Supplementary Information

New Air-stable Solution-processed Organic n-type Semiconductors Based on Sulphur-rich Core-expanded Naphthalene Diimdes

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1. TGA analysis of **1** and **2**

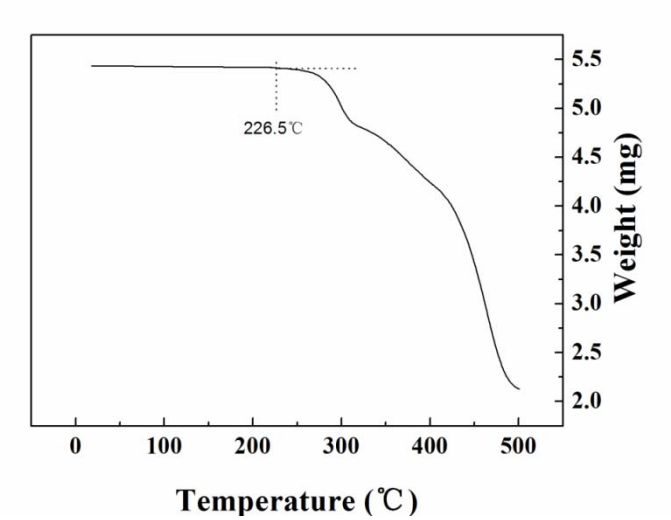


Figure S1. TGA analysis of **1**.

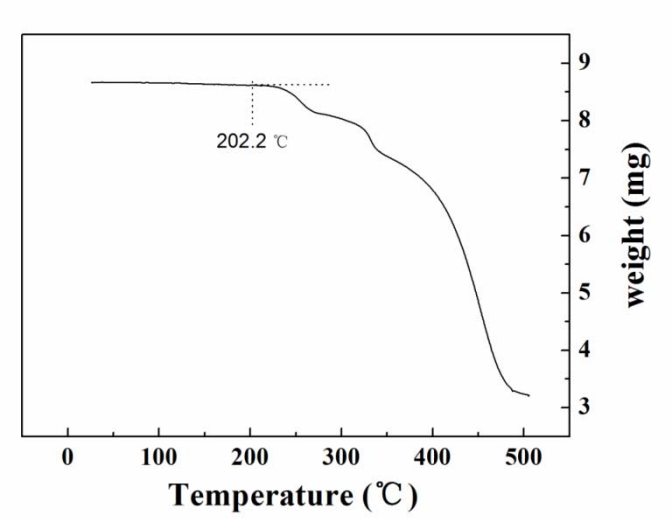


Figure S2. TGA analysis of **2**.

2. UV-Vis absorption spectrum of solution and thin film of compound **2**

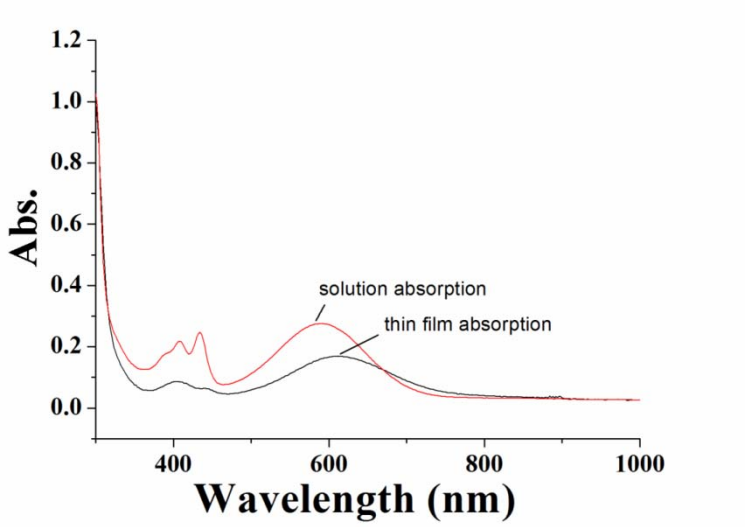


Figure S3. UV-Vis absorption of solution and thin film of compound **2**

3. Theoretical calculations for **1** and **2**

Compound **1**

Calculation method: B3LYP/6-31G (d) with Gaussian 03

Coordinates

	X	Y	Z
1 C	2.326295	0.717671	0.756839
2 C	2.326261	-0.717181	0.757025
3 C	1.149877	-1.403353	0.429854
4 C	-0.004279	-0.706189	-0.017988
5 C	-0.004318	0.706675	-0.017978
6 C	1.149886	1.403843	0.429717
7 C	-1.158025	-1.404676	-0.464479

8	C	-2.336516	-0.717253	-0.783479
9	C	-2.336595	0.717574	-0.783375
10	C	-1.158135	1.405102	-0.464373
11	C	-1.062364	2.874205	-0.659288
12	N	-0.00293	3.522322	-0.023026
13	C	1.050721	2.872218	0.614686
14	C	1.050643	-2.871712	0.614886
15	N	-0.002683	-3.521871	-0.023303
16	C	-1.062155	-2.873771	-0.659476
17	S	3.758456	1.670489	1.284244
18	C	5.055949	0.672332	0.612421
19	C	5.055897	-0.672306	0.612815
20	S	3.758209	-1.669905	1.285067
21	S	-3.775934	-1.666902	-1.29887
22	C	-5.062819	-0.672427	-0.601761
23	C	-5.062916	0.672228	-0.601574
24	S	-3.776212	1.667111	-1.298443
25	S	6.410989	1.469823	-0.189135
26	C	7.301385	-0.000449	-0.61903
27	S	6.410885	-1.470395	-0.188216
28	S	-6.401187	-1.470543	0.226511
29	C	-7.282746	-0.000435	0.675184

30	S	-6.401406	1.469923	0.22689
31	O	1.854671	3.514566	1.277308
32	O	-1.871394	3.498183	-1.332527
33	O	1.854335	-3.513988	1.277909
34	O	-1.871114	-3.497702	-1.332861
35	S	8.766059	-0.000736	-1.360562
36	S	-8.73216	-0.000639	1.446148
37	C	0.019766	4.992774	0.002388
38	C	0.020037	-4.992305	0.002068
39	H	-0.81444	5.347733	-0.596599
40	H	-0.067058	5.342598	1.032776
41	H	0.965585	5.350948	-0.40715
42	H	-0.813787	-5.347263	-0.597459
43	H	-0.067421	-5.342199	1.03238
44	H	0.966115	-5.350428	-0.406906

Total energies: 6125.0602015394 Hartrees

Compound **2**

Calculation method: B3LYP/6-31G (d) with Gaussian 03

Coordinates

	X	Y	Z
1 C	-2.350647	-0.717292	0.684436

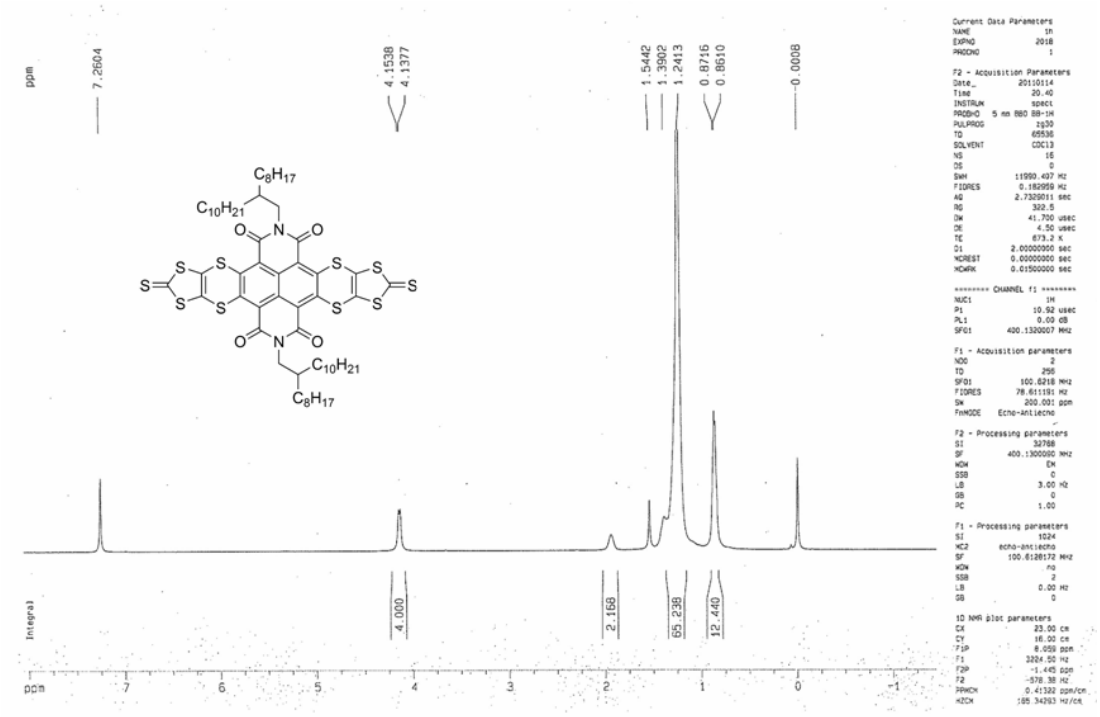
2	C	-2.350648	0.717322	0.684423
3	C	-1.164495	1.403965	0.396092
4	C	0.003509	0.706676	-0.013975
5	C	0.003504	-0.706661	-0.013977
6	C	-1.1645	-1.403941	0.396102
7	C	1.171094	1.405256	-0.422824
8	C	2.359102	0.717367	-0.702875
9	C	2.359097	-0.717365	-0.702875
10	C	1.171085	-1.405248	-0.422827
11	C	1.081782	-2.87419	-0.62153
12	N	0.001696	-3.52229	-0.020277
13	C	-1.07152	-2.872194	0.584704
14	C	-1.071522	2.872216	0.58468
15	N	0.00175	3.522306	-0.020223
16	C	1.081798	2.8742	-0.621518
17	S	-3.802404	-1.662603	1.16466
18	C	-5.075588	-0.671699	0.433828
19	C	-5.075589	0.671707	0.433803
20	S	-3.80241	1.662644	1.164599
21	S	3.817396	1.659815	-1.171016
22	C	5.079947	0.671691	-0.41847
23	C	5.079943	-0.671712	-0.41847

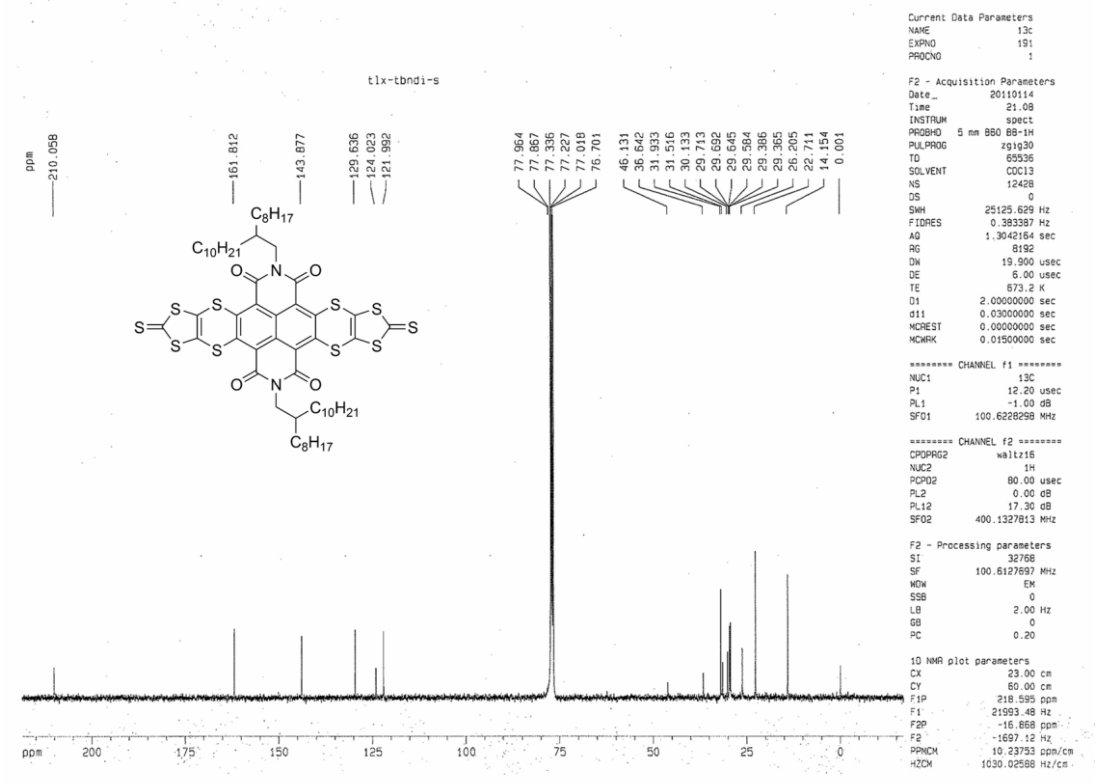
24 S	3.817384	-1.659823	-1.17102
25 S	-6.368221	-1.504221	-0.434098
26 C	-7.245025	-0.000026	-0.942328
27 S	-6.368226	1.504192	-0.434155
28 S	6.357212	1.504312	0.471671
29 C	7.224911	-0.000017	0.995289
30 S	6.357201	-1.504341	0.471673
31 O	-1.895292	-3.514751	1.222219
32 O	1.911836	-3.498287	-1.268531
33 O	-1.895339	3.514785	1.222125
34 O	1.91184	3.498289	-1.268546
35 O	-8.27454	-0.000039	-1.556404
36 O	8.243544	-0.000021	1.627246
37 C	-0.02192	-4.99244	0.00383
38 C	-0.021859	4.992456	0.003909
39 H	0.825222	-5.34716	-0.576922
40 H	0.042448	-5.343617	1.035519
41 H	-0.958833	-5.34991	-0.426186
42 H	0.826139	5.347181	-0.575589
43 H	0.040966	5.343517	1.035721
44 H	-0.958101	5.350039	-0.427499

Total energy: 5778.3460768110 Hartrees

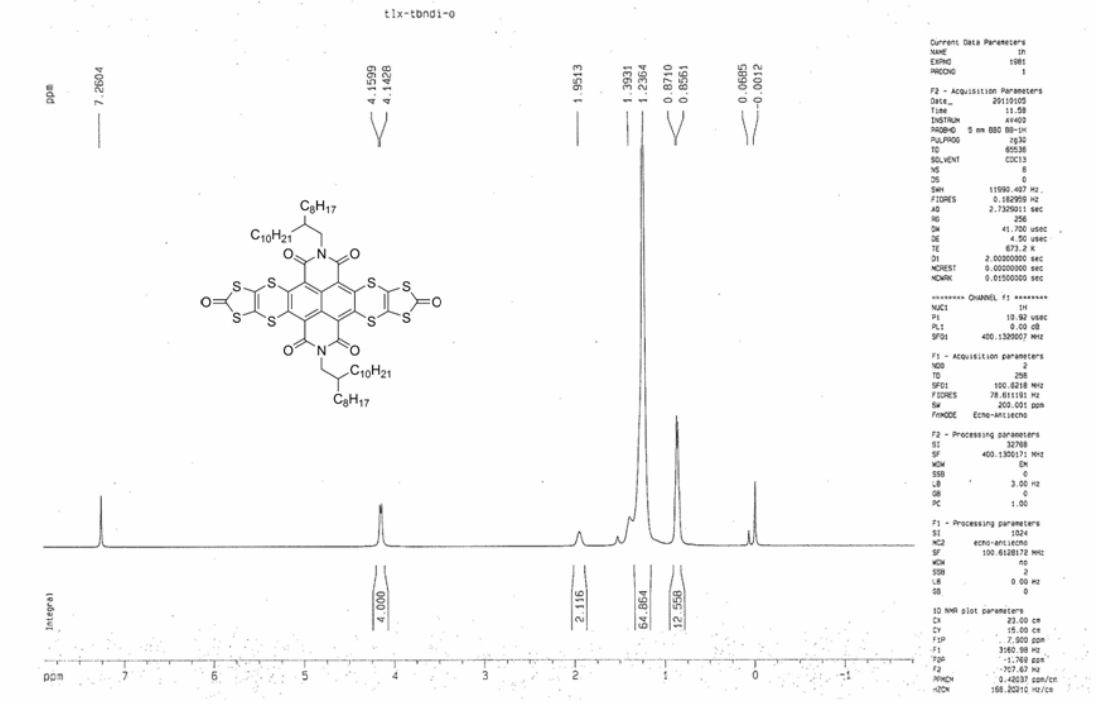
4. ^{1}H NMR & ^{13}C NMR of compound **1** and **2**

Compound **1**





Compound **2**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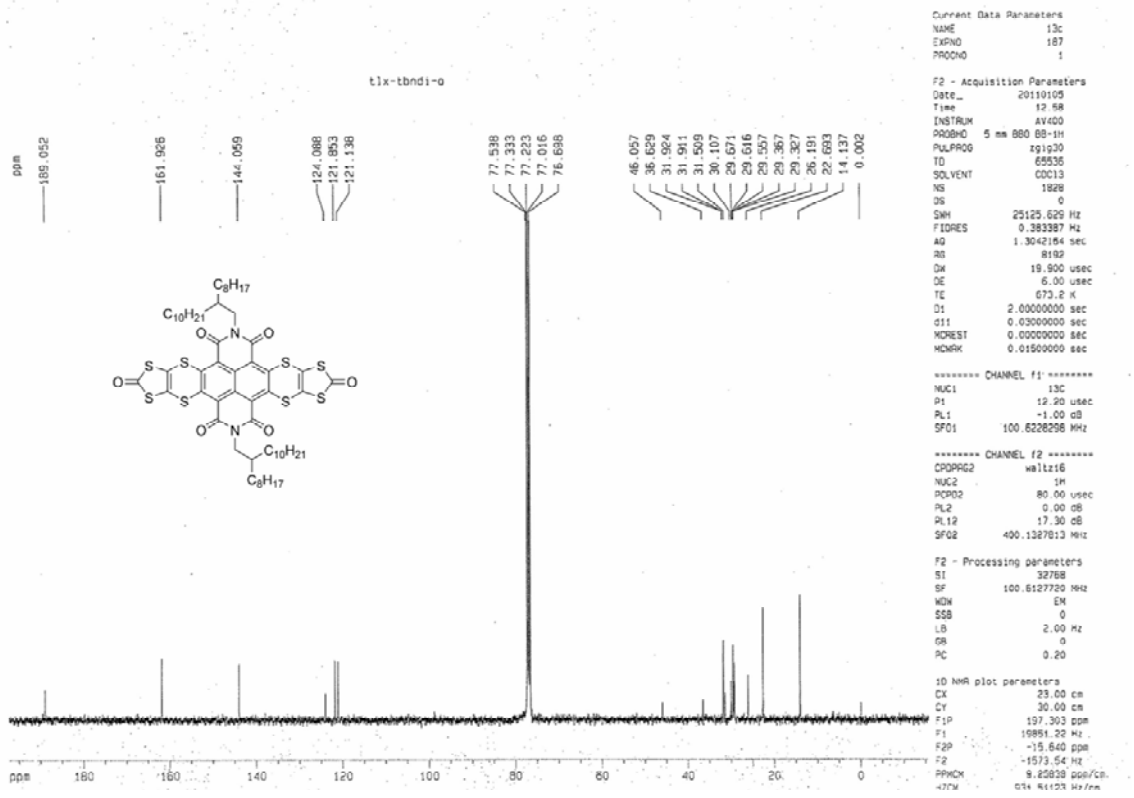
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