Boron-Bridged π–Conjugated Ladders as Efficient Electron-Transporting Emitters

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Content

Experimental section

General Procedure

All starting materials were purchased from Aldrich Chemical Co. and used without further purification. All experiments were performed under a nitrogen atmosphere using standard Schlenk techniques. ^{1}H NMR spectra of **H_2L1**–**H_2L4** were measured on Bruker AVANCE 300 MHz spectrometer with tetramethylsilane as the internal standard. Mass spectra were recorded on a Shimadzu AXIMA-CFR MALDITOF mass spectrometer. Elemental analyses were performed on a flash EA 1112 spectrometer.

2,5-bis(2-hydroxyphenyl)-thiazolo[5,4-d]thiazole (H$_2$L1). A mixture of dithiooxamide (0.5 g, 4.2 mmol), salicylaldehyde (5.1 g, 41.8 mmol) and phenol (1.5 g, 16.0 mmol) was heated to reflux temperature, and then it was cooled and diluted with ethanol after heating for 4 hours. The crude product was washed with ether and recrystallized from cyclohexanone to give yellow crystals (0.5 g, 38% yield). ^{1}H NMR (300 MHz, DMSO, ppm): δ 11.31 (s, 2 H), 8.25 (d, J = 7.2 Hz, 2 H), 7.36 (t, J = 6.9 Hz, 2 H), 7.07 (d, J = 8.1 Hz, 2 H), 7.01 (t, J = 7.5 Hz, 2 H). Ms m/z: 326.1 $[M]^+$ (calcd: 326.0). Anal. Calcd (%) for $C_{16}H_{10}N_2O_2S_2$: C, 58.88; H, 3.09; N, 8.58; S, 19.65. Found: C, 59.11; H, 3.19; N, 8.52; S, 19.54.

2,5-bis(2-hydroxy-5-fluorophenyl)thiazolo[5,4-d]thiazole (H$_2$L2). In the same manner described for **H_2L1**, compound **H_2L2** was provided as yellow crystals (30% yield) using 5-fluorosalicylaldehyde as the initial material. ^{1}H NMR (300 MHz, DMSO, ppm): δ 11.40 (s, 2 H), 7.98 (dd, J = 9.9 Hz, J = 3.3 Hz, 2 H), 7.24 (td, J = 8.4 Hz, J = 3.3 Hz, 2 H), 7.08 (dd, J = 9.0 Hz, J = 4.8 Hz, 2 H). Ms m/z: 362.1 $[M]^+$ (calcd: 362.0). Anal. Calcd (%) for $C_{16}H_8F_2N_2O_2S_2$: C, 53.03; H, 2.23; N, 7.73; S, 17.70. Found: C, 52.94; H, 2.31; N, 7.76; S, 17.82.

2,5-bis(2-hydroxy-5-methoxyphenyl)thiazolo[5,4-d]thiazole (H$_2$L3). In the same manner described for **H_2L1**, compound **H_2L3** was provided using 2-hydroxy-5-methoxybenzaldehyde as the initial material to give dark yellow solids (22% yield). ^{1}H NMR (300 MHz, DMSO, ppm): δ 10.91 (s, 2 H), 7.77 (s, 2 H), 6.99–6.98 (m, 4 H), 3.79 (s, 6 H). Ms m/z: 386.1 $[M]^+$ (calcd: 386.0). Anal. Calcd (%) for $C_{18}H_{14}N_2O_4S_2$: C, 55.94; H, 3.65; N, 7.25; S, 16.59. Found: C, 56.01; H, 3.67; N, 7.14; S, 16.45.

2,5-bis(2-hydroxy-4-methoxyphenyl)thiazolo[5,4-d]thiazole (H$_2$L4). In the same manner described for **H_2L1**, compound **H_2L4** was provided using 2-hydroxy-4-methoxybenzaldehyde as the initial material and purified by vacuum sublimation to give yellow solids (20% yield). ^{1}H NMR (300 MHz, DMSO, ppm): δ 11.30 (s, 2 H), 8.10 (d, J = 8.7 Hz, 2 H), 6.63–6.57 (m, 4 H), 3.80 (s, 6 H). Ms m/z: 386.1 $[M]^+$ (calcd: 386.0). Anal. Calcd (%) for $C_{18}H_{14}N_2O_4S_2$: C, 55.94; H, 3.65; N, 7.25; S, 16.59. Found: C, 56.20; H, 3.68; N, 7.28; S, 16.50.

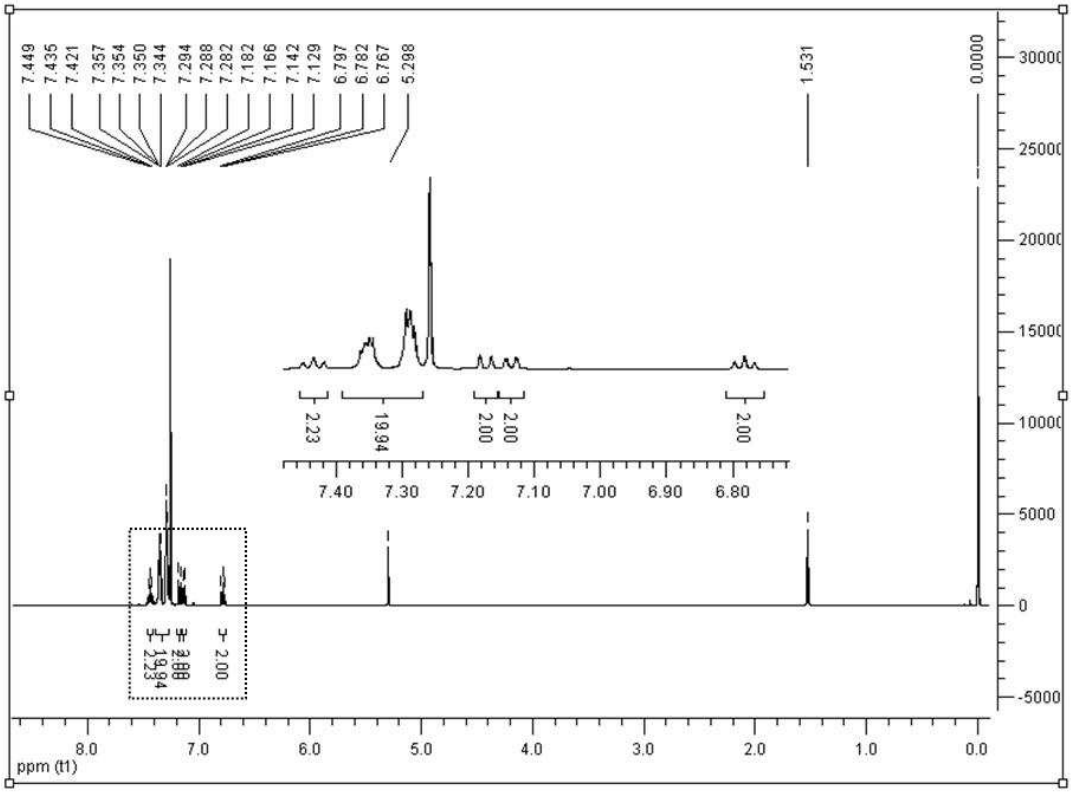

Fig. S1 ^{1}H NMR spectrum of complex **1**.

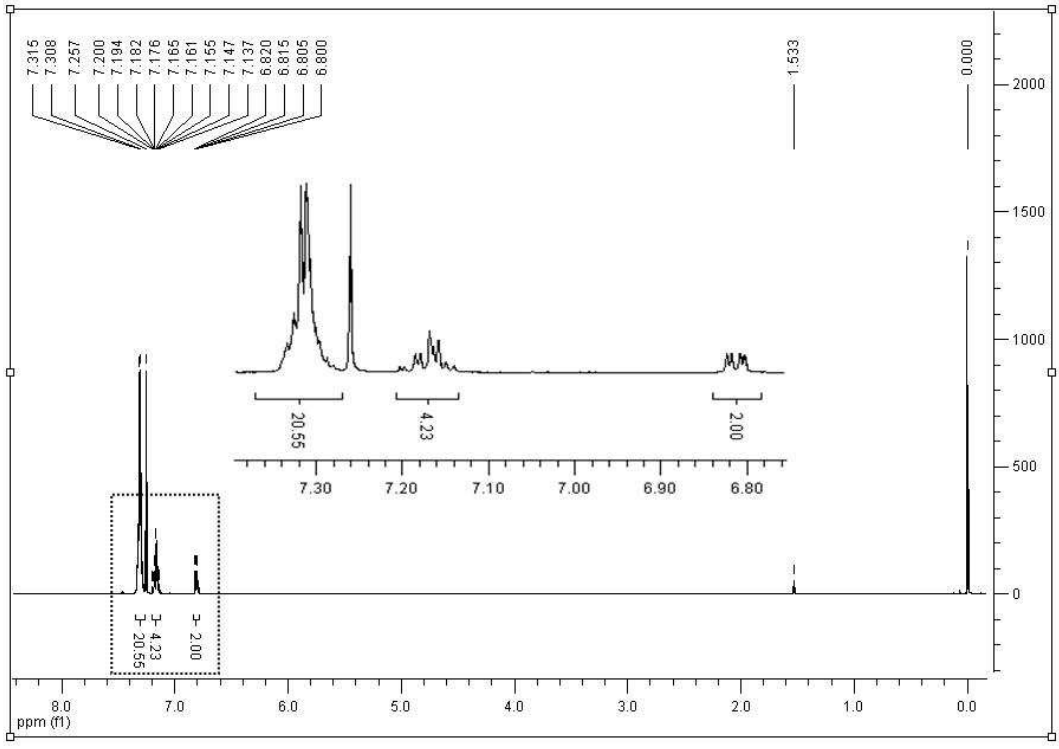

Fig. S2 ^{1}H NMR spectrum of complex **2**.

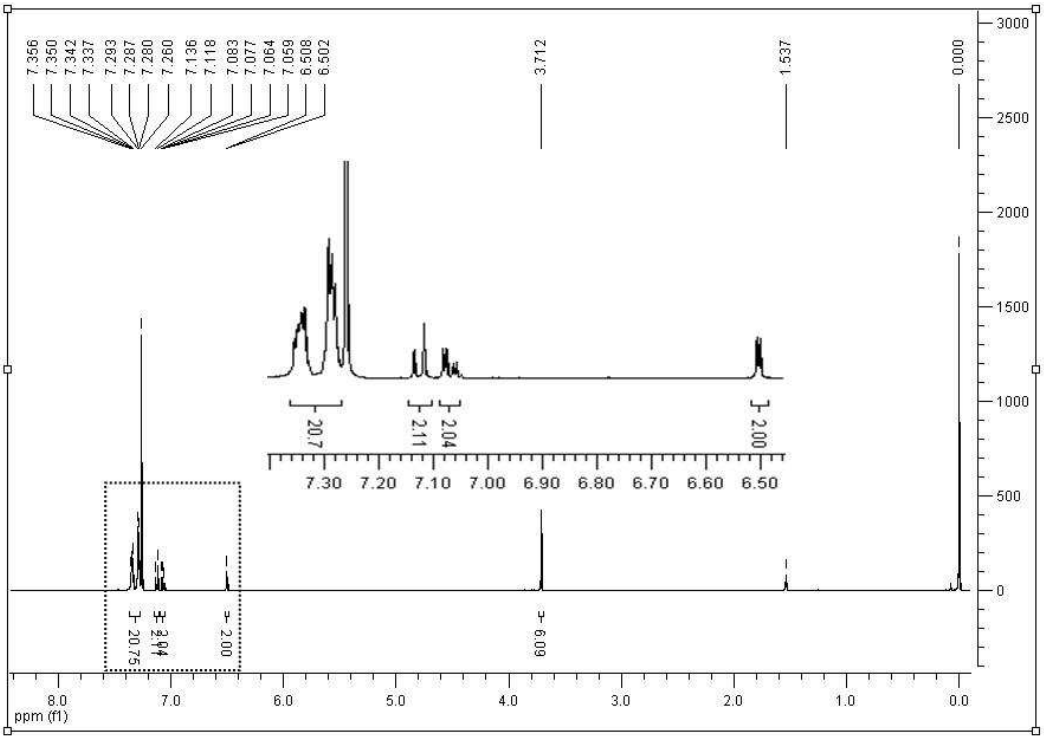

Fig. S3 ^{1}H NMR spectrum of complex **3**.

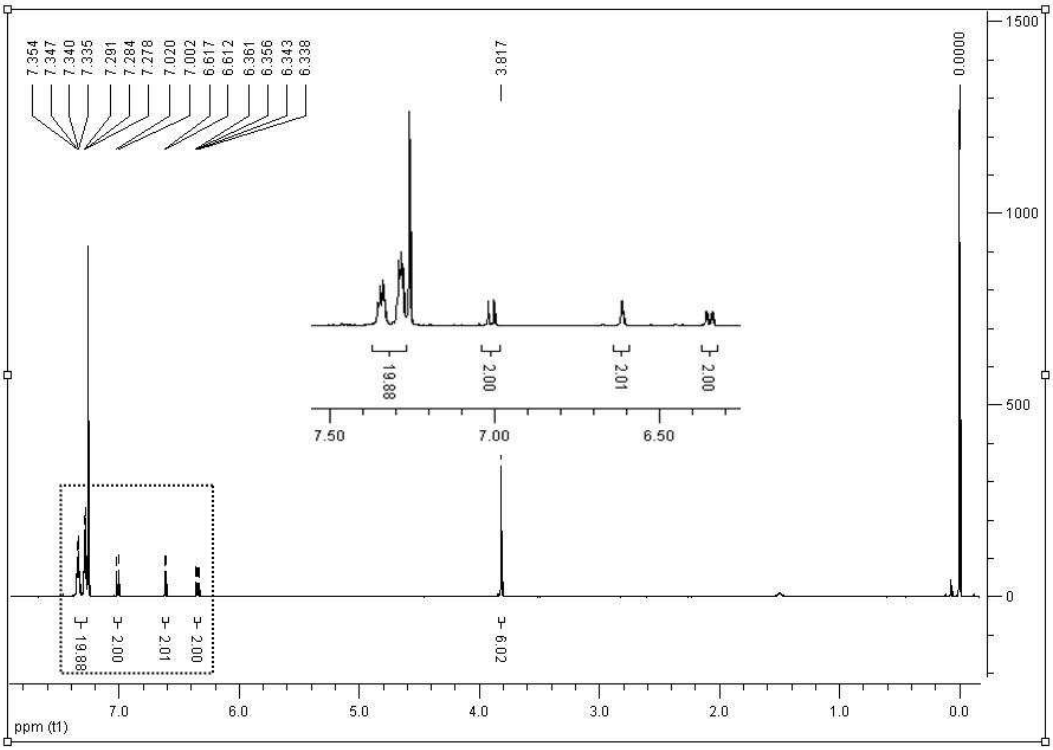

Fig. S4 ^{1}H NMR spectrum of complex **4**.

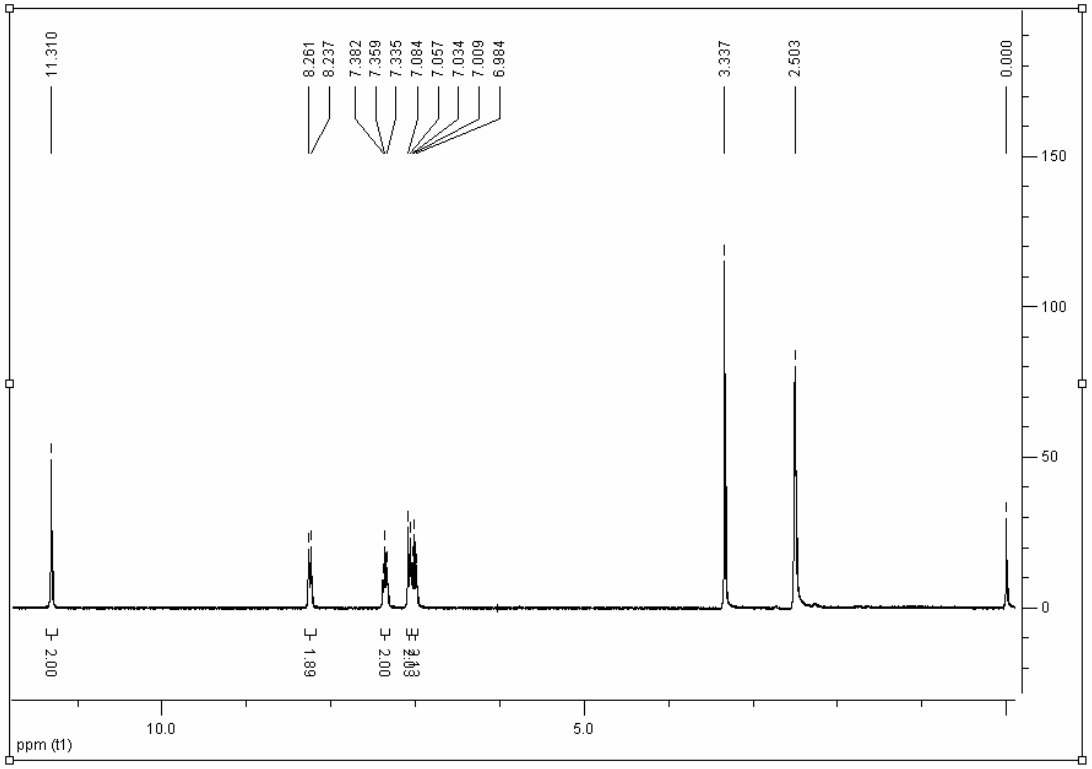

Fig. S5 ^{1}H NMR spectrum of compound **H_2L1**.

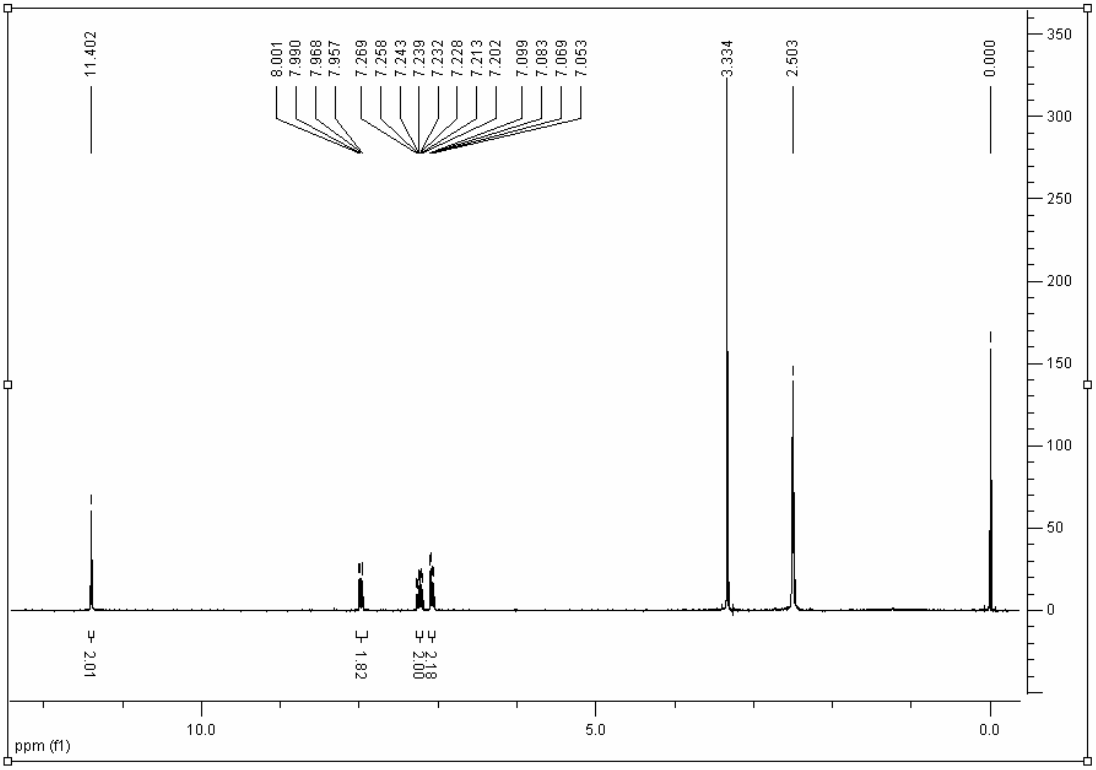

Fig. S6 ^{1}H NMR spectrum of compound **H_2L2**.

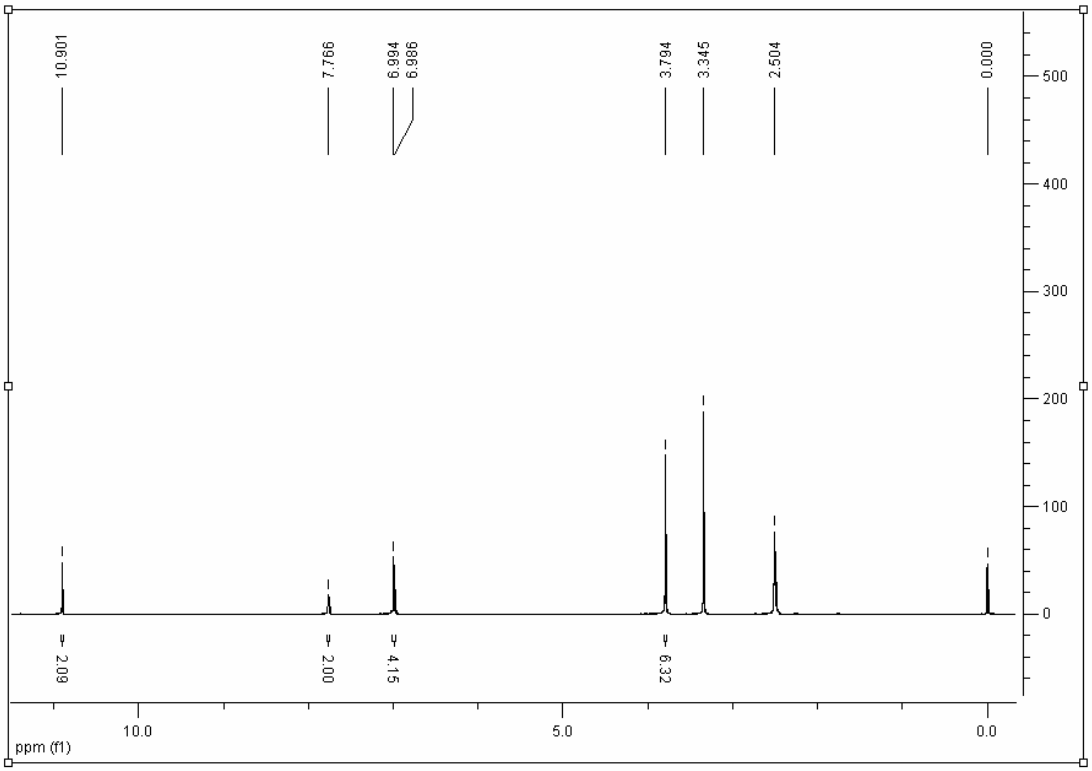

Fig. S7 ^{1}H NMR spectrum of compound **H_2L3**.

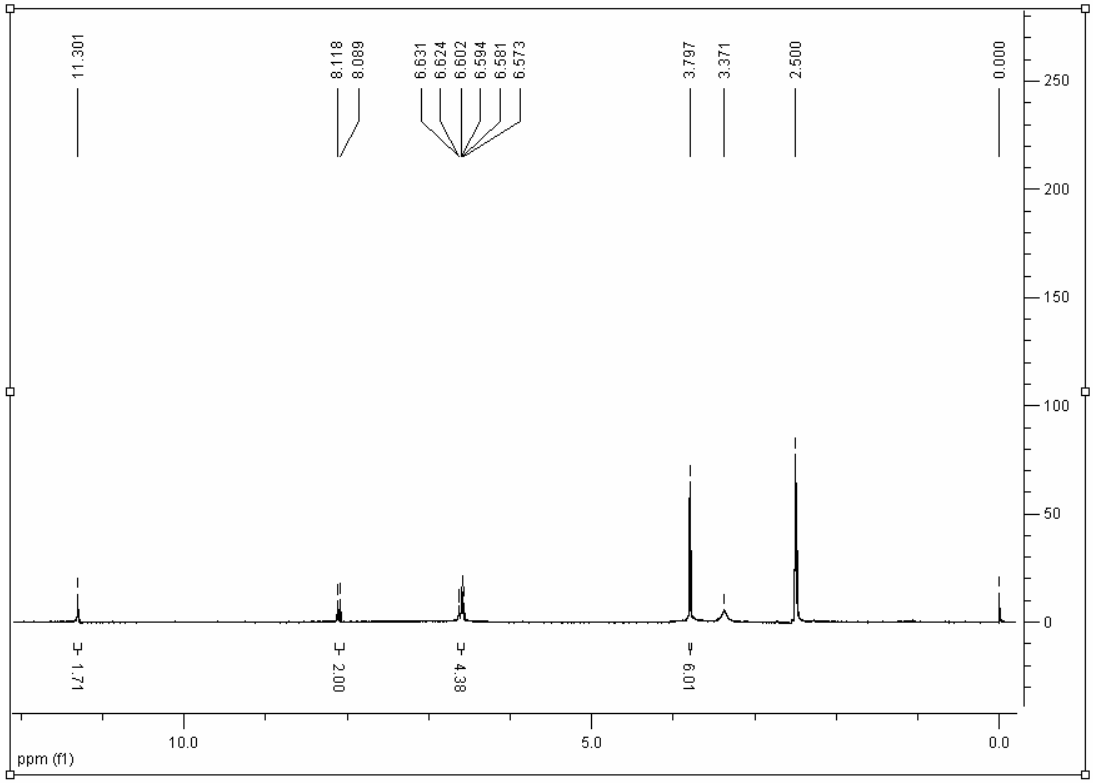

Fig. S8 ^{1}H NMR spectrum of compound **H_2L4**.

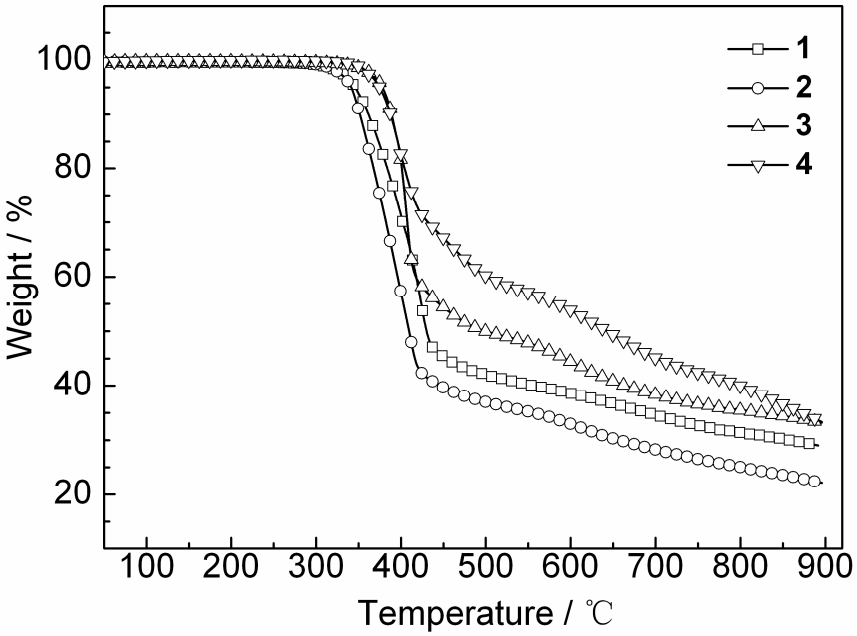

Figure S9. TGA curves of **1**–**4** at a heating rate of 10 °C/min.

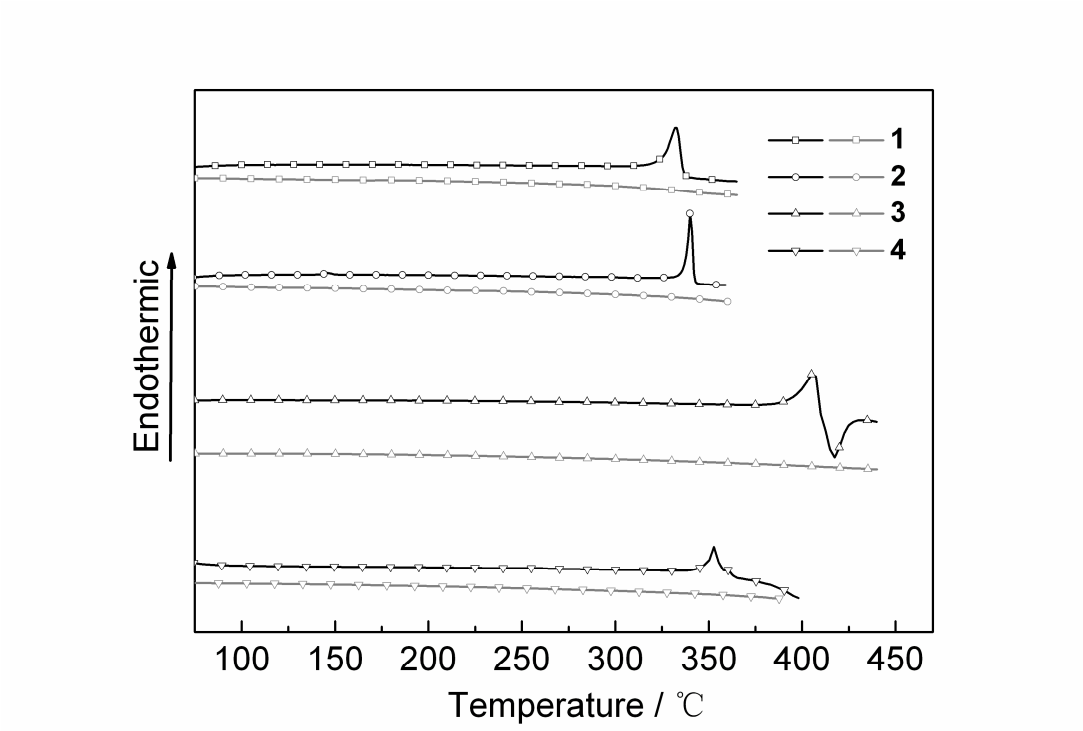

Figure S10. DSC curves of the first (black colour) and second (gray colour) heating segments of **1**–**4** at a heating rate of 10 °C/min.

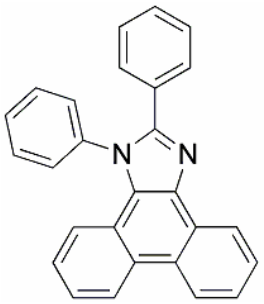

Figure S11. Molecular structure of BA(1,2-diphenyl-1H-phenanthro[9,10-d]imidazole).

Table S1. Crystal Data for Compounds **1–3**.

	1	**2**	**3**
formula	$C_{40}H_{28}B_2N_2O_2S_2$	$C_{40}H_{26}B_2F_2N_2O_2S_2$	$C_{42}H_{32}B_2N_2O_4S_2$
fw	654.4	690.39	714.47
crystal system	monoclinic	monoclinic	triclinic
space group	$P2_1/c$	$P2_1/c$	P_{-1}
a (Å)	8.5306(17)	11.485(2)	9.5072(19)
b (Å)	13.623(3)	15.432(3)	9.7261(19)
c (Å)	14.265(3)	9.831(2)	10.865(2)
α (deg)	90	90	105.12(3)
β (deg)	92.84(3)	98.21(3)	109.66(3)
γ (deg)	90	90	97.57(3)
V (Å^3)	1655.7(6)	1724.7(6)	886.3(3)
Z	2	2	1
D_c (g cm^{-3})	1.313	1.329	1.339
θ_{max} (deg)	27.47	27.48	27.47
no. of reflns meads	15727	15942	8760
no. of reflns used	3735	3868	4023
no. of parameters	217	226	236
R_{int}	0.0478	0.0362	0.0191
final R [I > 2σ(I)]			
R1	0.0568	0.0411	0.0416
wR	0.1423	0.1020	0.1250
R (all data)			
R1	0.1006	0.0563	0.0501
wR2	0.1632	0.1096	0.0312
GOF on F^2	1.013	1.040	1.102

Table S2. Selected Bond Lengths (Å) and Angles (deg) for **1**–**3**.

Complex **1**			
B(1)-O(1)	1.470(3)	C(1)-B(1)-N(1)	109.0(2)
B(1)-C(1)	1.604(4)	C(7)-B(1)-N(1)	107.1(2)
B(1)-C(7)	1.607(4)	C(19)-N(1)-C(20)	110.64(18)
B(1)-N(1)	1.659(3)	C(20)#1-C(20)-N(1)	114.6(3)
C(20)-N(1)	1.379(3)	C(20)#1-C(20)-S(1)#1	111.6(2)
C(20)-C(20)#1	1.360(4)	C(20)#1-S(1)-C(19)	89.00(11)
S(1)-C(20)#1	1.714(2)	C(18)-C(19)-S(1)	124.39(17)
C(19)-S(1)	1.735(2)	N(1)-C(19)-S(1)	114.12(18)
C(19)-N(1)	1.338(3)	N(1)-C(19)-C(18)	121.4(2)
C(13)-O(1)	1.342(3)	C(13)-C(18)-C(19)	117.2(2)
C(18)-C(19)	1.439(3)	O(1)-C(13)-C(18)	122.0(2)
O(1)-B(1)-C(1)	107.5(2)	C(19)-N(1)-B(1)	119.08(19)
O(1)-B(1)-C(7)	111.9(2)	C(20)-N(1)-B(1)	130.00(19)
C(1)-B(1)-C(7)	117.3(2)	C(13)-O(1)-B(1)	121.18(19)
O(1)-B(1)-N(1)	102.95(18)	N(1)-C(20)-S(1)#1	133.77(16)
Complex **2**			
S(1)-C(8)	1.7222(17)	C(10)#1-N(1)-B(1)	119.23(13)
S(1)-C(10)	1.7337(17)	C(8)-N(1)-B(1)	129.89(14)
O(1)-C(5)	1.339(2)	C(8)#1-C(8)-N(1)	114.68(19)
O(1)-B(1)	1.481(3)	C(8)#1-C(8)-S(1)	111.29(16)
N(1)-C(8)	1.370(2)	N(1)-C(8)-S(1)	134.02(12)
N(1)-B(1)	1.643(2)	N(1)#1-C(10)-C(11)	120.73(15)
C(8)-C(8)#1	1.362(3)	N(1)#1-C(10)-S(1)	114.76(12)
C(10)-C(11)	1.444(2)	O(1)-B(1)-C(20)	110.37(16)
C(11)-C(5)#1	1.405(3)	O(1)-B(1)-C(19)	111.86(16)
B(1)-C(19)	1.609(3)	C(20)-B(1)-C(19)	116.33(16)
C(20)-B(1)	1.598(3)	O(1)-B(1)-N(1)	102.51(14)
F(1)-C(13)	1.355(2)	C(20)-B(1)-N(1)	107.49(13)
C(10)-N(1)#1	1.324(2)	C(19)-B(1)-N(1)	107.20(15)
C(8)-S(1)-C(10)	88.41(8)	O(1)-C(5)-C(11)#1	121.95(16)
C(5)-O(1)-B(1)	118.22(16)	C(5)#1-C(11)-C(10)	116.48(16)
C(10)#1-N(1)-C(8)	110.83(13)	C(11)-C(10)-S(1)	124.38(14)

Complex **3**

S(1)-C(10)	1.7195(16)	C(8)#1-N(2)-B(2)	118.67(13)
S(1)-C(8)	1.7373(17)	C(10)-N(2)-B(2)	130.11(12)
O(2)-C(13)	1.345(2)	N(2)-C(10)-C(10)#1	114.74(17)
O(2)-B(2)	1.480(2)	N(2)-C(10)-S(1)	133.91(11)
N(2)-C(8)#1	1.331(2)	C(10)#1-C(10)-S(1)	111.35(15)
N(2)-C(10)	1.3660(19)	N(2)#1-C(8)-C(4)	120.58(14)
N(2)-B(2)	1.647(2)	N(2)#1-C(8)-S(1)	114.57(12)
C(10)-C(10)#1	1.368(3)	C(4)-C(8)-S(1)	124.84(13)
C(13)-C(4)#1	1.404(2)	O(2)-B(2)-N(2)	102.34(12)
C(8)-C(4)	1.445(2)	O(2)-C(13)-C(4)#1	122.06(15)
C(33)-B(2)	1.608(2)	C(33)-B(2)-N(2)	108.68(12)
C(37)-B(2)	1.611(2)	C(37)-B(2)-N(2)	106.23(12)
O(4)-C(2)	1.366(3)	O(2)-B(2)-C(33)	109.89(13)
O(4)-C(1)	1.370(4)	O(2)-B(2)-C(37)	112.52(13)
C(10)-S(1)-C(8)	88.50(8)	C(33)-B(2)-C(37)	116.13(13)
C(13)-O(2)-B(2)	116.40(12)	C(13)#1-C(4)-C(8)	116.34(15)
C(8)#1-N(2)-C(10)	110.85(13)	N(2)-C(10)-S(1)	133.91(11)
O(4)-C(2)-C(3)	125.2(2)	O(4)-C(2)-C(7)	114.96(18)
C(3)-C(4)-C(8)	122.68(15)	C(2)-O(4)-C(1)	119.0(2)

Table S3. Cartesian coordinates of complex **1** at the S_0 optimized geometry.

Atomic	Coordinates		
	x	y	z
B	1.65468	1.730946	2.27779
C	0.342095	2.195348	3.091698
C	-0.2724	1.323853	4.012189
H	0.167391	0.344185	4.186737
C	-1.41861	1.690575	4.716926
H	-1.86854	0.997074	5.423651
C	-1.98652	2.952239	4.518027
H	-2.87897	3.242685	5.067169
C	-1.39545	3.838541	3.617367
H	-1.82333	4.826699	3.464744
C	-0.24543	3.460875	2.91721
H	0.213008	4.166733	2.229079
C	2.463175	2.895033	1.497592
C	2.31273	3.2012	0.134839
H	1.636411	2.612714	-0.48324
C	3.01623	4.246388	-0.47048
H	2.876349	4.452003	-1.52932
C	3.899623	5.020337	0.28156
H	4.451626	5.832695	-0.18475
C	4.069198	4.740096	1.639473
H	4.756529	5.335616	2.236104
C	3.359454	3.695379	2.231643
H	3.505406	3.488432	3.289534
C	3.480671	0.141457	2.721537
C	4.630961	-0.12467	3.485637
H	4.735915	0.381319	4.439718
C	5.602535	-0.99251	3.010771
H	6.493415	-1.17095	3.607005
C	5.459701	-1.6345	1.766908
H	6.234756	-2.30009	1.401095
C	4.321112	-1.41054	1.014603
H	4.200238	-1.90417	0.053095
C	3.316602	-0.53464	1.4778
C	2.055875	-0.36568	0.810857
C	0.026001	0.503584	0.465908
N	1.19307	0.589665	1.174389
O	2.552344	0.964424	3.197332
S	1.452938	-1.42484	-0.46106
B	-1.65468	-1.73095	-2.27779
C	-0.3421	-2.19535	-3.0917

C	0.272396	-1.32385	-4.01219
H	-0.16739	-0.34419	-4.18674
C	1.418607	-1.69058	-4.71693
H	1.868543	-0.99707	-5.42365
C	1.986521	-2.95224	-4.51803
H	2.87897	-3.24269	-5.06717
C	1.395445	-3.83854	-3.61737
H	1.823326	-4.8267	-3.46474
C	0.24543	-3.46088	-2.91721
H	-0.21301	-4.16673	-2.22908
C	-2.46318	-2.89503	-1.49759
C	-2.31273	-3.2012	-0.13484
H	-1.63641	-2.61271	0.483244
C	-3.01623	-4.24639	0.470476
H	-2.87635	-4.452	1.529319
C	-3.89962	-5.02034	-0.28156
H	-4.45163	-5.8327	0.184745
C	-4.0692	-4.7401	-1.63947
H	-4.75653	-5.33562	-2.2361
C	-3.35945	-3.69538	-2.23164
H	-3.50541	-3.48843	-3.28953
C	-3.48067	-0.14146	-2.72154
C	-4.63096	0.124672	-3.48564
H	-4.73592	-0.38132	-4.43972
C	-5.60254	0.992512	-3.01077
H	-6.49342	1.170947	-3.60701
C	-5.4597	1.634495	-1.76691
H	-6.23476	2.300091	-1.4011
C	-4.32111	1.410544	-1.0146
H	-4.20024	1.904168	-0.0531
C	-3.3166	0.534639	-1.4778
C	-2.05588	0.365676	-0.81086
C	-0.026	-0.50358	-0.46591
N	-1.19307	-0.58967	-1.17439
O	-2.55234	-0.96442	-3.19733
S	-1.45294	1.424836	0.461055

Table S4. Cartesian coordinates of complex **2** at the S_0 optimized geometry.

Atomic	Coordinates		
	x	y	z
B	1.657936	1.730128	2.280271
C	0.343842	2.19474	3.089654
C	-0.27391	1.32453	4.009292
H	0.165804	0.345571	4.18788
C	-1.42351	1.692031	4.708075
H	-1.87604	0.999898	5.414412
C	-1.99158	2.952763	4.503614
H	-2.88688	3.243556	5.04777
C	-1.39723	3.837791	3.603812
H	-1.82541	4.825087	3.447105
C	-0.24371	3.459655	2.909727
H	0.217444	4.164499	2.222379
C	2.472358	2.891013	1.503001
C	2.330978	3.195381	0.138921
H	1.657128	2.607525	-0.48256
C	3.040132	4.238451	-0.4634
H	2.907267	4.442992	-1.5233
C	3.920208	5.011713	0.293166
H	4.476605	5.822334	-0.17079
C	4.080678	4.733324	1.652581
H	4.765066	5.328678	2.252649
C	3.36528	3.690834	2.241779
H	3.503517	3.485935	3.30115
C	3.482039	0.139978	2.712313
C	4.636254	-0.12429	3.4738
H	4.741071	0.375144	4.430935
C	5.615758	-0.98234	2.999995
H	6.517947	-1.1769	3.570986
C	5.451055	-1.6024	1.755058
C	4.325477	-1.39818	0.988495
H	4.23462	-1.8992	0.029548
C	3.321305	-0.5283	1.465236
C	2.05778	-0.36211	0.800972
C	0.02622	0.502903	0.467353
N	1.194998	0.590421	1.170921
O	2.549031	0.95362	3.197348
S	1.454863	-1.41977	-0.4707
B	-1.65794	-1.73013	-2.28027
C	-0.34384	-2.19474	-3.08965
C	0.273914	-1.32453	-4.00929

H	-0.1658	-0.34557	-4.18788
C	1.423512	-1.69203	-4.70808
H	1.87604	-0.9999	-5.41441
C	1.991583	-2.95276	-4.50361
H	2.886879	-3.24356	-5.04777
C	1.397229	-3.83779	-3.60381
H	1.825413	-4.82509	-3.44711
C	0.243707	-3.45966	-2.90973
H	-0.21744	-4.1645	-2.22238
C	-2.47236	-2.89101	-1.503
C	-2.33098	-3.19538	-0.13892
H	-1.65713	-2.60753	0.482564
C	-3.04013	-4.23845	0.463403
H	-2.90727	-4.44299	1.5233
C	-3.92021	-5.01171	-0.29317
H	-4.47661	-5.82233	0.170789
C	-4.08068	-4.73332	-1.65258
H	-4.76507	-5.32868	-2.25265
C	-3.36528	-3.69083	-2.24178
H	-3.50352	-3.48594	-3.30115
C	-3.48204	-0.13998	-2.71231
C	-4.63625	0.124294	-3.4738
H	-4.74107	-0.37514	-4.43094
C	-5.61576	0.982339	-3
H	-6.51795	1.176898	-3.57099
C	-5.45106	1.6024	-1.75506
C	-4.32548	1.398175	-0.9885
H	-4.23462	1.8992	-0.02955
C	-3.32131	0.528303	-1.46524
C	-2.05778	0.362108	-0.80097
C	-0.02622	-0.5029	-0.46735
N	-1.195	-0.59042	-1.17092
O	-2.54903	-0.95362	-3.19735
S	-1.45486	1.419767	0.470701
F	-6.4233	2.421439	-1.30288
F	6.423296	-2.42144	1.302883

Table S5. Cartesian coordinates of complex **3** at the S_0 optimized geometry.

Atomic	Coordinates		
	x	y	z
S	0.839484	-1.90948	-0.05731
O	-3.79656	-1.25604	1.28274
N	-1.66518	-0.55665	0.264162
C	-0.31205	-0.60747	0.072388
C	2.106571	-0.70737	-0.29102
C	-2.02033	-3.04558	1.087709
C	-3.34189	-2.08214	-1.11349
B	-2.74946	-1.80023	0.365687
C	3.477579	-1.02177	-0.57206
C	-4.2665	-0.02098	1.122869
C	4.00271	-2.3303	-0.43375
H	3.389358	-3.10224	0.018004
C	-2.68975	-1.758	-2.31461
H	-1.72891	-1.24618	-2.2898
C	-4.58426	-2.73582	-1.22345
H	-5.12205	-3.00146	-0.31593
C	-1.62551	-4.19957	0.387693
H	-1.83771	-4.27195	-0.67619
O	5.913489	-3.81597	-0.76427
C	-1.74648	-3.00851	2.468885
H	-2.05706	-2.13964	3.044888
C	5.292748	-2.60407	-0.85707
C	6.065753	-1.57271	-1.4385
H	7.072094	-1.81429	-1.76659
C	-5.56448	0.293553	1.572586
H	-6.15957	-0.50046	2.011378
C	-5.14677	-3.04598	-2.46161
H	-6.11062	-3.5478	-2.50934
C	-0.98094	-5.2622	1.028636
H	-0.69448	-6.1446	0.460842
C	-0.71778	-5.19552	2.397066
H	-0.22144	-6.0215	2.90104
C	-1.10599	-4.06322	3.118836
H	-0.91248	-4.00693	4.187629
C	-3.24061	-2.06593	-3.56196
H	-2.70755	-1.79708	-4.47117
C	-4.4742	-2.71183	-3.6395
H	-4.90868	-2.95142	-4.60695
C	5.187226	-4.89234	-0.19287
H	4.9043	-4.67935	0.846845

H	5.857822	-5.75288	-0.21555
H	4.283098	-5.12094	-0.77334
S	-0.83948	1.909479	0.057313
O	3.796554	1.256045	-1.28274
N	1.665179	0.556655	-0.26416
C	0.312053	0.607467	-0.07239
C	-2.10657	0.707372	0.291021
C	2.020327	3.045584	-1.08771
C	3.341891	2.082135	1.113487
B	2.749464	1.80023	-0.36569
C	-3.47758	1.021771	0.57206
C	4.266496	0.020976	-1.12287
C	-4.00271	2.330304	0.433744
H	-3.38936	3.102236	-0.01801
C	2.689747	1.757995	2.314605
H	1.728907	1.246184	2.289803
C	4.584262	2.735816	1.223453
H	5.122055	3.00146	0.315932
C	1.625511	4.199571	-0.38769
H	1.837704	4.271952	0.676192
O	-5.91349	3.815975	0.764268
C	1.746483	3.008512	-2.46888
H	2.057062	2.139645	-3.04489
C	-5.29275	2.604066	0.85707
C	-6.06575	1.572708	1.438498
H	-7.0721	1.814291	1.766588
C	5.564483	-0.29355	-1.57259
H	6.159564	0.500456	-2.01138
C	5.146771	3.045973	2.461611
H	6.110624	3.547791	2.509338
C	0.980936	5.262195	-1.02863
H	0.694476	6.144602	-0.46084
C	0.717776	5.195525	-2.39706
H	0.221439	6.021503	-2.90103
C	1.105988	4.063225	-3.11883
H	0.91248	4.006934	-4.18763
C	3.240611	2.065928	3.561962
H	2.707553	1.797074	4.471167
C	4.474202	2.711826	3.639498
H	4.908681	2.951417	4.606952
C	-5.18723	4.892336	0.192863
H	-4.9043	4.679347	-0.84685
H	-5.85782	5.752875	0.215542
H	-4.2831	5.120942	0.773339

Table S6. Cartesian coordinates of complex **4** at the S_0 optimized geometry.

Atomic	Coordinates		
	x	y	z
S	-0.74999	1.944132	0.119281
O	3.952608	1.016668	1.033599
N	1.704937	0.466225	0.175218
C	0.344456	0.586951	0.085397
C	-2.08818	0.814596	-0.09249
C	2.238781	2.874378	1.120681
C	3.315798	2.015241	-1.25078
B	2.844268	1.654096	0.254979
C	-3.45893	1.198785	-0.23897
C	4.358593	-0.22015	0.767435
C	-3.92894	2.503095	0.003071
H	-3.25546	3.245991	0.423724
C	2.579747	1.737367	-2.41425
H	1.626776	1.215643	-2.342
C	4.543054	2.684777	-1.42189
H	5.144566	2.914407	-0.54505
C	1.845413	4.092606	0.539045
H	1.976077	4.235129	-0.53086
C	2.073163	2.746357	2.513537
H	2.385747	1.824632	2.999443
C	-5.23608	2.862505	-0.27034
C	-6.11014	1.897098	-0.81924
C	5.669725	-0.59521	1.065879
H	6.353717	0.137886	1.477436
C	5.011029	3.054737	-2.6826
H	5.96551	3.567585	-2.77816
C	1.304196	5.130535	1.304169
H	1.014755	6.063237	0.825278
C	1.146367	4.973335	2.68127
H	0.729589	5.779001	3.281033
C	1.536451	3.775443	3.286813
H	1.424829	3.647675	4.36115
C	3.035964	2.104959	-3.68363
H	2.439487	1.870912	-4.56259
C	4.25604	2.765832	-3.82209
H	4.616843	3.052058	-4.80706
S	0.750054	-1.94416	-0.11922
O	-3.95254	-1.01665	-1.03363
N	-1.70489	-0.46625	-0.17517
C	-0.34441	-0.58698	-0.08533
C	2.088244	-0.81461	0.092517

C	-2.23879	-2.87442	-1.12061
C	-3.31586	-2.01521	1.250781
B	-2.84425	-1.6541	-0.25496
C	3.459002	-1.19878	0.238958
C	-4.35852	0.220167	-0.76748
C	3.929026	-2.50308	-0.00311
H	3.255546	-3.24599	-0.42374
C	-2.5798	-1.73747	2.414282
H	-1.62676	-1.21587	2.342068
C	-4.54321	-2.68459	1.42185
H	-5.14473	-2.91413	0.544991
C	-1.84496	-4.09244	-0.53885
H	-1.97525	-4.23478	0.531125
C	-2.07369	-2.74667	-2.51355
H	-2.38665	-1.82512	-2.99954
C	5.236185	-2.86247	0.270253
C	6.110243	-1.89705	0.819126
C	-5.66963	0.59525	-1.06598
H	-6.35362	-0.13783	-1.47756
C	-5.01126	-3.05453	2.682542
H	-5.96581	-3.56725	2.778058
C	-1.30378	-5.13042	-1.30394
H	-1.01398	-6.06296	-0.82495
C	-1.14646	-4.97348	-2.68112
H	-0.72971	-5.77918	-3.28086
C	-1.53701	-3.7758	-3.28679
H	-1.42579	-3.64824	-4.36119
C	-3.03609	-2.10503	3.683637
H	-2.43961	-1.87109	4.562622
C	-4.25626	-2.76575	3.822059
H	-4.61712	-3.05195	4.807007
O	7.406339	-2.14331	1.131149
O	-7.40622	2.143378	-1.13132
C	7.941054	-3.43902	0.887642
H	8.983187	-3.39207	1.206991
H	7.416593	-4.206	1.470954
H	7.898496	-3.69665	-0.17779
C	-7.94092	3.439098	-0.88783
H	-7.41643	4.206069	-1.47113
H	-8.98304	3.392165	-1.20722
H	-7.8984	3.696735	0.177598
H	-5.57145	3.870566	-0.06257
H	5.571557	-3.87052	0.062467