Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C.

Supporting Information

The influence of tetraphenylethylene moieties on the emissive properties of dipyrrolonaphthyridinediones

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Table of contents

1. Cyclic voltammetry

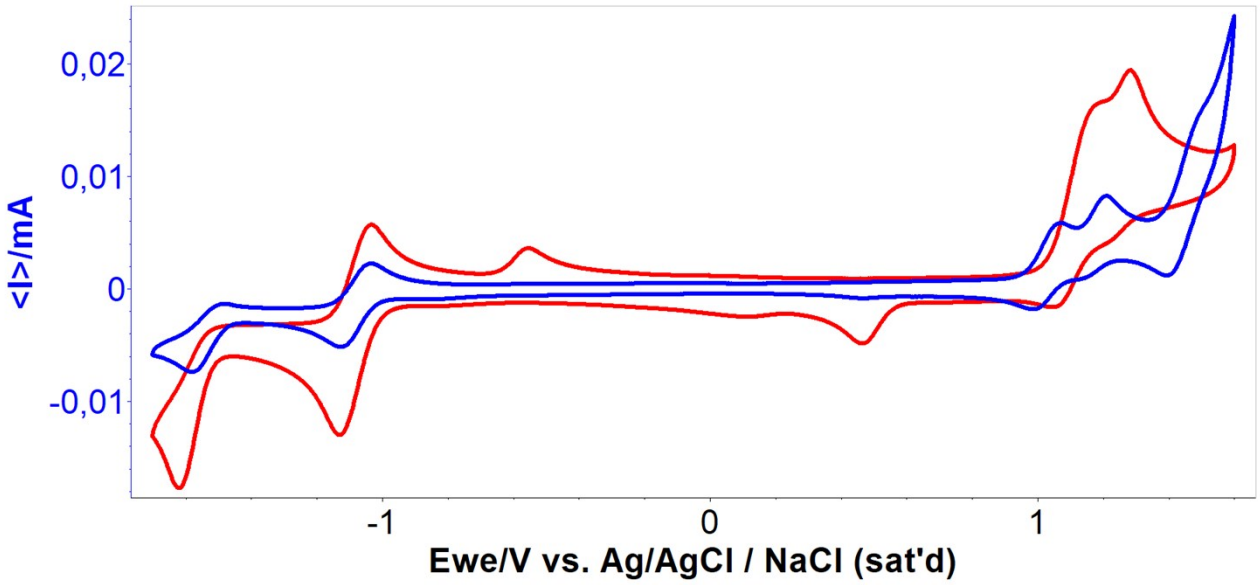


Figure S1. Cyclic voltammograms of **1** (blue) and **2** (red).

Table S1. Summary of electrochemical[a] properties of derivatives **1** and **2**.

Dye		Reduction			Oxidation	
		E_{red2} [V]	E_{red1} [V]	$E^{1/2}_{red1}$ [V]	E_{ox1} [V]	E_{ox2} [V]
1	E_{pa}	-1.482	-1.034	1.080	1.071	1.207
	E_{pc}	-1.582	-1.127		0.985	1.122
2	E_{pa}	-	-1.033	1.080	1.189	1.284
	E_{pc}	-1.620	-1.128		1.044	-

[a] Measurements conditions: compound (c = 0.1 - 0.2 mM); electrolyte (NBu_4ClO_4, c = 0.1 M); solvent: dry, degassed dichloromethane; potential sweep rate: 100 mV/s; working electrode: GC; auxiliary electrode: Pt wire; reference electrode: $Ag/AgCl/NaCl_{sat}$; all measurements were carried out at room temperature and under Ar atmosphere;

2. Computational details

Table S2. Transition energies and oscillator strengths (*f*) for molecular structures of **1** and **2** optimized in S_0 and S_1 electronic states (for the coordinates and vibrational frequencies, see Tables S5-S8). Structures were simplified by replacing alkyl chains with hydrogen. α – rotation angle of substituent plane in relations to the DPND core (in the case of TPE-DPND this angle concerns to the ring bonded with DPND), transition energy describes the absorption and fluorescence for S_0 and S_1 optimized structures, respectively, k_r is rate constant for radiative transition evaluated computationally. In last columns illustration for the geometry difference between C_i and C_2 isomers.

Molecule	**Symmetry**	***α*/ °**	**Transition energy /nm**	***f***	E_{HOMO}/ **eV**	E_{LUMO}/ **eV**	
S_0 state							
TPE-DPND (**1**)	C_i	43.5	628.1	1.0117	-4.988	-2.801	
	C_2	43.5	624.3	1.0329	-4.994	-2.797	
Ar-DPND (**2**)	C_i	45.4	543.9	0.7806	-5.186	-2.821	
	C_2	44.7	543.7	0.7875	-5.184	-2.823	
DPND	*Ci*	-	471.3	0.4560	-5.527	-2.894	
S_1 state							
					$10^{-8} \cdot k_r$ [s^{-1}]		
TPE-DPND (**1**)	C_i	34.0	705.5	1.2437	1.67		
	C_2	35.1	702.6	1.0810	1.46		
Ar-DPND (**2**)	C_i	35.9	599.5	0.8421	1.56		
	C_2	35.4	598.4	0.8458	1.57		
DPND	C_i	-	510.9	0.4586	1.17		

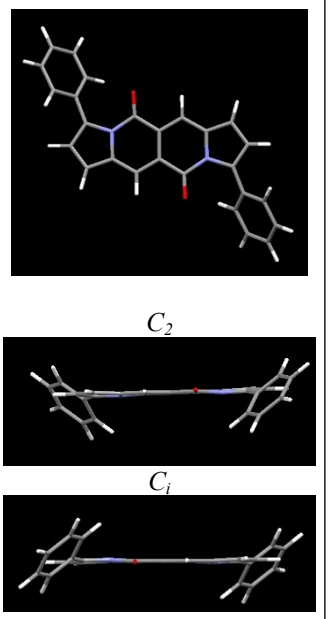
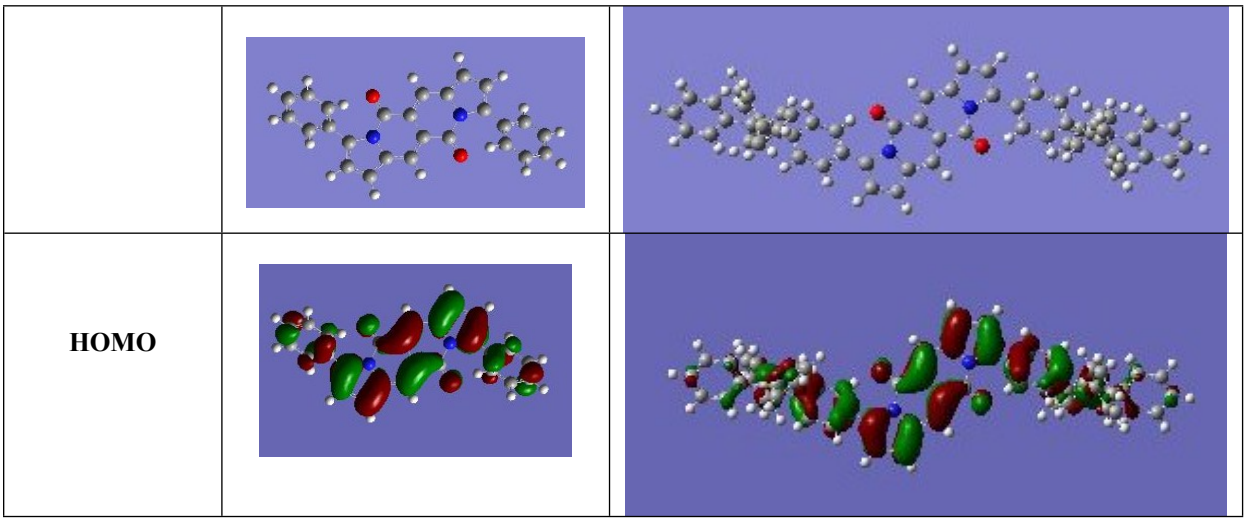
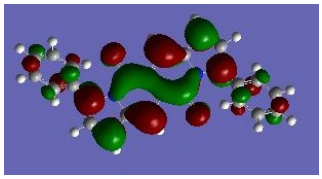
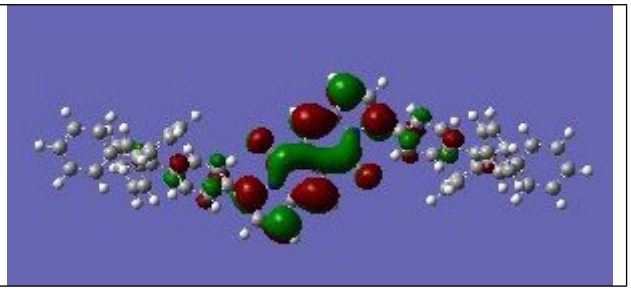


Table S3. HOMO and LUMO orbitals of **1** and **2**. Electronic configuration (HOMO, LUMO) describes $S_0 \rightarrow S_1$ and $S_1 \rightarrow S_0$ transitions.



LUMO		

Results of calculations for **1** and **2** are consistent with previously obtained results for DPND [1] and related molecules [2,3]. The electronic transitions between the S_0 and S_1 in molecules **1** and **2** are $\pi\pi^*$ transitions described by (HOMO, LUMO) configuration. HOMO and LUMO retain the features of the orbital of parent DPND molecule with some extension of π system on the substituents groups. The substitution of DPND by -Ar and -TPE at positions 3 and 9 mainly affects HOMO energy, causing a red shift in absorption and fluorescence. At the same time, the oscillator strength of the transition increases. In the excited state, the angle between the planes of the substituents and the central DPND plane decreases, which is accompanied by a slight increase in the strength of the transition oscillator.

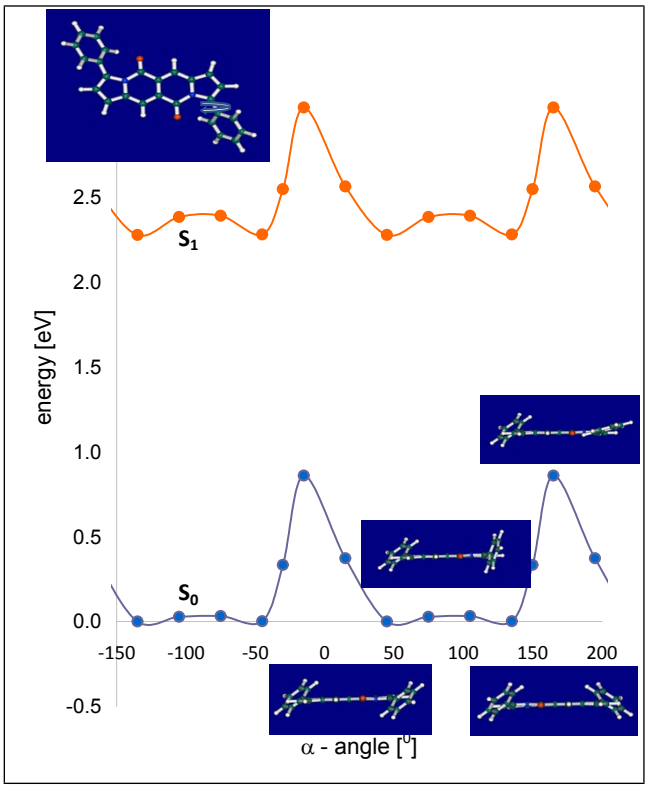


Figure S2. Restricted internal rotation of single -Ar group in Ar-DPND (**2**) molecule; α – rotation angle of substituent plane in relations to the DPND core plane. Inserts show the structure of a molecule in two minima and for two potential barriers. Two minima correspond to C_i and C_2 isomers. The rotation angle of the second substituent is constant (45˚).

The restricted internal rotation of the substituent at **1** and **2** occurs in a potential with two minima separated by a small barrier. These minima correspond to C_i and C_2 isomers. The height of the

barriers is controlled by steric factors, small for the perpendicular position (up to the DPND plane) position of the substituent and large for the parallel arrangement.

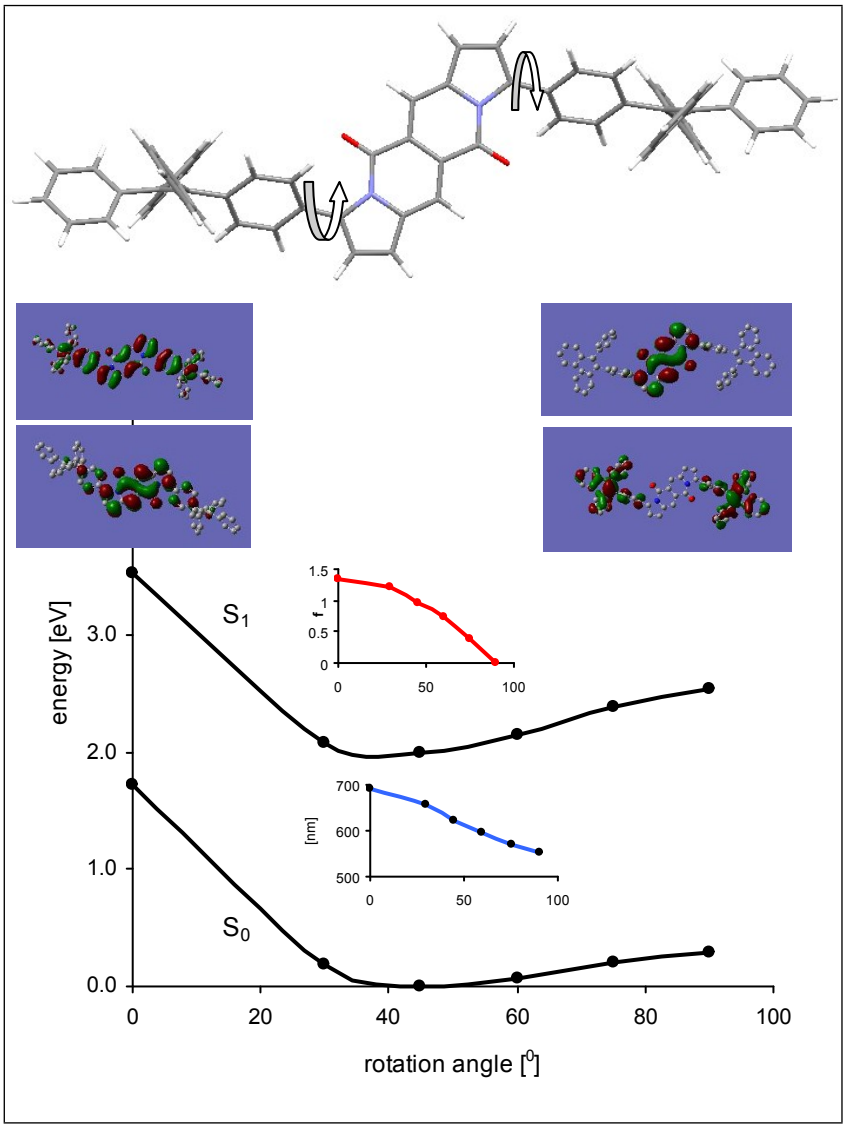
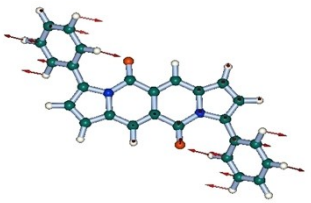
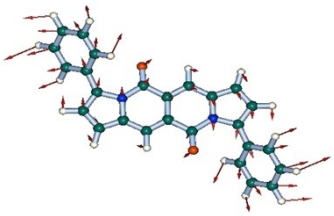
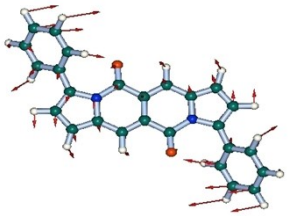
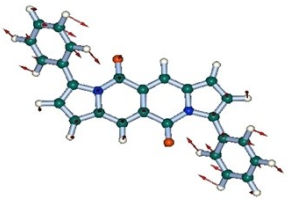
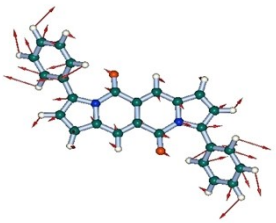
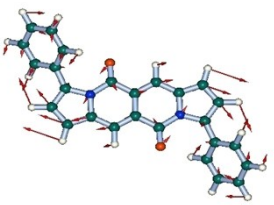
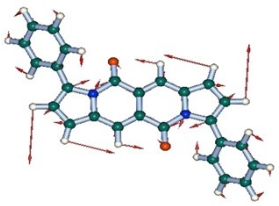


Figure S3. Internal rotation of both TPE groups in the molecule **1**, maintaining the symmetry of the molecule during rotation. With the perpendicular setting of substituents, the lowest excited state becomes the CT state with the zero oscillator strength. The inserts show the wavelength and oscillator strength of the transition as well as the electronic configurations corresponding to transitions in two extreme cases.

Table S4. Calculated Franck-Condon factors for vibronic transitions from $|S_1,0>$ state to $|S_0, n\cdot hv_i + m\cdot hv_k + \ldots.>$ states in **2** (n, m,… quantum numbers of hv_i, hv_k, … modes).

Initial vibronic state in excited S_1 electronic state	Final vibronic final state in ground S_0 electronic state	Energy of final vibronic state in relation to (0,0) transition [cm^{-1}]	FC factor	Shapes of some vibrations active in $S_1 \rightarrow S_0$ transition
<0|	|0>	0	0.663	
	|3^1>	-43	0.565	
	|5^1>	-52	0.677	
	|6^1>	-85	0.228	
	|3^2>	-85	0.240	
	|5^1;3^1>	-95	0.576	 3
	|5^2>	-105	0.345	
	|6^1;3^1>	-127	0.195	
	|3^3>	-128	0.068	
	|6^1;5^1>	-137	0.232	
	|5^1;3^2>	-138	0.245	 5
	|9^1>	-146	0.147	
	|5^2;3^1>	-147	0.293	
	|5^3>	-157	0.117	
	|6^2>	-169	0.039	
	|6^1;3^2>	-170	0.083	
	|6^1;5^1;3^1>	-180	0.198	
	|5^1;3^3>	-180	0.069	 6
	|9^1;3^1>	-189	0.126	
	|6^1;5^2>	-189	0.118	
	|5^2;3^2>	-190	0.125	
	|13^1>	-196	0.043	
	|9^1;5^1>	-199	0.151	 9
	|5^3;3^1>	-200	0.100	
	|5^4>	-209	0.030	
	|6^2;3^1>	-212	0.033	
	|6^1;3^3>	-213	0.024	
	|6^2;5^1>	-222	0.040	
	|6^1;5^1;3^2>	-222	0.085	 13
	|9^1;6^1>	-231	0.051	
	|9^1;3^2>	-232	0.054	
	|6^1;5^2;3^1>	-232	0.101	
	|5^2;3^3>	-233	0.035	
	|13^1;3^1>	-239	0.036	
	|9^1;5^1;3^1>	-242	0.128	 20
	|6^1;5^3>	-242	0.040	
	|5^3;3^2>	-242	0.042	
	|13^1;5^1>	-248	0.044	

|9^1;5^2>	-251	0.077	
|5^4;3^1>	-252	0.025	
|6^2;5^1;3^1>	-264	0.034	
|6^1;5^1;3^3>	-265	0.024	
|9^1;6^1;3^1>	-274	0.043	
|6^2;5^2>	-274	0.020	
|6^1;5^2;3^2>	-275	0.043	
|9^1;6^1;5^1>	-283	0.052	
|9^1;5^1;3^2>	-284	0.055	
|6^1;5^3;3^1>	-284	0.034	



86

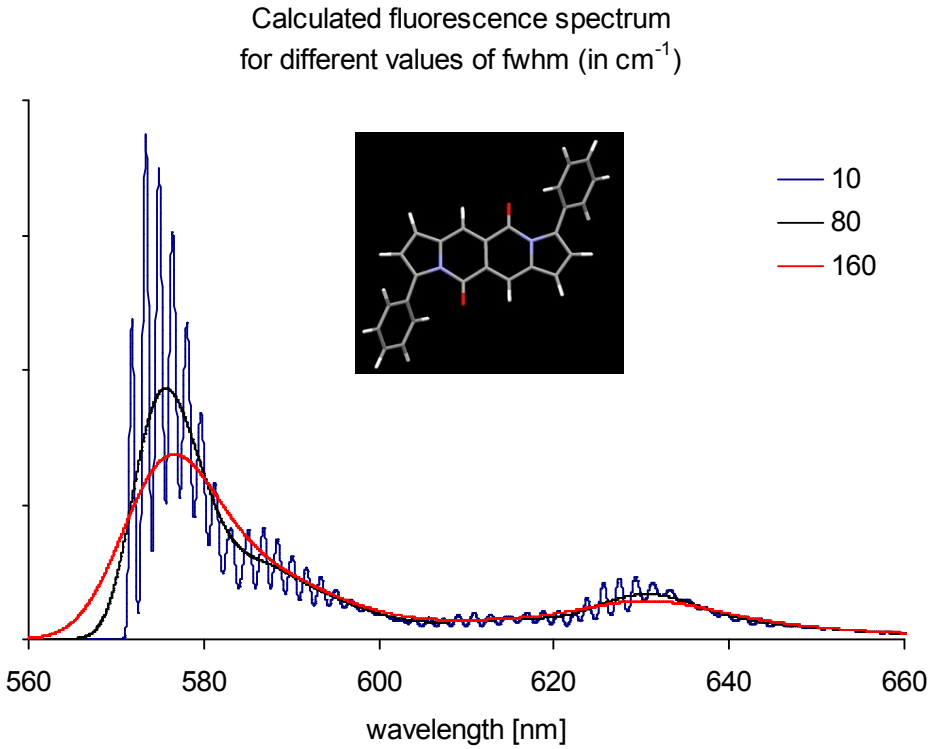


Figure S4. Simulation of fluorescence spectrum of **2** on the base of DFT and TDFT/6-31G(d,p) optimisations of **2** in ground S_0 and electronic excited S_1 states (see Table S8, S9 and Figure S5). Calculated energy of (0,0) transition is 17488 cm^{-1} (571.8 nm). Description of Franck-Condon factors in Table S4.

Table S5. Energies and oscillator strengths of electronic transition for different dimers of DPND. These dimers are formed by removing the monomer pairs from the DPND crystal [1]. At the top of the table, a symbolic description of HOMO and LUMO dimers as a combination of HOMO and LUMO, located on both monomers.

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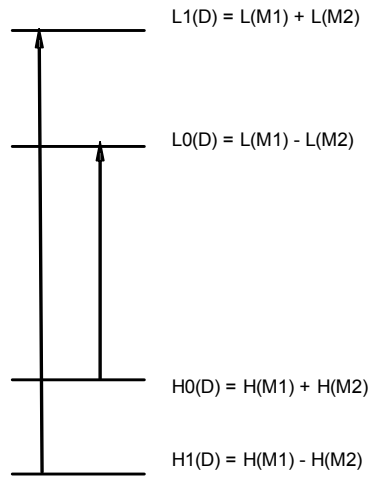
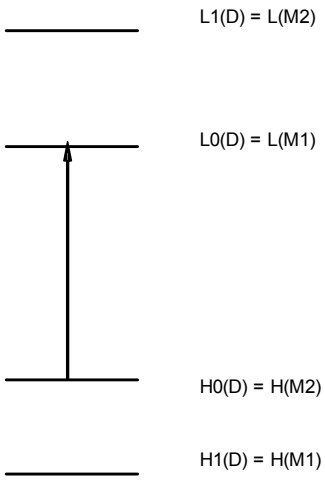
<tr><td colspan="2"> 
</td><td colspan="2"> 
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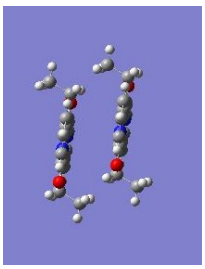
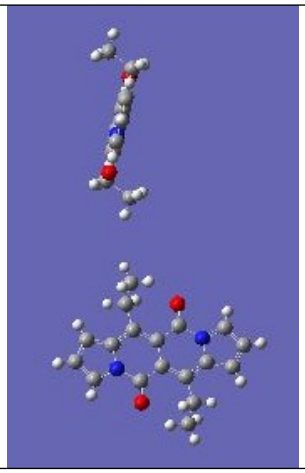
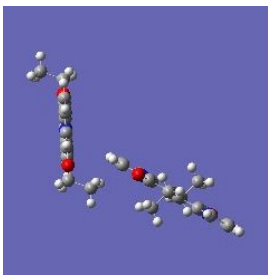
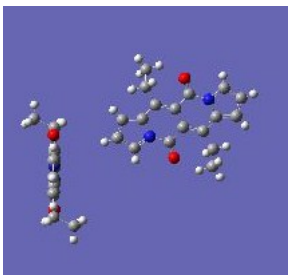
<tr><td>  </td><td>  </td><td>  </td><td>  </td></tr>
<tr><td>550.73 nm
$f = 0.0025$</td><td>482.40 nm
$f = 0.0002$</td><td>510.27 nm
$f = 0.0076$</td><td>489.29 nm
$f = 0.0000$</td></tr>
<tr><td>$\mu(S_0) = 0$
$\mu(S_1) = 0$</td><td>$\mu(S_0) = 0.1$
$\mu(S_1) = 0.1$</td><td>$\mu(S_0) = 0.3$
$\mu(S_1) = 36$</td><td>$\mu(S_0) = 0.2$
$\mu(S_1) = 57$</td></tr>
<tr><td colspan="4">monomer - 450.9 nm $f = 0.4239$ $\mu(S_0) = 0$ $\mu(S_1) = 0$</td></tr>
</table>

The four types of dimers removed from the DPND crystal are systems with low or zero oscillator strengths for the transition between the states S_0 and S_1, which makes the DPND ACQ-molecule. In the case of two dimers, the transition between S_0 and S_1 is an intermolecular CT transition, *i.e.* HOMO (monomer 2) → LUMO (monomer 1), in which the CT state has a high dipole moment.

Table S6. Cartesian coordinates of S_0 and S_1 for optimized structures of **1**.

S_0				S_1			
atom	x	y	z	atom	x	y	z
H	-14.9974	1.2589	-0.1925	H	-15.0667	0.9173	-0.0295
C	-13.9185	1.2065	-0.0796	C	-13.9847	0.9417	0.0603
H	-13.9607	-0.6143	1.0750	H	-13.8586	-0.9691	1.0528
H	-13.5475	3.0219	-1.1832	H	-13.7830	2.8680	-0.8888
C	-13.3358	0.1540	0.6286	C	-13.3053	-0.1193	0.6637
C	-13.1043	2.1961	-0.6339	C	-13.2638	2.0376	-0.4192
H	-10.8230	-4.4356	-2.4407	H	-10.5466	-4.2392	-2.7744

H	-9.5978	-4.6971	-0.2908	H	-9.2992	-4.5950	-0.6516
C	-10.4415	-3.5625	-1.9193	C	-10.2173	-3.3883	-2.1854
C	-11.9512	0.0847	0.7715	C	-11.9179	-0.0918	0.7756
H	-11.1513	-2.1627	-3.3981	H	-11.0186	-1.9235	-3.5507
C	-11.7206	2.1335	-0.4797	C	-11.8772	2.0730	-0.2943
C	-9.7526	-3.7085	-0.7138	C	-9.5152	-3.5875	-0.9950
C	-10.6281	-2.2866	-2.4542	C	-10.4858	-2.0879	-2.6187
H	-11.5049	-0.7365	1.3225	H	-11.3980	-0.9171	1.2497
H	-11.0942	2.9136	-0.9017	H	-11.3238	2.9311	-0.6625
C	-11.1179	1.0674	0.2111	C	-11.1744	1.0014	0.2909
C	-9.2553	-2.5882	-0.0504	C	-9.0835	-2.4953	-0.2455
C	-10.1406	-1.1656	-1.7847	C	-10.0671	-0.9960	-1.8624
H	-8.7100	-2.7099	0.8807	H	-8.5296	-2.6549	0.6743
C	-9.4549	-1.2952	-0.5653	C	-9.3655	-1.1794	-0.6572
H	-10.2885	-0.1771	-2.2064	H	-10.2752	0.0116	-2.2063
C	-9.6344	1.0221	0.3897	C	-9.6950	1.0583	0.4373
C	-8.8969	-0.1026	0.1438	C	-8.8796	-0.0171	0.1414
C	-9.0222	2.3041	0.8543	C	-9.1521	2.3605	0.9088
H	-10.4733	2.6206	2.4174	H	-10.6466	2.6250	2.4435
H	-7.4562	2.3266	-0.6257	H	-7.5521	2.4435	-0.5367
C	-9.5942	3.0202	1.9209	C	-9.7782	3.0603	1.9592
C	-7.9012	2.8552	0.2106	C	-8.0366	2.9555	0.2875
C	-7.4698	-0.2373	0.5595	C	-7.4709	-0.0963	0.5821
H	-7.7724	0.4458	2.5813	H	-7.8229	0.6371	2.5847
H	-6.8071	-1.0078	-1.3426	H	-6.7388	-0.9032	-1.2836
C	-9.0447	4.2269	2.3500	C	-9.2874	4.2893	2.3929
C	-7.3584	4.0676	0.6325	C	-7.5563	4.1908	0.7126
C	-7.0504	0.0710	1.8638	C	-7.0775	0.2706	1.8875
C	-6.5051	-0.7352	-0.3362	C	-6.4675	-0.5925	-0.2797
H	-9.4953	4.7566	3.1847	H	-9.7753	4.8031	3.2163
H	-6.4933	4.4754	0.1177	H	-6.6982	4.6321	0.2147
C	-7.9239	4.7560	1.7073	C	-8.1749	4.8607	1.7710
H	-7.4991	5.6998	2.0366	H	-7.7962	5.8224	2.1045
C	-5.7236	-0.0899	2.2459	C	-5.7588	0.1666	2.2935
C	-5.1755	-0.8800	0.0358	C	-5.1425	-0.6709	0.1133
H	-5.4241	0.1671	3.2573	H	-5.4889	0.4690	3.3002
H	-4.4578	-1.2496	-0.6853	H	-4.4011	-1.0265	-0.5879
C	-4.7552	-0.5559	1.3381	C	-4.7455	-0.2902	1.4163
H	-3.8269	-1.7171	3.7759	H	-3.8365	-1.0890	3.9961
C	-3.3952	-0.7985	1.8373	C	-3.3981	-0.4464	1.9419
O	-2.8627	0.6514	-0.6634	O	-2.8342	0.7006	-0.6980
C	-3.0870	-1.3834	3.0627	C	-3.0924	-0.8719	3.2427
N	-2.1810	-0.5621	1.1826	N	-2.1742	-0.3441	1.2560
C	-1.9464	0.1639	-0.0217	C	-1.9234	0.2412	-0.0128
C	-1.6928	-1.5235	3.1695	C	-1.7151	-1.0583	3.3634
H	-1.0064	1.2668	-2.2335	H	-0.9920	1.0142	-2.3772
C	-1.1281	-1.0121	2.0073	C	-1.1316	-0.7225	2.1318
H	-1.1378	-1.9574	3.9895	H	-1.1711	-1.4078	4.2293
C	-0.5274	0.2664	-0.4140	C	-0.5161	0.2358	-0.4339
C	-0.2160	0.8817	-1.5994	C	-0.2028	0.6928	-1.7092
C	0.2160	-0.8817	1.5994	C	0.2028	-0.6928	1.7092
C	0.5274	-0.2664	0.4140	C	0.5161	-0.2358	0.4339
H	1.1378	1.9574	-3.9895	H	1.1711	1.4078	-4.2293
C	1.1281	1.0121	-2.0073	C	1.1316	0.7225	-2.1318
H	1.0064	-1.2668	2.2335	H	0.9920	-1.0142	2.3772

C	1.6928	1.5235	-3.1695	C	1.7151	1.0583	-3.3634
C	1.9464	-0.1639	0.0217	C	1.9234	-0.2412	0.0128
N	2.1810	0.5621	-1.1826	N	2.1742	0.3441	-1.2560
C	3.0870	1.3834	-3.0627	C	3.0924	0.8719	-3.2427
O	2.8627	-0.6514	0.6634	O	2.8342	-0.7006	0.6980
C	3.3952	0.7985	-1.8373	C	3.3981	0.4464	-1.9419
H	3.8269	1.7171	-3.7759	H	3.8365	1.0890	-3.9961
C	4.7552	0.5559	-1.3381	C	4.7455	0.2902	-1.4163
H	4.4578	1.2496	0.6853	H	4.4011	1.0265	0.5879
H	5.4241	-0.1671	-3.2573	H	5.4889	-0.4690	-3.3002
C	5.1755	0.8800	-0.0358	C	5.1425	0.6709	-0.1133
C	5.7236	0.0899	-2.2459	C	5.7588	-0.1666	-2.2935
H	7.4991	-5.6998	-2.0366	H	7.7962	-5.8224	-2.1045
C	7.9239	-4.7560	-1.7073	C	8.1749	-4.8607	-1.7710
H	6.4933	-4.4754	-0.1177	H	6.6982	-4.6321	-0.2147
H	9.4953	-4.7566	-3.1847	H	9.7753	-4.8031	-3.2163
C	6.5051	0.7352	0.3362	C	6.4675	0.5925	0.2797
C	7.0504	-0.0710	-1.8638	C	7.0775	-0.2706	-1.8875
C	7.3584	-4.0676	-0.6325	C	7.5563	-4.1908	-0.7126
C	9.0447	-4.2269	-2.3500	C	9.2874	-4.2893	-2.3929
H	6.8071	1.0078	1.3426	H	6.7388	0.9032	1.2836
H	7.7724	-0.4458	-2.5813	H	7.8229	-0.6371	-2.5847
C	7.4698	0.2373	-0.5595	C	7.4709	0.0963	-0.5821
C	7.9012	-2.8552	-0.2106	C	8.0366	-2.9555	-0.2875
C	9.5942	-3.0202	-1.9209	C	9.7782	-3.0603	-1.9592
H	7.4562	-2.3266	0.6257	H	7.5521	-2.4435	0.5367
H	10.4733	-2.6206	-2.4174	H	10.6466	-2.6250	-2.4435
C	9.0222	-2.3041	-0.8543	C	9.1521	-2.3605	-0.9088
C	8.8969	0.1026	-0.1438	C	8.8796	0.0171	-0.1414
C	9.6344	-1.0221	-0.3897	C	9.6950	-1.0583	-0.4373
H	10.2885	0.1771	2.2064	H	10.2752	-0.0116	2.2063
C	9.4549	1.2952	0.5653	C	9.3655	1.1794	0.6572
H	8.7100	2.7099	-0.8807	H	8.5296	2.6549	-0.6743
C	10.1406	1.1656	1.7847	C	10.0671	0.9960	1.8624
C	9.2553	2.5882	0.0504	C	9.0835	2.4953	0.2455
C	11.1179	-1.0674	-0.2111	C	11.1744	-1.0014	-0.2909
H	11.0942	-2.9136	0.9017	H	11.3238	-2.9311	0.6625
H	11.5049	0.7365	-1.3225	H	11.3980	0.9171	-1.2497
C	10.6281	2.2866	2.4542	C	10.4858	2.0879	2.6187
C	9.7526	3.7085	0.7138	C	9.5152	3.5875	0.9950
C	11.7206	-2.1335	0.4797	C	11.8772	-2.0730	0.2943
H	11.1513	2.1627	3.3981	H	11.0186	1.9235	3.5507
C	11.9512	-0.0847	-0.7715	C	11.9179	0.0918	-0.7756
C	10.4415	3.5625	1.9193	C	10.2173	3.3883	2.1854
H	9.5978	4.6971	0.2908	H	9.2992	4.5950	0.6516
H	10.8230	4.4356	2.4407	H	10.5466	4.2392	2.7744
C	13.1043	-2.1961	0.6339	C	13.2638	-2.0376	0.4192
C	13.3358	-0.1540	-0.6286	C	13.3053	0.1193	-0.6637
H	13.5475	-3.0219	1.1832	H	13.7830	-2.8680	0.8888
H	13.9607	0.6143	-1.0750	H	13.8586	0.9691	-1.0528
C	13.9185	-1.2065	0.0796	C	13.9847	-0.9417	-0.0603
H	14.9974	-1.2589	0.1925	H	15.0667	-0.9173	0.0295

Table S7. Frequencies of vibrations of **1** in S_0 state.

mode	sym	freq	IR act	Mode	sym	freq	IR act	mode	sym	freq	IR act
1	AU	2.0	0.02	113	AU	739.9	3.54	225	AU	1296.2	41.26
2	AU	7.0	0.01	114	AU	752.2	7.96	226	AG	1299.7	0.00
3	AG	10.0	0.00	115	AG	753.2	0.00	227	AU	1300.1	3.24
4	AU	11.3	0.03	116	AU	770.1	65.86	228	AU	1323.4	63.98
5	AG	17.4	0.00	117	AG	771.0	0.00	229	AG	1325.5	0.00
6	AG	25.7	0.00	118	AG	773.1	0.00	230	AU	1328.8	18.46
7	AU	25.8	0.02	119	AU	778.4	9.62	231	AG	1330.1	0.00
8	AG	28.4	0.00	120	AG	780.9	0.00	232	AG	1330.9	0.00
9	AU	31.7	0.02	121	AU	781.6	31.56	233	AU	1333.9	12.44
10	AG	41.5	0.00	122	AG	793.3	0.00	234	AG	1334.9	0.00
11	AU	46.1	0.12	123	AU	793.7	22.64	235	AU	1336.3	5.24
12	AG	49.3	0.00	124	AG	804.7	0.00	236	AG	1337.1	0.00
13	AU	49.9	0.68	125	AU	808.9	81.48	237	AU	1347.3	0.63
14	AG	55.6	0.00	126	AG	824.6	0.00	238	AG	1347.3	0.00
15	AU	56.9	1.04	127	AU	837.6	2.89	239	AU	1349.6	87.47
16	AU	60.5	0.49	128	AG	841.8	0.00	240	AG	1360.6	0.00
17	AG	61.9	0.00	129	AU	846.8	17.14	241	AU	1360.6	3.06
18	AG	63.9	0.00	130	AU	849.1	8.12	242	AU	1361.4	8.44
19	AU	66.2	0.03	131	AG	849.2	0.00	243	AG	1361.4	0.00
20	AG	66.8	0.00	132	AG	860.1	0.00	244	AG	1361.8	0.00
21	AU	67.3	0.29	133	AU	860.1	0.40	245	AU	1361.8	1.53
22	AU	69.5	0.24	134	AU	861.7	1.90	246	AG	1369.1	0.00
23	AG	70.9	0.00	135	AG	861.7	0.00	247	AU	1392.7	31.61
24	AG	95.1	0.00	136	AU	862.4	2.65	248	AU	1411.1	197.11
25	AU	102.1	0.59	137	AG	862.4	0.00	249	AG	1423.1	0.00
26	AU	106.5	0.82	138	AG	868.4	0.00	250	AU	1451.2	68.48
27	AG	121.5	0.00	139	AU	868.5	22.64	251	AG	1452.4	0.00
28	AU	122.8	1.04	140	AG	879.5	0.00	252	AG	1454.4	0.00
29	AG	136.5	0.00	141	AU	880.0	12.56	253	AU	1482.6	2.56
30	AU	145.1	0.64	142	AU	888.9	4.77	254	AG	1482.6	0.00
31	AG	153.3	0.00	143	AG	889.0	0.00	255	AU	1483.1	11.21
32	AU	157.5	0.12	144	AG	928.7	0.00	256	AG	1483.1	0.00
33	AG	169.9	0.00	145	AU	930.3	4.25	257	AG	1485.0	0.00
34	AU	177.4	0.83	146	AG	930.4	0.00	258	AU	1485.0	18.78
35	AG	190.7	0.00	147	AU	934.3	16.53	259	AG	1508.7	0.00
36	AU	197.8	0.58	148	AU	936.4	2.18	260	AU	1509.2	628.28
37	AG	211.7	0.00	149	AG	936.4	0.00	261	AU	1531.2	18.17
38	AU	231.5	0.96	150	AU	937.8	8.92	262	AG	1531.2	0.00
39	AG	239.5	0.00	151	AG	937.9	0.00	263	AU	1534.4	14.56
40	AU	250.8	0.74	152	AG	938.9	0.00	264	AG	1534.4	0.00
41	AG	251.0	0.00	153	AU	954.9	17.43	265	AU	1535.3	45.36
42	AU	258.4	0.86	154	AG	973.5	0.00	266	AG	1535.3	0.00
43	AG	258.6	0.00	155	AU	973.7	0.45	267	AU	1549.1	165.18
44	AU	259.8	3.51	156	AG	974.4	0.00	268	AG	1556.0	0.00
45	AG	263.6	0.00	157	AU	974.4	2.35	269	AU	1564.0	292.75
46	AU	276.3	6.14	158	AU	975.6	1.24	270	AG	1590.5	0.00
47	AU	288.1	1.87	159	AG	975.6	0.00	271	AU	1594.1	63.08
48	AG	289.6	0.00	160	AG	976.1	0.00	272	AG	1597.8	0.00
49	AG	305.2	0.00	161	AU	976.1	0.56	273	AG	1609.4	0.00
50	AG	307.7	0.00	162	AG	976.9	0.00	274	AU	1610.2	0.85
51	AU	309.6	10.79	163	AU	976.9	1.69	275	AG	1622.6	0.00
52	AU	323.0	14.90	164	AU	992.9	9.01	276	AU	1627.8	1.39

53	AG	327.5	0.00	165	AG	993.0	0.00	277	AG	1627.8	0.00
54	AU	367.8	1.84	166	AU	997.6	1.42	278	AU	1628.9	7.50
55	AG	376.8	0.00	167	AG	997.6	0.00	279	AG	1628.9	0.00
56	AU	381.0	8.71	168	AG	997.9	0.00	280	AG	1634.7	0.00
57	AG	400.0	0.00	169	AU	997.9	1.23	281	AU	1634.7	0.88
58	AG	411.5	0.00	170	AU	1000.2	10.52	282	AU	1640.3	#####
59	AU	415.8	0.97	171	AG	1000.2	0.00	283	AU	1652.7	2.07
60	AG	416.1	0.00	172	AG	1015.5	0.00	284	AG	1652.7	0.00
61	AU	416.8	1.72	173	AU	1015.5	6.08	285	AG	1653.5	0.00
62	AG	417.1	0.00	174	AG	1015.9	0.00	286	AU	1653.6	9.34
63	AU	419.6	0.90	175	AU	1015.9	4.84	287	AU	1656.0	5.99
64	AG	419.8	0.00	176	AG	1016.1	0.00	288	AG	1656.0	0.00
65	AU	421.6	4.95	177	AU	1016.1	0.15	289	AG	1658.3	0.00
66	AG	423.2	0.00	178	AG	1017.1	0.00	290	AU	1658.3	12.41
67	AU	427.3	0.57	179	AU	1037.6	9.01	291	AG	1770.2	0.00
68	AU	451.9	1.89	180	AG	1040.5	0.00	292	AU	1774.8	806.83
69	AG	452.8	0.00	181	AU	1054.8	4.95	293	AU	3177.2	3.45
70	AU	470.8	5.41	182	AG	1054.8	0.00	294	AG	3177.2	0.00
71	AG	472.2	0.00	183	AU	1057.2	12.67	295	AU	3177.2	6.22
72	AU	490.0	2.89	184	AG	1057.2	0.00	296	AG	3177.3	0.00
73	AG	490.7	0.00	185	AU	1060.3	7.76	297	AU	3177.7	3.78
74	AU	519.6	11.89	186	AG	1060.4	0.00	298	AG	3177.7	0.00
75	AG	520.6	0.00	187	AG	1070.3	0.00	299	AU	3185.7	15.46
76	AU	540.0	14.83	188	AU	1073.7	113.98	300	AG	3185.7	0.00
77	AU	554.3	9.07	189	AU	1096.5	181.87	301	AG	3185.8	0.00
78	AG	560.6	0.00	190	AG	1108.2	0.00	302	AU	3185.8	7.00
79	AU	567.8	11.89	191	AU	1108.2	3.22	303	AU	3187.2	11.00
80	AG	577.5	0.00	192	AG	1109.7	0.00	304	AG	3187.2	0.00
81	AG	586.5	0.00	193	AU	1109.8	4.06	305	AU	3192.3	25.76
82	AU	587.2	26.61	194	AG	1110.3	0.00	306	AG	3192.3	0.00
83	AG	588.6	0.00	195	AU	1110.4	14.85	307	AU	3196.2	70.88
84	AU	598.9	37.72	196	AG	1124.1	0.00	308	AG	3196.2	0.00
85	AG	604.1	0.00	197	AU	1144.0	18.95	309	AU	3196.4	42.98
86	AU	630.7	2.17	198	AG	1146.9	0.00	310	AG	3196.4	0.00
87	AG	630.7	0.00	199	AU	1150.5	46.63	311	AG	3197.2	0.00
88	AU	632.4	1.90	200	AG	1156.7	0.00	312	AU	3197.2	37.98
89	AG	632.4	0.00	201	AU	1157.7	3.15	313	AU	3197.9	17.81
90	AU	635.7	3.96	202	AG	1179.2	0.00	314	AG	3197.9	0.00
91	AG	635.7	0.00	203	AU	1186.5	0.07	315	AG	3203.8	0.00
92	AG	642.9	0.00	204	AG	1186.5	0.00	316	AU	3203.8	109.05
93	AU	643.3	22.99	205	AU	1186.9	0.63	317	AU	3204.0	20.70
94	AU	649.8	14.75	206	AG	1186.9	0.00	318	AG	3204.0	0.00
95	AG	649.9	0.00	207	AU	1187.2	0.12	319	AU	3204.4	59.64
96	AG	657.9	0.00	208	AG	1187.2	0.00	320	AG	3204.4	0.00
97	AU	662.9	8.67	209	AU	1208.6	0.86	321	AU	3210.7	34.51
98	AU	671.9	4.91	210	AG	1208.6	0.00	322	AG	3210.7	0.00
99	AG	673.2	0.00	211	AU	1209.2	6.69	323	AU	3211.5	17.38
100	AG	679.1	0.00	212	AG	1209.2	0.00	324	AG	3211.5	0.00
101	AU	686.4	21.57	213	AU	1210.2	4.12	325	AU	3212.2	7.62
102	AG	691.4	0.00	214	AG	1210.2	0.00	326	AG	3212.2	0.00
103	AU	702.3	9.11	215	AU	1218.1	24.78	327	AU	3212.6	29.70
104	AG	703.3	0.00	216	AG	1218.5	0.00	328	AG	3212.6	0.00
105	AU	712.4	32.14	217	AU	1229.3	3.16	329	AG	3229.6	0.00
106	AG	712.7	0.00	218	AG	1233.6	0.00	330	AU	3229.8	4.37
107	AU	715.3	67.60	219	AU	1234.2	4.71	331	AG	3234.7	0.00

108	AG	715.5	0.00	220	AG	1234.7	0.00	332	AU	3234.7	12.10
109	AU	718.8	88.97	221	AU	1269.8	778.06	333	AU	3256.4	25.88
110	AG	719.0	0.00	222	AG	1280.6	0.00	334	AG	3256.4	0.00
111	AU	721.4	7.21	223	AU	1280.7	5.31	335	AU	3271.5	7.93
112	AG	727.7	0.00	224	AG	1281.9	0.00	336	AG	3271.5	0.00

Table S8 (S5)**.** Cartesian coordinates of S_0 and S_1 optimized structures of **2**.

S_0				S_1			
atom	x	y	z	atom	x	y	z
H	6.9153	-4.0593	1.6406	H	7.0835	-4.0010	1.4441
H	5.7808	-1.8623	1.6483	H	5.9317	-1.8250	1.5231
H	5.6409	0.1660	0.0712	H	5.6418	0.1516	0.2186
C	6.0836	-3.8803	0.9656	C	6.1850	-3.8468	0.8538
C	5.4482	-2.6398	0.9675	C	5.5404	-2.6164	0.8920
H	6.1382	-5.8562	0.1036	H	6.1746	-5.8461	0.0379
C	4.5606	0.1451	0.0652	C	4.5618	0.1385	0.1850
C	5.6463	-4.8880	0.1062	C	5.6728	-4.8835	0.0687
H	3.9713	2.2952	-0.0849	H	4.0068	2.2839	0.0197
C	4.3590	-2.3862	0.1152	C	4.3557	-2.3879	0.1529
C	3.6969	1.2510	-0.0306	C	3.7242	1.2418	0.0642
C	3.8053	-1.0228	0.0858	C	3.7960	-1.0425	0.1634
C	4.5693	-4.6450	-0.7501	C	4.5078	-4.6721	-0.6745
C	3.9300	-3.4093	-0.7483	C	3.8530	-3.4470	-0.6356
N	2.4615	-0.6411	0.0129	N	2.4545	-0.6490	0.0542
C	2.3955	0.7664	-0.0599	C	2.4009	0.7657	-0.0085
H	4.2256	-5.4229	-1.4254	H	4.1062	-5.4697	-1.2926
H	3.0962	-3.2337	-1.4162	H	2.9529	-3.3019	-1.2162
O	1.3760	-2.6582	0.3220	O	1.3376	-2.6559	0.3529
C	1.2977	-1.4527	0.1523	C	1.2830	-1.4422	0.1834
C	1.1509	1.4289	-0.1254	C	1.1802	1.4338	-0.0959
H	1.1246	2.5090	-0.2140	H	1.1512	2.5139	-0.1671
C	-0.0199	0.7181	-0.0704	C	-0.0135	0.7067	-0.0740
C	0.0199	-0.7181	0.0704	C	0.0135	-0.7067	0.0740
H	-1.1246	-2.5090	0.2140	H	-1.1512	-2.5139	0.1671
C	-1.1509	-1.4289	0.1254	C	-1.1802	-1.4338	0.0959
C	-1.2977	1.4527	-0.1523	C	-1.2830	1.4422	-0.1834
O	-1.3760	2.6582	-0.3220	O	-1.3376	2.6559	-0.3529
H	-3.0962	3.2337	1.4162	H	-2.9529	3.3019	1.2162
H	-4.2256	5.4229	1.4254	H	-4.1062	5.4697	1.2926
N	-2.4615	0.6411	-0.0129	N	-2.4545	0.6490	-0.0542
C	-2.3955	-0.7664	0.0599	C	-2.4009	-0.7657	0.0085
C	-3.9300	3.4093	0.7483	C	-3.8530	3.4470	0.6356
C	-4.5693	4.6450	0.7501	C	-4.5078	4.6721	0.6745
C	-3.8053	1.0228	-0.0858	C	-3.7960	1.0425	-0.1634
C	-3.6969	-1.2510	0.0306	C	-3.7242	-1.2418	-0.0642

C	-4.3590	2.3862	-0.1152	C	-4.3557	2.3879	-0.1529
H	-3.9713	-2.2952	0.0849	H	-4.0068	-2.2839	-0.0197
C	-5.6463	4.8880	-0.1062	C	-5.6728	4.8835	-0.0687
C	-4.5606	-0.1451	-0.0652	C	-4.5618	-0.1385	-0.1850
H	-6.1382	5.8562	-0.1036	H	-6.1746	5.8461	-0.0379
C	-5.4482	2.6398	-0.9675	C	-5.5404	2.6164	-0.8920
C	-6.0836	3.8803	-0.9656	C	-6.1850	3.8468	-0.8538
H	-5.6409	-0.1660	-0.0712	H	-5.6418	-0.1516	-0.2186
H	-5.7808	1.8623	-1.6483	H	-5.9317	1.8250	-1.5231
H	-6.9153	4.0593	-1.6406	H	-7.0835	4.0010	-1.4441

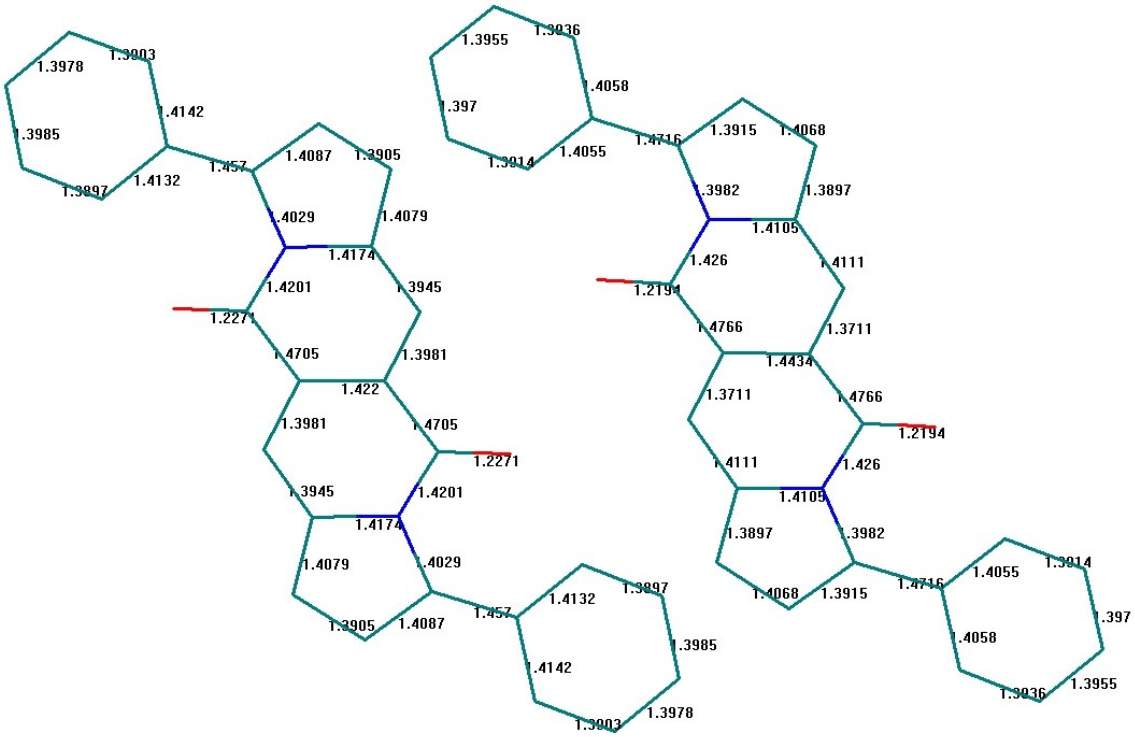


Figure S5. The length of the bonds in the ground state S_0 (left) and electronic excited state S_1(right) of the molecule **2**.

Table S9. Frequencies of vibrations of **2** in S_0 and S_1 electronic states

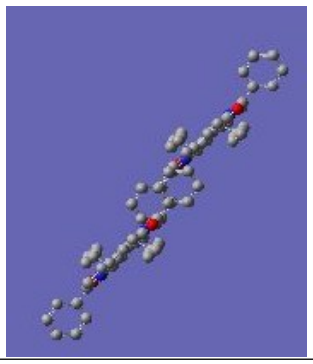
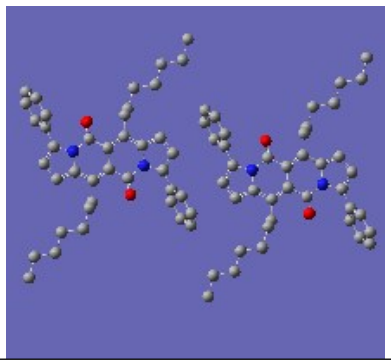
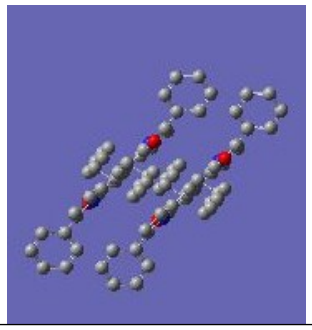
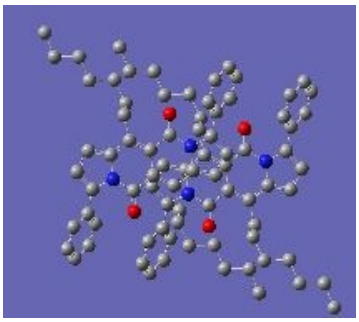
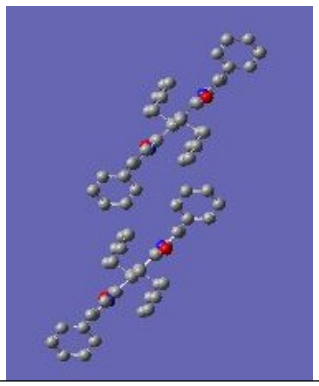
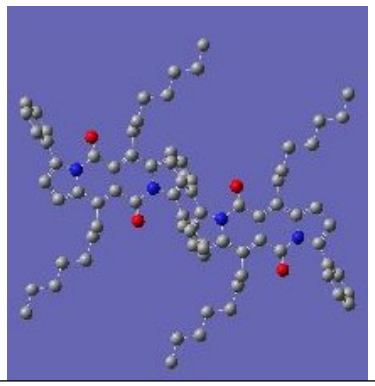
S_0				S_1			
mode	sym	freq [cm^{-1}]	IR act	Mode	Sym	freq [cm^{-1}]	IR act
1	AU	18.1	0.22	1	AU	16.5	0.67
2	AU	38.6	0.97	2	AU	40.2	1.53
3	AG	42.7	0.00	3	AG	41.7	0.00
4	AU	47.5	0.63	4	AU	48.8	2.81
5	AG	52.3	0.00	5	AG	57.7	0.00
6	AG	84.6	0.00	6	AG	90.7	0.00
7	AU	86.0	1.50	7	AU	96.3	6.00
8	AU	112.8	2.85	8	AU	108.5	3.56
9	AG	146.5	0.00	9	AU	146.9	62.25
10	AU	156.5	0.73	10	AG	154.5	0.00
11	AU	175.2	0.20	11	AU	177.9	33.31

12	AG	177.8	0.00	12	AG	184.5	0.00
13	AG	196.0	0.00	13	AG	201.5	0.00
14	AU	260.9	1.36	14	AU	239.2	216.46
15	AG	269.8	0.00	15	AG	258.2	0.00
16	AG	286.7	0.00	16	AU	280.1	0.00
17	AU	288.0	1.92	17	AU	296.5	22.98
18	AU	321.4	1.12	18	AU	309.4	15.01
19	AU	337.3	30.22	19	AG	337.3	16.18
20	AG	347.3	0.00	20	AU	339.5	0.00
21	AG	369.2	0.00	21	AG	363.9	0.00
22	AG	404.5	0.00	22	AG	401.8	0.00
23	AU	408.6	2.79	23	AU	402.3	14.81
24	AU	418.5	1.79	24	AG	414.7	74.26
25	AG	420.2	0.00	25	AG	422.4	0.00
26	AG	448.4	0.00	26	AU	447.8	26.00
27	AU	456.6	1.33	27	AU	452.4	0.00
28	AU	529.3	4.78	28	AU	512.1	264.65
29	AG	542.2	0.00	29	AG	529.6	0.00
30	AU	542.6	17.67	30	AG	529.8	100.01
31	AU	565.5	19.84	31	AG	537.3	0.00
32	AG	579.4	0.00	32	AU	556.8	33.96
33	AG	588.2	0.00	33	AU	582.8	0.00
34	AU	630.6	1.84	34	AG	627.3	2.71
35	AG	630.8	0.00	35	AU	627.4	0.00
36	AG	653.2	0.00	36	AG	654.4	0.00
37	AU	661.9	11.89	37	AU	664.0	4.15
38	AG	672.5	0.00	38	AG	665.0	71.30
39	AU	679.0	11.23	39	AU	666.9	0.00
40	AG	691.2	0.00	40	AG	671.0	0.00
41	AU	691.8	4.19	41	AU	683.9	50.81
42	AG	702.8	0.00	42	AG	695.6	0.00
43	AU	707.6	56.69	43	AU	697.6	92.81
44	AG	711.1	0.00	44	AG	706.9	0.00
45	AU	739.7	4.73	45	AG	715.0	12.19
46	AU	768.8	41.82	46	AU	746.2	1073.42
47	AG	773.1	0.00	47	AU	747.3	0.00
48	AG	774.2	0.00	48	AG	767.6	0.00
49	AU	784.0	36.20	49	AG	772.3	367.37
50	AG	808.1	0.00	50	AU	782.9	0.00
51	AU	811.8	57.26	51	AG	783.1	98.08
52	AG	824.7	0.00	52	AU	792.1	279.87
53	AU	843.3	9.26	53	AG	819.0	0.00
54	AG	852.9	0.00	54	AU	843.2	3.37
55	AU	853.0	2.01	55	AU	843.2	0.00
56	AU	887.6	3.72	56	AG	857.4	0.00
57	AG	887.7	0.00	57	AG	864.6	47.18
58	AG	928.3	0.00	58	AU	893.3	0.00
59	AU	930.9	2.97	59	AG	893.6	10.21
60	AG	931.5	0.00	60	AU	914.6	0.00
61	AU	935.3	14.98	61	AU	918.4	413.23
62	AG	940.1	0.00	62	AG	926.4	0.00
63	AU	955.6	3.97	63	AU	932.4	309.27
64	AU	971.7	2.73	64	AG	970.6	161.01
65	AG	971.7	0.00	65	AG	971.7	0.00
66	AG	996.1	0.00	66	AU	975.8	807.33

67	AU	996.2	0.55	67	AG	993.4	0.00
68	AG	1016.1	0.00	68	AU	993.5	1.17
69	AU	1016.2	6.67	69	AG	1008.7	0.00
70	AG	1018.0	0.00	70	AU	1011.9	10.17
71	AU	1055.1	3.38	71	AG	1013.1	0.00
72	AG	1057.3	0.00	72	AU	1052.9	6.35
73	AG	1069.7	0.00	73	AU	1054.9	0.00
74	AU	1072.0	76.59	74	AG	1083.0	0.00
75	AU	1098.5	137.74	75	AU	1084.0	39.24
76	AG	1111.1	0.00	76	AG	1108.4	228.95
77	AU	1111.2	10.76	77	AU	1112.5	0.00
78	AG	1125.9	0.00	78	AG	1114.3	22.70
79	AU	1148.9	44.71	79	AU	1122.0	0.00
80	AG	1178.8	0.00	80	AG	1167.9	0.00
81	AU	1188.5	0.46	81	AU	1187.7	67.20
82	AG	1188.5	0.00	82	AG	1188.3	0.00
83	AU	1213.0	26.36	83	AG	1189.5	77.82
84	AG	1213.3	0.00	84	AU	1215.1	79.66
85	AU	1228.9	2.75	85	AU	1216.1	0.00
86	AG	1234.8	0.00	86	AG	1219.8	2.98
87	AU	1271.9	623.33	87	AU	1221.0	0.00
88	AG	1282.9	0.00	88	AG	1244.7	505.37
89	AU	1295.9	25.99	89	AG	1284.4	30.09
90	AG	1327.4	0.00	90	AU	1288.1	0.00
91	AU	1327.7	77.50	91	AG	1330.8	0.00
92	AG	1333.0	0.00	92	AU	1335.8	27.54
93	AU	1348.5	104.78	93	AU	1345.4	0.00
94	AG	1364.1	0.00	94	AG	1347.1	0.00
95	AU	1364.6	5.92	95	AU	1363.5	3.68
96	AG	1369.5	0.00	96	AG	1370.6	0.00
97	AU	1392.7	19.37	97	AU	1371.6	5.02
98	AU	1412.3	173.13	98	AU	1390.8	3.37
99	AG	1425.7	0.00	99	AG	1425.9	0.00
100	AG	1454.1	0.00	100	AG	1466.9	0.00
101	AU	1486.6	72.08	101	AU	1469.2	13.97
102	AG	1487.3	0.00	102	AG	1485.8	0.00
103	AG	1510.9	0.00	103	AG	1488.9	121.26
104	AU	1510.9	250.98	104	AU	1498.5	39.17
105	AU	1545.9	38.20	105	AG	1502.6	0.00
106	AG	1550.2	0.00	106	AU	1537.1	0.00
107	AU	1565.5	283.86	107	AU	1538.0	17.62
108	AG	1598.1	0.00	108	AG	1545.3	0.00
109	AG	1620.0	0.00	109	AG	1574.9	98.35
110	AU	1630.8	64.80	110	AU	1587.2	0.00
111	AG	1633.0	0.00	111	AG	1610.5	40.13
112	AU	1642.5	1091.87	112	AU	1611.5	0.00
113	AU	1657.2	4.47	113	AU	1644.0	76.57
114	AG	1657.3	0.00	114	AG	1648.2	0.00
115	AG	1772.8	0.00	115	AG	1710.4	469.98
116	AU	1777.1	616.10	116	AU	1725.1	0.00
117	AU	3181.0	5.33	117	AG	3181.7	19.93
118	AG	3181.0	0.00	118	AU	3181.7	0.00
119	AU	3190.0	11.11	119	AG	3190.9	0.00
120	AG	3190.0	0.00	120	AU	3190.9	12.07
121	AU	3199.5	53.95	121	AG	3201.5	0.00

122	AG	3199.5	0.00	122	AU	3201.9	48.46
123	AU	3208.4	81.29	123	AG	3209.8	143.76
124	AG	3208.5	0.00	124	AU	3209.9	0.00
125	AG	3229.2	0.00	125	AG	3240.0	0.00
126	AU	3229.4	3.15	126	AU	3240.1	16.09
127	AG	3233.6	0.00	127	AG	3253.9	13.44
128	AU	3233.6	8.48	128	AG	3253.9	0.00
129	AU	3256.3	15.33	129	AU	3256.3	0.53
130	AG	3256.3	0.00	130	AG	3256.5	0.00
131	AU	3271.2	6.88	131	AU	3271.8	0.00
132	AG	3271.3	0.00	132	AU	3272.2	15.48

Table S10. Energies and oscillator strengths of four lowest energy electronic transitions ($S_0 \rightarrow S_i$, i = 1-4) for different dimers of DPND **1**, calculated by TD B3LYP/6-31G(d,p) method. The dimers are obtained by removing the monomer pairs from the DPND **1** crystal. The energies and oscillator strengths for two lowest excited state of DPND **1** monomer in crystal geometry are following: S_1(AU) 492.8 nm, f = 0.6126 and S_2(AG) 428.14 nm, f = 0.0000.

		S_1(AU) 516.34 nm; f=0.1395 S_2(AG) 515.19 nm f=0.0000 S_3(AU) 501.45 nm f=1.3115 S_4(AG) 485.94 nm f=0.0000
		S_1(AG) 576.11 nm f=0.0000 S_2(AU) 573.68 nm f=0.0156 S_3(AG) 509.96 nm f=0.0000 S_4(AU) 489.10 nm f=1.0334
		S_1(AU) 523.32 nm f=0.0014 S_2(AG) 523.31 nm f=0.0000 S_3(AU) 499.93 nm f=1.2839 S_4 (AG) 490.62 nm f=0.0000

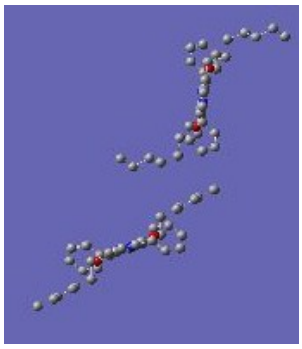
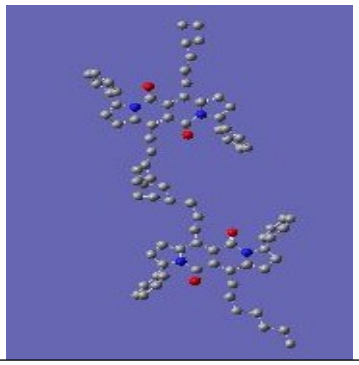
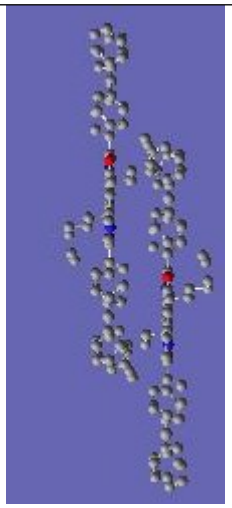
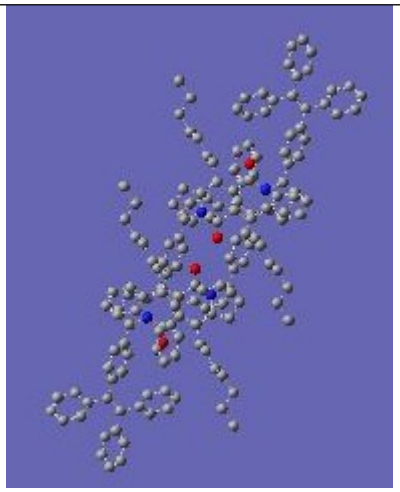
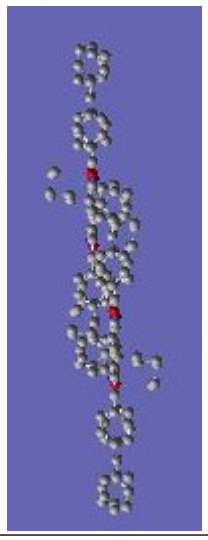
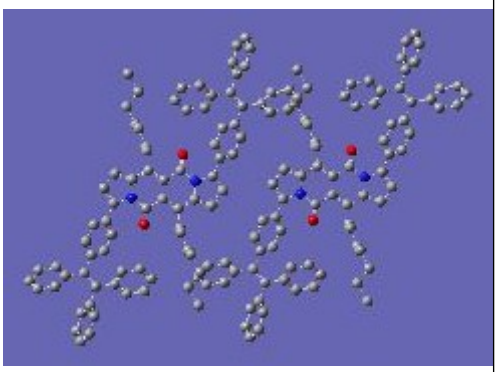
		502.97 nm f=0.0000 493.62 nm f=0.1916 493.08 nm f=0.0000 487.98 nm f=0.9785

Table S11. Energies and oscillator strengths of four lowest energy electronic transitions ($S_0 \rightarrow S_i$, I = 1-4) for different dimers of DPND **2**, calculated by TD B3LYP/6-31G(d,p) method. The dimers are obtained by removing the monomer pairs from the DPND **2** crystal. The energies and oscillator strengths for two lowest excited state of DPND **2** monomer in crystal geometry are following: S_1(AU) 552.5 nm; f = 0.4570 (HOMO → LUMO) and S_2(AG) 524.66 nm; f = 0.0000 (HOMO-1 → LUMO). Atom coordinates for dimer B are given in Table S12.

		S_1(AG) 587.28 nm f=0.0000 S_2(AU) 585.35 nm f=0.0313 S_3(AG) 561.28 nm f=0.0000 S_4(AU) 557.15 nm f=0.7373 A
		S_1(AU) 549.15 nm f=1.0472 S_2(AG) 544.04 nm f=0.0000 S_3(AU) 537.60 nm f=0.0009 S_4(AG) 537.50 nm f=0.0000

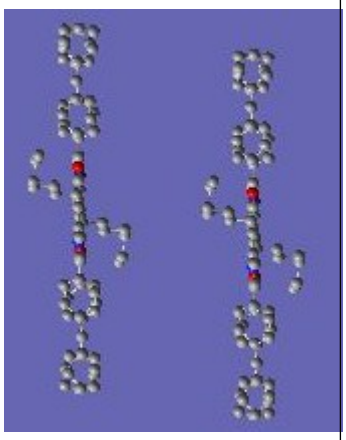
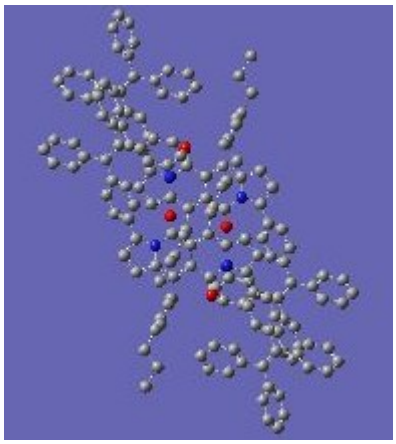
		B
		S_1(AG) 554.43 nm f=0.0000 S_2(AU) 550.70 nm f=0.8421 S_3(AG) 532.69 nm f=0.0000 S_4(AU) 532.69 nm f=0.0000 C

Table S12. Atom coordinates of dimer B of DPND **2** (see also Table S11).

	x	y	z		x	y	z		x	y	z		x	y	z
C	4.4051	-6.5160	-0.5998	C	0.9527	-5.1352	0.5998	C	-0.9527	5.1352	-0.5998	C	-4.4051	6.5160	0.5998
C	5.2059	-8.8331	-0.0464	C	0.1519	-2.8181	0.0464	C	-0.1519	2.8181	-0.0464	C	-5.2059	8.8331	0.0464
C	4.6253	-9.8905	0.6114	C	0.7326	-1.7606	-0.6114	C	-0.7326	1.7606	0.6114	C	-4.6253	9.8905	-0.6114
H	5.0086	-10.7539	0.7120	H	0.3493	-0.8972	-0.7120	H	-0.3493	0.8972	0.7120	H	-5.0086	10.7539	-0.7120
C	3.3751	-9.4924	1.1132	C	1.9828	-2.1588	-1.1132	C	-1.9828	2.1588	1.1132	C	-3.3751	9.4924	-1.1132
H	2.7722	-10.0348	1.6085	H	2.5856	-1.6163	-1.6085	H	-2.5856	1.6163	1.6085	H	-2.7722	10.0348	-1.6085
C	3.1804	-8.1775	0.7585	C	2.1775	-3.4736	-0.7585	C	-2.1775	3.4736	0.7585	C	-3.1804	8.1775	-0.7585
C	3.2840	-4.3544	-0.9803	C	2.0739	-7.2968	0.9803	C	-2.0739	7.2968	-0.9803	C	-3.2840	4.3544	0.9803
C	3.2523	-5.6137	-0.4089	C	2.1055	-6.0375	0.4089	C	-2.1055	6.0375	-0.4089	C	-3.2523	5.6137	0.4089
C	6.5203	-8.8509	-0.7017	C	-1.1624	-2.8003	0.7017	C	1.1624	2.8003	-0.7017	C	-6.5203	8.8509	0.7017
C	7.5541	-7.9783	-0.3573	C	-2.1963	-3.6729	0.3573	C	2.1963	3.6729	-0.3573	C	-7.5541	7.9783	0.3573
H	7.4105	-7.3133	0.3070	H	-2.0527	-4.3379	-0.3070	H	2.0527	4.3379	0.3070	H	-7.4105	7.3133	-0.3070
C	8.7793	-8.0742	-0.9726	C	-3.4214	-3.5770	0.9726	C	3.4214	3.5770	-0.9726	C	-8.7793	8.0742	0.9726
H	9.4743	-7.4752	-0.7275	H	-4.1165	-4.1760	0.7275	H	4.1165	4.1760	-0.7275	H	-9.4743	7.4752	0.7275
C	9.0173	-9.0405	-1.9542	C	-3.6595	-2.6107	1.9542	C	3.6595	2.6107	-1.9542	C	-9.0173	9.0405	1.9542
C	8.0071	-9.9409	-2.2548	C	-2.6493	-1.7103	2.2548	C	2.6493	1.7103	-2.2548	C	-8.0071	9.9409	2.2548
H	8.1648	-10.6342	-2.8856	H	-2.8070	-1.0169	2.8856	H	2.8070	1.0169	-2.8856	H	-8.1648	10.6342	2.8856
C	6.7628	-9.8357	-1.6395	C	-1.4049	-1.8155	1.6395	C	1.4049	1.8155	-1.6395	C	-6.7628	9.8357	1.6395
H	6.0735	-10.4487	-1.8665	H	-0.7156	-1.2024	1.8665	H	0.7156	1.2024	-1.8665	H	-6.0735	10.4487	1.8665
C	10.3075	-9.0640	-2.7089	C	-4.9497	-2.5872	2.7089	C	4.9497	2.5872	-2.7089	C	-10.3075	9.0640	2.7089
C	10.7127	-7.9627	-3.3951	C	-5.3548	-3.6884	3.3951	C	5.3548	3.6884	-3.3951	C	-10.7127	7.9627	3.3951
C	11.1071	-10.3121	-2.6328	C	-5.7493	-1.3390	2.6328	C	5.7493	1.3390	-2.6328	C	-11.1071	10.3121	2.6328
C	11.7350	-10.8733	-3.7421	C	-6.3771	-0.7778	3.7421	C	6.3771	0.7778	-3.7421	C	-11.7350	10.8733	3.7421
H	11.6042	-10.4891	-4.5999	H	-6.2463	-1.1620	4.5999	H	6.2463	1.1620	-4.5999	H	-11.6042	10.4891	4.5999
C	12.5453	-11.9852	-3.6067	C	-7.1874	0.3341	3.6067	C	7.1874	-0.3341	-3.6067	C	-12.5453	11.9852	3.6067
H	12.9742	-12.3530	-4.3703	H	-7.6163	0.7018	4.3703	H	7.6163	-0.7018	-4.3703	H	-12.9742	12.3530	4.3703
C	12.7344	-12.5643	-2.3696	C	-7.3766	0.9132	2.3696	C	7.3766	-0.9132	-2.3696	C	-12.7344	12.5643	2.3696
H	13.3127	-13.3117	-2.2767	H	-7.9549	1.6605	2.2767	H	7.9549	-1.6605	-2.2767	H	-13.3127	13.3117	2.2767
C	12.0841	-12.0539	-1.2719	C	-6.7262	0.4027	1.2719	C	6.7262	-0.4027	-1.2719	C	-12.0841	12.0539	1.2719

H	12.1915	-12.4666	-0.4231	H	-6.8337	0.8154	0.4231	H	6.8337	-0.8154	-0.4231	H	-12.1915	12.4666	0.4231
C	11.2699	-10.9382	-1.4022	C	-5.9121	-0.7129	1.4022	C	5.9121	0.7129	-1.4022	C	-11.2699	10.9382	1.4022
H	10.8169	-10.5985	-0.6398	H	-5.4590	-1.0527	0.6398	H	5.4590	1.0527	-0.6398	H	-10.8169	10.5985	0.6398
C	12.0531	-7.8633	-4.0375	C	-6.6952	-3.7879	4.0375	C	6.6952	3.7879	-4.0375	C	-12.0531	7.8633	4.0375
C	12.1529	-7.4997	-5.3751	C	-6.7950	-4.1515	5.3751	C	6.7950	4.1515	-5.3751	C	-12.1529	7.4997	5.3751
H	11.3618	-7.3456	-5.8782	H	-6.0039	-4.3055	5.8782	H	6.0039	4.3055	-5.8782	H	-11.3618	7.3456	5.8782
C	13.3855	-7.3588	-5.9853	C	-8.0276	-4.2924	5.9853	C	8.0276	4.2924	-5.9853	C	-13.3855	7.3588	5.9853
H	13.4330	-7.1297	-6.9063	H	-8.0752	-4.5215	6.9063	H	8.0752	4.5215	-6.9063	H	-13.4330	7.1297	6.9063
C	14.5458	-7.5493	-5.2655	C	-9.1880	-4.1018	5.2655	C	9.1880	4.1018	-5.2655	C	-14.5458	7.5493	5.2655
H	15.3919	-7.4358	-5.6822	H	-10.0341	-4.2154	5.6822	H	10.0341	4.2154	-5.6822	H	-15.3919	7.4358	5.6822
C	14.4670	-7.9072	-3.9291	C	-9.1091	-3.7440	3.9291	C	9.1091	3.7440	-3.9291	C	-14.4670	7.9072	3.9291
H	15.2632	-8.0451	-3.4286	H	-9.9053	-3.6061	3.4286	H	9.9053	3.6061	-3.4286	H	-15.2632	8.0451	3.4286
C	13.2331	-8.0657	-3.3216	C	-7.8752	-3.5854	3.3216	C	7.8752	3.5854	-3.3216	C	-13.2331	8.0657	3.3216
H	13.1894	-8.3161	-2.4057	H	-7.8316	-3.3351	2.4057	H	7.8316	3.3351	-2.4057	H	-13.1894	8.3161	2.4057
C	9.8706	-6.7419	-3.5009	C	-4.5127	-4.9092	3.5009	C	4.5127	4.9092	-3.5009	C	-9.8706	6.7419	3.5009
C	10.4238	-5.5069	-3.1758	C	-5.0659	-6.1443	3.1758	C	5.0659	6.1443	-3.1758	C	-10.4238	5.5069	3.1758
H	11.3375	-5.4573	-2.9204	H	-5.9796	-6.1939	2.9204	H	5.9796	6.1939	-2.9204	H	-11.3375	5.4573	2.9204
C	9.6700	-4.3535	-3.2171	C	-4.3122	-7.2977	3.2171	C	4.3122	7.2977	-3.2171	C	-9.6700	4.3535	3.2171
H	10.0612	-3.5208	-2.9797	H	-4.7033	-8.1304	2.9797	H	4.7033	8.1304	-2.9797	H	-10.0612	3.5208	2.9797
C	8.3372	-4.4096	-3.6067	C	-2.9793	-7.2415	3.6067	C	2.9793	7.2415	-3.6067	C	-8.3372	4.4096	3.6067
H	7.8144	-3.6166	-3.6337	H	-2.4565	-8.0346	3.6337	H	2.4565	8.0346	-3.6337	H	-7.8144	3.6166	3.6337
C	7.7795	-5.6167	-3.9511	C	-2.4217	-6.0345	3.9511	C	2.4217	6.0345	-3.9511	C	-7.7795	5.6167	3.9511
H	6.8711	-5.6545	-4.2245	H	-1.5132	-5.9967	4.2245	H	1.5132	5.9967	-4.2245	H	-6.8711	5.6545	4.2245
C	8.5313	-6.7801	-3.9020	C	-3.1735	-4.8710	3.9020	C	3.1735	4.8710	-3.9020	C	-8.5313	6.7801	3.9020
H	8.1353	-7.6085	-4.1446	H	-2.7774	-4.0427	4.1446	H	2.7774	4.0427	-4.1446	H	-8.1353	7.6085	4.1446
C	4.3263	-3.7761	-1.9065	C	1.0316	-7.8751	1.9065	C	-1.0316	7.8751	-1.9065	C	-4.3263	3.7761	1.9065
H	5.1818	-4.2554	-1.7724	H	0.1761	-7.3958	1.7724	H	-0.1761	7.3958	-1.7724	H	-5.1818	4.2554	1.7724
H	4.4730	-2.8238	-1.6769	H	0.8849	-8.8274	1.6769	H	-0.8849	8.8274	-1.6769	H	-4.4730	2.8238	1.6769
C	3.9199	-3.8793	-3.3796	C	1.4380	-7.7719	3.3796	C	-1.4380	7.7719	-3.3796	C	-3.9199	3.8793	3.3796
H	4.0374	-4.8136	-3.6828	H	1.3205	-6.8375	3.6828	H	-1.3205	6.8375	-3.6828	H	-4.0374	4.8136	3.6828
H	2.9611	-3.6501	-3.4660	H	2.3968	-8.0011	3.4660	H	-2.3968	8.0011	-3.4660	H	-2.9611	3.6501	3.4660
C	4.7324	-2.9605	-4.2813	C	0.6254	-8.6907	4.2813	C	-0.6254	8.6907	-4.2813	C	-4.7324	2.9605	4.2813

H	5.6794	-3.2493	-4.2581	H	-0.3216	-8.4019	4.2581	H	0.3216	8.4019	-4.2581	H	-5.6794	3.2493	4.2581
H	4.6910	-2.0402	-3.9175	H	0.6668	-9.6110	3.9175	H	-0.6668	9.6110	-3.9175	H	-4.6910	2.0402	3.9175
C	4.2675	-2.9310	-5.7350	C	1.0904	-8.7202	5.7350	C	-1.0904	8.7202	-5.7350	C	-4.2675	2.9310	5.7350
H	3.2980	-2.7296	-5.7583	H	2.0599	-8.9216	5.7583	H	-2.0599	8.9216	-5.7583	H	-3.2980	2.7296	5.7583
H	4.3984	-3.8276	-6.1323	H	0.9594	-7.8236	6.1323	H	-0.9594	7.8236	-6.1323	H	-4.3984	3.8276	6.1323
C	5.0193	-1.8851	-6.5941	C	0.3386	-9.7661	6.5941	C	-0.3386	9.7661	-6.5941	C	-5.0193	1.8851	6.5941
H	4.5268	-1.7568	-7.4442	H	0.8310	-9.8944	7.4442	H	-0.8310	9.8944	-7.4442	H	-4.5268	1.7568	7.4442
H	5.0211	-1.0198	-6.1143	H	0.3368	-10.6314	6.1143	H	-0.3368	10.6314	-6.1143	H	-5.0211	1.0198	6.1143
C	6.4024	-2.2604	-6.9011	C	-1.0446	-9.3908	6.9011	C	1.0446	9.3908	-6.9011	C	-6.4024	2.2604	6.9011
H	6.4010	-3.0377	-7.5139	H	-1.0431	-8.6134	7.5139	H	1.0431	8.6134	-7.5139	H	-6.4010	3.0377	7.5139
H	6.8598	-2.5305	-6.0666	H	-1.5019	-9.1206	6.0666	H	1.5019	9.1206	-6.0666	H	-6.8598	2.5305	6.0666
C	7.2002	-1.0754	-7.5693	C	-1.8423	-10.5758	7.5693	C	1.8423	10.5758	-7.5693	C	-7.2002	1.0754	7.5693
H	7.2328	-0.3140	-6.9514	H	-1.8749	-11.3371	6.9514	H	1.8749	11.3371	-6.9514	H	-7.2328	0.3140	6.9514
H	6.7508	-0.8048	-8.3975	H	-1.3929	-10.8463	8.3975	H	1.3929	10.8463	-8.3975	H	-6.7508	0.8048	8.3975
H	8.1126	-1.3690	-7.7731	H	-2.7547	-10.2821	7.7731	H	2.7547	10.2821	-7.7731	H	-8.1126	1.3690	7.7731
N	4.3083	-7.7679	0.0450	N	1.0495	-3.8832	-0.0450	N	-1.0495	3.8832	0.0450	N	-4.3083	7.7679	-0.0450
O	5.3947	-6.2699	-1.2552	O	-0.0369	-5.3813	1.2552	O	0.0369	5.3813	-1.2552	O	-5.3947	6.2699	1.2552

3. X-ray analysis

Table S13. Summary of crystal data for derivatives **1** and **2**.

Compound	**1**	**2**
Chemical formula	$C_{80}H_{72}N_2O_2$	$C_{40}H_{44}N_2O_2$
Formula weight (g·mol^{-1})	1093.39	584.77
Crystal system	Triclinic	Triclinic
Space group	P-1	P-1
a (Å) **b (Å)** **c (Å)** **α (°)** **β (°)** **γ (°)**	9.9509(9) 12.5238(11) 13.0711(12) 83.788(4) 81.296(3) 68.485(3)	5.6216(2) 10.3184(4) 27.8242(11) 88.5483(10) 87.7039(11) 81.9237(10)
Volume (Å^3)	1495.5(2)	1596.36(11)
Z	1	2
Density (Mg m^{-3})	1.214	1.217
Temperature (K)	100	200
F(000)	582	628
Crystal size (mm^3)	0.065 x 0.025 x 0.005	0.386 x 0.077 x 0.045
Meas. Refl.	18319	7312
Indep. Refl.	5476	6485
R(int)	0.0659	0.0913
Final R indices **[I > 2σ(I)]**	R = 0.0689 R_w = 0.1897	R = 0.1060 R_w = 0.3253
Goodness-of-fit	1.042	1.122
$\Delta\rho_{max}$, $\Delta\rho_{min}$ **(e Å^{-3})**	0.610, -0.462	0.411, -0.283

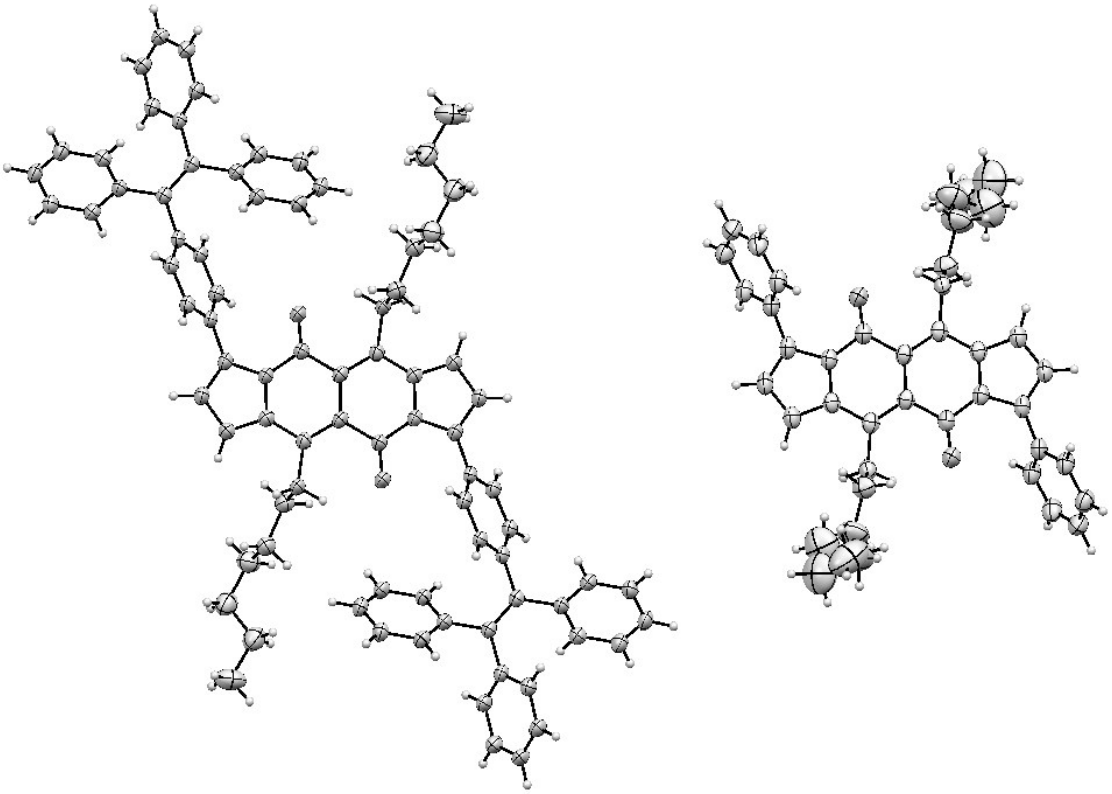


Figure S6. ORTEP at the 50 % probability level of the crystal structure of **1**(left) and **2** (right).

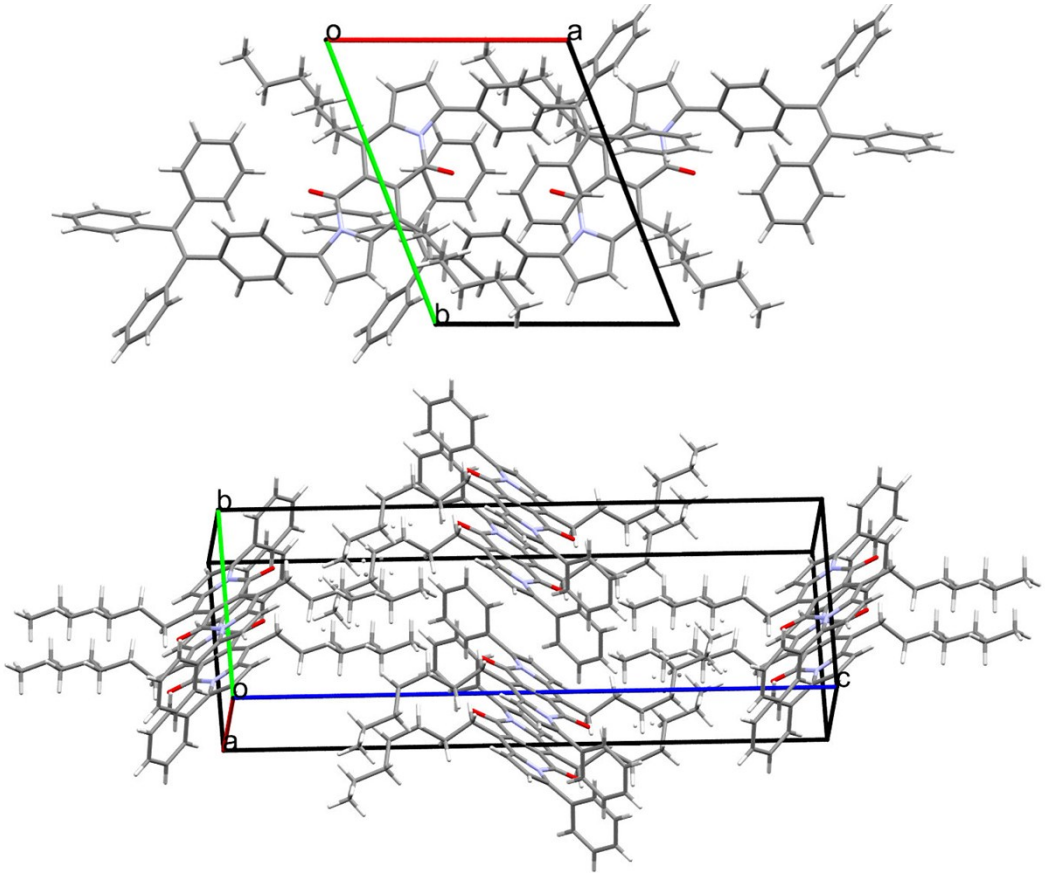


Figure S7. Crystal packing within unit cells for **1** (top) and **2** (bottom).

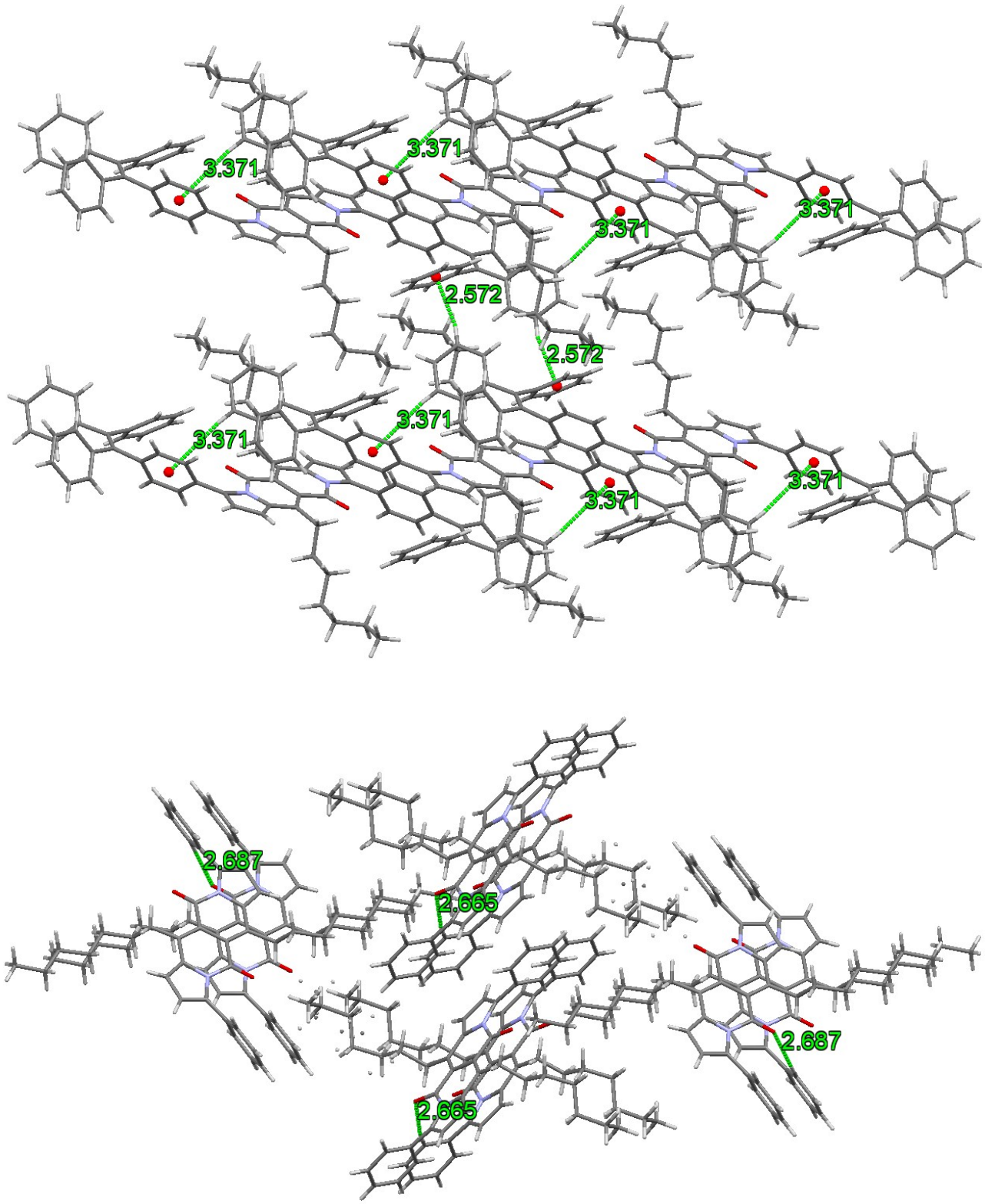
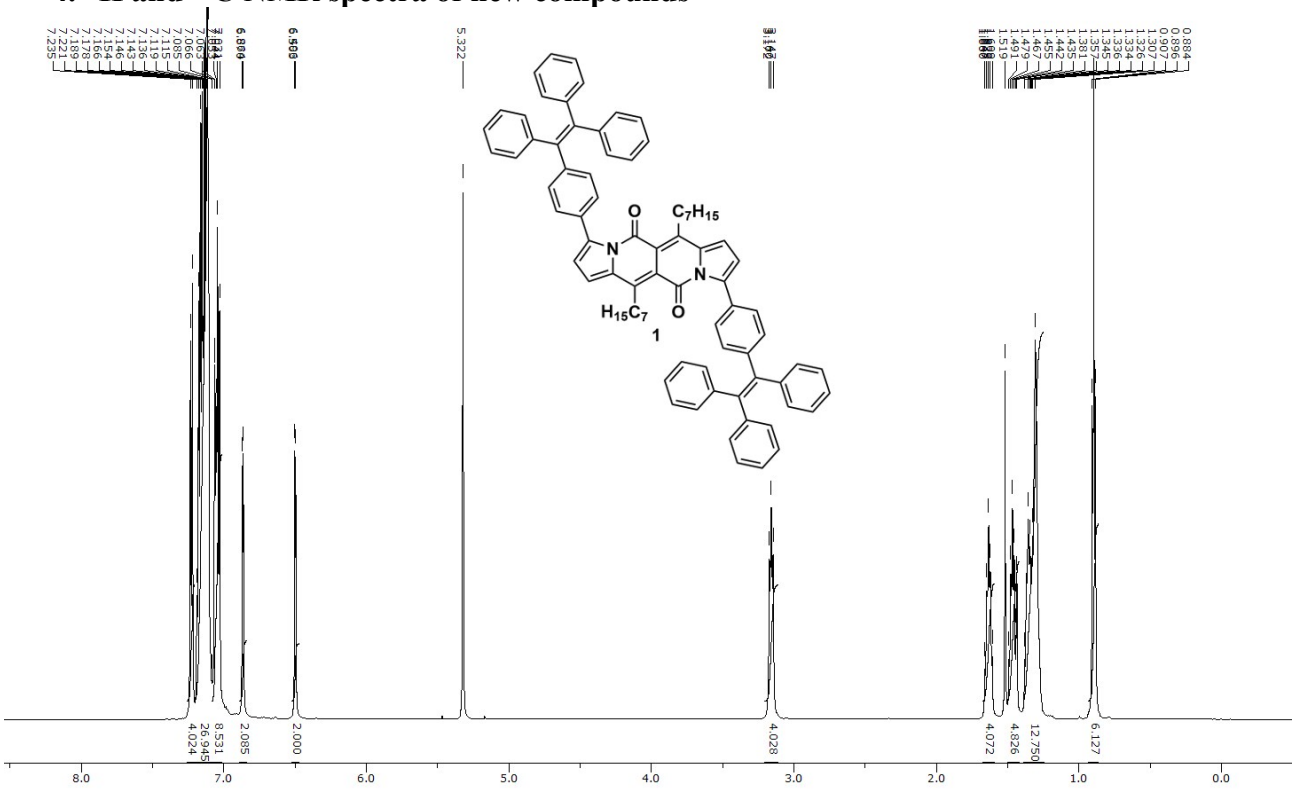
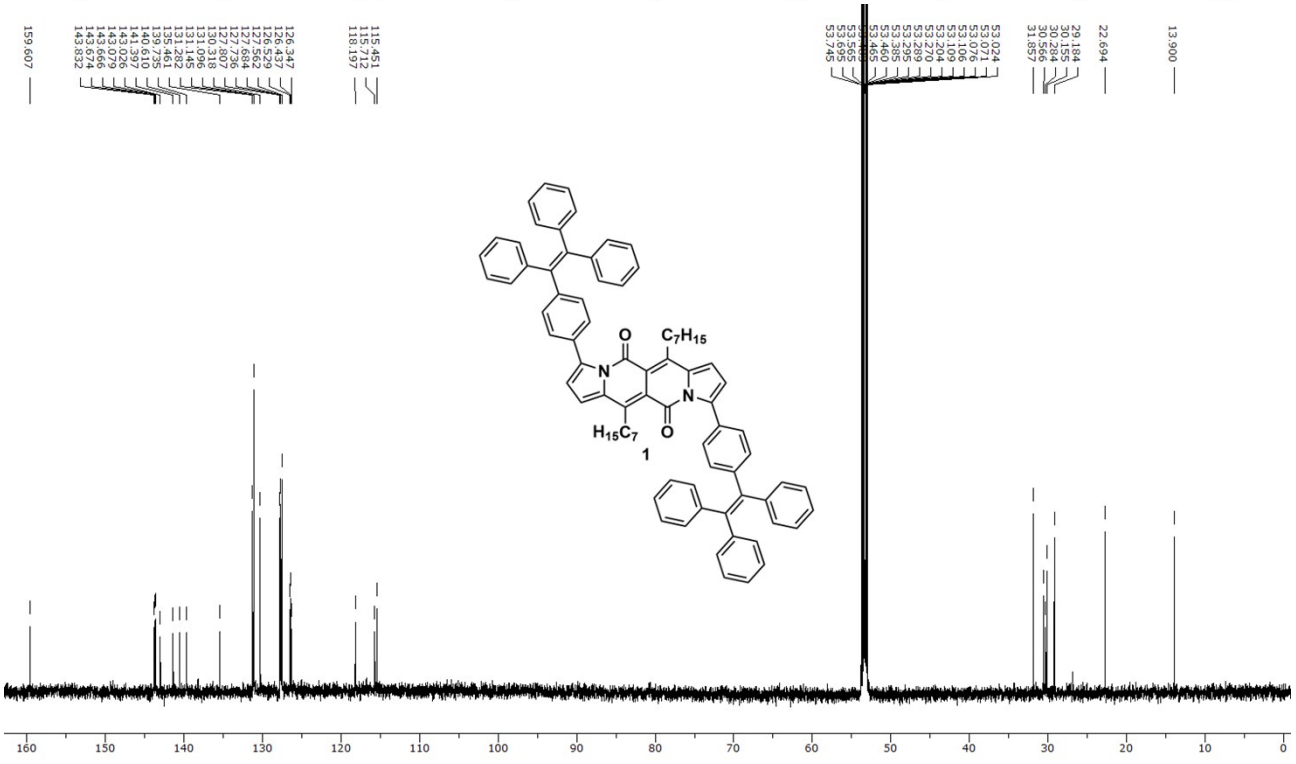
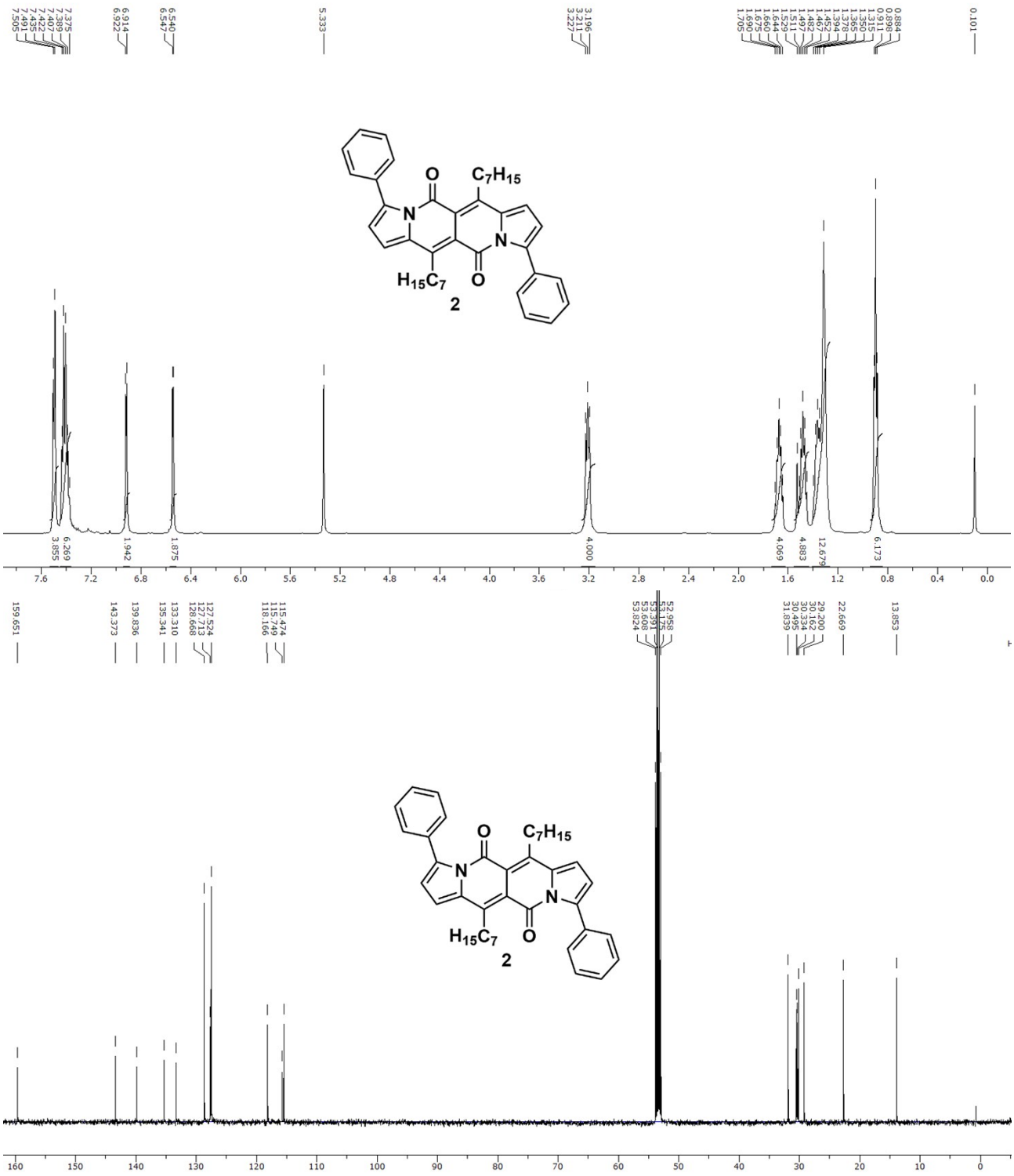


Figure S8. Interactions within crystal lattice for **1** (top) and **2** (bottom).

4. H and ^{13}C NMR spectra of new compounds







5. References

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