Supporting Information

Highly Efficient Carbazolylgold(III) Dendrimers Based on Thermally Activated Delayed Fluorescence and Their Application in Solution-Processed Organic Light-Emitting Devices

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Thermogravimetric Analysis

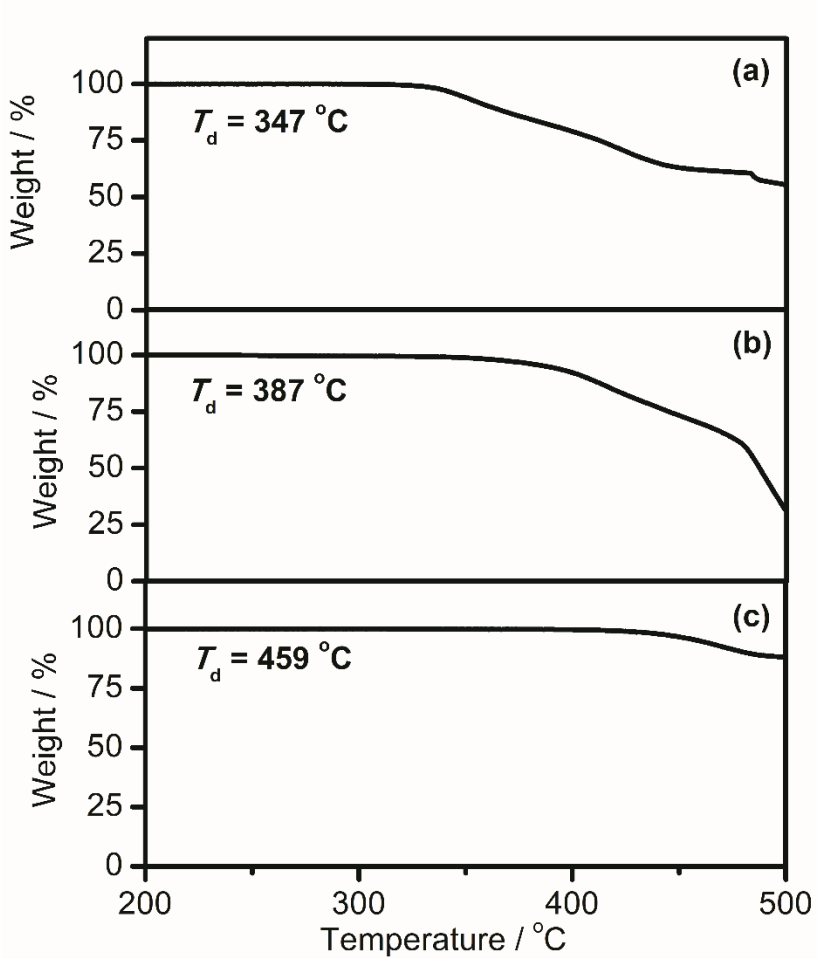

Figure S1. Thermogravimetric analysis (TGA) curves of (a) **1**, (b) **2** and (c) **3**.

Table S1. Thermal properties of **1**–**3**.

Complex	T_d[a] / °C
1	347
2	387
3	459

[a] T_d is defined as the temperature at which the material showed a 5 % weight loss.

Photophysical Properties

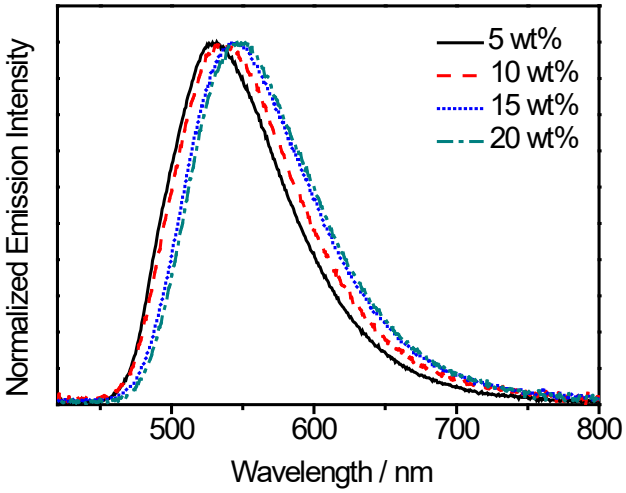

Figure S2. Normalized emission spectra of thin films of **1** doped into mCP at different concentrations (wt%) at 298 K.

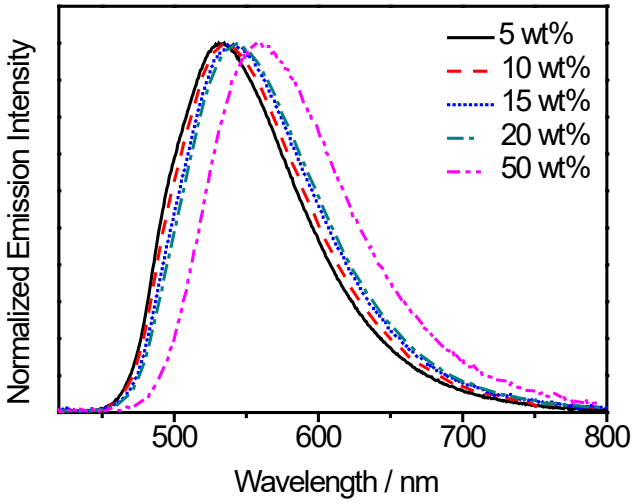

Figure S3. Normalized emission spectra of thin films of **2** doped into mCP at different concentrations (wt%) at 298 K.

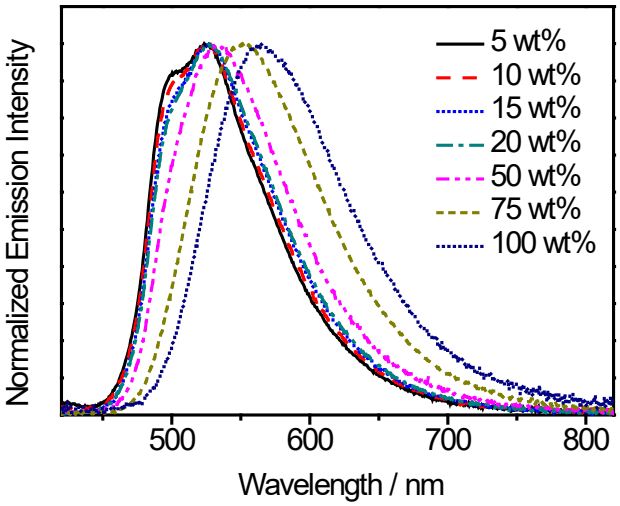

Figure S4. Normalized emission spectra of thin films of **3** doped into mCP at different concentrations (wt%) at 298 K.

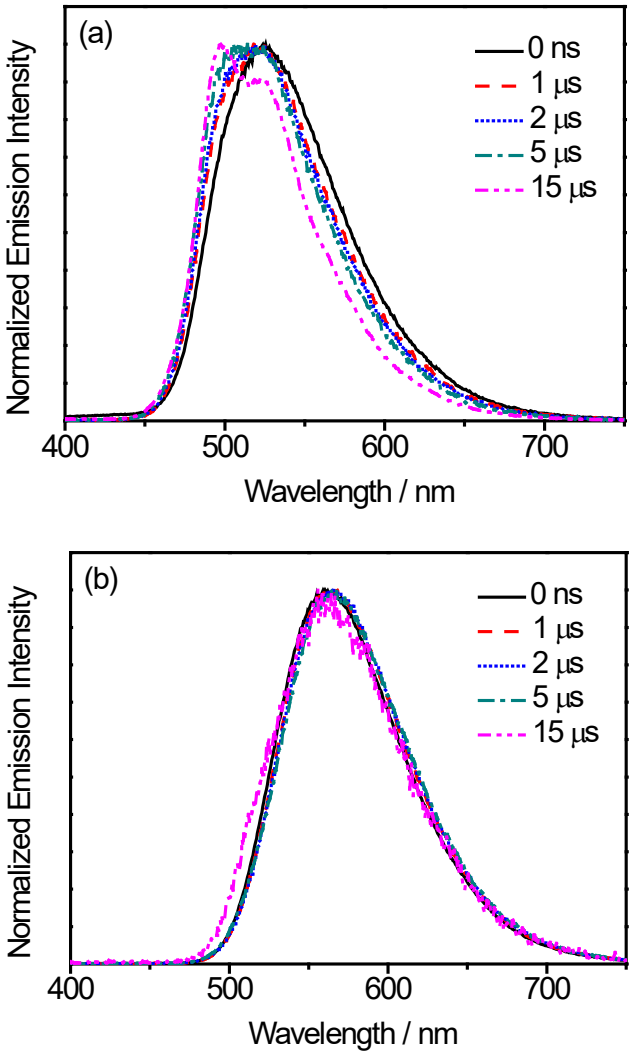

Figure S5. Normalized time-resolved emission spectra of (a) 20 wt% **3** doped into mCP thin film and (b) neat (non-doped) film of **3** at 298 K.

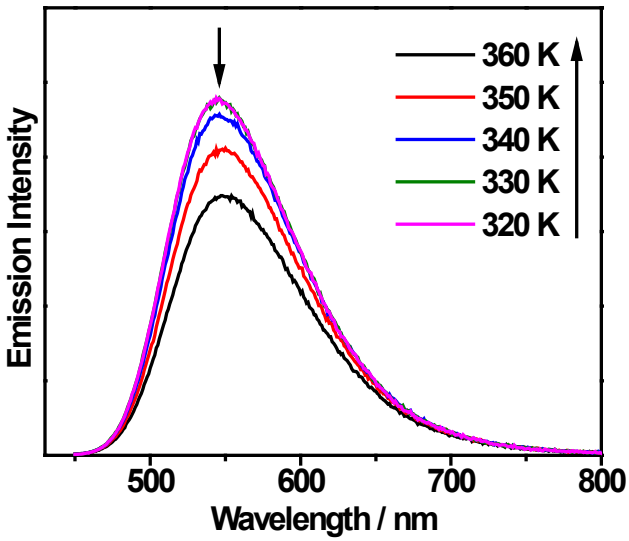

Figure S6. Emission spectra of 20 wt% **1** doped in mCP thin film upon increasing the temperature from 320 to 360 K.

Computational Studies

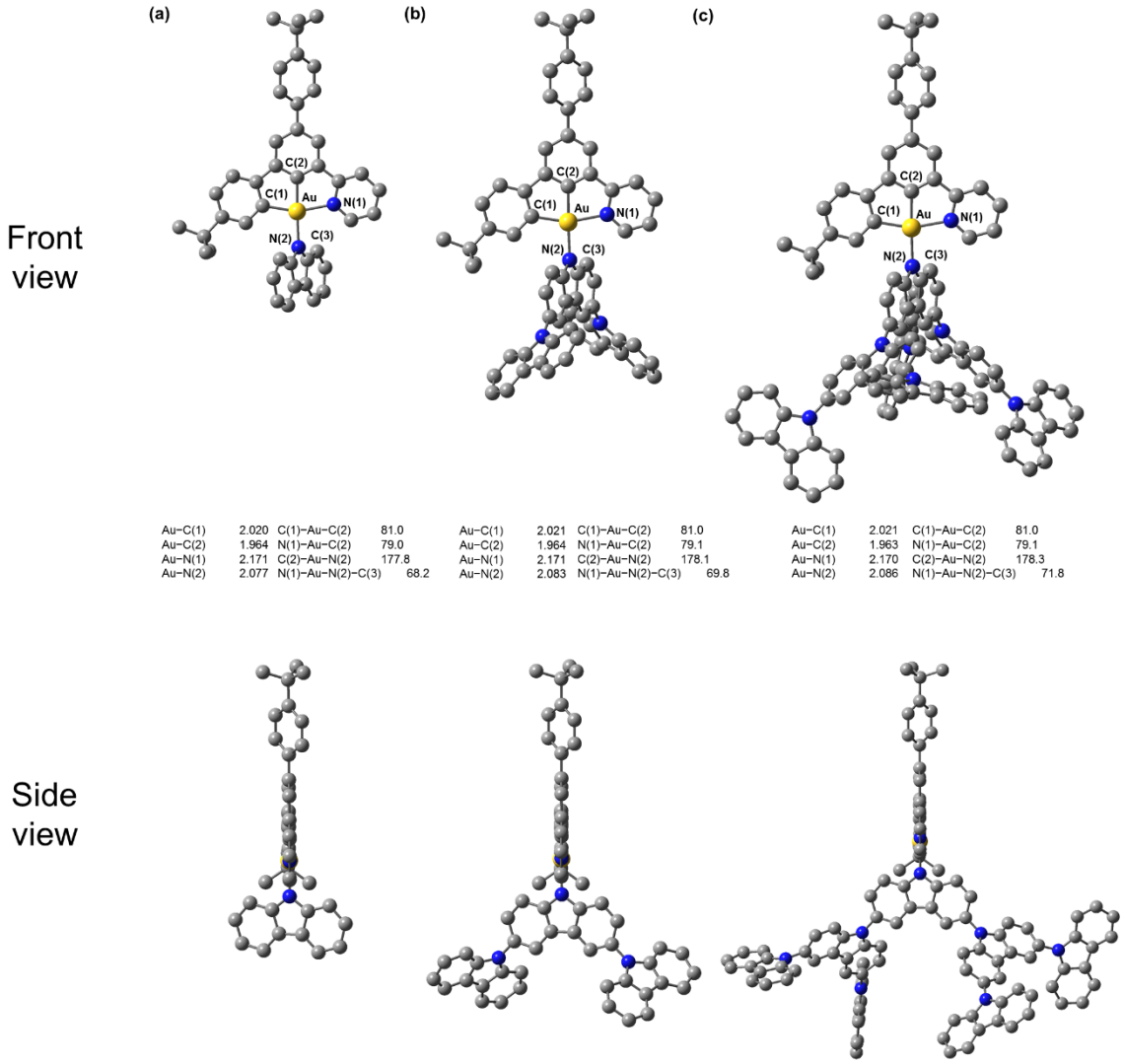

Figure S7. Optimized ground-state geometries (upper: front view; lower: side view) of (a) **1**, (b) **2** and (c) **3** at the PBE0 level of theory. The bond lengths and angles are in Angstroms and degrees, respectively. All hydrogen atoms are omitted for clarity.

Table S2. The first thirtieth singlet excited states (S_n) of **1**−**3** computed by TDDFT/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)	520	0.005	LLCT
	S_2	H−1→L (0.70)	411	0.000	LLCT
	S_3	H→L+1 (0.70)	409	0.003	LLCT
	S_4	H−2→L (0.69)	378	0.077	IL/ILCT
	S_5	H→L+2 (0.69)	358	0.013	LLCT
	S_6	H→L+3 (0.69)	355	0.025	LLCT
	S_7	H−1→L+1 (0.70)	340	0.001	LLCT
	S_8	H−3→L (0.68)	328	0.089	ILCT/IL
	S_9	H−2→L+1 (0.66)	320	0.106	ILCT/IL
	S_{10}	H→L+5 (0.62)	319	0.075	IL
	S_{11}	H−1→L+2 (0.70)	303	0.001	LLCT
	S_{12}	H−4→L (0.69)	301	0.009	LLCT
	S_{13}	H→L+4 (0.62)	297	0.003	LLCT
	S_{14}	H−1→L+3 (0.70)	294	0.003	LLCT
	S_{15}	H−3→L+1 (0.43)	291	0.048	ILCT/IL
		H−2→L+2 (0.31)			ILCT/IL
	S_{16}	H−2→L+3 (0.64)	291	0.007	IL
	S_{17}	H−5→L (0.63)	288	0.136	ILCT
	S_{18}	H−2→L+2 (0.59)	282	0.030	IL/ILCT
	S_{19}	H−7→L (0.47)	279	0.658	ILCT/IL
		H−3→L+1 (−0.38)			IL/ILCT
	S_{20}	H→L+7 (0.64)	278	0.004	LLCT
	S_{21}	H−1→L+5 (0.54)	277	0.102	IL
		H→L+9 (−0.34)			IL
	S_{22}	H−6→L (0.63)	270	0.005	ILCT
	S_{23}	H−5→L+1 (0.47)	266	0.116	ILCT/IL
		H−4→L+1 (0.35)			LLCT
	S_{24}	H→L+8 (0.61)	264	0.005	LMCT
		H→L+6 (−0.32)			LLCT
	S_{25}	H→L+6 (0.59)	262	0.001	LLCT
		H→L+8 (0.32)			LMCT
	S_{26}	H−9→L (0.53)	260	0.003	LLCT/ILCT
		H−8→L (0.36)			LLCT
	S_{27}	H−1→L+4 (0.61)	260	0.001	LLCT
	S_{28}	H−4→L+1 (0.61)	259	0.006	LLCT
	S_{29}	H−3→L+2 (0.65)	257	0.413	IL/ILCT
	S_{30}	H−2→L+4 (0.62)	254	0.503	IL/ILCT
2	S_1	H→L (0.69)	502	0.004	LLCT
	S_2	H−1→L (0.70)	424	0.000	LLCT
	S_3	H→L+1 (0.69)	398	0.001	LLCT
	S_4	H−6→L (0.56)	381	0.069	IL/ILCT
		H−2→L (0.40)			LLCT
	S_5	H−2→L (0.56)	376	0.013	LLCT
		H−6→L (−0.40)			IL/ILCT

	S_6	H−5→L (0.53)	360	0.000	LLCT
		H−4→L (−0.35)			LLCT
		H−3→L (−0.30)			LLCT
	S_7	H−4→L (0.58)	357	0.000	LLCT
		H−3→L (−0.37)			LLCT
	S_8	H−3→L (0.52)	356	0.000	LLCT
		H−5→L (0.42)			LLCT
	S_9	H→L+2 (0.53)	351	0.013	LLCT
		H−1→L+1 (−0.43)			LLCT
	S_{10}	H−1→L+1 (0.55)	349	0.006	LLCT
		H→L+2 (0.41)			LLCT
	S_{11}	H→L+3 (0.66)	347	0.016	LLCT
	S_{12}	H→L+4 (0.68)	341	0.048	IL
	S_{13}	H−7→L (0.68)	331	0.077	IL/ILCT
	S_{14}	H−6→L+1 (0.61)	321	0.099	IL/ILCT
		H−2→L+1 (0.30)			LLCT
	S_{15}	H−2→L+1 (0.62)	317	0.015	LLCT
	S_{16}	H→L+5 (0.54)	315	0.097	ILCT/IL
		H−1→L+5 (−0.31)			ILCT/IL
	S_{17}	H→L+6 (0.55)	314	0.060	ILCT/IL
		H−1→L+6 (0.31)			ILCT/IL
	S_{18}	H−1→L+2 (0.54)	311	0.019	LLCT
		H−1→L+4 (−0.37)			ILCT/IL
	S_{19}	H−1→L+2 (0.43)	309	0.046	LLCT
		H−1→L+4 (0.47)			ILCT/IL
	S_{20}	H−3→L+1 (0.47)	305	0.000	LLCT
		H−5→L+1 (−0.41)			LLCT
		H−4→L+1 (0.33)			LLCT
	S_{21}	H−4→L+1 (0.54)	306	0.000	LLCT
		H−3→L+1 (−0.44)			LLCT
	S_{22}	H−5→L+1 (0.56)	302	0.000	LLCT
		H−4→L+1 (0.31)			LLCT
	S_{23}	H−1→L+3 (0.61)	298	0.005	LLCT
		H−1→L+4 (0.31)			ILCT/IL
	S_{24}	H−6→L+3 (0.65)	295	0.000	IL
	S_{25}	H−7→L+1 (0.43)	292	0.046	ILCT/IL
		H−10→L (0.31)			LLCT
	S_{26}	H→L+7 (0.64)	291	0.007	LLCT
	S_{27}	H−10→L (0.52)	290	0.133	LLCT
	S_{28}	H→L+10 (0.48)	286	0.184	IL/ILCT
		H−2→L+2 (0.34)			LLCT
	S_{29}	H−2→L+2 (0.44)	286	0.154	LLCT
		H→L+10 (−0.37)			IL/ILCT
	S_{30}	H−1→L+5 (0.52)	284	0.006	ILCT/IL
		H→L+5 (0.36)			ILCT/IL
3	S_1	H→L (0.63)	477	0.003	LLCT
		H−4→L (0.30)			LLCT
	S_2	H−1→L (0.70)	432	0.000	LLCT
	S_3	H−4→L (0.61)	410	0.003	LLCT

	H→L (−0.31)			LLCT
S_4	H−3→L (0.69)	401	0.000	LLCT
S_5	H−2→L (0.70)	400	0.000	LLCT
S_6	H→L+1 (0.60)	382	0.015	LLCT
S_7	H−10→L (0.64)	381	0.067	IL/ILCT
S_8	H−9→L (0.65)	366	0.000	LLCT
S_9	H−1→L+1 (0.70)	355	0.000	LLCT
S_{10}	H−8→L (0.65)	350	0.000	LLCT
S_{11}	H−6→L (0.66)	350	0.000	LLCT
S_{12}	H−7→L (0.70)	350	0.000	LLCT
S_{13}	H−5→L (0.71)	349	0.000	LLCT
S_{14}	H→L+3 (0.56)	345	0.036	IL
	H−1→L+3 (−0.40)			IL
S_{15}	H→L+4 (0.52)	343	0.034	IL
	H−1→L+4 (0.44)			IL
S_{16}	H→L+5 (0.55)	341	0.014	IL
S_{17}	H−4→L+1 (0.62)	340	0.001	LLCT
S_{18}	H→L+2 (0.57)	337	0.010	LLCT
S_{19}	H→L+6 (0.49)	335	0.051	IL
	H−4→L+6 (0.33)			IL
	H−15→L (−0.31)			ILCT/IL
S_{20}	H−2→L+1 (0.53)	334	0.000	LLCT
	H−3→L+1 (0.44)			LLCT
S_{21}	H−3→L+1 (0.53)	334	0.000	LLCT
	H−2→L+1 (−0.46)			LLCT
S_{22}	H−15→L (0.56)	333	0.069	ILCT/IL
S_{23}	H−12→L (0.62)	331	0.001	LLCT
S_{24}	H−11→L (0.64)	329	0.005	LLCT
S_{25}	H−10→L+1 (0.65)	321	0.071	ILCT/IL
S_{26}	H−3→L+3 (0.67)	320	0.100	ILCT/IL
S_{27}	H−2→L+4 (0.67)	320	0.078	ILCT/IL
S_{28}	H−14→L (0.63)	320	0.000	LLCT
	H−13→L (−0.31)			LLCT
S_{29}	H−13→L (0.62)	319	0.000	LLCT
S_{30}	H−1→L+5 (0.51)	317	0.091	IL
	H−1→L+2 (0.37)			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.

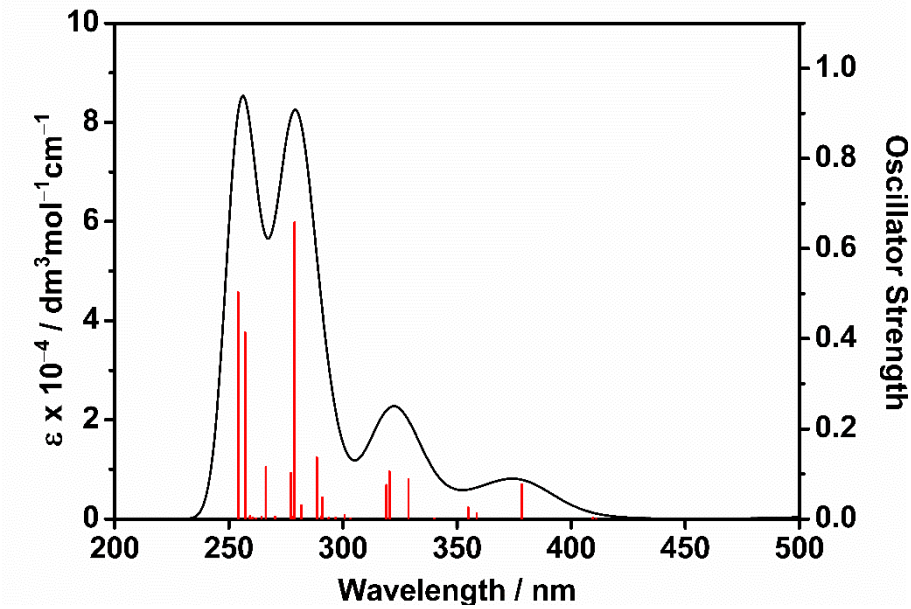

Figure S8. Simulated UV-vis spectrum of **1** computed by TDDFT/CPCM using toluene as the solvent.

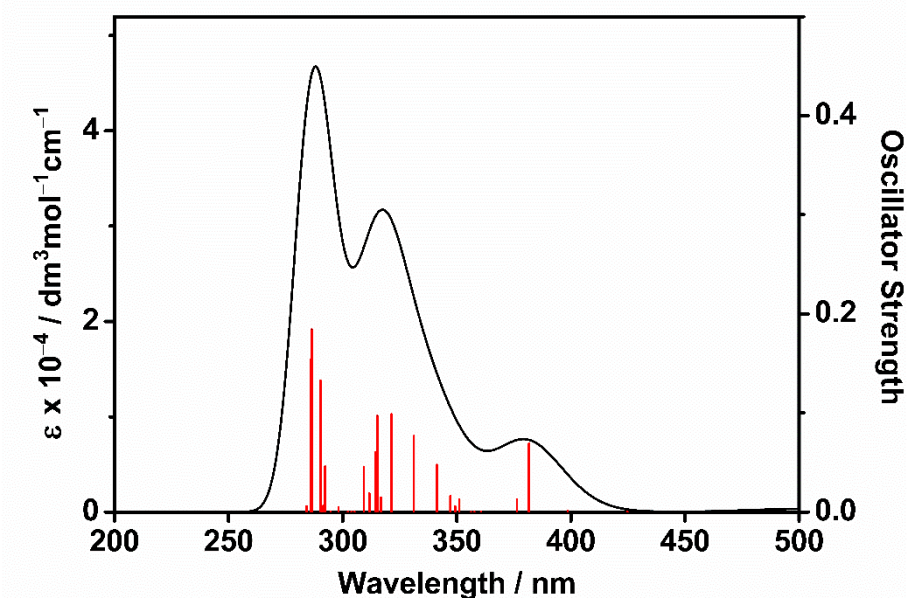

Figure S9. Simulated UV-vis spectrum of **2** computed by TDDFT/CPCM using toluene as the solvent.

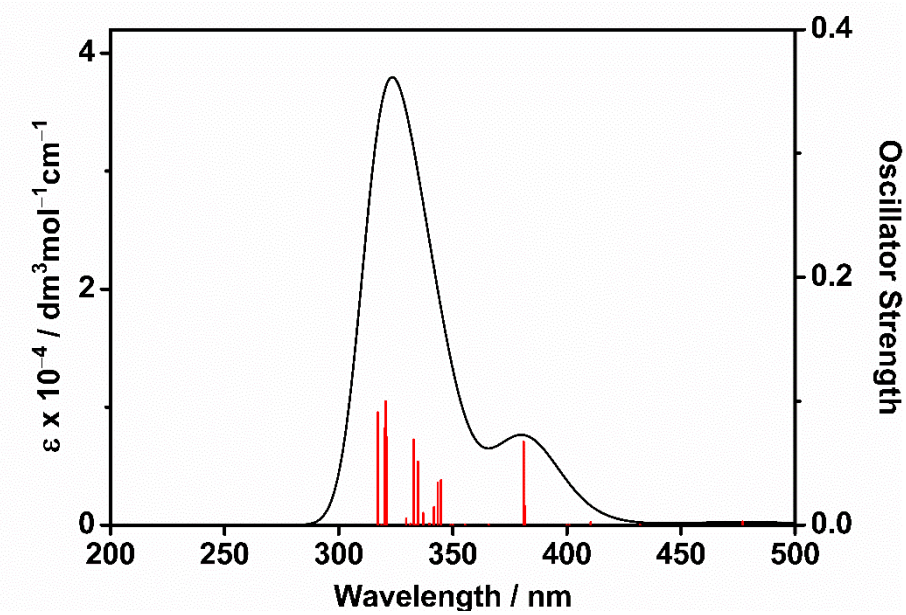

Figure S10. Simulated UV-vis spectrum of **3** computed by TDDFT/CPCM using toluene as the solvent.

Table S3. Relative energies of the optimized T_1 states of **1**−**3**.

Complex	$\Delta E(T_1-S_0)$ / cm^{-1} (λ / nm)[a]
1	18868 (530)
2	18719 (534)
3	19728 (507)

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

Table S4. Cartesian coordinates of the optimized ground-state geometry of **2**.

1	C	3.043353	-1.076440	1.807965	64	C	12.417765	-1.044037	-1.153023
2	C	1.668215	-0.895970	1.498329	65	H	12.048345	-2.015922	-0.812078
3	C	0.687324	-1.371269	2.349390	66	H	12.086366	-0.901655	-2.186845
4	C	1.019872	-2.050965	3.538591	67	H	13.512793	-1.082672	-1.148323
5	C	2.373754	-2.220471	3.832494	68	C	-0.101424	-2.573675	4.438497
6	C	3.373321	-1.741393	2.983283	69	C	-0.989644	-1.399520	4.882716
7	H	-0.355339	-1.221110	2.087012	70	H	-0.410032	-0.662359	5.448106
8	H	2.672251	-2.736314	4.738654	71	H	-1.446474	-0.887892	4.030298
9	H	4.416449	-1.894652	3.249201	72	H	-1.799115	-1.762636	5.525631
10	C	3.975137	-0.520728	0.815729	73	C	-0.949960	-3.586710	3.651012
11	C	5.368995	-0.503281	0.800970	74	H	-1.768453	-3.959901	4.276603
12	C	3.307390	0.083329	-0.250378	75	H	-1.391123	-3.142122	2.753586
13	C	6.066850	0.103978	-0.261001	76	H	-0.343628	-4.443246	3.338097
14	H	5.935437	-0.935769	1.621522	77	C	0.438393	-3.268541	5.691353
15	C	3.960271	0.694876	-1.315734	78	H	-0.398714	-3.622533	6.301449
16	C	5.360878	0.699141	-1.315708	79	H	1.055307	-4.138073	5.441017
17	H	5.918863	1.138145	-2.137826	80	H	1.034408	-2.588558	6.309340
18	C	7.547108	0.113894	-0.263452	81	H	0.440727	2.606331	-4.811772
19	C	8.280174	-0.995820	0.178561	82	H	2.884439	2.892314	-5.313716
20	C	8.265266	1.228813	-0.705258	83	H	4.560383	2.014268	-3.706958
21	C	9.667849	-0.982919	0.174406	84	C	-5.654012	-4.056563	0.065254
22	H	7.756150	-1.889885	0.506028	85	C	-4.880126	-4.576492	-1.984727
23	C	9.657633	1.235480	-0.707362	86	C	-5.843358	-3.510337	1.335249
24	H	7.730445	2.118502	-1.027627	87	C	-6.493489	-5.080073	-0.436272
25	C	10.394485	0.131890	-0.268114	88	C	-4.166886	-4.625328	-3.183180
26	H	10.194812	-1.869407	0.517274	89	C	-5.997218	-5.413785	-1.749958
27	H	10.167456	2.129281	-1.050831	90	C	-6.898624	-3.999216	2.095326
28	C	3.076361	1.264364	-2.345325	91	H	-5.188262	-2.732203	1.713608
29	C	3.500398	1.903867	-3.508564	92	C	-7.548451	-5.552444	0.349117
30	C	0.836899	1.593221	-2.962407	93	C	-4.584167	-5.538255	-4.143874
31	C	2.559235	2.393188	-4.406142	94	H	-3.317872	-3.971874	-3.356537
32	C	1.203269	2.238274	-4.135296	95	C	-6.395144	-6.323089	-2.733556
33	H	-0.201703	1.438162	-2.686859	96	C	-7.746602	-5.007455	1.610799
34	Au	1.343725	0.082223	-0.239799	97	H	-7.068918	-3.590385	3.087316
35	C	-1.588950	-0.946837	-0.449911	98	H	-8.202089	-6.337025	-0.022478
36	C	-1.526981	1.235431	-0.120564	99	C	-5.684499	-6.381867	-3.925186
37	C	-1.271706	-2.298870	-0.640183	100	H	-4.045979	-5.597379	-5.085750
38	C	-2.948525	-0.525823	-0.403014	101	H	-7.250571	-6.972551	-2.568171
39	C	-1.134419	2.563805	0.096338	102	H	-8.563412	-5.363870	2.231259
40	C	-2.908530	0.896564	-0.194746	103	H	-5.982148	-7.084590	-4.697712
41	C	-2.307882	-3.209499	-0.769453	104	C	-5.387936	4.586630	-0.688693
42	H	-0.237145	-2.629254	-0.667593	105	C	-4.622722	5.049566	1.378276
43	C	-3.979649	-1.453566	-0.562714	106	C	-5.588392	4.057002	-1.964017
44	C	-2.116630	3.534071	0.213466	107	C	-6.170116	5.660038	-0.198801
45	H	-0.083537	2.832032	0.167612	108	C	-3.932365	5.047946	2.591072
46	C	-3.884832	1.883797	-0.050710	109	C	-5.679430	5.956969	1.125745
47	C	-3.653831	-2.793686	-0.738085	110	C	-6.595718	4.614350	-2.741876
48	H	-2.091869	-4.266438	-0.893973	111	H	-4.978846	3.238108	-2.332270
49	H	-5.022159	-1.147757	-0.553169	112	C	-7.177619	6.201044	-1.001933
50	C	-3.483577	3.200946	0.144354	113	C	-4.310382	5.981725	3.547921
51	H	-1.840369	4.573813	0.361508	114	H	-3.131175	4.340368	2.778918
52	H	-4.943343	1.640946	-0.082999	115	C	-6.038791	6.885947	2.105853
53	N	-0.738786	0.120880	-0.285767	116	C	-7.386262	5.673625	-2.269432
54	N	1.743196	1.126912	-2.099971	117	H	-6.773788	4.219246	-3.738079
55	C	11.923902	0.102330	-0.254863	118	H	-7.787030	7.024411	-0.639217
56	C	12.533412	1.410274	-0.766328	119	C	-5.350117	6.894656	3.311643
57	H	12.240623	2.265243	-0.147748	120	H	-3.789263	6.002086	4.500926
58	H	13.625505	1.340344	-0.737869	121	H	-6.848046	7.588795	1.926930
59	H	12.242357	1.617848	-1.801494	122	H	-8.167004	6.083135	-2.903404
60	C	12.416068	-0.129562	1.183331	123	H	-5.618308	7.611534	4.081932
61	H	12.046088	-1.074516	1.592546	124	N	-4.682945	-3.760402	-0.880673
62	H	13.511060	-0.161406	1.207427	125	N	-4.455827	4.226500	0.274012
63	H	12.084056	0.676972	1.845227					

Table S5. Cartesian coordinates of the optimized ground-state geometry of **3**.

1	C	-6.103700	-1.068662	-1.918369	64	C	-15.398129	-2.034157	-0.539738
2	C	-4.729900	-0.875740	-1.610768	65	H	-15.087374	-1.593460	-1.491843
3	C	-3.763218	-1.015391	-2.589706	66	H	-14.990883	-3.049276	-0.489694
4	C	-4.108801	-1.357089	-3.912849	67	H	-16.491481	-2.105412	-0.546000
5	C	-5.461228	-1.543822	-4.202594	68	C	-3.001869	-1.511675	-4.957522
6	C	-6.446785	-1.402177	-3.223488	69	C	-2.225020	-0.189854	-5.077026
7	H	-2.721033	-0.863307	-2.326432	70	H	-2.885089	0.624692	-5.392860
8	H	-5.769788	-1.806590	-5.208564	71	H	-1.762675	0.099044	-4.128328
9	H	-7.489153	-1.556850	-3.491350	72	H	-1.426210	-0.288729	-5.820346
10	C	-7.019416	-0.884491	-0.782936	73	C	-2.042386	-2.629959	-4.515875
11	C	-8.407976	-0.991545	-0.719764	74	H	-1.233975	-2.743225	-5.246783
12	C	-6.340191	-0.559931	0.391928	75	H	-1.586993	-2.418434	-3.543439
13	C	-9.089436	-0.771391	0.492975	76	H	-2.568194	-3.587452	-4.439369
14	H	-8.981158	-1.268221	-1.600733	77	C	-3.555544	-1.870117	-6.339139
15	C	-6.976209	-0.336712	1.608706	78	H	-2.728438	-1.967910	-7.049476
16	C	-8.372026	-0.443048	1.651726	79	H	-4.095057	-2.823049	-6.327286
17	H	-8.919301	-0.250038	2.569962	80	H	-4.229797	-1.096119	-6.720850
18	C	-10.564477	-0.884680	0.544191	81	H	-3.423233	0.820744	5.389958
19	C	-11.363931	-0.421835	-0.509749	82	H	-5.851485	0.755327	6.025638
20	C	-11.211160	-1.455957	1.643912	83	H	-7.542578	0.219184	4.289424
21	C	-12.746601	-0.527738	-0.457083	84	C	2.773428	-3.840524	-1.350923
22	H	-10.897769	0.050725	-1.370275	85	C	2.220053	-4.853771	0.577054
23	C	-12.598916	-1.558961	1.690973	86	C	2.817757	-3.014985	-2.474817
24	H	-10.622043	-1.852728	2.466710	87	C	3.708621	-4.886330	-1.163119
25	C	-13.401913	-1.098288	0.643674	88	C	1.622756	-5.219911	1.783704
26	H	-13.327234	-0.146747	-1.292992	89	C	3.351915	-5.538459	0.073234
27	H	-13.051606	-2.018978	2.562888	90	C	3.824879	-3.237978	-3.401223
28	C	-6.082255	-0.001232	2.728262	91	H	2.096529	-2.216529	-2.613977
29	C	-6.489196	0.255479	4.036078	92	C	4.701095	-5.109947	-2.118119
30	C	-3.842672	0.328570	3.344036	93	C	2.162567	-6.295767	2.471786
31	C	-5.539581	0.554387	5.005397	94	H	0.756343	-4.689841	2.165032
32	C	-4.191944	0.592500	4.660883	95	C	3.895639	-6.603487	0.792230
33	H	-2.811333	0.341012	3.005071	96	C	4.758672	-4.277294	-3.231019
34	Au	-4.384306	-0.401623	0.323118	97	H	3.906797	-2.600908	-4.276392
35	C	-1.387381	-1.227010	0.157910	98	H	5.415470	-5.920630	-2.010233
36	C	-1.596741	0.957139	0.391422	99	C	3.291432	-6.982298	1.986758
37	C	-1.615300	-2.602915	0.015707	100	H	1.710905	-6.626192	3.402010
38	C	-0.059719	-0.710938	0.151937	101	H	4.777990	-7.129803	0.440558
39	C	-2.080154	2.265594	0.534039	102	C	2.062786	4.361892	1.602055
40	C	-0.195408	0.711718	0.310171	103	C	1.187151	5.215712	-0.283378
41	C	-0.523584	-3.441107	-0.139610	104	C	2.351225	3.577501	2.719261
42	H	-2.625740	-3.001686	0.009590	105	C	2.753825	5.571012	1.348770
43	C	1.030344	-1.572880	0.019321	106	C	0.447270	5.437835	-1.445329
44	C	-1.166626	3.303870	0.613455	107	C	2.192367	6.118553	0.138136
45	H	-3.147162	2.465422	0.584298	108	C	3.341312	4.020915	3.582660
46	C	0.710119	1.772059	0.370196	109	H	1.810186	2.657597	2.914218
47	C	0.790505	-2.933537	-0.132613	110	C	3.764982	5.987723	2.215332
48	H	-0.670431	-4.508547	-0.275009	111	C	0.727043	6.579125	-2.181203
49	H	2.051425	-1.201818	0.033746	112	H	-0.311129	4.734121	-1.771937
50	C	0.218337	3.062680	0.529316	113	C	2.442568	7.274321	-0.602556
51	H	-1.512067	4.325228	0.743191	114	C	4.050697	5.210658	3.333278
52	H	1.780990	1.607527	0.288286	115	H	3.578219	3.449539	4.474805
53	N	-2.306098	-0.216938	0.309580	116	H	4.327287	6.897917	2.029483
54	N	-4.757349	0.044991	2.413532	117	C	1.708887	7.496929	-1.763321
55	C	-14.928560	-1.193992	0.659457	118	H	0.188978	6.774546	-3.103574
56	C	-15.455028	-1.847372	1.939959	119	H	3.190761	7.995404	-0.287190
57	H	-15.176177	-1.277083	2.832363	120	N	1.881083	-3.830400	-0.291662
58	H	-16.548218	-1.892229	1.904711	121	N	1.119145	4.158635	0.608797
59	H	-15.085846	-2.871855	2.056005	122	C	5.551705	-4.738717	-5.552310
60	C	-15.527306	0.218762	0.557211	123	C	7.136862	-4.417802	-3.981086
61	H	-15.220645	0.725249	-0.362963	124	C	4.347393	-4.906362	-6.236675
62	H	-16.621731	0.166177	0.560382	125	C	6.800963	-4.859441	-6.205949
63	H	-15.213695	0.838844	1.403402	126	C	7.826822	-4.156545	-2.796940

127	C	7.815764	-4.654230	-5.199922
128	C	4.413249	-5.183804	-7.596667
129	H	3.394075	-4.825833	-5.724424
130	C	6.838195	-5.138713	-7.574529
131	C	9.215305	-4.148385	-2.849520
132	H	7.297980	-3.964610	-1.868993
133	C	9.212844	-4.641283	-5.224273
134	C	5.642890	-5.296672	-8.263421
135	H	3.490256	-5.318259	-8.153531
136	H	7.789759	-5.233789	-8.090478
137	C	9.905453	-4.390647	-4.047208
138	H	9.776821	-3.948451	-1.941366
139	H	9.748179	-4.822048	-6.152428
140	H	5.657036	-5.512842	-9.327446
141	H	10.991220	-4.378932	-4.051123
142	C	3.937921	-9.377989	2.270674
143	C	4.274126	-8.015521	4.035553
144	C	3.585646	-9.918356	1.033551
145	C	4.489570	-10.176611	3.300381
146	C	4.365895	-6.917928	4.892152
147	C	4.704700	-9.304411	4.430401
148	C	3.807437	-11.275979	0.837650
149	H	3.152597	-9.300786	0.253362
150	C	4.703115	-11.539222	3.076172
151	C	4.884992	-7.134833	6.162728
152	H	4.046381	-5.930186	4.575972
153	C	5.222670	-9.494472	5.714130
154	C	4.362756	-12.081262	1.843945
155	H	3.543132	-11.721672	-0.117088
156	H	5.127028	-12.164977	3.856845
157	C	5.307440	-8.408059	6.574868
158	H	4.967199	-6.297297	6.849648
159	H	5.557304	-10.478252	6.031822
160	H	4.524722	-13.138239	1.655215
161	H	5.707228	-8.541501	7.575588
162	C	6.190718	4.886418	4.577131
163	C	5.081765	6.814994	4.945716
164	C	6.608832	3.641316	4.106130
165	C	6.953379	5.619644	5.516813
166	C	4.151804	7.855085	4.949952
167	C	6.243533	6.854259	5.752684
168	C	7.802041	3.132384	4.604248
169	H	6.024998	3.091947	3.374696
170	C	8.149565	5.084291	6.001446
171	C	4.411060	8.947099	5.769170
172	H	3.257534	7.811931	4.336738
173	C	6.480141	7.964976	6.566772
174	C	8.566108	3.841080	5.544112
175	H	8.150296	2.164748	4.254331
176	H	8.745983	5.635632	6.723275
177	C	5.562938	9.007465	6.568504
178	H	3.703578	9.771172	5.789912
179	H	7.368497	8.009583	7.190910
180	H	9.493183	3.412510	5.912776
181	H	5.735007	9.877663	7.194769
182	C	1.017455	9.634320	-2.850947
183	C	3.163807	9.000781	-3.127474
184	C	-0.320560	9.729525	-2.466878
185	C	1.633985	10.627452	-3.648489
186	C	4.379169	8.315781	-3.112087
187	C	3.008070	10.221882	-3.825296
188	C	-1.039863	10.833556	-2.908058
189	H	-0.781720	8.969851	-1.844054
190	C	0.887265	11.727302	-4.078626
191	C	5.445870	8.882301	-3.799026
192	H	4.486760	7.373445	-2.584809
193	C	4.097674	10.769913	-4.507178
194	C	-0.447573	11.822905	-3.707887
195	H	-2.083806	10.931610	-2.624024
196	H	1.346830	12.497692	-4.691835
197	C	5.312432	10.097665	-4.487939
198	H	6.403578	8.369674	-3.802180
199	H	3.993425	11.707380	-5.046638
200	H	-1.040024	12.671697	-4.035977
201	H	6.168069	10.512496	-5.012187
202	N	5.060587	5.619275	4.239155
203	N	1.952359	8.655287	-2.542103
204	N	3.812093	-8.072305	2.727379
205	N	5.767365	-4.471206	-4.206959

Table S6. Cartesian coordinates of the optimized T_1 geometry of **2** computed by DFT/CPCM.

1	C	3.036476	-0.842263	1.891728	64	C	12.417620	-1.179309	-0.975703
2	C	1.662193	-0.694483	1.553462	65	H	12.035397	-2.097596	-0.519671
3	C	0.689759	-1.090509	2.460138	66	H	12.091147	-1.162093	-2.020730
4	C	1.021310	-1.644361	3.713325	67	H	13.512388	-1.229101	-0.960890
5	C	2.374470	-1.781487	4.023711	68	C	-0.098853	-2.069659	4.666222
6	C	3.369841	-1.385438	3.126352	69	C	-0.980803	-0.854075	4.996603
7	H	-0.358233	-0.972053	2.197336	70	H	-0.394388	-0.068032	5.483687
8	H	2.676310	-2.201832	4.977104	71	H	-1.435746	-0.425753	4.098221
9	H	4.414609	-1.506633	3.403122	72	H	-1.790724	-1.145636	5.675156
10	C	3.972363	-0.383459	0.854893	73	C	-0.957548	-3.153071	3.992109
11	C	5.364246	-0.377866	0.858372	74	H	-1.772909	-3.460612	4.657001
12	C	3.317237	0.120175	-0.270156	75	H	-1.403102	-2.796531	3.058143
13	C	6.068407	0.128662	-0.262496	76	H	-0.355535	-4.037906	3.760017
14	H	5.920291	-0.727148	1.723838	77	C	0.441960	-2.638191	5.981003
15	C	3.966945	0.635480	-1.408068	78	H	-0.393591	-2.926222	6.627505
16	C	5.378919	0.621772	-1.370923	79	H	1.056002	-3.529788	5.816153
17	H	5.948612	0.971260	-2.228306	80	H	1.043801	-1.902187	6.524408
18	C	7.548832	0.127029	-0.257794	81	H	0.409231	2.179028	-5.020999
19	C	8.273552	-0.927052	0.317173	82	H	2.878652	2.468852	-5.568213
20	C	8.284021	1.173950	-0.823533	83	H	4.556333	1.750725	-3.887939
21	C	9.661622	-0.928663	0.318654	84	C	-5.714858	-3.962699	0.112783
22	H	7.738778	-1.769607	0.747550	85	C	-4.596154	-4.916923	-1.614856
23	C	9.676534	1.166192	-0.822577	86	C	-6.094535	-3.189902	1.209945
24	H	7.758529	2.023421	-1.251865	87	C	-6.479275	-5.072530	-0.309361
25	C	10.402085	0.116655	-0.251631	88	C	-3.708676	-5.204753	-2.651224
26	H	10.177971	-1.772898	0.768820	89	C	-5.767628	-5.678834	-1.412052
27	H	10.195685	2.007787	-1.269348	90	C	-7.281765	-3.523170	1.853036
28	C	3.102508	1.091197	-2.456966	91	H	-5.484661	-2.366972	1.566378
29	C	3.494336	1.643181	-3.685216	92	C	-7.664703	-5.389544	0.353763
30	C	0.825370	1.344200	-3.111467	93	C	-3.997659	-6.297146	-3.461723
31	C	2.563911	2.043474	-4.621037	94	H	-2.828085	-4.598696	-2.833048
32	C	1.180467	1.884619	-4.317632	95	C	-6.037053	-6.769313	-2.239276
33	H	-0.217928	1.202932	-2.843404	96	C	-8.064763	-4.604736	1.428824
34	Au	1.363691	0.116849	-0.290481	97	H	-7.600908	-2.934204	2.707633
35	C	-1.588440	-0.965227	-0.407597	98	H	-8.260388	-6.241520	0.039073
36	C	-1.575383	1.231039	-0.226159	99	C	-5.143209	-7.077621	-3.257576
37	C	-1.217612	-2.310996	-0.517766	100	H	-3.319333	-6.544375	-4.272765
38	C	-2.960826	-0.583668	-0.376491	101	H	-6.935304	-7.362266	-2.093160
39	C	-1.188960	2.571692	-0.107691	102	H	-8.985869	-4.837701	1.953985
40	C	-2.952281	0.866444	-0.264674	103	H	-5.337096	-7.924863	-3.908036
41	C	-2.220534	-3.262822	-0.602422	104	C	-5.662430	4.280265	-0.756665
42	H	-0.170086	-2.596103	-0.513266	105	C	-4.540880	5.215492	0.979536
43	C	-3.954274	-1.535642	-0.468149	106	C	-6.046194	3.515411	-1.857967
44	C	-2.180470	3.535404	-0.024835	107	C	-6.415289	5.398129	-0.334993
45	H	-0.138181	2.845389	-0.100794	108	C	-3.655409	5.489290	2.021432
46	C	-3.934331	1.830277	-0.175518	109	C	-5.701880	5.992325	0.773109
47	C	-3.578769	-2.890555	-0.582451	110	C	-7.225984	3.865177	-2.505961
48	H	-1.964711	-4.315443	-0.651440	111	H	-5.444872	2.685955	-2.213755
49	H	-5.004690	-1.263994	-0.488530	112	C	-7.593380	5.731708	-1.003046
50	C	-3.542902	3.180149	-0.054373	113	C	-3.935217	6.582718	2.833762
51	H	-1.911748	4.584469	0.030610	114	H	-2.783293	4.871932	2.206061
52	H	-4.988066	1.571380	-0.160960	115	C	-5.962230	7.083553	1.602228
53	N	-0.770565	0.127750	-0.315755	116	C	-7.997688	4.955097	-2.082455
54	N	1.728438	0.947372	-2.176565	117	H	-7.548052	3.282695	-3.363895
55	C	11.931344	0.073645	-0.228584	118	H	-8.180070	6.590044	-0.688740
56	C	12.556073	1.301838	-0.895894	119	C	-5.070001	7.377840	2.626073
57	H	12.270514	2.229634	-0.388942	120	H	-3.258133	6.819152	3.649049
58	H	13.647605	1.225188	-0.856231	121	H	-6.852369	7.687914	1.453241
59	H	12.267656	1.382852	-1.949263	122	H	-8.913166	5.200997	-2.611542
60	C	12.418756	0.017073	1.228619	123	H	-5.256837	8.225484	3.278073
61	H	12.035920	-0.865260	1.750395	124	N	-4.571120	-3.871272	-0.685744
62	H	13.513509	-0.023484	1.261638	125	N	-4.523860	4.172472	0.047262
63	H	12.093412	0.903041	1.783759					

Table S7. Cartesian coordinates of the optimized T_1 geometry of **3** computed by DFT/CPCM.

1	C	-6.134596	-0.914605	-2.003807	64	C	-15.453353	-1.831741	-0.762089
2	C	-4.761506	-0.739082	-1.674142	65	H	-15.119940	-1.389942	-1.706021
3	C	-3.800449	-0.858043	-2.667535	66	H	-15.059954	-2.852338	-0.711298
4	C	-4.141894	-1.156195	-4.002290	67	H	-16.547560	-1.888645	-0.787595
5	C	-5.493453	-1.326985	-4.302748	68	C	-3.033398	-1.281143	-5.050769
6	C	-6.477798	-1.206756	-3.318128	69	C	-2.253595	0.041652	-5.133209
7	H	-2.753635	-0.718236	-2.410621	70	H	-2.913176	0.865193	-5.425891
8	H	-5.802750	-1.557383	-5.316650	71	H	-1.794675	0.303408	-4.174814
9	H	-7.521694	-1.344860	-3.590042	72	H	-1.452910	-0.035115	-5.877807
10	C	-7.058613	-0.754739	-0.871569	73	C	-2.073938	-2.413005	-4.645931
11	C	-8.446811	-0.850148	-0.841161	74	H	-1.266327	-2.508097	-5.380964
12	C	-6.394692	-0.468246	0.322692	75	H	-1.617558	-2.229387	-3.668138
13	C	-9.138966	-0.653533	0.379893	76	H	-2.602101	-3.370935	-4.594850
14	H	-9.007557	-1.102977	-1.736623	77	C	-3.584675	-1.597659	-6.443706
15	C	-7.032478	-0.263444	1.561076	78	H	-2.757378	-1.676118	-7.156771
16	C	-8.441295	-0.363788	1.553100	79	H	-4.127197	-2.548735	-6.459538
17	H	-9.004119	-0.186406	2.466058	80	H	-4.258085	-0.811921	-6.801849
18	C	-10.615999	-0.750078	0.407254	81	H	-3.450425	0.740532	5.336421
19	C	-11.396375	-0.273082	-0.655908	82	H	-5.909859	0.712337	5.992812
20	C	-11.292099	-1.320406	1.490857	83	H	-7.598716	0.241869	4.237661
21	C	-12.781320	-0.361638	-0.627340	84	C	2.855477	-3.676889	-1.219677
22	H	-10.909448	0.196703	-1.506392	85	C	1.894043	-5.063117	0.288311
23	C	-12.681872	-1.404306	1.516109	86	C	3.131988	-2.657863	-2.130766
24	H	-10.720810	-1.728877	2.320322	87	C	3.711750	-4.791905	-1.085384
25	C	-13.462969	-0.928566	0.459004	88	C	1.084860	-5.639533	1.266890
26	H	-13.342900	0.030629	-1.471551	89	C	3.097027	-5.677573	-0.123333
27	H	-13.153742	-1.862998	2.378874	90	C	4.304476	-2.746247	-2.867522
28	C	-6.161130	0.026930	2.661921	91	H	2.461822	-1.816645	-2.267907
29	C	-6.541043	0.266784	3.990280	92	C	4.870986	-4.880053	-1.851486
30	C	-3.883163	0.309740	3.300833	93	C	1.475741	-6.861703	1.794492
31	C	-5.604378	0.528164	4.968195	94	H	0.173295	-5.162394	1.608561
32	C	-4.226657	0.546821	4.604179	95	C	3.488887	-6.892263	0.433429
33	H	-2.844084	0.310630	2.983696	96	C	5.172371	-3.844175	-2.733723
34	Au	-4.446669	-0.324831	0.294908	97	H	4.564449	-1.953686	-3.561640
35	C	-1.425743	-1.182816	0.092554	98	H	5.525623	-5.743278	-1.783883
36	C	-1.594488	0.989686	0.415512	99	C	2.665708	-7.489452	1.385892
37	C	-1.700812	-2.542245	-0.099001	100	H	0.851271	-7.352112	2.534132
38	C	-0.084621	-0.702565	0.115861	101	H	4.424341	-7.365097	0.151039
39	C	-2.075243	2.290292	0.613117	102	C	2.283486	4.147870	1.537667
40	C	-0.195208	0.729716	0.336953	103	C	1.054010	5.345948	0.063786
41	C	-0.633483	-3.410791	-0.260879	104	C	2.756552	3.194309	2.438842
42	H	-2.726055	-2.896422	-0.142395	105	C	2.945081	5.383026	1.362469
43	C	0.973928	-1.574614	-0.037274	106	C	0.122343	5.775856	-0.880577
44	C	-1.155280	3.319444	0.727041	107	C	2.162570	6.145843	0.417062
45	H	-3.141487	2.479350	0.692974	108	C	3.919577	3.483126	3.137830
46	C	0.715200	1.760582	0.445425	109	H	2.225732	2.266247	2.619606
47	C	0.693430	-2.942016	-0.228377	110	C	4.121870	5.650966	2.056935
48	H	-0.816057	-4.463204	-0.448873	111	C	0.304363	7.029222	-1.446578
49	H	2.003940	-1.237249	0.018788	112	H	-0.707261	5.150495	-1.190545
50	C	0.227279	3.067970	0.642654	113	C	2.320122	7.410922	-0.143539
51	H	-1.496258	4.331288	0.916945	114	C	4.609097	4.693282	2.944382
52	H	1.782798	1.592013	0.346800	115	H	4.301149	2.773408	3.864639
53	N	-2.318999	-0.161548	0.271793	116	H	4.659034	6.583393	1.914561
54	N	-4.793087	0.058109	2.323004	117	C	1.384167	7.850832	-1.077246
55	C	-14.991037	-1.004985	0.449090	118	H	-0.389051	7.383573	-2.202323
56	C	-15.546907	-1.659264	1.716731	119	H	3.150628	8.050978	0.137217
57	H	-15.274680	-1.097943	2.616811	120	N	1.754231	-3.845976	-0.380456
58	H	-16.640102	-1.690742	1.663966	121	N	1.135517	4.130742	0.745804
59	H	-15.191088	-2.688485	1.832647	122	C	6.422868	-3.795366	-4.892868
60	C	-15.571604	0.415197	0.346094	123	C	7.642148	-4.061012	-3.009066
61	H	-15.241715	0.923369	-0.565106	124	C	5.392725	-3.658935	-5.823722
62	H	-16.666821	0.377375	0.330166	125	C	7.775830	-3.891612	-5.292852
63	H	-15.263909	1.025751	1.201375	126	C	8.072776	-4.176646	-1.687230

Table S8. Cartesian coordinates of the optimized S_1 geometry of **1** computed by TDA-TDDFT/CPCM.

1	C	-0.318867	1.948205	0.034197	64	H	-9.894429	-1.655206	0.472564
2	C	1.016259	1.459000	0.023030	65	C	-9.746744	1.803197	0.543949
3	C	2.073577	2.356576	0.034317	66	H	-9.294941	2.607256	-0.044866
4	C	1.864890	3.750740	0.056638	67	H	-10.833447	1.944131	0.524189
5	C	0.547435	4.208560	0.067298	68	H	-9.407435	1.913362	1.579178
6	C	-0.531726	3.320582	0.056140	69	C	-9.881925	0.297267	-1.457167
7	H	3.091579	1.975906	0.025528	70	H	-9.435157	1.057028	-2.105617
8	H	0.339627	5.273087	0.084635	71	H	-9.640070	-0.685504	-1.875022
9	H	-1.545375	3.714505	0.064806	72	H	-10.969843	0.424993	-1.492874
10	C	-1.349775	0.899562	0.019198	73	C	3.072782	4.691334	0.067625
11	C	-2.737150	1.022298	0.026044	74	C	3.927753	4.411273	1.314777
12	C	-0.805538	-0.384237	0.003542	75	H	3.350481	4.582625	2.229350
13	C	-3.542844	-0.139740	0.014242	76	H	4.290723	3.379062	1.335099
14	H	-3.209287	1.999479	0.071333	77	H	4.800923	5.073535	1.333443
15	C	-1.558560	-1.570321	-0.007906	78	C	3.919223	4.451209	-1.193593
16	C	-2.959653	-1.408974	-0.004805	79	H	4.792367	5.113765	-1.197177
17	H	-3.606852	-2.281232	-0.046357	80	H	4.281842	3.420172	-1.249144
18	C	-5.018017	-0.008470	0.016851	81	H	3.335787	4.651461	-2.098334
19	C	-5.658756	1.008848	-0.704598	82	C	2.660318	6.165643	0.092568
20	C	-5.829338	-0.890105	0.738032	83	H	3.555114	6.796739	0.099850
21	C	-7.041565	1.129927	-0.702229	84	H	2.070089	6.437358	-0.788892
22	H	-5.063535	1.700053	-1.295406	85	H	2.075712	6.408857	0.986020
23	C	-7.216450	-0.766229	0.735050					
24	H	-5.367827	-1.674065	1.332705					
25	C	-7.858943	0.246009	0.016542					
26	H	-7.492456	1.929866	-1.284173					
27	H	-7.797102	-1.473509	1.318108					
28	C	-0.795977	-2.790402	-0.032154					
29	C	-1.304581	-4.090591	-0.046951					
30	C	1.410479	-3.685877	-0.058344					
31	C	-0.469851	-5.192204	-0.068240					
32	H	-2.382934	-4.222985	-0.041156					
33	C	0.938511	-4.970464	-0.073537					
34	H	2.476317	-3.482189	-0.061812					
35	H	-0.875726	-6.197169	-0.080032					
36	H	1.640559	-5.796410	-0.089293					
37	Au	1.136954	-0.573586	-0.007475					
38	C	4.077471	-0.839525	-1.118711					
39	C	4.080270	-0.859100	1.086816					
40	C	3.684501	-0.787475	-2.462142					
41	C	5.446477	-0.971050	-0.746841					
42	C	3.690580	-0.830626	2.431910					
43	C	5.448295	-0.984110	0.709306					
44	C	4.679666	-0.870321	-3.431737					
45	H	2.637811	-0.683866	-2.728261					
46	C	6.419810	-1.051579	-1.721875					
47	C	4.688040	-0.931247	3.397444					
48	H	2.644565	-0.730954	2.702164					
49	C	6.423959	-1.082579	1.680368					
50	C	6.022955	-1.000275	-3.070421					
51	H	4.409000	-0.832886	-4.481427					
52	H	7.469953	-1.151926	-1.465699					
53	C	6.030391	-1.055342	3.030577					
54	H	4.419973	-0.912309	4.448297					
55	H	7.473432	-1.178808	1.419885					
56	H	6.779181	-1.062428	-3.846262					
57	H	6.788468	-1.131688	3.803340					
58	N	3.270701	-0.774836	-0.014278					
59	N	0.602724	-2.592652	-0.038914					
60	C	-9.379306	0.416249	-0.008821					
61	C	-10.095189	-0.641571	0.835288					
62	H	-9.800762	-0.588789	1.888786					
63	H	-11.176956	-0.479986	0.785299					

Table S9. Cartesian coordinates of the optimized S_1 geometry of **2** computed by TDA-TDDFT/CPCM.

1	C	3.032711	0.725531	1.938409	64	C	12.418939	-1.509487	0.108520
2	C	1.660714	0.596928	1.585876	65	H	12.035842	-1.866379	1.069368
3	C	0.683196	0.938426	2.508679	66	H	12.093220	-2.212646	-0.665067
4	C	1.008468	1.414086	3.795257	67	H	13.513659	-1.535601	0.154389
5	C	2.359811	1.530081	4.120638	68	C	-0.116161	1.781883	4.766735
6	C	3.360322	1.190380	3.205714	69	C	-0.974858	2.900539	4.152918
7	H	-0.362756	0.837572	2.230849	70	H	-0.373235	3.797351	3.971144
8	H	2.656725	1.890938	5.099607	71	H	-1.418824	2.595021	3.200315
9	H	4.403510	1.295251	3.494772	72	H	-1.791620	3.169603	4.832585
10	C	3.972503	0.337790	0.874972	73	C	-0.996780	0.547530	5.022696
11	C	5.365432	0.342277	0.879228	74	H	-1.810532	0.797731	5.713059
12	C	3.321787	-0.076930	-0.286581	75	H	-1.446151	0.170526	4.098842
13	C	6.070032	-0.068771	-0.276083	76	H	-0.410671	-0.263913	5.466575
14	H	5.918954	0.686962	1.747965	77	C	0.418259	2.274900	6.114177
15	C	3.972242	-0.493220	-1.460461	78	H	-0.420352	2.524600	6.772540
16	C	5.382182	-0.479467	-1.420434	79	H	1.018561	1.509614	6.617307
17	H	5.953768	-0.818458	-2.280622	80	H	1.032132	3.174910	6.003101
18	C	7.551163	-0.067382	-0.269598	81	H	0.423149	-1.831289	-5.165175
19	C	8.273783	-0.439698	0.872854	82	H	2.896428	-2.045817	-5.739945
20	C	8.287207	0.305789	-1.398607	83	H	4.566859	-1.419604	-4.012247
21	C	9.661915	-0.439301	0.877080	84	C	-5.662418	-3.968413	1.268776
22	H	7.737486	-0.757256	1.763171	85	C	-4.513126	-5.373416	-0.092399
23	C	9.679837	0.301716	-1.390486	86	C	-6.062647	-2.912475	2.087209
24	H	7.762721	0.628604	-2.294100	87	C	-6.408367	-5.164613	1.188206
25	C	10.403658	-0.069649	-0.253922	88	C	-3.611899	-5.940513	-0.992796
26	H	10.177178	-0.744522	1.784409	89	C	-5.676969	-6.058961	0.318837
27	H	10.200230	0.607254	-2.292268	90	C	-7.252901	-3.058537	2.791589
28	C	3.108485	-0.887720	-2.541770	91	H	-5.466095	-2.012691	2.190123
29	C	3.503820	-1.343586	-3.801184	92	C	-7.596868	-5.289594	1.906935
30	C	0.833219	-1.126739	-3.203900	93	C	-3.878604	-7.227823	-1.446040
31	C	2.577711	-1.692883	-4.765951	94	H	-2.737947	-5.401616	-1.341215
32	C	1.192993	-1.575343	-4.446116	95	C	-5.924227	-7.348757	-0.150738
33	H	-0.210782	-1.023187	-2.925655	96	C	-8.018194	-4.228238	2.699567
34	Au	1.369396	-0.089871	-0.306861	97	H	-7.588131	-2.248747	3.432532
35	C	-1.570005	-1.191773	-0.090456	98	H	-8.178692	-6.205185	1.853799
36	C	-1.589845	0.955424	-0.561277	99	C	-5.015868	-7.930464	-1.027067
37	C	-1.181946	-2.508034	0.196296	100	H	-3.189131	-7.692939	-2.143980
38	C	-2.950024	-0.840309	-0.173769	101	H	-6.816396	-7.885480	0.158413
39	C	-1.224974	2.280609	-0.833864	102	H	-8.942097	-4.309541	3.263654
40	C	-2.962651	0.577037	-0.489153	103	H	-5.192286	-8.934806	-1.399297
41	C	-2.169754	-3.457501	0.390652	104	C	-5.722166	3.669368	-1.930670
42	H	-0.132144	-2.768613	0.282644	105	C	-4.616521	5.074563	-0.534867
43	C	-3.929028	-1.793071	0.015576	106	C	-6.093119	2.617516	-2.767973
44	C	-2.230145	3.212404	-1.028776	107	C	-6.492992	4.849098	-1.839810
45	H	-0.179688	2.562923	-0.905185	108	C	-3.736473	5.644500	0.384559
46	C	-3.959052	1.511988	-0.679488	109	C	-5.789277	5.743681	-0.948281
47	C	-3.533852	-3.116646	0.300819	110	C	-7.278660	2.750432	-3.482713
48	H	-1.898494	-4.474630	0.650200	111	H	-5.477919	1.730981	-2.876437
49	H	-4.982841	-1.555120	-0.085801	112	C	-7.676361	4.960980	-2.569345
50	C	-3.587476	2.844500	-0.952010	113	C	-4.033748	6.918628	0.855556
51	H	-1.977034	4.237435	-1.275477	114	H	-2.855853	5.116941	0.733952
52	H	-5.008829	1.253219	-0.587094	115	C	-6.067017	7.020694	-0.460715
53	N	-0.770204	-0.111229	-0.324240	116	C	-8.067966	3.903490	-3.382014
54	N	1.731388	-0.781863	-2.244629	117	H	-7.591324	1.943605	-4.138645
55	C	11.932917	-0.084868	-0.205684	118	H	-8.277196	5.863763	-2.508684
56	C	12.559106	0.353281	-1.532302	119	C	-5.180133	7.605643	0.435096
57	H	12.272710	1.376112	-1.799021	120	H	-3.361419	7.385809	1.568735
58	H	13.650535	0.325864	-1.449315	121	H	-6.966130	7.544876	-0.771338
59	H	12.272634	-0.309685	-2.355545	122	H	-8.987399	3.974771	-3.954710
60	C	12.418883	0.871922	0.895462	123	H	-5.380455	8.600137	0.821448
61	H	12.036177	0.585538	1.879776	124	N	-4.511203	-4.099613	0.486397
62	H	13.513612	0.866023	0.947620	125	N	-4.582549	3.811213	-1.134256
63	H	12.092679	1.897493	0.693551					

Table S10. Cartesian coordinates of the optimized S_1 geometry of **3** computed by TDA-TDDFT/CPCM.

1	C	-6.191457	-0.370513	-2.051922	64	C	-15.459876	-1.793108	-0.892225
2	C	-4.811393	-0.280672	-1.719225	65	H	-15.163880	-1.071316	-1.659497
3	C	-3.876632	-0.090027	-2.726169	66	H	-15.055274	-2.770189	-1.176089
4	C	-4.253470	0.017922	-4.080293	67	H	-16.553700	-1.860998	-0.901315
5	C	-5.611894	-0.072499	-4.383790	68	C	-3.174819	0.226344	-5.146587
6	C	-6.569824	-0.263981	-3.384198	69	C	-2.413127	1.530204	-4.855815
7	H	-2.824176	-0.022768	-2.462649	70	H	-3.090345	2.390377	-4.879349
8	H	-5.947957	0.004982	-5.412280	71	H	-1.931784	1.508323	-3.873172
9	H	-7.619913	-0.329799	-3.659419	72	H	-1.632132	1.690352	-5.608011
10	C	-7.082713	-0.572471	-0.898942	73	C	-2.190634	-0.954866	-5.115715
11	C	-8.469046	-0.701855	-0.862909	74	H	-1.406475	-0.816390	-5.868969
12	C	-6.386320	-0.644583	0.307249	75	H	-1.704329	-1.052590	-4.140139
13	C	-9.121767	-0.897153	0.376508	76	H	-2.706107	-1.896936	-5.329753
14	H	-9.054433	-0.685243	-1.777747	77	C	-3.762917	0.321272	-6.557048
15	C	-6.984184	-0.837386	1.564103	78	H	-2.955829	0.469283	-7.282111
16	C	-8.389366	-0.960688	1.564232	79	H	-4.296607	-0.593061	-6.836870
17	H	-8.924762	-1.079343	2.502762	80	H	-4.453886	1.165373	-6.653002
18	C	-10.596523	-1.029464	0.414883	81	H	-3.297586	-0.907742	5.374072
19	C	-11.417550	-0.263744	-0.425034	82	H	-5.734030	-1.207987	6.056558
20	C	-11.227982	-1.921378	1.287390	83	H	-7.468588	-1.177363	4.279570
21	C	-12.799688	-0.386735	-0.385637	84	C	2.920139	-3.642401	-1.337193
22	H	-10.964817	0.456294	-1.101594	85	C	1.987257	-5.082942	0.136640
23	C	-12.615112	-2.039449	1.325038	86	C	3.175837	-2.595797	-2.222787
24	H	-10.623753	-2.552857	1.933432	87	C	3.798754	-4.742883	-1.229922
25	C	-13.437022	-1.276809	0.490512	88	C	1.189513	-5.698927	1.100441
26	H	-13.394327	0.235468	-1.049881	89	C	3.202052	-5.663496	-0.289549
27	H	-13.051964	-2.752560	2.016389	90	C	4.349751	-2.642236	-2.960972
28	C	-6.079686	-0.871708	2.682878	91	H	2.488686	-1.765195	-2.338933
29	C	-6.419971	-1.050558	4.025420	92	C	4.959482	-4.788615	-1.997440
30	C	-3.787981	-0.727424	3.315372	93	C	1.604792	-6.925386	1.598570
31	C	-5.457995	-1.068674	5.017745	94	H	0.268521	-5.248419	1.452789
32	C	-4.093668	-0.900634	4.638277	95	C	3.618140	-6.883104	0.237998
33	H	-2.760953	-0.597095	2.989108	96	C	5.239698	-3.725327	-2.853700
34	Au	-4.442835	-0.460554	0.273381	97	H	4.593643	-1.827833	-3.635345
35	C	-1.403500	-1.255395	0.035843	98	H	5.631627	-5.639654	-1.950758
36	C	-1.609619	0.899106	0.416888	99	C	2.807125	-7.519119	1.175670
37	C	-1.653560	-2.614818	-0.191230	100	H	0.990284	-7.445873	2.325847
38	C	-0.069142	-0.755493	0.076655	101	H	4.562824	-7.330266	-0.055209
39	C	-2.110972	2.188578	0.645784	102	C	2.212804	4.086665	1.644551
40	C	-0.203836	0.666019	0.336443	103	C	0.968410	5.309693	0.203900
41	C	-0.572278	-3.460915	-0.373157	104	C	2.697502	3.113966	2.518655
42	H	-2.671161	-2.988119	-0.243185	105	C	2.854666	5.337083	1.510089
43	C	1.004017	-1.606441	-0.097919	106	C	0.033821	5.752607	-0.731472
44	C	-1.209697	3.228397	0.790765	107	C	2.062653	6.116049	0.585486
45	H	-3.179551	2.360090	0.724186	108	C	3.853526	3.399628	3.230322
46	C	0.688500	1.708675	0.479327	109	H	2.180228	2.173135	2.670059
47	C	0.746598	-2.971810	-0.326551	110	C	4.024024	5.602904	2.217108
48	H	-0.737222	-4.511092	-0.587656	111	C	0.197438	7.025385	-1.258399
49	H	2.028308	-1.253891	-0.031367	112	H	-0.783515	5.123184	-1.064758
50	C	0.178084	3.001782	0.709475	113	C	2.202246	7.399432	0.063958
51	H	-1.568113	4.229195	1.004803	114	C	4.524089	4.626016	3.076629
52	H	1.759177	1.560687	0.381863	115	H	4.243360	2.674503	3.937166
53	N	-2.312858	-0.255530	0.240188	116	H	4.546229	6.547870	2.105550
54	N	-4.722199	-0.704986	2.329011	117	C	1.262392	7.852654	-0.859925
55	C	-14.963705	-1.378388	0.502685	118	H	-0.498365	7.390737	-2.006575
56	C	-15.468090	-2.408496	1.516819	119	H	3.021505	8.043630	0.367137
57	H	-15.171183	-2.151727	2.539181	120	N	1.823241	-3.853456	-0.502463
58	H	-16.562036	-2.445054	1.489020	121	N	1.067725	4.075408	0.848369
59	H	-15.097099	-3.414374	1.293405	122	C	6.489859	-3.596752	-5.009825
60	C	-15.561979	-0.009852	0.868523	123	C	7.713585	-3.883050	-3.131948
61	H	-15.269259	0.765074	0.153557	124	C	5.457453	-3.459490	-5.938038
62	H	-16.656641	-0.063384	0.874442	125	C	7.844818	-3.653234	-5.410599
63	H	-15.230791	0.307901	1.862661	126	C	8.145873	-4.022649	-1.812971

127	C	8.626847	-3.835435	-4.210564	190	C	0.085883	12.413935	-2.167401
128	C	5.806970	-3.358085	-7.279425	191	C	4.688738	9.766539	-3.014471
129	H	4.417768	-3.438906	-5.628244	192	H	3.920461	8.004689	-2.031204
130	C	8.168905	-3.548733	-6.765341	193	C	3.227749	11.696377	-3.155677
131	C	9.513570	-4.133306	-1.591867	194	C	-1.194191	12.382116	-1.630020
132	H	7.442713	-4.040362	-0.986780	195	H	-2.667925	11.232667	-0.556868
133	C	9.996506	-3.949068	-3.960845	196	H	0.455372	13.307535	-2.662714
134	C	7.146756	-3.397262	-7.693008	197	C	4.447437	11.087375	-3.420043
135	H	5.021968	-3.249443	-8.022207	198	H	5.645871	9.305189	-3.239792
136	H	9.205784	-3.590117	-7.087177	199	H	3.037183	12.715743	-3.479599
137	C	10.432439	-4.101372	-2.651242	200	H	-1.835348	13.254705	-1.709293
138	H	9.875998	-4.245134	-0.574067	201	H	5.221213	11.634708	-3.949655
139	H	10.709155	-3.914993	-4.780207	202	N	5.702571	4.870856	3.813384
140	H	7.383652	-3.313563	-8.749268	203	N	1.384335	9.144914	-1.414243
141	H	11.493916	-4.192996	-2.442231	204	N	3.195590	-8.765916	1.712507
142	C	3.507644	-9.905075	0.976504	205	N	6.421167	-3.735929	-3.626867
143	C	3.334817	-9.060890	3.065304					
144	C	3.481542	-10.100949	-0.404391					
145	C	3.850494	-10.948252	1.867528					
146	C	3.165026	-8.231352	4.173980					
147	C	3.741168	-10.408453	3.202361					
148	C	3.824239	-11.360102	-0.882620					
149	H	3.198814	-9.302897	-1.083013					
150	C	4.191169	-12.204556	1.360593					
151	C	3.390370	-8.781500	5.430276					
152	H	2.872844	-7.192295	4.062945					
153	C	3.961136	-10.936601	4.476706					
154	C	4.179808	-12.402430	-0.013825					
155	H	3.812917	-11.538466	-1.953970					
156	H	4.456834	-13.015188	2.033425					
157	C	3.780388	-10.119951	5.585197					
158	H	3.263315	-8.157251	6.310004					
159	H	4.273239	-11.970302	4.596909					
160	H	4.443754	-13.373207	-0.422163					
161	H	3.946122	-10.517381	6.581892					
162	C	6.835257	4.062192	3.824492					
163	C	5.928690	5.961355	4.648917					
164	C	7.089298	2.885206	3.120103					
165	C	7.803652	4.639550	4.677873					
166	C	5.075981	7.014216	4.980875					
167	C	7.224027	5.852472	5.205297					
168	C	8.327908	2.281037	3.300943					
169	H	6.351086	2.457225	2.449897					
170	C	9.040736	4.012225	4.841906					
171	C	5.551704	7.972873	5.867699					
172	H	4.074419	7.082382	4.569224					
173	C	7.677960	6.829680	6.094137					
174	C	9.294589	2.832457	4.154628					
175	H	8.550450	1.362950	2.764901					
176	H	9.793983	4.444685	5.494538					
177	C	6.839372	7.888279	6.417351					
178	H	4.907858	8.803662	6.141409					
179	H	8.671187	6.758666	6.528645					
180	H	10.251306	2.333105	4.273473					
181	H	7.179221	8.656187	7.105526					
182	C	0.397579	10.126630	-1.410261					
183	C	2.510698	9.651804	-2.056344					
184	C	-0.881935	10.093142	-0.855490					
185	C	0.895363	11.280921	-2.057654					
186	C	3.728379	9.029393	-2.331739					
187	C	2.245156	10.977301	-2.471194					
188	C	-1.666983	11.233441	-0.978536					
189	H	-1.252471	9.212516	-0.341219					

Table S11. Cartesian coordinates of the optimized T_1 geometry of **1** computed by TDA-TDDFT/CPCM.

1	C	-0.318442	1.947748	0.032574	64	H	-9.894540	-1.653493	0.473562
2	C	1.016609	1.458488	0.021548	65	C	-9.746078	1.804918	0.542884
3	C	2.074071	2.355964	0.031741	66	H	-9.294172	2.608536	-0.046453
4	C	1.865461	3.750141	0.052877	67	H	-10.832754	1.946055	0.523132
5	C	0.548040	4.208082	0.063424	68	H	-9.406661	1.915643	1.578017
6	C	-0.531160	3.320183	0.053304	69	C	-9.881685	0.297813	-1.457329
7	H	3.092054	1.975309	0.023020	70	H	-9.434776	1.057082	-2.106257
8	H	0.340314	5.272637	0.079850	71	H	-9.640071	-0.685265	-1.874600
9	H	-1.544787	3.714161	0.061801	72	H	-10.969574	0.425762	-1.493060
10	C	-1.349388	0.899219	0.018688	73	C	3.073458	4.690624	0.062732
11	C	-2.736676	1.022196	0.025297	74	C	3.928725	4.411544	1.309898
12	C	-0.805115	-0.384675	0.004380	75	H	3.351729	4.583798	2.224477
13	C	-3.542642	-0.139634	0.014274	76	H	4.291561	3.379302	1.331049
14	H	-3.208625	1.999512	0.069779	77	H	4.801992	5.073700	1.327731
15	C	-1.558580	-1.570432	-0.006420	78	C	3.919538	4.449337	-1.198508
16	C	-2.959598	-1.408947	-0.003811	79	H	4.792697	5.111866	-1.202912
17	H	-3.606887	-2.281152	-0.045027	80	H	4.282122	3.418245	-1.253242
18	C	-5.017781	-0.008085	0.016709	81	H	3.335862	4.648803	-2.103265
19	C	-5.658317	1.008903	-0.705384	82	C	2.661139	6.164995	0.086515
20	C	-5.829269	-0.889107	0.738454	83	H	3.556003	6.796002	0.093010
21	C	-7.041099	1.130279	-0.703052	84	H	2.070708	6.436012	-0.795024
22	H	-5.062972	1.699611	-1.296650	85	H	2.076802	6.409046	0.979915
23	C	-7.216352	-0.764935	0.735429					
24	H	-5.367910	-1.672781	1.333622					
25	C	-7.858643	0.246996	0.016310					
26	H	-7.491835	1.929943	-1.285492					
27	H	-7.797142	-1.471715	1.318956					
28	C	-0.796305	-2.790832	-0.029389					
29	C	-1.305292	-4.090752	-0.041727					
30	C	1.409948	-3.686998	-0.054541					
31	C	-0.470929	-5.192809	-0.061333					
32	H	-2.383693	-4.222718	-0.035199					
33	C	0.937360	-4.971318	-0.067355					
34	H	2.475823	-3.483734	-0.058653					
35	H	-0.877073	-6.197673	-0.071096					
36	H	1.639190	-5.797498	-0.081909					
37	Au	1.137562	-0.574191	-0.006851					
38	C	4.075612	-0.845132	-1.118182					
39	C	4.079683	-0.854770	1.087686					
40	C	3.681885	-0.799680	-2.461539					
41	C	5.444851	-0.973073	-0.746388					
42	C	3.690860	-0.820788	2.432800					
43	C	5.447518	-0.979461	0.709825					
44	C	4.676661	-0.885673	-3.431272					
45	H	2.634863	-0.698637	-2.727461					
46	C	6.417847	-1.056930	-1.721552					
47	C	4.689146	-0.915317	3.398127					
48	H	2.644826	-0.721629	2.703299					
49	C	6.424068	-1.071961	1.680663					
50	C	6.020295	-1.012315	-3.070050					
51	H	4.405414	-0.853348	-4.480984					
52	H	7.468228	-1.154829	-1.465399					
53	C	6.031440	-1.039029	3.030934					
54	H	4.421734	-0.891941	4.449060					
55	H	7.473491	-1.167785	1.419827					
56	H	6.776206	-1.077093	-3.845988					
57	H	6.790154	-1.110619	3.803532					
58	N	3.269133	-0.776766	-0.013459					
59	N	0.602340	-2.593291	-0.037090					
60	C	-9.378968	0.417560	-0.009078					
61	C	-10.095028	-0.639598	0.835709					
62	H	-9.800499	-0.586268	1.889151					
63	H	-11.176760	-0.477786	0.785714					

Table S12. Cartesian coordinates of the optimized T_1 geometry of **2** computed by TDA-TDDFT/CPCM.

1	C	3.024058	1.069336	1.763751	64	C	12.416665	-1.460544	0.432794
2	C	1.653789	0.870199	1.438748	65	H	12.028057	-1.630220	1.441533
3	C	0.672653	1.369666	2.282392	66	H	12.094164	-2.296558	-0.196508
4	C	0.992121	2.079824	3.457382	67	H	13.511086	-1.477870	0.488779
5	C	2.341962	2.262800	3.757142	68	C	-0.137262	2.617513	4.340111
6	C	3.346207	1.763546	2.923070	69	C	-0.999447	3.596604	3.524905
7	H	-0.372245	1.211437	2.029288	70	H	-0.401015	4.446343	3.179497
8	H	2.634636	2.802361	4.651582	71	H	-1.438899	3.115158	2.645528
9	H	4.388182	1.925829	3.189021	72	H	-1.819624	3.984306	4.140088
10	C	3.968677	0.494807	0.793392	73	C	-1.013084	1.449104	4.821999
11	C	5.361459	0.501667	0.803320	74	H	-1.830127	1.820769	5.451049
12	C	3.323352	-0.128606	-0.274229	75	H	-1.457892	0.902549	3.984770
13	C	6.071910	-0.116589	-0.251705	76	H	-0.424646	0.738826	5.412080
14	H	5.910626	1.001760	1.595903	77	C	0.390917	3.358190	5.571654
15	C	3.979969	-0.754575	-1.347210	78	H	-0.450624	3.723214	6.169643
16	C	5.389661	-0.733113	-1.303196	79	H	0.993248	2.704266	6.210973
17	H	5.965478	-1.225837	-2.082415	80	H	1.001102	4.224169	5.294256
18	C	7.552952	-0.113977	-0.237454	81	H	0.452560	-2.722179	-4.781209
19	C	8.268788	-0.268307	0.958264	82	H	2.928970	-3.041668	-5.289768
20	C	8.295587	0.043350	-1.411920	83	H	4.589094	-2.121970	-3.687702
21	C	9.656839	-0.267612	0.970098	84	C	-5.667072	-3.928376	1.497241
22	H	7.727221	-0.415220	1.888993	85	C	-4.527403	-5.411995	0.213284
23	C	9.688163	0.040492	-1.395358	86	C	-6.060468	-2.826789	2.256661
24	H	7.776413	0.194704	-2.354667	87	C	-6.417059	-5.124663	1.487073
25	C	10.405249	-0.114201	-0.205639	88	C	-3.631617	-6.031963	-0.657155
26	H	10.166752	-0.399514	1.921143	89	C	-5.691897	-6.069130	0.666774
27	H	10.213813	0.173622	-2.335214	90	C	-7.248294	-2.928979	2.972773
28	C	3.121997	-1.340070	-2.343220	91	H	-5.460548	-1.924781	2.306820
29	C	3.524817	-2.010604	-3.499952	92	C	-7.602917	-5.205098	2.216392
30	C	0.850943	-1.687850	-2.969648	93	C	-3.904307	-7.341873	-1.036080
31	C	2.604552	-2.523359	-4.394833	94	H	-2.757443	-5.516521	-1.038871
32	C	1.218220	-2.347588	-4.111348	95	C	-5.945318	-7.382382	0.271525
33	H	-0.194682	-1.533267	-2.723467	96	C	-8.017620	-4.099408	2.949742
34	Au	1.370871	-0.151698	-0.298500	97	H	-7.578270	-2.083330	3.568527
35	C	-1.570012	-1.245625	-0.025663	98	H	-8.187640	-6.120374	2.217254
36	C	-1.586882	0.874198	-0.608494	99	C	-5.042235	-8.015737	-0.573946
37	C	-1.185662	-2.546291	0.330563	100	H	-3.219120	-7.848021	-1.709240
38	C	-2.949578	-0.894826	-0.122773	101	H	-6.838179	-7.897550	0.613577
39	C	-1.219343	2.182751	-0.948135	102	H	-8.939396	-4.145742	3.521206
40	C	-2.959767	0.504225	-0.510992	103	H	-5.223466	-9.038820	-0.888324
41	C	-2.175833	-3.480489	0.578619	104	C	-5.716830	3.534448	-2.087952
42	H	-0.136809	-2.806275	0.428596	105	C	-4.601762	4.997787	-0.761377
43	C	-3.930912	-1.832297	0.121417	106	C	-6.094551	2.446211	-2.874165
44	C	-2.223017	3.107329	-1.182877	107	C	-6.483619	4.719682	-2.048306
45	H	-0.173429	2.457680	-1.036502	108	C	-3.716437	5.605851	0.128170
46	C	-3.954795	1.431741	-0.742156	109	C	-5.773841	5.651480	-1.200830
47	C	-3.539248	-3.140188	0.475930	110	C	-7.282426	2.550057	-3.589768
48	H	-1.906776	-4.482978	0.891827	111	H	-5.482682	1.553431	-2.943424
49	H	-4.984250	-1.595880	0.011911	112	C	-7.669526	4.801740	-2.777821
50	C	-3.580793	2.748032	-1.080803	113	C	-4.008046	6.900967	0.541973
51	H	-1.968267	4.118664	-1.479482	114	H	-2.836188	5.091785	0.498344
52	H	-5.004803	1.180868	-0.631969	115	C	-6.045590	6.950322	-0.770747
53	N	-0.768172	-0.181394	-0.319002	116	C	-8.067600	3.709302	-3.539476
54	N	1.743347	-1.185371	-2.076537	117	H	-7.600405	1.714859	-4.206481
55	C	11.934171	-0.120299	-0.146382	118	H	-8.267389	5.708279	-2.756331
56	C	12.568723	0.060895	-1.527857	119	C	-5.153677	7.572187	0.094621
57	H	12.286016	1.015949	-1.983117	120	H	-3.331717	7.397691	1.231022
58	H	13.659600	0.048426	-1.434684	121	H	-6.944023	7.463004	-1.101889
59	H	12.285552	-0.744268	-2.214052	122	H	-8.989053	3.757177	-4.111368
60	C	12.414454	1.026253	0.758555	123	H	-5.349372	8.583866	0.436150
61	H	12.023973	0.930423	1.776255	124	N	-4.519194	-4.107458	0.719167
62	H	13.508773	1.029484	0.819047	125	N	-4.573938	3.708710	-1.303130
63	H	12.091858	1.995741	0.364857					

Table S13. Cartesian coordinates of the optimized T_1 geometry of **3** computed by TDA-TDDFT/CPCM.

1	C	-6.184844	-0.408850	-2.053449	64	C	-15.459430	-1.788178	-0.892721
2	C	-4.805845	-0.312913	-1.718247	65	H	-15.159173	-1.086411	-1.676733
3	C	-3.867359	-0.147341	-2.726186	66	H	-15.055612	-2.772806	-1.150423
4	C	-4.239378	-0.071554	-4.083803	67	H	-16.553338	-1.854315	-0.904269
5	C	-5.596875	-0.167355	-4.389778	68	C	-3.156606	0.109373	-5.150956
6	C	-6.558477	-0.333545	-3.389208	69	C	-2.394255	1.419026	-4.889521
7	H	-2.815733	-0.074895	-2.460845	70	H	-3.070220	2.279209	-4.936628
8	H	-5.929287	-0.114135	-5.420993	71	H	-1.916474	1.420692	-3.904909
9	H	-7.607704	-0.404517	-3.666407	72	H	-1.610347	1.559657	-5.642588
10	C	-7.080284	-0.582279	-0.899135	73	C	-2.174166	-1.072000	-5.087534
11	C	-8.466931	-0.708144	-0.864875	74	H	-1.387089	-0.952994	-5.841069
12	C	-6.387984	-0.627349	0.310804	75	H	-1.691555	-1.146529	-4.108083
13	C	-9.124399	-0.872621	0.376490	76	H	-2.690157	-2.018353	-5.280397
14	H	-9.049111	-0.711980	-1.781901	77	C	-3.739511	0.170331	-6.565444
15	C	-6.990746	-0.789213	1.569638	78	H	-2.929599	0.299315	-7.290995
16	C	-8.396146	-0.909420	1.567884	79	H	-4.273537	-0.749883	-6.824579
17	H	-8.934930	-1.004622	2.507147	80	H	-4.428864	1.012781	-6.684687
18	C	-10.599548	-1.001006	0.412833	81	H	-3.317334	-0.783673	5.392801
19	C	-11.416044	-0.254585	-0.448599	82	H	-5.756820	-1.061269	6.073668
20	C	-11.235930	-1.869947	1.304739	83	H	-7.485316	-1.065949	4.290268
21	C	-12.798551	-0.373984	-0.411248	84	C	2.910904	-3.645966	-1.327582
22	H	-10.959520	0.447787	-1.140990	85	C	1.976574	-5.081573	0.150087
23	C	-12.623422	-1.984348	1.340297	86	C	3.167966	-2.601552	-2.215359
24	H	-10.635332	-2.486570	1.968273	87	C	3.787434	-4.747985	-1.218854
25	C	-13.440816	-1.240968	0.484234	88	C	1.178388	-5.694001	1.115784
26	H	-13.389533	0.232732	-1.092833	89	C	3.189826	-5.665428	-0.276005
27	H	-13.064168	-2.679320	2.047467	90	C	4.341114	-2.651824	-2.954512
28	C	-6.090169	-0.799789	2.692122	91	H	2.482411	-1.769748	-2.332402
29	C	-6.435493	-0.947519	4.037059	92	C	4.947398	-4.797535	-1.987349
30	C	-3.800170	-0.647761	3.329047	93	C	1.591635	-6.920262	1.616069
31	C	-5.476935	-0.945974	5.032953	94	H	0.258577	-5.240911	1.467925
32	C	-4.110974	-0.790493	4.654348	95	C	3.603897	-6.884830	0.253708
33	H	-2.771658	-0.528019	3.003522	96	C	5.228934	-3.736538	-2.845954
34	Au	-4.443952	-0.447133	0.279271	97	H	4.586085	-1.839241	-3.630692
35	C	-1.407199	-1.248399	0.045168	98	H	5.617946	-5.649773	-1.939522
36	C	-1.609213	0.907183	0.423529	99	C	2.792432	-7.517247	1.193367
37	C	-1.659952	-2.607518	-0.180031	100	H	0.976747	-7.438044	2.344961
38	C	-0.072092	-0.750845	0.084219	101	H	4.547371	-7.334572	-0.039463
39	C	-2.107949	2.197940	0.650793	102	C	2.221272	4.089956	1.639144
40	C	-0.203991	0.671348	0.342035	103	C	0.976500	5.312334	0.198195
41	C	-0.580257	-3.455812	-0.361752	104	C	2.705715	3.118275	2.514511
42	H	-2.678269	-2.979084	-0.230583	105	C	2.865636	5.338591	1.500254
43	C	0.999505	-1.603954	-0.089748	106	C	0.040997	5.755082	-0.736332
44	C	-1.204614	3.236374	0.792919	107	C	2.073400	6.117097	0.575463
45	H	-3.176157	2.371489	0.729987	108	C	3.863992	3.403020	3.222885
46	C	0.690410	1.712578	0.481968	109	H	2.186674	2.178976	2.669344
47	C	0.739465	-2.969106	-0.316390	110	C	4.037204	5.603444	2.203986
48	H	-0.747229	-4.505987	-0.574704	111	C	0.206504	7.026124	-1.266855
49	H	2.024465	-1.253155	-0.024298	112	H	-0.778505	5.126760	-1.066349
50	C	0.182636	3.007090	0.710242	113	C	2.214906	7.398830	0.050375
51	H	-1.560956	4.238194	1.005612	114	C	4.537005	4.627486	3.064697
52	H	1.760677	1.562457	0.383334	115	H	4.253799	2.678700	3.930570
53	N	-2.314823	-0.246439	0.249181	116	H	4.561313	6.546941	2.088963
54	N	-4.731189	-0.644257	2.339148	117	C	1.274239	7.851883	-0.872745
55	C	-14.967726	-1.339428	0.493210	118	H	-0.490007	7.391201	-2.014507
56	C	-15.477820	-2.342826	1.530996	119	H	3.036327	8.041857	0.350173
57	H	-15.184206	-2.060949	2.547681	120	N	1.814390	-3.853142	-0.491441
58	H	-16.571722	-2.378112	1.500015	121	N	1.074398	4.079374	0.845500
59	H	-15.107937	-3.354679	1.334340	122	C	6.477200	-3.615808	-5.003632
60	C	-15.564826	0.038913	0.822327	123	C	7.702296	-3.899236	-3.126259
61	H	-15.268136	0.795177	0.089240	124	C	5.444088	-3.479076	-5.931139
62	H	-16.659596	-0.012573	0.825545	125	C	7.831644	-3.675890	-5.405651
63	H	-15.236697	0.380950	1.809395	126	C	8.135645	-4.036124	-1.807344

127	C	8.614559	-3.856270	-4.205924
128	C	5.792399	-3.381948	-7.273154
129	H	4.404775	-3.455664	-5.620289
130	C	8.154512	-3.575635	-6.761009
131	C	9.503350	-4.148769	-1.587314
132	H	7.433257	-4.050333	-0.980426
133	C	9.984255	-3.971835	-3.957265
134	C	7.131682	-3.424758	-7.688021
135	H	5.006834	-3.273823	-8.015417
136	H	9.190978	-3.619800	-7.083810
137	C	10.421215	-4.121431	-2.647695
138	H	9.866594	-4.258558	-0.569582
139	H	10.696144	-3.941342	-4.777430
140	H	7.367634	-3.344346	-8.744749
141	H	11.482726	-4.214515	-2.439500
142	C	3.486980	-9.905344	0.998611
143	C	3.319298	-9.055999	3.085693
144	C	3.458497	-10.104218	-0.381808
145	C	3.828563	-10.947355	1.891498
146	C	3.153072	-8.223517	4.192704
147	C	3.722505	-10.404259	3.225255
148	C	3.797432	-11.365269	-0.857699
149	H	3.176842	-9.306943	-1.061793
150	C	4.165453	-12.205620	1.386882
151	C	3.378838	-8.771338	5.449937
152	H	2.863236	-7.184017	4.079662
153	C	3.942959	-10.930022	4.500510
154	C	4.151663	-12.406531	0.012930
155	H	3.784199	-11.545994	-1.928633
156	H	4.430120	-13.015396	2.061138
157	C	3.765797	-10.110389	5.607374
158	H	3.254543	-8.144776	6.328416
159	H	4.252664	-11.964217	4.622659
160	H	4.412665	-13.378859	-0.393609
161	H	3.931964	-10.505943	6.604745
162	C	6.848787	4.060259	3.808033
163	C	5.948463	5.963217	4.630531
164	C	7.098460	2.881166	3.105613
165	C	7.820640	4.637429	4.657602
166	C	5.098917	7.018703	4.962271
167	C	7.245004	5.852780	5.183798
168	C	8.336236	2.274734	3.284575
169	H	6.357587	2.453291	2.438280
170	C	9.056795	4.007797	4.819821
171	C	5.579022	7.978340	5.845666
172	H	4.096458	7.088134	4.553019
173	C	7.703358	6.831018	6.069232
174	C	9.306322	2.825964	4.134514
175	H	8.555409	1.354983	2.750000
176	H	9.812668	4.440084	5.469526
177	C	6.867918	7.892179	6.392192
178	H	4.937707	8.811167	6.119122
179	H	8.697554	6.758834	6.501327
180	H	10.262270	2.324817	4.251981
181	H	7.211221	8.660911	7.077727
182	C	0.413843	10.126470	-1.427510
183	C	2.524259	9.644517	-2.077126
184	C	-0.864443	10.097780	-0.869646
185	C	0.912904	11.277569	-2.079586
186	C	3.739773	9.018309	-2.353489
187	C	2.260969	10.969396	-2.495377
188	C	-1.647007	11.239607	-0.994330
189	H	-1.235907	9.219618	-0.351841
190	C	0.105913	12.412205	-2.190907
191	C	4.700296	9.751028	-3.040740
192	H	3.930084	7.994065	-2.050270
193	C	3.243686	11.683991	-3.184363
194	C	-1.172965	12.385137	-1.650431
195	H	-2.646955	11.242557	-0.570320
196	H	0.476391	13.303384	-2.689831
197	C	4.461251	11.071210	-3.449765
198	H	5.655767	9.286659	-3.266912
199	H	3.054838	12.702834	-3.510923
200	H	-1.812193	13.259034	-1.730873
201	H	5.235100	11.615035	-3.982874
202	N	5.717810	4.871325	3.798078
203	N	1.398190	9.142350	-1.430809
204	N	3.178821	-8.763770	1.732462
205	N	6.409676	-3.751049	-3.620251

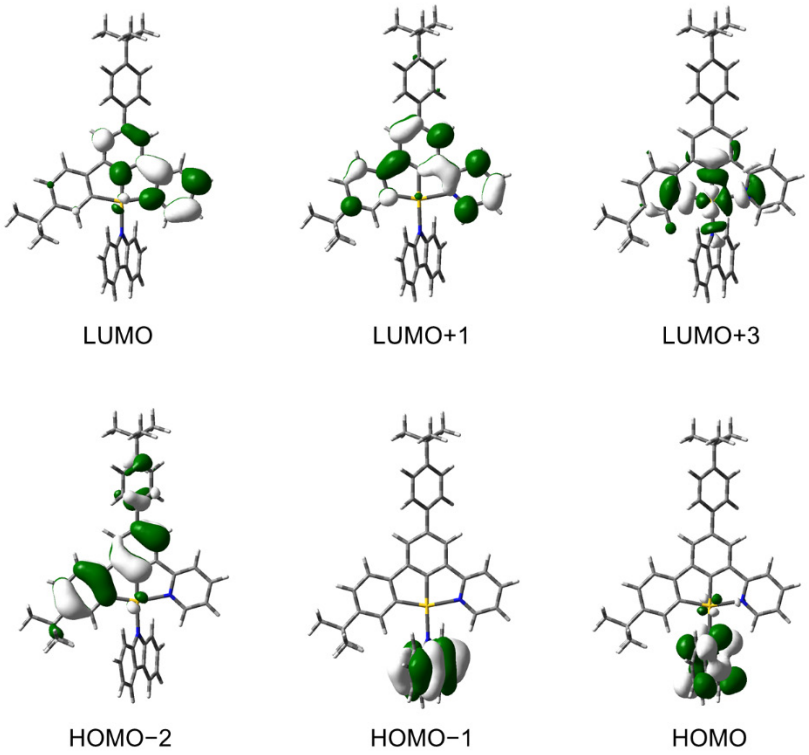

Figure S11. Spatial plots (isovalue = 0.03) of selected molecular orbitals of **1** at the optimized ground-state geometry.

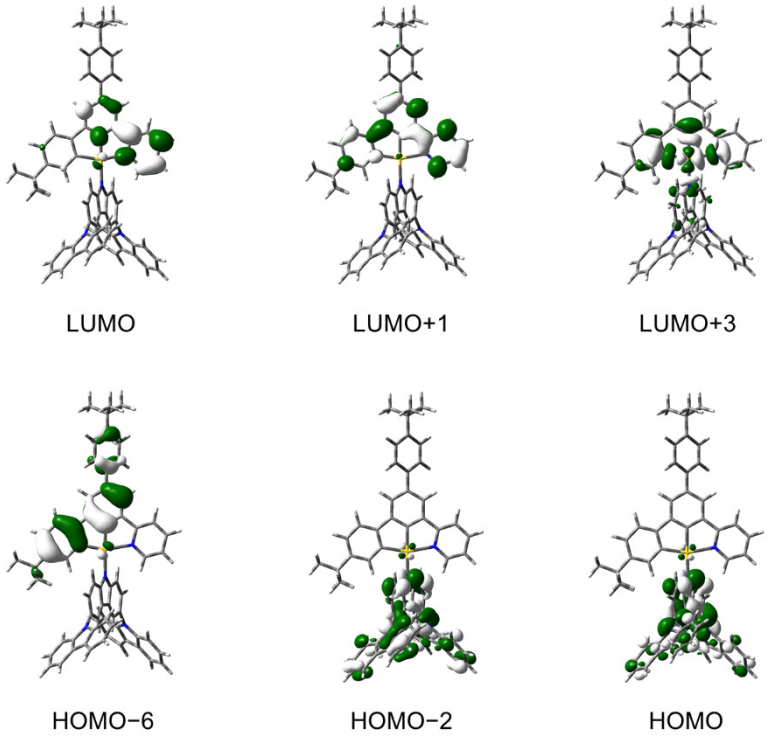

Figure S12. Spatial plots (isovalue = 0.03) of selected molecular orbitals of **2** at the

optimized ground-state geometry.

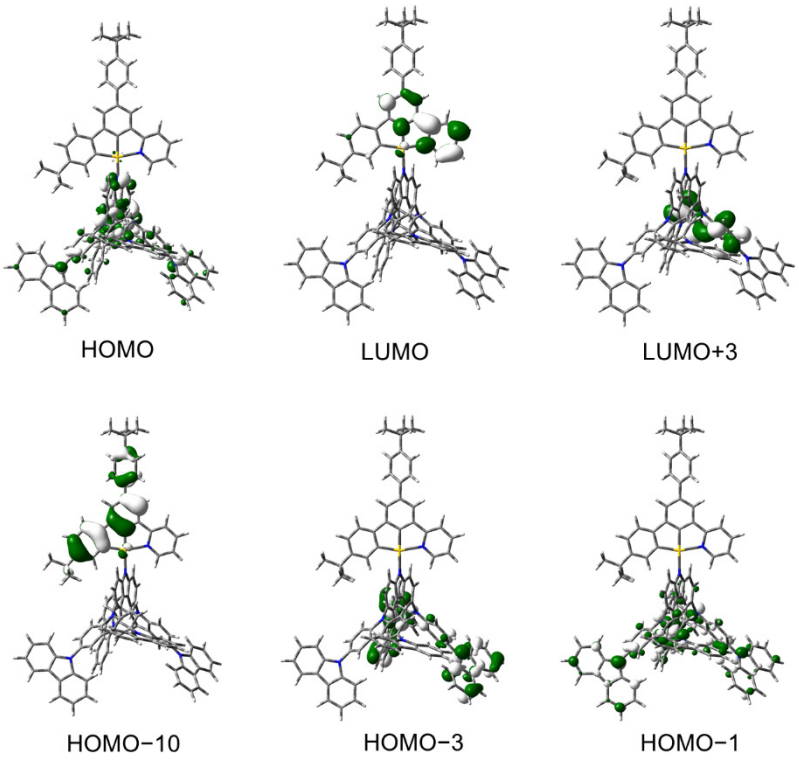

Figure S13. Spatial plots (isovalue = 0.03) of selected molecular orbitals of **3** at the optimized ground-state geometry.

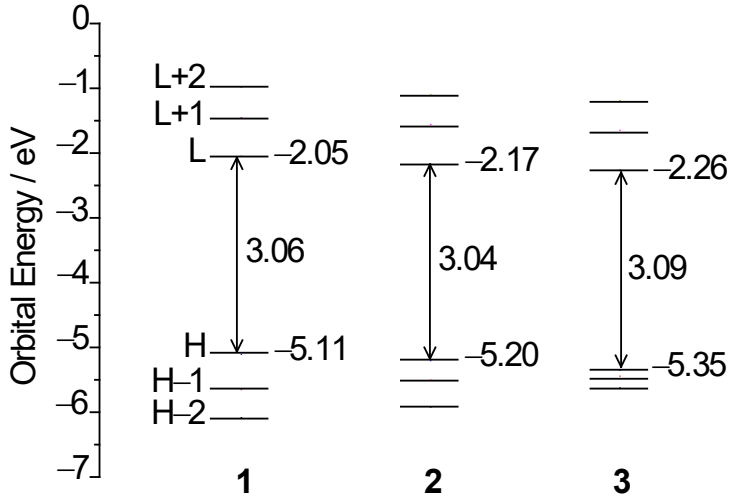

Figure S14. Orbital energy diagram of **1**–**3**.

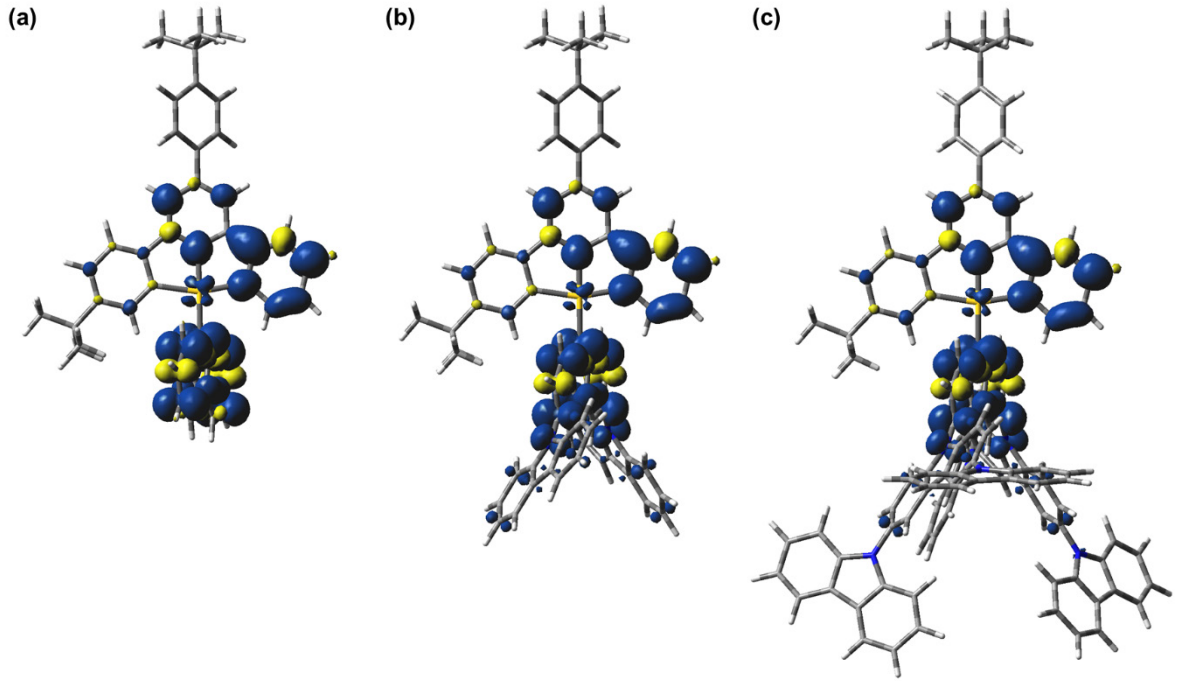

Figure S15. Plots of spin density (isovalue = 0.002) of the T_1 of (a) **1,** (b) **2** and (c) **3**.

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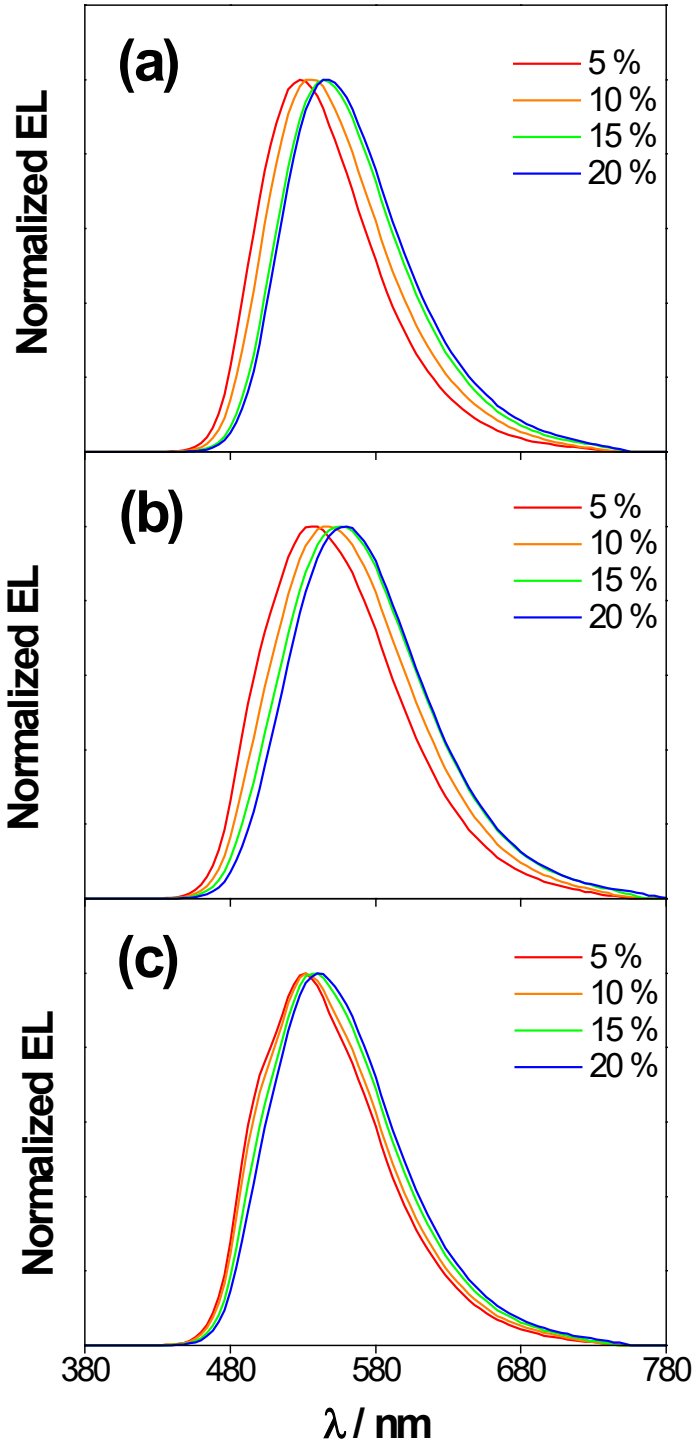

Figure S16. Normalized EL spectra of the solution-processed OLEDs based on **1**–**3**.

Table S14. Key parameters of the solution-processed OLEDs based on **1**−**3**.

Complex	Conc. / wt%	CE[a] / cd A^{-1}	PE[b] / lm W^{-1}	EQE_{max}[c] / %	EQE[d] / %	λ_{max}[e] / nm	CIE[f] (x, y)
1	5	18.8	4.5	5.6	5.5	528	0.33, 0.58
	10	35.9	13.7	10.6	10.5	536	0.36, 0.58
	15	35.5	15.6	10.5	10.3	544	0.39, 0.57
	20	40.0	15.7	11.9	10.0	548	0.40, 0.57
2	5	7.2	2.0	2.2	2.0	540	0.36, 0.56
	10	14.9	4.4	4.6	4.6	544	0.39, 0.55
	15	26.5	9.5	8.4	8.4	556	0.42, 0.54
	20	27.1	10.4	8.7	8.0	560	0.43, 0.54
3	5	41.2	32.1	12.5	6.4	532	0.33, 0.57
	10	45.9	32.7	13.9	8.8	532	0.35, 0.57
	15	47.2	33.3	14.3	10.4	540	0.36, 0.57
	20	52.6	41.3	15.8	12.2	540	0.38, 0.57

[a] CE represents maximum current efficiency.
[b] PE represents maximum power efficiency.
[c] EQE_{max} represents maximum external quantum efficiency.
[d] EQE represents external quantum efficiency at luminance of 500 cd m^{-2}.
[e] λ_{max} represents peak maximum.
[f] CIE coordinates are taken at a luminance of 100 cd m^{-2}.

Table S15. Summary of the EL performance of some representative TADF-based solution-processed OLEDs.

EML	CE[a] / cd A^{-1}	PE[b] / lm W^{-1}	EQE_{max}[c] / %	λ_{max}[d] / nm	Ref.
3:CBP	52.6	41.3	15.8	540	This work
2PXZ-OXD:PVK:OXD-7	16.2	5.3	7.5	547	1
CDE1:CzSi	38.9	17.3	12.0		2
4CzIPN:CBP/B4PyMPM	39.0	48.0	12.0	525	3
TB-3PXZ:CzSi	41.5	32.6	13.9		4
TXO-PhCz:DCzDCN:SimCP2	55.6	47.2	18.9	532	5
t4CzIPN:Xm-mCP	76.5	51.8	22.0	532	6
DACT-II:DCzPPy	111.9	89.9	30.8	530	7

[a] CE represents maximum current efficiency.
[b] PE represents maximum power efficiency.
[c] EQE_{max} represents maximum external quantum efficiency.
[d] λ_{max} represents peak maximum.

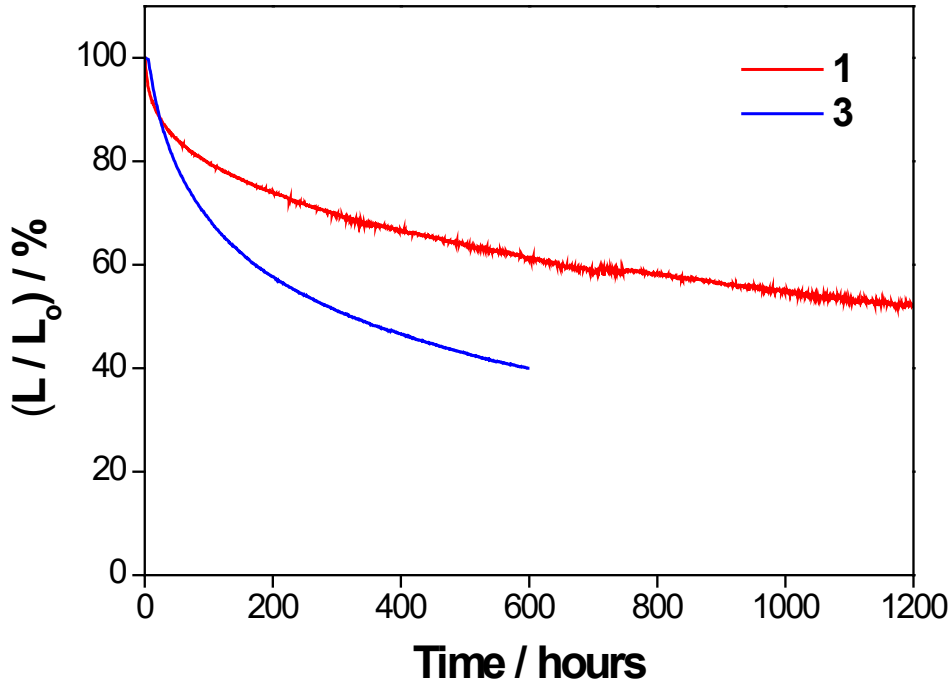

Figure S17. Relative luminance, L/L_0, of the solution-processed OLEDs based on **1** and **3**.

Table S16. Lifetime data of the solution-processed OLEDs based on **1** and **3**.

Complex	L_0[a] / cd m^{-2}	Lifetime / hours		
		LT_{70}[b] at 1,000 cd m^{-2}	LT_{70} at 100 cd m^{-2}	LT_{50}[c] at 100 cd m^{-2}
1	689	6	295	1305
3	850	2	94	322

[a] L_0 is defined as the initial luminance.
[b] LT_{70} is defined as the operational lifetime at 70 % of initial luminance.
[c] LT_{50} is defined as the operational lifetime at 50 % of initial luminance.

Experimental Details

Materials and Reagents. All solvents were purified and distilled using standard procedures before use. The carbazole-based dendrimers were prepared by Ullmann coupling reaction according to previously reported procedures,[8] and [Au{4-^{t}BuC^C(4-^{t}BuC$_6$H$_4$)^N}Cl] was prepared according to literature procedures.[9,10] **1**−**3** were synthesized by reacting the corresponding carbazole ligands with [Au{4-^{t}BuC^C(4-^{t}BuC$_6$H$_4$)^N}Cl] in the presence of sodium hydride in degassed tetrahydrofuran.[10] Tetra-*n*-butylammonium hexafluorophosphate (Aldrich, 98 %) was recrystallized more than three times from hot absolute ethanol before use. All reactions were performed under anaerobic conditions using standard Schlenk techniques under nitrogen atmosphere unless specified otherwise.

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. ^{1}H and ^{13}C{^{1}H} NMR spectra were recorded on a Bruker Avance 600 (600 MHz for ^{1}H and 150 MHz for ^{13}C nuclei) Fourier-transform NMR spectrometer with chemical shifts reported relative to tetramethylsilane (δ = 0 ppm) with the residual solvent peak(s) in dimethyl sulfoxide (δ = 2.50 ppm) or dichloromethane (δ = 5.32 ppm) used as internal reference. High-resolution ESI mass spectra were recorded on Bruker maXis II^{TM} High Resolution LC-QTOF Mass Spectrometer. Thermogravimetric analyses were performed with Q50 TGA (TA instruments), in which the decomposition temperature, T_d, is defined as the temperature at which the sample shows a 5 % weight loss. Steady-state excitation and emission spectra were recorded on a Horiba Scientific FluoroMax-4 spectrofluorometer equipped with a R928P PMT detector. Solid-state photophysical measurements were performed by loading the solid sample into a quartz tube inside a quartz-walled Dewar flask. Excited-state lifetimes of solution, solid, glass samples and thin films were measured using a conventional laser system. Liquid nitrogen was placed into the quartz-walled optical Dewar flask for low temperature (77 K) photophysical measurements. 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 and analyzed with a program for exponential fits. Relative luminescence quantum yields were measured by the optical dilute method reported by Demas and Crosby.[11] A degassed solution of quinine sulfate in 0.5 M H_2SO_4 (Φ_{lum}=0.546, excitation wavelength at 365 nm) was used as

the reference,[11] while the absolute photoluminescence quantum yields (PLQYs) of thin films were measured on a Hamamatsu C9920-03 Absolute PLQY Measurement System. Cyclic voltammetry was performed with a CH Instruments Model CHI620E (CH Instruments, Inc.). All solutions for electrochemical measurements were purged with pre-purified argon gas prior to measurement.

Synthesis and Characterization.

[Au{4-^{t}BuC^C(4-^{t}BuC$_6$H$_4$)^N}{(Cbz)−(Cbz)$_2$}] (**2**). A mixture of [Au{4-^{t}BuC^C(4-^{t}BuC$_6$H$_4$)^N}Cl] (277 mg, 0.43 mmol), [(Cbz)−(Cbz)$_2$] (233 mg, 0.47 mmol) and sodium hydride (15 mg, 0.64 mmol) in degassed tetrahydrofuran (50 mL) was refluxed for 4 h. The reaction mixture was then concentrated, and the crude product was washed with minimal amount of acetone. Subsequent recrystallization of the crude product by slow diffusion of diethyl ether vapor into a concentrated tetrahydrofuran solution of the complex gave a yellow solid. Yield: 237 mg, 50 %. ^{1}H NMR (600 MHz, DMSO-d$_6$, 298 K, δ/ppm) δ 8.62 (d, J = 8.0 Hz, 1H, pyridyl proton), 8.53−8.49 (m, 3H, pyridyl proton and carbazolyl protons), 8.37−8.36 (m, 1H, pyridyl proton), 8.23 (d, J = 8.0 Hz, 4H, carbazolyl protons), 8.12 (s, 1H, −C$_6$H$_2$−), 7.96 (d, J = 8.5 Hz, 2H, carbazolyl protons), 7.85 (s, 1H, −C$_6$H$_2$−), 7.80 (d, J = 8.0 Hz, 2H, −C$_6$H$_4$−), 7.72−7.71 (m, 1H, pyridyl proton), 7.70 (d, J = 6.0 Hz, 1H, −C$_6$H$_3$−), 7.60 (d, J = 8.0 Hz, 2H, −C$_6$H$_4$−), 7.56−7.32 (m, 10H, carbazolyl protons), 7.26−7.19 (m, 4H, carbazolyl protons), 7.18−7.17 (m, 1H, −C$_6$H$_3$−), 6.42 (d, J = 2.0 Hz, 1H, −C$_6$H$_3$−), 1.35 (s, 9H, −^{t}Bu), 0.94 (s, 9H, −^{t}Bu).^{13}C{^{1}H} NMR (150 MHz, DMSO-d$_6$, 298 K, δ/ppm): δ 163.76, 163.72, 152.05, 150.58, 150.37, 150.28, 149.31, 148.38, 147.66, 142.65, 142.13, 141.52, 141.42, 137.27, 130.54, 126.85, 126.03, 125.92, 125.67, 125.58, 124.78, 123.86, 122.60, 122.25, 122.02, 121.59, 121.12, 12.40, 119.50, 119.39, 115.34, 109.69, 34.39, 34.35, 31.14, 30.62. Elemental analyses: Found (%): C 70.74, H 4.89, N 4.78. Calcd for C$_{67}$H$_{53}$AuN$_4$·1.5 H$_2$O: C 70.70, H 4.96, N 4.92.

[Au{4-^{t}BuC^C(4-^{t}BuC$_6$H$_4$)^N}{(Cbz)−(Cbz)$_2$−(Cbz)$_4$}] (**3**). This complex was synthesized with a procedure similar to that of **2**, except that [(Cbz)−(Cbz)$_2$−(Cbz)$_4$] (118 mg, 0.10 mmol) was used instead of [(Cbz)−(Cbz)$_2$]. Yellow crystals. Yield: 90 mg, 49 %. ^{1}H NMR (600 MHz, CD$_2$Cl$_2$, 298 K, δ/ppm) δ 8.62 (d, J = 2.5 Hz, 2H, carbazolyl protons), 8.56 (d, J = 5.0 Hz, 1H, pyridyl proton), 8.33 (d, J = 1.0 Hz, 4H, carbazolyl protons), 8.17−8.12 (m, 9H, pyridyl proton and carbazolyl protons), 8.07 (d, J = 8.5 Hz, 2H, carbazolyl protons), 7.78−7.67 (m, 10H, −C$_6$H$_4$−, −C$_6$H$_2$− protons and carbazolyl protons), 7.64−7.57 (m, 6H, −C$_6$H$_4$− and carbazolyl

protons), 7.50−7.48 (m, 1H, pyridyl proton), 7.46−7.38 (m, 18H, $-C_6H_3-$ protons, carbazolyl protons), 7.29−7.23 (m, 9H, pyridyl proton and carbazolyl protons), 6.82 (d, J = 2.5 Hz, 1H, $-C_6H_3-$), 1.41 (s, 9H, $-^t$Bu), 1.06 (s, 9H, $-^t$Bu). $^{13}C\{^1H\}$ NMR (150 MHz, CD_2Cl_2, 298 K, δ/ppm): δ 165.24, 165.11, 152.59, 152.12, 151.86, 151.78, 150.20, 149.55, 148.64, 142.93, 142.64, 142.43, 142.38, 142.25, 138.55, 132.08, 130.26, 127.39, 126.94, 126.61, 126.54, 126.49, 126.43, 125.68, 125.45, 124.85, 124.09, 123.57, 122.76, 122.65, 121.51, 121.20, 120.70, 120.14, 120.07, 115.95, 112.13, 110.32, 35.34, 35.11, 31.66, 31.28. Elemental analyses: Found (%): C 77.20, H 4.56, N 6.27. Calcd for $C_{115}H_{81}AuN_8 \cdot H_2O$: C 77.17, H 4.67, N 6.26.

Computational Details. All calculations were carried out with the Gaussian 09 suite of programs.[4] By density functional theory (DFT), the ground-state (S_0) geometries of **1**−**3** were fully optimized in toluene with the hybrid Perdew, Burke, and Ernzerhof (PBE0) functional,[12] in conjunction with the conductor-like polarizable continuum model (CPCM).[13] Time-dependent density functional theory[14] (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**. 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**. Vibrational frequency calculations were then performed on the stationary points to verify that each was a minimum (NIMAG = 0) on the potential energy surface (PES). In order to gain further insights into the excited states involved in TADF, the geometries of the lowest-lying singlet excited state (S_1) and the lowest-lying triplet excited state (T_1) were optimized using TDDFT with the Tamm-Dancoff approximation (TDA) method.[15] The Cartesian coordinates of the optimized S_0, T_1 and S_1 geometries of the complexes are given in **Tables S4−S13**, while that of the optimized S_0 and T_1 geometries of **1** are reported in the previous literature.[10] For all the calculations, the effective core potentials (ECPs) and the associated basis set were used to describe Au[16] with f-type polarization functions (ζ = 1.050),[17] while the 6-31G(d,p) basis set[11] was applied for all other atoms. All the DFT and TDDFT calculations were carried out with a pruned (99,590) grid for numerical integration. To calculate the rate constants of fluorescence (k_f) and phosphorescence (k_p) of **1**, the geometries of the S_1 and T_1 states have been optimized in toluene at the PBE0/TZP level by TDDFT using the Amsterdam Density Functional (ADF) program,[19] with spin-orbit coupling (SOC) included in the TDDFT calculation of the T_1 state. The computed k_f and k_p values were used to determine the average radiative decay rate constant ($k_{r,avg}$) by the equation of the two-level model,[20] and the rate constants of intersystem crossing (ISC) and reverse ISC

(RISC) were calculated by the following equation,[21]

$$k_{ISC\ or\ RISC} = \frac{2\pi}{\hbar}|V_{SOC}|^2 \times \rho_{FCWD}$$

where $|V_{SOC}|^2$ is the coupling term of the matrix representation of the SOC operator ($\hat{H}_{SOC}$), and ρ_{FCWD} is the Frank-Condon-weighted density of states which describes the thermokinetic barrier associated with the $T_1 \rightarrow S_1$ transition.[22]

$$\rho_{FCWD}^{SCMT} = \frac{1}{\sqrt{4\pi\lambda k_B T}} exp\left(-\frac{(\Delta E_{ST} + \lambda)^2}{4\lambda k_B T}\right)$$

where k_B is the Boltzmann constant, T is the temperature, and λ is the reorganization energy,

$$\lambda = E_{S1/T1} - E_{S1/S1}$$

in which $E_{S1/T1}$ and $E_{S1/S1}$ are the energies of the S_1 state at the optimized T_1 and S_1 geometries, respectively.

OLED Fabrication and Characterization. Solution-processed organic light-emitting devices (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) layer was spin-coated onto the ITO-coated glass substrates as the hole-transporting layer. After that, the emissive layer was formed by mixing gold(III) dendrimer with 1,3-bis(carbazol-9-yl)benzene (mCP) to prepare a 10 mg cm^{-3} solution in chloroform and spin-coating onto the PEDOT:PSS layer to give a 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 30 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 LiF (1 nm)/Al (120 nm) was used as the metal cathode. The emissive area of each pixel was 0.1 cm^2. Current density−voltage−luminance characteristics and electroluminescence (EL) spectra were measured simultaneously with a programmable Keithley model 2420 power source and a Photoresearch PR-655 spectrometer. The operational lifetime of the solution-processed devices were measured by a McScience M6000 OLED lifetime test system.

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