Electronic supplementary information for

Conformation Change Significantly Affected the Optical and Electronic Properties of Arylsulfonamide-Substituted Anthraquinones

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1. Comparison of UV-Vis spectra of *N*-Me derivatives 1-4 and *N*-H derivatives 5-8

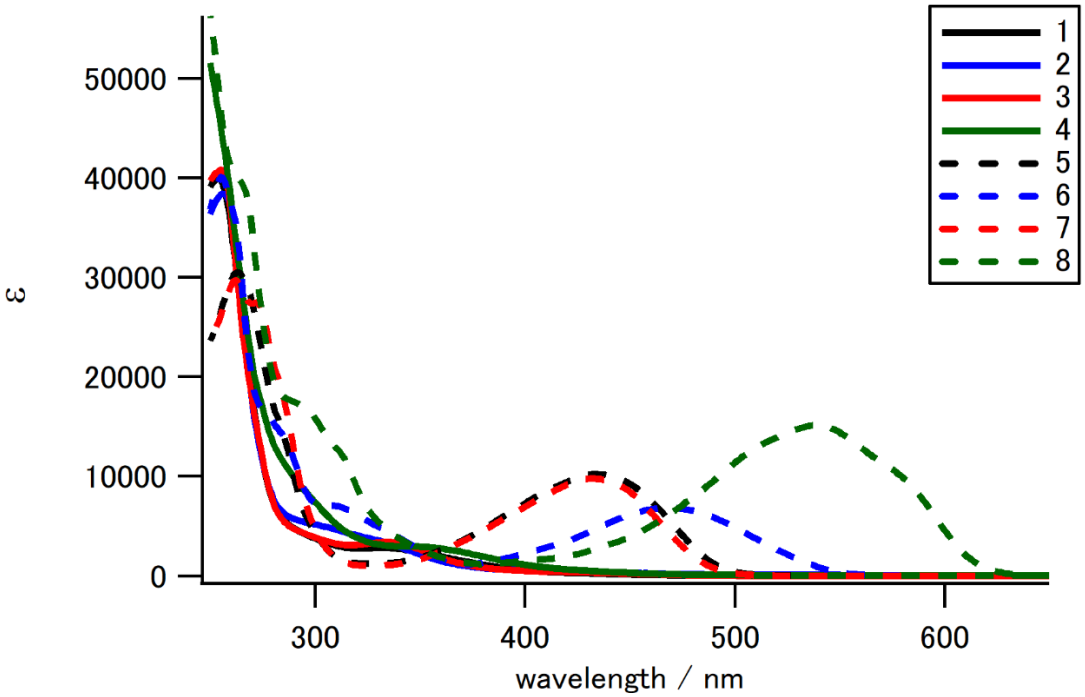


Figure S1 UV-Vis spectra of **1-4** (bold line) and **5-8** (dotted line) in CH_2Cl_2.

2. Comparison of reduction potentials of *N*-Me derivatives 1-4 and *N*-H derivatives 5-8

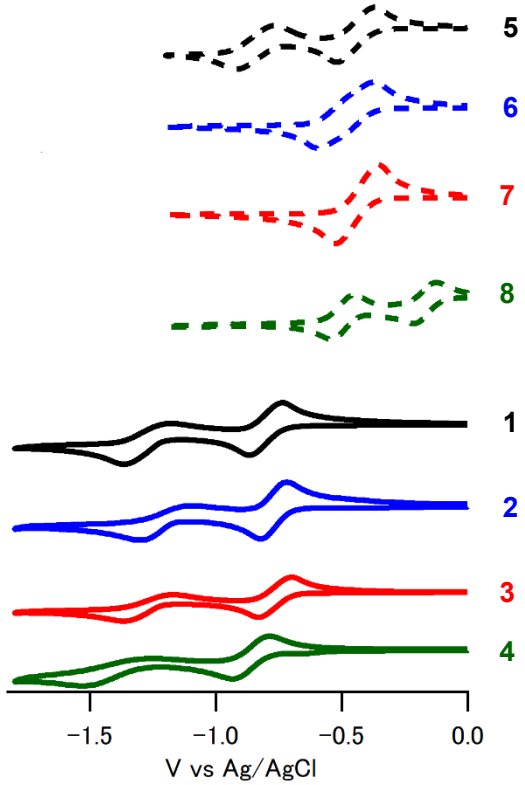


Figure S2 Cyclic voltammograms of **1-8** in CH_2Cl_2 (0.1 M Bu_4NBF_4, 100 mV/sec).

3. ORTEP drawing of 1

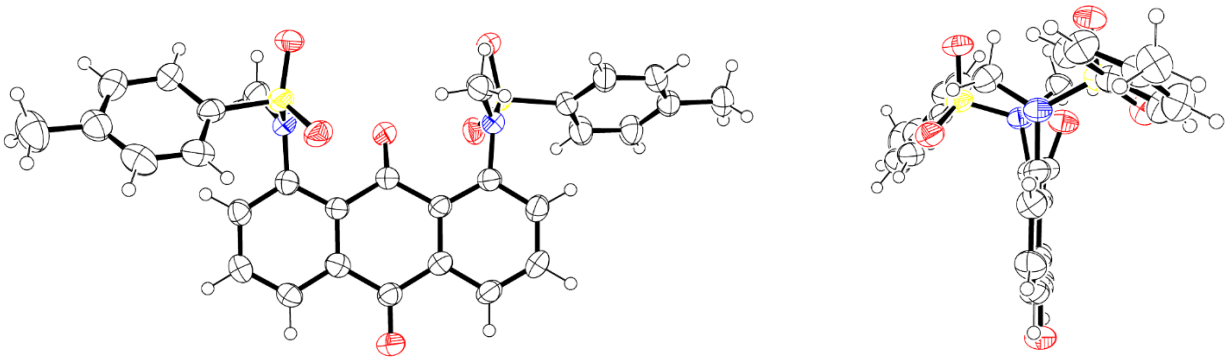


Figure S3 ORTEP drawing of **1**. Front view (left) and side view (right). Displacement ellipsoids are drawn at the 50% probability level.

4. HOMO, LUMO and oscillator strength of the HOMO-LUMO transition of 1-8

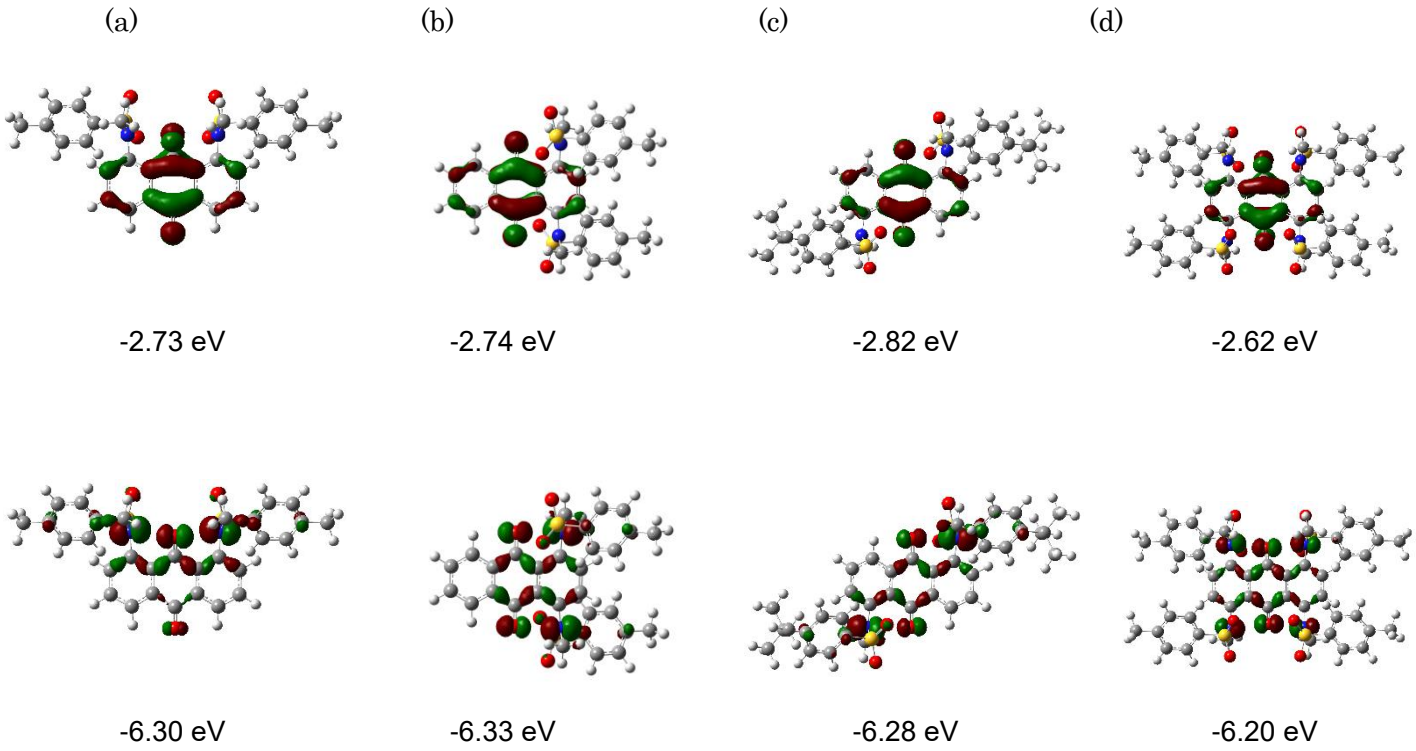


Figure S4 LUMO (top), HOMO (bottom) and their energies for (a) **1**, (b) **2**, (c) **3**, and (d) **4**.
Atomic orbital coefficients of 2py orbital of nitrogen atoms (y axis defined as perpendicular to the anthraquinone plane). HOMO: **1**: 0.04484, -0.04488, **2**: 0.29211, -0.29190, **3**: 0.15059, -0.14513, **4**: 0.02196, 0.02196, -0.02195, -0.02196; LUMO: **1**: 0.00282, 0.00283, **2**: -0.00495, -0.00497, **3**: 0.00231, -0.00280, **4**: 0.00167, -0.00167, -0.00167, 0.00167.
Oscillator strength of the HOMO-LUMO transition: **1**: 0.0078, **2**: 0.0004, **3**: 0.0000, **4**: 0.0000.

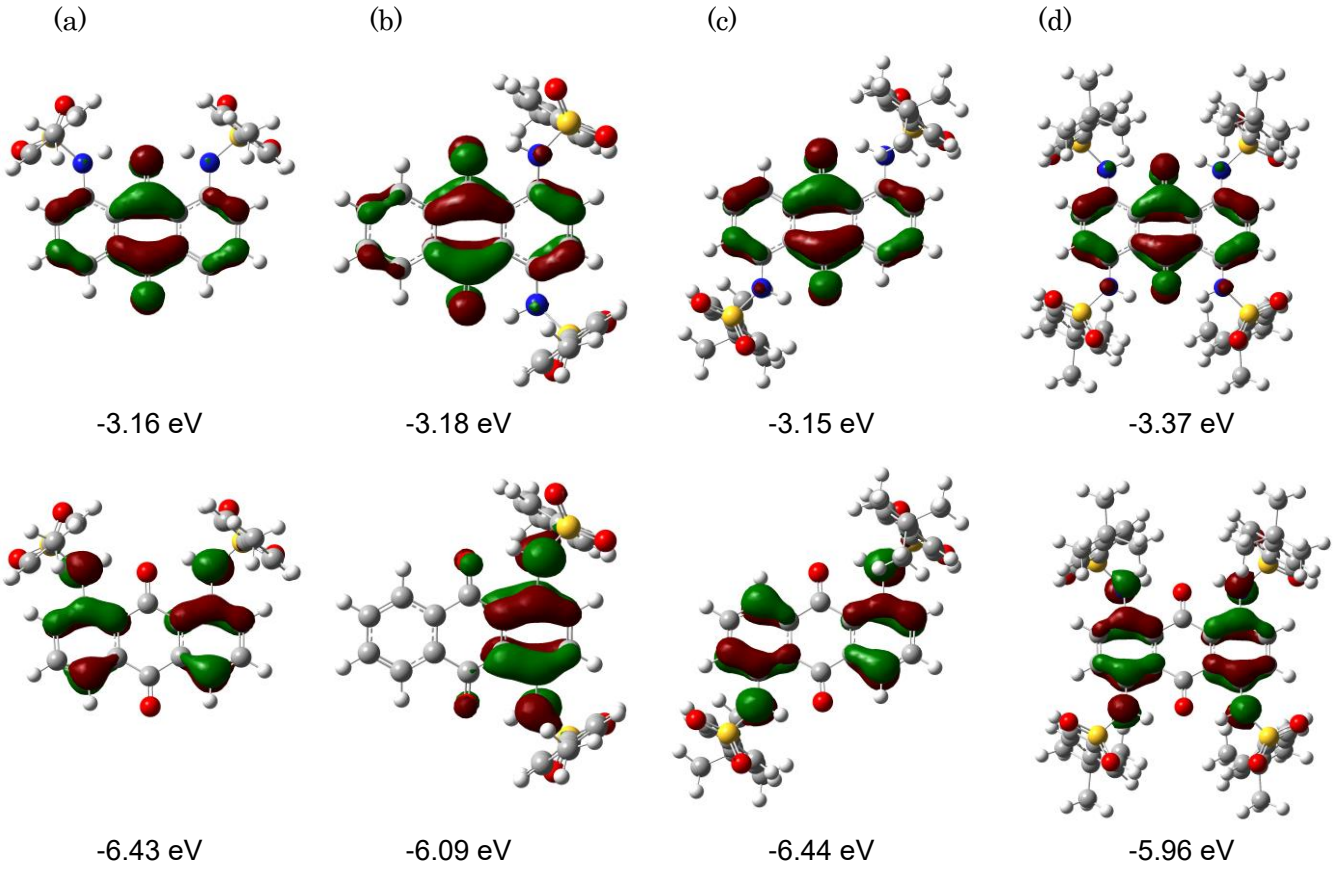


Figure S5 LUMO (top), HOMO (bottom) and their energies for (a) **5**, (b) **6**, (c) **7**, and (d) **8**.
Atomic orbital coefficients of 2py orbital of nitrogen atoms (y axis defined as perpendicular to the anthraquinone plane). HOMO: **5**: -0.16150, 0.16474, **6**: -0.07353, -0.07330, **7**: 0.22514, 0.22522, **8**: 0.05006, 0.04984, 0.04999, 0.04980; LUMO: **5**: -0.04127, -0.04204, **6**: 0.02465, 0.02455, **7**: 0.06217, -0.06217, **8**: -0.02273, -0.02264, 0.02270, 0.02263.
Oscillator strength of the HOMO-LUMO transition: **5**: 0.1891, **6**: 0.1428, **7**: 0.2421, **8**: 0.3188.

5. Solid state UV-Vis spectra of 1-4

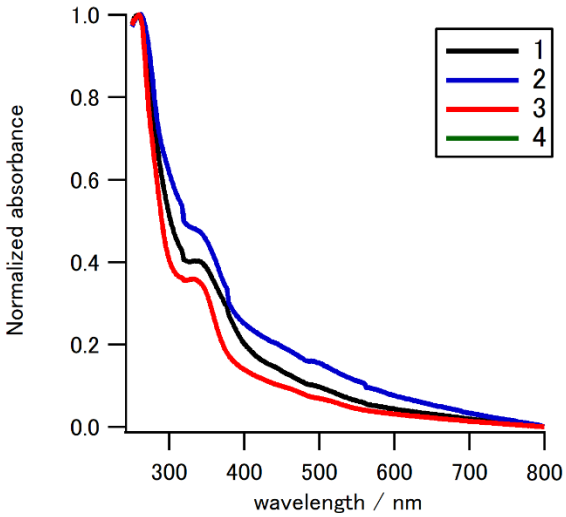


Figure S6 Normalized UV-Vis spectra of **1-4** in the solid state. The absorption of **4** overlapped with that of **3**.

6. Experimental section

General methods. Commercially available reagents and solvents were used as received. Compounds **5-8** were prepared by as described in the literature.[S1] ^{1}H (400 MHz) and ^{13}C (100 MHz) NMR spectra were recorded on a Bruker Avance III 400 NMR spectrometer. Chemical shifts (δ) are expressed in ppm with reference to tetramethylsilane (^{1}H 0.00 ppm) or residual nondeuterated solvent ($CDCl_3$; ^{13}C 77.0 ppm) as an internal standard. Mass spectra were recorded on a JMS-700 spectrometer at the NMR and MS Laboratory, Graduate School of Agriculture, Tohoku University. Elemental analyses were performed on a Microcoder JM10 at the Elementary Analysis Laboratory, Institute of Multidisciplinary Research for Advanced Materials, Tohoku University. IR spectra were measured on a Thermo Scientific NICOLET 6700 FT-IR spectrometer.

Preparation of 1.[S1]

To a suspension of NaH (60% in oil, 333 mg, 8.33 mmol) in dry DMF (20 mL) was added **5** (303 mg, 554 μmol) under N_2. The mixture was stirred at rt for 45 min. To the resulting solution was added MeI (700 μL, 11.0 mmol) at this temperature. The mixture was stirred at rt for 12 h. The mixture was diluted with an excess amount of water. The resulting precipitate was collected by filtration, washed with water, and then dried under vacuum. Recrystallization from EtOH gave **1** (171 mg, 54%) as an orange crystalline solid.

Mp: 236-237 °C. ^{1}H NMR (400 MHz): δ 8.24 (dd, J = 7.8, 1.3 Hz, 2H), 7.70 (d, J = 7.8 Hz, 4H), 7.63 (t, J = 7.6 Hz, 2H), 7.47 (dd, J = 7.8, 1.3 Hz, 2H), 7.31 (d, J = 7.8 Hz, 4H), 3.24 (s, 6H), 2.43 (s, 6H). ^{13}C NMR (100 MHz): δ 182.6, 182.3, 143.5, 140.3, 136.0, 134.6, 133.6, 133.0, 129.6, 127.9, 126.9, 38.8, 21.6. IR: 3072, 2948, 2919, 1680, 1585, 1495, 1461, 1436, 1400, 1345, 1318, 1249, 1216, 1188, 1150, 1089, 1020, 1011, 957, 871, 850, 802, 752, 730, 688, 675, 651, 581, 563, 545, 517 cm^{-1}. HRMS (FAB) calcd for $C_{30}H_{27}N_2O_6S_2$: 575.1311 [$(M+H)^+$]; found: 575.1309. Anal. Calcd for $C_{30}H_{26}N_2O_6S_2$: C, 62.70 H, 4.56; N, 4.87. Found: C, 62.55 H, 4.73; N, 4.78.

Preparation of 2.

A mixture of **6** (200 mg, 366 μmol), K_2CO_3 (506 mg, 3.66 mmol) and MeI (455 μL, 7.32 mmol) in DMF (10 mL) was stirred at 50 °C for 13.5 h in a sealed glass pressure vessel. After cooling to rt, the mixture was diluted with H_2O. The resulting precipitate was collected by filtration, washed with H_2O, and then dried under vacuum. Recrystallization from $CHCl_3$/EtOH gave **2** (195 mg, 93%) as a yellow solid.

Mp: 228-229 °C (decomp.). ^{1}H NMR (400 MHz, 50 °C): δ 7.92 (br s, 2H), 7.68 (dd, J = 5.7, 3.2 Hz, 2H), 7.57 (t, J = 8.2 Hz, 4H), 7.42 (s, 2H), 7.23 (d, J = 8.2 Hz, 4H), 3.35 (s, 6H), 2.39 (s, 6H). IR: 1670, 1590, 1463, 1348, 1322, 1305, 1254, 1201, 1156, 1087, 931, 910, 877, 809, 795, 727, 713, 679, 636, 596, 549, 516 cm^{-1}. HRMS (FAB) calcd for $C_{30}H_{27}N_2O_6S_2$: 575.1311 [$(M+H)^+$]; found: 575.1310. Anal. Calcd for $C_{30}H_{26}N_2O_6S_2$: C, 62.70 H, 4.56; N, 4.87. Found: C, 62.88 H, 4.57; N, 4.82.

Preparation of 3.

To a suspension of NaH (60% in oil, 380 mg, 9.51 mmol) in dry DMF (30 mL) was added **7** (400 mg, 634 μmol) under N_2. The mixture was stirred at rt for 45 min. To the resulting solution was added MeI (790 μL, 12.7 mmol) at this temperature. The mixture was stirred at rt for 16.5 h. The mixture was diluted with an excess amount of water. The resulting precipitate was collected by filtration, washed with water, and then dried under vacuum. Recrystallization from $CHCl_3$/EtOH gave **3** (177 mg, 42%) as a yellow solid.

Mp: 268-270 °C (decomp.). ^{1}H NMR (400 MHz, 50 °C): δ 8.08 (br d, J = 7.8 Hz, 2H), 7.65(t, J = 7.8 Hz, 2H), 7.63 (d, J = 8.5 Hz, 4H), 7.50 (d, J = 7.8 Hz, 2H), 7.44 (d, J = 8.5 Hz, 4H), 3.35 (s, 6H), 1.33 (s, 18H). IR: 3076, 2957, 1675, 1596, 1580, 1457, 1438, 1400, 1349, 1310, 1267, 1190, 1158, 1112, 1085, 1018, 877, 825, 807, 773, 756, 710, 626, 581, 552 cm^{-1}. HRMS (FAB) calcd for $C_{36}H_{39}N_2O_6S_2$: 659.2250 [(M+H)$^+$]; found: 659.2250. Anal. Calcd for $C_{36}H_{38}N_2O_6S_2$: C, 65.60 H, 5.81; N, 4.25. Found: C, 62.60 H, 5.86; N, 4.22.

Preparation of 4.

To a suspension of NaH (60% in oil, 304 mg, 7.60 mmol) in dry DMF (30 mL) was added **8** (400 mg, 380 μmol) under N_2. The mixture was stirred at rt for 45 min. To the resulting solution was added MeI (710 μL, 11.4 mmol) at this temperature. The mixture was stirred at rt for 17 h. The mixture was diluted with an excess amount of water. The resulting precipitate was collected by filtration, washed with water, and then dried under vacuum. Recrystallization from $CHCl_3$/EtOH gave **4** (264 mg, 63%) as a yellow solid.

Mp: 253-255 °C (decomp.). ^{1}H NMR (400 MHz): δ 7.76 (d, J = 8.6 Hz, 8H), 7.56 (d, J = 8.6 Hz, 8H), 7.25 (s, 4H), 3.20 (s, 12H), 1.37 (s, 36H). IR: 2964, 2871, 1702, 1595, 1477, 1397, 1349, 1333, 1307, 1269, 1217, 1160, 1111, 1085, 1042, 936, 888, 865, 842, 812, 793, 762, 671, 630, 601, 580, 547 cm^{-1}. HRMS (FAB) calcd for $C_{58}H_{69}N_4O_{10}S_4$: 1109.3897 [(M+H)$^+$]; found: 1109.3899. Anal. Calcd for $C_{58}H_{68}N_4O_{10}S_4$: C, 62.79 H, 6.18; N, 5.05. Found: C, 62.57 H, 6.13; N, 5.00.

X-ray structural analysis. Crystallographic data for single crystals were collected using a diffractometer equipped with a rotating anode fitted with a multilayer confocal optic using Cu-Kα (λ = 1.54187 Å) radiation. Structure refinements were carried out using the full-matrix least-squares method on F^2. Calculations were performed using the Crystal Structure and SHELEX software packages.[S3] Parameters were refined using anisotropic temperature factors, except for the hydrogen atom.

Crystal data of 1: A single-crystalline sample was obtained by recrystallization from $CHCl_3$/hexane. $C_{30}H_{22}N_2O_6S_2$, M = 570.63, P2$_1$/c (#14), a = 9.9499(4) Å, b = 9.6309(4) Å, c = 27.2708(11) Å, β = 93.901(7) °, V = 2607.20(19) Å^3, Z= 4, Dc= 1.454 g cm^{-3}. Independent reflections 4693 (all), T = 100 K, μ= 22.745 cm^{-1}, R = 6.15%. CCDC 2013362.

Crystal data of 2 · $(CHCl_3)_2$: A single-crystalline sample was obtained by recrystallization from $CHCl_3$/hexane. $C_{32}H_{28}Cl_6N_2O_6S_2$, M = 813.42, C2/c (#15), a = 52.9762(19) Å, b = 15.1879(5) Å, c = 13.2000(5) Å, β = 102.745(7) °, V = 10359.0(7) Å^3, Z= 12, Dc= 1.565 g cm^{-3}. Independent reflections 9364 (all), T = 100K, μ= 60.76 cm^{-1}, R = 5.41%. CCDC 2013365.

Crystal structures of **5-8** have already in published in the literature.[S2]

5·(MeCN)	CCDC 1550096
5·(EtCN)	CCDC 1550093
6	CCDC 1550105
7	CCDC 1550102
8·$(Fluorobenzene)_2$	CCDC 1550149
8·$(Benzonitrile)_2$	CCDC 1576397

7. ^{1}H NMR spectra of 1-4

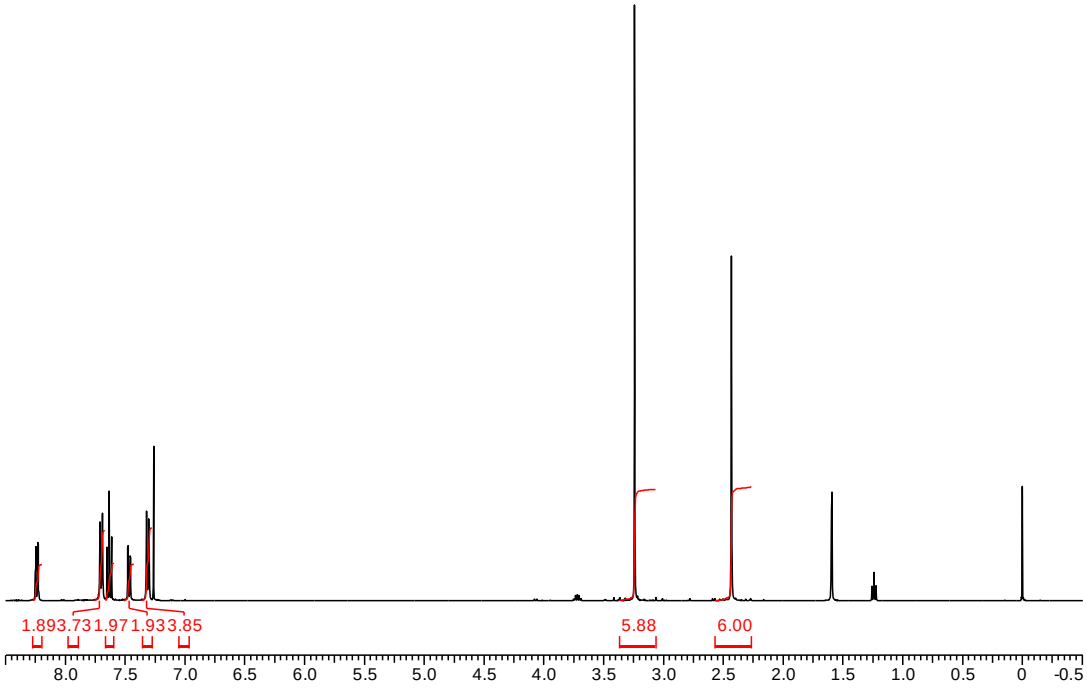


Figure S7 ^{1}H NMR spectrum of **1**.

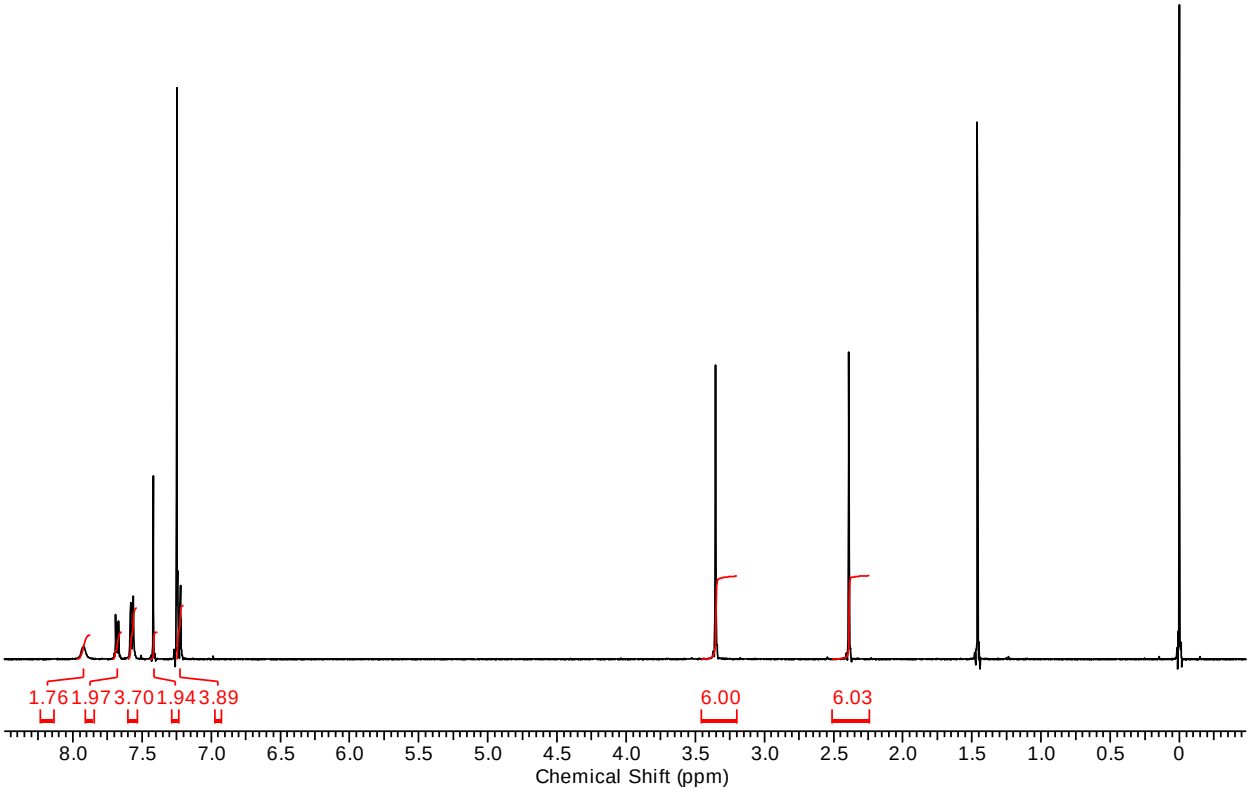


Figure S8 ^{1}H NMR spectrum of **2**.

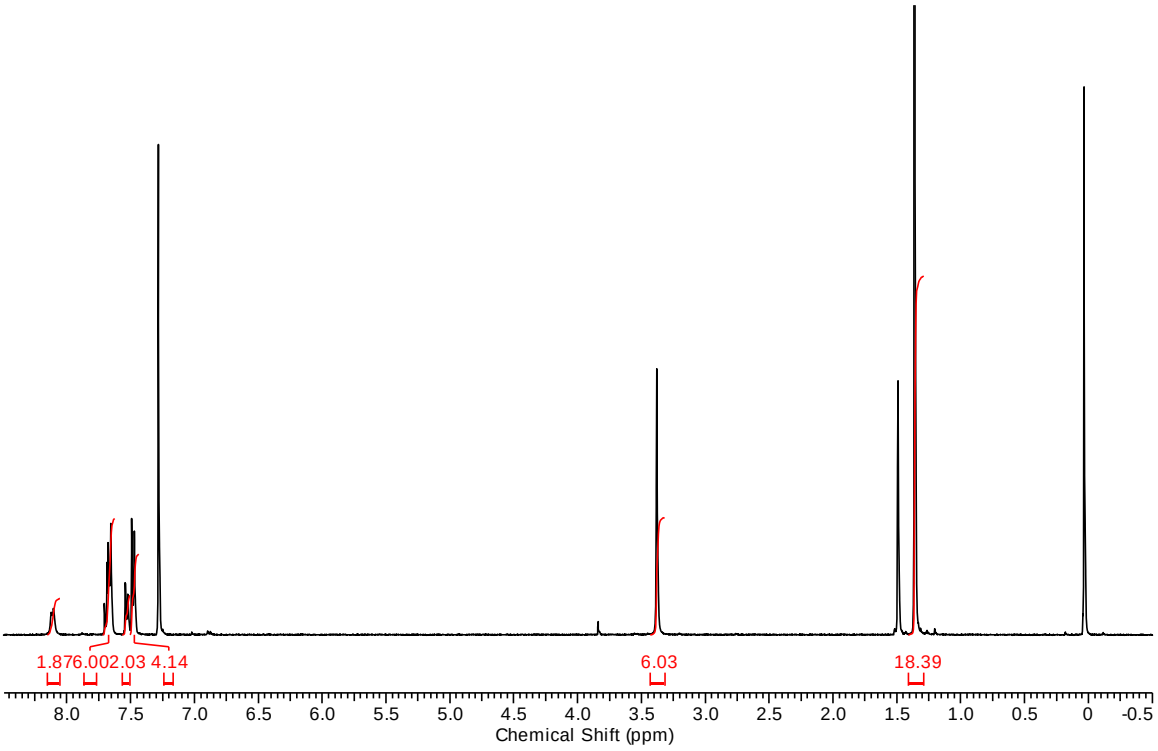


Figure S9 ^{1}H NMR spectrum of **3**.

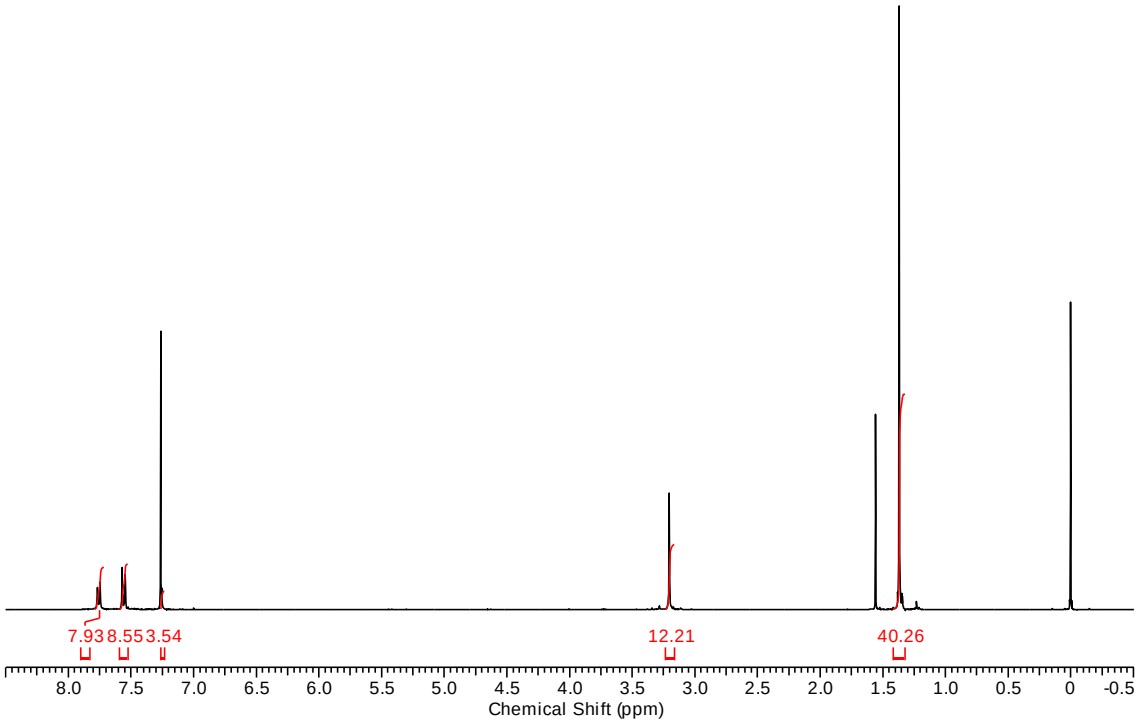


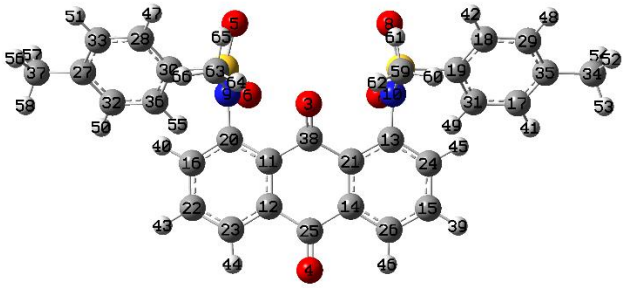
Figure S10 ^{1}H NMR spectrum of **4**.

8. Cartesian Coordinates for optimized structures 1-4

a. Optimized structure of **1**

E(RB3LYP) = -2515.94134656 a.u.

Number of imaginary frequency: 0



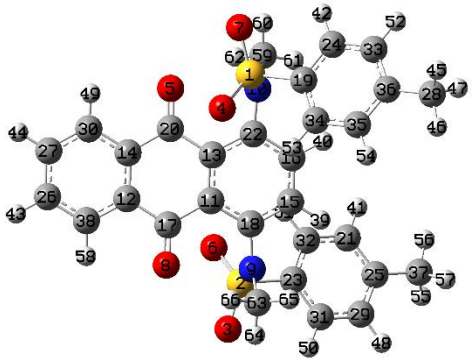
Atom No.	Element	Cartesian Coorinates		
		X	Y	Z
1	S	-2.751827	-1.418072	0.079166
2	S	2.751590	-1.418108	0.079991
3	O	0.000117	0.567903	1.972344
4	O	0.000441	5.051277	-0.773200
5	O	2.417336	-2.615363	0.851430
6	O	2.046088	-1.028263	-1.139489
7	O	-2.046805	-1.028250	-1.140595
8	O	-2.417433	-2.615438	0.850370
9	N	2.582075	-0.117639	1.144218
10	N	-2.581563	-0.117730	1.143472
11	C	1.282624	1.885517	0.470806
12	C	1.277754	3.168557	-0.111779
13	C	-2.515012	1.207343	0.608491
14	C	-1.277021	3.168560	-0.112053
15	C	-3.679577	3.128258	-0.335494
16	C	3.696492	1.843725	0.211731
17	C	-6.329154	-1.056589	-1.823464
18	C	-5.363856	-2.239268	0.512278
19	C	-4.496969	-1.553763	-0.342301
20	C	2.515572	1.207383	0.609147
21	C	-1.282029	1.885492	0.470480
22	C	3.680365	3.128228	-0.334698
23	C	2.470081	3.787570	-0.503517
24	C	-3.695837	1.843734	0.210882
25	C	0.000394	3.900988	-0.349050
26	C	-2.469254	3.787595	-0.504039
27	C	7.221551	-1.730907	-0.978958
28	C	5.363625	-2.239928	0.511873
29	C	-6.717519	-2.318029	0.190749
30	C	4.496529	-1.554042	-0.342213
31	C	-4.972614	-0.965720	-1.516782
32	C	6.328273	-1.056729	-1.823871
33	C	6.717136	-2.318835	0.189829

Atom No.	Element	Cartesian Coorinates		
		X	Y	Z
34	C	-8.683928	-1.852786	-1.337620
35	C	-7.222252	-1.730372	-0.978013
36	C	4.971833	-0.965746	-1.516684
37	C	8.683089	-1.853563	-1.339040
38	C	0.000229	1.340171	1.025625
39	H	-4.610330	3.603286	-0.632256
40	H	4.636116	1.313895	0.330040
41	H	-6.699106	-0.603477	-2.740298
42	H	-4.976768	-2.722855	1.403012
43	H	4.611181	3.603228	-0.631305
44	H	2.414834	4.781089	-0.935209
45	H	-4.635512	1.313957	0.329002
46	H	-2.413906	4.781124	-0.935694
47	H	4.976772	-2.723690	1.402615
48	H	-7.392232	-2.853853	0.854146
49	H	-4.280054	-0.461222	-2.181922
50	H	6.697971	-0.603403	-2.740697
51	H	7.392002	-2.854963	0.852829
52	H	-9.308319	-1.971388	-0.446173
53	H	-9.037165	-0.973961	-1.887257
54	H	-8.858997	-2.727855	-1.977426
55	H	4.279128	-0.460941	-2.181441
56	H	9.308153	-1.968129	-0.447518
57	H	8.858463	-2.731082	-1.975399
58	H	9.035266	-0.976665	-1.892391
59	C	-2.888940	-0.288256	2.564714
60	H	-3.925483	-0.009153	2.803529
61	H	-2.713267	-1.330280	2.834053
62	H	-2.195934	0.331995	3.136586
63	C	2.889144	-0.288106	2.565522
64	H	2.195671	0.331734	3.137292
65	H	2.713942	-1.330243	2.834727
66	H	3.925480	-0.008495	2.804618

b. Optimized structure of **2**

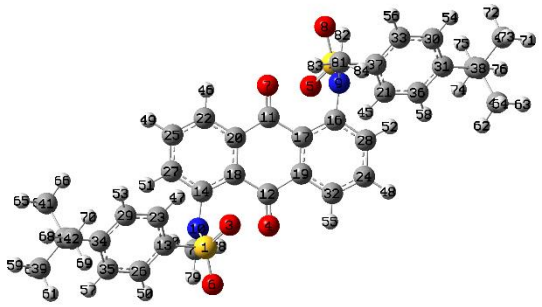
E(RB3LYP) = -2515.94229569 a.u.

Number of imaginary frequency: 0



Atom No.	Element	Cartesian Coorinates		
		X	Y	Z
1	S	3.902684	0.230832	-0.448976
2	S	-3.902816	0.231067	0.448748
3	O	-4.950253	0.599458	1.403088
4	O	3.530578	1.080487	0.684792
5	O	1.968497	2.591975	-1.826979
6	O	-3.530604	1.080574	-0.685090
7	O	4.950049	0.599080	-1.403453
8	O	-1.968484	2.592211	1.826841
9	N	-2.498366	-0.046946	1.338678
10	N	2.498164	-0.047271	-1.338750
11	C	-0.599128	1.276765	0.377930
12	C	-0.546751	3.844682	0.438376
13	C	0.599076	1.276699	-0.377988
14	C	0.547102	3.844621	-0.438325
15	C	-0.619558	-1.151870	0.316463
16	C	0.619336	-1.151934	-0.316324
17	C	-1.130678	2.571767	0.934947
18	C	-1.234620	0.045978	0.678939
19	C	4.351731	-1.371675	0.231569
20	C	1.130764	2.571640	-0.935005
21	C	-4.190415	-3.014980	-1.982491
22	C	1.234465	0.045840	-0.678931
23	C	-4.351824	-1.371520	-0.231621
24	C	5.183305	-2.222830	-0.501786
25	C	-5.013581	-3.891410	-1.264591
26	C	-0.545835	6.261470	0.438569
27	C	0.546630	6.261408	-0.438310
28	C	5.377654	-5.250174	1.814673
29	C	-5.506019	-3.472469	-0.018380
30	C	1.090416	5.058457	-0.877552
31	C	-5.183389	-2.222606	0.501824
32	C	-3.856898	-1.757712	-1.477495
33	C	5.505972	-3.472623	0.018560

Atom No.	Element	Cartesian Coorinates		
		X	Y	Z
34	C	3.856831	-1.757733	1.477495
35	C	4.190386	-3.014935	1.982636
36	C	5.013568	-3.891426	1.264831
37	C	-5.377551	-5.250265	-1.814243
38	C	-1.089846	5.058581	0.877702
39	H	-1.121549	-2.085320	0.550986
40	H	1.121269	-2.085432	-0.550784
41	H	-3.812003	-3.314197	-2.956815
42	H	5.586969	-1.895263	-1.453983
43	H	-0.970777	7.202616	0.776305
44	H	0.971747	7.202505	-0.775963
45	H	6.464327	-5.359691	1.915007
46	H	4.932296	-5.417374	2.799999
47	H	5.034430	-6.053219	1.150684
48	H	-6.159973	-4.131949	0.547648
49	H	1.935737	5.031362	-1.556574
50	H	-5.587079	-1.894941	1.453976
51	H	-3.239366	-1.072853	-2.048509
52	H	6.159924	-4.132159	-0.547405
53	H	3.239290	-1.072823	2.048437
54	H	3.811993	-3.314049	2.956999
55	H	-6.464252	-5.360218	-1.913761
56	H	-4.932854	-5.417237	-2.799906
57	H	-5.033498	-6.053213	-1.150560
58	H	-1.935176	5.031584	1.556717
59	C	2.538140	-0.211256	-2.793683
60	H	3.577577	-0.174898	-3.119856
61	H	2.095560	-1.171671	-3.085043
62	H	2.001836	0.612711	-3.272197
63	C	-2.538470	-0.210937	2.793589
64	H	-3.577865	-0.173539	3.119781
65	H	-2.096800	-1.171758	3.085021
66	H	-2.001382	0.612533	3.272079



c. Optimized structure of **3**

E(RB3LYP) = -2751.81851735 a.u.

Number of imaginary frequency: 0

Atom No.	Element	Cartesian Coorinates		
		X	Y	Z
1	S	-4.284243	1.878759	-0.318031
2	S	4.284380	-1.829799	0.411457
3	O	-3.512131	1.337292	-1.439372
4	O	-1.081074	2.482747	0.355759
5	O	3.587897	-1.241578	1.558105
6	O	-4.573379	3.307603	-0.176219
7	O	1.075283	-2.428591	-0.073988
8	O	4.527809	-3.268740	0.287668
9	N	3.467072	-1.346404	-0.987040
10	N	-3.527518	1.388550	1.110323
11	C	0.624383	-1.295565	0.034594
12	C	-0.652090	1.347493	0.195133
13	C	-5.861849	1.016146	-0.322870
14	C	-2.746070	0.190745	1.088692
15	C	-9.661379	-1.113821	-0.327439
16	C	2.688803	-0.147000	-0.937681
17	C	1.361385	-0.088660	-0.441886
18	C	-1.404860	0.136010	0.632455
19	C	0.709694	1.160986	-0.407515
20	C	-0.750585	-1.112001	0.608933
21	C	6.071735	0.229706	0.916697
22	C	-1.391007	-2.266449	1.076146
23	C	-5.981600	-0.209913	-0.980657
24	C	2.626423	2.240784	-1.407962
25	C	-2.691215	-2.197268	1.556960
26	C	-6.958099	1.574884	0.331517
27	C	-3.365529	-0.975447	1.546208
28	C	3.296426	1.016745	-1.417003
29	C	-7.204966	-0.873905	-0.965438
30	C	8.158746	-0.976536	-0.482934
31	C	8.378747	0.278375	0.104656
32	C	1.340257	2.313738	-0.891297
33	C	6.926503	-1.623753	-0.385005
34	C	-8.328921	-0.343772	-0.306722
35	C	-8.176016	0.893832	0.336231
36	C	7.308564	0.859514	0.808460
37	C	5.883315	-1.013295	0.308450
38	C	9.727272	1.014996	0.016187
39	C	-10.770689	-0.390145	0.459140
40	C	9.515429	2.395927	-0.649550
41	C	-9.457002	-2.512078	0.303797
42	C	-10.134646	-1.275628	-1.791895

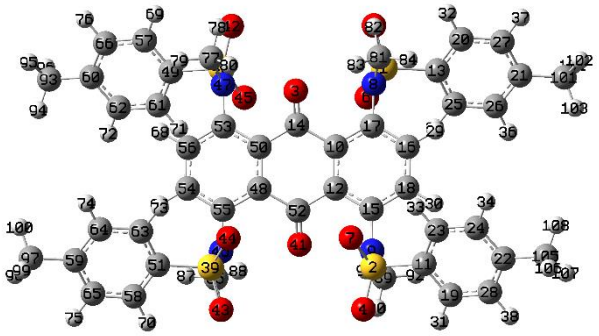
Atom No.	Element	Cartesian Coorinates		
		X	Y	Z
43	C	10.766970	0.237334	-0.812635
44	C	10.295594	1.213835	1.441791
45	H	5.263867	0.681872	1.481844
46	H	-0.845082	-3.202473	1.041743
47	H	-5.130686	-0.621887	-1.512186
48	H	3.114521	3.131338	-1.793508
49	H	-3.187882	-3.089721	1.926842
50	H	-6.866427	2.542682	0.813512
51	H	-4.392348	-0.905518	1.891163
52	H	4.310988	0.942418	-1.795511
53	H	-7.282793	-1.822176	-1.489366
54	H	8.955864	-1.474398	-1.023002
55	H	0.797663	3.251082	-0.843135
56	H	6.783175	-2.604712	-0.825973
57	H	-9.016087	1.351395	0.846007
58	H	7.440402	1.822470	1.293312
59	H	-11.693238	-0.979791	0.419632
60	H	-10.506672	-0.261812	1.515113
61	H	-10.993522	0.596691	0.038043
62	H	8.818916	3.021872	-0.082074
63	H	10.468137	2.934785	-0.715810
64	H	9.116979	2.286110	-1.664712
65	H	-10.398025	-3.074744	0.290223
66	H	-8.710063	-3.101227	-0.238289
67	H	-9.126860	-2.428924	1.345676
68	H	-11.080628	-1.829439	-1.825617
69	H	-10.295184	-0.298883	-2.261959
70	H	-9.406217	-1.822964	-2.398960
71	H	11.703052	0.805089	-0.854324
72	H	10.994658	-0.739345	-0.370936
73	H	10.431325	0.078212	-1.843780
74	H	9.619978	1.800261	2.073047
75	H	10.462201	0.249812	1.935495
76	H	11.254929	1.743440	1.397586
77	C	-3.410805	2.296701	2.254930
78	H	-2.381831	2.653326	2.356012
79	H	-4.056585	3.158135	2.084780
80	H	-3.724596	1.780601	3.169587
81	C	3.278488	-2.273359	-2.106564
82	H	3.934292	-3.132248	-1.963898
83	H	2.246062	-2.633274	-2.139193
84	H	3.534976	-1.771243	-3.046336

d. Optimized structure of **4**

(Terminal *t*Bu groups were replaced with Me groups)

E(RB3LYP) = -4343.10074070 a.u.

Number of imaginary frequency: 0



Atom No.	Element	Cartesian Coorinates		
		X	Y	Z
1	S	2.737041	3.891947	0.397802
2	S	2.737066	-3.891969	-0.397673
3	O	-0.000180	1.721907	1.999042
4	O	2.393399	-5.017635	-1.266409
5	O	2.393420	5.017619	1.266547
6	O	2.045349	3.610759	-0.859259
7	O	2.045449	-3.610798	0.859433
8	N	2.556077	2.503349	1.341059
9	N	2.556042	-2.503363	-1.340905
10	C	1.292058	0.596755	0.374257
11	C	4.487109	-4.058607	-0.011357
12	C	1.292051	-0.596784	-0.374047
13	C	4.487060	4.058588	0.011377
14	C	-0.000165	1.080952	0.959487
15	C	2.517439	-1.234219	-0.683695
16	C	3.714157	0.616837	0.323815
17	C	2.517454	1.234198	0.683863
18	C	3.714151	-0.616849	-0.323693
19	C	5.343980	-4.673866	-0.928538
20	C	5.343986	4.673856	0.928500
21	C	7.233673	4.292242	-0.576129
22	C	7.233760	-4.292254	0.575974
23	C	4.983088	-3.571027	1.196366
24	C	8.738238	4.444994	-0.861825
25	C	6.345463	-3.690667	1.479220
26	C	8.738345	-4.444998	0.861571
27	C	4.982964	3.571004	-1.196375
28	C	6.345320	3.690648	-1.479316
29	C	6.698483	4.780915	0.630184
30	C	6.698496	-4.780922	-0.630307
31	C	9.109751	5.947322	-0.862216
32	C	9.140158	3.850079	-2.224792
33	C	9.109864	-5.947324	0.861957
34	C	9.546012	3.717087	0.239371
35	C	9.546042	-3.717101	-0.239688
36	C	9.140354	-3.850064	2.224504
37	H	4.652346	1.108408	0.559985
38	H	4.652334	-1.108411	-0.559900

Atom No.	Element	Cartesian Coorinates		
		X	Y	Z
73	N	-2.556371	2.503479	1.340852
74	C	-1.292391	-0.596800	-0.373994
75	C	-4.486944	4.058837	0.010757
76	C	-1.292388	0.596781	0.374229
77	C	-4.487039	-4.058830	-0.010733
78	C	-0.000179	-1.080972	-0.959266
79	C	-2.517779	1.234262	0.683786
80	C	-3.714486	-0.616863	-0.323616
81	C	-2.517782	-1.234260	-0.683581
82	C	-3.714484	0.616889	0.323781
83	C	-5.343901	4.674312	0.927718
84	C	-5.343943	-4.674272	-0.927765
85	C	-7.233610	-4.292688	0.576900
86	C	-7.233474	4.292709	-0.577060
87	C	-4.982778	3.571159	-1.196981
88	C	-8.738162	-4.445503	0.862635
89	C	-6.345094	3.690912	-1.480078
90	C	-8.738005	4.445536	-0.862899
91	C	-4.982946	-3.571178	1.196986
92	C	-6.345282	-3.690924	1.479991
93	C	-6.698418	-4.781427	-0.629390
94	C	-6.698356	4.781474	0.629252
95	C	-9.109635	-5.947833	0.863121
96	C	-9.140087	-3.850523	2.225573
97	C	-9.109464	5.947870	-0.863417
98	C	-9.545977	-3.717680	-0.238594
99	C	-9.545903	3.717727	0.238279
100	C	-9.139843	3.850553	-2.225861
101	H	-4.652677	-1.108440	-0.559767
102	H	-4.652672	1.108487	0.559898
103	H	-4.946149	5.087942	1.848532
104	H	-4.946136	-5.087881	-1.848564
105	H	-4.303308	3.123046	-1.914074
106	H	-6.704968	3.312726	-2.430120
107	H	-4.303518	-3.123091	1.914135
108	H	-6.705215	-3.312758	2.430020
109	H	-7.348079	-5.268875	-1.350345
110	H	-7.348058	5.268950	1.350151

39	H	4.946118	-5.087439	-1.849331
40	H	4.946180	5.087433	1.849315
41	H	4.303682	-3.123093	1.913630
42	H	6.705457	-3.312566	2.429251
43	H	4.303514	3.123064	-1.913594
44	H	6.705256	3.312544	-2.429368
45	H	7.348158	5.268243	1.351207
46	H	7.348128	-5.268242	-1.351375
47	H	8.892692	6.422798	0.099895
48	H	10.180761	6.072293	-1.062061
49	H	8.553804	6.488975	-1.635604
50	H	8.926196	2.776628	-2.282148
51	H	8.626949	4.347339	-3.055528
52	H	10.217141	3.979946	-2.378709
53	H	8.892749	-6.422812	-0.100134
54	H	10.180887	-6.072288	1.061738
55	H	8.553967	-6.488970	1.635386
56	H	9.341911	4.125145	1.234786
57	H	9.307189	2.647502	0.259902
58	H	10.621378	3.820895	0.051534
59	H	9.341880	-4.125176	-1.235083
60	H	9.307208	-2.647519	-0.260221
61	H	10.621421	-3.820896	-0.051917
62	H	8.926391	-2.776613	2.281862
63	H	8.627201	-4.347316	3.055281
64	H	10.217348	-3.979924	2.378352
65	S	-2.737070	-3.892010	-0.397289
66	S	-2.737001	3.892008	0.397430
67	O	-0.000211	-1.721946	-1.998810
68	O	-2.393349	5.017720	1.266111
69	O	-2.393374	-5.017707	-1.265972
70	O	-2.045325	-3.610639	0.859702
71	O	-2.045179	3.610603	-0.859510
72	N	-2.556366	-2.503463	-1.340672

111	H	-8.892604	-6.423370	-0.098966
112	H	-10.180635	-6.072821	1.063012
113	H	-8.553650	-6.489434	1.636521
114	H	-8.926170	-2.777060	2.282859
115	H	-8.626836	-4.347711	3.056327
116	H	-10.217061	-3.980426	2.379521
117	H	-8.892486	6.423409	0.098681
118	H	-10.180451	6.072867	-1.063375
119	H	-8.553426	6.489460	-1.636786
120	H	-9.341869	-4.125802	-1.233979
121	H	-9.307182	-2.648092	-0.259196
122	H	-10.621338	-3.821510	-0.050734
123	H	-9.341857	4.125849	1.233677
124	H	-9.307123	2.648136	0.258900
125	H	-10.621250	3.821569	0.050347
126	H	-8.925924	2.777089	-2.283130
127	H	-8.626538	4.347738	-3.056584
128	H	-10.216807	3.980457	-2.379879
129	C	-2.850295	2.546700	2.774477
130	H	-2.651557	3.555719	3.137065
131	H	-3.890317	2.267265	2.997189
132	H	-2.166022	1.861260	3.278318
133	C	2.849968	2.546343	2.774702
134	H	2.651470	3.555373	3.137394
135	H	2.165509	1.861014	3.278445
136	H	3.889913	2.266624	2.997405
137	C	-2.850200	-2.546651	-2.774316
138	H	-2.651458	-3.555667	-3.136911
139	H	-3.890201	-2.267191	-2.997092
140	H	-2.165879	-1.861215	-3.278099
141	C	2.849849	-2.546340	-2.774566
142	H	2.651339	-3.555368	-3.137257
143	H	2.165352	-1.861012	-3.278260
144	H	3.889777	-2.266607	-2.997329

9. Reference

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S2. T. Takeda, S. Noro, T. Nakamura, Y. Suzuki, J. Kawamata, T. Akutagawa *CrystEngComm* 2018, **20**, 17-24.