445208	2.816272	-1.709410
31	1	0	5.144406	4.228793	1.645133
32	1	0	5.181055	-4.282366	-1.642779
33	9	0	2.549251	-2.005507	1.286101
34	9	0	2.543199	1.933297	-1.299485

35	6	0	-6.412064	-0.566797	0.081091
36	6	0	-6.371129	0.781034	-0.070449
37	6	0	-4.251528	0.042492	0.017841
38	7	0	-5.099417	-0.999873	0.133034
39	7	0	-5.034066	1.135868	-0.104361
40	1	0	-7.239009	-1.260949	0.155813
41	1	0	-7.154651	1.522477	-0.154693
42	6	0	-4.517957	2.471600	-0.254635
43	6	0	-4.312095	3.235221	0.902905
44	6	0	-4.205277	2.919173	-1.545326
45	6	0	-3.752834	4.501922	0.734004
46	6	0	-3.648101	4.193939	-1.655289
47	1	0	-3.570456	5.127653	1.606695
48	1	0	-3.389294	4.581746	-2.640008
49	6	0	-4.677930	-2.369649	0.256195
50	6	0	-4.523649	-3.118158	-0.918213
51	6	0	-4.419724	-2.873725	1.537556
52	6	0	-4.106138	-4.441585	-0.775130
53	6	0	-4.001683	-4.202300	1.621899
54	1	0	-3.977082	-5.061286	-1.661892
55	1	0	-3.791991	-4.636301	2.599075
56	6	0	-4.427492	2.075073	-2.783280
57	1	0	-4.971450	1.162579	-2.491993
58	6	0	-4.627436	2.711171	2.288574
59	1	0	-5.252094	1.809655	2.186268
60	6	0	-4.777714	-2.541067	-2.294813
61	1	0	-5.076651	-1.486714	-2.183731
62	6	0	-4.551680	-2.033692	2.790312
63	1	0	-4.942219	-1.042477	2.509436
64	6	0	-3.421992	4.975132	-0.529511
65	1	0	-2.986854	5.966828	-0.638141
66	6	0	-3.850536	-4.978573	0.480012
67	1	0	-3.527649	-6.014122	0.569346
68	6	0	-3.342441	2.301824	3.009682
69	1	0	-2.671369	3.163792	3.131928
70	1	0	-3.568737	1.908194	4.009647
71	1	0	-2.793163	1.526895	2.452259
72	6	0	-3.094768	1.639807	-3.392335
73	1	0	-3.259768	1.017962	-4.282178
74	1	0	-2.496907	2.509325	-3.699923
75	1	0	-2.496927	1.054582	-2.675208
76	6	0	-5.284535	2.804287	-3.815901
77	1	0	-6.241252	3.130434	-3.388855

78	1	0	-4.774061	3.693274	-4.210071
79	1	0	-5.497378	2.145916	-4.667688
80	6	0	-5.416581	3.716814	3.122991
81	1	0	-4.816854	4.604841	3.363709
82	1	0	-6.322543	4.054231	2.604231
83	1	0	-5.717432	3.263248	4.075742
84	6	0	-3.185670	-1.816137	3.440207
85	1	0	-3.277031	-1.182922	4.332484
86	1	0	-2.735410	-2.768507	3.752700
87	1	0	-2.487084	-1.324758	2.744167
88	6	0	-3.507001	-2.559694	-3.142000
89	1	0	-3.160885	-3.585457	-3.328624
90	1	0	-3.689879	-2.090296	-4.117613
91	1	0	-2.689189	-2.015156	-2.647512
92	6	0	-5.923971	-3.268516	-2.994347
93	1	0	-5.680766	-4.325503	-3.168778
94	1	0	-6.845493	-3.233625	-2.398023
95	1	0	-6.131704	-2.811720	-3.970431
96	6	0	-5.539557	-2.650400	3.777882
97	1	0	-6.525164	-2.801609	3.319006
98	1	0	-5.188732	-3.624931	4.143586
99	1	0	-5.666073	-1.998094	4.651316

2^{+} (UM06/ SDD(Au), 6-31G(d)(H, C, N, F, Cl)) in dichloromethane

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	79	0	-2.688864	0.000594	-0.013357
2	17	0	5.806867	-0.678958	-2.170434
3	17	0	6.831127	4.574701	-2.361889
4	17	0	5.800540	0.674566	2.167265
5	17	0	6.842334	-4.574951	2.365438
6	17	0	3.043015	-2.858471	-0.995430
7	17	0	3.030667	2.841166	0.989343
8	7	0	-0.563447	-0.009318	-0.013093
9	6	0	6.201714	1.958723	-2.101682
10	6	0	2.268648	-0.009388	-0.007704
11	6	0	1.498246	0.588800	-1.021976

12	6	0	0.118895	0.577672	-1.009770
13	6	0	0.115057	-0.597218	0.985662
14	6	0	1.494373	-0.608823	1.002882
15	6	0	3.711622	-0.006869	-0.003868
16	6	0	4.452742	-1.123889	0.595596
17	6	0	4.217866	-2.466940	0.233772
18	6	0	5.467069	-0.921958	1.552460
19	6	0	6.204122	-1.961528	2.101404
20	6	0	5.929336	-3.258615	1.693762
21	6	0	4.936215	-3.527366	0.760582
22	6	0	4.450530	1.113617	-0.600059
23	6	0	5.467230	0.916070	-1.555107
24	6	0	5.921516	3.254421	-1.693268
25	6	0	4.925603	3.518820	-0.761813
26	6	0	4.209881	2.455341	-0.237533
27	1	0	6.968268	1.760212	-2.845539
28	1	0	-0.440310	1.041019	-1.817724
29	1	0	-0.447285	-1.060173	1.791668
30	1	0	6.968566	-1.759593	2.846510
31	1	0	4.735481	-4.544433	0.435560
32	1	0	4.720674	4.534876	-0.436245
33	9	0	2.103919	1.169603	-2.046776
34	9	0	2.096163	-1.190168	2.029648
35	6	0	-6.851418	0.680424	0.164945
36	6	0	-6.860096	-0.623529	-0.200885
37	6	0	-4.709832	0.013161	-0.014767
38	7	0	-5.521058	1.053915	0.274297
39	7	0	-5.534969	-1.015815	-0.306925
40	1	0	-7.652370	1.381055	0.359977
41	1	0	-7.670395	-1.313165	-0.396557
42	6	0	-5.096386	-2.337349	-0.660916
43	6	0	-4.879757	-2.632082	-2.009759
44	6	0	-4.900888	-3.269605	0.362817
45	6	0	-4.451583	-3.920972	-2.323395
46	6	0	-4.471465	-4.543352	-0.003369
47	6	0	-4.246192	-4.887260	-1.337614
48	1	0	-4.275416	-4.177632	-3.369270
49	1	0	-4.310602	-5.289836	0.776190
50	6	0	-5.064640	2.360148	0.661112
51	6	0	-4.832903	2.610278	2.016650
52	6	0	-4.867615	3.321671	-0.334626
53	6	0	-4.389443	3.884454	2.366806
54	6	0	-4.421756	4.578878	0.067492

55	6	0	-4.182548	4.879011	1.409913
56	1	0	-4.202374	4.106413	3.418686
57	1	0	-4.258802	5.347480	-0.689802
58	6	0	-3.819205	-6.276546	-1.704707
59	1	0	-3.186826	-6.722004	-0.927284
60	1	0	-4.690397	-6.934920	-1.828328
61	1	0	-3.264740	-6.291267	-2.650457
62	6	0	-5.132469	-2.904905	1.798174
63	1	0	-4.445155	-2.111955	2.127912
64	1	0	-6.151361	-2.529473	1.965832
65	1	0	-4.981311	-3.771899	2.450171
66	6	0	-5.085834	-1.597184	-3.074153
67	1	0	-6.094349	-1.163449	-3.034170
68	1	0	-4.377309	-0.762900	-2.965729
69	1	0	-4.943556	-2.029033	-4.070554
70	6	0	-5.035503	1.543683	3.050135
71	1	0	-6.032480	1.087437	2.980903
72	1	0	-4.305385	0.729234	2.933002
73	1	0	-4.919866	1.952151	4.059799
74	6	0	-3.739312	6.252225	1.816250
75	1	0	-3.108201	6.715262	1.048108
76	1	0	-4.603164	6.914786	1.966349
77	1	0	-3.177955	6.232850	2.757859
78	6	0	-5.115621	3.004447	-1.778341
79	1	0	-4.453775	2.201030	-2.133589
80	1	0	-6.145927	2.664256	-1.950830
81	1	0	-4.942363	3.884686	-2.406639

3^{+} (UM06/ SDD(Au), 6-31G(d)(H, C, N, F, Cl)) in dichloromethane

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	79	0	-2.939282	0.000008	-0.000020
2	17	0	5.554289	-0.830789	-2.118361
3	17	0	6.583102	4.393523	-2.693969
4	17	0	5.554259	0.830794	2.118380
5	17	0	6.583069	-4.393516	2.694010
6	17	0	2.792364	-2.911458	-0.787532

7	17	0	2.792348	2.911457	0.787514
8	7	0	-0.810142	0.000003	-0.000024
9	6	0	5.952038	1.804495	-2.242278
10	6	0	2.022167	-0.000001	-0.000012
11	6	0	1.250068	0.513682	-1.058151
12	6	0	-0.129377	0.502926	-1.042766
13	6	0	-0.129387	-0.502922	1.042724
14	6	0	1.250058	-0.513682	1.058120
15	6	0	3.465500	0.000000	-0.000004
16	6	0	4.204076	-1.072444	0.679223
17	6	0	3.965366	-2.437130	0.414383
18	6	0	5.218267	-0.804963	1.619715
19	6	0	5.952010	-1.804490	2.242306
20	6	0	5.673285	-3.126790	1.929102
21	6	0	4.679812	-3.459243	1.016953
22	6	0	4.204083	1.072445	-0.679222
23	6	0	5.218287	0.804966	-1.619700
24	6	0	5.673309	3.126795	-1.929076
25	6	0	4.679821	3.459245	-1.016942
26	6	0	3.965367	2.437131	-0.414384
27	1	0	6.717034	1.551662	-2.971143
28	1	0	-0.689406	0.898587	-1.885429
29	1	0	-0.689423	-0.898583	1.885383
30	1	0	6.716994	-1.551655	2.971181
31	1	0	4.476178	-4.496468	0.765668
32	1	0	4.476183	4.496471	-0.765659
33	9	0	1.853415	1.007288	-2.128870
34	9	0	1.853395	-1.007288	2.128844
35	6	0	-7.101914	0.602497	0.310420
36	6	0	-7.101913	-0.602528	-0.310378
37	6	0	-4.966903	0.000001	-0.000007
38	7	0	-5.780742	0.955757	0.501355
39	7	0	-5.780741	-0.955768	-0.501349
40	1	0	-7.924545	1.230009	0.624781
41	1	0	-7.924545	-1.230049	-0.624721
42	6	0	-5.321475	2.230044	1.077467
43	6	0	-5.451044	3.357055	0.059900
44	6	0	-6.046460	2.553115	2.376424
45	1	0	-4.253313	2.072892	1.300180
46	6	0	-4.932411	4.664551	0.649173
47	1	0	-6.513213	3.466591	-0.218123
48	1	0	-4.903484	3.087915	-0.855713
49	6	0	-5.510852	3.857843	2.958851

50	1	0	-7.125256	2.667860	2.180172
51	1	0	-5.932657	1.721079	3.085389
52	6	0	-5.641460	4.999768	1.956808
53	1	0	-5.054329	5.476027	-0.080242
54	1	0	-3.849188	4.570807	0.835961
55	1	0	-6.043120	4.093551	3.889600
56	1	0	-4.449518	3.726613	3.228716
57	1	0	-5.239338	5.929160	2.381961
58	1	0	-6.710083	5.182320	1.753546
59	6	0	-5.321461	-2.230046	-1.077472
60	6	0	-5.450926	-3.357049	-0.059884
61	6	0	-6.046513	-2.553161	-2.376381
62	1	0	-4.253319	-2.072856	-1.300251
63	6	0	-4.932280	-4.664534	-0.649172
64	1	0	-6.513074	-3.466622	0.218205
65	1	0	-4.903322	-3.087878	0.855694
66	6	0	-5.510891	-3.857876	-2.958825
67	1	0	-7.125292	-2.667946	-2.180062
68	1	0	-5.932786	-1.721131	-3.085364
69	6	0	-5.641395	-4.999794	-1.956760
70	1	0	-5.054123	-5.476004	0.080261
71	1	0	-3.849072	-4.570751	-0.836026
72	1	0	-6.043207	-4.093615	-3.889538
73	1	0	-4.449578	-3.726610	-3.228756
74	1	0	-5.239265	-5.929175	-2.381926
75	1	0	-6.709999	-5.182383	-1.753431

4^{+} (UM06/ SDD(Au), 6-31G(d)(H, C, N, F, Cl)) in dichloromethane

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	79	0	-2.207704	-0.000252	-0.000264
2	17	0	6.325825	0.461137	-2.233356
3	17	0	7.268755	5.220694	0.067685
4	17	0	6.325378	-0.460926	2.233598
5	17	0	7.270022	-5.220292	-0.067138
6	17	0	3.521528	-2.050957	-2.245569
7	17	0	3.520532	2.050376	2.245183

8	7	0	-0.089827	-0.000522	-0.000519
9	6	0	6.674841	2.765827	-0.926092
10	6	0	2.759531	-0.000314	-0.000364
11	6	0	1.977616	1.017667	-0.591369
12	6	0	0.595667	1.002353	-0.584697
13	6	0	0.595748	-1.003308	0.583709
14	6	0	1.977684	-1.018434	0.590512
15	6	0	4.207036	-0.000174	-0.000153
16	6	0	4.946352	-1.277315	-0.010916
17	6	0	4.695804	-2.293201	-0.965976
18	6	0	5.960292	-1.572205	0.930574
19	6	0	6.675294	-2.765539	0.926437
20	6	0	6.382588	-3.717393	-0.043905
21	6	0	5.393036	-3.493958	-0.997345
22	6	0	4.946062	1.277159	0.010843
23	6	0	5.960137	1.572313	-0.930414
24	6	0	6.381685	3.717579	0.044212
25	6	0	5.391981	3.493876	0.997430
26	6	0	4.695047	2.292949	0.965869
27	1	0	7.433502	2.950862	-1.676977
28	1	0	0.035984	1.799369	-1.059124
29	1	0	0.036100	-1.800332	1.058167
30	1	0	7.433827	-2.950374	1.677502
31	1	0	5.178411	-4.232114	-1.760668
32	1	0	5.177014	4.231953	1.760732
33	9	0	2.578035	2.036287	-1.212278
34	9	0	2.578190	-2.036940	1.211529
35	6	0	-4.224086	0.000073	0.000063
36	7	0	-4.991784	1.087787	-0.134430
37	7	0	-4.992260	-1.087191	0.135119
38	6	0	-4.516215	-2.435003	0.300490
39	6	0	-4.332175	-3.234586	-0.846545
40	6	0	-4.273351	-2.918467	1.602758
41	6	0	-3.872069	-4.543407	-0.659884
42	6	0	-3.814943	-4.234905	1.732651
43	1	0	-3.714137	-5.182153	-1.524759
44	1	0	-3.613110	-4.634555	2.722924
45	6	0	-4.515167	2.435337	-0.300158
46	6	0	-4.330339	3.234873	0.846755
47	6	0	-4.272554	2.918623	-1.602534
48	6	0	-3.869680	4.543472	0.659887
49	6	0	-3.813410	4.234785	-1.732644
50	1	0	-3.711218	5.182204	1.524676

51	1	0	-3.611619	4.634240	-2.723003
52	6	0	-4.480888	-2.066434	2.848594
53	1	0	-4.857726	-1.086808	2.534780
54	6	0	-4.600672	-2.722973	-2.256347
55	1	0	-4.994738	-1.703402	-2.181300
56	6	0	-4.598737	2.723489	2.256674
57	1	0	-4.992225	1.703670	2.181890
58	6	0	-4.481119	2.066691	-2.848262
59	1	0	-4.858490	1.087332	-2.534249
60	6	0	-3.614314	-5.040523	0.614936
61	1	0	-3.258843	-6.060212	0.737934
62	6	0	-3.612017	5.040374	-0.615035
63	1	0	-3.256037	6.059864	-0.738198
64	6	0	-3.302215	-2.646087	-3.079861
65	1	0	-2.853676	-3.638070	-3.211885
66	1	0	-3.508281	-2.235986	-4.075812
67	1	0	-2.562092	-2.001773	-2.589762
68	6	0	-3.154301	-1.821922	3.590174
69	1	0	-3.319953	-1.175623	4.460360
70	1	0	-2.717173	-2.761306	3.949091
71	1	0	-2.420801	-1.334155	2.936240
72	6	0	-5.531628	-2.685414	3.787998
73	1	0	-6.485913	-2.843473	3.272440
74	1	0	-5.198399	-3.653590	4.179995
75	1	0	-5.710487	-2.023480	4.643387
76	6	0	-5.661277	-3.572983	-2.978459
77	1	0	-5.316538	-4.602519	-3.130454
78	1	0	-6.597586	-3.613269	-2.410017
79	1	0	-5.878558	-3.146219	-3.964576
80	6	0	-3.155037	1.821243	-3.590403
81	1	0	-3.321538	1.175112	-4.460553
82	1	0	-2.717331	2.760302	-3.949459
83	1	0	-2.421654	1.332888	-2.936781
84	6	0	-3.300420	2.647614	3.080466
85	1	0	-2.852714	3.639939	3.212738
86	1	0	-3.506397	2.237275	4.076336
87	1	0	-2.559626	2.003969	2.590504
88	6	0	-5.659948	3.573176	2.978303
89	1	0	-5.315856	4.603009	3.129756
90	1	0	-6.596264	3.612603	2.409810
91	1	0	-5.877021	3.146786	3.964629
92	6	0	-5.531867	2.686377	-3.787212
93	1	0	-6.485786	2.845215	-3.271212

94	1	0	-5.198084	3.654274	-4.179427
95	1	0	-5.711642	2.024518	-4.642467
96	6	0	-6.437154	0.761215	-0.123240
97	1	0	-6.887202	1.035794	-1.082531
98	1	0	-6.941522	1.321807	0.668792
99	6	0	-6.437475	-0.759900	0.124653
100	1	0	-6.887159	-1.034259	1.084179
101	1	0	-6.942497	-1.320308	-0.667095

5^{+} (UM06/ SDD(Au), 6-31G(d)(H, C, N, F, Cl)) in dichloromethane

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	79	0	-3.402320	0.000074	0.000044
2	17	0	5.093384	0.101604	-2.270287
3	17	0	6.112116	5.111623	-0.677103
4	17	0	5.093440	-0.101735	2.270249
5	17	0	6.111841	-5.111804	0.676996
6	17	0	2.324716	-2.338565	-1.902513
7	17	0	2.324912	2.338619	1.902545
8	7	0	-1.275760	0.000089	0.000078
9	6	0	5.485051	2.561151	-1.314817
10	6	0	1.556010	0.000040	0.000044
11	6	0	0.784226	0.895944	-0.762126
12	6	0	-0.595158	0.879783	-0.752944
13	6	0	-0.595171	-0.879623	0.753089
14	6	0	0.784213	-0.895829	0.762240
15	6	0	2.999387	0.000002	0.000014
16	6	0	3.737979	-1.255682	0.184022
17	6	0	3.497891	-2.395182	-0.612005
18	6	0	4.752968	-1.394016	1.151262
19	6	0	5.484944	-2.561300	1.314749
20	6	0	5.204418	-3.642413	0.492213
21	6	0	4.211070	-3.574662	-0.476428
22	6	0	3.738045	1.255642	-0.184026
23	6	0	4.753014	1.393910	-1.151298
24	6	0	5.204614	3.642286	-0.492280
25	6	0	4.211293	3.574599	0.476394

26	6	0	3.498050	2.395161	0.612001
27	1	0	6.250146	2.626718	-2.083488
28	1	0	-1.154436	1.580294	-1.366373
29	1	0	-1.154458	-1.580117	1.366530
30	1	0	6.250060	-2.626917	2.083395
31	1	0	4.006693	-4.420354	-1.127159
32	1	0	4.006986	4.420307	1.127126
33	9	0	1.388121	1.778407	-1.543450
34	9	0	1.388096	-1.778310	1.543554
35	6	0	-7.566359	0.434318	0.546265
36	6	0	-7.566309	-0.434372	-0.546365
37	6	0	-5.429836	0.000037	-0.000004
38	7	0	-6.232413	0.676579	0.851886
39	7	0	-6.232336	-0.676552	-0.851928
40	6	0	-5.801432	-1.534400	-1.940786
41	1	0	-4.708912	-1.561606	-1.957671
42	1	0	-6.187135	-2.548457	-1.791363
43	1	0	-6.169169	-1.140047	-2.894092
44	6	0	-5.801605	1.534457	1.940757
45	1	0	-6.169356	1.140086	2.894051
46	1	0	-4.709088	1.561730	1.957686
47	1	0	-6.187364	2.548491	1.791315
48	6	0	-8.748527	0.891818	1.119361
49	6	0	-8.748423	-0.891947	-1.119511
50	1	0	-8.750353	-1.569897	-1.970046
51	1	0	-8.750538	1.569765	1.969897
52	6	0	-9.930122	0.437555	0.548819
53	1	0	-10.880086	0.767891	0.962840
54	6	0	-9.930071	-0.437761	-0.549020
55	1	0	-10.879996	-0.768158	-0.963079

$[Au^{I}(F_2PyBTM)PPh_3]^+$ (UM06 / SDD(Au), 6-31G(d)(H, C, N, F, P, Cl)) in dichloromethane

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	79	0	2.615159	-0.027043	0.039128
2	17	0	-5.909936	0.273921	2.254443
3	17	0	-6.882384	5.165913	0.302512

4	17	0	-5.868201	-0.233782	-2.274939
5	17	0	-6.973768	-5.111238	-0.361681
6	17	0	-3.181880	-2.220481	2.075924
7	17	0	-3.092413	2.196362	-2.040390
8	15	0	4.926200	-0.002101	0.001291
9	7	0	0.471025	-0.038960	0.056992
10	6	0	-6.279061	2.662495	1.124071
11	6	0	-2.360206	-0.016938	0.029999
12	6	0	-1.586434	0.937591	0.716836
13	6	0	-0.207117	0.911536	0.719534
14	6	0	-0.209160	-0.980627	-0.615965
15	6	0	-1.588543	-0.985257	-0.639636
16	6	0	-3.802662	-0.002989	0.012719
17	6	0	-4.555233	-1.259879	-0.096603
18	6	0	-4.341413	-2.346049	0.777779
19	6	0	-5.559700	-1.450694	-1.066157
20	6	0	-6.305129	-2.617215	-1.160644
21	6	0	-6.050001	-3.643643	-0.263220
22	6	0	-5.068564	-3.522828	0.712226
23	6	0	-4.532099	1.269021	0.103426
24	6	0	-5.553785	1.481834	1.049925
25	6	0	-5.984134	3.681056	0.229672
26	6	0	-4.983079	3.538894	-0.722604
27	6	0	-4.277356	2.348229	-0.768291
28	6	0	5.663873	-0.551464	1.567449
29	6	0	5.099506	-1.645512	2.232750
30	6	0	5.683907	-2.124908	3.398918
31	6	0	6.826124	-1.510506	3.908354
32	6	0	7.387785	-0.420507	3.250155
33	6	0	6.811449	0.060306	2.078448
34	6	0	5.593595	1.655722	-0.327911
35	6	0	4.975917	2.761936	0.265437
36	6	0	5.504326	4.034062	0.081661
37	6	0	5.597648	-1.085040	-1.294712
38	6	0	6.682488	-1.931056	-1.053701
39	6	0	7.194035	-2.709975	-2.088105
40	6	0	6.630955	-2.641955	-3.358546
41	6	0	5.551539	-1.794643	-3.602595
42	6	0	5.031815	-1.020047	-2.573419
43	6	0	6.740650	1.831711	-1.106832
44	6	0	6.645606	4.206985	-0.698283
45	6	0	7.262149	3.108605	-1.290739
46	1	0	-7.050004	2.787304	1.879434

47	1	0	0.353555	1.663130	1.268568
48	1	0	0.350174	-1.741428	-1.153487
49	1	0	-7.060684	-2.725095	-1.933989
50	1	0	-4.883617	-4.325184	1.421021
51	1	0	-4.766826	4.335235	-1.429406
52	1	0	4.203337	-2.124211	1.834485
53	1	0	5.243864	-2.975966	3.914505
54	1	0	7.278852	-1.883219	4.825036
55	1	0	8.279363	0.059109	3.648655
56	1	0	7.257264	0.910845	1.563532
57	1	0	4.080652	2.626593	0.874332
58	1	0	5.021206	4.892682	0.543355
59	1	0	7.130037	-1.983436	-0.061571
60	1	0	8.037148	-3.370999	-1.898205
61	1	0	7.033504	-3.253044	-4.163967
62	1	0	5.110983	-1.741242	-4.595993
63	1	0	4.185914	-0.357223	-2.764132
64	1	0	7.229008	0.973320	-1.567924
65	1	0	7.055277	5.204206	-0.846207
66	1	0	8.153796	3.244229	-1.899288
67	9	0	-2.188422	1.891548	1.410591
68	9	0	-2.191893	-1.930025	-1.344628

Extracted results of TD-DFT calculation.

1^{+} (UM06/ SDD(Au), 6-31G(d)(H, C, N, F, Cl)) in dichloromethane

```
Excitation energies and oscillator strengths:

Excited State   1:  2.068-A     2.2454 eV  552.17 nm  f=0.0543  <S**2>=0.820
   236A ->238A       0.10499
   230B ->236B      -0.12635
   233B ->236B       0.96879
 This state for optimization and/or second-order correction.
 Total Energy, E(TD-HF/TD-DFT) =  -5000.69013090
 Copying the excited state density for this state as the 1-particle RhoCI density.

 Excited State   2:  2.062-A     2.3036 eV  538.23 nm  f=0.0053  <S**2>=0.813
   228B ->236B      -0.15309
   232B ->236B       0.97392

 Excited State   3:  2.059-A     2.4082 eV  514.83 nm  f=0.0079  <S**2>=0.810
   230B ->236B       0.89492
   231B ->236B       0.40159
   233B ->236B       0.13076

 Excited State   4:  2.087-A     2.4777 eV  500.39 nm  f=0.0502  <S**2>=0.839
   236A ->237A       0.20535
   224B ->236B      -0.10661
   227B ->236B       0.17473
   228B ->236B       0.91240
   232B ->236B       0.18562

 Excited State   5:  2.069-A     2.4961 eV  496.70 nm  f=0.0001  <S**2>=0.820
   235B ->236B       0.99446

 Excited State   6:  2.069-A     2.5095 eV  494.07 nm  f=0.0000  <S**2>=0.821
   234B ->236B       0.99544

 Excited State   7:  2.081-A     2.7809 eV  445.84 nm  f=0.0007  <S**2>=0.833
   226B ->236B       0.16102
   229B ->236B       0.12738
   230B ->236B      -0.38929
   231B ->236B       0.89235

 Excited State   8:  2.070-A     2.8533 eV  434.52 nm  f=0.0001  <S**2>=0.821
```

```
   229B ->236B       0.98993
   231B ->236B      -0.10408

Excited State   9:  2.103-A     2.8869 eV  429.47 nm  f=0.1623  <S**2>=0.856
   227A ->237A       0.11569
   236A ->237A       0.80997
   218B ->236B      -0.11786
   224B ->236B      -0.32871
   227B ->236B      -0.34504
   228B ->236B      -0.16662

Excited State  10:  2.233-A     2.9989 eV  413.44 nm  f=0.0095  <S**2>=0.997
   225A ->237A      -0.18985
   236A ->238A       0.11525
   236A ->239A      -0.10843
   225B ->236B       0.94873
   225B ->237B       0.10558

Excited State  11:  2.116-A     3.0775 eV  402.87 nm  f=0.1361  <S**2>=0.870
   236A ->237A       0.33588
   227B ->236B       0.88771
   228B ->236B      -0.26653

Excited State  12:  2.105-A     3.3080 eV  374.81 nm  f=0.0007  <S**2>=0.858
   226B ->236B       0.97511
   231B ->236B      -0.15092

Excited State  13:  2.958-A     3.4158 eV  362.97 nm  f=0.0655  <S**2>=1.937
   229A ->242A      -0.21383
   232A ->239A      -0.10893
   232A ->241A      -0.22705
   233A ->237A       0.21673
   236A ->238A       0.62122
   236A ->239A       0.23302
   236A ->241A      -0.11790
   228B ->238B      -0.20633
   230B ->242B      -0.18019
   232B ->238B       0.11123
   232B ->239B       0.12751
   232B ->241B       0.16576
   233B ->236B      -0.15931
   233B ->237B      -0.25842
   233B ->252B      -0.12513
```

```
 Excited State  14:  2.590-A     3.4335 eV  361.10 nm  f=0.0857  <S**2>=1.427
   227A ->237A      -0.17392
   228A ->237A      -0.11381
   232A ->242A      -0.13085
   233A ->238A       0.15606
   236A ->237A       0.27205
   236A ->248A       0.11938
   236A ->250A      -0.10411
   218B ->236B       0.11929
   224B ->236B       0.73235
   227B ->236B      -0.21418
   228B ->237B      -0.14384
   232B ->242B      -0.12617
   233B ->238B      -0.16007

 Excited State  15:  3.056-A     3.6854 eV  336.42 nm  f=0.0420  <S**2>=2.085
   229A ->238A       0.11990
   229A ->239A       0.15798
   229A ->241A       0.25518
   232A ->242A       0.31186
   233A ->238A      -0.21316
   233A ->241A       0.17329
   236A ->237A       0.25690
   224B ->236B       0.45267
   228B ->236B       0.11856
   228B ->237B       0.22366
   230B ->238B      -0.14585
   230B ->239B      -0.14660
   230B ->241B      -0.20208
   232B ->242B       0.28703
   233B ->238B       0.24945
   233B ->241B      -0.15306
```

2^{+} (UM06/ SDD(Au), 6-31G(d)(H, C, N, F, Cl)) in dichloromethane

```
Excitation energies and oscillator strengths:

 Excited State   1:  2.180-A     2.4839 eV  499.15 nm  f=0.0493  <S**2>=0.938
   212A ->214A      -0.17301
   199B ->212B       0.10852
   204B ->212B       0.24695
```

```
   205B ->212B       0.90255
   205B ->213B       0.12739
This state for optimization and/or second-order correction.
Total Energy, E(TD-HF/TD-DFT) =  -4763.34957774
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State   2:  2.173-A     2.5583 eV  484.64 nm  f=0.0185  <S**2>=0.930
   212A ->213A      -0.17956
   200B ->212B       0.10872
   203B ->212B      -0.50976
   206B ->212B       0.63456
   207B ->212B      -0.46332

Excited State   3:  2.147-A     2.7068 eV  458.04 nm  f=0.0202  <S**2>=0.902
   212A ->213A       0.18257
   203B ->212B       0.73351
   206B ->212B       0.53751
   207B ->212B      -0.25656

Excited State   4:  2.099-A     2.7226 eV  455.39 nm  f=0.0072  <S**2>=0.851
   201B ->212B      -0.10072
   204B ->212B       0.93735
   205B ->212B      -0.27956

Excited State   5:  2.095-A     2.8338 eV  437.52 nm  f=0.0006  <S**2>=0.847
   208B ->212B       0.46186
   210B ->212B      -0.14968
   211B ->212B       0.86482

Excited State   6:  2.100-A     2.8358 eV  437.22 nm  f=0.0010  <S**2>=0.852
   202B ->212B      -0.15568
   208B ->212B       0.80508
   210B ->212B      -0.26456
   211B ->212B      -0.49458

Excited State   7:  2.092-A     2.8434 eV  436.04 nm  f=0.0001  <S**2>=0.844
   208B ->212B       0.29596
   210B ->212B       0.95031

Excited State   8:  2.091-A     2.8573 eV  433.92 nm  f=0.0000  <S**2>=0.843
   209B ->212B       0.99487

Excited State   9:  2.309-A     2.9958 eV  413.85 nm  f=0.0107  <S**2>=1.083
```

```
   201A ->213A       0.19448
   201B ->212B       0.93786
   201B ->213B      -0.15465

Excited State  10:  2.184-A     3.0903 eV  401.20 nm  f=0.1578  <S**2>=0.942
   202A ->213A       0.16750
   212A ->213A       0.77054
   180B ->212B      -0.14279
   200B ->212B      -0.40007
   203B ->212B      -0.31512
   206B ->212B       0.12551

Excited State  11:  2.141-A     3.2008 eV  387.35 nm  f=0.0288  <S**2>=0.896
   212A ->213A      -0.17697
   206B ->212B       0.50441
   207B ->212B       0.82530

Excited State  12:  2.365-A     3.2840 eV  377.54 nm  f=0.0131  <S**2>=1.149
   204A ->219A      -0.11313
   205A ->215A       0.11158
   212A ->214A       0.26920
   202B ->212B       0.84688
   202B ->213B      -0.10861
   203B ->214B      -0.10617
   204B ->218B       0.10305
   205B ->212B       0.15137
   205B ->213B      -0.11187
   208B ->212B       0.17359

Excited State  13:  2.856-A     3.3147 eV  374.04 nm  f=0.0723  <S**2>=1.789
   202A ->214A      -0.12578
   204A ->219A      -0.22072
   205A ->215A       0.21870
   206A ->213A      -0.17677
   206A ->226A       0.11917
   212A ->214A       0.51376
   202B ->212B      -0.46466
   203B ->214B      -0.19697
   204B ->212B       0.11656
   204B ->218B       0.19851
   205B ->212B       0.22384
   205B ->213B      -0.17379
   205B ->228B      -0.10411
```

```
   206B ->216B       0.16801

 Excited State  14:  3.045-A     3.3474 eV  370.39 nm  f=0.0829  <S**2>=2.069
   202A ->213A      -0.21550
   204A ->214A      -0.14765
   204A ->215A       0.20769
   205A ->219A      -0.23355
   206A ->214A      -0.25950
   212A ->213A       0.17927
   212A ->224A       0.12759
   212A ->226A      -0.15696
   180B ->212B       0.11587
   200B ->212B       0.48518
   201B ->219B       0.12105
   203B ->212B      -0.20804
   203B ->213B       0.20946
   204B ->214B       0.14564
   204B ->216B       0.19742
   205B ->214B       0.23474
   205B ->216B      -0.11773
   206B ->212B       0.11028
   206B ->218B       0.19076
   207B ->212B       0.12194
   207B ->218B      -0.11388

 Excited State  15:  3.479-A     3.4836 eV  355.91 nm  f=0.0000  <S**2>=2.776
   208A ->222A      -0.32158
   208A ->224A       0.12475
   209A ->227A      -0.30576
   210A ->225A       0.27287
   210A ->228A      -0.14548
   211A ->220A       0.38167
   208B ->222B      -0.34944
   209B ->226B       0.30572
   210B ->224B      -0.28273
   210B ->227B       0.12751
   211B ->220B      -0.38181
```

3^{+} (UM06/ SDD(Au), 6-31G(d)(H, C, N, F, Cl)) in dichloromethane

```
Excitation energies and oscillator strengths:
```

```
Excited State   1:  2.180-A     2.4859 eV  498.74 nm  f=0.0504  <S**2>=0.938
   194A ->196A      -0.17270
   183B ->194B       0.10775
   190B ->194B       0.24654
   191B ->194B       0.90631
   191B ->195B       0.12850
This state for optimization and/or second-order correction.
Total Energy, E(TD-HF/TD-DFT) =  -4534.89007263
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State   2:  2.173-A     2.5629 eV  483.76 nm  f=0.0177  <S**2>=0.930
   194A ->195A      -0.17990
   185B ->194B       0.10761
   189B ->194B      -0.51367
   192B ->194B       0.78517

Excited State   3:  2.149-A     2.7076 eV  457.92 nm  f=0.0197  <S**2>=0.904
   194A ->195A       0.18296
   189B ->194B       0.73730
   192B ->194B       0.59322

Excited State   4:  2.099-A     2.7261 eV  454.81 nm  f=0.0075  <S**2>=0.851
   190B ->194B       0.93847
   191B ->194B      -0.27888

Excited State   5:  2.316-A     3.0033 eV  412.83 nm  f=0.0115  <S**2>=1.091
   187A ->195A       0.19696
   187B ->194B       0.93741
   187B ->195B      -0.15750

Excited State   6:  2.103-A     3.0338 eV  408.68 nm  f=0.0000  <S**2>=0.855
   193B ->194B       0.99336

Excited State   7:  2.187-A     3.0866 eV  401.68 nm  f=0.1721  <S**2>=0.946
   188A ->195A       0.16746
   194A ->195A       0.78602
   162B ->194B       0.13945
   185B ->194B      -0.39327
   189B ->194B      -0.30689

Excited State   8:  2.172-A     3.2089 eV  386.38 nm  f=0.0006  <S**2>=0.930
   188B ->194B       0.96864
   188B ->195B      -0.13383
```

```
Excited State   9:  3.016-A     3.3106 eV  374.51 nm  f=0.0863  <S**2>=2.024
   188A ->196A      -0.14160
   190A ->201A       0.24548
   191A ->197A      -0.24506
   192A ->195A      -0.20120
   192A ->203A       0.10912
   192A ->205A      -0.13768
   194A ->196A       0.57235
   188B ->194B      -0.15777
   189B ->196B      -0.22245
   190B ->194B       0.13780
   190B ->200B       0.22142
   191B ->194B       0.26055
   191B ->195B      -0.20246
   191B ->206B       0.13793
   192B ->196B       0.12672
   192B ->197B       0.21289

Excited State  10:  3.065-A     3.3416 eV  371.04 nm  f=0.0997  <S**2>=2.099
   188A ->195A      -0.21796
   190A ->196A      -0.15019
   190A ->197A       0.20556
   191A ->201A      -0.24000
   192A ->196A      -0.26400
   194A ->195A       0.19973
   194A ->203A      -0.15181
   194A ->205A       0.16267
   162B ->194B      -0.11426
   185B ->194B       0.49303
   187B ->201B      -0.12332
   189B ->194B      -0.20035
   189B ->195B       0.21206
   189B ->206B      -0.11227
   190B ->196B       0.14737
   190B ->197B       0.19258
   191B ->196B       0.23610
   191B ->197B      -0.12085
   192B ->200B       0.22390

Excited State  11:  2.695-A     3.7103 eV  334.16 nm  f=0.1831  <S**2>=1.566
   190A ->197A      -0.22200
   191A ->201A       0.26065
```

```
   192A ->196A       0.11594
   194A ->195A       0.47925
   185B ->194B       0.57347
   187B ->201B      -0.11791
   189B ->194B       0.11700
   190B ->196B      -0.11921
   190B ->197B      -0.21323
   191B ->196B      -0.14197
   191B ->197B       0.10330
   192B ->200B      -0.24841

Excited State  12:  2.809-A     3.9442 eV  314.34 nm  f=0.0497  <S**2>=1.723
   190A ->201A      -0.24820
   191A ->197A       0.28311
   192A ->201A       0.16200
   194A ->196A       0.64790
   194A ->197A      -0.17889
   183B ->194B       0.26488
   189B ->197B      -0.13266
   190B ->200B      -0.26429
   191B ->200B       0.15736
   192B ->197B      -0.30452

Excited State  13:  2.561-A     3.9845 eV  311.16 nm  f=0.0093  <S**2>=1.390
   190A ->201A      -0.14793
   192A ->201A      -0.15803
   194A ->197A       0.85415
   189B ->197B       0.10003
   190B ->195B       0.12186
   190B ->200B      -0.14010
   191B ->200B      -0.10859
   192B ->196B      -0.20705
   192B ->197B      -0.10195

Excited State  14:  2.094-A     4.0565 eV  305.64 nm  f=0.0001  <S**2>=0.846
   186B ->194B       0.99478

Excited State  15:  2.396-A     4.1111 eV  301.59 nm  f=0.0077  <S**2>=1.185
   187A ->195A      -0.23862
   188A ->197A      -0.10695
   188A ->200A       0.10781
   192A ->195A      -0.12408
   194A ->196A      -0.12370
```

```
   194A ->197A      -0.11676
   194A ->199A      -0.41632
   194A ->200A       0.67689
   183B ->194B       0.33548
```

4^{+} (UM06/ SDD(Au), 6-31G(d)(H, C, N, F, Cl)) in dichloromethane

```
Excitation energies and oscillator strengths:

 Excited State   1:  2.175-A     2.4740 eV  501.15 nm  f=0.0490  <S**2>=0.933
   237A ->239A      -0.17009
   224B ->237B      -0.10853
   229B ->237B      -0.25217
   230B ->237B       0.89488
   230B ->238B      -0.12794
   232B ->237B      -0.11995
 This state for optimization and/or second-order correction.
 Total Energy, E(TD-HF/TD-DFT) =  -5000.22826960
 Copying the excited state density for this state as the 1-particle RhoCI density.

 Excited State   2:  2.167-A     2.5473 eV  486.74 nm  f=0.0191  <S**2>=0.924
   237A ->238A       0.17136
   225B ->237B      -0.10303
   228B ->237B       0.50453
   231B ->237B       0.79375

 Excited State   3:  2.146-A     2.6957 eV  459.93 nm  f=0.0216  <S**2>=0.901
   237A ->238A       0.17862
   228B ->237B       0.74724
   231B ->237B      -0.58063

 Excited State   4:  2.098-A     2.7096 eV  457.58 nm  f=0.0071  <S**2>=0.851
   226B ->237B       0.10141
   229B ->237B       0.93385
   230B ->237B       0.28878

 Excited State   5:  2.095-A     2.7456 eV  451.58 nm  f=0.0000  <S**2>=0.848
   235B ->237B       0.18939
   236B ->237B       0.97704

 Excited State   6:  2.095-A     2.7649 eV  448.42 nm  f=0.0000  <S**2>=0.847
   235B ->237B       0.97998
```

```
   236B ->237B      -0.19011

Excited State   7:  2.123-A     2.8375 eV  436.94 nm  f=0.0006  <S**2>=0.877
   227B ->237B       0.22874
   232B ->237B      -0.17674
   234B ->237B       0.93998

Excited State   8:  2.308-A     2.9889 eV  414.82 nm  f=0.0110  <S**2>=1.082
   226A ->238A      -0.19276
   237A ->242A      -0.10592
   226B ->237B       0.93628
   226B ->238B       0.14666

Excited State   9:  2.097-A     3.0481 eV  406.76 nm  f=0.0000  <S**2>=0.849
   233B ->237B       0.99716

Excited State  10:  2.183-A     3.0807 eV  402.46 nm  f=0.1840  <S**2>=0.941
   227A ->238A       0.16336
   237A ->238A       0.79079
   200B ->237B       0.13827
   214B ->237B      -0.11227
   225B ->237B      -0.38542
   228B ->237B      -0.30240

Excited State  11:  2.125-A     3.1219 eV  397.15 nm  f=0.0005  <S**2>=0.879
   227B ->237B      -0.22137
   232B ->237B       0.93154
   234B ->237B       0.23982

Excited State  12:  3.026-A     3.3050 eV  375.14 nm  f=0.0802  <S**2>=2.040
   227A ->239A      -0.14397
   229A ->243A       0.24474
   230A ->238A      -0.19704
   230A ->251A      -0.12390
   231A ->240A      -0.24254
   231A ->242A       0.11228
   237A ->239A       0.57549
   228B ->239B      -0.22486
   229B ->237B      -0.14237
   229B ->243B      -0.22274
   230B ->237B       0.27146
   230B ->238B       0.20054
   230B ->252B       0.12263
```

```
   231B ->239B      -0.13204
   231B ->240B       0.22012

Excited State  13:  3.060-A     3.3376 eV  371.48 nm  f=0.1003  <S**2>=2.091
   226A ->242A      -0.10386
   227A ->238A      -0.21522
   229A ->239A       0.15089
   229A ->240A      -0.20543
   230A ->239A      -0.26238
   231A ->243A       0.23409
   237A ->238A       0.19265
   237A ->247A      -0.13634
   237A ->251A       0.14948
   200B ->237B      -0.11514
   225B ->237B       0.49622
   228B ->237B      -0.19174
   228B ->238B      -0.20671
   229B ->239B      -0.14876
   229B ->240B       0.19923
   230B ->239B       0.23568
   230B ->240B       0.11726
   231B ->243B      -0.22298

Excited State  14:  2.141-A     3.3783 eV  367.00 nm  f=0.0022  <S**2>=0.896
   227B ->237B       0.92903
   227B ->238B       0.10529
   232B ->237B       0.26786
   234B ->237B      -0.18398

Excited State  15:  3.479-A     3.4736 eV  356.94 nm  f=0.0000  <S**2>=2.776
   233A ->245A      -0.25248
   233A ->249A      -0.15102
   234A ->245A      -0.15481
   234A ->249A      -0.18397
   235A ->250A       0.33064
   235A ->252A      -0.19096
   236A ->241A       0.10157
   236A ->250A       0.19822
   236A ->252A      -0.22158
   233B ->245B      -0.25737
   233B ->246B      -0.10093
   233B ->247B       0.15282
   234B ->245B      -0.15785
```

```
   234B ->246B      -0.10706
   234B ->247B       0.18633
   235B ->250B      -0.32577
   235B ->251B       0.20412
   236B ->241B      -0.10201
   236B ->250B      -0.19399
   236B ->251B       0.23690
```

5^{+} (UM06/ SDD(Au), 6-31G(d)(H, C, N, F, Cl)) in dichloromethane

```
Excitation energies and oscillator strengths:

 Excited State   1:  2.177-A     2.4815 eV  499.64 nm  f=0.0514  <S**2>=0.935
   169A ->172A       0.17207
   159B ->169B      -0.10924
   164B ->169B      -0.24943
   165B ->169B       0.90657
   165B ->170B      -0.12873
 This state for optimization and/or second-order correction.
 Total Energy, E(TD-HF/TD-DFT) =  -4297.99464495
 Copying the excited state density for this state as the 1-particle RhoCI density.

 Excited State   2:  2.170-A     2.5595 eV  484.41 nm  f=0.0178  <S**2>=0.927
   169A ->170A       0.17790
   160B ->169B       0.10909
   163B ->169B      -0.50852
   166B ->169B       0.78999

 Excited State   3:  2.149-A     2.7032 eV  458.66 nm  f=0.0203  <S**2>=0.904
   169A ->170A      -0.18505
   163B ->169B       0.74111
   166B ->169B       0.58703

 Excited State   4:  2.098-A     2.7199 eV  455.84 nm  f=0.0076  <S**2>=0.850
   164B ->169B       0.93832
   165B ->169B       0.28163

 Excited State   5:  2.096-A     2.9742 eV  416.86 nm  f=0.0001  <S**2>=0.848
   168B ->169B       0.99671

 Excited State   6:  2.321-A     3.0079 eV  412.19 nm  f=0.0119  <S**2>=1.097
   161A ->170A      -0.20131
```

```
   161B ->169B       0.93671
   161B ->170B       0.15949

Excited State   7:  2.091-A     3.0733 eV  403.42 nm  f=0.0000  <S**2>=0.843
   167B ->169B       0.99783

Excited State   8:  2.187-A     3.0795 eV  402.61 nm  f=0.1844  <S**2>=0.945
   162A ->170A       0.16609
   169A ->170A       0.79461
   146B ->169B      -0.13737
   153B ->169B       0.11028
   160B ->169B       0.38106
   163B ->169B       0.31030

Excited State   9:  2.475-A     3.2873 eV  377.16 nm  f=0.0200  <S**2>=1.281
   164A ->176A      -0.13728
   165A ->173A      -0.13529
   166A ->170A       0.11867
   169A ->172A       0.32593
   162B ->169B       0.80278
   162B ->170B       0.11205
   163B ->172B       0.12988
   164B ->175B      -0.12487
   165B ->169B      -0.16460
   165B ->170B      -0.13465
   166B ->173B       0.12205

Excited State  10:  2.779-A     3.3175 eV  373.73 nm  f=0.0677  <S**2>=1.680
   162A ->172A       0.11652
   164A ->176A       0.20584
   165A ->173A       0.20419
   166A ->170A      -0.16705
   166A ->181A      -0.11432
   169A ->172A      -0.47808
   162B ->169B       0.56569
   163B ->172B      -0.18500
   164B ->169B      -0.11232
   164B ->175B       0.18488
   165B ->169B       0.20932
   165B ->170B       0.16069
   165B ->183B       0.11750
   166B ->172B       0.10553
   166B ->173B      -0.18124
```

```
Excited State  11:  3.063-A     3.3421 eV  370.98 nm  f=0.0999  <S**2>=2.095
   162A ->170A       0.22077
   164A ->172A       0.15191
   164A ->173A      -0.20293
   165A ->176A      -0.23848
   166A ->172A      -0.26259
   169A ->170A      -0.18882
   169A ->179A      -0.15243
   169A ->181A      -0.16265
   146B ->169B      -0.11767
   160B ->169B       0.50123
   161B ->176B      -0.12417
   163B ->169B      -0.19415
   163B ->170B      -0.21266
   163B ->183B      -0.11255
   164B ->172B      -0.14952
   164B ->173B       0.19455
   165B ->172B       0.23500
   165B ->173B       0.11858
   166B ->175B      -0.22284

Excited State  12:  3.479-A     3.4571 eV  358.64 nm  f=0.0000  <S**2>=2.775
   167A ->171A      -0.53054
   167A ->178A       0.32569
   167A ->185A      -0.16829
   168A ->182A      -0.25504
   167B ->171B       0.53070
   167B ->178B      -0.32587
   167B ->185B       0.16827
   168B ->181B       0.25517

Excited State  13:  2.703-A     3.7069 eV  334.47 nm  f=0.1900  <S**2>=1.576
   164A ->173A       0.22030
   164A ->174A      -0.10346
   165A ->176A       0.26183
   166A ->172A       0.11712
   169A ->170A      -0.47123
   160B ->169B       0.57645
   161B ->176B      -0.11847
   163B ->169B       0.12081
   164B ->172B       0.12183
   164B ->173B      -0.21633
```

```
   165B ->172B      -0.14343
   165B ->173B      -0.10313
   166B ->175B       0.24923

 Excited State  14:  3.479-A     3.9087 eV  317.20 nm  f=0.0000  <S**2>=2.776
   168A ->171A       0.66116
   168A ->178A      -0.21885
   168B ->171B      -0.66106
   168B ->178B       0.21883

 Excited State  15:  2.809-A     3.9446 eV  314.31 nm  f=0.0490  <S**2>=1.723
   164A ->176A       0.24723
   165A ->173A       0.28063
   165A ->174A      -0.12031
   166A ->176A       0.16438
   169A ->172A       0.64457
   169A ->173A      -0.17786
   169A ->174A       0.10276
   159B ->169B       0.27811
   163B ->173B      -0.13235
   164B ->175B       0.26293
   165B ->175B       0.15933
   166B ->173B      -0.30645
```

$[Au^{I}(F_2PyBTM)PPh_3]^+$ (UM06 / SDD(Au), 6-31G(d)(H, C, N, F, P, Cl)) in dichloromethane

```
Excitation energies and oscillator strengths:

 Excited State   1:  2.174-A     2.4732 eV  501.31 nm  f=0.0506  <S**2>=0.931
   199A ->201A       0.16229
   185B ->199B      -0.10960
   193B ->199B      -0.25022
   196B ->199B       0.90779
   196B ->200B      -0.12806
 This state for optimization and/or second-order correction.
 Total Energy, E(TD-HF/TD-DFT) =  -4875.56532464
 Copying the excited state density for this state as the 1-particle RhoCI density.

 Excited State   2:  2.164-A     2.5449 eV  487.19 nm  f=0.0199  <S**2>=0.921
   199A ->200A      -0.16530
   186B ->199B       0.10791
   192B ->199B       0.50180
```

```
   197B ->199B       0.79712

Excited State   3:  2.144-A     2.6904 eV  460.84 nm  f=0.0233  <S**2>=0.899
   199A ->200A      -0.17236
   192B ->199B       0.74916
   197B ->199B      -0.57628

Excited State   4:  2.097-A     2.7077 eV  457.89 nm  f=0.0074  <S**2>=0.850
   193B ->199B       0.93748
   196B ->199B       0.28070

Excited State   5:  2.108-A     2.8711 eV  431.84 nm  f=0.0006  <S**2>=0.861
   187B ->199B      -0.12922
   198B ->199B       0.98810

Excited State   6:  2.312-A     2.9923 eV  414.35 nm  f=0.0119  <S**2>=1.086
   188A ->200A      -0.18257
   199A ->206A      -0.10397
   188B ->199B       0.93895
   188B ->200B       0.15070

Excited State   7:  2.192-A     3.0884 eV  401.45 nm  f=0.1919  <S**2>=0.951
   189A ->200A       0.15938
   199A ->200A       0.79682
   168B ->199B       0.11566
   186B ->199B      -0.37400
   192B ->199B       0.29194

Excited State   8:  3.044-A     3.3051 eV  375.13 nm  f=0.0806  <S**2>=2.067
   189A ->201A      -0.13655
   193A ->207A      -0.24815
   196A ->200A       0.20426
   196A ->212A      -0.10777
   196A ->216A      -0.11519
   197A ->204A      -0.17100
   197A ->205A       0.17854
   197A ->206A      -0.11421
   199A ->201A       0.55643
   199A ->202A      -0.14915
   192B ->201B       0.17089
   192B ->202B      -0.15343
   193B ->199B       0.13793
   193B ->207B      -0.22378
```

```
   196B ->199B      -0.26237
   196B ->200B      -0.20789
   196B ->216B      -0.13851
   197B ->201B       0.10713
   197B ->205B       0.22554

Excited State   9:  2.239-A     3.3212 eV  373.31 nm  f=0.0205  <S**2>=1.003
   186B ->199B       0.17140
   195B ->199B       0.93222

Excited State  10:  2.130-A     3.3270 eV  372.66 nm  f=0.0043  <S**2>=0.884
   194B ->199B       0.98311

Excited State  11:  2.938-A     3.3469 eV  370.44 nm  f=0.0725  <S**2>=1.909
   189A ->200A      -0.19905
   193A ->201A      -0.13554
   193A ->204A      -0.13383
   193A ->205A       0.13954
   196A ->201A       0.23497
   197A ->207A      -0.22014
   199A ->200A       0.14675
   199A ->212A      -0.13614
   199A ->216A      -0.12375
   186B ->199B       0.44991
   188B ->208B       0.10606
   192B ->199B       0.18990
   192B ->200B       0.19489
   192B ->216B       0.10140
   193B ->201B       0.11059
   193B ->205B       0.18814
   194B ->199B       0.16611
   195B ->199B      -0.35334
   196B ->201B      -0.16550
   196B ->202B       0.14843
   196B ->205B       0.10295
   197B ->207B      -0.20648

Excited State  12:  3.476-A     3.4715 eV  357.15 nm  f=0.0000  <S**2>=2.770
   190A ->204A      -0.13386
   190A ->205A      -0.11234
   190A ->210A      -0.11278
   191A ->203A       0.18636
   191A ->210A      -0.11474
```

```
   192A ->208A       0.11798
   192A ->211A      -0.15884
   192A ->215A      -0.10543
   195A ->211A      -0.10057
   195A ->214A      -0.11054
   195A ->215A      -0.21634
   198A ->202A       0.22636
   198A ->203A       0.10468
   198A ->204A      -0.12285
   198A ->208A      -0.12280
   198A ->210A      -0.10724
   198A ->211A      -0.10178
   189B ->204B       0.16626
   189B ->210B       0.10666
   190B ->203B      -0.19383
   190B ->204B       0.10748
   190B ->210B       0.11860
   191B ->206B      -0.11268
   191B ->211B       0.15947
   195B ->211B       0.10095
   195B ->212B       0.12108
   195B ->214B       0.20179
   198B ->201B      -0.14390
   198B ->202B      -0.18627
   198B ->203B      -0.10869
   198B ->204B       0.13229
   198B ->206B       0.12544
   198B ->210B       0.10701
   198B ->211B       0.10544

Excited State  13:  3.414-A     3.4799 eV  356.29 nm  f=0.0000  <S**2>=2.664
   190A ->202A       0.13145
   190A ->204A       0.15129
   190A ->205A       0.18426
   190A ->208A      -0.10460
   190A ->209A      -0.12055
   190A ->211A      -0.11597
   192A ->214A      -0.17468
   194A ->208A       0.14949
   194A ->211A      -0.13681
   194A ->214A       0.18977
   198A ->204A      -0.17900
   198A ->205A      -0.19488
```

```
   198A ->209A       0.12795
   189B ->202B      -0.10793
   189B ->204B      -0.24459
   189B ->206B       0.11291
   189B ->209B       0.11413
   189B ->211B       0.11710
   191B ->199B       0.22580
   191B ->212B       0.16974
   194B ->206B      -0.13769
   194B ->211B       0.13741
   194B ->212B      -0.18895
   198B ->204B       0.26927
   198B ->209B      -0.12018

Excited State  14:  3.460-A     3.4819 eV  356.08 nm  f=0.0000  <S**2>=2.742
   190A ->203A      -0.12109
   191A ->202A      -0.14318
   191A ->203A       0.21719
   191A ->209A      -0.13847
   191A ->211A       0.11158
   192A ->215A       0.15008
   194A ->211A      -0.14416
   194A ->214A      -0.11441
   194A ->215A       0.12423
   194A ->216A       0.11653
   195A ->208A      -0.13299
   195A ->211A       0.12327
   198A ->203A      -0.26019
   198A ->210A       0.13340
   189B ->203B       0.13176
   190B ->202B       0.11362
   190B ->203B      -0.20777
   190B ->204B      -0.10329
   190B ->209B       0.13948
   190B ->211B      -0.11171
   191B ->199B       0.10848
   191B ->214B      -0.14010
   191B ->215B      -0.11002
   194B ->211B       0.14423
   194B ->214B      -0.11687
   194B ->215B      -0.13396
   195B ->206B       0.12852
   195B ->211B      -0.12485
```

```
   198B ->203B       0.26347
   198B ->210B      -0.12756

Excited State  15:  2.205-A     3.5056 eV  353.67 nm  f=0.0001  <S**2>=0.966
   191B ->199B       0.96428
```