Supporting Information

Molecular Design of Efficient Yellow- to Red-Emissive Alkynylgold(III) Complexes for the Realization of Thermally Activated Delayed Fluorescence (TADF) and Their Applications in Solution-Processed Organic Light-Emitting Devices

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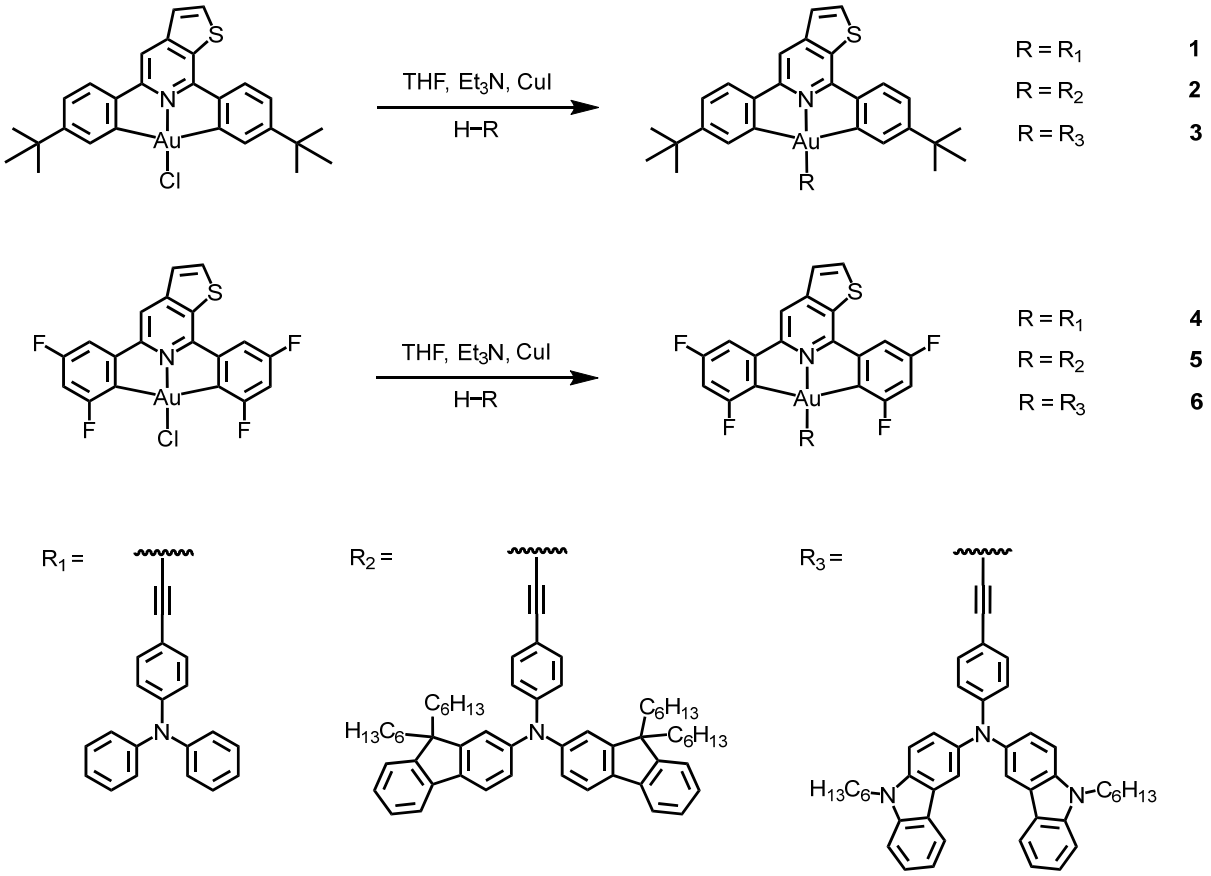


Scheme S1. Synthetic routes for the gold(III) complexes.

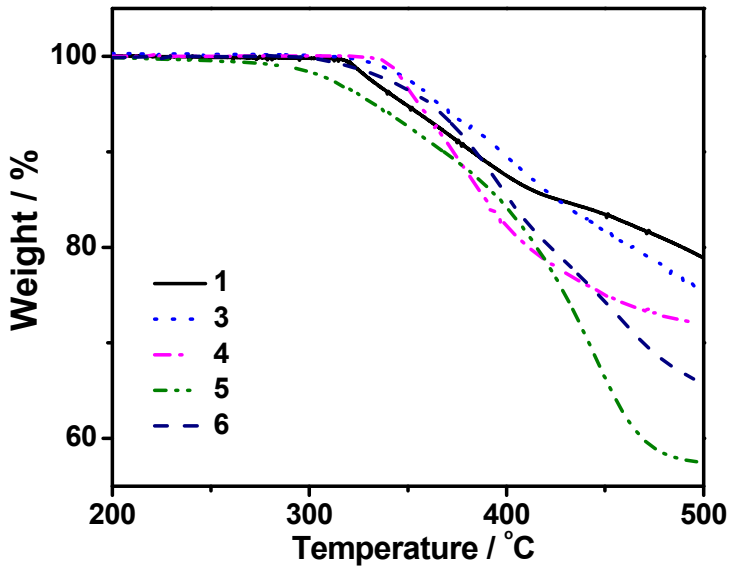


Figure S1. Thermogravimetric analysis (TGA) traces of **1**, **3**−**6**.

Table S1. Thermal properties of **1**, **3**−**6**.

Complex	T_d [a] / °C
1	347
3	365
4	354
5	332
6	363

[a] Decomposition temperature (T_d) is defined as the temperature at which the complex shows a 5 % weight loss.

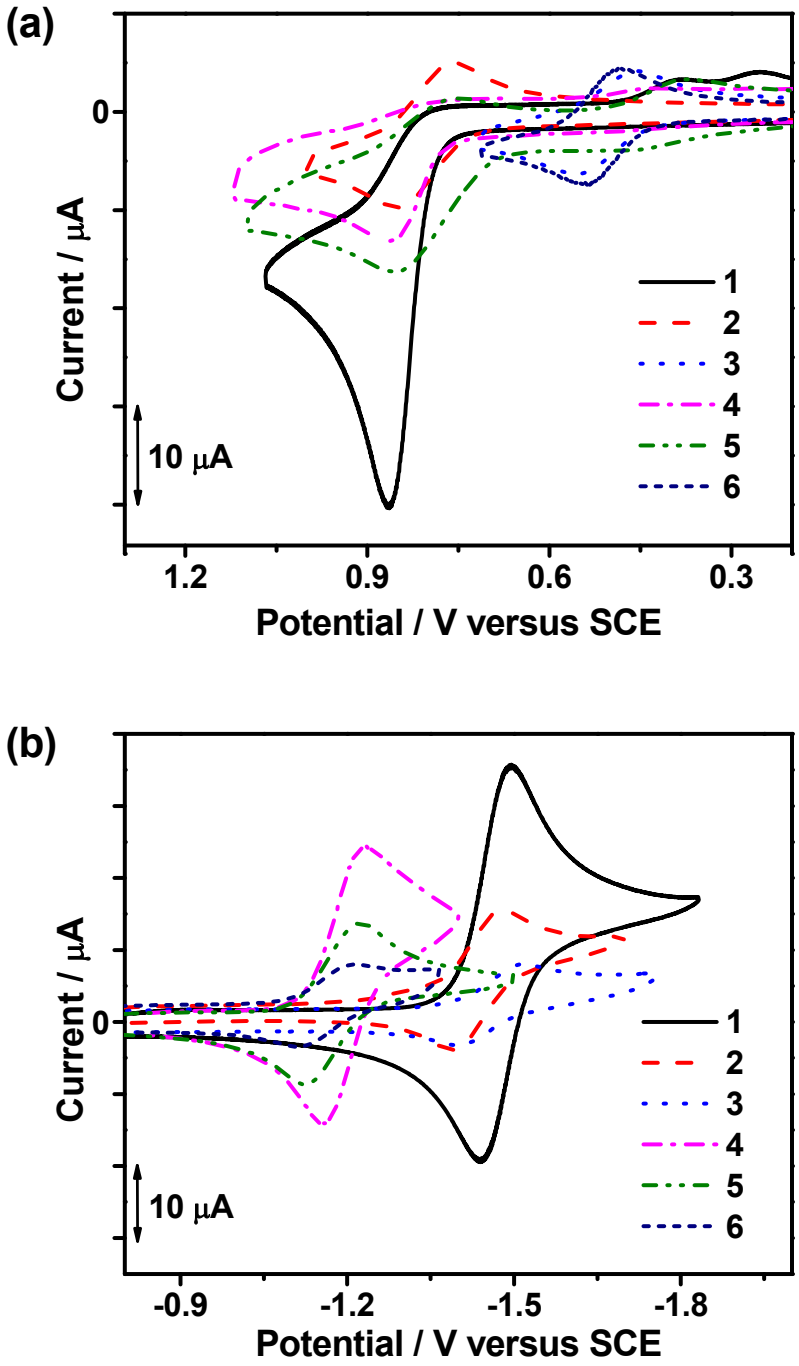


Figure S2. Cyclic voltammograms for the (a) oxidation and (b) reduction scans of **1**−**6** in dichloromethane (0.1 M $^{n}Bu_4NPF_6$).

Table S2. Electrochemical data of **1**−**6**.[a]

Complex	Oxidation $E_{1/2}$[b] / V *vs.* SCE (ΔE_p / mV)[c] [E_{pa}, V *vs.* SCE][d]	Reduction $E_{1/2}$[b] / V *vs.* SCE (ΔE_p / mV)[c]	E_{HOMO} / eV[e]	E_{LUMO} / eV[f]	E_{HOMO}−E_{LUMO} / eV
1	[+0.87]	−1.46 (58)	−5.21	−2.88	2.33
2	+0.80 (90)	−1.43 (90)	−5.14	−2.91	2.23
3	+0.54 (85), +1.04 (85)	−1.45 (87)	−4.88	−2.89	1.99
4	[+0.86]	−1.19 (63)	−5.20	−3.15	2.05
5	+0.81 (96)	−1.19 (96)	−5.15	−3.15	2.00
6	+0.51 (85), +1.05 (85)	−1.16 (85)	−4.85	−3.18	1.67

[a] In CH_2Cl_2 solution with 0.1 M $^nBu_4NPF_6$ as supporting electrolyte at 298 K working electrode, glassy carbon; scan rate = 100 mV s^{-1} .

[b] $E_{1/2} = (E_{pa} + E_{pc})/2$; E_{pa} and E_{pc} are the peak anodic and peak cathodic potentials, respectively.

[c] $\Delta E_p = (E_{pa} - E_{pc})$.

[d] E_{pa} refers to the anodic peak potential for the irreversible oxidation waves.

[e] E_{HOMO} levels were calculated from electrode potentials, i.e., $E_{HOMO} = -[E_{pa}$ (*vs.* $Fc^+/Fc) + 4.80]$ eV or $E_{HOMO} = -[E_{1/2}^{ox}$ (*vs.* $Fc^+/Fc) + 4.80]$ eV. $E^\circ(Fc^+/Fc)$ = +0.46 V *vs.* SCE in CH_2Cl_2 (0.1 M $^nBu_4NPF_6$). From ref. 1.

[f] E_{LUMO} levels were calculated from electrode potentials, i.e., $E_{LUMO} = -[E_{pc}$ (*vs.* $Fc^+/Fc) + 4.80]$ eV or $E_{LUMO} = -[E_{1/2}^{red}$ (*vs.* $Fc^+/Fc) + 4.80]$ eV. $E^\circ(Fc^+/Fc)$ = +0.46 V *vs.* SCE in CH_2Cl_2 (0.1 M $^nBu_4NPF_6$). From ref. 1.

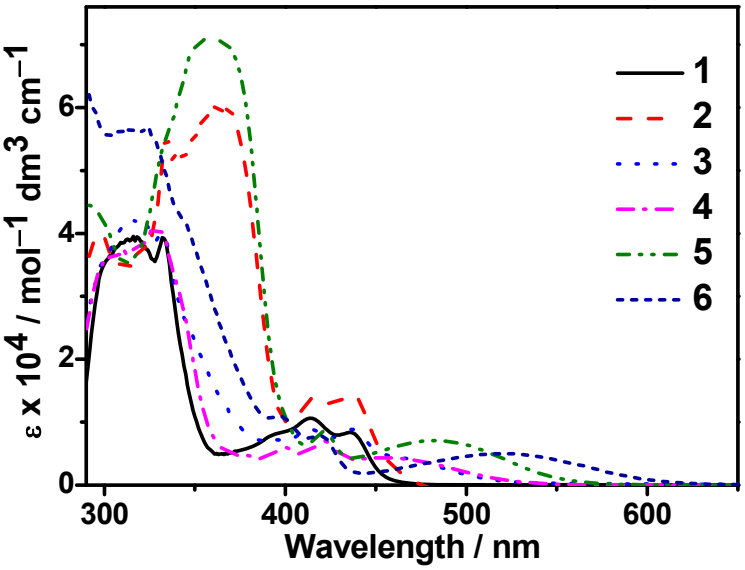


Figure S3. UV−Visible absorption spectra of **1**−**6** in toluene at 298 K.

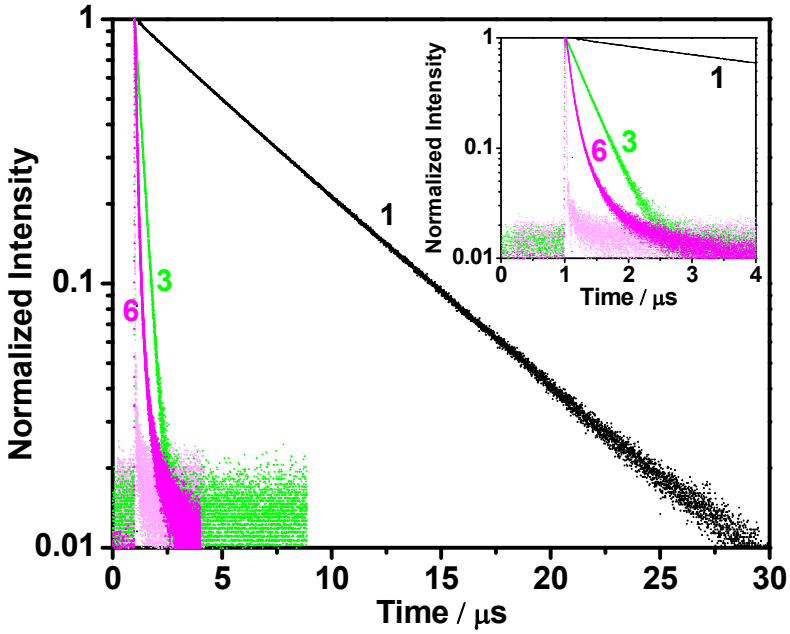


Figure S4. Time-resolved photoluminescence decay profiles of **1**, **3** and **6** in toluene at 298 K.

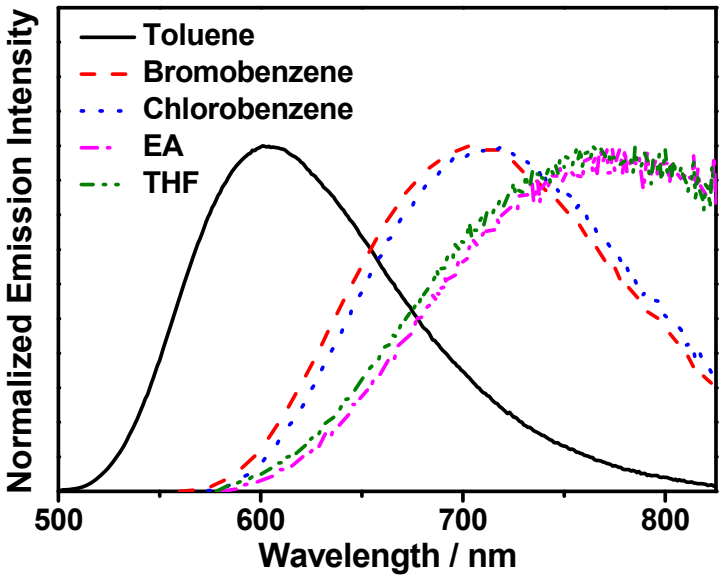


Figure S5. Normalized solvent-dependent emission spectra of **3** in various solvents at 298 K.

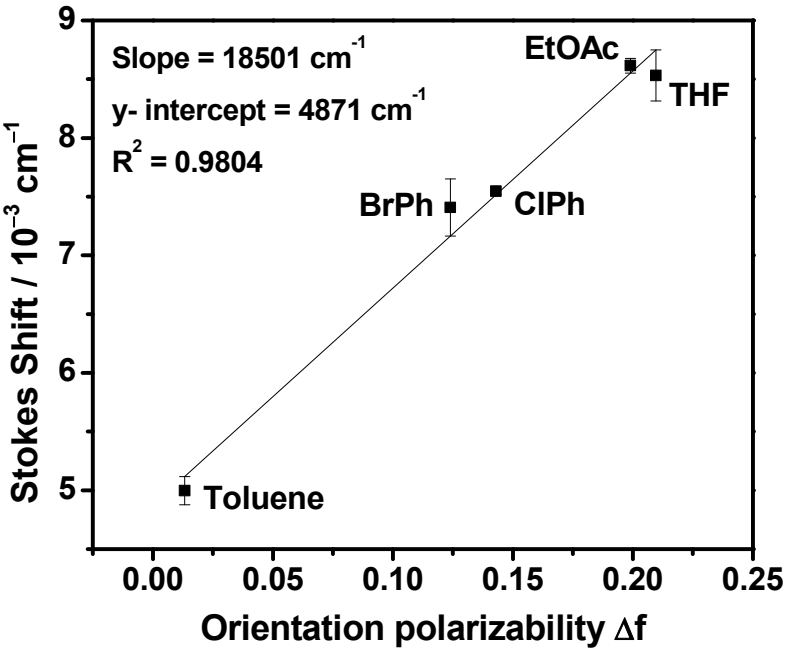


Figure S6. Lippert-Mataga plot of **3** in various solvents at 298 K.

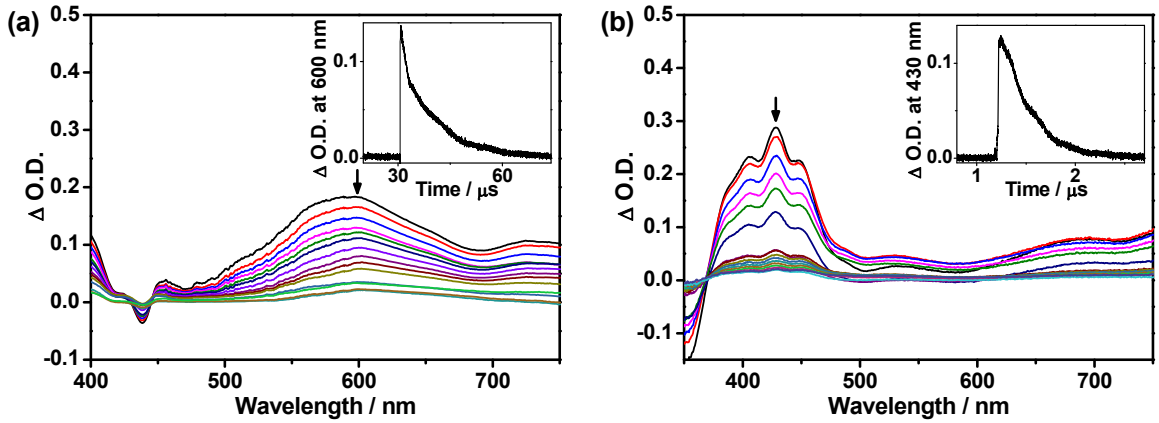


Figure S7. Transient absorption spectra of (a) **1** in degassed toluene at 298 K at decay times of 0−10 μs and the decay trace monitored at 600 nm in the inset and (b) **3** in degassed toluene at 298 K at decay times of 0−1 μs and the decay trace monitored at 430 nm in the inset.

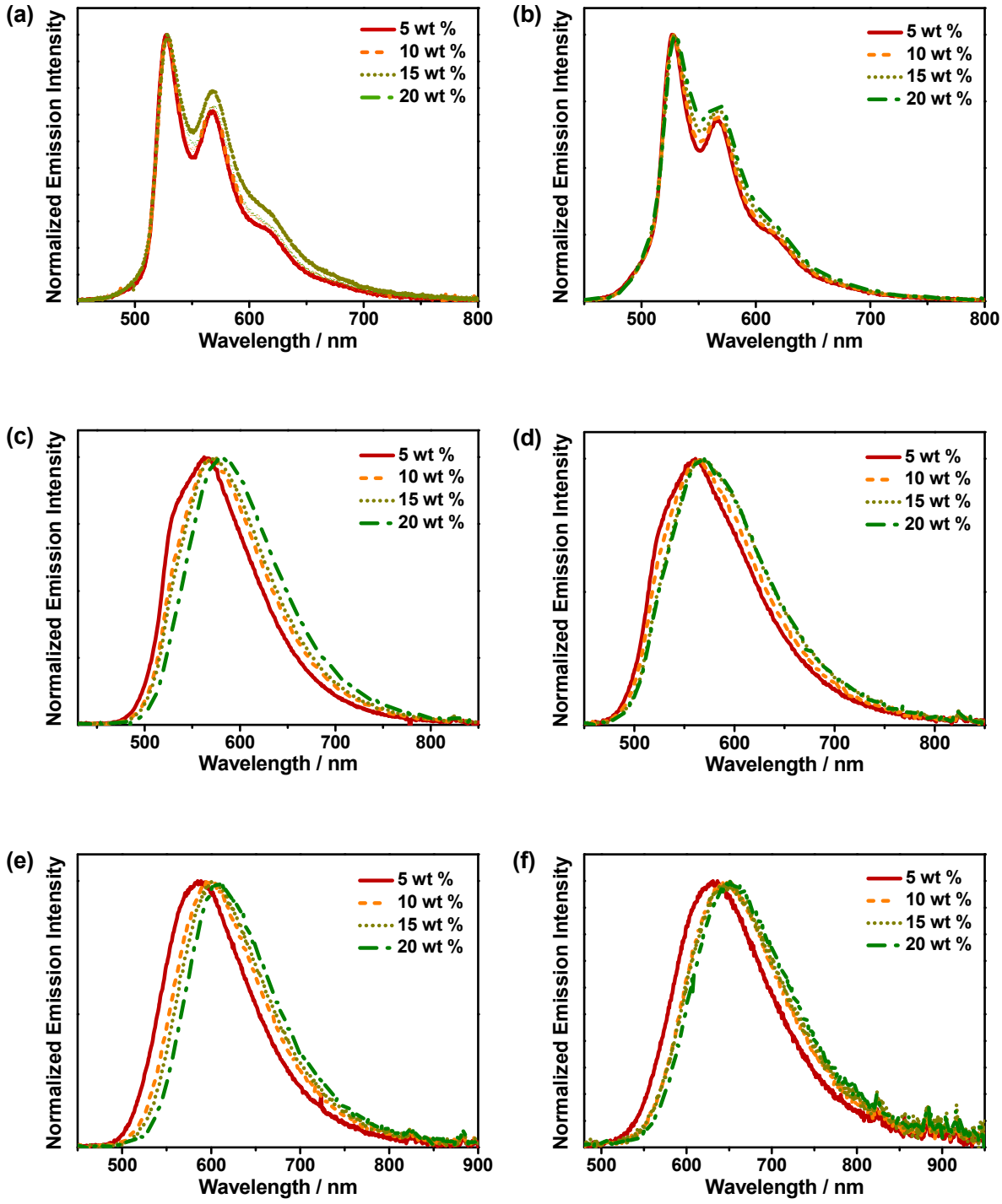


Figure S8. Normalized emission spectra of doped mCP thin films of (a) **1**, (b) **2**, (c) **3**, (d) **4**, (e) **5** and (f) **6** at different concentrations.

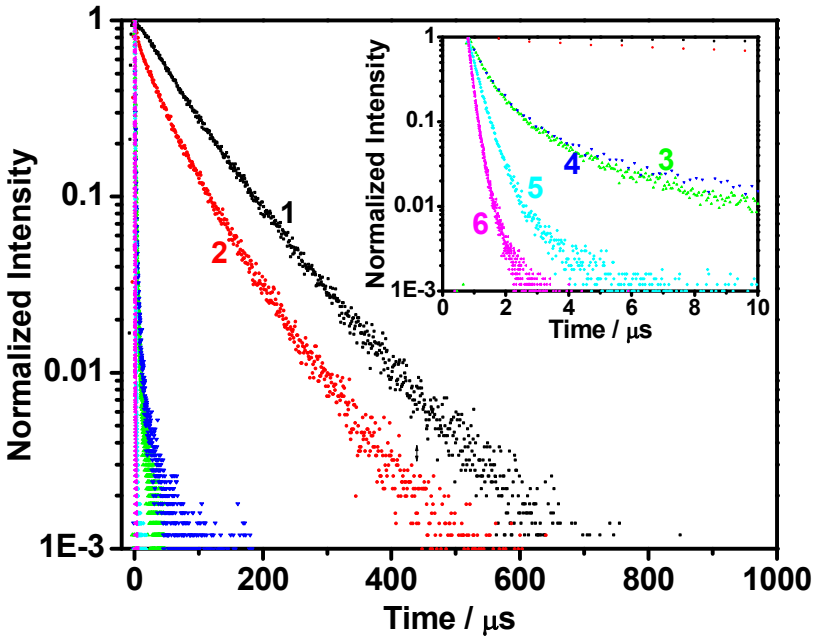


Figure S9. Time-resolved photoluminescence decay profiles of **1**−**6** in 10 wt % doped mCP thin film at 298 K and the decay profiles of **3**−**6** from 0 to 10 μs in the inset.

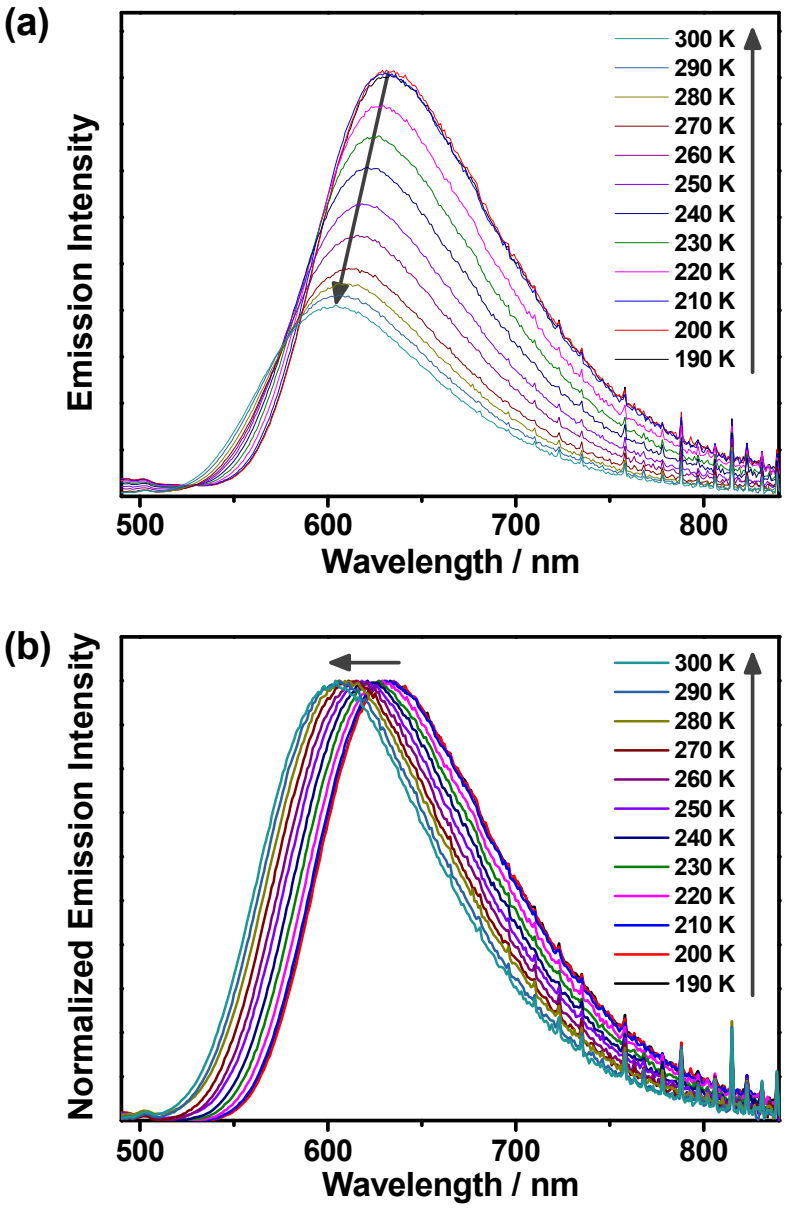


Figure S10. (a) Emission spectra and (b) normalized emission spectra of **3** in degassed toluene upon increasing temperature from 190 K to 300 K.

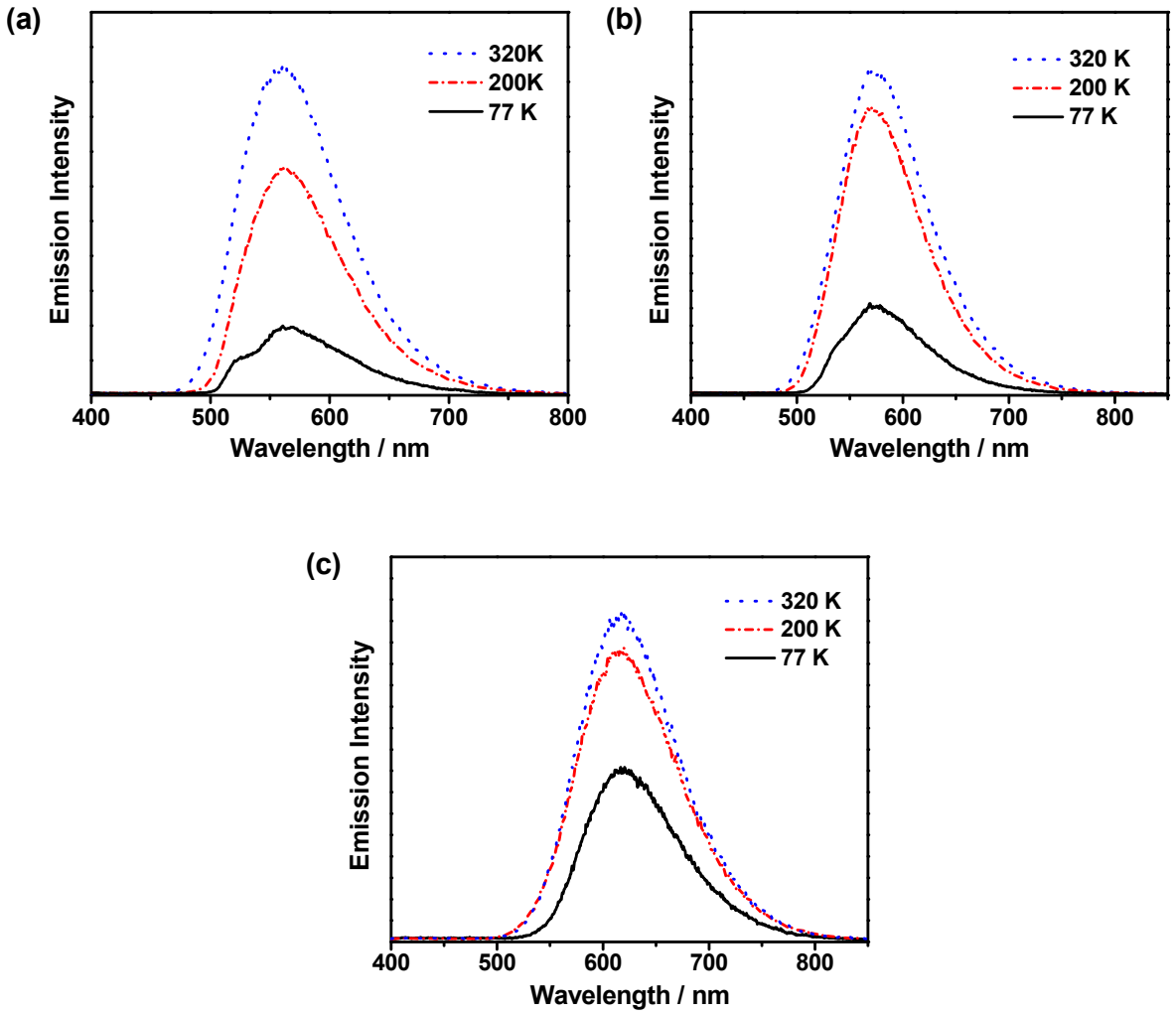


Figure S11. Emission spectra of (a) **4**, (b) **5** and (c) **6** in 5 wt % doped mCP thin film at 77, 200 and 320 K.

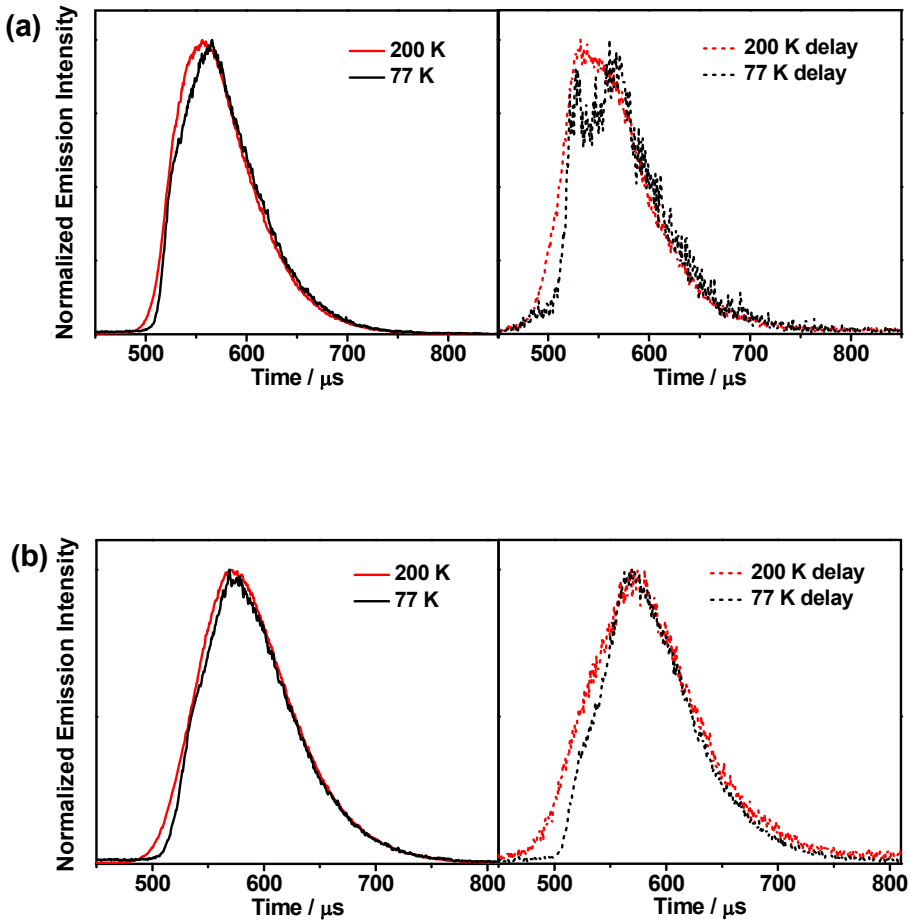


Figure S12. Time-resolved emission spectra of (a) **3** and (b) **5** recorded at delay times of 0 μs (prompt) and 5 μs (delayed) in 5 wt % doped mCP thin film at 77 and 200 K.

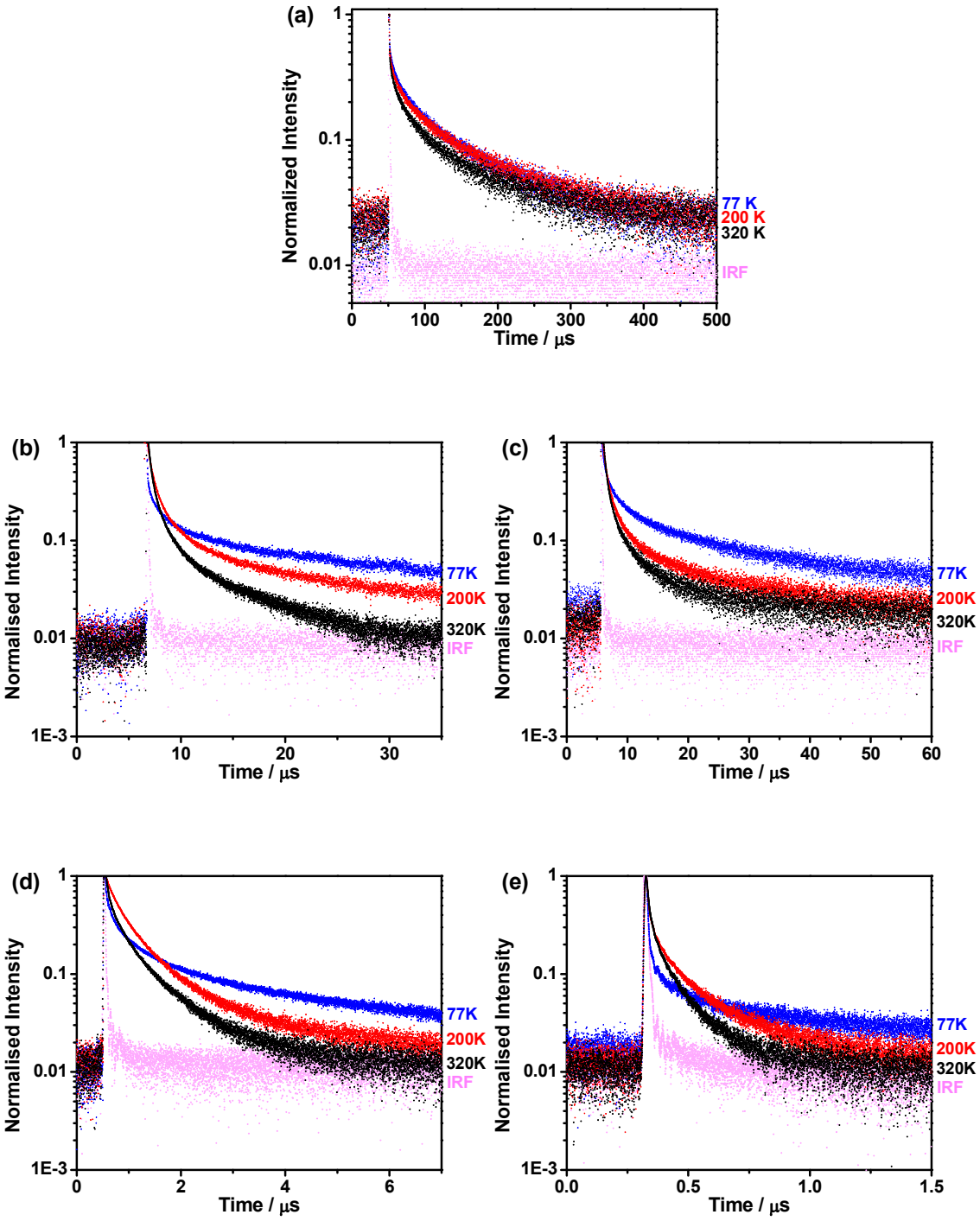


Figure S13. Time-resolved photoluminescence decay profiles of (a) **1**, (b) **3**, (c) **4**, (d) **5** and (e) **6** in 5 wt % doped mCP thin film at 77, 200 and 320 K respectively.

Table S3. Emission lifetime (μs) of **1**, **3**, **4**, **5** and **6** in 5 wt % doped mCP thin film at various temperature.

Temperature (K)	**1**	**3**	**4**	**5**	**6**
77	92.51	34.05	21.30	5.73	0.32
100	-	25.95	17.09	4.35	0.29
120	92.08	19.38	14.09	3.46	0.25
140	-	14.90	12.22	2.53	0.24
160	91.55	11.23	11.21	2.02	0.21
180	-	9.30	10.26	1.43	0.20
200	89.99	7.64	9.25	1.02	0.19
220	-	6.21	8.79	0.78	0.17
240	88.33	5.65	7.67	0.70	0.17
260	-	5.01	7.17	0.62	0.15
280	86.98	4.68	6.98	0.55	0.15
300	-	4.00	6.09	0.51	0.15
320	85.09	3.80	5.64	0.47	0.15
340	-	3.60	5.34	0.45	0.15
360	-	3.41	4.97	0.44	0.15

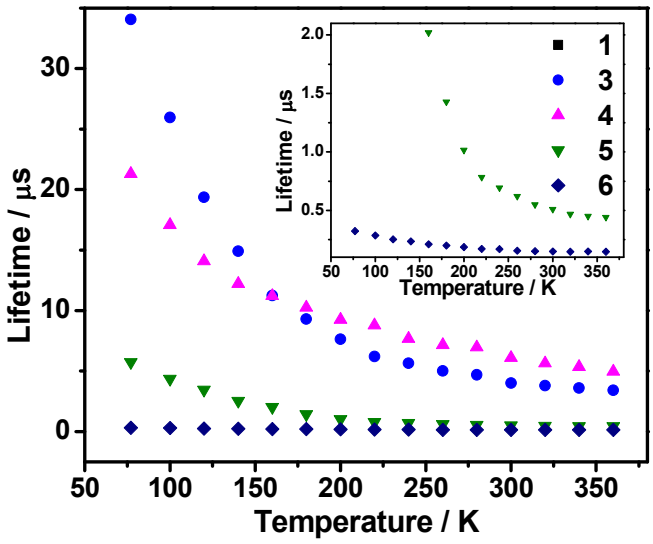
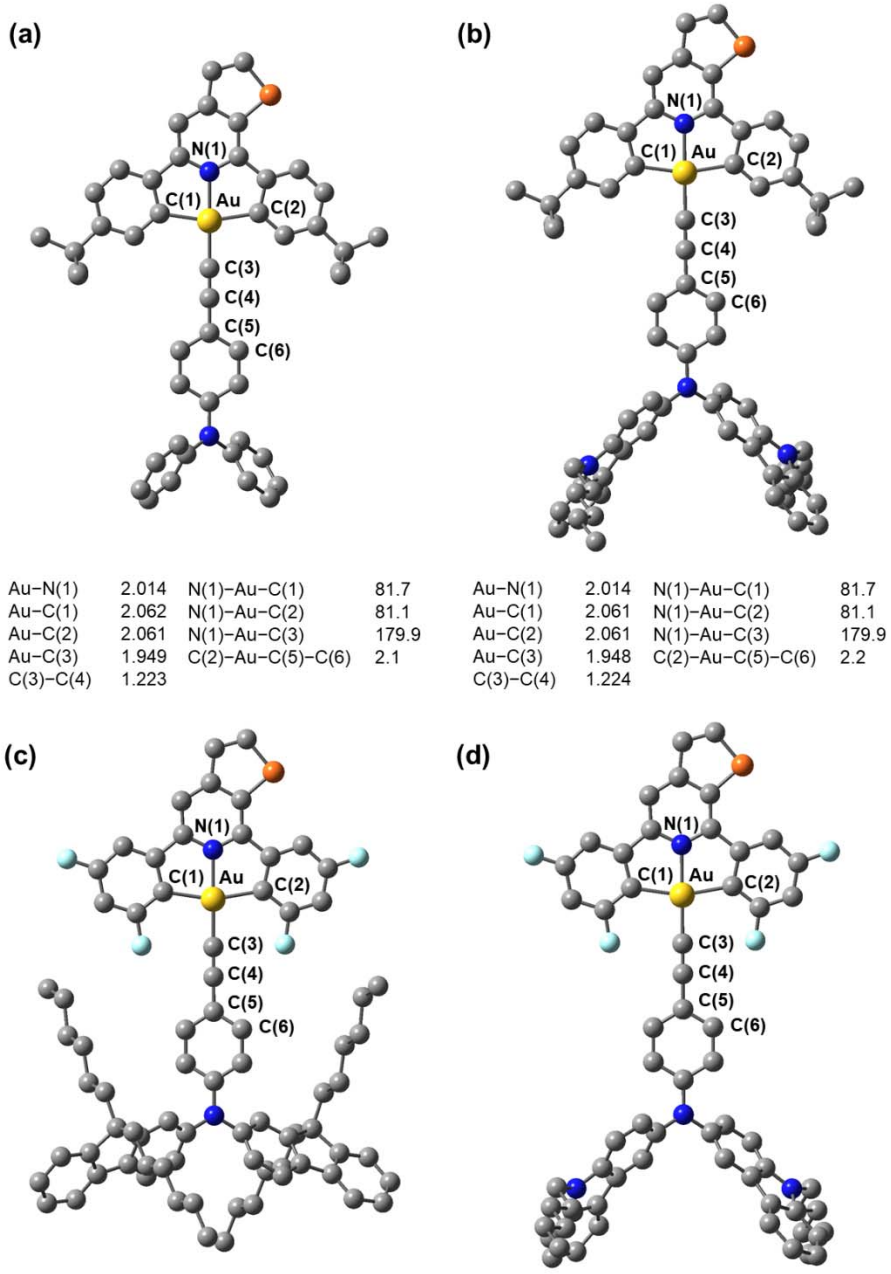


Figure S14. Plot of the emission lifetime of **1**, **3**, **4**, **5** and **6** in 5 wt % doped mCP thin film against temperature.



Au–N(1)	2.014	N(1)–Au–C(1)	81.7
Au–C(1)	2.062	N(1)–Au–C(2)	81.1
Au–C(2)	2.061	N(1)–Au–C(3)	179.9
Au–C(3)	1.949	C(2)–Au–C(5)–C(6)	2.1
C(3)–C(4)	1.223		

Au–N(1)	2.014	N(1)–Au–C(1)	81.7
Au–C(1)	2.061	N(1)–Au–C(2)	81.1
Au–C(2)	2.061	N(1)–Au–C(3)	179.9
Au–C(3)	1.948	C(2)–Au–C(5)–C(6)	2.2
C(3)–C(4)	1.224		

Au–N(1)	2.022	N(1)–Au–C(1)	81.3
Au–C(1)	2.066	N(1)–Au–C(2)	80.5
Au–C(2)	2.066	N(1)–Au–C(3)	179.9
Au–C(3)	1.945	C(2)–Au–C(5)–C(6)	18.1
C(3)–C(4)	1.220		

Au–N(1)	2.023	N(1)–Au–C(1)	81.3
Au–C(1)	2.065	N(1)–Au–C(2)	80.5
Au–C(2)	2.064	N(1)–Au–C(3)	179.8
Au–C(3)	1.946	C(2)–Au–C(5)–C(6)	1.7
C(3)–C(4)	1.221		

Figure S15. Optimized ground-state geometries with selected structural parameters of (a) **1**, (b) **3**, (c) **5** and (d) **6** at the PBE0 level of theory. The bond lengths and angles are in Angstroms and degrees, respectively. All hydrogen atoms are omitted for clarity.

Table S4. First twenty-five singlet excited states (S_n) of **1**, **3**, **5** and **6** computed by DDFT/CPCM using toluene as the solvent.

Complex	S_n	Excitation[a] (Coefficient)[b]	Vertical excitation wavelength / nm	*f*[c]	Character[d]
1	S_1	H→L (0.70)	485	0.218	LLCT
	S_2	H−1→L (0.69)	402	0.123	IL/ILCT
	S_3	H→L+1 (0.70)	375	0.072	LLCT
	S_4	H−2→L (0.68)	372	0.000	LLCT/ILCT
	S_5	H→L+2 (0.52)	337	0.703	IL/ILCT
		H−3→L (0.41)			LLCT
	S_6	H−3→L (0.54)	329	0.146	LLCT
		H→L+2 (−0.40)			IL/ILCT
	S_7	H−4→L (0.68)	322	0.116	ILCT/IL
	S_8	H→L+4 (0.69)	314	0.022	IL
	S_9	H−5→L (0.47)	311	0.089	ILCT/IL
		H−1→L+1 (−0.44)			IL
	S_{10}	H−5→L (0.51)	310	0.269	ILCT/IL
		H−1→L+1 (0.39)			IL
	S_{11}	H→L+6 (0.69)	305	0.277	ILCT/IL
	S_{12}	H−2→L+1 (0.67)	303	0.000	LLCT/ILCT
	S_{13}	H−8→L (0.56)	293	0.363	ILCT/IL
		H−1→L+1 (−0.35)			IL
	S_{14}	H−9→L (0.63)	292	0.009	LLCT/ILCT
	S_{15}	H→L+5 (0.64)	292	0.001	LLCT
	S_{16}	H→L+3 (0.62)	284	0.071	LLCT/IL
	S_{17}	H−12→L (0.45)	279	0.086	IL
		H−3→L+1 (−0.42)			LLCT
	S_{18}	H−6→L (0.59)	278	0.012	LLCT
		H→L+9 (0.26)			IL
	S_{19}	H−3→L+1 (0.50)	276	0.069	LLCT
		H−12→L (0.41)			IL
	S_{20}	H→L+7 (0.47)	273	0.023	LLCT
		H→L+8 (−0.44)			IL/ILCT
	S_{21}	H→L+8 (0.46)	272	0.017	IL/ILCT
		H→L+7 (0.44)			LLCT
	S_{22}	H→L+9 (0.47)	272	0.030	IL
		H−6→L (−0.36)			LLCT
		H→L+10 (−0.34)			IL
	S_{23}	H−4→L+1 (0.53)	271	0.027	IL/ILCT
	S_{24}	H−7→L (0.61)	269	0.008	LLCT
	S_{25}	H−5→L+1 (0.55)	268	0.110	IL/ILCT

3	S_1	H→L (0.70)	554	0.213	LLCT
	S_2	H→L+1 (0.70)	417	0.045	LLCT
	S_3	H−3→L (0.68)	401	0.131	IL/ILCT
	S_4	H→L+2 (0.70)	388	0.037	IL/ILCT
	S_5	H−2→L (0.66)	379	0.171	LLCT
	S_6	H−6→L (0.69)	375	0.003	LLCT/ILCT
	S_7	H−1→L (0.71)	366	0.002	LLCT
	S_8	H→L+3 (0.62)	361	0.151	IL
		H→L+4 (0.30)			IL
	S_9	H→L+4 (0.56)	348	0.775	IL
	S_{10}	H−5→L (0.64)	338	0.016	LLCT
	S_{11}	H−4→L (0.70)	335	0.001	LLCT
	S_{12}	H−8→L (0.67)	322	0.112	ILCT/IL
	S_{13}	H−9→L (0.43)	311	0.075	ILCT/IL
		H−3→L+1 (−0.41)			IL
	S_{14}	H→L+6 (0.66)	311	0.017	LLCT
	S_{15}	H−9→L (0.51)	310	0.251	ILCT/IL
		H−3→L+1 (0.37)			IL
	S_{16}	H→L+8 (0.66)	309	0.309	IL/ILCT
	S_{17}	H−2→L+1 (0.65)	308	0.014	LLCT
	S_{18}	H→L+5 (0.51)	305	0.127	LLCT/IL
		H−6→L+1 (0.32)			LLCT/IL
	S_{19}	H−6→L+1 (0.61)	305	0.031	LLCT/IL
	S_{20}	H−1→L+1 (0.70)	300	0.003	LLCT
	S_{21}	H→L+9 (0.48)	299	0.230	IL/ILCT
		H−2→L+2 (−0.37)			IL/ILCT
	S_{22}	H−1→L+2 (0.50)	297	0.081	IL
		H−7→L (0.31)			LLCT
	S_{23}	H−7→L (0.39)	296	0.032	LLCT
		H−1→L+2 (−0.37)			IL
		H−11→L (−0.31)			ILCT/IL
	S_{24}	H−12→L (0.67)	294	0.004	LLCT/ILCT
	S_{25}	H→L+9 (0.39)	293	0.051	IL/ILCT
		H−2→L+2 (0.38)			IL/ILCT
5	S_1	H→L (0.70)	609	0.161	LLCT
	S_2	H→L+1 (0.70)	454	0.028	LLCT
	S_3	H−1→L (0.62)	406	0.062	LLCT
	S_4	H−4→L (0.65)	393	0.040	IL
	S_5	H−3→L (0.55)	380	0.326	LLCT/ILCT
	S_6	H→L+3 (0.70)	375	0.880	IL/ILCT
	S_7	H−2→L (0.70)	369	0.025	LLCT
	S_8	H→L+2 (0.58)	369	0.386	IL

	S_9	H→L+4 (0.68)	343	0.003	LLCT
	S_{10}	H−7→L (0.62)	336	0.212	ILCT/IL
	S_{11}	H→L+7 (0.69)	330	0.039	IL
	S_{12}	H−1→L+1 (0.65)	329	0.012	LLCT
	S_{13}	H→L+5 (0.64)	322	0.002	LLCT/IL
	S_{14}	H−11→L (0.58)	321	0.031	ILCT/IL
	S_{15}	H−3→L+1 (0.64)	311	0.025	LLCT/ILCT
	S_{16}	H−5→L (0.55)	309	0.009	LLCT
	S_{17}	H−6→L (0.59)	307	0.004	LLCT
		H−9→L (0.34)			LLCT
	S_{18}	H−5→L (0.41)	306	0.058	LLCT
		H−4→L+1 (−0.40)			IL
	S_{19}	H−2→L+1 (0.69)	306	0.005	LLCT
	S_{20}	H→L+6 (0.57)	303	0.074	LLCT/IL
		H→L+8 (−0.32)			IL
	S_{21}	H−8→L (0.44)	302	0.106	LLCT
		H−4→L+1 (0.33)			IL
	S_{22}	H−9→L (0.57)	301	0.002	LLCT
		H−6→L (−0.37)			LLCT
	S_{23}	H→L+8 (0.53)	297	0.003	IL
		H→L+6 (0.36)			LLCT/IL
	S_{24}	H−13→L (0.46)	291	0.050	ILCT/IL
		H−10→L (−0.39)			LLCT
	S_{25}	H−13→L (0.44)	289	0.276	ILCT/IL
		H−10→L (0.39)			LLCT
6	S_1	H→L (0.70)	662	0.213	LLCT
	S_2	H→L+1 (0.70)	486	0.029	LLCT
	S_3	H−2→L (0.67)	425	0.109	LLCT
	S_4	H−1→L (0.71)	410	0.002	LLCT
	S_5	H−5→L (0.69)	401	0.000	LLCT/ILCT
	S_6	H−6→L (0.69)	393	0.044	IL
	S_7	H→L+2 (0.70)	389	0.037	IL/ILCT
	S_8	H−4→L (0.65)	376	0.091	LLCT
	S_9	H−3→L (0.71)	371	0.001	LLCT
	S_{10}	H→L+5 (0.58)	363	0.383	IL/ILCT
		H→L+3 (−0.37)			LLCT
	S_{11}	H→L+4 (0.68)	358	0.000	LLCT
	S_{12}	H→L+3 (0.47)	356	0.367	LLCT
		H→L+5 (0.36)			IL/ILCT
		H→L+6 (−0.31)			LLCT/IL
	S_{13}	H−2→L+1 (0.67)	344	0.003	LLCT
	S_{14}	H−8→L (0.69)	336	0.210	ILCT/IL
	S_{15}	H−1→L+1 (0.70)	334	0.001	LLCT

S_{16}	H→L+6 (0.57)	329	0.294	LLCT/IL
	H→L+3 (0.33)			LLCT
S_{17}	H−5→L+1 (0.69)	324	0.000	LLCT/ILCT
S_{18}	H−9→L (0.54)	323	0.006	LLCT
	H−7→L (−0.39)			LLCT
S_{19}	H−10→L (0.33)	318	0.008	ILCT/IL
	H−7→L (0.54)			LLCT
S_{20}	H−4→L+1 (0.65)	311	0.009	LLCT
S_{21}	H→L+8 (0.68)	310	0.308	IL/ILCT
S_{22}	H−3→L+1 (0.70)	307	0.002	LLCT
S_{23}	H−9→L (0.67)	305	0.015	LLCT
S_{24}	H−6→L+1 (0.57)	305	0.223	IL
S_{25}	H→L+7 (0.66)	302	0.084	IL/LLCT

[a] Orbitals involved in the major excitation (H = HOMO and L = LUMO).

[b] The coefficients in the configuration interaction (CI) expansion that are less than 0.3 are not listed.

[c] Oscillator strengths.

[d] Character of the transition.

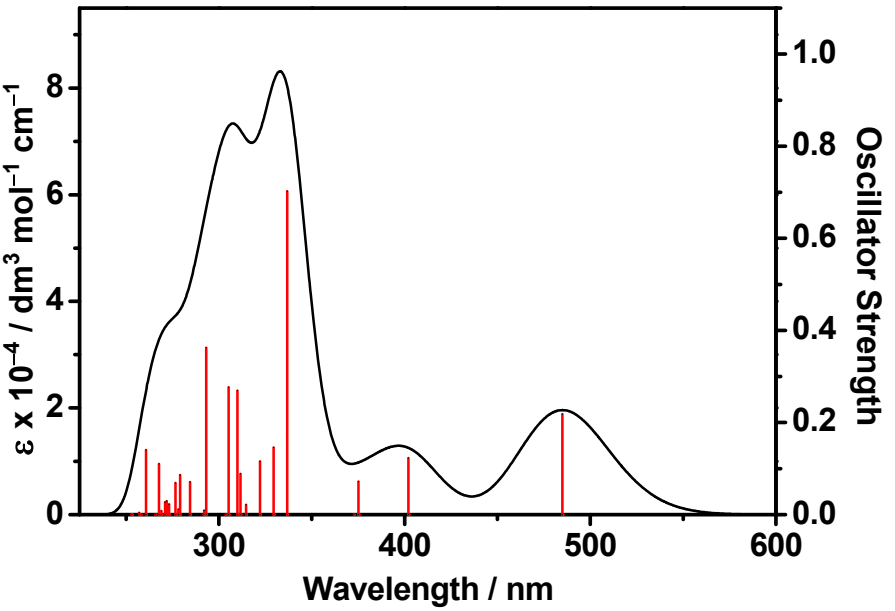


Figure S16. Simulated UV-vis spectrum of **1** computed by TDDFT/CPCM using toluene as the solvent.

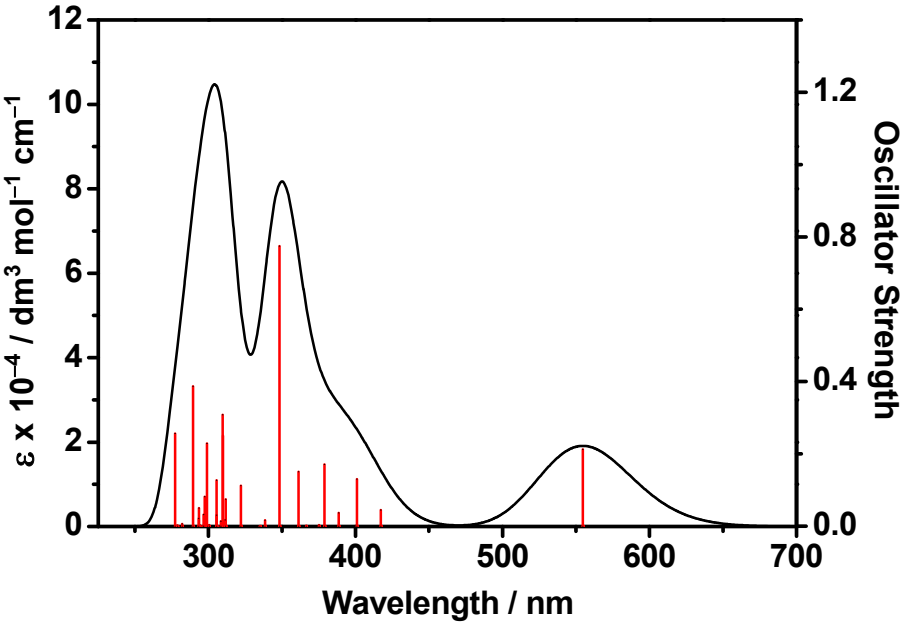


Figure S17. Simulated UV-vis spectrum of **3** computed by TDDFT/CPCM using toluene as the solvent.

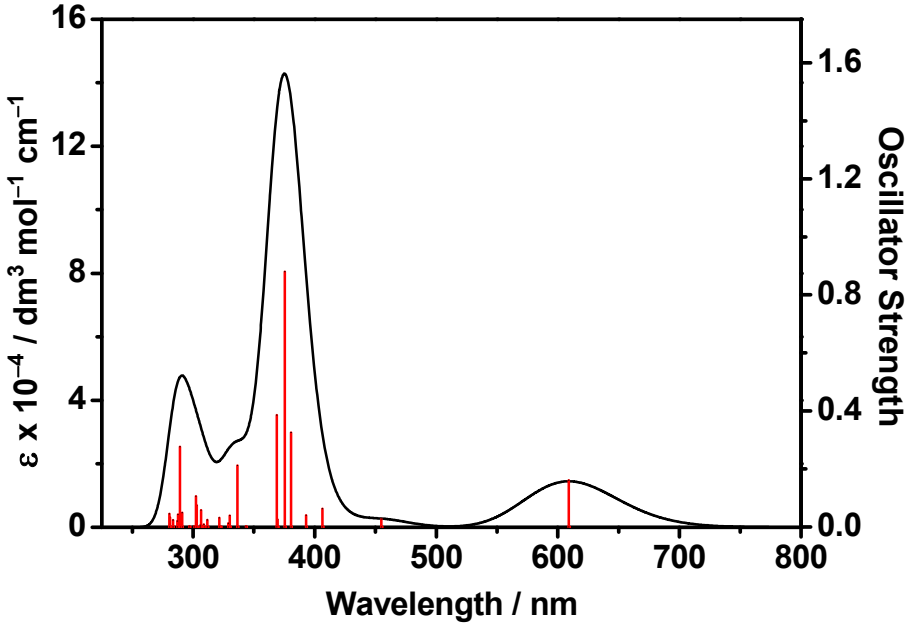


Figure S18. Simulated UV-vis spectrum of **5** computed by TDDFT/CPCM using toluene as the solvent.

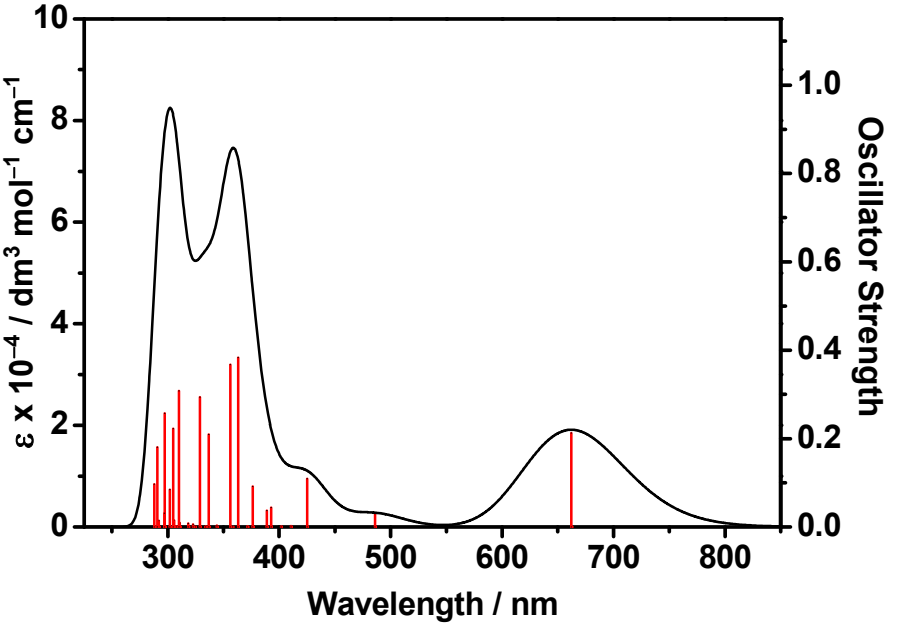


Figure S19. Simulated UV-vis spectrum of **6** computed by TDDFT/CPCM using toluene as the solvent.

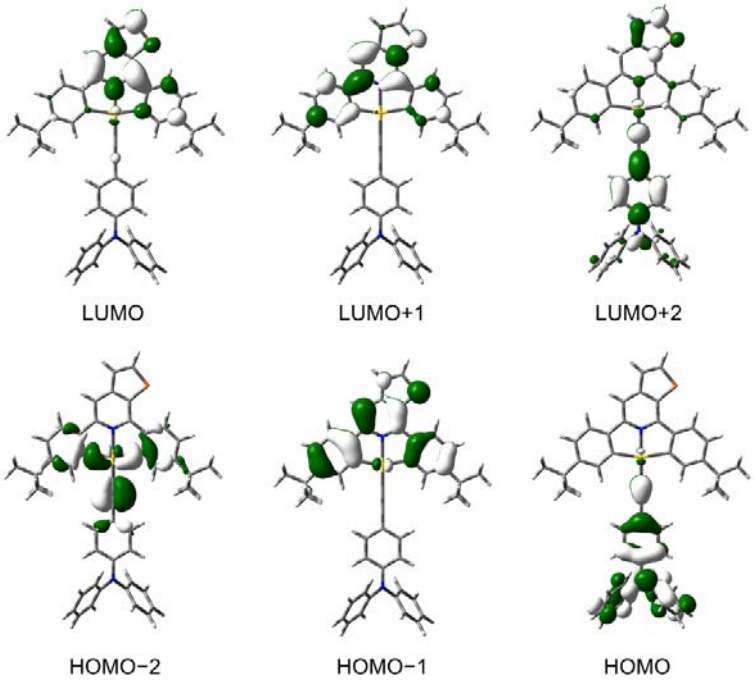


Figure S20. Spatial plots (isovalue = 0.03) of selected molecular orbitals of **1** at the optimized ground-state geometry.

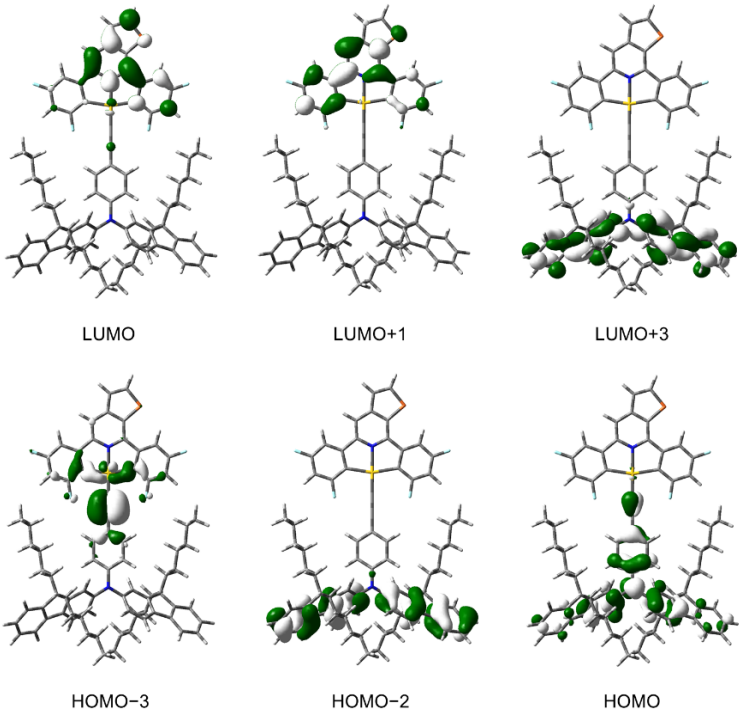


Figure S21. Spatial plots (isovalue = 0.03) of selected molecular orbitals of **5** at the optimized ground-state geometry.

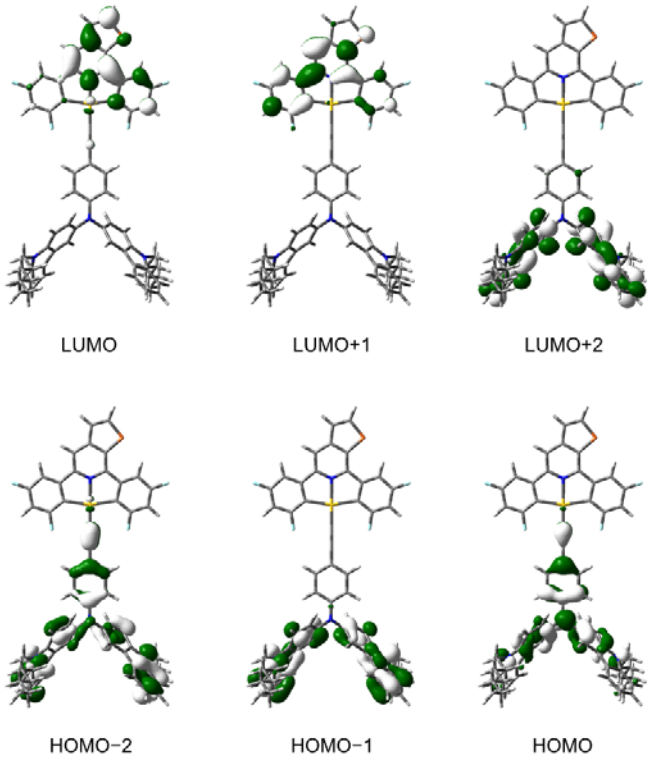


Figure S22. Spatial plots (isovalue = 0.03) of selected molecular orbitals of **6** at the optimized ground-state geometry.

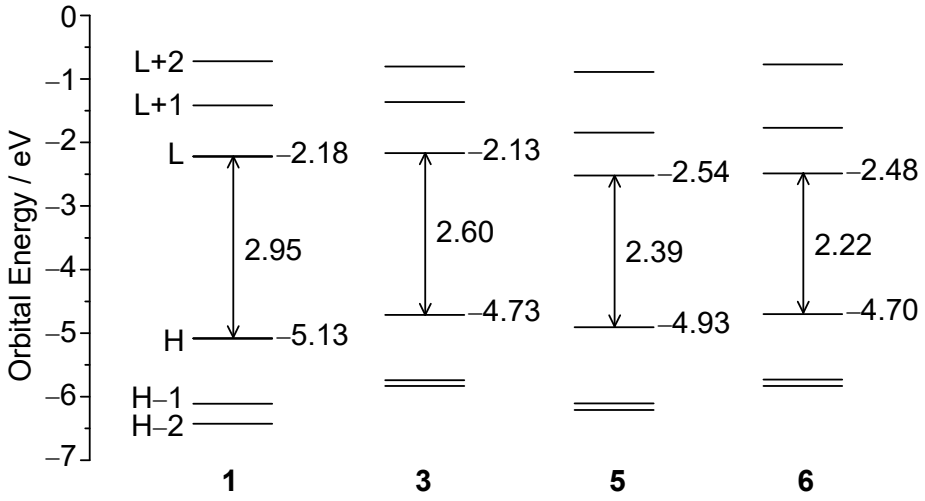


Figure S23. Orbital energy diagram of **1**, **3**, **5** and **6**.

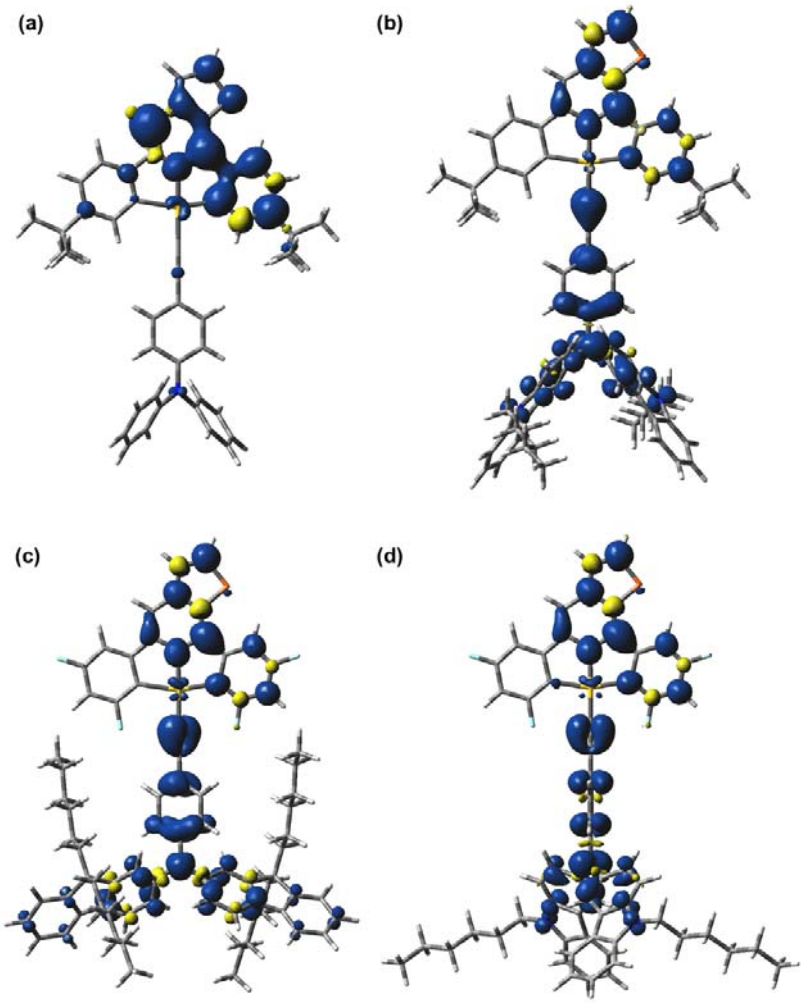
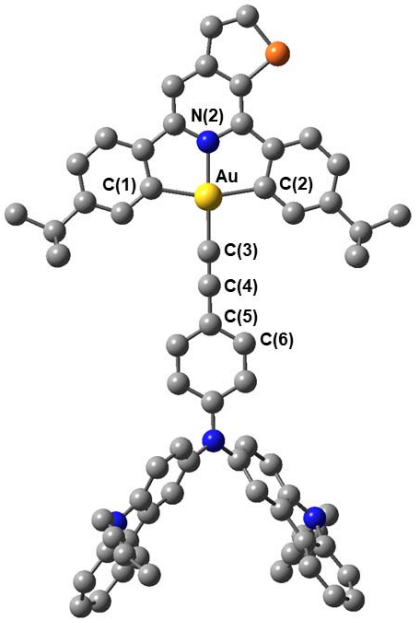


Figure S24. Plots of spin density (isovalue = 0.002) of the T_1 states of (a) **1**, (b) **3**, (c) **5** and (d) **6**.



Au−N(1)	1.995 (0.003)	N(1)−Au−C(1)	81.1 (−0.1)
Au−C(1)	2.091 (0.001)	N(1)−Au−C(2)	80.9 (0.0)
Au−C(2)	2.080 (0.000)	N(1)−Au−C(3)	179.6 (+0.1)
Au−C(3)	1.975 (0.009)	C(2)−Au−C(5)−C(6)	3.0 (−2.5)
C(3)−C(4)	1.231 (−0.005)		

Figure S25. Selected structural parameters of the optimized T_1 geometry of **3**. The bond lengths and angles are in Armstrong and degrees, respectively. The changes in bond lengths and angles from the optimized T_1 to S_1 geometries are shown in the brackets, in which, the positive and negative values indicate bond elongation and contraction, respectively, and the differences in bond angles. All hydrogen atoms are omitted for clarity.

Table S5. Relative energies of the optimized T_1 and S_1 states of **1**, **3**, **5** and **6**.

Complex	$\Delta E(T_1-S_0)$ / cm^{-1} (λ / nm)[a]	$\Delta E(S_1-S_0)$ / cm^{-1} (λ / nm)[b]
1	19307 (518)	---
3	15854 (631)	17382 (575)
5	15942 (627)	15991 (625)
6	14206 (704)	14305 (699)

[a] Energy difference between the T_1 and S_0 states at the corresponding optimized geometry in toluene.

[b] Energy difference between the S_1 and S_0 states at the corresponding optimized geometry in toluene.

Table S6. Cartesian coordinates of the optimized ground-state geometry of **1** optimized with PBE0 functional.

1	C	-4.685669	1.570570	0.107197	61	H	-2.454511	-6.792311	-1.407445
2	C	-6.063357	1.697853	0.107778	62	C	-0.275793	-5.341103	0.861179
3	C	-6.844196	0.538466	0.012555	63	H	0.273719	-4.401320	0.969676
4	C	-6.223231	-0.733446	-0.082162	64	H	-0.884015	-5.481436	1.760806
5	C	-4.823106	-0.834692	-0.080251	65	H	0.456674	-6.154696	0.814510
6	H	-8.934332	1.296292	0.057551	66	N	6.689958	-0.244346	-0.011606
7	H	-6.534137	2.671123	0.180240	67	C	5.283415	-0.172687	-0.000256
8	C	-8.272610	0.440783	-0.004776	68	C	7.354989	-1.283852	0.678595
9	C	-8.700553	-0.842075	-0.107942	69	C	8.458256	-1.925130	0.101278
10	H	-9.722815	-1.196693	-0.142691	70	C	6.922896	-1.683699	1.949602
11	C	-3.687603	2.647028	0.197775	71	C	9.117324	-2.938761	0.787903
12	C	-2.319866	2.266670	0.178790	72	H	8.793854	-1.622884	-0.885903
13	C	-4.025870	3.996611	0.299616	73	C	7.577404	-2.710800	2.620369
14	C	-1.351023	3.257019	0.263697	74	H	6.072965	-1.185116	2.405242
15	C	-3.031177	4.966575	0.383141	75	C	8.680138	-3.342052	2.048079
16	H	-5.066885	4.309626	0.315226	76	H	9.971326	-3.425873	0.325603
17	C	-1.676069	4.621046	0.367500	77	H	7.229349	-3.008574	3.605492
18	H	-0.307304	2.953999	0.248272	78	H	9.192970	-4.138811	2.578204
19	H	-3.329660	6.006202	0.461545	79	C	7.444553	0.719686	-0.719255
20	C	-3.961067	-2.023001	-0.166443	80	C	8.618942	1.245625	-0.166186
21	C	-2.556763	-1.790283	-0.140087	81	C	7.030989	1.158560	-1.983510
22	C	-4.431274	-3.334262	-0.269712	82	C	9.364881	2.184584	-0.869929
23	C	-1.696813	-2.875054	-0.218163	83	H	8.941031	0.912895	0.815699
24	C	-3.541233	-4.401696	-0.345688	84	C	7.774001	2.111442	-2.671340
25	H	-5.493263	-3.556031	-0.293018	85	H	6.125584	0.748842	-2.420454
26	C	-2.158931	-4.199374	-0.321694	86	C	8.946695	2.627534	-2.123238
27	H	-0.627785	-2.680180	-0.197184	87	H	10.273278	2.582602	-0.426404
28	H	-3.947368	-5.403923	-0.424466	88	H	7.439012	2.440963	-3.650868
29	Au	-2.130591	0.219929	0.019701	89	H	9.528014	3.366210	-2.666633
30	C	2.459248	-0.026893	0.016562	90	S	-7.415920	-1.996096	-0.189274
31	C	3.122348	-1.265502	-0.034299	91	C	-0.184682	0.114976	0.022956
32	C	3.246951	1.136836	0.060454	92	C	1.036551	0.047604	0.021248
33	C	4.505894	-1.338927	-0.049944					
34	H	2.535154	-2.178021	-0.077693					
35	C	4.630656	1.067300	0.059732					
36	H	2.757328	2.104911	0.109972					
37	H	4.995980	-2.305836	-0.103818					
38	H	5.218416	1.978522	0.107000					
39	N	-4.141764	0.326012	0.014561					
40	C	-0.556701	5.659823	0.458160					
41	C	0.322631	5.568257	-0.800299					
42	H	0.772983	4.577193	-0.909892					
43	H	-0.262925	5.773352	-1.702574					
44	H	1.134809	6.301941	-0.746767					
45	C	-1.094659	7.089259	0.565695					
46	H	-1.708423	7.227094	1.462223					
47	H	-0.256848	7.791240	0.627667					
48	H	-1.693727	7.365914	-0.308409					
49	C	0.301864	5.372087	1.701261					
50	H	-0.298585	5.435729	2.614731					
51	H	0.750915	4.375168	1.662845					
52	H	1.114417	6.103546	1.775733					
53	C	-1.152912	-5.347951	-0.402237					
54	C	-0.263124	-5.154209	-1.641722					
55	H	-0.862160	-5.159298	-2.558274					
56	H	0.286359	-4.208929	-1.604026					
57	H	0.469717	-5.966027	-1.708890					
58	C	-1.835132	-6.714514	-0.507603					
59	H	-1.073892	-7.499356	-0.561738					
60	H	-2.464451	-6.923917	0.363908					

Table S7. Cartesian coordinates of the optimized ground-state geometry of **3** optimized with PBE0 functional.

1	C	-8.091035	-1.267543	-0.821488	61	H	-5.617647	5.140299	4.657363
2	C	-9.471875	-1.343778	-0.864650	62	C	-3.482747	4.974478	1.934402
3	C	-10.218887	-0.370186	-0.188590	63	H	-2.961626	4.203391	1.359294
4	C	-9.561494	0.666829	0.521739	64	H	-4.086823	5.564291	1.237111
5	C	-8.158967	0.720807	0.550013	65	H	-2.726249	5.634710	2.373099
6	H	-12.329956	-0.952183	-0.575314	66	N	3.330101	0.016813	-0.009777
7	H	-9.970623	-2.137531	-1.408113	67	C	1.931804	-0.019218	-0.023563
8	C	-11.643957	-0.259592	-0.102646	68	S	-10.717298	1.734390	1.265360
9	C	-12.034805	0.808483	0.636191	69	C	-3.550126	-0.161285	-0.084925
10	H	-13.046384	1.122812	0.859643	70	C	-2.327116	-0.129485	-0.070133
11	C	-7.124289	-2.176930	-1.455300	71	C	4.023336	1.251874	0.080481
12	C	-5.746101	-1.891780	-1.267447	72	C	3.666687	2.320177	-0.767150
13	C	-7.501350	-3.283395	-2.216840	73	C	5.074081	1.400993	0.984046
14	C	-4.806189	-2.729204	-1.852362	74	C	4.322890	3.540985	-0.715372
15	C	-6.534994	-4.104682	-2.790248	75	H	2.855910	2.175936	-1.474529
16	H	-8.550994	-3.519631	-2.373261	76	C	5.764631	2.611863	1.031663
17	C	-5.170433	-3.847915	-2.622175	77	H	5.349444	0.573835	1.631618
18	H	-3.754281	-2.500499	-1.702049	78	C	5.375434	3.682533	0.190727
19	H	-6.863176	-4.956305	-3.376036	79	H	4.030010	4.347151	-1.380856
20	C	-7.262914	1.683119	1.208625	80	C	6.874536	3.094207	1.818164
21	C	-5.865902	1.460608	1.047497	81	C	7.101180	4.433611	1.413132
22	C	-7.694866	2.775633	1.964486	82	C	7.680195	2.525508	2.807412
23	C	-4.974850	2.337304	1.647397	83	C	8.122941	5.201807	1.975231
24	C	-6.774164	3.637450	2.553488	84	C	8.694174	3.287974	3.372380
25	H	-8.749978	2.981742	2.112362	85	H	7.516603	1.500059	3.127494
26	C	-5.398247	3.440431	2.410010	86	C	8.909349	4.611080	2.956967
27	H	-3.912025	2.152854	1.514780	87	H	8.305954	6.224198	1.659062
28	H	-7.150983	4.473555	3.131960	88	H	9.329615	2.858239	4.140802
29	Au	-5.497696	-0.207152	-0.105696	89	H	9.710746	5.188137	3.409634
30	C	-0.903419	-0.093053	-0.053851	90	C	4.085270	-1.183070	-0.081399
31	C	-0.207669	0.939957	0.598708	91	C	3.775693	-2.258464	0.775436
32	C	-0.141148	-1.088589	-0.690141	92	C	5.149041	-1.288595	-0.975591
33	C	1.176469	0.976412	0.620199	93	C	4.494200	-3.444425	0.743853
34	H	-0.771317	1.717031	1.107035	94	H	2.952038	-2.147595	1.473940
35	C	1.243139	-1.052987	-0.681815	95	C	5.900801	-2.463063	-1.003658
36	H	-0.652654	-1.893721	-1.209773	96	H	5.386912	-0.455580	-1.630505
37	H	1.686350	1.778586	1.143570	97	C	5.560568	-3.541981	-0.151893
38	H	1.805281	-1.827370	-1.193408	98	H	4.237221	-4.256879	1.416443
39	N	-7.511482	-0.251664	-0.124845	99	C	7.040713	-2.896840	-1.775339
40	C	-4.081409	-4.728205	-3.238188	100	C	7.333781	-4.217038	-1.350559
41	C	-3.196760	-5.299227	-2.117215	101	C	7.823849	-2.299446	-2.765756
42	H	-2.718125	-4.506900	-1.534062	102	C	8.399650	-4.937463	-1.893747
43	H	-3.785760	-5.914623	-1.429140	103	C	8.881543	-3.014640	-3.312063
44	H	-2.405829	-5.926333	-2.543822	104	H	7.609273	-1.288366	-3.101051
45	C	-4.660273	-5.899125	-4.037030	105	C	9.162530	-4.318919	-2.876910
46	H	-5.279017	-5.555662	-4.872895	106	H	8.633387	-5.944635	-1.562508
47	H	-3.843016	-6.496178	-4.454405	107	H	9.500126	-2.562107	-4.081148
48	H	-5.265859	-6.560922	-3.408688	108	H	9.997192	-4.858747	-3.315156
49	C	-3.217942	-3.877583	-4.184834	109	N	6.179684	4.777890	0.442798
50	H	-3.822304	-3.461529	-4.997663	110	N	6.422868	-4.596962	-0.383392
51	H	-2.740380	-3.044557	-3.660506	111	C	6.127511	6.038707	-0.262163
52	H	-2.426884	-4.492592	-4.628509	112	H	5.081047	6.241558	-0.516382
53	C	-4.358967	4.366483	3.042630	113	H	6.432297	6.828862	0.432998
54	C	-3.474866	3.552646	4.002637	114	C	6.440269	-5.843987	0.347616
55	H	-4.073371	3.110493	4.805916	115	H	5.406479	-6.101397	0.603906
56	H	-2.952996	2.741608	3.486152	116	H	6.792395	-6.629677	-0.329986
57	H	-2.718699	4.201507	4.458538	117	C	7.304718	-5.799713	1.605643
58	C	-5.000870	5.510747	3.831664	118	H	8.330029	-5.528415	1.323260
59	H	-4.217078	6.142183	4.262239	119	H	6.939533	-4.998069	2.260342
60	H	-5.623976	6.146255	3.193437	120	C	7.304810	-7.126303	2.357018

121	H	6.273189	-7.394195	2.626653
122	H	7.661079	-7.924426	1.690047
123	C	8.164314	-7.101686	3.616825
124	H	9.195803	-6.833276	3.347780
125	H	7.808370	-6.303910	4.284080
126	C	8.169348	-8.426367	4.373449
127	H	7.137984	-8.693210	4.640961
128	H	8.524341	-9.222477	3.705088
129	C	9.030591	-8.391866	5.629826
130	H	8.677125	-7.626710	6.329988
131	H	9.017320	-9.352978	6.153277
132	H	10.073556	-8.159316	5.387358
133	C	6.995107	6.072676	-1.518381
134	H	8.034352	5.856337	-1.239593
135	H	6.678717	5.265895	-2.191884
136	C	6.916548	7.413936	-2.238876
137	H	5.870629	7.626030	-2.503111
138	H	7.224606	8.215986	-1.552871
139	C	7.775257	7.471307	-3.498203
140	H	8.821396	7.259809	-3.235058
141	H	7.467876	6.669682	-4.184688
142	C	7.698851	8.811790	-4.222366
143	H	6.652835	9.021604	-4.483692
144	H	8.005253	9.611531	-3.534582
145	C	8.559237	8.860774	-5.478874
146	H	8.252721	8.092508	-6.197514
147	H	8.486271	9.831655	-5.978851
148	H	9.614823	8.687050	-5.241769

Table S8. Cartesian coordinates of the optimized ground-state geometry of **5** optimized with PBE0 functional.

1	C	-7.698488	-1.430730	-0.651183	61	C	6.881367	5.875088	1.402430
2	C	-9.076299	-1.531438	-0.696241	62	C	5.124831	7.329931	-0.249996
3	C	-9.842863	-0.480455	-0.179524	63	H	2.333558	6.335675	-0.987238
4	C	-9.203315	0.658268	0.376365	64	H	1.950251	4.630461	-1.129416
5	C	-7.801847	0.727822	0.406387	65	C	2.153860	5.305264	0.901285
6	H	-11.940405	-1.143645	-0.499322	66	H	3.950543	6.073336	-2.750430
7	H	-9.561761	-2.401546	-1.121085	67	H	3.529813	4.372050	-2.859958
8	C	-11.268958	-0.379617	-0.126840	68	C	5.648381	4.756389	-2.907033
9	C	-11.680548	0.780616	0.441822	69	C	6.984068	7.261858	1.306300
10	H	-12.697764	1.112592	0.606434	70	H	7.561240	5.317559	2.041323
11	C	-6.723126	-2.420692	-1.138450	71	C	6.113622	7.984879	0.488894
12	C	-5.350404	-2.096359	-0.984051	72	H	4.451946	7.899982	-0.886456
13	C	-7.142007	-3.620139	-1.721711	73	H	2.510750	4.370648	1.353320
14	C	-4.445314	-3.043897	-1.446086	74	H	2.644712	6.119432	1.450131
15	C	-6.176213	-4.510209	-2.156714	75	C	0.640528	5.393925	1.079933
16	H	-8.187346	-3.878920	-1.845256	76	H	6.366227	5.454469	-2.457306
17	C	-4.822683	-4.248676	-2.030759	77	H	5.942014	3.753503	-2.570460
18	C	-6.924517	1.793664	0.923644	78	C	5.755876	4.830762	-4.427366
19	C	-5.525182	1.566769	0.804055	79	H	7.748333	7.785544	1.873728
20	C	-7.428615	2.965236	1.498708	80	H	6.206099	9.065534	0.427062
21	C	-4.697595	2.570850	1.286826	81	H	0.268010	6.325172	0.629294
22	C	-6.534379	3.917445	1.956383	82	H	0.167390	4.575396	0.518199
23	H	-8.485012	3.172607	1.607793	83	C	0.191539	5.320838	2.535598
24	C	-5.165459	3.748094	1.862837	84	H	5.457794	5.833701	-4.765747
25	Au	-5.112091	-0.251465	-0.085076	85	H	5.035995	4.133263	-4.879437
26	C	-0.528264	-0.085898	-0.038346	86	C	7.154397	4.519179	-4.950236
27	C	0.154929	0.805571	0.807021	87	H	0.598497	4.408149	2.994785
28	C	0.234183	-0.923672	-0.870877	88	H	0.626004	6.160583	3.096755
29	C	1.539427	0.849676	0.829070	89	C	-1.325243	5.330615	2.704133
30	H	-0.418663	1.454647	1.461889	90	H	7.875046	5.215926	-4.498445
31	C	1.618277	-0.864369	-0.868678	91	H	7.453377	3.516014	-4.613767
32	H	-0.277988	-1.613358	-1.535074	92	C	7.266830	4.594300	-6.469790
33	H	2.049227	1.531285	1.502680	93	H	-1.734509	6.234464	2.231929
34	H	2.189275	-1.505774	-1.532616	94	H	-1.754482	4.479963	2.157207
35	N	-7.132861	-0.320941	-0.109249	95	C	-1.762349	5.273488	4.163101
36	N	3.702108	0.071920	-0.001718	96	H	6.967028	5.596682	-6.804544
37	C	2.293266	0.019492	-0.013715	97	H	6.546593	3.897615	-6.919833
38	S	-10.382118	1.805885	0.940597	98	C	8.667563	4.282546	-6.982096
39	C	-3.168360	-0.182860	-0.063533	99	H	-1.375901	6.130857	4.725561
40	C	-1.949463	-0.138403	-0.051564	100	H	-2.853088	5.278589	4.261275
41	H	-4.078960	-4.958328	-2.374865	101	H	-1.390877	4.365164	4.650543
42	H	-4.478254	4.504645	2.224235	102	H	8.979244	3.273447	-6.689853
43	F	-7.013298	5.039592	2.506610	103	H	8.720843	4.343741	-8.073733
44	F	-3.367282	2.442619	1.212491	104	H	9.402742	4.984751	-6.573130
45	F	-6.561859	-5.663596	-2.717061	105	C	4.445068	-1.121187	-0.134614
46	F	-3.128050	-2.828341	-1.340559	106	C	5.576889	-1.167524	-0.962916
47	C	4.352563	1.315370	0.151755	107	C	4.027455	-2.279238	0.539806
48	C	5.461671	1.439909	1.002461	108	C	6.268941	-2.358887	-1.153252
49	C	3.863150	2.444083	-0.524254	109	H	5.892993	-0.264061	-1.475292
50	C	6.058756	2.678172	1.213881	110	C	4.705937	-3.466312	0.332101
51	H	5.834408	0.558904	1.515835	111	H	3.160276	-2.232701	1.192786
52	C	4.446473	3.676957	-0.295443	112	C	5.819973	-3.518586	-0.522925
53	H	3.014658	2.338057	-1.194596	113	H	7.131060	-2.379753	-1.814594
54	C	5.536347	3.805987	0.582297	114	C	4.395407	-4.835380	0.911653
55	H	6.903678	2.758231	1.892652	115	C	6.284033	-4.904426	-0.589340
56	C	4.044228	5.023698	-0.870951	116	C	5.447982	-5.690234	0.225323
57	C	5.892556	5.222348	0.668136	117	C	2.951240	-5.272622	0.582514
58	C	5.015392	5.949695	-0.157510	118	C	4.568575	-4.856404	2.449503
59	C	2.564958	5.347274	-0.567102	119	C	7.334408	-5.485341	-1.297983
60	C	4.244033	5.072243	-2.404844	120	C	5.659878	-7.057468	0.332048

121	H	2.787131	-6.272555	1.007012
122	H	2.272892	-4.600347	1.126342
123	C	2.567970	-5.272880	-0.893986
124	H	4.346025	-5.874215	2.799143
125	H	3.794184	-4.209356	2.884444
126	C	5.934687	-4.429193	2.974351
127	C	7.540142	-6.859514	-1.187478
128	H	7.982850	-4.882310	-1.928173
129	C	6.710461	-7.640661	-0.381256
130	H	5.019359	-7.672461	0.960019
131	H	2.861978	-4.317124	-1.347078
132	H	3.130555	-6.051199	-1.425729
133	C	1.069829	-5.477839	-1.102447
134	H	6.712430	-5.074327	2.545643
135	H	6.157078	-3.410016	2.632176
136	C	6.018409	-4.480012	4.497137
137	H	8.353451	-7.327696	-1.734885
138	H	6.883413	-8.710673	-0.308076
139	H	0.759703	-6.431318	-0.651062
140	H	0.524097	-4.693483	-0.558086
141	C	0.647797	-5.450159	-2.567720
142	H	5.795320	-5.500242	4.841463
143	H	5.236366	-3.838157	4.927884
144	C	7.377085	-4.051351	5.041831
145	H	0.994811	-4.513014	-3.026868
146	H	1.156277	-6.259095	-3.111716
147	C	-0.859968	-5.575505	-2.767986
148	H	8.160060	-4.692351	4.611752
149	H	7.600680	-3.030943	4.698746
150	C	7.466107	-4.100869	6.563970
151	H	-1.210542	-6.503324	-2.295090
152	H	-1.363768	-4.754765	-2.239335
153	C	-1.268079	-5.564516	-4.236383
154	H	7.243005	-5.120815	6.905478
155	H	6.682795	-3.460828	6.992249
156	C	8.826547	-3.669635	7.097824
157	H	-0.806206	-6.395428	-4.781426
158	H	-2.352960	-5.652448	-4.357398
159	H	-0.955184	-4.635256	-4.725510
160	H	9.059952	-2.641529	6.798913
161	H	8.863773	-3.714521	8.190918
162	H	9.624516	-4.313380	6.710950

Table S9. Cartesian coordinates of the optimized ground-state geometry of **6** optimized with PBE0 functional.

1	C	8.207107	-1.216223	0.876897	63	C	-4.340082	-3.518749	-0.343814
2	C	9.585556	-1.310573	0.917361	64	H	-2.799054	-2.302156	-1.202565
3	C	10.342925	-0.377899	0.199238	65	C	-5.773709	-2.354123	1.263198
4	C	9.693577	0.637492	-0.550177	66	H	-5.280979	-0.284005	1.660598
5	C	8.291706	0.704145	-0.569710	67	C	-5.415760	-3.521454	0.546108
6	H	12.445728	-0.976047	0.601530	68	H	-4.069386	-4.401079	-0.915421
7	H	10.078053	-2.087449	1.489429	69	C	-6.919226	-2.705350	2.067863
8	C	11.767950	-0.293584	0.103346	70	C	-7.197305	-4.068600	1.796640
9	C	12.169429	0.736809	-0.681489	71	C	-7.718126	-2.003841	2.973746
10	H	13.183540	1.028146	-0.923872	72	C	-8.263522	-4.730500	2.409184
11	C	7.240517	-2.094132	1.557517	73	C	-8.776201	-2.660145	3.588982
12	C	5.865720	-1.803760	1.362178	74	H	-7.515266	-0.958648	3.190990
13	C	7.668774	-3.159230	2.355699	75	C	-9.042096	-4.008708	3.305885
14	C	4.967662	-2.641344	2.011799	76	H	-8.485773	-5.771384	2.194890
15	C	6.709776	-3.946478	2.967863	77	H	-9.406872	-2.126748	4.293739
16	H	8.716126	-3.390076	2.513076	78	H	-9.877348	-4.501437	3.795511
17	C	5.354370	-3.710759	2.813536	79	N	-6.088366	4.677933	-0.960803
18	C	7.405343	1.653935	-1.266049	80	N	-6.272723	-4.550074	0.889643
19	C	6.008714	1.451538	-1.088340	81	C	-6.062658	6.002811	-0.383388
20	C	7.897733	2.697839	-2.057306	82	H	-5.023569	6.242849	-0.131518
21	C	5.170753	2.344941	-1.740549	83	H	-6.362332	6.716709	-1.158660
22	C	6.993825	3.544759	-2.674893	84	C	-6.266557	-5.876377	0.314949
23	H	8.951941	2.883840	-2.215474	85	H	-6.621203	-6.578337	1.077814
24	C	5.626727	3.392851	-2.534634	86	H	-5.226319	-6.150729	0.106479
25	Au	5.609637	-0.165179	0.131931	87	C	-6.955183	6.148615	0.847049
26	C	1.022571	-0.057217	0.079209	88	H	-7.986148	5.892402	0.571290
27	C	0.322884	0.897619	-0.679188	89	H	-6.643370	5.415523	1.601999
28	C	0.269042	-0.985853	0.818486	90	C	-6.906772	7.554467	1.434905
29	C	-1.061387	0.921003	-0.705182	91	H	-7.208900	8.282131	0.668085
30	H	0.886046	1.618564	-1.264376	92	H	-5.869275	7.804941	1.698697
31	C	-1.115294	-0.960495	0.806034	93	C	-7.793424	7.721584	2.664696
32	H	0.790330	-1.725855	1.418446	94	H	-8.831065	7.471821	2.401396
33	H	-1.577240	1.658847	-1.310881	95	H	-7.492319	6.993794	3.431521
34	H	-1.673400	-1.679561	1.396680	96	C	-7.748259	9.126302	3.257971
35	N	7.631616	-0.226704	0.145379	97	H	-8.048051	9.852259	2.490092
36	N	-3.208241	0.015551	0.019039	98	H	-6.710810	9.374125	3.520165
37	C	-1.809587	-0.007569	0.039807	99	C	-8.637246	9.283954	4.485269
38	S	10.862098	1.653893	-1.341997	100	H	-8.586647	10.299199	4.891026
39	C	3.664851	-0.111498	0.112677	101	H	-9.685162	9.074034	4.243458
40	C	2.444676	-0.084825	0.096940	102	H	-8.338304	8.592334	5.280836
41	C	-3.909618	1.228446	-0.207867	103	C	-7.111646	-5.995881	-0.951299
42	C	-3.573332	2.381487	0.529721	104	H	-8.144308	-5.705882	-0.718710
43	C	-4.947743	1.273987	-1.136651	105	H	-6.745228	-5.274937	-1.693309
44	C	-4.238742	3.584193	0.344119	106	C	-7.084450	-7.403884	-1.535375
45	H	-2.771066	2.318052	1.258366	107	H	-7.442182	-8.119581	-0.781327
46	C	-5.646653	2.467172	-1.318609	108	H	-6.045496	-7.688625	-1.754974
47	H	-5.206725	0.381961	-1.699357	109	C	-7.923459	-7.544809	-2.801338
48	C	-5.279097	3.621938	-0.586117	110	H	-8.962456	-7.260230	-2.582467
49	H	-3.961552	4.457123	0.926952	111	H	-7.566289	-6.829360	-3.555604
50	C	-6.747559	2.855966	-2.167059	112	C	-7.899799	-8.951799	-3.390472
51	C	-6.991648	4.227357	-1.904440	113	H	-8.256058	-9.665380	-2.635224
52	C	-7.531711	2.181671	-3.105881	114	H	-6.860935	-9.234617	-3.607813
53	C	-8.010349	4.924197	-2.557760	115	C	-8.740372	-9.083053	-4.654441
54	C	-8.542197	2.872699	-3.761753	116	H	-8.706548	-10.100541	-5.056309
55	H	-7.354161	1.130711	-3.317324	117	H	-9.790031	-8.837547	-4.457945
56	C	-8.775270	4.228950	-3.486605	118	H	-8.384715	-8.404017	-5.437415
57	H	-8.206912	5.971656	-2.350468	119	H	4.615378	-4.336635	3.300327
58	H	-9.160924	2.360821	-4.492572	120	H	4.931206	4.064718	-3.024250
59	H	-9.573669	4.749057	-4.008339	121	F	7.461398	4.544546	-3.432699
60	C	-3.956120	-1.173898	0.219448	122	F	3.844065	2.230039	-1.626404
61	C	-3.629797	-2.338372	-0.504642	123	F	7.104270	-4.970618	3.735740
62	C	-5.029802	-1.184585	1.108093	124	F	3.650958	-2.445504	1.887927

Table S10. Cartesian coordinates of the optimized ground-state geometry of **3** optimized with M06 functional.

1	C	-8.102916	-1.280128	-0.872024	61	H	-5.844906	5.090358	4.741613
2	C	-9.479747	-1.391719	-0.920169	62	C	-3.715178	5.070611	2.016871
3	C	-10.252202	-0.448834	-0.229922	63	H	-3.157814	4.335917	1.424250
4	C	-9.629038	0.593549	0.500051	64	H	-4.346872	5.648544	1.330566
5	C	-8.229764	0.686487	0.534750	65	H	-2.987707	5.756696	2.470252
6	H	-12.337359	-1.092300	-0.641363	66	N	3.317066	0.039656	0.005524
7	H	-9.960484	-2.190310	-1.477922	67	C	1.916240	0.020424	-0.015212
8	C	-11.678724	-0.383422	-0.150327	68	S	-10.822737	1.620383	1.261022
9	C	-12.108739	0.657310	0.602831	69	C	-3.557249	-0.080208	-0.095679
10	H	-13.132059	0.936257	0.825418	70	C	-2.334835	-0.047925	-0.074714
11	C	-7.112654	-2.154919	-1.516965	71	C	4.028052	1.268087	0.083617
12	C	-5.739947	-1.848627	-1.327266	72	C	3.717332	2.314532	-0.805090
13	C	-7.465406	-3.256638	-2.295143	73	C	5.054037	1.421279	1.012426
14	C	-4.783369	-2.654514	-1.923501	74	C	4.397182	3.522675	-0.770344
15	C	-6.483313	-4.049045	-2.880839	75	H	2.922171	2.161010	-1.531531
16	H	-8.512583	-3.511507	-2.454963	76	C	5.766849	2.617766	1.044577
17	C	-5.125212	-3.767481	-2.709482	77	H	5.294461	0.604059	1.690943
18	H	-3.732290	-2.406211	-1.770070	78	C	5.423757	3.667737	0.161815
19	H	-6.795411	-4.899921	-3.480375	79	H	4.143568	4.318035	-1.468033
20	C	-7.364647	1.662731	1.214142	80	C	6.868720	3.096632	1.842624
21	C	-5.959606	1.492096	1.062519	81	C	7.141542	4.414000	1.404226
22	C	-7.834459	2.727545	1.985330	82	C	7.635367	2.535839	2.864181
23	C	-5.101582	2.384919	1.681450	83	C	8.174269	5.168635	1.959783
24	C	-6.947017	3.608274	2.595537	84	C	8.660024	3.285048	3.425956
25	H	-8.898553	2.898711	2.130400	85	H	7.433140	1.523719	3.210472
26	C	-5.565624	3.459294	2.458890	86	C	8.923638	4.586043	2.974102
27	H	-4.028356	2.238748	1.553727	87	H	8.392380	6.176481	1.612413
28	H	-7.356593	4.422707	3.186502	88	H	9.268006	2.860699	4.221144
29	Au	-5.522593	-0.161461	-0.126572	89	H	9.735213	5.152883	3.424913
30	C	-0.911135	-0.021486	-0.055000	90	C	4.061577	-1.170356	-0.048103
31	C	-0.210334	1.011018	0.588046	91	C	3.753916	-2.220929	0.836683
32	C	-0.161726	-1.032126	-0.678252	92	C	5.114864	-1.300997	-0.949304
33	C	1.173320	1.032364	0.613719	93	C	4.463861	-3.412041	0.824376
34	H	-0.773834	1.799153	1.085281	94	H	2.936289	-2.084672	1.541314
35	C	1.221819	-1.012381	-0.665167	95	C	5.857449	-2.479698	-0.958360
36	H	-0.687491	-1.837058	-1.189924	96	H	5.352222	-0.480300	-1.624703
37	H	1.694545	1.834671	1.130426	97	C	5.517186	-3.534947	-0.080757
38	H	1.780922	-1.798589	-1.166690	98	H	4.211960	-4.211046	1.518513
39	N	-7.555883	-0.257776	-0.155788	99	C	6.990629	-2.934325	-1.726195
40	C	-4.019252	-4.608676	-3.339633	100	C	7.283529	-4.243507	-1.276258
41	C	-3.108553	-5.162189	-2.236936	101	C	7.769573	-2.358428	-2.729917
42	H	-2.634244	-4.363181	-1.655263	102	C	8.347694	-4.974954	-1.802648
43	H	-3.675810	-5.794075	-1.541907	103	C	8.825782	-3.084625	-3.262690
44	H	-2.310197	-5.772854	-2.678799	104	H	7.552224	-1.352492	-3.084928
45	C	-4.569125	-5.787786	-4.139284	105	C	9.108639	-4.377627	-2.799646
46	H	-5.204371	-5.456999	-4.970738	106	H	8.580818	-5.976248	-1.446231
47	H	-3.736994	-6.360169	-4.567191	107	H	9.443610	-2.648283	-4.043670
48	H	-5.152142	-6.471691	-3.509398	108	H	9.944729	-4.926257	-3.227611
49	C	-3.194677	-3.729548	-4.287899	109	N	6.246456	4.755587	0.404543
50	H	-3.824388	-3.320837	-5.088259	110	N	6.371661	-4.603336	-0.298381
51	H	-2.727215	-2.887755	-3.764014	111	C	6.279541	5.973502	-0.374843
52	H	-2.394736	-4.321461	-4.751986	112	H	5.252307	6.210115	-0.685794
53	C	-4.561420	4.404847	3.109072	113	H	6.593817	6.794722	0.284343
54	C	-3.647295	3.607193	4.047278	114	C	6.410858	-5.819703	0.483143
55	H	-4.229867	3.116866	4.837324	115	H	5.381233	-6.077601	0.768247
56	H	-3.084056	2.832907	3.513505	116	H	6.758843	-6.634724	-0.166773
57	H	-2.921867	4.278362	4.525468	117	C	7.293443	-5.707745	1.717087
58	C	-5.240483	5.503283	3.923995	118	H	8.313697	-5.437429	1.403550
59	H	-4.477778	6.152106	4.371527	119	H	6.932478	-4.874931	2.340333
60	H	-5.886596	6.134349	3.300624	120	C	7.318796	-6.993301	2.527023

121	H	6.291961	-7.259462	2.827220
122	H	7.669554	-7.822486	1.890763
123	C	8.197972	-6.899131	3.763705
124	H	9.224832	-6.633569	3.463394
125	H	7.848389	-6.068760	4.398840
126	C	8.225975	-8.182353	4.579960
127	H	7.198788	-8.443721	4.876893
128	H	8.573035	-9.008960	3.941268
129	C	9.109476	-8.072333	5.811132
130	H	8.761752	-7.269747	6.473888
131	H	9.122489	-9.000860	6.391889
132	H	10.144954	-7.839342	5.532146
133	C	7.195350	5.881540	-1.586032
134	H	8.212708	5.632320	-1.246690
135	H	6.867954	5.042064	-2.218811
136	C	7.214452	7.168315	-2.394193
137	H	6.190454	7.412641	-2.721390
138	H	7.530192	8.004037	-1.748242
139	C	8.128070	7.094701	-3.607066
140	H	9.152095	6.851188	-3.279642
141	H	7.813719	6.257720	-4.251835
142	C	8.149930	8.379226	-4.421465
143	H	7.125633	8.618410	-4.745769
144	H	8.461495	9.212401	-3.773110
145	C	9.068435	8.290076	-5.628464
146	H	8.756368	7.480897	-6.300871
147	H	9.076716	9.219376	-6.208070
148	H	10.100891	8.079479	-5.321869

Table S11. Cartesian coordinates of the optimized ground-state geometry of **5** optimized with M06 functional.

1	C	-7.668957	-1.641320	-0.637824	61	C	6.463857	6.146156	1.567432
2	C	-9.042276	-1.783900	-0.637549	62	C	4.604238	7.462548	-0.086106
3	C	-9.821514	-0.756583	-0.093390	63	H	1.902796	6.223549	-0.818330
4	C	-9.203587	0.401141	0.443877	64	H	1.689248	4.486556	-0.986759
5	C	-7.806205	0.517678	0.426140	65	C	1.859547	5.145615	1.050293
6	H	-11.898438	-1.498753	-0.346053	66	H	3.537279	6.155812	-2.600641
7	H	-9.517864	-2.671152	-1.044674	67	H	3.278556	4.421307	-2.740519
8	C	-11.245925	-0.708081	0.008893	68	C	5.349535	5.005176	-2.770665
9	C	-11.682024	0.431249	0.597709	69	C	6.446208	7.536903	1.487363
10	H	-12.705680	0.724107	0.799768	70	H	7.184192	5.639740	2.208018
11	C	-6.681509	-2.604569	-1.152743	71	C	5.524793	8.191276	0.669751
12	C	-5.313531	-2.251551	-1.043236	72	H	3.887163	7.977839	-0.725339
13	C	-7.083152	-3.814595	-1.724887	73	H	2.317572	4.243985	1.488592
14	C	-4.397234	-3.163344	-1.544323	74	H	2.272397	5.998694	1.611295
15	C	-6.107443	-4.677689	-2.190090	75	C	0.352459	5.075550	1.246395
16	H	-8.126145	-4.104247	-1.817789	76	H	6.002853	5.762916	-2.310300
17	C	-4.757741	-4.379274	-2.113680	77	H	5.741394	4.028074	-2.446435
18	C	-6.948095	1.610374	0.920767	78	C	5.445992	5.109233	-4.284925
19	C	-5.545514	1.426004	0.785499	79	H	7.157439	8.119170	2.069070
20	C	-7.470480	2.776417	1.490065	80	H	5.524332	9.277910	0.621197
21	C	-4.736250	2.454245	1.239399	81	H	-0.123058	5.963889	0.798255
22	C	-6.594257	3.756226	1.922961	82	H	-0.042150	4.209874	0.686884
23	H	-8.531452	2.966877	1.609631	83	C	-0.063417	4.957429	2.703608
24	C	-5.222787	3.624655	1.810204	84	H	5.052117	6.085881	-4.611947
25	Au	-5.081716	-0.396343	-0.121014	85	H	4.790925	4.352920	-4.748215
26	C	-0.482425	-0.202981	0.021246	86	C	6.862858	4.936953	-4.808029
27	C	0.149465	0.753501	0.831987	87	H	0.405394	4.061202	3.144591
28	C	0.326141	-1.066724	-0.734013	88	H	0.336097	5.812928	3.273044
29	C	1.528516	0.847362	0.884773	89	C	-1.571331	4.882448	2.895715
30	H	-0.465235	1.419259	1.435203	90	H	7.518869	5.692373	-4.344699
31	C	1.707058	-0.958823	-0.705005	91	H	7.257312	3.960110	-4.482598
32	H	-0.149637	-1.817277	-1.366800	92	C	6.963114	5.042206	-6.322178
33	H	1.997295	1.586525	1.531564	93	H	-2.032777	5.786864	2.467825
34	H	2.314324	-1.618561	-1.322700	94	H	-1.969736	4.036901	2.313746
35	N	-7.123600	-0.509580	-0.116554	95	C	-1.968591	4.739321	4.355676
36	N	3.736215	0.133075	0.129649	96	H	6.567342	6.018060	-6.642931
37	C	2.331130	0.002610	0.103784	97	H	6.306038	4.287359	-6.780669
38	S	-10.404633	1.509808	1.062356	98	C	8.384939	4.867900	-6.828884
39	C	-3.119981	-0.313068	-0.084153	99	H	-1.607432	5.589678	4.948179
40	C	-1.901813	-0.277000	-0.036086	100	H	-3.055650	4.682919	4.485426
41	H	-4.005562	-5.070797	-2.483979	101	H	-1.536119	3.829894	4.791793
42	H	-4.548608	4.406958	2.147991	102	H	8.786699	3.887675	-6.542118
43	F	-7.094020	4.869004	2.464759	103	H	8.445945	4.945954	-7.919825
44	F	-3.408568	2.353557	1.134448	104	H	9.049947	5.629853	-6.402616
45	F	-6.478873	-5.839105	-2.734275	105	C	4.555865	-1.002336	-0.066364
46	F	-3.090506	-2.891680	-1.494604	106	C	5.637627	-0.950930	-0.955714
47	C	4.313545	1.417835	0.266972	107	C	4.246808	-2.201024	0.589429
48	C	5.393130	1.618693	1.137049	108	C	6.375916	-2.094046	-1.240814
49	C	3.769705	2.502432	-0.433507	109	H	5.868673	-0.009320	-1.449464
50	C	5.901124	2.894987	1.354035	110	C	4.960161	-3.341501	0.276411
51	H	5.808088	0.763257	1.666144	111	H	3.407920	-2.231820	1.284756
52	C	4.254839	3.771716	-0.189713	112	C	6.015475	-3.301558	-0.647920
53	H	2.938239	2.338036	-1.118494	113	H	7.194358	-2.044744	-1.957115
54	C	5.311152	3.980319	0.710660	114	C	4.696494	-4.757608	0.744767
55	H	6.724000	3.038280	2.052376	115	C	6.501193	-4.666021	-0.848044
56	C	3.737345	5.083278	-0.741701	116	C	5.719999	-5.531838	-0.063272
57	C	5.544386	5.420052	0.815723	117	C	3.245507	-5.165338	0.427114
58	C	4.616583	6.078910	-0.009754	118	C	4.933361	-4.919932	2.258147
59	C	2.241525	5.253830	-0.418623	119	C	7.520157	-5.165981	-1.653882
60	C	3.925323	5.178827	-2.267831	120	C	5.953259	-6.897748	-0.081982

121	H	3.103187	-6.221144	0.708976
122	H	2.587367	-4.585838	1.095829
123	C	2.791042	-4.943862	-1.008427
124	H	4.713645	-5.965755	2.530148
125	H	4.185614	-4.307369	2.788424
126	C	6.322873	-4.551577	2.753035
127	C	7.750072	-6.539934	-1.668773
128	H	8.127336	-4.498486	-2.263369
129	C	6.973897	-7.399992	-0.892008
130	H	5.351368	-7.573385	0.525971
131	H	3.075965	-3.928794	-1.328762
132	H	3.317136	-5.632192	-1.687925
133	C	1.285441	-5.094752	-1.166922
134	H	7.077256	-5.171914	2.244260
135	H	6.550377	-3.509249	2.478380
136	C	6.464786	-4.718706	4.258011
137	H	8.542075	-6.947023	-2.293513
138	H	7.166088	-8.470275	-0.917917
139	H	0.987595	-6.141215	-0.990139
140	H	0.782301	-4.502223	-0.383634
141	C	0.772154	-4.630366	-2.520116
142	H	6.229562	-5.759572	4.535977
143	H	5.712707	-4.095812	4.770000
144	C	7.849855	-4.361126	4.772369
145	H	1.017083	-3.559899	-2.644142
146	H	1.308512	-5.151715	-3.329845
147	C	-0.727790	-4.823295	-2.687716
148	H	8.602387	-4.984925	4.262235
149	H	8.086835	-3.320964	4.493719
150	C	7.994613	-4.525642	6.277584
151	H	-0.955634	-5.900673	-2.690224
152	H	-1.244727	-4.406389	-1.810611
153	C	-1.266467	-4.167582	-3.947996
154	H	7.754980	-5.564544	6.551670
155	H	7.241675	-3.901504	6.782846
156	C	9.384392	-4.165958	6.775443
157	H	-0.752150	-4.542774	-4.842218
158	H	-2.339691	-4.347059	-4.084711
159	H	-1.118732	-3.080113	-3.913896
160	H	9.630248	-3.123781	6.534712
161	H	9.477707	-4.287543	7.860105
162	H	10.146803	-4.798065	6.302496

Table S12. Cartesian coordinates of the optimized ground-state geometry of **6** optimized with M06 functional.

1	C	8.201900	-1.253379	0.955097	63	C	-4.445233	-3.502796	-0.438674
2	C	9.575826	-1.340859	1.062397	64	H	-2.916232	-2.332369	-1.388441
3	C	10.361733	-0.416476	0.365195	65	C	-5.770328	-2.281645	1.216872
4	C	9.749725	0.585148	-0.430006	66	H	-5.209445	-0.217505	1.561906
5	C	8.351335	0.649029	-0.516633	67	C	-5.473870	-3.464739	0.501780
6	H	12.436438	-1.012648	0.883454	68	H	-4.226891	-4.402834	-1.009614
7	H	10.046991	-2.107323	1.670357	69	C	-6.887854	-2.590550	2.075002
8	C	11.788168	-0.334553	0.338586	70	C	-7.214972	-3.946807	1.838595
9	C	12.231850	0.680388	-0.440981	71	C	-7.627079	-1.853157	3.000058
10	H	13.258462	0.966516	-0.637646	72	C	-8.273572	-4.568374	2.500133
11	C	7.209606	-2.126066	1.603333	73	C	-8.677387	-2.468758	3.667013
12	C	5.841479	-1.856955	1.348003	74	H	-7.383727	-0.809313	3.190868
13	C	7.610959	-3.174486	2.435528	75	C	-8.994042	-3.811382	3.415309
14	C	4.923193	-2.690850	1.969017	76	H	-8.532855	-5.607337	2.306874
15	C	6.634250	-3.961363	3.017703	77	H	-9.264283	-1.906308	4.389002
16	H	8.654421	-3.394414	2.643126	78	H	-9.824799	-4.271821	3.945476
17	C	5.284779	-3.743199	2.802612	79	N	-6.029081	4.738490	-0.947171
18	C	7.499171	1.589101	-1.266942	80	N	-6.339425	-4.469489	0.902236
19	C	6.095242	1.393360	-1.164276	81	C	-5.991230	6.032538	-0.302748
20	C	8.029565	2.625961	-2.041856	82	H	-4.944330	6.265243	-0.062031
21	C	5.291174	2.275297	-1.867942	83	H	-6.309759	6.789467	-1.033030
22	C	7.159311	3.465019	-2.714524	84	C	-6.410199	-5.795334	0.329173
23	H	9.091603	2.817544	-2.148778	85	H	-6.757357	-6.487942	1.108640
24	C	5.787198	3.314456	-2.647282	86	H	-5.389705	-6.113615	0.073291
25	Au	5.619063	-0.221976	0.069466	87	C	-6.853813	6.103216	0.948357
26	C	1.017160	-0.113457	-0.112085	88	H	-7.893104	5.857050	0.680772
27	C	0.330597	0.839072	-0.881654	89	H	-6.525105	5.324592	1.654046
28	C	0.258069	-1.032962	0.628552	90	C	-6.793516	7.468930	1.611841
29	C	-1.052272	0.872513	-0.911874	91	H	-7.111657	8.241764	0.892862
30	H	0.906258	1.552089	-1.468852	92	H	-5.747700	7.708211	1.865643
31	C	-1.125507	-0.997559	0.612053	93	C	-7.650443	7.561390	2.864220
32	H	0.779026	-1.771568	1.235036	94	H	-8.696716	7.324457	2.610577
33	H	-1.565262	1.610512	-1.523942	95	H	-7.334384	6.786873	3.582087
34	H	-1.694064	-1.707818	1.207488	96	C	-7.589093	8.925912	3.533441
35	N	7.661777	-0.275245	0.180323	97	H	-7.902932	9.696083	2.812329
36	N	-3.207606	0.003568	-0.178078	98	H	-6.542655	9.158141	3.783713
37	C	-1.806611	-0.042177	-0.159218	99	C	-8.450438	9.003540	4.782683
38	S	10.959340	1.594900	-1.186583	100	H	-8.398154	9.989261	5.257301
39	C	3.658415	-0.173233	-0.031625	101	H	-9.503314	8.802562	4.547274
40	C	2.439316	-0.143218	-0.075078	102	H	-8.134346	8.259324	5.524688
41	C	-3.889379	1.238678	-0.354360	103	C	-7.313493	-5.872517	-0.892386
42	C	-3.521026	2.358646	0.414571	104	H	-8.324174	-5.537512	-0.612108
43	C	-4.945345	1.327267	-1.257865	105	H	-6.952340	-5.160048	-1.650169
44	C	-4.171306	3.575962	0.281748	106	C	-7.369823	-7.273907	-1.477313
45	H	-2.703976	2.256012	1.125460	107	H	-7.725389	-7.979362	-0.708345
46	C	-5.629521	2.534276	-1.385810	108	H	-6.351030	-7.604242	-1.738723
47	H	-5.229907	0.453020	-1.841581	109	C	-8.262185	-7.372528	-2.704148
48	C	-5.226981	3.656381	-0.625133	110	H	-9.280630	-7.040402	-2.444171
49	H	-3.873085	4.429480	0.886960	111	H	-7.905629	-6.668379	-3.473642
50	C	-6.747689	2.964389	-2.189912	112	C	-8.322082	-8.774604	-3.290887
51	C	-6.968708	4.326621	-1.876628	113	H	-8.678539	-9.473815	-2.519090
52	C	-7.567081	2.329895	-3.123999	114	H	-7.302784	-9.103088	-3.545315
53	C	-7.999763	5.054512	-2.469197	115	C	-9.214690	-8.857294	-4.517631
54	C	-8.590563	3.051637	-3.722789	116	H	-9.251332	-9.870657	-4.931651
55	H	-7.406081	1.282787	-3.374666	117	H	-10.242766	-8.558526	-4.276507
56	C	-8.801625	4.398449	-3.394549	118	H	-8.857358	-8.186653	-5.309372
57	H	-8.177007	6.097935	-2.216487	119	H	4.531740	-4.371080	3.268389
58	H	-9.238551	2.569855	-4.450846	120	H	5.119079	3.982218	-3.181982
59	H	-9.613300	4.942885	-3.872035	121	F	7.665403	4.454896	-3.453967
60	C	-3.977774	-1.164322	0.073212	122	F	3.963792	2.154589	-1.820486
61	C	-3.715362	-2.342875	-0.650330	123	F	7.004404	-4.966811	3.815387
62	C	-5.007024	-1.134564	1.010570	124	F	3.614929	-2.506978	1.782380

Table S13. Cartesian coordinates of the optimized T_1 geometry of **1** computed by DFT/CPCM.

1	C	-4.670537	1.532155	0.104522	61	H	-2.381309	-6.789842	-1.407307
2	C	-6.071961	1.662856	0.105411	62	C	-0.224030	-5.311300	0.865760
3	C	-6.872223	0.483640	0.009169	63	H	0.311712	-4.363867	0.976190
4	C	-6.245918	-0.773213	-0.083890	64	H	-0.830775	-5.462243	1.764573
5	C	-4.818969	-0.899914	-0.084232	65	H	0.519911	-6.114460	0.817149
6	H	-8.947030	1.254363	0.055200	66	N	6.700619	-0.228804	-0.011058
7	H	-6.536471	2.638314	0.177944	67	C	5.294865	-0.160704	-0.000503
8	C	-8.291188	0.393377	-0.007241	68	C	7.368244	-1.270104	0.674060
9	C	-8.740731	-0.891876	-0.109921	69	C	8.472204	-1.906308	0.092474
10	H	-9.757776	-1.255880	-0.144854	70	C	6.937967	-1.675635	1.943902
11	C	-3.709924	2.626106	0.195611	71	C	9.133713	-2.921647	0.774022
12	C	-2.330922	2.259202	0.177513	72	H	8.805695	-1.599364	-0.893951
13	C	-4.072669	3.974296	0.297045	73	C	7.595419	-2.703964	2.609692
14	C	-1.380208	3.266120	0.263495	74	H	6.087905	-1.180083	2.402550
15	C	-3.093809	4.954096	0.380799	75	C	8.698566	-3.330674	2.033114
16	H	-5.118073	4.270531	0.311635	76	H	9.987958	-3.405479	0.308841
17	C	-1.729841	4.624132	0.366249	77	H	7.249475	-3.006381	3.594094
18	H	-0.331172	2.982503	0.249578	78	H	9.213534	-4.128623	2.559333
19	H	-3.403017	5.990273	0.458660	79	C	7.454163	0.740764	-0.712263
20	C	-3.976539	-2.029355	-0.166459	80	C	8.625617	1.267070	-0.153314
21	C	-2.541222	-1.786307	-0.138753	81	C	7.042399	1.183658	-1.975742
22	C	-4.419276	-3.378328	-0.273205	82	C	9.370527	2.211404	-0.850739
23	C	-1.674918	-2.859570	-0.215340	83	H	8.945622	0.930942	0.828073
24	C	-3.514218	-4.413497	-0.346320	84	C	7.784782	2.141337	-2.657374
25	H	-5.477466	-3.616020	-0.298546	85	H	6.139716	0.772632	-2.417023
26	C	-2.117732	-4.193440	-0.319939	86	C	8.954340	2.658352	-2.103358
27	H	-0.608349	-2.651598	-0.192955	87	H	10.276466	2.610294	-0.403091
28	H	-3.898183	-5.424767	-0.426249	88	H	7.452026	2.473930	-3.636580
29	Au	-2.125114	0.213397	0.019078	89	H	9.535100	3.400969	-2.641932
30	C	2.469564	-0.022106	0.015289	90	S	-7.429477	-2.017118	-0.188431
31	C	3.136875	-1.259575	-0.032560	91	C	-0.174484	0.109052	0.021396
32	C	3.255309	1.144037	0.056544	92	C	1.048308	0.048252	0.019814
33	C	4.520036	-1.329535	-0.047013					
34	H	2.551977	-2.173590	-0.074483					
35	C	4.638640	1.078258	0.055647					
36	H	2.763077	2.110824	0.104175					
37	H	5.012562	-2.295281	-0.098857					
38	H	5.224007	1.991070	0.101295					
39	N	-4.112603	0.319899	0.014904					
40	C	-0.629035	5.680788	0.457477					
41	C	0.253189	5.599843	-0.800295					
42	H	0.720283	4.616471	-0.907262					
43	H	-0.333952	5.794360	-1.703770					
44	H	1.052422	6.347297	-0.745502					
45	C	-1.187926	7.102361	0.562788					
46	H	-1.804015	7.233138	1.458706					
47	H	-0.359754	7.815466	0.624904					
48	H	-1.789193	7.370205	-0.312480					
49	C	0.231623	5.405686	1.702615					
50	H	-0.371014	5.460290	2.615119					
51	H	0.697306	4.416591	1.665032					
52	H	1.031314	6.150970	1.777047					
53	C	-1.100903	-5.328025	-0.399055					
54	C	-0.209193	-5.123385	-1.636769					
55	H	-0.805219	-5.137820	-2.555089					
56	H	0.326932	-4.170557	-1.598071					
57	H	0.534819	-5.925462	-1.699974					
58	C	-1.764915	-6.703691	-0.506174					
59	H	-0.993079	-7.478161	-0.559142					
60	H	-2.392770	-6.922243	0.364148					

Table S14. Cartesian coordinates of the optimized T_1 geometry of **3** computed by DFT/CPCM.

1	C	-8.033639	-1.060110	-1.029734	61	H	-5.402618	4.149261	5.562636
2	C	-9.402323	-1.111308	-1.072253	62	C	-3.304884	4.488226	2.831064
3	C	-10.153639	-0.271593	-0.204828	63	H	-2.811053	3.835844	2.104085
4	C	-9.468246	0.598820	0.683322	64	H	-3.908877	5.211950	2.273716
5	C	-8.070207	0.647078	0.722986	65	H	-2.526960	5.038305	3.374229
6	H	-12.260874	-0.749787	-0.680177	66	N	3.363857	0.010754	-0.010829
7	H	-9.911328	-1.780885	-1.756717	67	C	1.972648	-0.022788	-0.034390
8	C	-11.567184	-0.165137	-0.085408	68	S	-10.614588	1.515193	1.631702
9	C	-11.963803	0.744039	0.850274	69	C	-3.483303	-0.143514	-0.120705
10	H	-12.969416	1.017799	1.138633	70	C	-2.249561	-0.122155	-0.106342
11	C	-7.088307	-1.839356	-1.838472	71	C	4.043899	1.243190	0.065929
12	C	-5.705156	-1.603858	-1.609487	72	C	3.577734	2.342032	-0.691026
13	C	-7.471718	-2.778169	-2.798475	73	C	5.176760	1.364798	0.880775
14	C	-4.774132	-2.321215	-2.355822	74	C	4.215603	3.566338	-0.640401
15	C	-6.516282	-3.479048	-3.527375	75	H	2.717817	2.207222	-1.338538
16	H	-8.524820	-2.972857	-2.987837	76	C	5.828153	2.587991	0.939543
17	C	-5.147126	-3.267215	-3.323374	77	H	5.517598	0.516935	1.466267
18	H	-3.717945	-2.134016	-2.174076	78	C	5.339710	3.691134	0.184963
19	H	-6.855402	-4.199823	-4.264030	79	H	3.855797	4.393148	-1.243424
20	C	-7.172574	1.441455	1.533110	80	C	6.984886	3.066199	1.659271
21	C	-5.771347	1.238876	1.315011	81	C	7.139296	4.425985	1.302293
22	C	-7.563240	2.382331	2.501481	82	C	7.882777	2.477095	2.551293
23	C	-4.856729	1.972529	2.060314	83	C	8.177440	5.203794	1.813917
24	C	-6.618873	3.097495	3.227243	84	C	8.916163	3.248170	3.067592
25	H	-8.613195	2.570978	2.703277	85	H	7.776016	1.434270	2.836089
26	C	-5.244199	2.914326	3.028118	86	C	9.058109	4.594433	2.700183
27	H	-3.797739	1.802249	1.877928	87	H	8.302906	6.244760	1.533771
28	H	-6.974213	3.811990	3.962810	88	H	9.623826	2.806445	3.762098
29	Au	-5.429559	-0.175209	-0.141038	89	H	9.875963	5.176109	3.114974
30	C	-0.850832	-0.090369	-0.083177	90	C	4.104680	-1.187549	-0.062937
31	C	-0.152197	0.895050	0.665840	91	C	3.667357	-2.307334	0.680320
32	C	-0.080665	-1.040904	-0.806389	92	C	5.268544	-1.254442	-0.839417
33	C	1.221316	0.932552	0.687833	93	C	4.365405	-3.499188	0.653769
34	H	-0.724672	1.615159	1.241229	94	H	2.780798	-2.214069	1.298573
35	C	1.293102	-1.012658	-0.780903	95	C	5.980279	-2.444519	-0.873661
36	H	-0.597789	-1.787426	-1.400188	96	H	5.587356	-0.391370	-1.415022
37	H	1.737755	1.675351	1.286851	97	C	5.521359	-3.569575	-0.133113
38	H	1.865005	-1.729645	-1.360685	98	H	4.026416	-4.342023	1.246555
39	N	-7.406736	-0.202369	-0.153738	99	C	7.182556	-2.866027	-1.552984
40	C	-4.067325	-4.018989	-4.106533	100	C	7.391500	-4.216214	-1.187385
41	C	-3.179185	-4.804602	-3.127424	101	C	8.079837	-2.234295	-2.415993
42	H	-2.694600	-4.143323	-2.402523	102	C	8.483416	-4.942345	-1.661711
43	H	-3.769685	-5.538029	-2.568339	103	C	9.166657	-2.954040	-2.895338
44	H	-2.393642	-5.342000	-3.671899	104	H	7.931472	-1.198260	-2.706936
45	C	-4.659279	-5.009340	-5.113308	105	C	9.362294	-4.291262	-2.519628
46	H	-5.281680	-4.505459	-5.860340	106	H	8.650700	-5.975466	-1.374503
47	H	-3.850277	-5.520678	-5.645942	107	H	9.874689	-2.478684	-3.566886
48	H	-5.267739	-5.774784	-4.620105	108	H	10.221348	-4.832329	-2.905056
49	C	-3.200798	-3.010485	-4.878911	109	N	6.127959	4.785822	0.422438
50	H	-3.807235	-2.441244	-5.591162	110	N	6.369923	-4.624537	-0.341171
51	H	-2.716416	-2.296042	-4.206369	111	C	5.983609	6.086885	-0.199816
52	H	-2.415830	-3.532179	-5.439261	112	H	4.918184	6.255544	-0.387024
53	C	-4.178652	3.685855	3.809773	113	H	6.290971	6.843472	0.529875
54	C	-3.291650	2.695607	4.582921	114	C	6.269094	-5.930098	0.280222
55	H	-3.886466	2.116390	5.296953	115	H	5.207561	-6.151132	0.431684
56	H	-2.795782	1.988670	3.910547	116	H	6.638264	-6.671852	-0.435923
57	H	-2.514811	3.231987	5.141128	117	C	7.032500	-6.030625	1.598287
58	C	-4.789438	4.665107	4.816136	118	H	8.087257	-5.785438	1.420214
59	H	-3.990955	5.192620	5.349130	119	H	6.648589	-5.271984	2.292299
60	H	-5.412939	5.417870	4.322192	120	C	6.918690	-7.415797	2.225520

121	H	5.859133	-7.656787	2.391344
122	H	7.295048	-8.169087	1.519014
123	C	7.676126	-7.537893	3.543834
124	H	8.735556	-7.296018	3.378176
125	H	7.300078	-6.784578	4.250511
126	C	7.568047	-8.921433	4.177474
127	H	6.508989	-9.161578	4.341726
128	H	7.942882	-9.672917	3.469592
129	C	8.327967	-9.034302	5.493124
130	H	7.950872	-8.316515	6.230080
131	H	8.234595	-10.034994	5.926099
132	H	9.395351	-8.831219	5.351610
133	C	6.785601	6.229616	-1.490789
134	H	7.844379	6.035251	-1.277354
135	H	6.462918	5.455978	-2.199257
136	C	6.625954	7.610127	-2.118306
137	H	5.562201	7.800123	-2.319693
138	H	6.940984	8.377919	-1.397548
139	C	7.421051	7.774135	-3.409613
140	H	8.484670	7.582916	-3.208377
141	H	7.106159	7.006556	-4.130700
142	C	7.267949	9.153520	-4.043031
143	H	6.204771	9.342997	-4.243029
144	H	7.581515	9.919193	-3.320711
145	C	8.066151	9.308532	-5.331439
146	H	7.749768	8.576461	-6.082780
147	H	7.939282	10.305355	-5.764821
148	H	9.136650	9.156709	-5.153776

Table S15. Cartesian coordinates of the optimized T_1 geometry of **5** computed by DFT/CPCM.

1	C	-7.699906	-1.551887	-0.356315	61	C	6.811691	5.755288	1.765342
2	C	-9.064461	-1.658351	-0.370773	62	C	5.106123	7.312798	0.145748
3	C	-9.849944	-0.511329	-0.075208	63	H	2.354334	6.389810	-0.780757
4	C	-9.201718	0.712486	0.226988	64	H	1.959232	4.702421	-1.031577
5	C	-7.802535	0.813090	0.239465	65	C	2.056622	5.269835	1.040313
6	H	-11.936147	-1.232782	-0.238429	66	H	4.043562	6.183232	-2.474445
7	H	-9.547592	-2.600641	-0.602076	67	H	3.625150	4.491485	-2.682142
8	C	-11.268370	-0.402688	-0.035344	68	C	5.745466	4.869677	-2.609850
9	C	-11.701852	0.848971	0.283104	69	C	6.922773	7.142490	1.750075
10	H	-12.718066	1.205289	0.381446	70	H	7.468780	5.157605	2.391083
11	C	-6.734246	-2.621040	-0.631292	71	C	6.076840	7.914495	0.949085
12	C	-5.361083	-2.264701	-0.546227	72	H	4.455797	7.923781	-0.475105
13	C	-7.134621	-3.922199	-0.961066	73	H	2.379132	4.311324	1.468674
14	C	-4.448565	-3.279554	-0.805939	74	H	2.519660	6.051407	1.656367
15	C	-6.161623	-4.871130	-1.205337	75	C	0.535707	5.363541	1.131200
16	H	-8.178602	-4.206548	-1.030906	76	H	6.441198	5.550257	-2.102480
17	C	-4.806704	-4.580858	-1.135216	77	H	6.027600	3.854401	-2.300409
18	C	-6.946572	1.939896	0.512076	78	C	5.920748	5.002176	-4.120023
19	C	-5.534688	1.691291	0.433890	79	H	7.671505	7.630576	2.366895
20	C	-7.421257	3.227109	0.841288	80	H	6.176434	8.996090	0.952131
21	C	-4.697041	2.764122	0.693047	81	H	0.199592	6.325264	0.718435
22	C	-6.512328	4.234345	1.084318	82	H	0.092941	4.588814	0.488455
23	H	-8.475222	3.463915	0.913479	83	C	-0.009141	5.201090	2.546232
24	C	-5.138712	4.042474	1.019724	84	H	5.636879	6.017405	-4.432015
25	Au	-5.120322	-0.267274	-0.053626	85	H	5.222389	4.323208	-4.630098
26	C	-0.551728	-0.092046	-0.034357	86	C	7.341741	4.710122	-4.590988
27	C	0.136830	0.809741	0.821493	87	H	0.366120	4.259285	2.973584
28	C	0.218758	-0.935799	-0.879355	88	H	0.385319	6.001849	3.188029
29	C	1.507963	0.875130	0.823934	89	C	-1.534179	5.203392	2.605843
30	H	-0.443658	1.444248	1.483013	90	H	8.040606	5.389386	-4.082096
31	C	1.590681	-0.891638	-0.862001	91	H	7.627164	3.694824	-4.279626
32	H	-0.299319	-1.614241	-1.549025	92	C	7.520788	4.842232	-6.100237
33	H	2.021485	1.554112	1.496153	93	H	-1.909261	6.139963	2.170295
34	H	2.166492	-1.527265	-1.526125	94	H	-1.922000	4.396203	1.970515
35	N	-7.102032	-0.349558	-0.059042	95	C	-2.080654	5.044132	4.019090
36	N	3.649966	0.075887	-0.004628	96	H	7.235441	5.856729	-6.409702
37	C	2.264100	0.020519	-0.014120	97	H	6.821500	4.163816	-6.607478
38	S	-10.386284	1.952235	0.549001	98	C	8.942986	4.548664	-6.561385
39	C	-3.176557	-0.187293	-0.047517	99	H	-1.749133	5.862365	4.668374
40	C	-1.944883	-0.146482	-0.043710	100	H	-3.175088	5.034807	4.025262
41	H	-4.057146	-5.340038	-1.326712	101	H	-1.739528	4.105599	4.470522
42	H	-4.442662	4.850787	1.209276	102	H	9.242516	3.528991	-6.294127
43	F	-6.970551	5.460136	1.397130	103	H	9.043647	4.650775	-7.646445
44	F	-3.357837	2.605817	0.634123	104	H	9.658934	5.234618	-6.094902
45	F	-6.533622	-6.123049	-1.521987	105	C	4.401984	-1.099826	-0.216143
46	F	-3.125464	-3.029059	-0.744065	106	C	5.513834	-1.076950	-1.073142
47	C	4.303960	1.306337	0.219131	107	C	4.002002	-2.290960	0.413084
48	C	5.405364	1.367672	1.087912	108	C	6.200369	-2.250460	-1.351354
49	C	3.816440	2.465551	-0.408260	109	H	5.801024	-0.143729	-1.546947
50	C	5.991970	2.590786	1.380341	110	C	4.691552	-3.453372	0.135285
51	H	5.761724	0.457744	1.560008	111	H	3.160646	-2.279115	1.100149
52	C	4.406405	3.677998	-0.115535	112	C	5.776134	-3.445017	-0.764050
53	H	2.985912	2.390679	-1.104466	113	H	7.038874	-2.233494	-2.041129
54	C	5.478330	3.751315	0.796057	114	C	4.434081	-4.849558	0.670508
55	H	6.821548	2.636834	2.079525	115	C	6.253113	-4.815228	-0.917714
56	C	4.039963	5.052938	-0.642305	116	C	5.460954	-5.651575	-0.109246
57	C	5.838945	5.154709	0.965755	117	C	2.979876	-5.300380	0.413662
58	C	4.988203	5.929936	0.155872	118	C	4.703782	-4.926426	2.194537
59	C	2.550513	5.379133	-0.398988	119	C	7.280745	-5.339586	-1.702054
60	C	4.318645	5.166671	-2.162332	120	C	5.693282	-7.019728	-0.085052

121	H	2.862737	-6.319562	0.805137
122	H	2.326435	-4.667889	1.030654
123	C	2.498171	-5.248082	-1.032946
124	H	4.514094	-5.960305	2.513215
125	H	3.948680	-4.309366	2.700647
126	C	6.094395	-4.502908	2.654104
127	C	7.506456	-6.712592	-1.672835
128	H	7.892536	-4.694614	-2.326800
129	C	6.719151	-7.545421	-0.873082
130	H	5.089487	-7.677654	0.534844
131	H	2.745186	-4.270491	-1.468423
132	H	3.033475	-5.994642	-1.633671
133	C	0.991925	-5.470328	-1.142991
134	H	6.852321	-5.123720	2.159310
135	H	6.289927	-3.469197	2.338992
136	C	6.265106	-4.607969	4.166959
137	H	8.299634	-7.141951	-2.277667
138	H	6.908291	-8.614973	-0.865013
139	H	0.731597	-6.451690	-0.721719
140	H	0.476215	-4.727430	-0.517277
141	C	0.457374	-5.372456	-2.567872
142	H	6.070355	-5.642190	4.484831
143	H	5.503627	-3.990492	4.664697
144	C	7.649410	-4.185672	4.648352
145	H	0.757849	-4.407534	-3.002536
146	H	0.928753	-6.144574	-3.192626
147	C	-1.060710	-5.506041	-2.651009
148	H	8.411420	-4.803167	4.151535
149	H	7.845284	-3.151249	4.330810
150	C	7.825244	-4.289192	6.160204
151	H	-1.361689	-6.465647	-2.208144
152	H	-1.526355	-4.726636	-2.033356
153	C	-1.593932	-5.412427	-4.075228
154	H	7.630291	-5.322949	6.475984
155	H	7.062513	-3.673105	6.655400
156	C	9.210496	-3.863882	6.631057
157	H	-1.180295	-6.206273	-4.707397
158	H	-2.684698	-5.499565	-4.100866
159	H	-1.328118	-4.453261	-4.533778
160	H	9.418566	-2.823334	6.357488
161	H	9.309828	-3.947829	7.717793
162	H	9.990149	-4.485545	6.176753

Table S16. Cartesian coordinates of the optimized T_1 geometry of **6** computed by DFT/CPCM.

1	C	8.158149	1.256570	0.857596	63	C	-4.135218	-3.555456	0.655105
2	C	9.523011	1.338782	0.909182	64	H	-2.609454	-2.553201	-0.462308
3	C	10.300356	0.369660	0.215545	65	C	-5.732346	-2.057424	1.774387
4	C	9.641075	-0.653755	-0.509871	66	H	-5.384234	0.061894	1.539542
5	C	8.240969	-0.730821	-0.558195	67	C	-5.263487	-3.363109	1.460328
6	H	12.392383	0.961989	0.627260	68	H	-3.789382	-4.547206	0.383819
7	H	10.012812	2.127846	1.468132	69	C	-6.901784	-2.231609	2.602278
8	C	11.717394	0.268791	0.136996	70	C	-7.082562	-3.627320	2.744345
9	C	12.141151	-0.785502	-0.615443	71	C	-7.791170	-1.350291	3.220131
10	H	13.154062	-1.091540	-0.838013	72	C	-8.138919	-4.156213	3.485808
11	C	7.201154	2.159367	1.505439	73	C	-8.842288	-1.871447	3.963079
12	C	5.827320	1.864906	1.301746	74	H	-7.663800	-0.276080	3.120617
13	C	7.604850	3.252381	2.283042	75	C	-9.010233	-3.258345	4.091239
14	C	4.915622	2.715258	1.912399	76	H	-8.284775	-5.226732	3.588803
15	C	6.633895	4.050166	2.856258	77	H	-9.543717	-1.201022	4.449714
16	H	8.649716	3.490352	2.448453	78	H	-9.841571	-3.642174	4.675117
17	C	5.277716	3.808228	2.689958	79	N	-6.218037	4.128379	-2.123069
18	C	7.376831	-1.669672	-1.223075	80	N	-6.075866	-4.291336	2.058569
19	C	5.968206	-1.449664	-1.060050	81	C	-6.164313	5.570876	-1.995823
20	C	7.832362	-2.757121	-1.999626	82	H	-5.115321	5.860697	-1.875397
21	C	5.113274	-2.338232	-1.688945	83	H	-6.495247	6.004044	-2.945684
22	C	6.908202	-3.592243	-2.590252	84	C	-5.955745	-5.730067	1.933643
23	H	8.882973	-2.968091	-2.154705	85	H	-6.282043	-6.177356	2.878593
24	C	5.536698	-3.417141	-2.459283	86	H	-4.893101	-5.972657	1.830140
25	Au	5.561259	0.192807	0.111683	87	C	-7.005359	6.107326	-0.840341
26	C	0.987477	0.079047	0.049496	88	H	-8.046281	5.787743	-0.977027
27	C	0.252501	0.748687	-0.963393	89	H	-6.659224	5.650806	0.095814
28	C	0.259768	-0.624282	1.044622	90	C	-6.936285	7.626929	-0.735673
29	C	-1.120790	0.723736	-0.979167	91	H	-7.274658	8.074184	-1.681055
30	H	0.796134	1.270785	-1.743530	92	H	-5.889496	7.937857	-0.609731
31	C	-1.113213	-0.661875	1.027609	93	C	-7.769831	8.185592	0.413114
32	H	0.807843	-1.122312	1.837285	94	H	-8.816768	7.875035	0.287418
33	H	-1.665814	1.219002	-1.775425	95	H	-7.432296	7.738082	1.358699
34	H	-1.653913	-1.182384	1.810592	96	C	-7.704635	9.705736	0.523502
35	N	7.548171	0.251092	0.144647	97	H	-8.040858	10.151056	-0.422528
36	N	-3.218453	-0.016097	-0.000265	98	H	-6.657882	10.013981	0.648278
37	C	-1.834517	0.014844	0.015828	99	C	-8.540014	10.255529	1.672882
38	S	10.814312	-1.703257	-1.262480	100	H	-8.475808	11.346500	1.729899
39	C	3.615891	0.136576	0.079697	101	H	-9.596603	9.990047	1.555744
40	C	2.383232	0.111095	0.066459	102	H	-8.203510	9.851819	2.634305
41	C	-3.956643	1.071896	-0.521512	103	C	-6.753632	-6.303974	0.765600
42	C	-3.576658	2.390959	-0.191546	104	H	-7.809475	-6.029359	0.884452
43	C	-5.066237	0.829188	-1.337618	105	H	-6.412054	-5.834407	-0.165746
44	C	-4.277013	3.479140	-0.678202	106	C	-6.617567	-7.819378	0.665682
45	H	-2.732759	2.545477	0.472740	107	H	-6.952479	-8.279126	1.606296
46	C	-5.781464	1.911848	-1.830600	108	H	-5.556416	-8.085250	0.558245
47	H	-5.344372	-0.189950	-1.586815	109	C	-7.406697	-8.415324	-0.495668
48	C	-5.378000	3.236960	-1.507376	110	H	-8.467910	-8.149378	-0.388759
49	H	-3.981891	4.485313	-0.400157	111	H	-7.072274	-7.955783	-1.436568
50	C	-6.939857	2.034188	-2.682988	112	C	-7.275049	-9.931546	-0.600736
51	C	-7.179769	3.420536	-2.829292	113	H	-7.608386	-10.388846	0.340591
52	C	-7.776136	1.114424	-3.318696	114	H	-6.214155	-10.195262	-0.706636
53	C	-8.243407	3.902198	-3.592213	115	C	-8.066273	-10.518708	-1.762807
54	C	-8.834068	1.588582	-4.083144	116	H	-7.954768	-11.606071	-1.815674
55	H	-7.603028	0.046908	-3.216282	117	H	-9.135069	-10.298197	-1.664644
56	C	-9.061211	2.966672	-4.215019	118	H	-7.730604	-10.103031	-2.719406
57	H	-8.434985	4.965211	-3.698138	119	H	4.530234	4.445359	3.148034
58	H	-9.494707	0.887800	-4.583887	120	H	4.829084	-4.086537	-2.933172
59	H	-9.896841	3.313313	-4.815786	121	F	7.349802	-4.627125	-3.329312
60	C	-3.918996	-1.136222	0.504749	122	F	3.780159	-2.184459	-1.573318
61	C	-3.473634	-2.436829	0.183431	123	F	7.010145	5.101747	3.604384
62	C	-5.055664	-0.943652	1.296569	124	F	3.596005	2.500750	1.765899

Table S17. Cartesian coordinates of the optimized S_1 geometry of **3** computed by TDDFT/CPCM.M.

1	C	-8.053058	-1.066589	-1.006064	61	H	-5.400491	4.230799	5.511317
2	C	-9.419644	-1.110094	-1.045192	62	C	-3.303686	4.529180	2.782349
3	C	-10.164346	-0.249907	-0.186364	63	H	-2.803551	3.868018	2.064304
4	C	-9.469258	0.629416	0.687007	64	H	-3.909460	5.244372	2.211428
5	C	-8.075102	0.670324	0.723452	65	H	-2.527819	5.091046	3.321010
6	H	-12.264192	-0.729110	-0.657209	66	N	3.417272	0.014493	0.000725
7	H	-9.938237	-1.787785	-1.718542	67	C	2.006782	-0.024800	-0.024690
8	C	-11.571535	-0.134574	-0.067342	68	S	-10.612456	1.572473	1.629300
9	C	-11.971976	0.789535	0.853873	69	C	-3.436631	-0.158932	-0.119393
10	H	-12.976596	1.072841	1.138963	70	C	-2.210755	-0.137636	-0.104626
11	C	-7.116071	-1.868284	-1.807599	71	C	4.081231	1.248488	0.084025
12	C	-5.728900	-1.650495	-1.595467	72	C	3.567440	2.364780	-0.617003
13	C	-7.519258	-2.814413	-2.748500	73	C	5.247397	1.364897	0.855947
14	C	-4.814558	-2.390691	-2.335834	74	C	4.193845	3.591897	-0.561704
15	C	-6.580301	-3.540367	-3.474860	75	H	2.679244	2.235794	-1.229264
16	H	-8.579256	-2.996033	-2.925724	76	C	5.885268	2.590489	0.919148
17	C	-5.208799	-3.345317	-3.285406	77	H	5.620872	0.506450	1.409677
18	H	-3.750360	-2.215783	-2.165365	78	C	5.352636	3.705560	0.215564
19	H	-6.937207	-4.268568	-4.199018	79	H	3.801092	4.434819	-1.124085
20	C	-7.171461	1.473141	1.519452	80	C	7.069389	3.062368	1.597694
21	C	-5.768995	1.268910	1.311139	81	C	7.198751	4.428408	1.267923
22	C	-7.559249	2.428894	2.471964	82	C	8.011497	2.458266	2.428169
23	C	-4.855220	2.009162	2.044305	83	C	8.254910	5.201438	1.741105
24	C	-6.614726	3.153468	3.189432	84	C	9.064966	3.224174	2.910019
25	H	-8.611171	2.623968	2.670125	85	H	7.923388	1.406317	2.692199
26	C	-5.242559	2.965939	2.997756	86	C	9.182171	4.577421	2.567346
27	H	-3.791976	1.834482	1.866589	87	H	8.358838	6.250994	1.476169
28	H	-6.972533	3.880814	3.914595	88	H	9.809517	2.770669	3.558804
29	Au	-5.420832	-0.183906	-0.136196	89	H	10.018552	5.154381	2.953921
30	C	-0.796564	-0.102269	-0.078733	90	C	4.149399	-1.182497	-0.061361
31	C	-0.114782	0.781611	0.782629	91	C	3.677663	-2.323193	0.629403
32	C	-0.034781	-0.946741	-0.911633	92	C	5.338438	-1.238197	-0.804013
33	C	1.264495	0.822831	0.810894	93	C	4.368234	-3.516230	0.591736
34	H	-0.696715	1.424470	1.438451	94	H	2.768955	-2.240059	1.219167
35	C	1.344786	-0.911750	-0.886756	95	C	6.040440	-2.429242	-0.849746
36	H	-0.554414	-1.620115	-1.588884	96	H	5.680218	-0.361861	-1.350190
37	H	1.783202	1.491137	1.494016	97	C	5.549205	-3.570213	-0.157867
38	H	1.925355	-1.549359	-1.549089	98	H	4.006581	-4.377990	1.146392
39	N	-7.418862	-0.200348	-0.145274	99	C	7.262639	-2.839707	-1.499952
40	C	-4.146614	-4.120899	-4.061531	100	C	7.453444	-4.197770	-1.166950
41	C	-3.268059	-4.906459	-3.080755	101	C	8.191894	-2.187833	-2.308544
42	H	-2.760931	-4.245586	-2.367831	102	C	8.557804	-4.915942	-1.616025
43	H	-3.870814	-5.620305	-2.505026	103	C	9.293533	-2.898919	-2.766067
44	H	-2.497738	-5.470341	-3.624787	104	H	8.056732	-1.141394	-2.574629
45	C	-4.755563	-5.113603	-5.049661	105	C	9.470973	-4.245032	-2.420907
46	H	-5.376315	-4.610419	-5.801800	106	H	8.708395	-5.959199	-1.348644
47	H	-3.954925	-5.643918	-5.580881	107	H	10.028908	-2.407623	-3.397568
48	H	-5.372695	-5.866143	-4.542613	108	H	10.343918	-4.778687	-2.788364
49	C	-3.272467	-3.140360	-4.852263	109	N	6.138622	4.802648	0.446073
50	H	-3.878431	-2.568147	-5.566182	110	N	6.395358	-4.625891	-0.369368
51	H	-2.765193	-2.424270	-4.194970	111	C	5.974333	6.108321	-0.166357
52	H	-2.502381	-3.684145	-5.416666	112	H	4.899934	6.292005	-0.297253
53	C	-4.177556	3.742591	3.766594	113	H	6.328561	6.863648	0.547433
54	C	-3.296652	2.765580	4.554356	114	C	6.281644	-5.939234	0.238036
55	H	-3.897284	2.195616	5.274593	115	H	5.214739	-6.174016	0.347089
56	H	-2.796242	2.046350	3.894715	116	H	6.685597	-6.675633	-0.469133
57	H	-2.520731	3.309813	5.110714	117	C	6.994935	-6.028357	1.578162
58	C	-4.783626	4.735056	4.756674	118	H	8.054899	-5.765874	1.438898
59	H	-3.982271	5.268170	5.284313	119	H	6.576601	-5.270083	2.258135
60	H	-5.405333	5.484957	4.251254	120	C	6.876251	-7.409894	2.200508

121	H	5.812082	-7.666967	2.327249
122	H	7.287136	-8.162230	1.507850
123	C	7.585625	-7.515228	3.541057
124	H	8.649719	-7.257558	3.413140
125	H	7.175966	-6.760716	4.232349
126	C	7.471742	-8.894162	4.173060
127	H	6.407994	-9.147168	4.298361
128	H	7.879031	-9.644435	3.478390
129	C	8.187107	-8.982946	5.510421
130	H	7.775012	-8.259852	6.225584
131	H	8.099188	-9.978911	5.957064
132	H	9.256026	-8.760550	5.400104
133	C	6.709994	6.229637	-1.491827
134	H	7.777412	6.013840	-1.330898
135	H	6.339362	5.454191	-2.180066
136	C	6.543765	7.605116	-2.116660
137	H	5.472092	7.817339	-2.261798
138	H	6.910672	8.373726	-1.417219
139	C	7.271125	7.740607	-3.444815
140	H	8.342140	7.524276	-3.299180
141	H	6.902959	6.972028	-4.143915
142	C	7.114499	9.115268	-4.076945
143	H	6.043960	9.327894	-4.218391
144	H	7.482160	9.879256	-3.375168
145	C	7.846529	9.233473	-5.402965
146	H	7.472538	8.497199	-6.125581
147	H	7.728676	10.226490	-5.849279
148	H	8.921139	9.050522	-5.276546

Table S18. Cartesian coordinates of the optimized S_1 geometry of **5** computed by TDDFT/CPCM.

1	C	-7.635893	-1.475708	-0.567143	61	C	6.769395	5.861063	1.664493
2	C	-8.999131	-1.580311	-0.578010	62	C	4.911472	7.345116	0.146679
3	C	-9.776242	-0.490774	-0.092432	63	H	2.171524	6.261460	-0.641993
4	C	-9.122200	0.669242	0.391321	64	H	1.885761	4.554818	-0.936267
5	C	-7.724840	0.767656	0.402278	65	C	2.075050	5.054183	1.144853
6	H	-11.856203	-1.186067	-0.345806	66	H	3.780679	6.220507	-2.445061
7	H	-9.491547	-2.474679	-0.949230	67	H	3.479519	4.504148	-2.679984
8	C	-11.190212	-0.391935	-0.020208	68	C	5.565289	5.039682	-2.686545
9	C	-11.625983	0.791451	0.495251	69	C	6.796839	7.250731	1.675800
10	H	-12.641811	1.125792	0.660836	70	H	7.485090	5.288851	2.251705
11	C	-6.676003	-2.490274	-1.026806	71	C	5.875630	7.985940	0.925538
12	C	-5.300127	-2.163110	-0.913070	72	H	4.199475	7.927352	-0.437066
13	C	-7.089505	-3.718721	-1.552830	73	H	2.500011	4.109096	1.522081
14	C	-4.399035	-3.123000	-1.347103	74	H	2.512333	5.849960	1.767834
15	C	-6.127122	-4.620085	-1.964889	75	C	0.565070	5.018946	1.327497
16	H	-8.138259	-3.986998	-1.649147	76	H	6.234973	5.766405	-2.200503
17	C	-4.769808	-4.352661	-1.875251	77	H	5.943593	4.043084	-2.407184
18	C	-6.864038	1.836376	0.842261	78	C	5.654845	5.204691	-4.195959
19	C	-5.451599	1.625470	0.691177	79	H	7.539389	7.771980	2.274673
20	C	-7.332796	3.044902	1.398315	80	H	5.911972	9.072417	0.949614
21	C	-4.614545	2.646609	1.096950	81	H	0.126443	5.968236	0.979270
22	C	-6.422817	4.007378	1.780889	82	H	0.142461	4.237389	0.672710
23	H	-8.386122	3.258581	1.547931	83	C	0.130785	4.750703	2.759133
24	C	-5.051476	3.849762	1.644550	84	H	5.272540	6.198995	-4.479392
25	Au	-5.031694	-0.248696	-0.109554	85	H	4.986992	4.477177	-4.685948
26	C	-0.422637	-0.088016	-0.079833	86	C	7.066863	5.035260	-4.732871
27	C	0.247344	0.811327	0.778205	87	H	0.549054	3.783973	3.090107
28	C	0.346677	-0.930334	-0.911679	88	H	0.568373	5.509093	3.429365
29	C	1.623061	0.870345	0.803669	89	C	-1.381312	4.731566	2.929204
30	H	-0.346096	1.451558	1.427456	90	H	7.734640	5.763849	-4.244175
31	C	1.723014	-0.879185	-0.887602	91	H	7.450738	4.041440	-4.448325
32	H	-0.169915	-1.615713	-1.580417	92	C	7.160379	5.198448	-6.242322
33	H	2.131065	1.546778	1.487843	93	H	-1.787301	5.709118	2.624585
34	H	2.307984	-1.512286	-1.551526	94	H	-1.818271	3.997017	2.235900
35	N	-7.034673	-0.336173	-0.091889	95	C	-1.811464	4.413625	4.351180
36	N	3.782922	0.079192	-0.004439	96	H	6.774987	6.190656	-6.522331
37	C	2.379504	0.024137	-0.029583	97	H	6.491824	4.470113	-6.726245
38	S	-10.304139	1.850180	0.918911	98	C	8.577479	5.027131	-6.762866
39	C	-3.052612	-0.175317	-0.110190	99	H	-1.423205	5.156793	5.059574
40	C	-1.829343	-0.141098	-0.101519	100	H	-2.902334	4.393792	4.451404
41	H	-4.028147	-5.077179	-2.199568	101	H	-1.433177	3.432275	4.665161
42	H	-4.353975	4.627499	1.940135	102	H	8.969207	4.031915	-6.516636
43	F	-6.881436	5.153386	2.308415	103	H	8.633326	5.146481	-7.850163
44	F	-3.279874	2.514786	0.966046	104	H	9.253619	5.764536	-6.311793
45	F	-6.514466	-5.799689	-2.470040	105	C	4.521488	-1.109560	-0.137962
46	F	-3.077675	-2.885544	-1.264296	106	C	5.677165	-1.135900	-0.938175
47	C	4.423528	1.318744	0.160004	107	C	4.049822	-2.280861	0.479627
48	C	5.549488	1.424746	0.995860	108	C	6.328844	-2.334481	-1.179198
49	C	3.882451	2.457741	-0.461748	109	H	6.016106	-0.217242	-1.410446
50	C	6.099219	2.666653	1.268003	110	C	4.696926	-3.467783	0.227923
51	H	5.943319	0.529634	1.470664	111	H	3.170512	-2.236648	1.120579
52	C	4.427277	3.687785	-0.177795	112	C	5.821562	-3.509376	-0.619489
53	H	3.029610	2.354274	-1.130913	113	H	7.197537	-2.356400	-1.833176
54	C	5.519347	3.805762	0.704526	114	C	4.317258	-4.853235	0.702453
55	H	6.943517	2.747592	1.948707	115	C	6.220974	-4.899909	-0.776942
56	C	3.955189	5.045583	-0.649325	116	C	5.332990	-5.700764	-0.035850
57	C	5.804266	5.220558	0.888551	117	C	2.861899	-5.179629	0.320519
58	C	4.878419	5.959754	0.129874	118	C	4.472380	-4.994306	2.230220
59	C	2.467472	5.253215	-0.311990	119	C	7.255651	-5.472018	-1.515712
60	C	4.146536	5.218163	-2.169937	120	C	5.474302	-7.079387	-0.032322

121	H	2.631972	-6.202381	0.658302
122	H	2.207790	-4.517984	0.912358
123	C	2.506944	-5.033163	-1.152039
124	H	4.180511	-6.020388	2.506399
125	H	3.733585	-4.332079	2.710316
126	C	5.854716	-4.695599	2.788402
127	C	7.391290	-6.855428	-1.507246
128	H	7.942353	-4.852651	-2.089590
129	C	6.508238	-7.651923	-0.773924
130	H	4.792355	-7.708656	0.538394
131	H	2.877249	-4.066853	-1.532822
132	H	3.020230	-5.806382	-1.744676
133	C	1.005646	-5.107540	-1.386588
134	H	6.597508	-5.365866	2.328089
135	H	6.156976	-3.672115	2.513594
136	C	5.911783	-4.845931	4.300928
137	H	8.189761	-7.323756	-2.077203
138	H	6.629806	-8.732439	-0.781964
139	H	0.621471	-6.078053	-1.032405
140	H	0.507088	-4.344196	-0.764531
141	C	0.606299	-4.899313	-2.838136
142	H	5.607341	-5.868157	4.579426
143	H	5.169645	-4.176240	4.765831
144	C	7.287239	-4.554177	4.878592
145	H	0.968152	-3.912413	-3.176045
146	H	1.119932	-5.638375	-3.475132
147	C	-0.896020	-4.990462	-3.062156
148	H	8.029680	-5.223280	4.413079
149	H	7.592288	-3.531467	4.601002
150	C	7.349615	-4.705876	6.390845
151	H	-1.244864	-5.986342	-2.746506
152	H	-1.408056	-4.272137	-2.404400
153	C	-1.293232	-4.737404	-4.506597
154	H	7.044095	-5.727491	6.663635
155	H	6.605889	-4.037945	6.851652
156	C	8.730218	-4.410491	6.952185
157	H	-0.825757	-5.466789	-5.180625
158	H	-2.377968	-4.799419	-4.648034
159	H	-0.974316	-3.738915	-4.832112
160	H	9.040467	-3.385080	6.713815
161	H	8.764078	-4.523143	8.041101
162	H	9.481417	-5.086335	6.524010

Table S19. Cartesian coordinates of the optimized S_1 geometry of **6** computed by TDDFT/CPCM.

1	C	8.091965	-0.878451	1.245370	63	C	-4.186058	-3.574834	-0.169170
2	C	9.454239	-0.950749	1.340564	64	H	-2.616404	-2.342436	-0.939832
3	C	10.248245	-0.281843	0.366283	65	C	-5.905735	-2.363934	1.108580
4	C	9.610137	0.439145	-0.673321	66	H	-5.608830	-0.241183	1.349643
5	C	8.213912	0.508010	-0.762183	67	C	-5.373770	-3.568470	0.571916
6	H	12.317574	-0.725392	0.992588	68	H	-3.792878	-4.488706	-0.606473
7	H	9.933366	-1.506419	2.141634	69	C	-7.122626	-2.725236	1.797293
8	C	11.663554	-0.230248	0.280234	70	C	-7.269329	-4.120060	1.639916
9	C	12.117602	0.497679	-0.778492	71	C	-8.079500	-2.004540	2.509488
10	H	13.138473	0.697721	-1.076486	72	C	-8.356093	-4.808887	2.170160
11	C	7.118532	-1.502292	2.153489	73	C	-9.164241	-2.685169	3.046995
12	C	5.745630	-1.294460	1.859680	74	H	-7.978503	-0.928983	2.640250
13	C	7.523016	-2.265061	3.254131	75	C	-9.297612	-4.069155	2.876186
14	C	4.836802	-1.889165	2.722393	76	H	-8.472310	-5.882056	2.038330
15	C	6.553426	-2.822454	4.064118	77	H	-9.920563	-2.140146	3.605472
16	H	8.570022	-2.433173	3.492023	78	H	-10.157957	-4.578312	3.303267
17	C	5.199303	-2.652925	3.824774	79	N	-6.096769	4.706155	-1.011195
18	C	7.368601	1.173915	-1.720869	80	N	-6.190489	-4.613695	0.910841
19	C	5.951326	1.043945	-1.527590	81	C	-5.916606	6.083188	-0.589414
20	C	7.860829	1.924844	-2.808354	82	H	-4.839214	6.276418	-0.504680
21	C	5.131517	1.677408	-2.441815	83	H	-6.280986	6.734081	-1.395127
22	C	6.967431	2.522728	-3.671244	84	C	-6.023949	-5.992917	0.490831
23	H	8.919438	2.059623	-3.004597	85	H	-6.412382	-6.638770	1.289369
24	C	5.592800	2.423394	-3.523789	86	H	-4.948294	-6.202522	0.424864
25	Au	5.500368	-0.110028	0.146772	87	C	-6.626039	6.394672	0.719162
26	C	0.878492	-0.016369	0.034265	88	H	-7.697677	6.167694	0.610314
27	C	0.179449	0.715081	-0.944917	89	H	-6.246244	5.720759	1.502659
28	C	0.140324	-0.732908	0.995956	90	C	-6.438389	7.843106	1.139597
29	C	-1.201857	0.731612	-0.964502	91	H	-6.812031	8.508205	0.344168
30	H	0.748841	1.256725	-1.695849	92	H	-5.362559	8.062620	1.234505
31	C	-1.240892	-0.721575	0.980828	93	C	-7.139780	8.174595	2.447082
32	H	0.681483	-1.285205	1.759938	94	H	-8.215528	7.953823	2.351845
33	H	-1.738288	1.280040	-1.735313	95	H	-6.766612	7.508503	3.242101
34	H	-1.807790	-1.259139	1.737376	96	C	-6.956666	9.623028	2.874011
35	N	7.506512	-0.170882	0.225941	97	H	-7.328345	10.284130	2.076391
36	N	-3.336107	0.024714	-0.019009	98	H	-5.881422	9.838914	2.966171
37	C	-1.920920	0.011995	-0.000774	99	C	-7.663216	9.939285	4.181279
38	S	10.810289	1.159845	-1.728049	100	H	-7.525089	10.983858	4.479582
39	C	3.516330	-0.055174	0.078764	101	H	-8.742101	9.756050	4.099594
40	C	2.295263	-0.033610	0.054027	102	H	-7.285222	9.307864	4.995298
41	C	-4.015728	1.231321	-0.239316	103	C	-6.714775	-6.292973	-0.830290
42	C	-3.495339	2.429869	0.304520	104	H	-7.784856	-6.051049	-0.739839
43	C	-5.198257	1.245987	-0.995838	105	H	-6.311945	-5.623729	-1.606234
44	C	-4.128803	3.637994	0.106600	106	C	-6.540106	-7.743502	-1.249106
45	H	-2.594086	2.382579	0.909258	107	H	-6.935663	-8.404099	-0.460538
46	C	-5.844071	2.451834	-1.200042	108	H	-5.465936	-7.977543	-1.326650
47	H	-5.577135	0.324260	-1.431483	109	C	-7.224468	-8.064502	-2.568170
48	C	-5.302817	3.649017	-0.656065	110	H	-8.298717	-7.830152	-2.489975
49	H	-3.729289	4.546440	0.549410	111	H	-6.830094	-7.402327	-3.356190
50	C	-7.042897	2.830816	-1.910654	112	C	-7.052901	-9.514668	-2.994019
51	C	-7.170555	4.228002	-1.758067	113	H	-7.445310	-10.171913	-2.203162
52	C	-7.998592	2.123647	-2.637726	114	H	-5.979124	-9.743930	-3.069574
53	C	-8.237429	4.932564	-2.307594	115	C	-7.742741	-9.820629	-4.312612
54	C	-9.063542	2.819959	-3.194462	116	H	-7.612893	-10.866488	-4.610131
55	H	-7.912058	1.046426	-2.765067	117	H	-8.820421	-9.624130	-4.247566
56	C	-9.178351	4.206115	-3.028101	118	H	-7.344247	-9.192995	-5.119749
57	H	-8.339285	6.007628	-2.179451	119	H	4.451070	-3.098823	4.472435
58	H	-9.818702	2.285663	-3.764739	120	H	4.908320	2.902191	-4.215728
59	H	-10.023446	4.727692	-3.470367	121	F	7.447466	3.235295	-4.703524
60	C	-4.040706	-1.171192	0.184564	122	F	3.794964	1.596457	-2.320212
61	C	-3.529672	-2.376574	-0.352446	123	F	6.930296	-3.555651	5.121932
62	C	-5.236971	-1.168070	0.918859	124	F	3.517917	-1.743055	2.516054

Table S20. Cartesian coordinates of the optimized T_1 geometry of **3** computed by TDDFT/CPCM.

1	C	-8.062635	-1.085978	-0.980002	61	H	-5.403865	4.360708	5.404922
2	C	-9.430341	-1.129681	-1.016103	62	C	-3.333690	4.626312	2.651851
3	C	-10.172913	-0.249787	-0.180402	63	H	-2.833966	3.956216	1.941945
4	C	-9.479765	0.651497	0.670431	64	H	-3.951747	5.324694	2.073376
5	C	-8.084704	0.692946	0.704540	65	H	-2.558397	5.205717	3.172214
6	H	-12.274578	-0.741448	-0.639279	66	N	3.387428	0.017661	-0.001096
7	H	-9.949519	-1.824133	-1.671712	67	C	1.987550	-0.018269	-0.028330
8	C	-11.581760	-0.132328	-0.065026	68	S	-10.622598	1.617891	1.587763
9	C	-11.979481	0.814592	0.832040	69	C	-3.459542	-0.152008	-0.121991
10	H	-12.984461	1.104710	1.109720	70	C	-2.229203	-0.128588	-0.108221
11	C	-7.127493	-1.906771	-1.761163	71	C	4.063381	1.251226	0.081780
12	C	-5.740155	-1.684321	-1.554888	72	C	3.589276	2.355506	-0.660990
13	C	-7.531611	-2.875924	-2.678572	73	C	5.202777	1.368398	0.888189
14	C	-4.825952	-2.444082	-2.275330	74	C	4.228051	3.578224	-0.608696
15	C	-6.593105	-3.619861	-3.386074	75	H	2.721308	2.222737	-1.301340
16	H	-8.591603	-3.061265	-2.851712	76	C	5.854722	2.588709	0.947658
17	C	-5.221079	-3.421578	-3.200559	77	H	5.549810	0.514858	1.466517
18	H	-3.761674	-2.266751	-2.108553	78	C	5.359790	3.694350	0.204958
19	H	-6.950069	-4.365255	-4.092368	79	H	3.865314	4.413579	-1.202010
20	C	-7.181283	1.516962	1.480059	80	C	7.023230	3.059110	1.652668
21	C	-5.779961	1.310617	1.272729	81	C	7.181696	4.416826	1.299587
22	C	-7.570636	2.493294	2.410557	82	C	7.930577	2.459882	2.524952
23	C	-4.865973	2.072016	1.984608	83	C	8.234176	5.184496	1.790990
24	C	-6.626910	3.237491	3.107580	84	C	8.979027	3.220683	3.024568
25	H	-8.622567	2.688972	2.607814	85	H	7.819129	1.414704	2.806771
26	C	-5.254293	3.049723	2.915149	86	C	9.125883	4.565270	2.658453
27	H	-3.802755	1.897047	1.807820	87	H	8.361348	6.226920	1.508247
28	H	-6.984407	3.980334	3.816765	88	H	9.696603	2.770583	3.705449
29	Au	-5.433930	-0.179580	-0.136045	89	H	9.957914	5.138745	3.059606
30	C	-0.824744	-0.093108	-0.083590	90	C	4.126261	-1.181249	-0.059666
31	C	-0.137026	0.852904	0.715692	91	C	3.681553	-2.307545	0.667928
32	C	-0.057349	-1.000084	-0.854519	92	C	5.294871	-1.243415	-0.829344
33	C	1.237811	0.893190	0.742004	93	C	4.377679	-3.499265	0.635017
34	H	-0.718888	1.540112	1.325005	94	H	2.788474	-2.216399	1.280462
35	C	1.317651	-0.967293	-0.826723	95	C	6.004256	-2.432197	-0.869221
36	H	-0.577327	-1.716871	-1.485357	96	H	5.619758	-0.373818	-1.396538
37	H	1.755575	1.606428	1.378532	97	C	5.537737	-3.561427	-0.143819
38	H	1.897235	-1.651613	-1.441340	98	H	4.036022	-4.351609	1.216561
39	N	-7.429291	-0.197181	-0.140571	99	C	7.213388	-2.847140	-1.539708
40	C	-4.159715	-4.219666	-3.954589	100	C	7.421817	-4.197746	-1.185321
41	C	-3.294201	-4.991967	-2.951940	101	C	8.118226	-2.205167	-2.383795
42	H	-2.787650	-4.320684	-2.248428	102	C	8.520936	-4.916345	-1.647863
43	H	-3.906296	-5.690119	-2.366915	103	C	9.213371	-2.916997	-2.854619
44	H	-2.524042	-5.571788	-3.479040	104	H	7.968714	-1.164939	-2.666373
45	C	-4.769742	-5.227110	-4.927025	105	C	9.409000	-4.255195	-2.487714
46	H	-5.383850	-4.734493	-5.691525	106	H	8.685696	-5.953171	-1.363923
47	H	-3.969531	-5.771705	-5.444124	107	H	9.929676	-2.433004	-3.513227
48	H	-5.393414	-5.966843	-4.409280	108	H	10.276757	-4.789925	-2.866031
49	C	-3.272813	-3.261659	-4.758665	109	N	6.154089	4.788039	0.438410
50	H	-3.869461	-2.698490	-5.487449	110	N	6.387202	-4.617506	-0.355587
51	H	-2.762803	-2.537284	-4.112734	111	C	6.028294	6.079251	-0.210792
52	H	-2.504123	-3.822896	-5.307493	112	H	4.960727	6.276954	-0.375126
53	C	-4.190124	3.850759	3.659854	113	H	6.375862	6.847793	0.492285
54	C	-3.292819	2.897222	4.457815	114	C	6.296569	-5.918019	0.280651
55	H	-3.881184	2.334655	5.193795	115	H	5.233797	-6.160062	0.413838
56	H	-2.789509	2.171284	3.807916	116	H	6.694312	-6.666001	-0.418078
57	H	-2.518432	3.460116	4.997207	117	C	7.033722	-5.975344	1.609596
58	C	-4.796950	4.856057	4.636435	118	H	8.089648	-5.710398	1.446158
59	H	-3.995804	5.404763	5.147970	119	H	6.623303	-5.204993	2.280772
60	H	-5.428089	5.592192	4.122587	120	C	6.933053	-7.343891	2.262894

121	H	5.872357	-7.603816	2.411586
122	H	7.337086	-8.108623	1.579772
123	C	7.663382	-7.418058	3.594264
124	H	8.724179	-7.158322	3.444973
125	H	7.260601	-6.651153	4.275924
126	C	7.565574	-8.784014	4.256347
127	H	6.504975	-9.039389	4.402029
128	H	7.966666	-9.546663	3.571595
129	C	8.300227	-8.841844	5.584951
130	H	7.894774	-8.105907	6.290766
131	H	8.223518	-9.828732	6.053356
132	H	9.366389	-8.616833	5.454919
133	C	6.799364	6.156061	-1.519409
134	H	7.859979	5.934570	-1.324557
135	H	6.438654	5.364797	-2.194839
136	C	6.663198	7.514288	-2.187624
137	H	5.597605	7.731643	-2.366556
138	H	7.019153	8.299713	-1.501261
139	C	7.425323	7.605418	-3.499994
140	H	8.490739	7.386757	-3.320665
141	H	7.069635	6.818583	-4.185146
142	C	7.294447	8.961431	-4.176638
143	H	6.229299	9.176254	-4.351667
144	H	7.649381	9.743883	-3.488765
145	C	8.060594	9.035577	-5.486513
146	H	7.700510	8.279733	-6.195898
147	H	7.960249	10.015265	-5.965450
148	H	9.130512	8.850678	-5.327322

Table S21. Cartesian coordinates of the optimized T_1 geometry of **5** computed by TDDFT/CPCM.

1	C	-7.646762	-1.492121	-0.566804	61	C	6.753288	5.861042	1.678320
2	C	-9.009902	-1.597794	-0.589414	62	C	4.936787	7.346560	0.114398
3	C	-9.793506	-0.507741	-0.120674	63	H	2.195104	6.276832	-0.695342
4	C	-9.147092	0.658388	0.358851	64	H	1.899651	4.568730	-0.973973
5	C	-7.750510	0.760379	0.379646	65	C	2.072337	5.089867	1.103238
6	H	-11.870016	-1.211851	-0.384806	66	H	3.825003	6.209649	-2.478417
7	H	-9.496966	-2.496819	-0.956670	67	H	3.510589	4.494350	-2.702839
8	C	-11.208874	-0.413433	-0.060081	68	C	5.600978	5.010702	-2.691271
9	C	-11.651039	0.772181	0.443225	69	C	6.794273	7.251003	1.675652
10	H	-12.669268	1.104733	0.597907	70	H	7.453672	5.288521	2.283563
11	C	-6.682327	-2.510540	-1.002726	71	C	5.893665	7.987148	0.902510
12	C	-5.308145	-2.181299	-0.874515	72	H	4.239952	7.928918	-0.487445
13	C	-7.088272	-3.746833	-1.517087	73	H	2.486022	4.145381	1.494401
14	C	-4.400507	-3.148735	-1.278106	74	H	2.510906	5.888336	1.721785
15	C	-6.120171	-4.654146	-1.900468	75	C	0.560573	5.069518	1.273025
16	H	-8.135425	-4.017038	-1.624596	76	H	6.272132	5.734827	-2.203438
17	C	-4.763946	-4.385950	-1.792445	77	H	5.966810	4.012813	-2.400300
18	C	-6.896262	1.838141	0.813174	78	C	5.707341	5.163482	-4.200856
19	C	-5.483196	1.624044	0.685266	79	H	7.531973	7.771018	2.281713
20	C	-7.373860	3.056176	1.338879	80	H	5.940063	9.073479	0.915588
21	C	-4.651268	2.653739	1.083528	81	H	0.133148	6.019642	0.913282
22	C	-6.469896	4.025801	1.716941	82	H	0.136588	4.286360	0.621065
23	H	-8.429422	3.273846	1.464868	83	C	0.112750	4.817061	2.703389
24	C	-5.096575	3.864908	1.603171	84	H	5.337498	6.159285	-4.495500
25	Au	-5.053358	-0.257808	-0.090405	85	H	5.037205	4.438822	-4.692050
26	C	-0.456395	-0.088799	-0.053058	86	C	7.122633	4.976396	-4.723118
27	C	0.219997	0.851724	0.762658	87	H	0.523588	3.851527	3.046961
28	C	0.315485	-0.971858	-0.847787	88	H	0.549054	5.579492	3.369813
29	C	1.592119	0.911991	0.780756	89	C	-1.400615	4.807158	2.863067
30	H	-0.371259	1.517601	1.387140	90	H	7.792921	5.702128	-4.233624
31	C	1.688226	-0.920438	-0.828227	91	H	7.494165	3.981075	-4.427665
32	H	-0.202633	-1.683853	-1.486605	92	C	7.231506	5.127378	-6.232804
33	H	2.100138	1.618411	1.433527	93	H	-1.800442	5.782772	2.544497
34	H	2.269742	-1.583481	-1.465088	94	H	-1.836896	4.066440	2.175782
35	N	-7.051580	-0.345183	-0.096212	95	C	-1.840484	4.507608	4.286179
36	N	3.747492	0.082994	0.003027	96	H	6.858350	6.121168	-6.523637
37	C	2.352809	0.025402	-0.014626	97	H	6.560239	4.401973	-6.717409
38	S	-10.336734	1.838791	0.869903	98	C	8.651467	4.938415	-6.739291
39	C	-3.082348	-0.179618	-0.079197	99	H	-1.452399	5.257134	4.987903
40	C	-1.855259	-0.141757	-0.070512	100	H	-2.931891	4.494013	4.381549
41	H	-4.017772	-5.116685	-2.091616	101	H	-1.468323	3.528314	4.613587
42	H	-4.403418	4.647733	1.895819	102	H	9.031195	3.941310	-6.482161
43	F	-6.935265	5.181395	2.215395	103	H	8.718235	5.049074	-7.826907
44	F	-3.315702	2.519540	0.973546	104	H	9.330743	5.672535	-6.287567
45	F	-6.499603	-5.841043	-2.393682	105	C	4.496708	-1.102400	-0.147548
46	F	-3.080708	-2.911160	-1.176115	106	C	5.627824	-1.118285	-0.979017
47	C	4.393669	1.324326	0.174684	107	C	4.058840	-2.273627	0.491135
48	C	5.501341	1.427029	1.031432	108	C	6.290006	-2.310408	-1.229731
49	C	3.875889	2.460255	-0.468369	109	H	5.943212	-0.197187	-1.463036
50	C	6.057874	2.667422	1.302990	110	C	4.712917	-3.455469	0.226419
51	H	5.880130	0.531643	1.518153	111	H	3.197662	-2.236504	1.157022
52	C	4.424478	3.689772	-0.182484	112	C	5.814422	-3.487613	-0.649252
53	H	3.035810	2.357641	-1.153984	113	H	7.142450	-2.324592	-1.905145
54	C	5.499967	3.805795	0.718244	114	C	4.359460	-4.843435	0.714253
55	H	6.891239	2.746642	1.997426	115	C	6.229421	-4.875378	-0.807250
56	C	3.970082	5.047606	-0.671578	116	C	5.370352	-5.682631	-0.040493
57	C	5.795853	5.221435	0.893241	117	C	2.901223	-5.187816	0.358853
58	C	4.890677	5.961309	0.111738	118	C	4.542331	-4.977133	2.239137
59	C	2.480344	5.269961	-0.351756	119	C	7.253768	-5.439094	-1.565533
60	C	4.178615	5.206269	-2.191009	120	C	5.530041	-7.059372	-0.030784

121	H	2.688123	-6.211303	0.705551
122	H	2.249996	-4.529811	0.958062
123	C	2.519827	-5.053303	-1.108205
124	H	4.267057	-6.005340	2.524584
125	H	3.804663	-4.321497	2.730068
126	C	5.930629	-4.660580	2.772167
127	C	7.408622	-6.820987	-1.550644
128	H	7.918832	-4.814864	-2.159441
129	C	6.554116	-7.624061	-0.791937
130	H	4.869617	-7.693284	0.559969
131	H	2.874086	-4.085412	-1.500340
132	H	3.031372	-5.824173	-1.705307
133	C	1.015722	-5.145049	-1.317353
134	H	6.672423	-5.325780	2.303041
135	H	6.217188	-3.635682	2.486090
136	C	6.014427	-4.801345	4.284351
137	H	8.200327	-7.282246	-2.135767
138	H	6.690018	-8.702939	-0.795130
139	H	0.648209	-6.118231	-0.952902
140	H	0.519209	-4.384759	-0.689865
141	C	0.590472	-4.947308	-2.763065
142	H	5.723824	-5.824570	4.573920
143	H	5.274084	-4.135538	4.757703
144	C	7.396445	-4.494012	4.837762
145	H	0.937606	-3.958763	-3.111353
146	H	1.100897	-5.684372	-3.404886
147	C	-0.914168	-5.053629	-2.963966
148	H	8.137002	-5.159925	4.364756
149	H	7.688226	-3.470667	4.548519
150	C	7.484233	-4.634988	6.349793
151	H	-1.248900	-6.051691	-2.639992
152	H	-1.423924	-4.337832	-2.301382
153	C	-1.334150	-4.809135	-4.403547
154	H	7.191234	-5.657119	6.634219
155	H	6.742634	-3.969835	6.818025
156	C	8.871176	-4.324978	6.887123
157	H	-0.869912	-5.536930	-5.081481
158	H	-2.420138	-4.880656	-4.529972
159	H	-1.028066	-3.809217	-4.736871
160	H	9.169470	-3.298838	6.636904
161	H	8.923235	-4.429883	7.976108
162	H	9.620812	-4.997824	6.451553

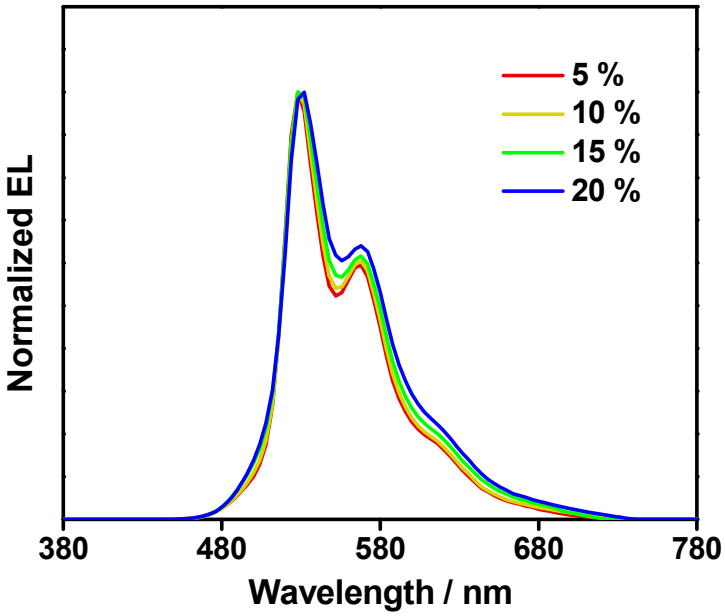


Figure S26. Normalized EL spectra of solution-processed devices made with **1** at a luminance of 100 cd m^{-2}.

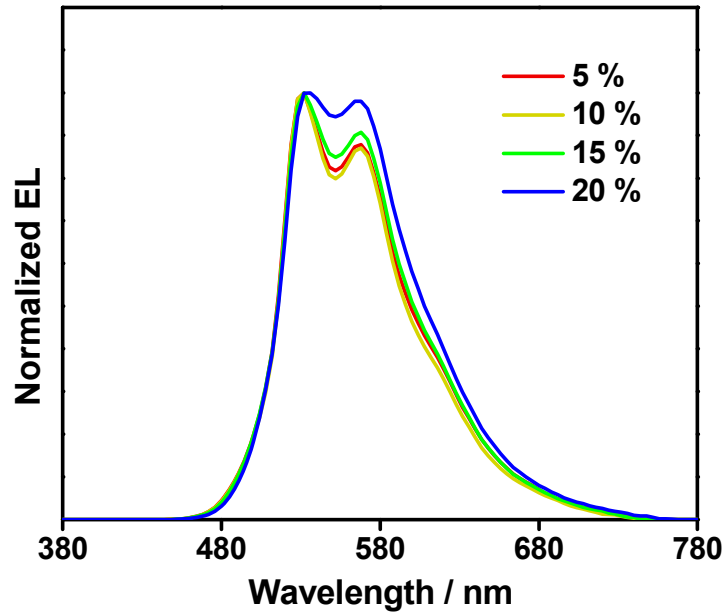


Figure S27. Normalized EL spectra of solution-processed devices made with **2** at a luminance of 100 cd m^{-2}.

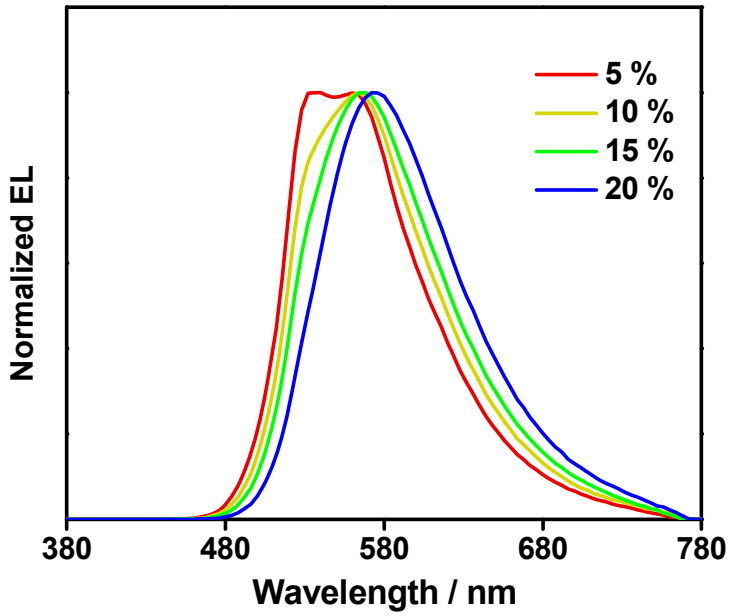


Figure S28. Normalized EL spectra of solution-processed devices made with **3** at a luminance of 100 cd m^{-2}.

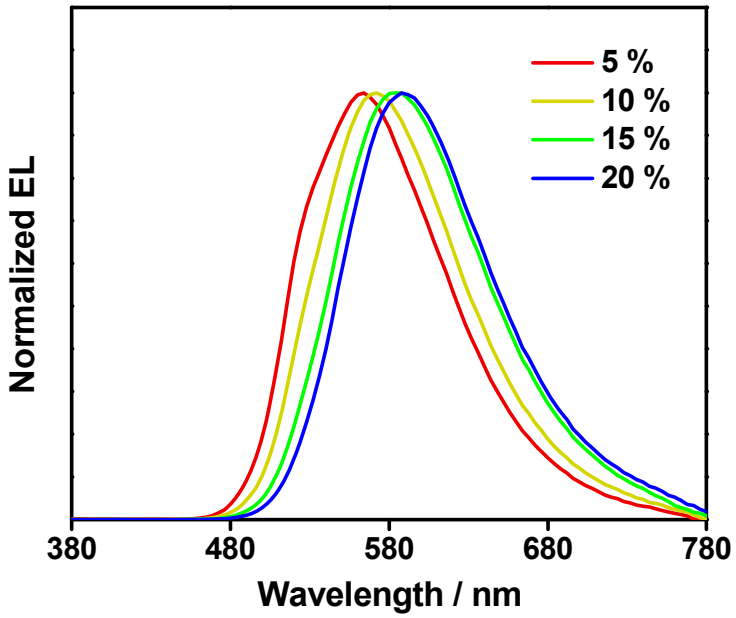


Figure S29. Normalized EL spectra of solution-processed devices made with **4** at a luminance of 100 cd m^{-2}.

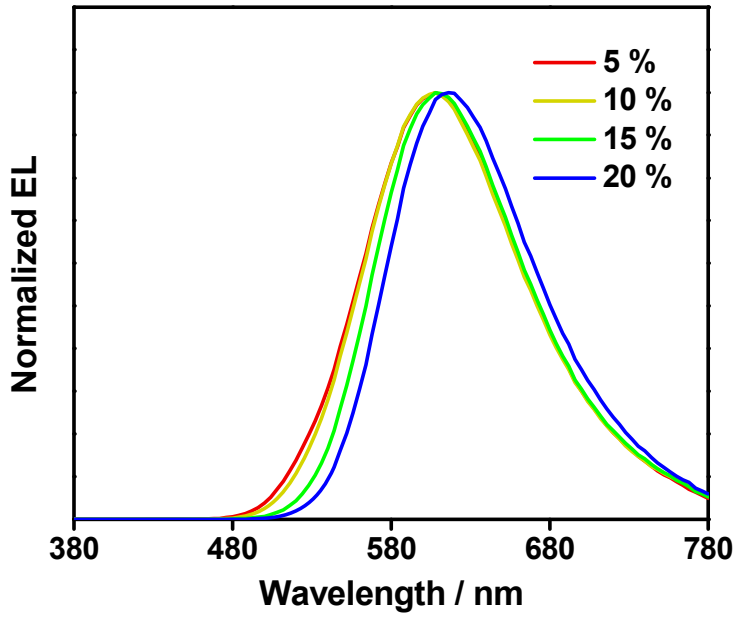


Figure S30. Normalized EL spectra of solution-processed devices made with **5** at a luminance of 100 cd m^{-2}.

Table S22. Key parameters of the solution-processed OLEDs based on **1**−**5**.

Complex	Conc. [wt%]	CE[a] [cd A^{-1}]	PE[b] [lm W^{-1}]	EQE[c] [%]	λ_{max}[d]	CIE[e] [x, y]
1	5	26.8	10.5	7.2	528	0.36, 0.61
	10	37.0	18.2	10.0	528	0.37, 0.60
	15	28.0	17.5	7.7	528	0.37, 0.60
	20	21.4	13.4	6.0	532	0.38, 0.59
2	5	11.8	3.4	3.4	532	0.40, 0.57
	10	15.1	5.4	4.4	532	0.40, 0.57
	15	25.4	11.6	7.4	532	0.41, 0.57
	20	30.1	18.5	8.9	532	0.42, 0.56
3	5	14.5	2.9	4.4	560	0.41, 0.56
	10	17.7	5.6	5.6	564	0.44, 0.54
	15	22.8	11.2	7.5	564	0.46, 0.53
	20	22.2	12.4	8.0	572	0.49, 0.50
4	5	9.3	2.7	3.0	564	0.44, 0.54
	10	10.6	3.5	3.7	572	0.47, 0.51
	15	11.9	4.6	4.7	588	0.51, 0.48
	20	12.3	5.2	5.2	588	0.53, 0.48
5	5	3.8	0.8	1.9	608	0.55, 0.44
	10	4.1	1.1	2.1	608	0.55, 0.44
	15	8.5	4.0	4.9	608	0.58, 0.42
	20	7.9	4.4	5.3	616	0.60, 0.40

[a] CE represents maximum current efficiency.

[b] PE represents maximum power efficiency.

[c] EQE represents maximum external quantum efficiency.

[d] λ_{max} represents peak maximum.

[e] CIE coordinates are taken at a current density of 100 cd m^{-2}.

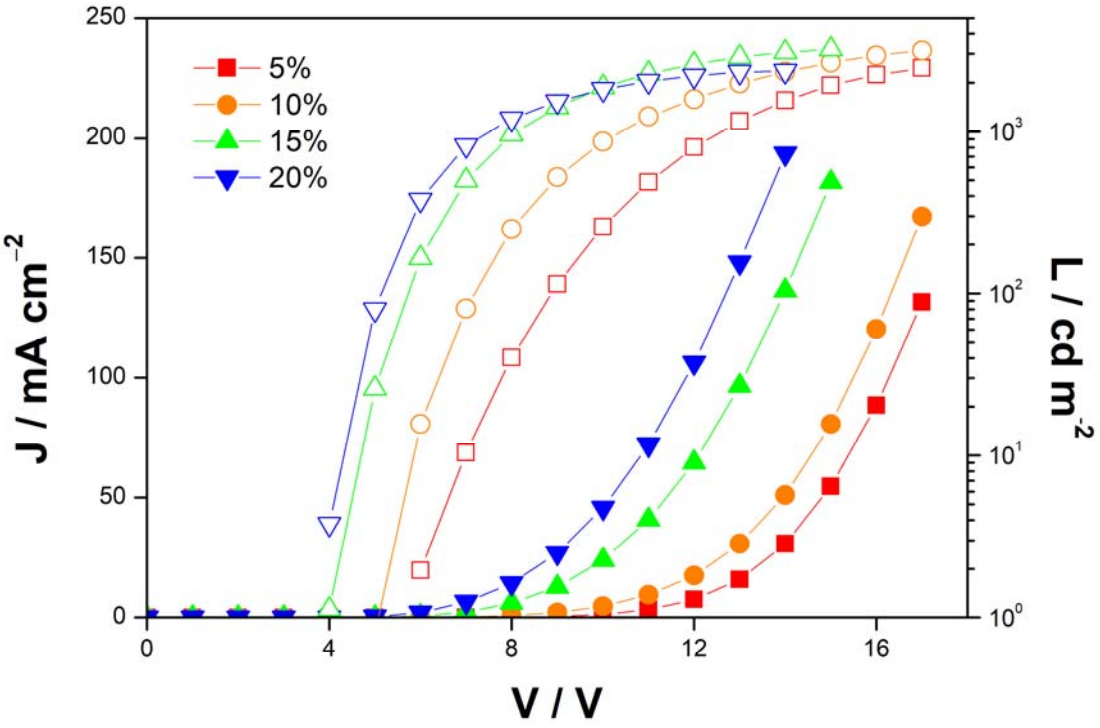


Figure S31. Current density–voltage–luminance (*J*–*V*–*L*) characteristics of solution-processed devices made with **1**.

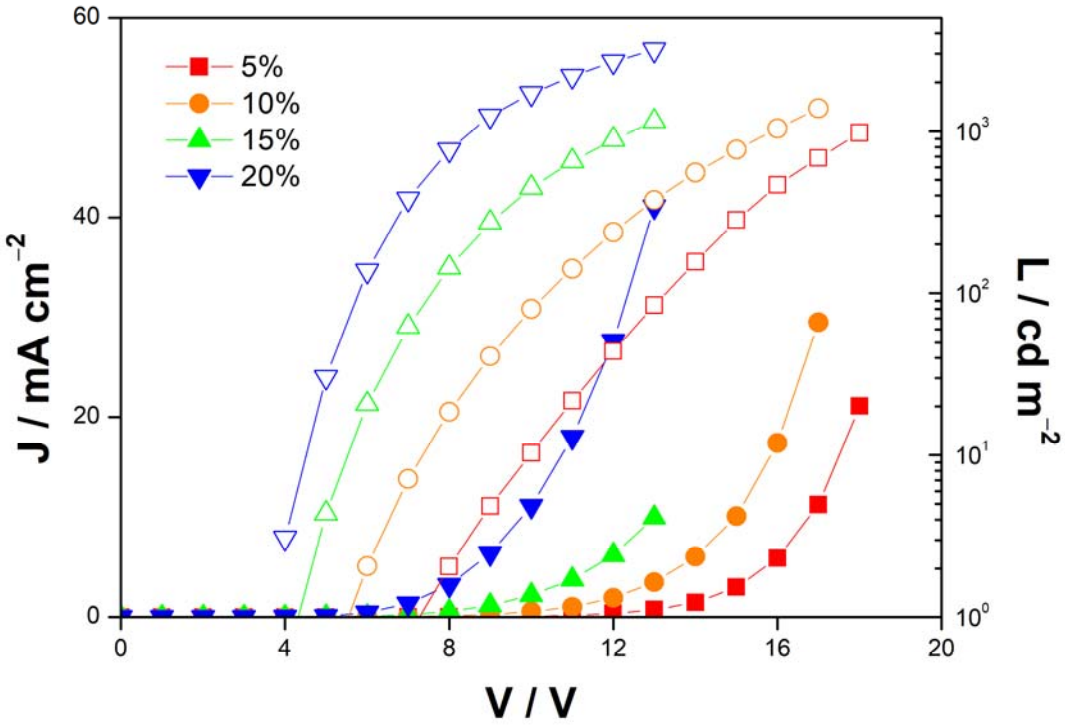


Figure S32. *J–V–L* characteristics of solution-processed devices made with **2**.

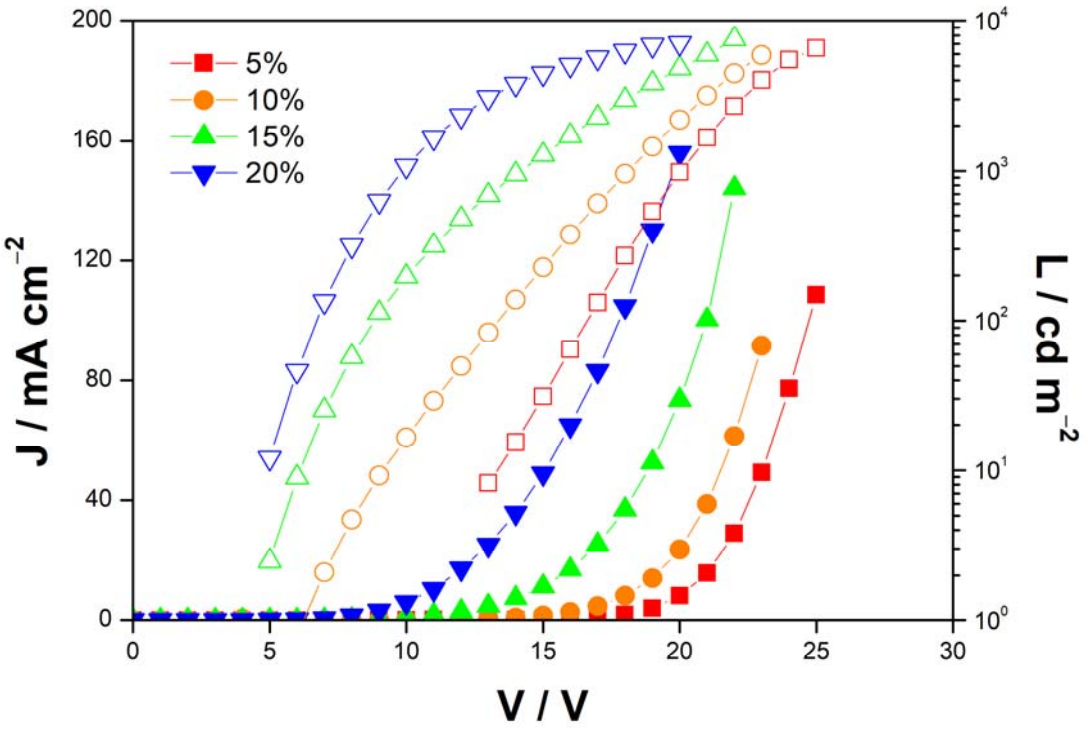


Figure S33. *J–V–L* characteristics of solution-processed devices made with **3**.

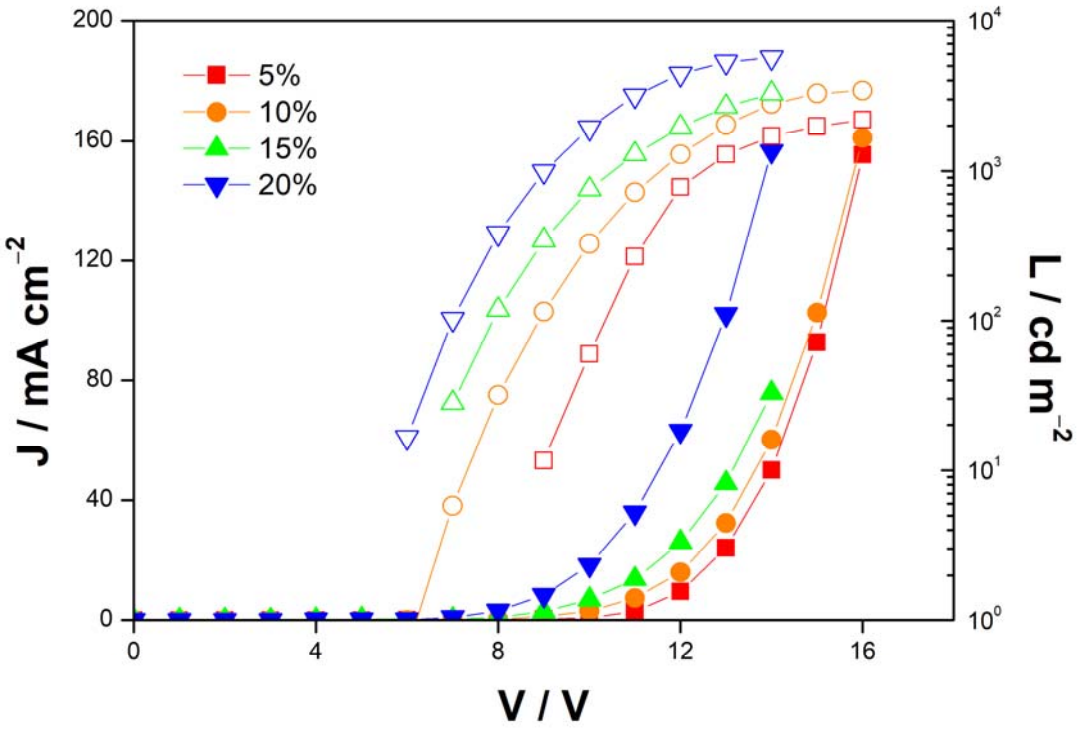


Figure S34. *J–V–L* characteristics of solution-processed devices made with **4**.

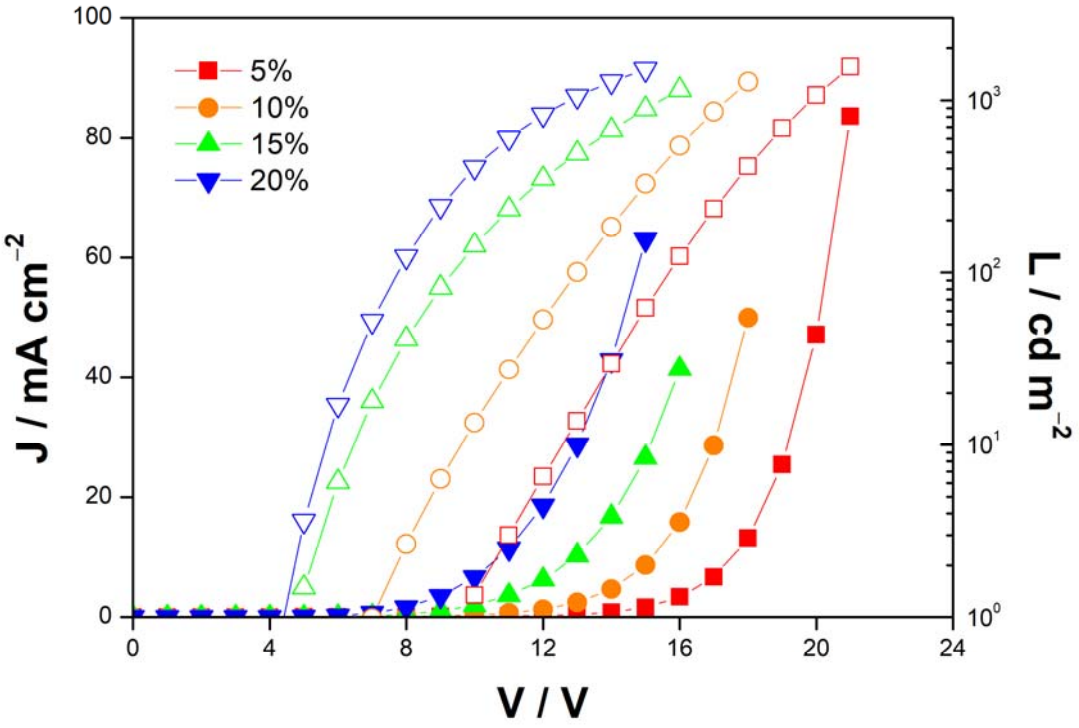


Figure S35. *J–V–L* characteristics of solution-processed devices made with **5**.

Materials and reagents. Potassium tetrachloroaurate(III) was purchased from Strem or Matrix Scientific. Tetrahydrofuran for reactions were purified by the Innovative Technology, Inc. PureSolv MD 5 Solvent Purification System before use. All other reagents were of analytical grade and were used as received. Tetra-*n*-butylammonium hexafluorophosphate (Aldrich, 98 %) was recrystallized for no less than three times from hot absolute ethanol prior to use. All reactions were performed under anaerobic and anhydrous conditions using standard Schlenk techniques under an inert atmosphere of nitrogen.

Physical measurements and instrumentation. The UV−vis absorption spectra were recorded on a Cary 60 UV−vis (Agilent Technology) spectrophotometer equipped with a Xenon flash lamp. Transient absorption measurements were performed on a LP980 laser flash photolysis spectrometer (Edinburgh Instruments Ltd., Livingston, U.K.) at ambient temperature. The excitation source was the 355-nm output (third harmonic) of a Nd:YAG laser (Spectra-Physics Quanta-Ray Lab130 Pulsed Nd:YAG Laser), and the probe light source was a Xe900 450W xenon arc lamp. The transient absorption spectra were detected by an image intensified CCD camera (Andor) with PC plug-in controller, fully operated by L900 spectrometer software. The absorption kinetics were detected by a Hamamatsu R928 photomultiplier tube and recorded on a Tektronix model TDS3012B (100 MHz, 1.25 GS/s) digital oscilloscope and analyzed using the same software for exponential fit. ^{1}H and ^{13}C{^{1}H} and ^{19}F{^{1}H} nuclear magnetic resonance (NMR) spectra were recorded on Bruker AVANCE 400 or 500 (400 MHz and 500 MHz for ^{1}H, respectively; 100 MHz or 125 MHz for ^{13}C, respectively; and 470 MHz or 376 MHz for ^{19}F nucleus, respectively) fourier-transform NMR spectrometers. All ^{1}H and ^{13}C chemical shift data were reported relative to tetramethylsilane, with the residual NMR solvent peak used as internal reference. ^{19}F chemical shift data were reported with reference to trifluoroacetic acid (δ = 76.55 ppm). Splitting of the ^{13}C signal due to ^{19}F–^{13}C coupling was not determined; instead

all of them were reported as individual singlet signals. High-resolution electrospray ionization (HR-ESI) mass spectra were recorded on Bruker maXis II^{TM} High Resolution LC-QTOF Mass Spectrometer. Fourier transform infrared (FT-IR) measurements were performed with a PerkinElmer Spectrum Two system (PerkinElmer, Buckinghamshire, UK) at a wavenumber range of 400−4000 cm^{-1}. Elemental analyses were performed on the Carlo Erba 1106 elemental analyzer at the Institute of Chemistry, Chinese Academy of Sciences in Beijing. Steady-state excitation and emission spectra were recorded on a Horiba Scientific FluoroMax-4 fluorescence spectrofluorometer equipped with a R928P PMT detector. Liquid nitrogen was placed into the quartz-walled optical Dewar flask for low temperature (77 K) photophysical measurements. Solid-state photophysical measurements were performed with solid sample loaded into a quartz tube inside a quartz-walled Dewar flask. Low temperature (77 K) photophysical measurements were done by placing liquid nitrogen into the optical Dewar flask. Excited-state lifetimes of solution and glass samples were measured with a conventional laser system. The excitation source used was the 355-nm output (third harmonic, 8 ns) of a Spectra-Physics Quanta-Ray Q-switched GCR-150 pulsed Nd:YAG laser (10 Hz). Luminescence decay signals were detected by a Hamamatsu R928 photomultiplier tube, recorded on a Tektronix model TDS-620A (500 MHz, 2 GSs^{-1}) digital oscilloscope, with a 50 Ω load resistor and analyzed with a program for exponential fits. Relative photoluminescence quantum yields in solution were measured by the optical dilute method reported by Demas and Crosby.[2] A degassed solution of $[Ru(bpy)_3]Cl_2$ in MeCN has been used as reference (Φ_{lum} = 0.06, excitation wavelength at 436 nm),[2] whereas absolute photoluminescence quantum yields (PLQYs) in thin films were measured on a Hamamatsu C9920−03 absolute PLQY measurement system. Excited-state lifetimes of thin films were measured on an Edinburgh Instruments LP980 Spectrometer. Variable-temperature emission spectra were obtained using the Edinburgh Instruments FS5 Spectrofluorometer with an Oxford Instrument OptistatDN2

cryostat for temperatures in the range of 77 K to 320 K. The solution sample was degassed by bubbling with nitrogen. Solution samples and thin films were placed in a quartz cell inside the cryostat and maintained at the desired temperature until equilibrium was reached before recording the spectrum. Cyclic voltammetry was performed with a CH Instruments Model CHI620E (CH Instruments, Inc.). All solutions for electrochemical measurements were purged with prepurified argon gas prior to measurement. Thermal analyses were performed on a TGA Q50 (TA Instruments), in which T_d is defined as the temperature at which the sample shows a 5 % weight loss.

Synthesis and characterization. The cyclometalating ligands, 4-^{t}BuC^N^{THPY}^C^{t}Bu-4 and 3,5-F_2C^N^{THPY}^CF_2-3,5, and the respective precursor gold compounds, [Au{4-^{t}BuC^N^{THPY}^C^{t}Bu-4}Cl] and [Au{3,5-F_2C^N^{THPY}^CF_2-3,5}Cl], were prepared by slight modifications of the literature procedures.[3–7] H−C≡C−C_6H_4−N(C_6H_5)$_2$-*p*, H−C≡C−C_6H_4−N[$C_{13}H_7$(C_6H_{13})$_2$]$_2$, H−C≡C−C_6H_4−N[$C_{12}H_7$N(C_6H_{13})]$_2$ and the alkynylgold(III) complexes were synthesized by modifying a lourterature procedure for bis-cyclometalated diarylpyridine alkynylgold(III) complexes previously reported by us.[4–7]

4-^{t}BuC^N^{THPY}^C^{t}Bu-4. Yield: 540 mg (90 %). ^{1}H NMR (500 MHz, $CDCl_3$, 298 K, relative to Me_4Si, δ/ppm): δ 8.18−8.16 (d, J = 8.5 Hz, 2H, phenyl protons), 8.14−8.12 (d, J = 8.5 Hz, 2H, phenyl protons), 8.07 (s, 1H, thienopyridyl proton), 7.72−7.71 (d, J = 5.4 Hz, 1H, thienopyridyl proton), 7.59−7.58 (d, J = 8.5 Hz, 2H, phenyl protons), 7.53−7.51 (d, J = 8.5 Hz, 2H, phenyl protons), 7.47−7.46 (d, J = 5.4 Hz, 1H, thienopyridyl proton), 1.40 (s, 9H, −^{t}Bu), 1.38 (s, 9H, −^{t}Bu). ^{13}C{^{1}H} NMR (150 MHz, $CDCl_3$, 298 K, relative to Me_4Si, δ/ppm): δ 152.65, 152.42, 151.81, 151.53, 147.48, 137.18, 137.13, 132.20, 131.94, 128.26, 126.84, 125.70, 125.68, 123.86, 112.57, 34.88, 34.73, 31.47, 31.44. HRMS (positive ESI) calcd for

$C_{27}H_{29}NS$: *m/z* = 399.2015 $[M]^+$; found 399.2044 $[M]^+$. Elemental analysis calculated for $C_{27}H_{29}NS \cdot H_2O$ (%): C, 77.65; H, 7.48; N, 3.35; found: C, 77.68; H, 7.13; N, 3.43.

[Au{4-^{t}BuC^N^{THPY}^C^{t}Bu-4}Cl]. Yield: 300 mg (38 %). ^{1}H NMR (500 MHz, $CDCl_3$, 298 K, relative to Me_4Si, δ/ppm): δ 8.09 (d, *J* = 2.2 Hz, 1H, phenyl proton), 8.01 (d, *J* = 2.2 Hz, 1H, phenyl proton), 7.99−7.98 (d, *J* = 5.4 Hz, 1H, thienopyridyl proton), 7.90−7.89 (d, *J* = 8.3 Hz, 1H, phenyl proton), 7.51−7.50 (d, *J* = 8.3 Hz, 1H, phenyl proton), 7.48−7.47 (d, *J* = 5.4 Hz, 1H, thienopyridyl proton), 7.47 (s, 1H, thienopyridyl proton), 7.40−7.38 (dd, *J* = 8.3 and 2.2 Hz, 1H, phenyl proton), 7.30−7.28 (dd, *J* = 8.3 and 2.2 Hz, 1H, phenyl proton), 1.41 (s, 9H, −^{t}Bu), 1.39 (s, 9H, −^{t}Bu). No $^{13}C\{^1H\}$ NMR signals were recorded due to the low solubility of the complex. HRMS (positive ESI) calcd for $C_{27}H_{28}AuClNS$: *m/z* = 630.1291 $[M+H]^+$; found 630.1268 $[M+H]^+$.

3,5-F$_2$C^N^{THPY}^CF$_2$-3,5. Yield: 540 mg (93 %). ^{1}H NMR (500 MHz, $CDCl_3$, 298 K, relative to Me_4Si, δ/ppm): δ 8.41 (s, 1H, thienopyridyl proton), 7.82−7.80 (d, *J* = 5.4 Hz, 1H, thienopyridyl proton), 7.76−7.74 (m, 2H, phenyl proton), 7.73−7.71 (m, 2H, phenyl protons), 7.54−7.53 (d, *J* = 5.4 Hz, 1H, thienopyridyl proton), 7.00−6.95 (tt, *J* = 8.7 and 2.4 Hz, 1H, phenyl proton), 6.89−6.85 (tt, *J* = 8.7 and 2.4 Hz, 1H, phenyl proton). $^{13}C\{^1H\}$ NMR (150 MHz, $CDCl_3$, 298 K, relative to Me_4Si, δ/ppm): δ 148.01, 133.58, 133.05, 124.18, 114.22, 111.71, 111.65, 111.55, 111.49, 109.94, 109.89, 109.78, 109.73, 105.23, 105.02, 104.82, 104.25, 104.04, 103.84. $^{19}F\{^1H\}$ NMR (470 MHz, $CDCl_3$, 298 K, relative to CF_3COOH, δ/ppm): δ −108.67, −109.53. HRMS (positive ESI) calcd for $C_{19}H_{10}F_4NS$: *m/z* = 360.0465 $[M+H]^+$; found 360.0567 $[M+H]^+$. Elemental analysis calculated for $C_{19}H_9F_4NS$ (%): C, 63.51; H, 2.52; N, 3.90; found: C, 63.49; H, 2.50; N, 3.87.

[Au{3,5-F_2C^N^{THPY}^CF_2-3,5}Cl]. Yield: 350 mg (40 %). ^{1}H NMR (500 MHz, DMSO-d_6, 298 K, relative to Me_4Si, δ/ppm): δ 8.68 (s, 1H, thienopyridyl proton), 8.63−8.62 (d, J = 5.4 Hz, 1H, thienopyridyl proton), 7.73−7.71 (m, 2H, thienopyridyl proton and phenyl proton), 7.56−7.55 (d, J = 8.2, 1H, phenyl proton), 7.27−7.24 (m, 1H, phenyl proton), 7.08−7.05 (m, 1H, phenyl proton). No $^{13}C\{^1H\}$ NMR signals were recorded due to the low solubility of the complex. $^{19}F\{^1H\}$ NMR (470 MHz, DMSO-d_6, 298 K, relative to CF_3COOH, δ/ppm): −91.87, −93.41, −110.56, −111.32. HRMS (positive ESI) calcd for $C_{19}H_8AuClF_4NS$: m/z = 589.9662 $[M+H]^+$; found 589.9682 $[M+H]^+$.

[Au{4-^{t}BuC^$N^{THPY}^{C}^t$Bu-4}{C≡C−C_6H_4−$N(C_6H_5)_2$-p}] (**1**). A mixture of [Au{4-^{t}BuC^$N^{THPY}^{C}^t$Bu-4}Cl] (70 mg, 0.11 mmol), copper(I) iodide (3 mg, 0.02 mmol), triethylamine (2 mL) and (4-ethynylphenyl)diphenylamine (45 mg, 0.17 mmol) in a degassed THF (20 mL) solution was stirred at room temperature for 4 h. After removing the solvent, the crude product was purified by column chromatography on silica gel (70−230 mesh) using hexane-ethyl acetate (10:1, v/v) as the eluent. Subsequent recrystallization by diffusion of diethyl ether vapor into a concentrated THF solution of the product gave **1** as a yellow solid. Yield: 62 mg (65 %). ^{1}H NMR (500 MHz, $CDCl_3$, 298 K, relative to Me_4Si, δ/ppm): δ 8.33−8.32 (d, J = 2.2 Hz, 1H, phenyl proton of 4-^{t}BuC^$N^{THPY}^{C}^t$Bu-4), 8.26−8.25 (d, J = 2.2 Hz, 1H, phenyl proton of 4-^{t}BuC^$N^{THPY}^{C}^t$Bu-4), 7.94−7.92 (m, 2H, phenyl and thienopyridyl protons of 4-^{t}BuC^$N^{THPY}^{C}^t$Bu-4), 7.80 (s, 1H, thienopyridyl proton of 4-^{t}BuC^$N^{THPY}^{C}^t$Bu-4), 7.56−7.54 (d, J = 8.3 Hz, 1H, phenyl proton of 4-^{t}BuC^$N^{THPY}^{C}^t$Bu-4), 7.51−7.50 (d, J = 8.7 Hz, 2H, phenyl protons of −C≡C−C_6H_4−), 7.46−7.45 (d, J = 5.4 Hz, 1H, thienopyridyl proton of 4-^{t}BuC^$N^{THPY}^{C}^t$Bu-4), 7.40−7.38 (dd, J = 8.3 and 2.2 Hz, 1H, phenyl proton of 4-^{t}BuC^$N^{THPY}^{C}^t$Bu-4), 7.30−7.27 (m, 5H, phenyl proton of 4-^{t}BuC^$N^{THPY}^{C}^t$Bu-4 and phenyl protons of −$N(C_6H_5)_2$), 7.15−7.13 (m, 4H,

phenyl protons of −N(C_6H_5)$_2$), 7.06−7.04 (m, 4H, phenyl protons of −C≡C−C_6H_4− and phenyl protons of −N(C_6H_5)$_2$), 1.42 (s, 9H, −^{t}Bu), 1.40 (s, 9H, −^{t}Bu). ^{13}C{^{1}H} NMR (150 MHz, $CDCl_3$, 298 K, relative to Me_4Si, δ/ppm): δ 168.33, 165.76, 160.37, 158.56, 155.10, 153.86, 150.33, 147.79, 146.98, 146.72, 146.45, 136.49, 133.50, 133.46, 133.00, 129.41, 127.90, 127.62, 124.68, 124.24, 124.04, 123.79, 123.45, 123.39, 123.09, 120.94, 110.36, 100.43, 92.03, 35.54, 35.41, 31.47, 31.39. HRMS (positive ESI) calcd for $C_{47}H_{41}AuN_2S$: *m/z* = 862.2651 $[M]^+$; found 862.2604 $[M]^+$. IR (thin film): 2155 cm^{-1} ν(C≡C). Elemental analysis calculated for $C_{47}H_{41}AuN_2S$ (%): C, 65.42; H, 4.79; N, 3.25; found: C, 65.66; H, 4.74; N, 3.42.

[Au{4-^{t}BuC^N^{THPY}^C^{t}Bu-4}{C≡C−C_6H_4−N[$C_{13}H_7$(C_6H_{13})$_2$]$_2$}] (**2**). This complex was synthesized by a procedure similar to that of **1**, except that H−C≡C−C_6H_4−N[$C_{13}H_7$(C_6H_{13})$_2$]$_2$ (64 mg, 0.11 mmol) was used instead of (4-ethynylphenyl)diphenylamine. Subsequent recrystallization by diffusion of diethyl ether vapor into a concentrated THF solution of the product gave **2** as a yellow solid. Yield: 90 mg (59 %). ^{1}H NMR (400 MHz, acetone-d_6, 298 K, relative to Me_4Si, δ/ppm): δ 8.41−8.39 (d, J = 5.4 Hz, 1H, thienopyridyl proton of 4-^{t}BuC^N^{THPY}^C^{t}Bu-4), 8.35−8.34 (d, J = 2.1 Hz, 1H, phenyl proton of 4-^{t}BuC^N^{THPY}^C^{t}Bu-4), 8.30 (s, 1H, thienopyridyl proton of 4-^{t}BuC^N^{THPY}^C^{t}Bu-4), 8.26−8.25 (d, J = 2.1 Hz, 1H, phenyl proton of 4-^{t}BuC^N^{THPY}^C^{t}Bu-4), 8.04−8.02 (d, J = 8.3 Hz, 1H, phenyl proton of 4-^{t}BuC^N^{THPY}^C^{t}Bu-4), 7.80−7.78 (d, J = 8.2 Hz, 1H, phenyl proton of 4-^{t}BuC^N^{THPY}^C^{t}Bu-4), 7.77−7.73 (m, 5H, thienopyridyl proton of 4-^{t}BuC^N^{THPY}^C^{t}Bu-4 and fluorenyl protons), 7.52−7.49 (m, 3H, phenyl proton of 4-^{t}BuC^N^{THPY}^C^{t}Bu-4 and phenyl protons of −C≡C−C_6H_4−), 7.44−7.43 (d, J = 6.7 Hz, 2H, fluorenyl protons), 7.39−7.36 (dd, J = 8.2 and 2.1 Hz, 1H, phenyl proton of 4-^{t}BuC^N^{THPY}^C^{t}Bu-4), 7.36−7.27 (m, 6H, fluorenyl protons), 7.13−7.11 (m, 4H, phenyl

protons of −C≡C−C_6H_4− and fluorenyl protons), 2.00−1.94 (m, 8H, −CH_2−), 1.42 (s, 9H, −CH_3), 1.40 (s, 9H, −CH_3), 1.20−1.08 (m, 24H, −CH_2−), 0.82−0.78 (t, J = 7.1 Hz, 12H, −CH_3), 0.77−0.62 (m, 8H, −CH_2−). $^{13}C\{^1H\}$ NMR (150 MHz, $CDCl_3$, 298 K, δ/ppm): δ 168.37, 165.78, 160.34, 158.55, 155.08, 153.85, 152.24, 150.73, 150.31, 147.07, 146.98, 146.46, 141.10, 136.56, 136.49, 133.49, 132.98, 127.89, 127.64, 126.88, 126.43, 124.26, 124.06, 123.82, 123.62, 123.48, 122.87, 122.78, 120.47, 119.23, 110.37, 91.99, 55.23, 40.46, 35.53, 35.40, 31.73, 31.45, 31.36, 29.83, 23.96, 22.70, 14.24. HRMS (positive ESI) calcd for $C_{85}H_{97}AuN_2S$: m/z = 1373.6954 $[M]^+$; found 1373.7057 $[M]^+$. IR (thin film): 2165 cm^{-1} ν(C≡C). Elemental analysis calculated for $C_{85}H_{97}AuN_2S$ (%): C, 74.21; H, 7.11; N, 2.04; found: C, 73.90; H, 7.11; N, 2.09.

[Au{4-^{t}BuC^N^{THPY}^C^{t}Bu-4}{C≡C−C_6H_4−N[$C_{12}H_7N(C_6H_{13})]_2$}] (**3**). This complex was synthesized by a procedure similar to that of **1**, except that H−C≡C−C_6H_4−N[$C_{12}H_7N(C_6H_{13})]_2$ (70 mg, 0.11 mmol) was used instead of (4-ethynylphenyl)diphenylamine. Subsequent recrystallization by diffusion of diethyl ether vapor into a concentrated THF solution of the product gave **3** as a yellow solid. Yield: 80 mg (60 %). ^1H NMR (400 MHz, DMSO-d_6, 298 K, δ/ppm): δ 8.51−8.50 (d, J = 5.4 Hz, 1H, thienopyridyl proton of 4-^{t}BuC^N^{THPY}^C^{t}Bu-4), 8.41 (s, 1H, thienopyridyl proton of 4-^{t}BuC^N^{THPY}^C^{t}Bu-4), 8.15−8.14 (d, J = 2.1 Hz, 1H, phenyl proton of 4-^{t}BuC^N^{THPY}^C^{t}Bu-4), 8.10−8.09 (m, 4H, carbazolyl protons), 8.05 (d, J = 2.1 Hz, 1H, phenyl proton of 4-^{t}BuC^N^{THPY}^C^{t}Bu-4), 7.97−7.95 (d, J = 8.3 Hz, 1H, phenyl proton of 4-^{t}BuC^N^{THPY}^C^{t}Bu-4), 7.82−7.80 (d, J = 8.3 Hz, 1H, phenyl proton of 4-^{t}BuC^N^{THPY}^C^{t}Bu-4), 7.74−7.73 (d, J = 5.4 Hz, 1H, thienopyridyl proton of 4-^{t}BuC^N^{THPY}^C^{t}Bu-4), 7.66−7.64 (d, J = 8.8 Hz, 2H, carbazolyl protons), 7.60−7.58 (d, J = 8.3 Hz, 2H, carbazolyl protons), 7.51−7.49 (dd, J = 8.3 and 2.1 Hz, 1H, phenyl proton of

4-^{t}BuC^N^{THPY}^C^{t}Bu-4), 7.46−7.39 (m, 4H, carbazolyl protons), 7.36−7.33 (dd, J = 8.3 and 2.1 Hz, 1H, phenyl proton of 4-^{t}BuC^N^{THPY}^C^{t}Bu-4), 7.31−7.28 (d, J = 8.7 Hz, 2H, phenyl protons of −C≡C−C_6H_4−), 7.15−7.12 (t, J = 7.6 Hz, 2H, carbazolyl protons), 6.79−6.77 (d, J = 8.7 Hz, 2H, phenyl protons of −C≡C−C_6H_4−), 4.41−4.37 (t, J = 6.9 Hz, 4H, −NCH_2−), 1.80−1.77 (m, 4H, −CH_2−), 1.33 (s, 9H, −^{t}Bu), 1.31 (s, 9H, −^{t}Bu), 1.30−1.20 (m, 12H, −CH_2−), 0.83−0.79 (d, J = 7.0 Hz, 6H, −CH_3). $^{13}C\{^1H\}$ NMR (150 MHz, THF-d_8, 298 K, δ/ppm): δ 169.35, 166.60, 160.75, 159.34, 155.08, 153.73, 151.59, 149.80, 147.83, 147.40, 141.85, 140.93, 138.29, 137.85, 134.02, 133.92, 133.02, 128.48, 127.96, 126.17, 125.70, 124.98, 124.63, 124.10, 123.80, 123.50, 121.07, 119.76, 119.12, 118.99, 118.75, 111.30, 110.20, 109.35, 100.77, 91.53, 43.49, 35.79, 35.66, 32.42, 31.52, 31.41, 29.79, 27.64, 23.30, 14.19. HRMS (positive ESI) calcd for $C_{71}H_{71}AuN_4S$: m/z = 1208.5060 $[M]^+$; found 1208.5047 $[M]^+$. IR (thin film): 2163 cm^{-1} ν(C≡C). Elemental analysis calculated for $C_{71}H_{71}AuN_4S$ (%): C, 70.51; H, 5.92; N, 4.63; found: C, 70.25; H, 5.93; N, 4.69.

[Au{3,5-F_2C^N^{THPY}^CF_2-3,5}{C≡C−C_6H_4−N(C_6H_5)$_2$-p}] (**4**). This complex was synthesized by a procedure similar to that of **1**, except that [Au{3,5-F_2C^N^{THPY}^CF_2-3,5}Cl] (64 mg, 0.11 mmol) was used instead of [Au{4-^{t}BuC^N^{THPY}^C^{t}Bu-4}Cl]. Subsequent recrystallization by diffusion of diethyl ether vapor into a concentrated THF solution of the product gave **4** as a yellow solid. Yield: 50 mg (56 %). ^1H NMR (500 MHz, $CDCl_3$, 298 K, relative to Me_4Si, δ/ppm): δ 7.97−7.95 (d, J = 5.4 Hz, 1H, thienopyridyl proton of 3,5-F_2C^N^{THPY}^CF_2-3,5), 7.87 (s, 1H, thienopyridyl proton of 3,5-F_2C^N^{THPY}^CF_2-3,5), 7.50−7.46 (m, 2H, thienopyridyl proton of 3,5-F_2C^N^{THPY}^CF_2-3,5 and phenyl proton of 3,5-F_2C^N^{THPY}^CF_2-3,5), 7.38−7.37 (d, J = 8.3 Hz, 2H, phenyl protons of −C≡C−C_6H_4−), 7.29−7.27 (m, 4H, phenyl protons of −N(C_6H_5)$_2$), 7.14−7.12 (m, 4H, phenyl protons of −N(C_6H_5)$_2$), 7.09−7.08 (d, J = 8.5, 1H, phenyl proton of 3,5-F_2C^N^{THPY}^CF_2-3,5), 7.05−7.02

(m, 4H, phenyl protons of −C≡C−C_6H_4− and phenyl protons of −N(C_6H_5)$_2$), 6.83−6.80 (m, 1H, phenyl proton of 3,5-F_2C^N^{THPY}^CF_2-3,5), 6.70−6.66 (m, 1H, phenyl proton of 3,5-F_2C^N^{THPY}^CF_2-3,5). No $^{13}C\{^1H\}$ NMR signals were recorded due to the low solubility of the complex. $^{19}F\{^1H\}$ NMR (470 MHz, $CDCl_3$, 298 K, relative to CF_3COOH, δ/ppm): −85.41, −86.71, −110.90, −111.47. HRMS (positive ESI) calcd for $C_{39}H_{22}AuF_4N_2S$: *m/z* = 823.1100 $[M+H]^+$; found 823.1096 $[M+H]^+$. IR (thin film): 2135 cm^{-1} ν(C≡C). Elemental analysis calculated for $C_{39}H_{21}AuF_4N_2S\cdot\frac{1}{2}H_2O$ (%): C, 56.33; H, 2.67; N, 3.37; found: C, 56.40; H, 2.78; N, 3.29.

[Au{3,5-F_2C^N^{THPY}^CF_2-3,5}{C≡C−C_6H_4−N[$C_{13}H_7$(C_6H_{13})$_2$]$_2$}] (**5**). This complex was synthesized by a procedure similar to that of **2**, except that [Au{3,5-F_2C^N^{THPY}^CF_2-3,5}Cl] (64 mg, 0.11 mmol) was used instead of [Au{4-^{t}BuC^N^{THPY}^C^{t}Bu-4}Cl]. Subsequent recrystallization by diffusion of diethyl ether vapor into a concentrated THF solution of the product gave **5** as a red solid. Yield: 90 mg (62 %). ^1H NMR (500 MHz, acetone-d_6, 298 K, δ/ppm): δ 8.32−8.30 (m, 2H, thienopyridyl proton and thienopyridyl proton of 3,5-F_2C^N^{THPY}^CF_2-3,5), 7.76−7.73 (m, 4H, fluorenyl protons), 7.58−7.57 (d, *J* = 5.4 Hz, 1H, thienopyridyl proton of 3,5-F_2C^N^{THPY}^CF_2-3,5), 7.47−7.43 (m, 3H, phenyl proton of 3,5-F_2C^N^{THPY}^CF_2-3,5 and fluorenyl protons), 7.35−7.28 (m, 9H, phenyl proton of 3,5-F_2C^N^{THPY}^CF_2-3,5, phenyl protons of −C≡C−C_6H_4− and fluorenyl protons), 7.13−7.10 (dd, *J* = 8.1 and 2.0 Hz, 2H, fluorenyl protons), 7.09−7.07 (d, *J* = 8.6 Hz, 2H, phenyl protons of −C≡C−C_6H_4−), 6.85−6.81 (m, 1H, phenyl proton of 3,5-F_2C^N^{THPY}^CF_2-3,5), 6.70−6.67 (m, 1H, phenyl proton of 3,5-F_2C^N^{THPY}^CF_2-3,5), 2.00−1.94 (m, 8H, −CH_2−), 1.20−1.16 (m, 8H, −CH_2−), 1.11−1.10 (m, 16H, −CH_2−), 0.84−0.81 (t, *J* = 7.1 Hz, 12H, −CH_3), 0.77−0.62 (m, 8H, −CH_2−). $^{13}C\{^1H\}$ NMR (150 MHz, $CDCl_3$, 298 K, relative to Me_4Si, δ/ppm): δ 152.22, 150.69, 150.41, 146.99, 141.09, 136.97, 136.53, 133.14, 130.17, 126.92, 126.46,

124.48, 123.52, 122.88, 122.68, 120.47, 120.39, 119.24, 119.14, 113.57, 55.23, 40.50, 31.77, 29.87, 24.00, 22.75, 14.25. $^{19}F\{^{1}H\}$ NMR (376 MHz, acetone-d_6, 298 K, relative to CF_3COOH, δ/ppm): −86.08, −87.10, −112.36, −113.04. HRMS (positive ESI) calcd for $C_{77}H_{78}AuF_4N_2S$: m/z = 1335.5482 $[M+H]^+$; found 1335.5471 $[M+H]^+$. IR (thin film): 2159 cm^{-1} ν(C≡C). Elemental analysis calculated for $C_{77}H_{77}AuF_4N_2S{\cdot}H_2O$ (%): C, 68.33; H, 5.88; N, 2.07; found: C, 68.39; H, 5.76; N, 2.30.

[Au{3,5-F_2C^N^{THPY}^CF_2-3,5}{C≡C−C_6H_4−N[$C_{12}H_7N(C_6H_{13})]_2$}] (**6**). This complex was synthesized by a procedure similar to that of **3**, except that [Au{3,5-F_2C^N^{THPY}^CF_2-3,5}Cl] (64 mg, 0.11 mmol) was used instead of [Au{4-^{t}BuC^$N^{THPY}^{C}^t$Bu-4}Cl]. Subsequent recrystallization by diffusion of diethyl ether vapor into a concentrated THF solution of the product gave **6** as a brown solid. Yield: 70 mg (55 %). ^{1}H NMR (500 MHz, THF-d_8, 298 K, relative to Me_4Si, δ/ppm): δ 8.44 (s, 1H, thienopyridyl proton of 3,5-F_2C^N^{THPY}^CF_2-3,5), 8.37−8.36 (d, J = 5.4 Hz, 1H, thienopyridyl proton of 3,5-F_2C^N^{THPY}^CF_2-3,5), 7.98−7.96 (m, 4H, carbazolyl protons), 7.69−7.67 (d, J = 5.4 Hz, 1H, thienopyridyl proton of 3,5-F_2C^N^{THPY}^CF_2-3,5), 7.66−7.64 (dd, J = 9.5 and 2.2 Hz, 1H, phenyl proton of 3,5-F_2C^N^{THPY}^CF_2-3,5), 7.51−7.49 (dd, J = 9.5 and 2.2 Hz, 1H, phenyl proton of 3,5-F_2C^N^{THPY}^CF_2-3,5), 7.47−7.44 (m, 4H, carbazolyl protons), 7.38−7.33 (m, 4H, carbazolyl protons), 7.26−7.25 (d, J = 8.7 Hz, 2H, phenyl protons of −C≡C−C_6H_4−), 7.08−7.05 (t, J = 7.2 Hz, 2H, carbazolyl protons), 7.03−7.00 (m, 1H, phenyl proton of 3,5-F_2C^N^{THPY}^CF_2-3,5), 6.92−6.90 (d, J = 8.7 Hz, 2H, phenyl protons of −C≡C−C_6H_4−), 6.87−6.83 (m, 1H, phenyl proton of 3,5-F_2C^N^{THPY}^CF_2-3,5), 4.38−4.36 (t, J = 6.9 Hz, 4H, −NCH_2−), 1.90−1.87 (m, 4H, −CH_2−), 1.47−1.44 (m, 4H, −CH_2−), 1.35−1.33 (m, 8H, −CH_2−), 0.90−0.87 (d, J = 7.1 Hz, 6H, −CH_3). No $^{13}C\{^{1}H\}$ NMR signals were recorded due to the low solubility of the complex. $^{19}F\{^{1}H\}$ NMR (376 MHz, THF-d_8, 298 K, relative to

CF_3COOH, δ/ppm): −85.00, −86.69, −112.66, −113.27. HRMS (positive ESI) calcd for $C_{63}H_{51}AuF_4N_4S$: *m/z* = 1168.3431 $[M]^+$; found 1168.3540 $[M]^+$. IR (thin film): 2164 cm^{-1} ν(C≡C). Elemental analysis calculated for $C_{63}H_{51}AuF_4N_4S$ (%): C, 64.72; H, 4.40; N, 4.79; found: C, 64.42; H, 4.63; N, 4.71.

Computational Details. All calculations were carried out with the Gaussian 09 suite of programs.[8] By density functional theory (DFT), the ground-state (S_0) geometries of complexes **1**, **3**, **5** and **6** were fully optimized in toluene with the hybrid Perdew, Burke, and Ernzerhof (PBE0) functional,[9–11] in conjunction with the conductor-like polarizable continuum model (CPCM).[12,13] Time-dependent density functional theory[14–16] (TDDFT) calculations at the same level associated with CPCM were then carried out on the optimized S_0 geometries to compute the singlet-singlet transitions in the electronic absorption spectra of **1**, **3**, **5** and **6**. In order to investigate the nature of the emissive states, the geometries of the lowest-lying triplet excited states (T_1) were optimized with the unrestricted UPBE0/CPCM method for **1**, **3**, **5** and **6**. On the basis of the optimized S_0 and T_1 geometries, vibrational frequencies were calculated and all stationary points were verified to be minima on the potential energy surface, as there are no imaginary frequencies observed (NIMAG = 0). In order to gain further insights into the excited states involved in the thermally activated delayed fluorescence (TADF) and to compute the ΔE_{ST} value, the geometries of the S_0, the lowest singlet excited state (S_1) and the T_1 states of **3**, **5** and **6** were optimized using TDDFT with the M06 functional.[17,18] The Cartesian coordinates of the optimized S_0, S_1 and T_1 geometries of **1**, **3**, **5** and **6** are given in **Tables S12**−**S20**. For all the calculations, the Stuttgart effective core potentials (ECPs) and the associated basis set were used to describe Au[19] with f-type polarization functions (ζ = 1.050),[20] while the 6-31G(d,p) basis set[21–23] was applied for all other atoms. All the DFT and TDDFT calculations were carried out with a pruned (99,590) grid for numerical integration.

OLED fabrication and measurements. Solution-processed OLEDs were fabricated on patterned indium tin oxide (ITO)-coated glass substrates. The substrates were cleaned with Decon 90, rinsed with deionized water, then dried in an oven, and finally treated in an ultraviolet ozone chamber. A 40-nm-thick poly(ethylenedioxythiophene):poly(styrene sulfonic acid (PEDOT:PSS) was spin-coated onto the ITO-coated glass substrates as hole-transporting layer. After that, the emissive layer was formed by mixing the corresponding gold(III) complex with mCP to prepare a 10 mg cm^{-3} solutions in chloroform and spin-coating onto PEDOT:PSS layer to give 30-nm-thick uniform thin film. Onto this, a 5-nm-thick tris(2,4,6-trimethyl-3-(pyridin-3-yl)phenyl)borane (3TPYMB) and a 40-nm-thick 1,3,5-tri[(3-pyridyl)phen-3-yl]benzene (TmPyPB) were evaporated as a hole-blocking layer and an electron-transporting layer, respectively; while a LiF/Al was used as the metal cathode. All the films were sequentially deposited at a rate of 0.1−0.2 nm s^{-1} without vacuum break. A shadow mask was used to define the cathode and to make four 0.1 cm^2 devices on each substrate. Current density−voltage−luminance characteristics and EL spectra were measured simultaneously with a programmable Keithley model 2420 power source and a Photoresearch PR-655 spectrometer under ambient conditions.

^{1}H and ^{13}C{^{1}H} NMR spectra of the cyclometalating ligands and the gold(III) complexes.

4-^{t}BuC^N^{THPY}^C^{t}Bu-4

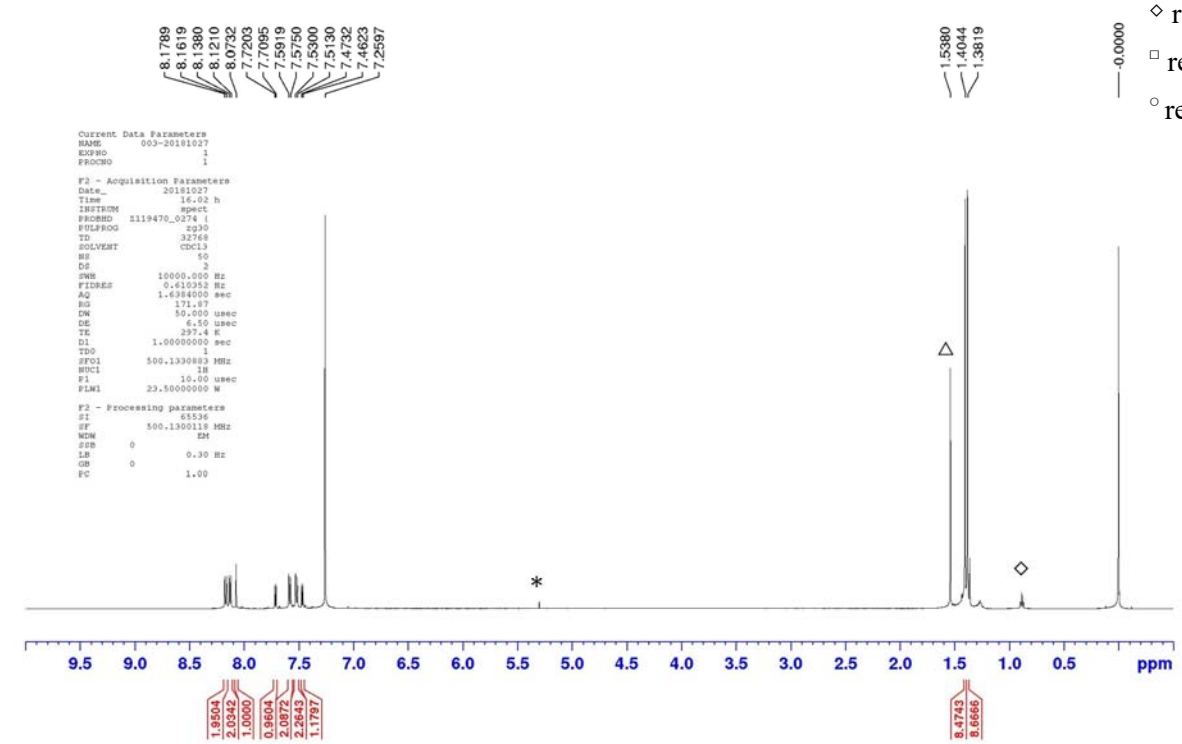
* residual CH_2Cl_2

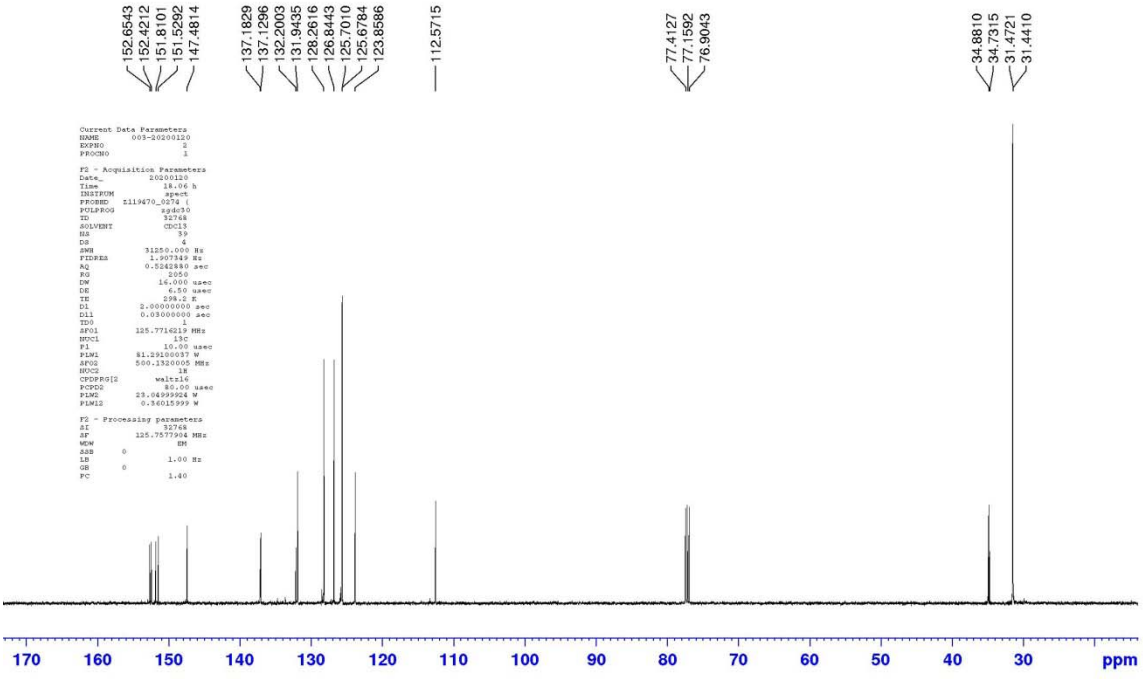
△ residual H_2O

◇ residual C_6H_{14}

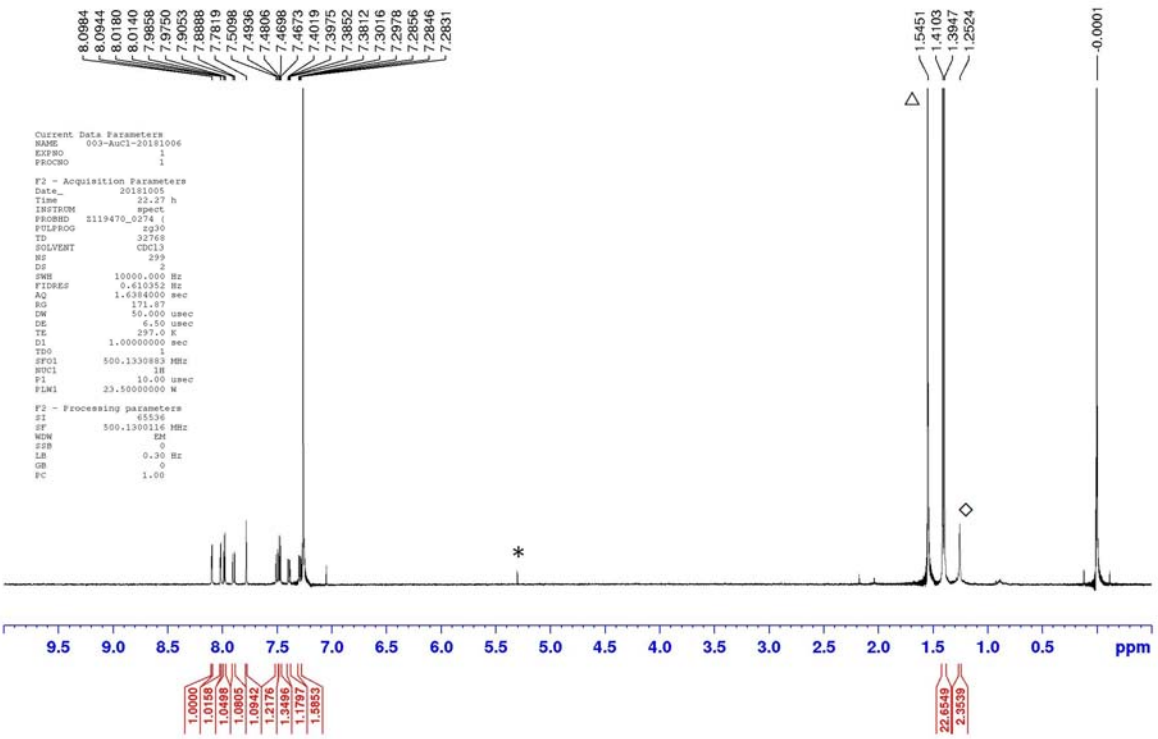
□ residual Et_2O

○ residual $(CH_2)_4O$

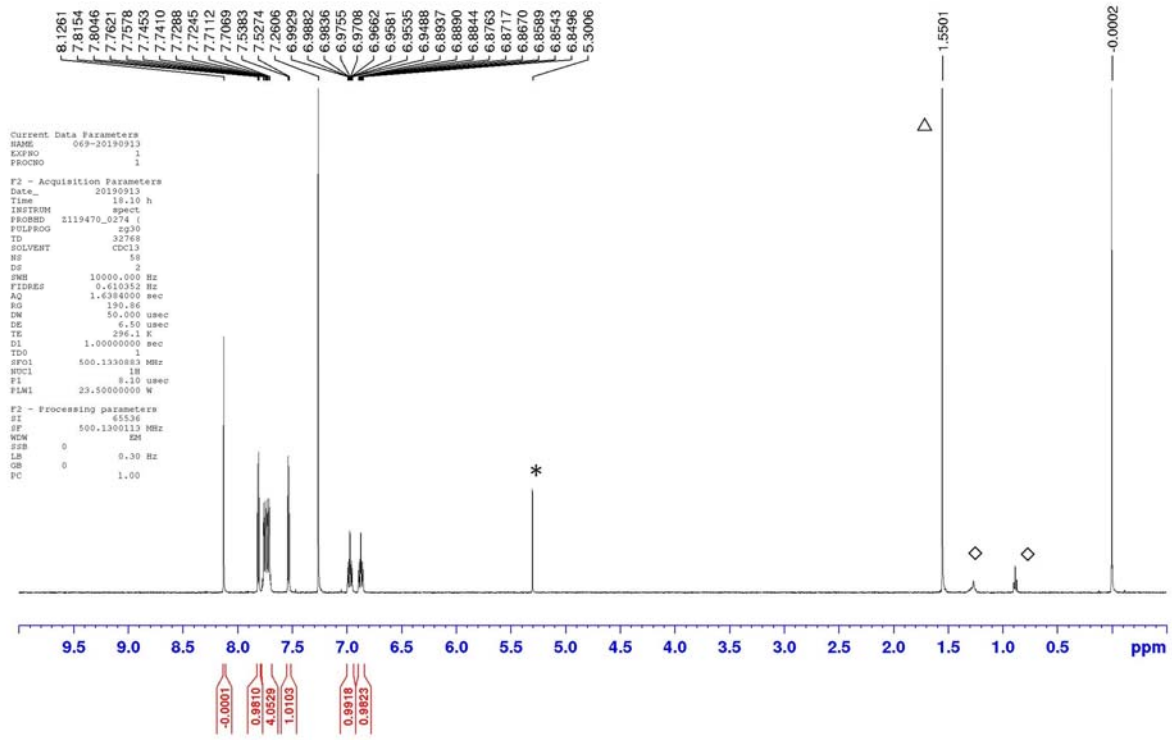


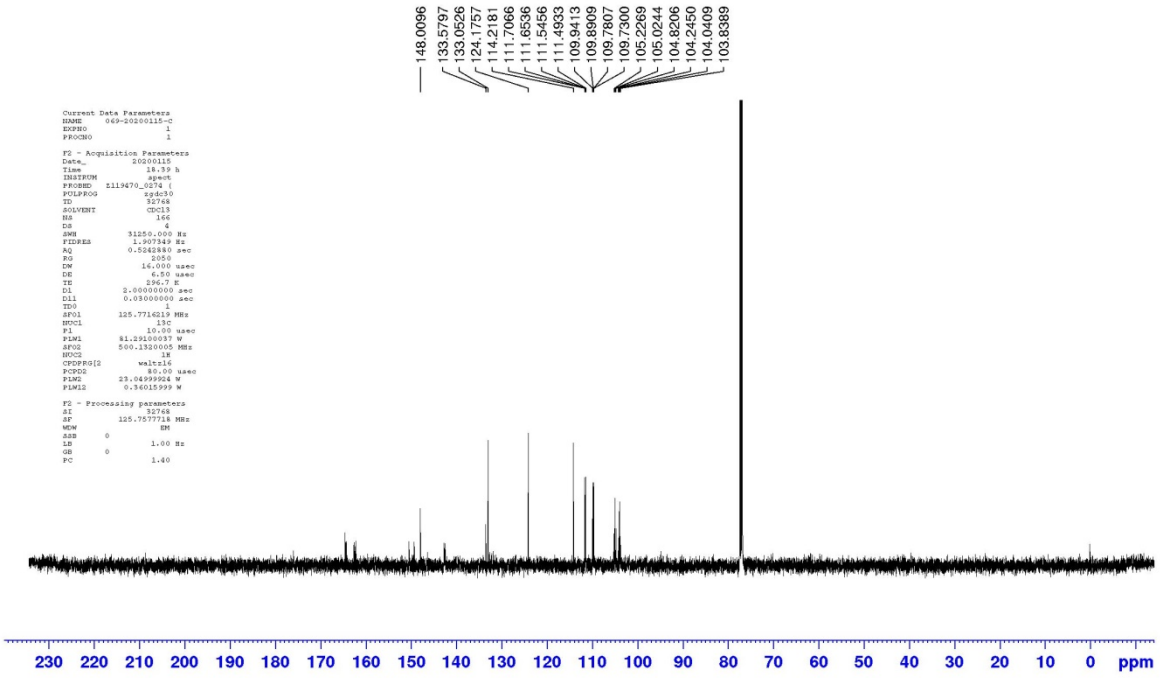


[Au{4-^{t}BuC^N^{THPY}^C^{t}Bu-4}Cl]

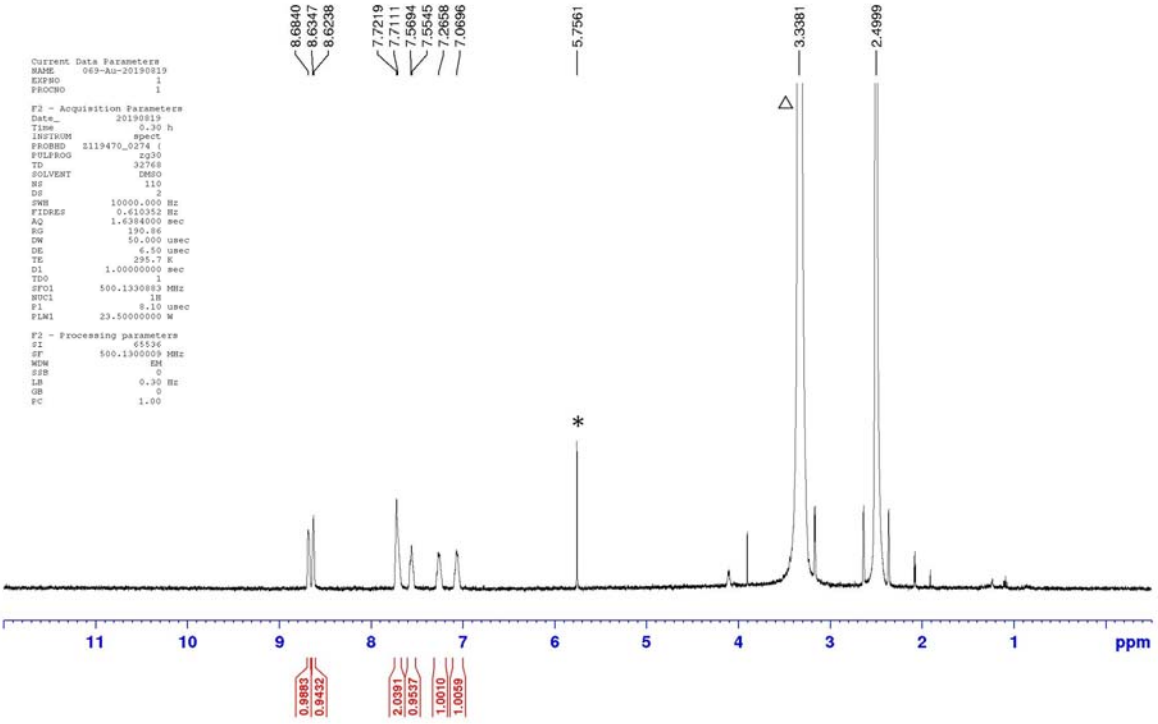


3,5-F_2C^N^{THPY}^CF_2-3,5





[Au{3,5-F_2C^N^{THPY}^CF_2-3,5}Cl]



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LB 0.30 Hz
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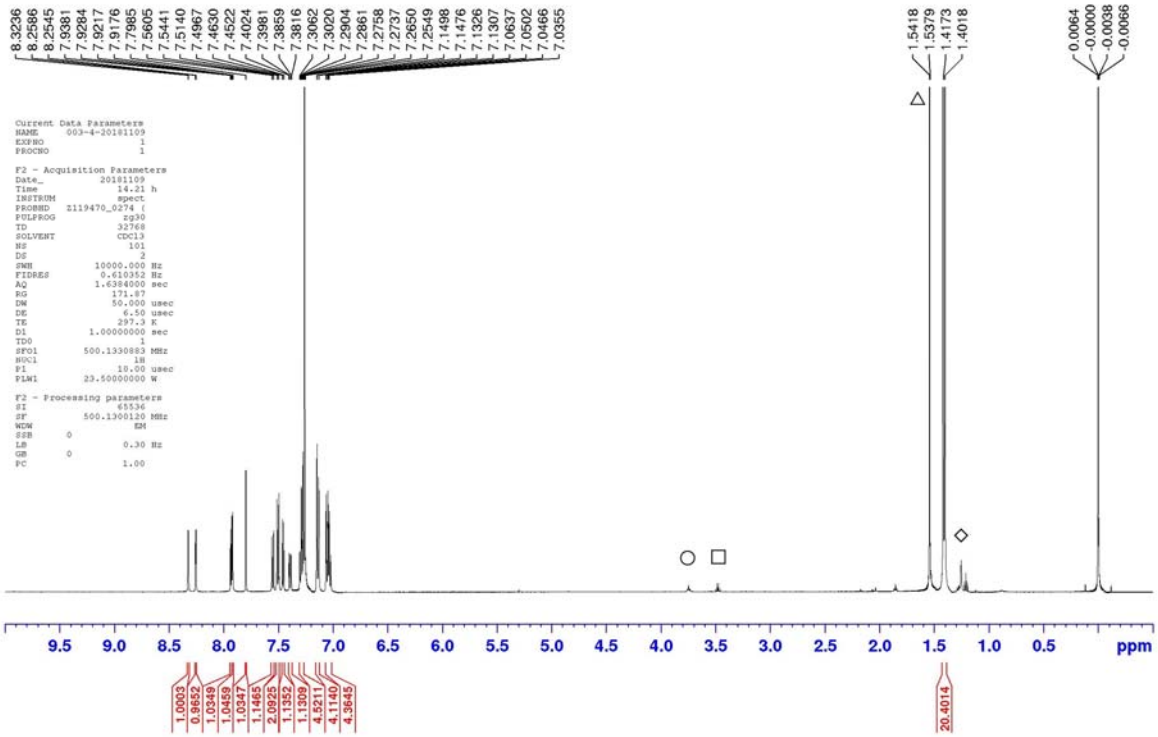
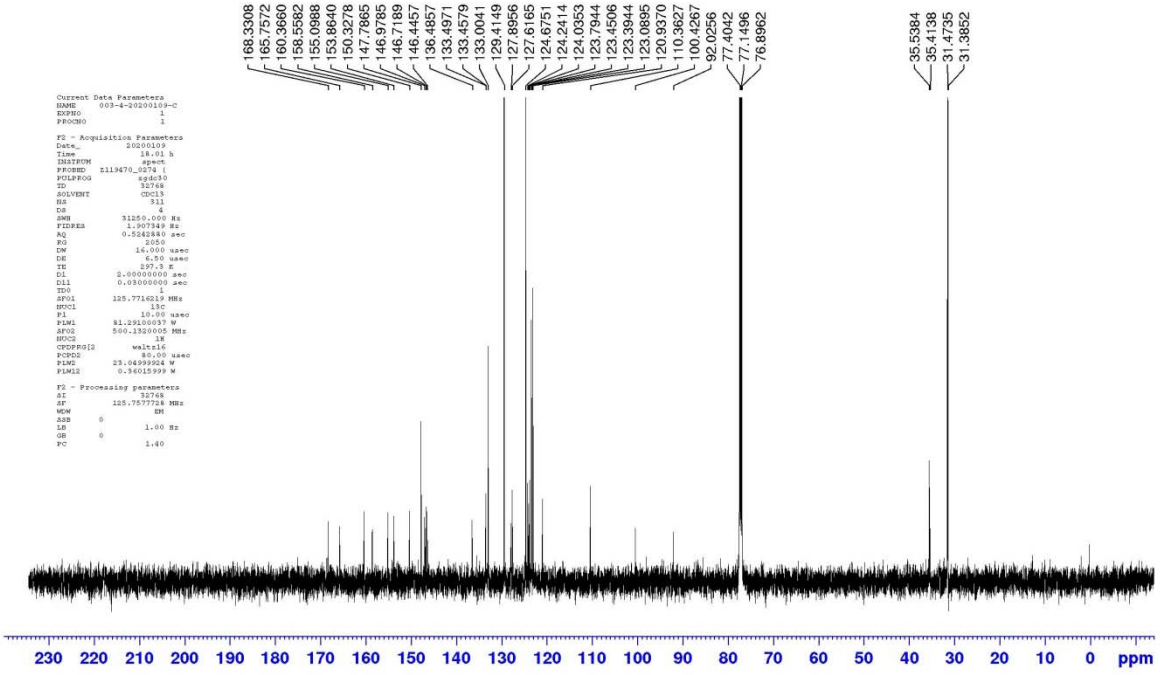
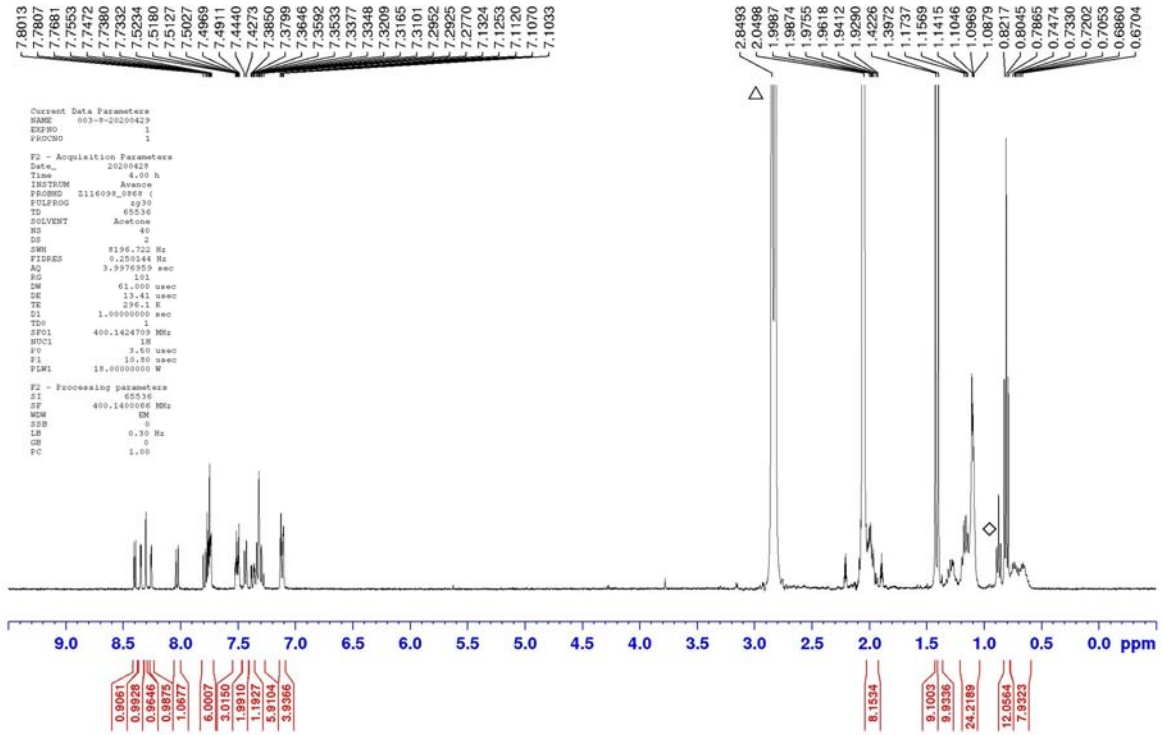
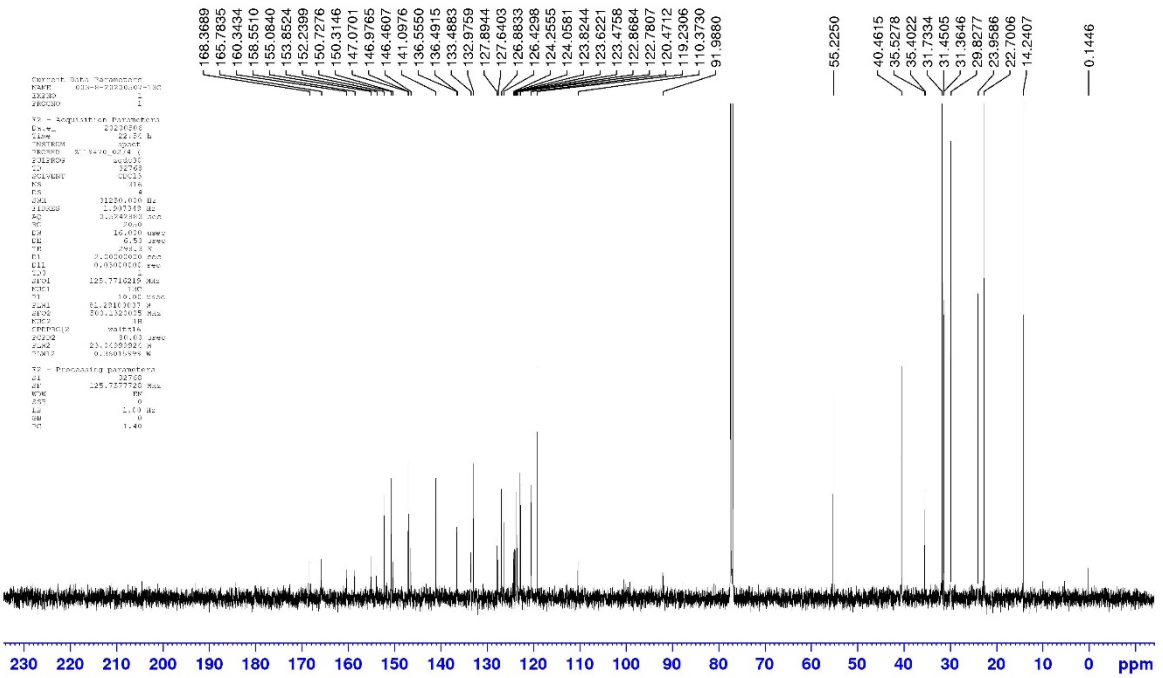
[Au{4-^{t}BuC^N^{THPY}^C^{t}Bu-4}{C≡C−C_6H_4−$N(C_6H_5)_2$-*p*}] (**1**)



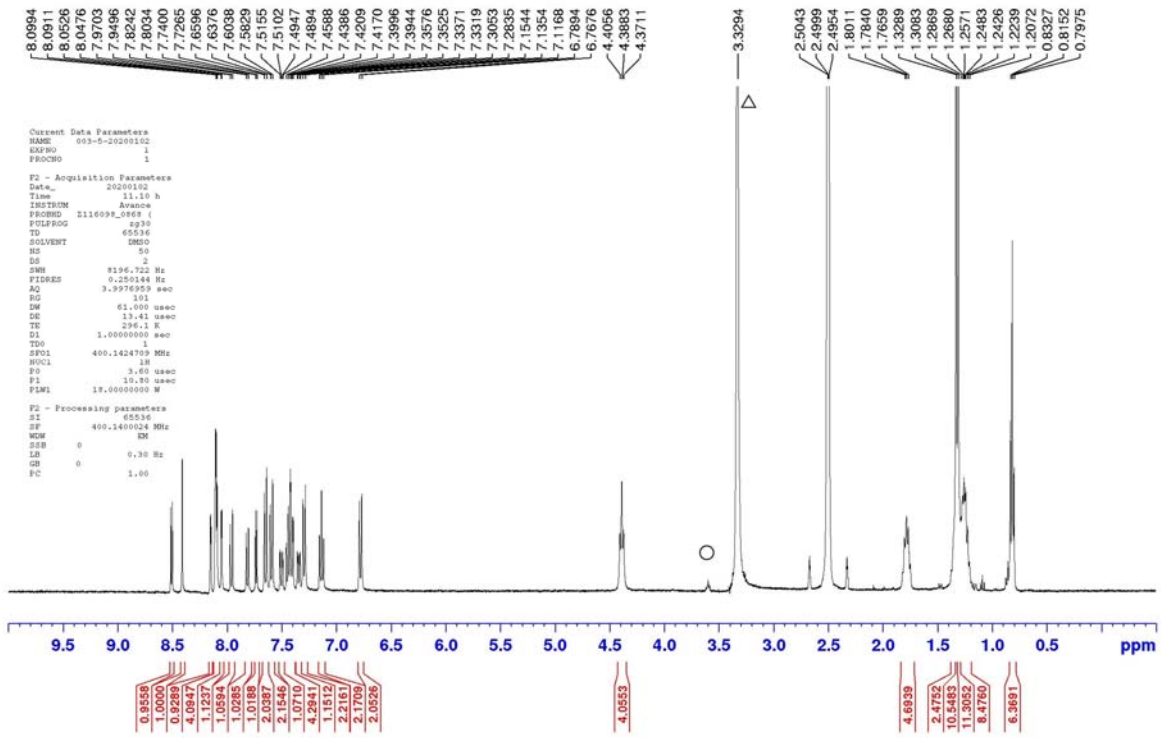


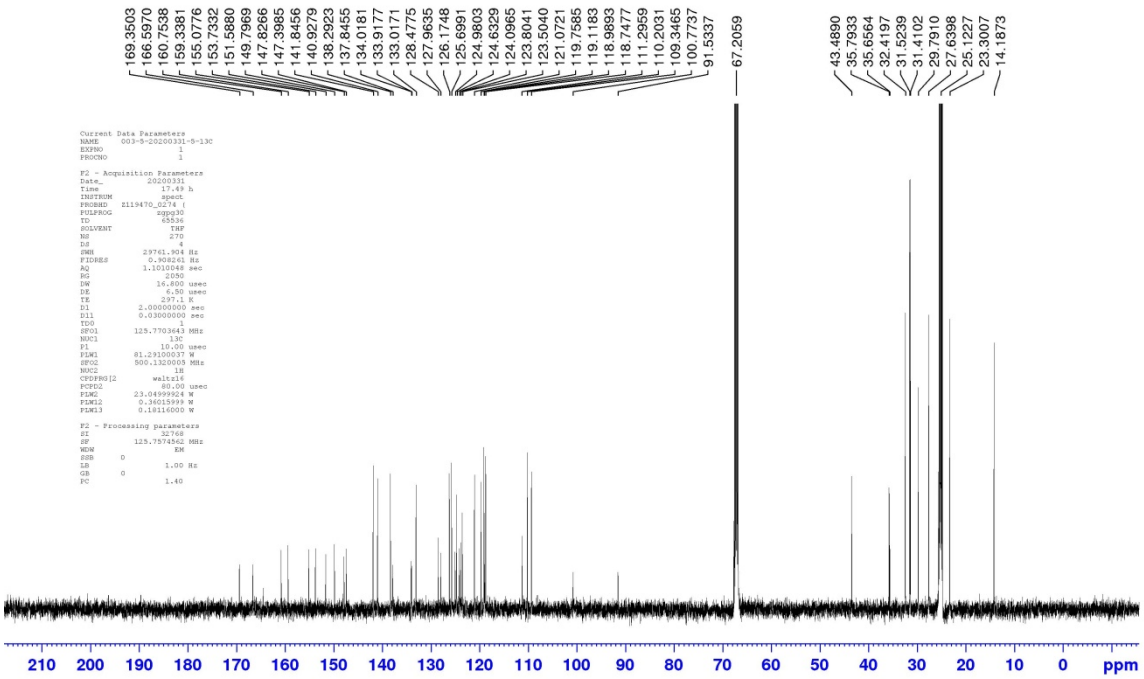
[Au{4-^{t}BuC^N^{THPY}^C^{t}Bu-4}{C≡C−C_6H_4−N[$C_{13}H_7(C_6H_{13})_2]_2$}] (**2**)



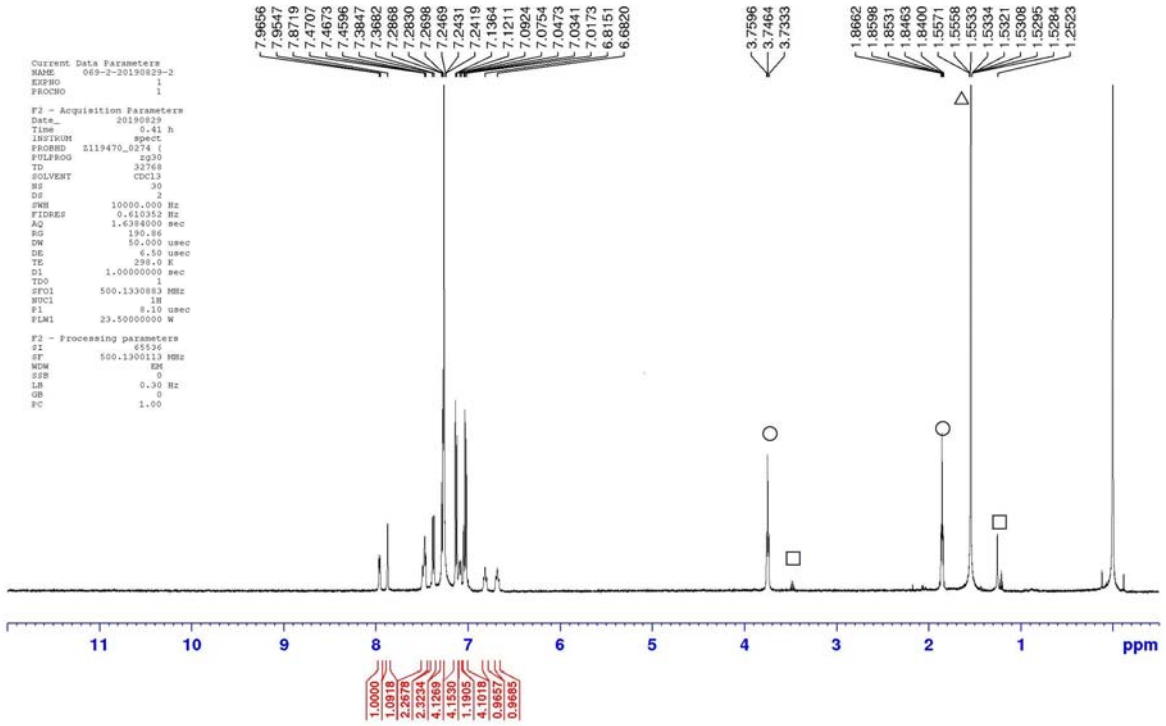


[Au{4-^{t}BuC^N^{THPY}^C^{t}Bu-4}{C≡C−C_6H_4−N[$C_{12}H_7N(C_6H_{13})]_2$}] (**3**)

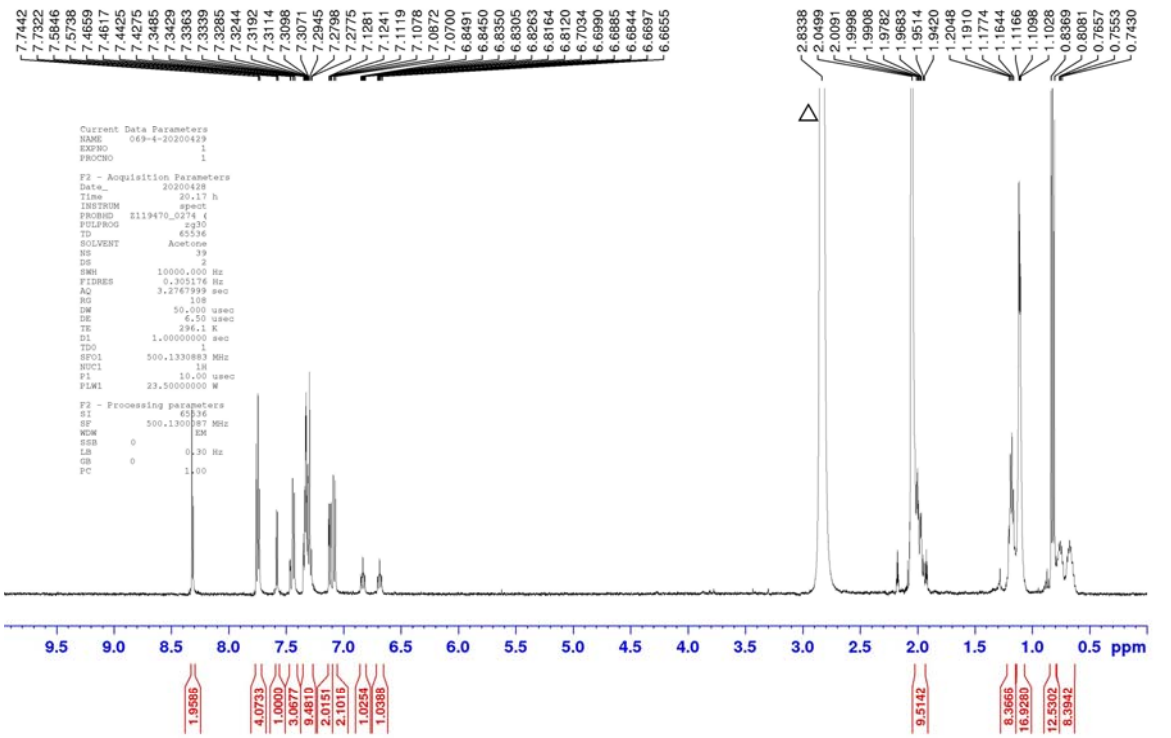


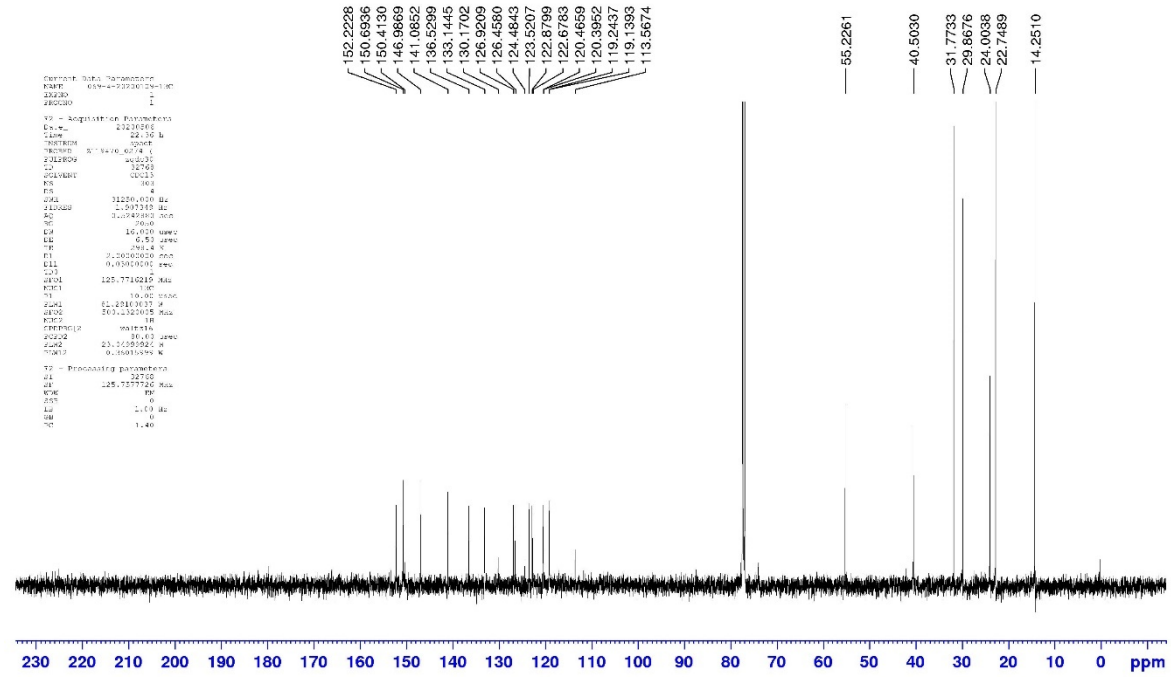


[Au{3,5-F_2C^N^{THPY}^CF_2-3,5}{C≡C−C_6H_4−N(C_6H_5)$_2$-*p*}] (**4**)

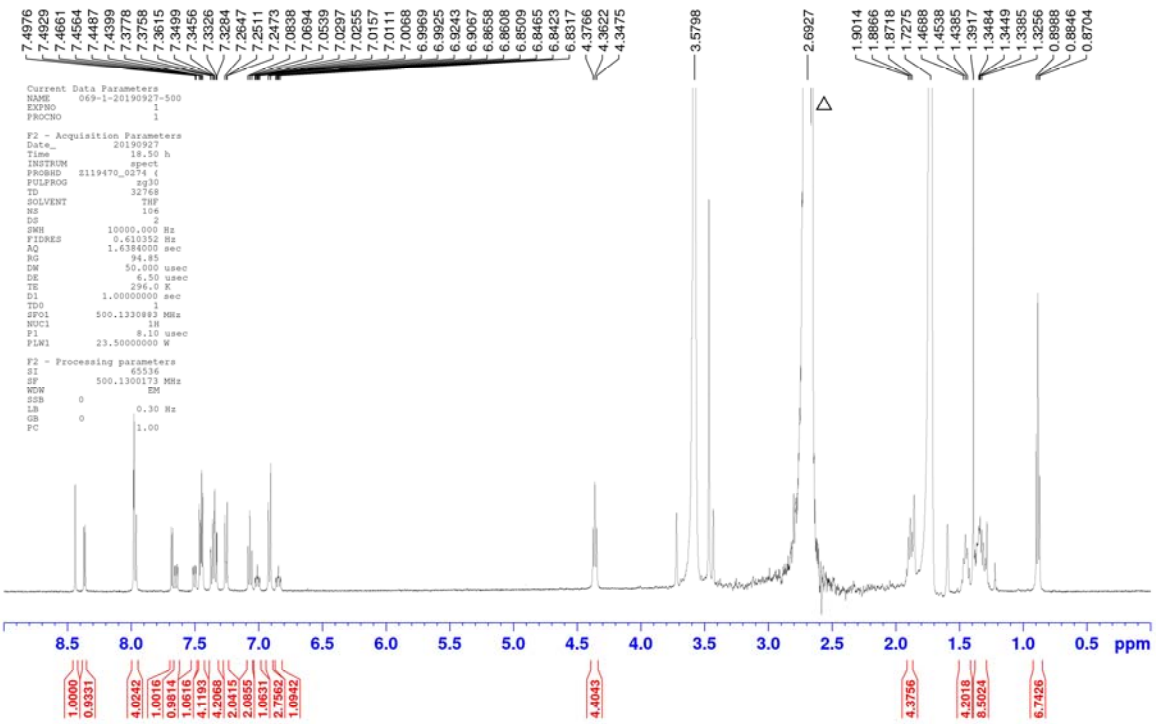


[Au{3,5-F_2C^N^{THPY}^CF_2-3,5}{C≡C−C_6H_4−N[$C_{13}H_7(C_6H_{13})_2]_2$}] (**5**)





[Au{3,5-F_2C^N^{THPY}^CF_2-3,5}{C≡C−C_6H_4−N[$C_{12}H_7N(C_6H_{13})]_2$}] (**6**)



References

1. N. G. Connelly and W. E. Geiger, *Chem. Rev.*, 1996, **96**, 877−910.
2. G. A. Crosby and J. N. Demas, *J. Phys. Chem.*, 1971, **75**, 991−1024.
3. V. K.-M. Au, K. M.-C. Wong, D. P.-K. Tsang, M.-Y. Chan, N. Zhu and V. W.-W. Yam, *J. Am. Chem. Soc.*, 2010, **132**, 14273−14278.
4. M.-C. Tang, C.-H. Lee, M. Ng, Y.-C. Wong, M.-Y. Chan and V. W.-W. Yam, *Angew. Chem. Int. Ed.*, 2018, **57**, 5463−5466.
5. L.-K. Li, M.-C. Tang, W.-L. Cheung, S.-L. Lai, M. Ng, C. K.-M. Chan, M.-Y. Chan and V. W.-W. Yam, *Chem. Mater.*, 2019, **31**, 6706−6714.
6. C.-H. Lee, M.-C. Tang, W.-L. Cheung, S.-L. Lai, M.-Y. Chan and V. W.-W. Yam, *Chem. Sci.*, 2018, **9**, 6228−6232.
7. M.-C. Tang, L. H.-Y. Lo, W.-L. Cheung, S.-L. Lai, M.-Y. Chan and V. W.-W. Yam, *Chem. Commun.*, 2019, **55**, 13844−13847.
8. M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. Montgomery, J. A., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski and D. J. Fox, Gaussian 09 (Revision D.01). Gaussian, Inc.: Wallingford CT, 2013: 2013.

9. J. P. Perdew, K. Burke and M. Ernzerhof, *Phys. Rev. Lett.*, 1996, **77**, 3865.
10. J. P. Perdew, K. Burke and M. Ernzerhof, *Phys. Rev. Lett.*, 1997, **78**, 1396.
11. C. Adamo and V. Barone, *J. Chem. Phys.*, 1999, **110**, 6158.
12. V. Barone and M. Cossi, *J. Phys. Chem. A*, 1998, **102**, 1995.
13. M. Cossi, N. Rega, G. Scalmani and V. Barone, *J. Comput. Chem.*, 2003, **24**, 669.
14. R. Bauernschmitt and R. Ahlrichs, *J. Chem. Phys.*, 1996, **256**, 454.
15. M. E. Casida, C. Jamorski, K. C. Casida and D. R. Salahub, *J. Chem. Phys.*, 1998, **108**, 4439.
16. R. E. Stratmann, G. E. Scuseria and M. J. Frisch, *J. Chem. Phys.*, 1998, **109**, 8218.
17. Y. Zhao and D. G. Truhlar, *Theor. Chem. Acc.*, 2008, **120**, 215.
18. Y. Zhao and D. G. Truhlar, *Acc. Chem. Res.*, 2008, **41**, 157.
19. D. Andrae, U. Häußermann, M. Dolg, H. Stoll and H. Preuß, *Theor. Chim. Acc*, 1990, **77**, 123.
20. A. W. Ehlers, M. Böhme, S. Dapprich, A. Gobbi, A. Höllwarth, V. Jonas, K. F. Köhler, R. Stegmann, A. Veldkamp and G. Frenking, *J. Chem. Phys.*, 1993, **208**, 111.
21. W. J. Hehre, R. Ditchfield and J. A. Pople, *J. Chem. Phys.*, 1972, **56**, 2257.
22. P. C. Hariharan and J. A. Pople, *Theor. Chim. Acc*, 1973, **28**, 213.
23. M. M. Francl, W. J. Pietro, W. J. Hehre, J. S. Binkley, M. S. Gordon, D. J. DeFrees and J. A. Pople, *J. Chem. Phys.*, 1982, **77**, 3654.