

**Supplementary Information (ESI) for**  
**Towards Red–Light *o*-Carborane Derivatives with both**  
**Aggregation Induced Emission and Thermally Activated**  
**Delayed Fluorescence Combining Quantum Chemistry**  
**Calculation with Molecular Dynamics Simulation**

Ying-Chen Duan,<sup>a</sup> Ying Gao,<sup>a</sup> Yun Geng,<sup>\*a</sup> Yong Wu,<sup>b</sup>  
Guo-Gang Shan,<sup>\*a</sup> Liang Zhao,<sup>a</sup> Min Zhang<sup>a</sup> and Zhong-Min Su<sup>\*a, c, d</sup>

<sup>a</sup>Institute of Functional Material Chemistry, Faculty of Chemistry, Northeast Normal University, Changchun 130024, P. R. China  
E-mail: [gengy575@nenu.edu.cn](mailto:gengy575@nenu.edu.cn); [shangg187@nenu.edu.cn](mailto:shangg187@nenu.edu.cn); [zmsu@nenu.edu.cn](mailto:zmsu@nenu.edu.cn)

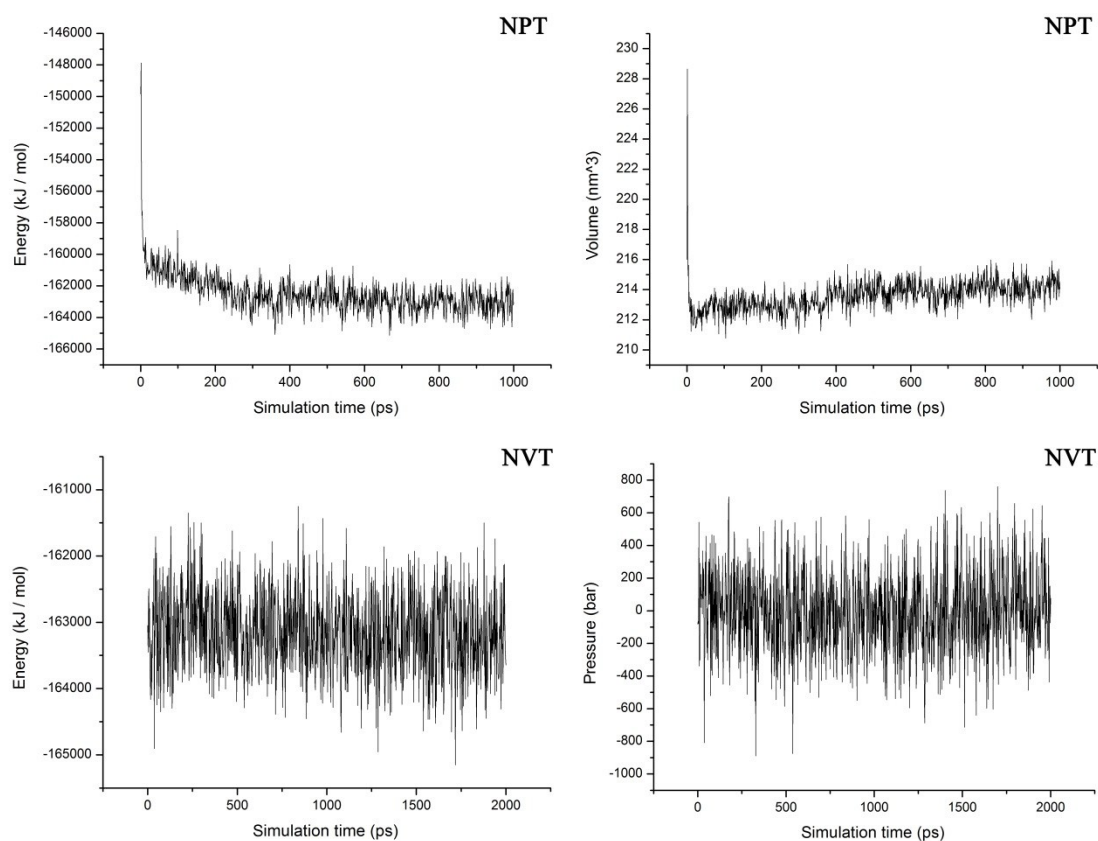
<sup>b</sup>School of Pharmaceutical Sciences, Changchun University of Chinese Medicine, 1035 Boshuo Road, Changchun, 130117, P. R. China

<sup>c</sup>School of Chemistry & Environmental Engineering, Changchun University of Science and Technology, Changchun, 130022, P. R. China

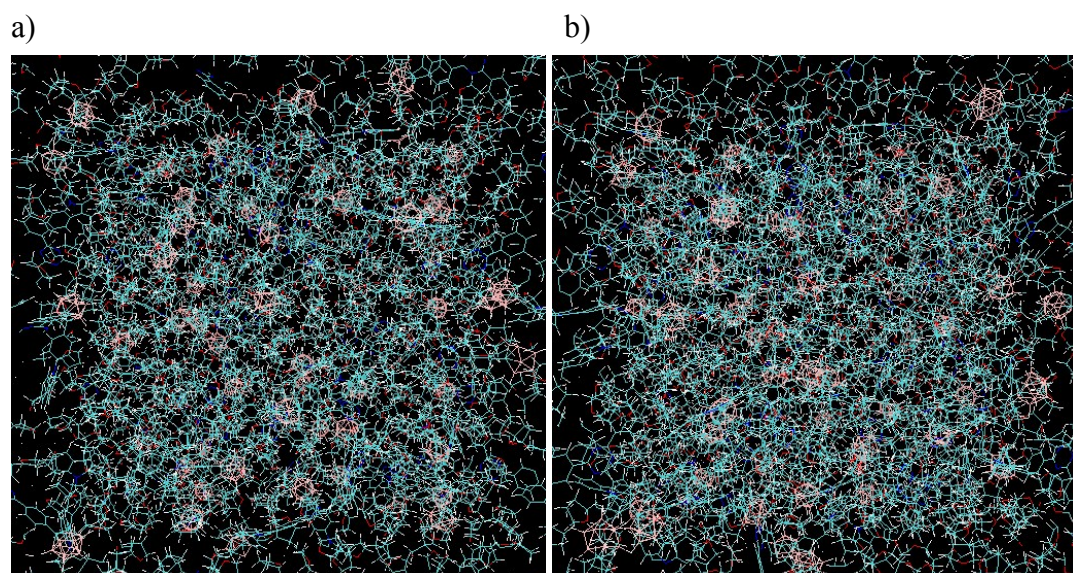
<sup>d</sup>Jilin Provincial Science and Technology Innovation Center of Optical Materials and Chemistry, Changchun, 130022, P. R. China

**Table S1** Selected bond lengths (Å) and dihedral angles (°) of **1** at  $S_0$  state calculated by different functionals compared with the experimental values of the X-ray diffraction crystal structure, together with their differences ( $\Delta$ ).

	Expt.	B3LYP P	CAM- B3LYP	PBE0	TPSS H	$\Delta$ (B3LYP )	$\Delta$ (CAM- B3LYP)	$\Delta$ (PBE0 )	$\Delta$ (TPSSH )
C1–C2	1.713			1.705					
	6	1.7599	1.7022	6	1.7383	0.0463	-0.0114	-0.0080	0.0247
C1–C3	1.505			1.502					
	3	1.5071	1.5074	2	1.5067	0.0018	0.0021	-0.0030	0.0015
C2–C5	1.503			1.501					
	7	1.5060	1.5057	1	1.5043	0.0023	0.0020	-0.0025	0.0007
C2–C1–C3–C 4	105.3 4	97.80	105.83	106.4 2	106.02	-7.54	0.49	1.08	0.68
C1–C2–C5–C 6	125.3 8	100.21	103.39	106.9 1	103.11	-25.17	-21.98	-18.46	-22.27



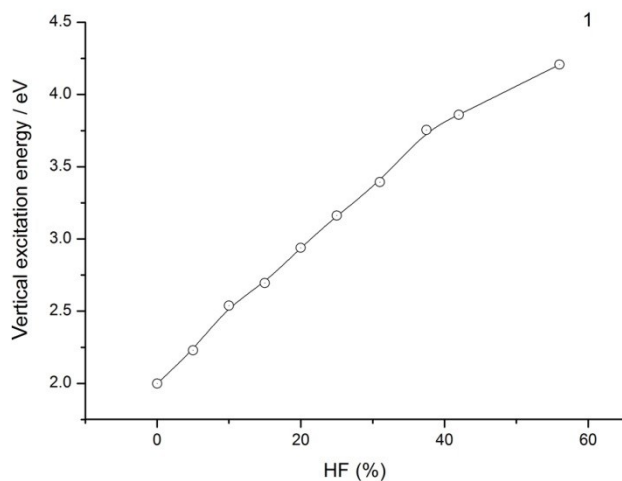
**Fig. S1** The plots of energy versus simulation time and volume versus simulation time in NPT process as well as energy versus simulation time and pressure versus simulation time in NVT process for **1**.



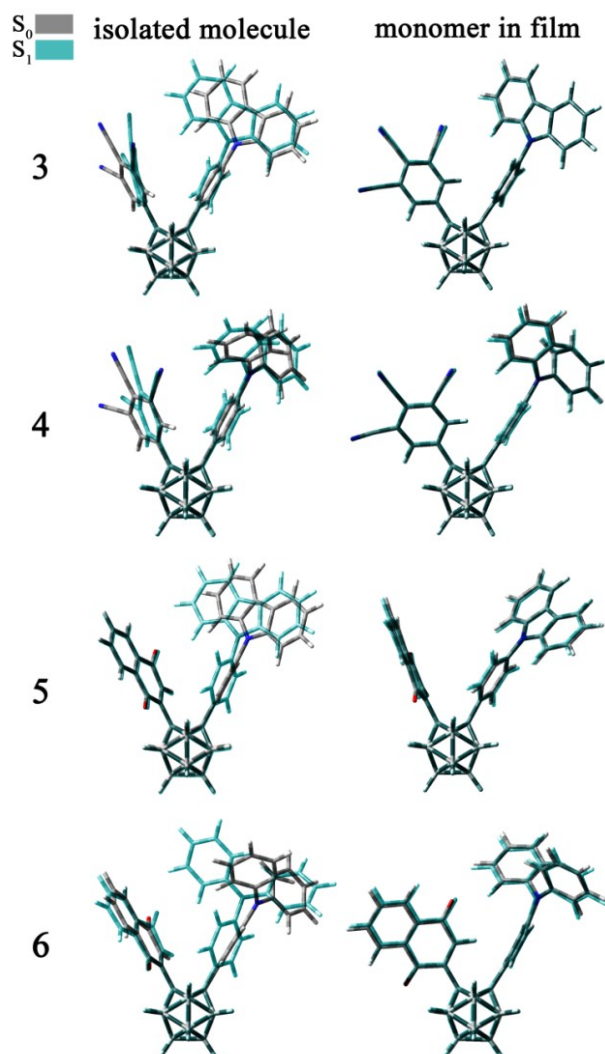
**Fig. S2** Position change of molecules in the 1/THF solution model before (a) and after (b) MD simulation.

**Table S2** Overlap integrals of the norms of HOMO and LUMO for **1-6** at their  $T_1$  states, respectively.

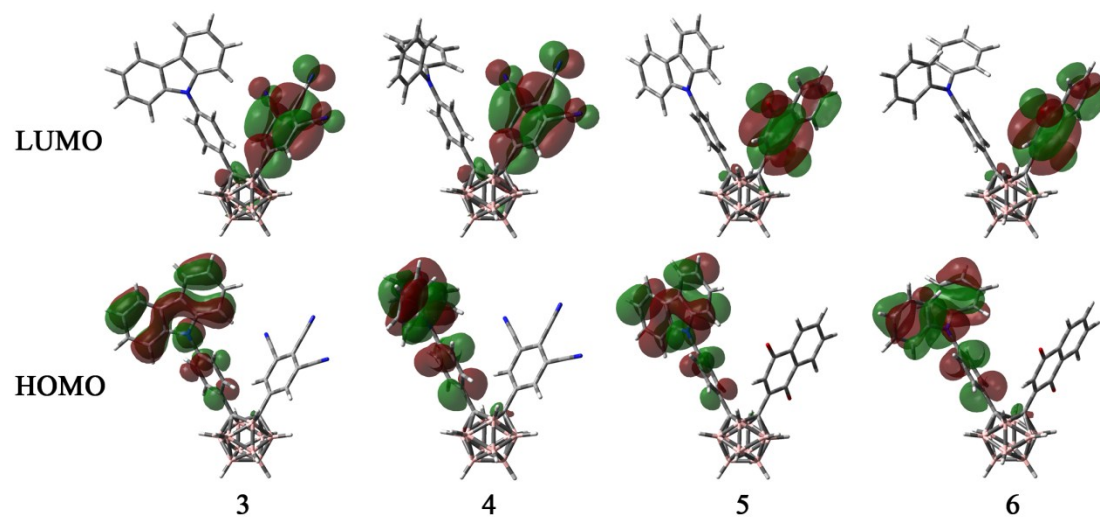
	<b>1</b>	<b>2</b>	<b>3</b>	<b>4</b>	<b>5</b>	<b>6</b>
Overlap integral	0.065	0.370	0.060	0.091	0.057	0.077



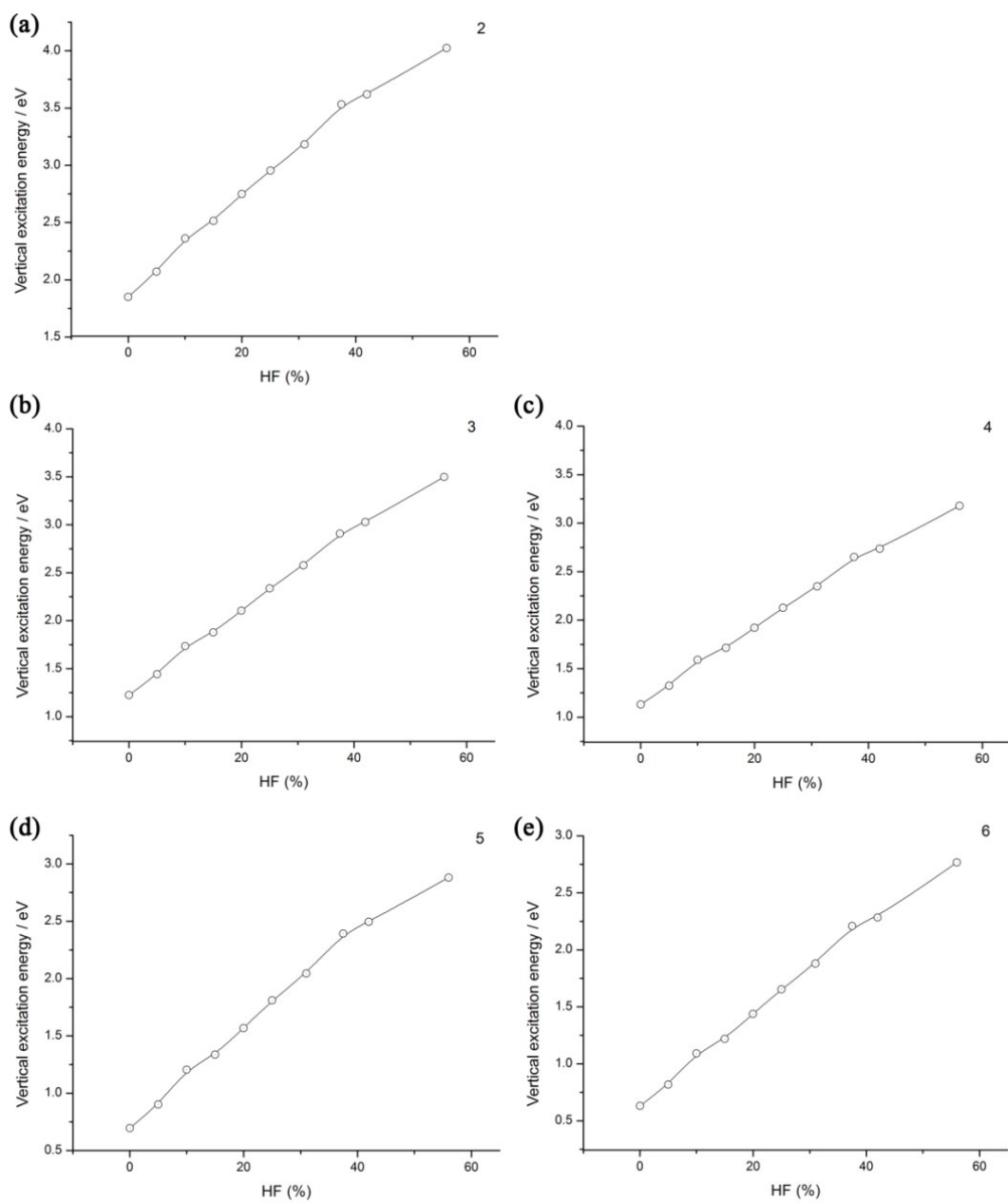
**Fig. S3** The calculated vertical excitation energies  $E_{VA}(S_1)/\text{eV}$  of  $S_0 \rightarrow S_1$  transition versus HF% for **1**.



**Fig. S4** Structural changes from  $S_0$  (in grey) to  $S_1$  (in cyan) states for single **3-6** molecules in isolated state and cluster in film.



**Fig. S5** Calculated frontier molecular orbital diagrams of **3-6**.



**Fig. S6** The calculated vertical excitation energies  $E_{VA}(S_1)/\text{eV}$  of  $S_0 \rightarrow S_1$  transition versus HF% for **2-6**.

**Table S3** Vertical excitation energies  $E(S_1)/\text{eV}$  of  $S_0 \rightarrow S_1$  transition for **3-6** calculated by different functionals with various HF percent, coupled with the values calculated by OHF[ $E_{VA}(S_1, \text{OHF})$ ] and the corresponding  $\Delta E_{ST}/\text{eV}$  [ $q$  denotes the CT amount in the excitation process and  $E_{VA}(T_1, \text{BLYP})$  is the vertical excitation energy of  $S_0 \rightarrow T_1$  transition].

Functional	HF(100%)	<b>3</b>	<b>4</b>	<b>5</b>	<b>6</b>
		$E_{VA}(S_1)$			
BLYP	5	1.224	1.132	0.696	0.631
MPWLYP1M	10	1.442	1.325	0.902	0.818
TPSSh	15	1.735	1.590	1.206	1.092
B3LYP*	20	1.877	1.714	1.337	1.219
B3LYP	25	2.105	1.922	1.567	1.438
PBE0	31	2.338	2.128	1.811	1.655
MPW1B95	33.33	2.578	2.348	2.045	1.880
PBE38	37.5	2.909	2.652	2.392	2.208
BMK	42	3.028	2.737	2.495	2.284
M062X	56	3.499	3.178	2.881	2.766
$42q$		39.56	37.84	39.44	38.56
$E_{VA}(S_1, \text{OHF})$		2.940	2.640	2.430	2.220
$E_{VA}(T_1, \text{BLYP})$		1.221	1.123	0.681	0.606
$\Delta E_{ST}$		0.009	0.023	0.052	0.090

**Table S4** Calculated C1–C2, C1–C3 and C2–C5 bond lengths (Å), C2–C1–C3–C4 dihedral angles and C1–C2–C5–C6 dihedral angles (°) of **1** before and after replacing the carborane moiety with phenyl moiety in  $S_0$  state at the PBE0/6-31G\* level.

	<b>1</b>	<b>1-Ph</b>
C1–C2	1.7056	1.4135
C1–C3	1.5022	1.4839
C2–C5	1.5011	1.4736
C2–C1–C3–C4	106.42	132.42
C1–C2–C5–C6	106.91	129.65

**Table S5** Relative energy (eV) of **1** when the C2–C1–C3–C4 dihedral angle and the C1–C2–C5–C6 dihedral angle (°) respectively change between 10° and 180° (the lowest energy point is set as the zero of energy, where the dihedral angles are both 100°).

1 C1–C2–C5–C6	C2–C1–C3–C4																		
	10	20	30	40	50	60	70	80	90	100	110	120	130	140	150	160	170	180	
10	11.295	5.722	2.970	1.660	1.027	0.703	0.530	0.459	0.480	0.606	0.886	1.431	2.561	5.008	10.11 1				
20	5.705	2.940	1.579	0.906	0.576	0.413	0.338	0.328	0.387	0.543	0.878	1.582	3.144	6.832					11.772
30	2.951	1.573	0.847	0.483	0.316	0.242	0.212	0.217	0.270	0.411	0.735	1.472	3.287	9.046			9.690	5.889	
40	1.645	0.900	0.483	0.282	0.195	0.159	0.144	0.146	0.174	0.273	0.530	1.146	2.636	5.973	8.322	6.416	4.733	2.987	
50	1.016	0.573	0.319	0.199	0.150	0.129	0.117	0.109	0.117	0.174	0.335	0.718	1.485	2.540	3.096	2.956	2.391	1.656	
60	0.694	0.413	0.250	0.172	0.139	0.123	0.111	0.096	0.086	0.115	0.201	0.390	0.716	1.111	1.407	1.491	1.335	1.028	
70	0.520	0.340	0.227	0.164	0.132	0.115	0.099	0.079	0.065	0.075	0.116	0.204	0.345	0.530	0.718	0.835	0.828	0.697	
80	0.439	0.330	0.238	0.166	0.121	0.097	0.080	0.057	0.037	0.042	0.064	0.108	0.177	0.277	0.404	0.511	0.556	0.512	
90	0.469	0.419	0.305	0.191	0.121	0.084	0.059	0.036	0.015	0.013	0.029	0.059	0.099	0.159	0.246	0.338	0.406	0.427	
100	0.714	0.680	0.454	0.279	0.169	0.104	0.064	0.031	0.007	0.000	0.013	0.037	0.065	0.106	0.173	0.261	0.359	0.457	
110	1.296	1.050	0.756	0.527	0.328	0.184	0.101	0.050	0.019	0.008	0.019	0.038	0.061	0.094	0.155	0.256	0.412	0.656	
120	1.851	1.658	1.484	1.150	0.714	0.373	0.183	0.091	0.046	0.027	0.034	0.052	0.075	0.111	0.183	0.327	0.623	1.195	
130	2.699	3.182	3.330	2.666	1.490	0.703	0.329	0.164	0.089	0.056	0.058	0.075	0.103	0.153	0.262	0.520	1.108	1.974	
140	5.069	6.928	9.197	6.000	2.531	1.095	0.514	0.266	0.155	0.103	0.097	0.118	0.160	0.247	0.444	0.908	1.788	2.868	
150	10.237			8.192	3.046	1.376	0.693	0.388	0.240	0.171	0.162	0.197	0.278	0.445	0.805	1.543	2.842	5.185	
160				6.265	2.885	1.449	0.805	0.492	0.333	0.263	0.271	0.351	0.516	0.837	1.476	2.762	5.349	10.249	
170			9.412	4.586	2.316	1.288	0.795	0.536	0.406	0.370	0.435	0.602	0.914	1.515	2.746	5.333	10.496		
180		11.34	5.677	2.877	1.598	0.990	0.670	0.499	0.435	0.470	0.620	0.918	1.479	2.632	5.112	10.156			



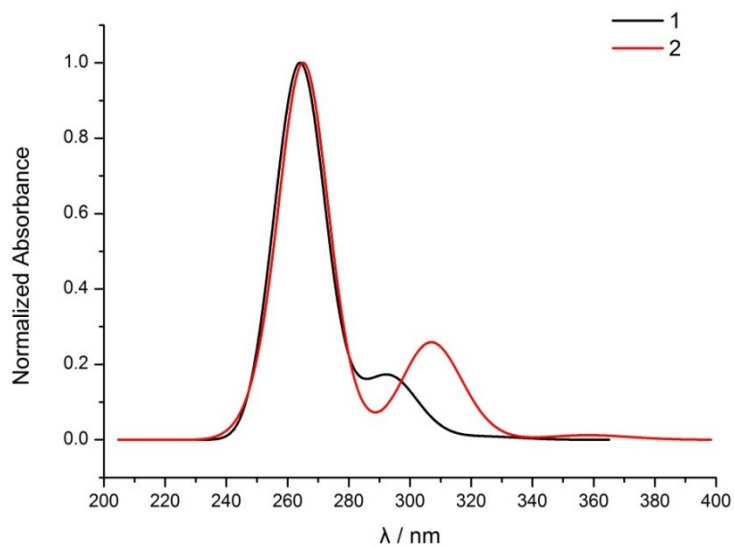
**Table S6** Relative energy (eV) of **1-Ph** when the C2–C1–C3–C4 dihedral angle and the C1–C2–C5–C6 dihedral angle (°) respectively change between 10° and 180° (the lowest energy point is set as the zero of energy, where the dihedral angles are both 130°).

1-Ph C1–C2–C5–C6	C2–C1–C3–C4																	
	10	20	30	40	50	60	70	80	90	100	110	120	130	140	150	160	170	180
10	21.371	11.151	5.720	3.083	1.811	1.171	0.847	0.701	0.685	0.788	1.030	1.494	2.414	4.371	8.578	16.459		
20	11.183	5.701	3.038	1.686	1.002	0.661	0.516	0.488	0.556	0.726	1.054	1.704	3.098	6.145	12.701			20.140
30	5.745	3.050	1.625	0.861	0.485	0.321	0.278	0.308	0.398	0.574	0.915	1.656	3.367	7.855			17.063	10.800
40	3.115	1.709	0.872	0.418	0.213	0.142	0.143	0.183	0.259	0.397	0.691	1.388	3.169	8.790			8.512	5.450
50	1.843	1.025	0.498	0.219	0.103	0.075	0.088	0.122	0.174	0.262	0.467	0.979	2.198	4.566	6.065	5.282	4.251	2.912
60	1.199	0.684	0.338	0.152	0.079	0.068	0.084	0.110	0.142	0.187	0.297	0.575	1.142	1.922	2.445	2.540	2.267	1.733
70	0.864	0.533	0.295	0.154	0.095	0.087	0.100	0.122	0.143	0.160	0.202	0.315	0.541	0.856	1.157	1.351	1.350	1.146
80	0.706	0.507	0.331	0.200	0.132	0.114	0.122	0.139	0.152	0.156	0.162	0.192	0.274	0.423	0.619	0.805	0.889	0.830
90	0.695	0.592	0.433	0.278	0.181	0.143	0.138	0.148	0.157	0.152	0.142	0.137	0.161	0.236	0.369	0.523	0.637	0.686
100	0.848	0.804	0.618	0.416	0.270	0.189	0.156	0.152	0.150	0.139	0.120	0.102	0.102	0.140	0.231	0.364	0.532	0.725
110	1.212	1.154	0.966	0.722	0.487	0.305	0.200	0.159	0.140	0.119	0.093	0.067	0.054	0.073	0.144	0.314	0.656	1.018
120	1.669	1.792	1.737	1.466	1.038	0.604	0.321	0.192	0.135	0.099	0.066	0.034	0.016	0.030	0.139	0.492	1.065	1.287
130	2.509	3.227	3.542	3.373	2.347	1.204	0.560	0.281	0.161	0.100	0.055	0.017	0.000	0.047	0.294	0.846	1.211	1.592
140	4.509	6.408	8.274		4.869	2.009	0.884	0.436	0.241	0.143	0.082	0.042	0.047	0.167	0.521	0.941	1.492	2.504
150	8.870	13.147			6.264	2.504	1.180	0.632	0.379	0.246	0.171	0.143	0.194	0.385	0.745	1.351	2.490	4.528
160	16.952				5.329	2.559	1.359	0.815	0.542	0.398	0.335	0.351	0.479	0.773	1.345	2.457	4.587	8.768

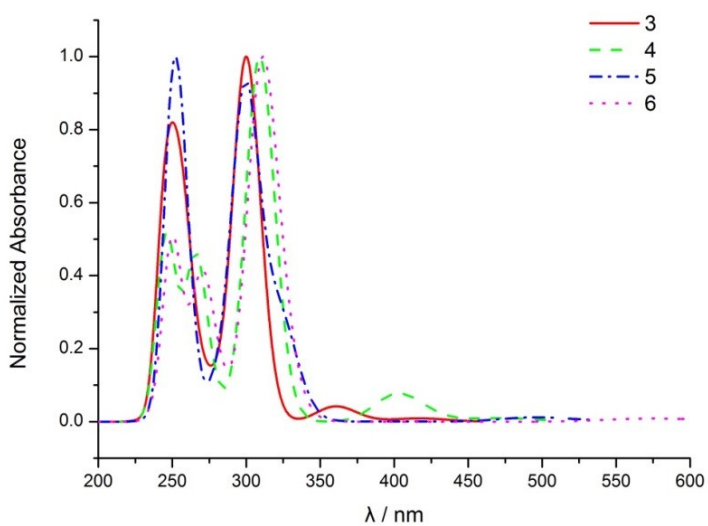
---

170	16.914	8.485	4.224	2.245	1.339	0.896	0.664	0.559	0.555	0.665	0.935	1.462	2.498	4.589	8.793	17.031
180	19.890	5.346	2.848	1.694	1.127	0.835	0.700	0.685	0.789	1.041	1.536	2.501	4.519	8.749	16.992	

---



**Fig. S7** The simulated absorption spectra of **1** and **2** in THF media by using TD-DFT/PBE38 method.



**Fig. S8** The simulated absorption spectra of **3-6** in THF media by using TD-DFT/PBE38 method.