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Thiophene Derivatives as Electrode Materials for High-Performance Sodium-Ion Batteries

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Experimental section

The synthesis procedure of STTDC was shown in **Figure S2**.

Synthesis of STTDC

Sodium thieno[3,2-*b*]thiophene-2,5-dicarboxylate (STTDC) was prepared by using thieno[3,2-b]thiophene (TT) as a precursor through the procedure illustrated in **Figure S2**. First, 2,5-dibromothieno[3,2-*b*]thiophene (DBTT) was synthesized by one step reaction of TT with N-bromosuccinimide (NBS).[1] DBTT should be stored in dark and at low temperature. Then, 1.42 g of DBTT and 1.62 g of dried copper (I) cyanide were dissolved in 20 mL of dry DMF. After refluxed under nitrogen for 70 h, the reaction mixture was poured into ice-water. The solid precipitation was collected by filtration and washed with water. The solid was stirred in water containing ethylene-

diamine (50 mL) for 1 h. Finally, thieno[3,2-*b*]thiophene-2,5-dicarbonitrile (TTDC) was prepared by filtration, washing with water and drying.[2]

0.41 g of TTDC was dispersed in NaOH aqueous solution (1.28 g NaOH dissolved in 20 mL H_2O). The mixture was refluxed under vigorously stirring for 35 h. After cooling down to room temperature, active carbon was added. The whole mixture was refluxed for an additional 1 h. Subsequently, the mixture was filtered and washed with NaOH solution and then water. 6 M HCl was added to the filtrate dropwise to give white precipitate. After filtered and washed by water, the precipitate was dried at 65 °C to obtain 2,5-thieno[3,2-b]thiophene dicarboxylic acid (TTDCA). The ^{1}H and ^{13}C NMR spectrums were shown in **Figure S3**.

^{1}H-NMR (400 MHz, DMSO-*d*6): δ 13.5, 8.2 (s, 2H)

^{13}C-NMR (75 MHz, DMSO-*d*6): δ 126.8, 139.9, 142.7, 163.5

TTDCA (0.50 g) and NaOH (0.23 g) were added into 15 mL methyl alcohol (MeOH) at room temperature under constant magnetic stirring for overnight. The mixture was filtered and washed with MeOH three times. After dried in vacuum at 80 °C for 10 h, sodium thieno[3,2-b]thiophene-2,5-dicarboxylate (STTDC) was obtained.

Characterization

Scanning electron microscopy (SEM) observation was performed on a FEI Nova NanoSEM 2300. ^{1}H and ^{13}C NMR spectra were recorded on a Bruker 400 spectrometer. In situ diffuse reflectance infrared Fourier transform spectroscopy (DRIFTs) analyses were performed on an FTIR spectrometer (PerkinElmer Frontier FT-IR Spectrometer) from 4000 to 650 cm^{-1}.

The working electrodes were made by mixing 60 wt% the active material, 30 wt% conducting agent (Super P) and 10 wt% binder (sodium alginate, SA). Then the slurry was spread onto a copper foil and dried at 80 °C for 24 h in a vacuum drying oven. The electrode was cut into discs of 12 mm in diameter and pressed at 6 MPa. The mass loading of STTDC is about 0.2 mg cm^{-2}. A CR2016 type coin half-cell battery was assembled in an Ar-filled glove-box. Sodium metal was used as the counter electrode, and glass-fiber (GF) as the separator, and 1.0 M $NaClO_4$ in a mixture of ethylene carbonate (EC) and propylene carbonate (PC) (1:1 in volume) with fluoroethylene carbonate (FEC, 5 wt%) as the electrolyte.

Solid-state sodium-ion batteries are assembled as follows: PEO (molecular weights M_n=600000) and $NaClO_4$ were dissolved in tetrahydrofuran at a molar ratio of EO:Na=8:1. The Al_2O_3 nano powder and PEO($NaClO_4$)/THF solution with weight ratio of 4:1 (based on the solid content) were mixed homogeneously, and the mixture was cast to form a solid electrolyte film in an argon-filled glovebox. The solid electrolyte film was cut into the discs of 19 mm in diameter. A CR2016 type coin solid-state sodium-ion battery was assembled in an Ar-filled glovebox. Thioindigo was used as working electrode, and sodium metal as the counter electrode, and PEO-$NaClO_4$-Al_2O_3 as solid-state electrolyte. Galvanostatic charge-discharge experiments were conducted on a NEWARE cell testing system (CT-4800, Shenzheng, China). The AC impedance measurements and CV (cyclic voltammetry) were carried out using an Autolab PGSTAT302N. A.C. impedance spectrums were measured with a frequency range from 0.1 Hz to100 KHz. CV measurement was performed within the

range of 0.01-3 V at a scanning rate of 0.1 mV s^{-1}.

Computational Methods

The first-principles calculations were conducted within the formalism of spin-polarization density functional theory (DFT). The quantum chemical calculation analyses of the LUMO/HOMO of Na_x-STTDC (x=0, 2, 4, 6). By using the Gaussian 09 package, the quantum chemical calculations at the level of M06/6-31G+ (d, p) were carried out to obtain molecular orbital distributions of Na_x-STTDC (x=0, 2, 4, 6).

Based on the change of Gibbs free energy, the intercalation/deintercalation voltages of Na_x-STTDC (x=0, 2, 4, 6) were further calculated with the reference to Na metal. The equation of $V^{Na_{x+2}C_8H_2O_4S_2} = -\frac{G_{Na_{x+2+n}C_8H_2O_4S_2} - G_{Na_{x+2}C_8H_2O_4S_2} - G_{nNa}}{n}$ is used to obtain the discharge voltage,[3, 4] where G is the Gibbs free energy.

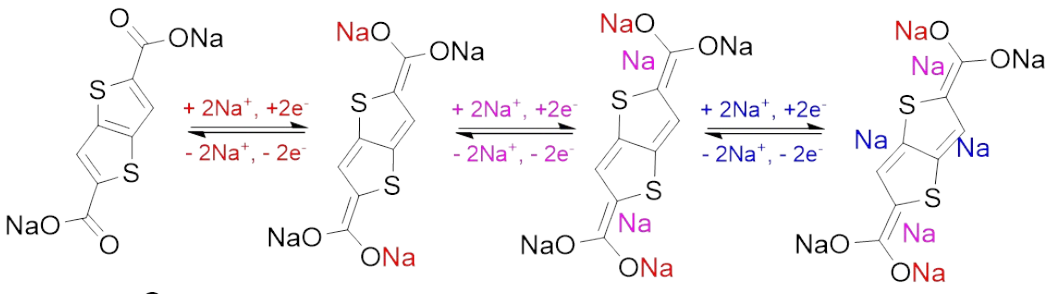


Figure S1 Molecular structure and reversible Na-ion insertion/extraction mechanism of STTDC.

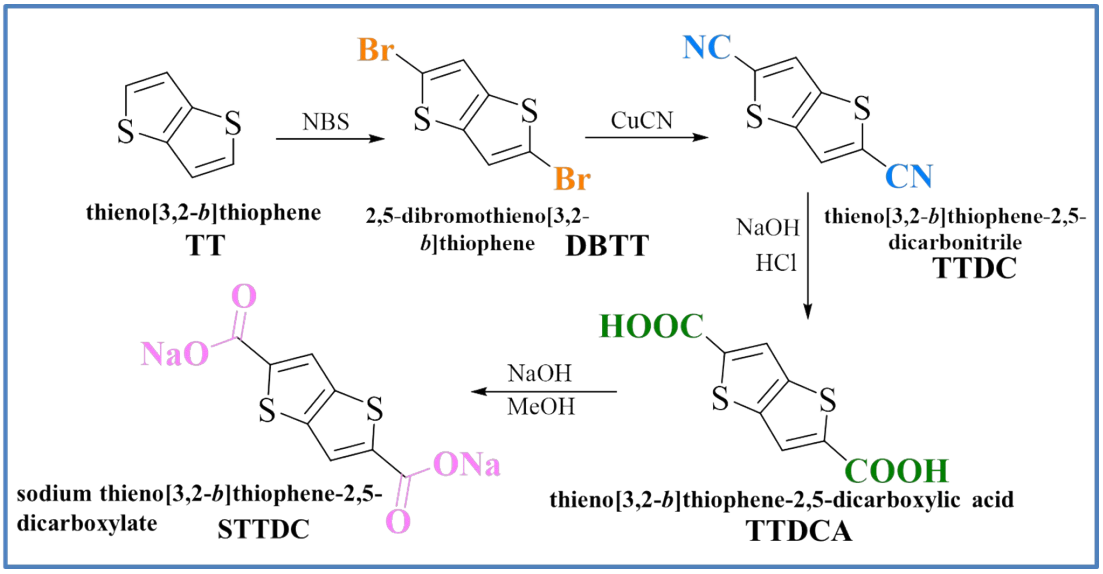


Figure S2 Synthesis route diagram of the STTDC

Thieno[3,2-b]thiophene-2,5-dicarboxylic acid (TTDCA)

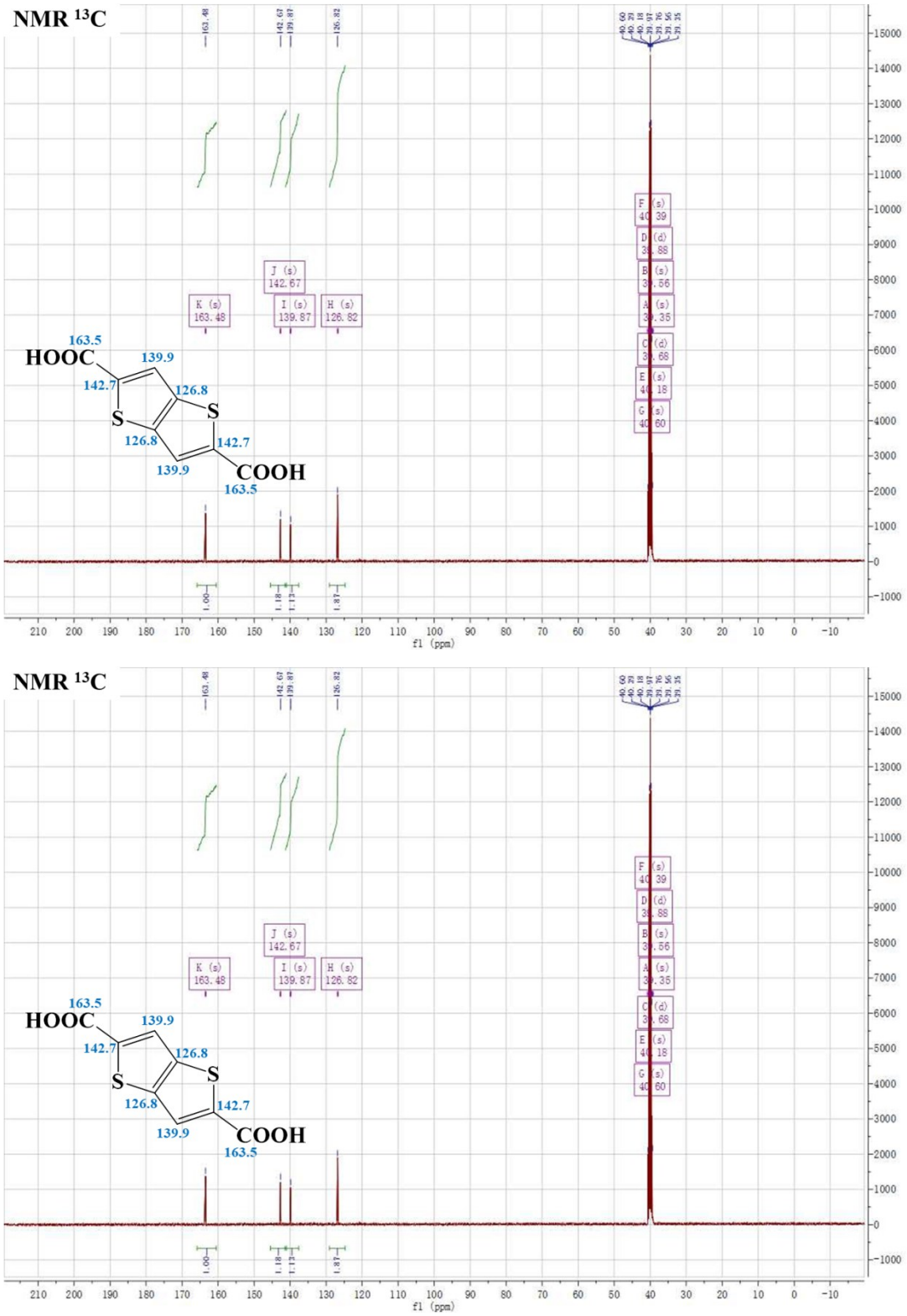


Figure S3 ^{1}H (top) and ^{13}C (bottom) NMR spectra of TTDCA

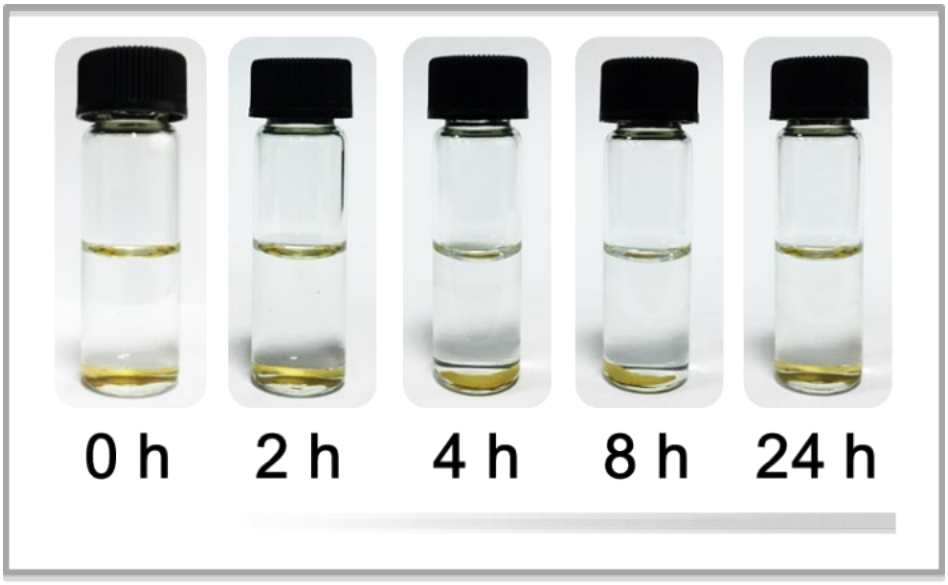


Figure S4 The dissolvability test of STTDC in electrolyte.

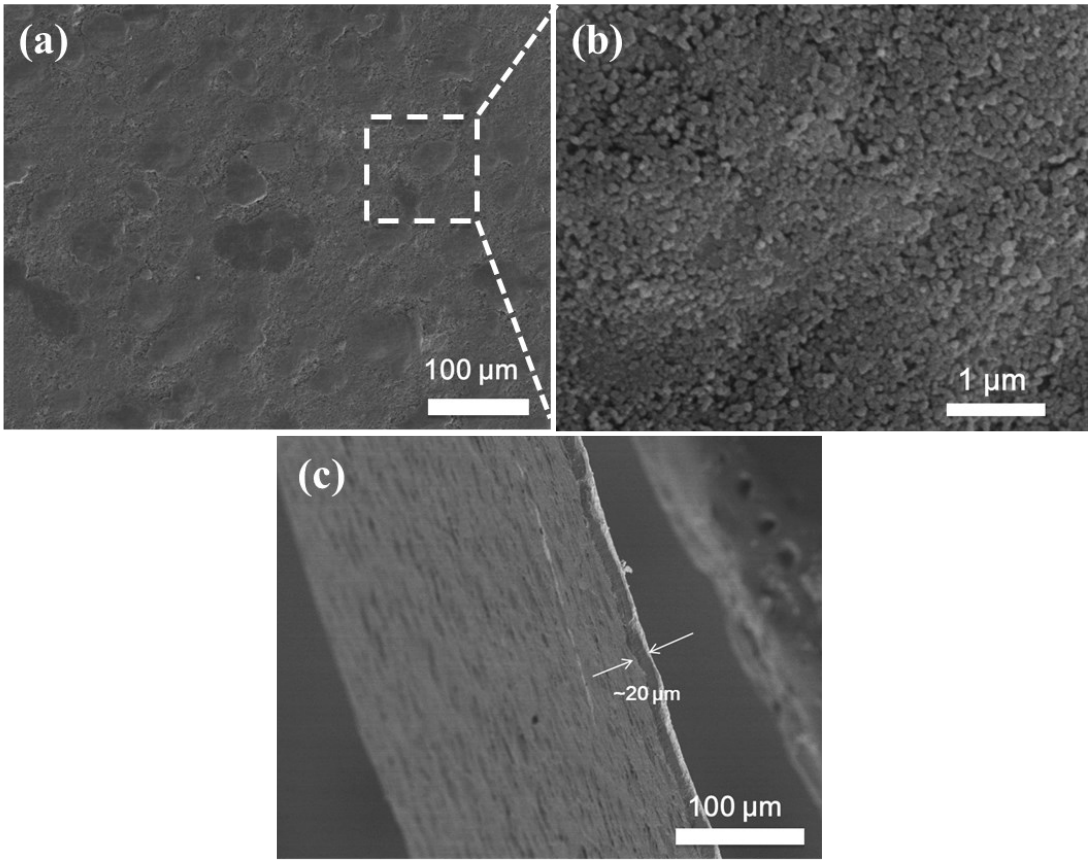


Figure S5 (a-b) Top- and (c) side-view SEM images of the STTDC electrode after recrystallization.

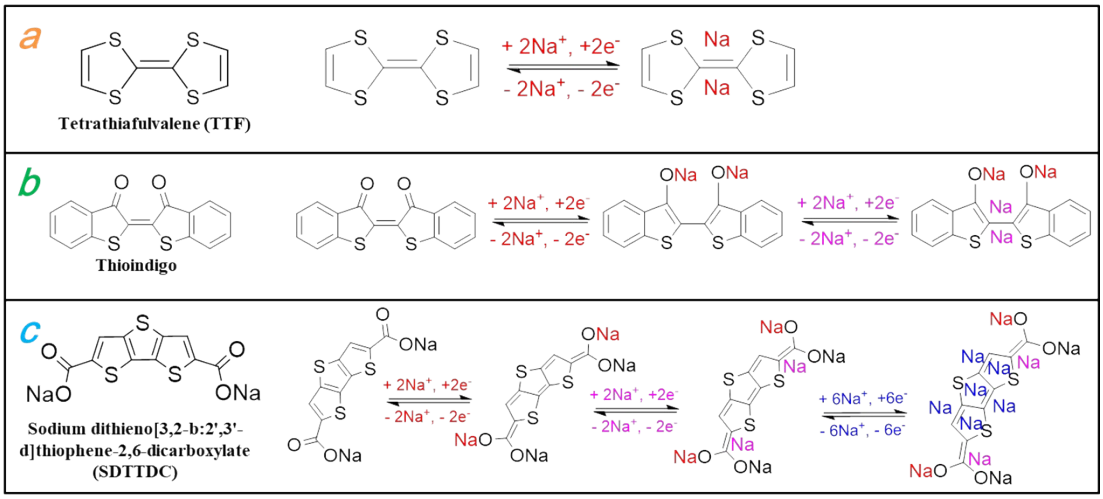


Figure S6 Molecular structure and reversible Na-ion insertion/extraction mechanism of tetrathiafulvalene, thioindigo and sodium dithieno[3,2-b:2',3'-d]thiophene-2,6-dicarboxylate.

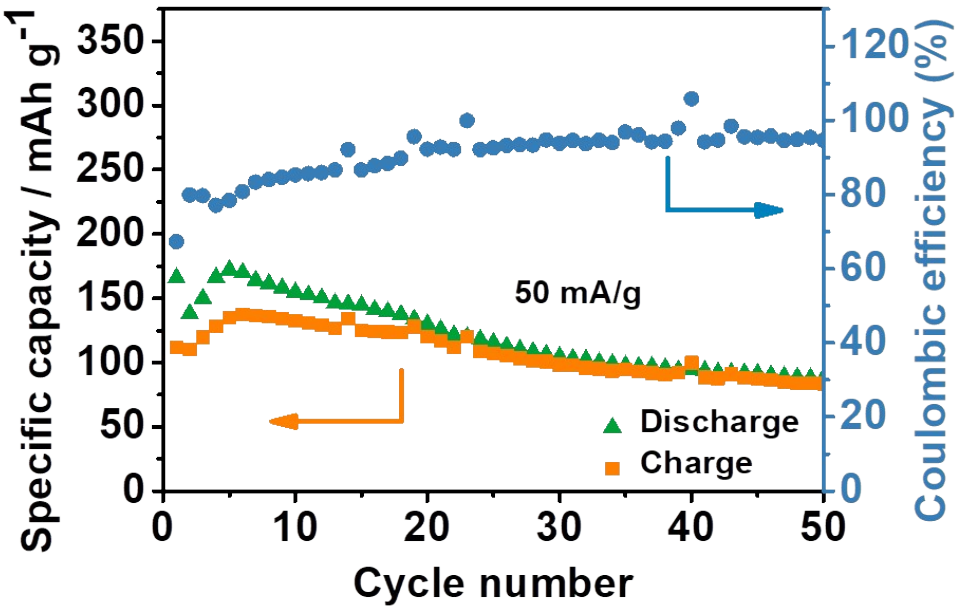


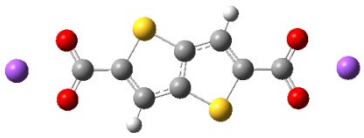
Figure S7 Cycling performance of thioindigo at a current density of 50 mA g^{-1} under 55 °C. The test was performed with a solid-state sodium-ion battery assembled with PEO-$NaClO_4$-Al_2O_3 as the solid-state electrolyte.

Table S1 Coordinates of molecular structures

All coordinates are reported as XYZ Cartesian coordinates. Converged geometries and the thermochemistriy were also obtained from M06/6-31+G(d,p) level of theory. They are stated in Hartrees units. All energies reported were calculated using the GAUSSIAN 09 Revision-D.01 computational chemistry package.

STTDC

Table S1a

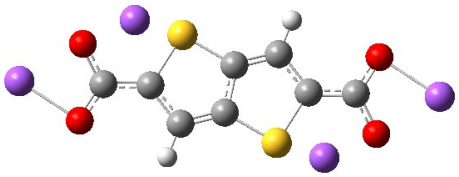


Standard orientation

Center Number	Element Symbol	Coordinates (Angstroms) X	Y	Z
1	C	-2.28365	0.045518	0.000024
2	C	-1.42697	1.115092	0.000007
3	C	-0.07658	0.694224	-0.000014
4	C	0.076586	-0.69422	-0.000001
5	C	2.283653	-0.04552	-0.000063
6	C	1.426968	-1.11509	-0.000031
7	H	-1.78928	2.137517	-0.000002
8	H	1.789283	-2.13752	-0.000032
9	S	-1.46263	-1.50055	0.000047
10	S	1.462634	1.500556	-0.000056
11	C	-3.76263	0.090337	0.000025
12	O	-4.39082	-1.01047	0.000195
13	O	-4.32116	1.226957	0.000146
14	C	3.76263	-0.09033	-0.000102
15	O	4.390822	1.010466	-0.000162
16	O	4.321154	-1.22696	-0.000128
17	Na	-6.25717	0.172038	0.000286
18	Na	6.257169	-0.17205	-0.000221

Electronic Energy (EE) =-1727.678830

Table S1b

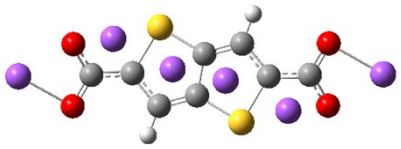


Standard orientation

Center Number	Element Symbol	Coordinates (Angstroms) X	Y	Z
1	C	-2.34441	0.219859	0.007397
2	C	-1.32896	1.145919	-0.40913
3	C	-0.06309	0.662598	-0.28176
4	C	0.063286	-0.66293	0.281268
5	C	2.34453	-0.22043	-0.00845
6	C	1.329132	-1.14637	0.408383
7	H	-1.61123	2.106316	-0.83123
8	H	1.611398	-2.10677	0.830481
9	S	-1.54398	-1.23177	0.789239
10	S	1.544219	1.23147	-0.78967
11	C	-3.74025	0.376359	-0.01189
12	O	-4.51069	-0.68646	0.242193
13	O	-4.29625	1.494895	-0.32523
14	C	3.74036	-0.37621	0.012277
15	O	4.510564	0.686868	-0.24131
16	O	4.2966	-1.49453	0.326187
17	Na	-6.16711	0.734607	0.401326
18	Na	6.167055	-0.73413	-0.40137
19	Na	-3.29247	-1.94163	-1.08764
20	Na	3.291671	1.941734	1.088075

Electronic Energy (EE) =-2052.224078

Table S1c

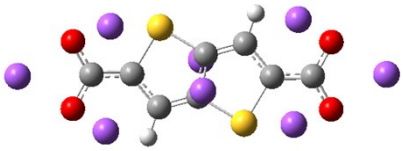


Standard orientation

Center Number	Element Symbol	Coordinates (Angstroms) X	Y	Z
1	C	-2.32016	0.440253	0.102841
2	C	-1.33479	0.848931	-0.86418
3	C	-0.06774	0.423633	-0.58232
4	C	0.080395	-0.40489	0.602284
5	C	2.330909	-0.4223	-0.08401
6	C	1.346112	-0.8378	0.878737
7	H	-1.63727	1.419652	-1.73838
8	H	1.648097	-1.41398	1.749443
9	S	-1.49354	-0.51968	1.444952
10	S	1.503797	0.527983	-1.43081
11	C	-3.72288	0.352537	-0.11258
12	O	-4.42694	-0.51832	0.578408
13	O	-4.28711	1.096938	-0.98743
14	C	3.734875	-0.34733	0.119586
15	O	4.440821	0.514946	-0.58252
16	O	4.301803	-1.09206	0.992693
17	Na	-6.22635	0.368236	-0.35148
18	Na	6.240459	-0.4233	0.291448
19	Na	-3.11695	-2.29961	0.010899
20	Na	3.133192	2.293605	-0.00513
21	Na	-0.90227	2.340116	1.289063
22	Na	0.809748	-2.32168	-1.29014

Electronic Energy (EE) =-2376.787777

Table S1d



Standard orientation

Center Number	Element Symbol	Coordinates (Angstroms) X	Y	Z
1	C	-2.24934	0.452986	-0.50443
2	C	-1.3284	-0.44778	-1.13735
3	C	-0.0808	-0.44657	-0.56322
4	C	0.081183	0.445913	0.564292
5	C	2.249723	-0.45353	0.505494
6	C	1.328856	0.447278	1.138254
7	H	-1.63215	-1.07179	-1.97525
8	H	1.632715	1.071305	1.976116
9	S	-1.36095	1.491204	0.695498
10	S	1.361386	-1.49168	-0.69452
11	C	-3.6538	0.445404	-0.5423
12	O	-4.33669	1.20848	0.267079
13	O	-4.27554	-0.39911	-1.31867
14	C	3.654235	-0.44504	0.542692
15	O	4.337326	-1.20734	-0.26714
16	O	4.27565	0.399841	1.318894
17	Na	-6.21711	0.363034	-0.56129
18	Na	6.217345	-0.36035	0.560941
19	Na	-3.57986	0.255894	2.218608
20	Na	3.579693	-0.25678	-2.21895
21	Na	0.60465	2.025922	-1.62403
22	Na	-0.60658	-2.02761	1.623416
23	Na	3.649959	2.301318	0.193896
24	Na	-3.65023	-2.30132	-0.19609

Electronic Energy (EE) =-2701.393836

Table S2 Electrochemical performance of organic electrode materials reported.

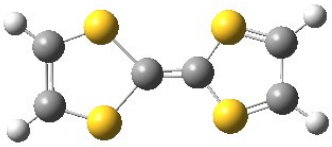
No.	Carbon additives (wt%)	Discharge capacity 1st/2nd (mAh g^{-1})	Rates	Capacity (mAh g^{-1})/ Cycle number	Ref.
1	40%SP	1195/284	100 mA g^{-1}	249/100	5
2	40%SP	375/290	50 mA g^{-1}	204/50	6
3	40%SP	799.9/503	0.1 A g^{-1}	391/400	7
4	37.5%CB	700/233	30 mA g^{-1}	202/5	8
5	30%SP	191/233	0.02 C	90/100	9
6	20%SP	~850/534	100 mA g^{-1}	440/100	10
7	20%CB	230	0.01 A g^{-1}	180/40	11
8	35%SP	801/240	10 mA g^{-1}	200/50	12
9	50%AB	133/	200 mA g^{-1}	~140/500	13
10	30%AB	351/201	25 mA g^{-1}	131/120	14
11	20%SP	150/138	200 mA g^{-1}	108/300	15
12	30%KB	275/-	25mA g^{-1}	130/100	16
13	30%CB	1100/320	500 mA g^{-1}	95/100	17
14	30%AB	126/121	100 mA g^{-1}	105/50	18
15	30%SP	~295/295(100th)	200 mA g^{-1}	210/1400	19
16	28.6%SP	430/208	0.1 C	170/150	20
17	40%AB	248/240	250 mA g^{-1}	105/100	21
18	30%SP	697/425	50 mA g^{-1} 2 A g^{-1}	425/40 286/4000	Our work

Table S3 Coordinates of molecular structures

All coordinates are reported as XYZ Cartesian coordinates. Converged geometries and the thermochemistriy were also obtained from M06/6-31+G(d,p) level of theory. They are stated in Hartrees units. All energies reported were calculated using the GAUSSIAN 09 Revision-D.01 computational chemistry package.

Table S3a

a Tetrathiafulvalene

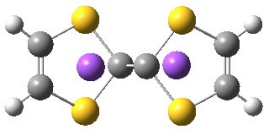


Standard orientation

Center Number	Element Symbol	Coordinates (Angstroms) X	Y	Z
1	C	0.6749020	0.0000370	-0.0002110
2	C	-3.1836500	0.6682130	0.0004530
3	C	-3.1836410	-0.6682500	0.0004810
4	H	-4.0763590	1.2849650	0.0007240
5	H	-4.0763400	-1.2850180	0.0007540
6	C	-0.6747210	-0.0000090	-0.0001710
7	S	-1.6378830	1.4953570	-0.0002470
8	S	-1.6378600	-1.4953760	-0.0000680
9	S	1.6376000	1.4954370	-0.0001800
10	S	1.6376550	-1.4953720	-0.0003570
11	C	3.1841000	-0.6682440	0.0005570
12	H	4.0765470	-1.2853580	0.0009430
13	C	3.1842270	0.6681540	0.0005960
14	H	4.0766540	1.2852780	0.0009800

Electronic Energy (EE) =-1823.455762

Table S3b



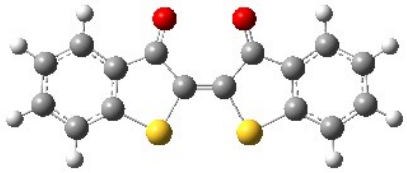
Standard orientation

Center Number	Element Symbol	Coordinates (Angstroms) X	Y	Z
1	C	0.4084510	-0.0077290	0.6649180
2	C	-2.9387350	0.6756050	0.0554580
3	C	-2.9404000	-0.6694240	0.0389410
4	H	-3.7692080	1.2890200	0.4010830
5	H	-3.7726240	-1.2891600	0.3687610
6	C	-0.4092320	0.0096220	-0.6635290
7	S	-1.5226890	1.4496920	-0.7159320
8	S	-1.5254170	-1.4274790	-0.7506450
9	S	1.5230910	1.4307330	0.7532680
10	S	1.5254290	-1.4470160	0.7132710
11	C	2.9405470	-0.6684570	-0.0566940
12	H	3.7719520	-1.2804870	-0.4025170
13	C	2.9386110	0.6763790	-0.0389010
14	H	3.7682850	1.2994170	-0.3688390
15	Na	-1.3553530	-0.0387460	2.2009500
16	Na	1.3553100	0.0196870	-2.2008620

Electronic Energy (EE) =-2148.021803

Table S4a

b Thioindigo

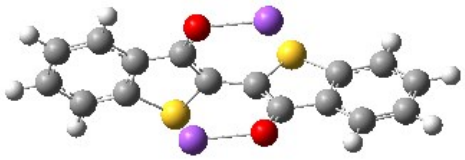


Standard orientation

Center Number	Element Symbol	Coordinates (Angstroms) X	Y	Z
1	C	3.1216020	-0.7717070	-0.0239250
2	C	3.0293790	0.6156430	0.0353320
3	C	4.1795670	1.3989300	0.0535760
4	C	5.4202130	0.7740190	0.0023130
5	C	5.4996060	-0.6204090	-0.0601760
6	C	4.3529840	-1.4120250	-0.0718210
7	C	1.6476690	1.1315390	0.0960380
8	H	4.0776170	2.4808470	0.1069610
9	H	6.3308360	1.3668420	0.0118200
10	H	6.4746140	-1.1006290	-0.0998290
11	H	4.4235780	-2.4959840	-0.1173580
12	C	0.6798560	-0.0281280	0.0088680
13	C	-0.6798560	-0.0281280	-0.0088670
14	C	-1.6476690	1.1315390	-0.0960360
15	C	-3.0293790	0.6156430	-0.0353320
16	C	-3.1216020	-0.7717070	0.0239250
17	C	-4.1795670	1.3989300	-0.0535770
18	C	-4.3529840	-1.4120250	0.0718210
19	C	-5.4202130	0.7740190	-0.0023140
20	H	-4.0776170	2.4808470	-0.1069630
21	C	-5.4996060	-0.6204090	0.0601750
22	H	-4.4235780	-2.4959840	0.1173580
23	H	-6.3308360	1.3668420	-0.0118220
24	H	-6.4746140	-1.1006290	0.0998280
25	O	1.3552230	2.2989820	0.2340090
26	O	-1.3552230	2.2989820	-0.2340080
27	S	-1.5433820	-1.5731320	0.0250900
28	S	1.5433820	-1.5731320	-0.0250900

Electronic Energy (EE) =-1560.788762

Table S4b

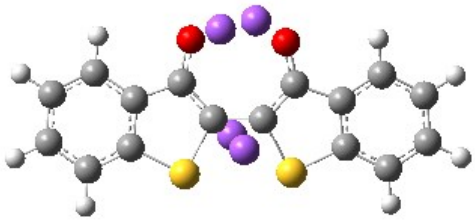


Standard orientation

Center Number	Element Symbol	Coordinates (Angstroms) X	Y	Z
1	C	-3.1940280	0.7694280	-0.3966950
2	C	-2.9295260	-0.2683100	0.5150820
3	C	-3.9917470	-0.9882630	1.0742860
4	C	-5.2931940	-0.6647010	0.7248940
5	C	-5.5464540	0.3777360	-0.1818550
6	C	-4.5059250	1.1015230	-0.7472370
7	C	-1.5035320	-0.4772270	0.7802920
8	H	-3.7640580	-1.7834040	1.7818070
9	H	-6.1265820	-1.2132480	1.1578630
10	H	-6.5729670	0.6254380	-0.4433970
11	H	-4.7049340	1.9129860	-1.4444400
12	C	-0.7236810	0.4170130	0.0336250
13	C	0.7235000	0.4183080	-0.0476480
14	C	1.5058180	-0.4850990	-0.7804560
15	C	2.9308420	-0.2727260	-0.5123360
16	C	3.1917250	0.7755010	0.3886040
17	C	3.9954030	-0.9994640	-1.0581840
18	C	4.5021930	1.1116650	0.7405950
19	C	5.2954090	-0.6721370	-0.7068700
20	H	3.7705130	-1.8029020	-1.7571870
21	C	5.5450300	0.3810380	0.1884410
22	H	4.6984260	1.9312510	1.4290260
23	H	6.1305120	-1.2261760	-1.1294190
24	H	6.5704600	0.6315360	0.4515320
25	O	-1.0681380	-1.4102640	1.5501180
26	O	1.0729980	-1.4275080	-1.5401640
27	S	1.7161050	1.5442740	0.9476930
28	S	-1.7208080	1.5322920	-0.9696270
29	Na	1.0734380	-1.2936770	1.8382070
30	Na	-1.0712580	-1.3194200	-1.8256340

Electronic Energy (EE) =-1885.487911

Table S4c



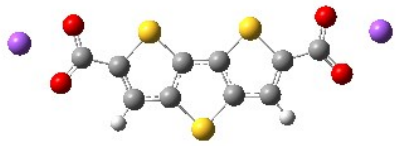
Standard orientation

Center Number	Element Symbol	Coordinates (Angstroms) X	Y	Z
1	C	-3.1345420	-1.0199140	0.1312990
2	C	-3.0218680	0.3506560	-0.1336700
3	C	-4.1823010	1.1166710	-0.2844160
4	C	-5.4208470	0.5053430	-0.1614820
5	C	-5.5153340	-0.8676580	0.1077260
6	C	-4.3725670	-1.6450250	0.2525290
7	C	-1.6485960	0.8346210	-0.2444430
8	H	-4.0839540	2.1780880	-0.5020020
9	H	-6.3294410	1.0921030	-0.2743080
10	H	-6.4936910	-1.3324910	0.2049810
11	H	-4.4432800	-2.7105560	0.4594800
12	C	-0.7279160	-0.2046380	-0.0253670
13	C	0.7275780	-0.2044210	0.0244950
14	C	1.6484130	0.8344670	0.2447230
15	C	3.0216230	0.3504310	0.1334700
16	C	3.1342530	-1.0198450	-0.1329870
17	C	4.1820720	1.1161680	0.2854850
18	C	4.3722590	-1.6449230	-0.2545190
19	C	5.4206070	0.5048720	0.1622640
20	H	4.0837600	2.1773270	0.5043340
21	C	5.5150570	-0.8678230	-0.1084660
22	H	4.4429450	-2.7102400	-0.4625730
23	H	6.3292130	1.0914180	0.2760960
24	H	6.4934000	-1.3326560	-0.2058530
25	O	-1.3847430	2.0794290	-0.4878680
26	O	1.3849620	2.0789730	0.4902300
27	S	1.5575980	-1.7818580	-0.2723430
28	S	-1.5579620	-1.7822930	0.2694380
29	Na	0.5126360	2.5418560	-1.5885300
30	Na	-0.5123650	2.5352340	1.5933880
31	Na	-0.1811820	-0.8771890	-2.6181200
32	Na	0.1825260	-0.8842350	2.6175870

Electronic Energy (EE) =-2210.028215

Table S5a

c Sodium dithieno[3,2-b:2',3'-d]thiophene-2,6-dicarboxylate

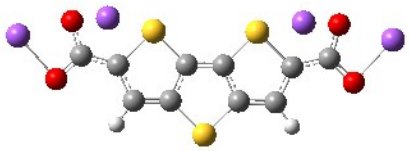


Standard orientation

Center Number	Element Symbol	Coordinates (Angstroms) X	Y	Z
1	C	-0.7085740	0.0040770	-0.0000030
2	C	-1.2380250	1.2939330	0.0000580
3	C	-3.1778180	0.0586730	-0.0000160
4	S	-1.9560200	-1.1960360	-0.0000880
5	S	0.0000600	2.5363520	0.0001180
6	C	1.2380850	1.2939510	0.0000270
7	C	0.7086670	0.0040200	-0.0000150
8	C	2.6501230	1.3239810	0.0000180
9	H	3.2811700	2.2064010	0.0001020
10	S	1.9559510	-1.1960610	-0.0000010
11	C	3.1778300	0.0585920	0.0000370
12	C	4.6094130	-0.3123930	0.0000050
13	O	4.9042040	-1.5450340	-0.0000220
14	O	5.4627820	0.6229840	-0.0000130
15	C	-4.6094500	-0.3122440	-0.0000280
16	O	-4.9042770	-1.5448910	0.0005140
17	O	-5.4628020	0.6231570	-0.0005640
18	C	-2.6500390	1.3240580	0.0000500
19	H	-3.2809930	2.2065450	0.0001050
20	Na	-7.0232450	-0.9269430	0.0000090
21	Na	7.0231930	-0.9267520	-0.0000810

Electronic Energy (EE) =-2202.000048

Table S5b

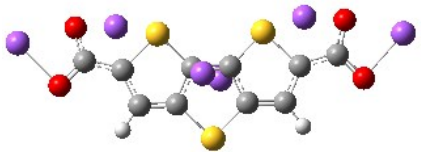


Standard orientation

Center Number	Element Symbol	Coordinates (Angstroms) X	Y	Z
1	C	-0.6795950	0.2150550	-0.0461930
2	C	-1.2665760	1.5279310	-0.0941580
3	C	-3.2277170	0.2524970	-0.2122460
4	S	-1.9226810	-1.0202430	-0.2285470
5	S	0.0000740	2.7764860	0.0004340
6	C	1.2666160	1.5278190	0.0948700
7	C	0.6795480	0.2149820	0.0468640
8	C	2.6272930	1.5513640	0.2044570
9	H	3.2525290	2.4384410	0.2432670
10	S	1.9225170	-1.0205040	0.2287970
11	C	3.2276350	0.2521920	0.2131610
12	C	4.5934750	-0.0902790	0.1602610
13	O	4.9324110	-1.3467090	-0.1312750
14	O	5.5130910	0.7878240	0.3352080
15	C	-4.5936340	-0.0898230	-0.1597490
16	O	-4.9328170	-1.3462670	0.1315080
17	O	-5.5130780	0.7883200	-0.3351730
18	C	-2.6272640	1.5515970	-0.2036320
19	H	-3.2524160	2.4387410	-0.2422450
20	Na	-6.9513240	-0.7972600	-0.5530320
21	Na	6.9517350	-0.7978630	0.5504310
22	Na	-3.5555210	-1.4399760	1.8473480
23	Na	3.5556360	-1.4371150	-1.8480120

Electronic Energy (EE) =-2526.546989

Table S5c

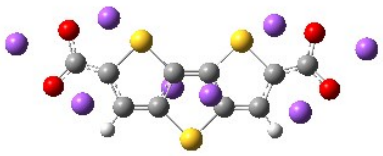


Standard orientation

Center Number	Element Symbol	Coordinates (Angstroms) X	Y	Z
1	C	-0.6870000	0.1621170	-0.0110730
2	C	-1.2728200	1.4794900	-0.1275780
3	C	-3.2113600	0.1912690	-0.3210890
4	S	-1.9050210	-1.0709370	-0.3658620
5	S	-0.0000180	2.7429190	-0.0015630
6	C	1.2728800	1.4797330	0.1262260
7	C	0.6870850	0.1621630	0.0117780
8	C	2.6308340	1.4907060	0.3247540
9	H	3.2617390	2.3733000	0.3786110
10	S	1.9052410	-1.0702410	0.3682080
11	C	3.2115500	0.1918930	0.3208240
12	C	4.5796210	-0.1669730	0.1890380
13	O	4.8782230	-1.4023370	-0.1613240
14	O	5.5019230	0.6976350	0.3705690
15	C	-4.5794890	-0.1673690	-0.1893680
16	O	-4.8782990	-1.4022320	0.1625310
17	O	-5.5016930	0.6970270	-0.3725090
18	C	-2.6306860	1.4901140	-0.3267100
19	H	-3.2616090	2.3725960	-0.3821760
20	Na	-6.9788870	-0.8806960	-0.3204190
21	Na	6.9791370	-0.8801800	0.3192430
22	Na	-3.4334200	-1.4689070	1.9247890
23	Na	3.4326400	-1.4726450	-1.9223680
24	Na	-0.2893620	0.4868780	-2.5406730
25	Na	0.2891410	0.4907000	2.5408870

Electronic Energy (EE) =-2851.106564

Table S5d

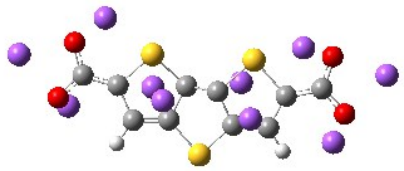


Standard orientation

Center Number	Element Symbol	Coordinates (Angstroms) X	Y	Z
1	C	0.6383840	0.0072760	0.2483170
2	C	1.2032950	1.3259610	0.4180230
3	C	3.1165960	0.0404260	0.8162660
4	S	1.8259560	-1.2235960	0.6845110
5	S	-0.0001030	2.5915410	0.0007610
6	C	-1.2041520	1.3271430	-0.4180070
7	C	-0.6390570	0.0079850	-0.2527330
8	C	-2.5462100	1.3444540	-0.6988590
9	H	-3.1495290	2.2393170	-0.8351910
10	S	-1.8273090	-1.2216060	-0.6905220
11	C	-3.1180910	0.0428000	-0.8169030
12	C	-4.4751090	-0.3304090	-0.7466970
13	O	-4.7971010	-1.5889630	-0.6405690
14	O	-5.3975480	0.5868820	-0.6831980
15	C	4.4736560	-0.3327510	0.7477520
16	O	4.7957130	-1.5910670	0.6386590
17	O	5.3964050	0.5845630	0.6887490
18	C	2.5448870	1.3424970	0.7011970
19	H	3.1478490	2.2369840	0.8415230
20	Na	6.9328970	-1.0103940	0.5581680
21	Na	-6.9339940	-1.0087130	-0.5541540
22	Na	3.7758140	-1.9723140	-1.4002430
23	Na	-3.7735950	-1.9763450	1.3954040
24	Na	-1.4491910	0.7219460	2.2936540
25	Na	1.4532980	0.7289880	-2.2945190
26	Na	-4.8290300	1.3746570	1.4085860
27	Na	4.8310780	1.3784150	-1.4015860

Electronic Energy (EE) =-3175.709375

Table S5e

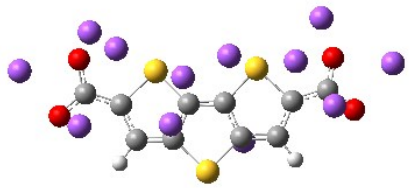


Standard orientation

Center Number	Element Symbol	Coordinates (Angstroms) X	Y	Z
1	C	-0.6865720	0.0042620	0.2726730
2	C	-1.2646760	1.3147000	-0.0136020
3	C	-3.2354920	0.0746590	-0.3608830
4	S	-1.9314670	-1.2228030	-0.3198250
5	S	-0.0003460	2.5765240	0.0035120
6	C	1.2640390	1.3148020	0.0163420
7	C	0.6863290	0.0055990	-0.2771440
8	C	2.5802400	1.3735040	0.3915130
9	H	3.1274210	2.2849920	0.6243220
10	S	1.9310630	-1.2243170	0.3107390
11	C	3.2345730	0.0733930	0.3610070
12	C	4.5601570	-0.2654390	0.6669310
13	O	4.9119500	-1.5251610	0.7483940
14	O	5.4742960	0.6643340	0.7702200
15	C	-4.5614700	-0.2633540	-0.6658510
16	O	-4.9129170	-1.5228820	-0.7520930
17	O	-5.4762070	0.6664480	-0.7636050
18	C	-2.5814800	1.3750710	-0.3867030
19	H	-3.1290640	2.2876560	-0.6141890
20	Na	-7.0201230	-0.9242650	-1.0208460
21	Na	7.0185520	-0.9267040	1.0234470
22	Na	-4.2454070	-2.1756840	1.2952920
23	Na	4.2485910	-2.1709850	-1.3027250
24	Na	2.5084600	0.5642290	-2.3211650
25	Na	-2.5066460	0.5562230	2.3227600
26	Na	5.5839730	1.3855530	-1.3722160
27	Na	-5.5830240	1.3810560	1.3807840
28	Na	0.9436500	0.1056070	2.4424050
29	Na	-0.9423200	0.1187690	-2.4450070

Electronic Energy (EE) =-3500.261887

Table S5f



Standard orientation

Center Number	Element Symbol	Coordinates (Angstroms) X	Y	Z
1	C	-0.6805960	-0.0359720	0.4446630
2	C	-1.2790850	-0.0189360	1.7501060
3	C	-3.2057510	0.1184250	0.4294310
4	S	-1.8929560	0.0227270	-0.8206120
5	S	-0.0009440	-0.0251520	3.0096060
6	C	1.2778150	-0.0095470	1.7507490
7	C	0.6800670	0.0297900	0.4455190
8	C	2.6455790	-0.1047590	1.7506950
9	H	3.2806340	-0.2009780	2.6286420
10	S	1.8931430	-0.0068340	-0.8199680
11	C	3.2052630	-0.1250360	0.4291460
12	C	4.5134780	-0.4433430	0.0050150
13	O	4.6983190	-0.8000450	-1.2481790
14	O	5.5145700	-0.2782300	0.7978760
15	C	-4.5136210	0.4436390	0.0099710
16	O	-4.6980820	0.8191720	-1.2379400
17	O	-5.5150380	0.2665490	0.7997840
18	C	-2.6468730	0.0758420	1.7507940
19	H	-3.2824100	0.1562820	2.6299890
20	Na	-6.9790700	0.4085910	-0.9201520
21	Na	6.9784220	-0.3918110	-0.9240160
22	Na	-4.4825850	-1.2188280	-2.5087940
23	Na	4.4870790	1.2542530	-2.4965680
24	Na	1.1794330	3.0540700	-0.9248450
25	Na	-1.1720100	-3.0397170	-0.9709810
26	Na	5.0005710	2.0163830	0.9274860
27	Na	-5.0059900	-2.0301750	0.8971530
28	Na	1.0858590	-2.8038320	1.5223640
29	Na	-1.0864320	2.7786420	1.5594980
30	Na	3.1154670	-2.5731350	-1.4007790
31	Na	-3.1172810	2.5958000	-1.3650840

Electronic Energy (EE) =-3824.825356

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