Electronic Supplementary Information

for

N-oxide containing conjugated semiconducting polymer with enhanced electron mobility via direct (hetero)arylation polymerization

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1. Materials and Methods

1.1 Materials

2-Bromo-4-methylthiazole (Bidepharm, 97%), bis(1,5-cyclooctadiene)nickel(0) ($Ni(cod)_2$, Bidepharm, 97%), 2,2'-bipyridine (Bidepharm, 97%), 3-chloroperoxybenzoic acid (*m*-CPBA, Adamas-Beta, 85%), thiophene-2-carbonitrile (Adamas-Beta, ≥97%), diisopropyl succinate (Adamas-Beta, 97%), *tert*-amyl alcohol (Adamas-Beta, 99%), potassium carbonate (K_2CO_3, Adamas-Beta, 99.99%), iron(III) chloride ($FeCl_3$, Adamas-Beta, 97%), elemental sodium (Na, Aladdin, 98%), 15-(3-iodopropyl)nonacosane (LYN Design Optoelectronic Material Co., Ltd., 97%), N-bromosuccinimide (NBS, Adamas-Beta, 98%), anhydrous sodium sulfate (Na_2SO_4, Adamas-Beta, ≥99%), chloroform-D ($CDCl_3$, Adamas-Beta, D, 99.8%), pivalic acid (PivOH, TCI, 99%), cesium carbonate (Cs_2CO_3, Adamas-Beta, 99.9%), trans-bis(acetato)bis[o-(di-o-tolylphosphino)benzyl]dipalladium(II) (Hermann's catalyst, Adamas-Beta, ≥98%), tris(2-methoxyphenyl)phosphine (P(*o*-MeOPh)$_3$, Bidephram, 98%), *n*-Octadecyltrichlorosilane (OTS-18, 98%, J&K). silicon wafer (Guangzhou Fangdao Semiconductor Co., Ltd.).

1,2-Dichloroethane (DCE, Adamas-Beta, 99%), dichloromethane (DCM, General-Reagent, ≥99.5%), petroleum ether (PE, General-Reagent), *N,N'*-dimethylformamide (DMF, General-Reagent, ≥99.5%), hexane (General-Reagent, ≥99.5%), methanol (MeOH, General-Reagent, ≥99.5%), ethanol (EtOH, General-Reagent, 95%), acetic acid (General-Reagent, ≥99.5%), silica gel (General-Reagent, 200 – 300 mesh), toluene (Guangzhou Chemical Reagent Factory, ≥99.5%), acetone (Guangzhou Chemical Reagent Factory, AR), chloroform ($CHCl_3$, Guangzhou Chemical Reagent Factory, AR). DMF and toluene were dried by solvent drying system prior to use.

1.2 Chemical structure and optoelectronic property characterization

^{1}H NMR and ^{13}C NMR spectra were measured on a Jeol ECZR500R spectrometer. All ^{1}H NMR chemical shifts were referenced to $CDCl_3$ at 7.26 ppm and all ^{13}C NMR chemical shifts were referenced to $CDCl_3$ at 77.16 ppm.

Matrix assisted laser desorption ionization time of flight (MALDI-TOF) mass spectrometry (MS) was performed on a Bruker autoflex III smartbean mass spectrometer using dithranol as matrix.

Molecular weights of the polymers were determined were determined by Agilent Technologies PL-GPC220 high temperature chromatograph running in 1,2,4-trichlorobenzene (TCB) at 150 °C. The concentration of the solution for GPC measurement is 0.1 mg mL^{-1}, the flow rate of the TCB eluent is 1.0 mL min^{-1}.

UV-vis-NIR absorption spectroscopy was recorded on Shimadzu UV3600Plus UV-vis-NIR spectrometer. Solutions of the polymers were prepared in $CHCl_3$ (1×10^{-5} M) and thin films of the polymers were prepared by spin coating 10 mg mL^{-1} $CHCl_3$ solutions on glass substrates.

Film cyclic voltammetry (CV) measurements were carried out on a CHI600E electrochemical work station in acetonitrile containing 0.1 M anhydrous acetonitrile tetrabutylammonium hexafluorophosphate (n-Bu_4NPF_6) as a supporting electrolyte. Glassy carbon electrode was used as a working electrode and a platinum wire as a counter electrode, and all potentials were recorded versus Ag/AgCl as a reference electrode (scan rate: 50 mV s^{-1}). The polymers were deposited on the electrode. Potentials were referenced to the ferrocene/ferrocenium (Fc/Fc^{+}) couple by using ferrocene as standard. The oxidation potential of ferrocene was set at − 4.80 eV with respect to zero vacuum level. The oxidation potential of ferrocene was 0.42 V ($E_{Fc/Fc+}$ = 0.42V). The LUMO energy levels were calculated according to the equation of $E_{LUMO} = -[4.8 + e(E_{re} - E_{Fc/Fc+})]$ (eV).

Atomic force microscopy (AFM) studies of thin films were performed with Oxford Instruments Asylum Research Cypher VRS.

The grazing incidence wide-angle X-ray scattering (GIWAXS) measurements were performed on an in-house Xenocs Xeuss 2.0 beamline. The incident X-ray has a wavelength of 1.34 Å and an incident angle of 0.2 °. The data is collected by a Pilatus3R 1M detector.

1.3 DFT Calculations

The structures of small molecules at ground states were optimized with the B3LYP functional and the 6-311++G** basis set via the Gaussian 16 software. The structures of trimers at ground states were optimized with the B3LYP functional and the 6-31+G* basis set via the Gaussian 16 software. Vibrational frequency calculations were performed at the same level to ensure that the optimized structures have real frequencies and are thermodynamically stable. The highest occupied molecular orbital energy (E_{HOMO}), the lowest unoccupied molecular orbital energy (E_{LUMO}), and the corresponding ground-state HOMO−LUMO energy gap in this work were represented using the Multiwfn 3.7 program package.

The calculations of the energy barriers of C-H bond were performed with Gaussian 09. Geometry optimizations of all the ground state and transition structures were carried out at the B3LYP level of theory[1, 2] with the TZVP[3] basis set (DZVP for palladium). The same method was previously used by Fagnou and co-workers to explain the selectivity of Pd-catalyzed direct arylation.[4] Vibrational frequencies were computed at the same level to verify that optimized structures are local minimums or transition states and to evaluate zero-point vibrational energies (ZPE) and thermal corrections at 298 K. The three-dimensional structures were visualized utilizing CYLview.

2. Supplementary Figures

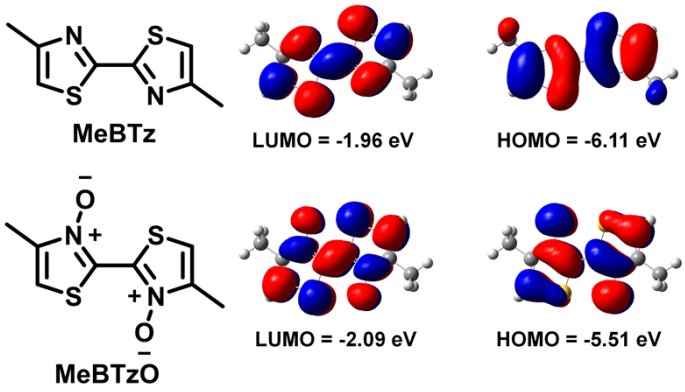


Fig. S1 DFT-derived (B3LYP/6-311++G**) HOMO/LUMO energy levels of monomers MeBTz and MeBTzO.

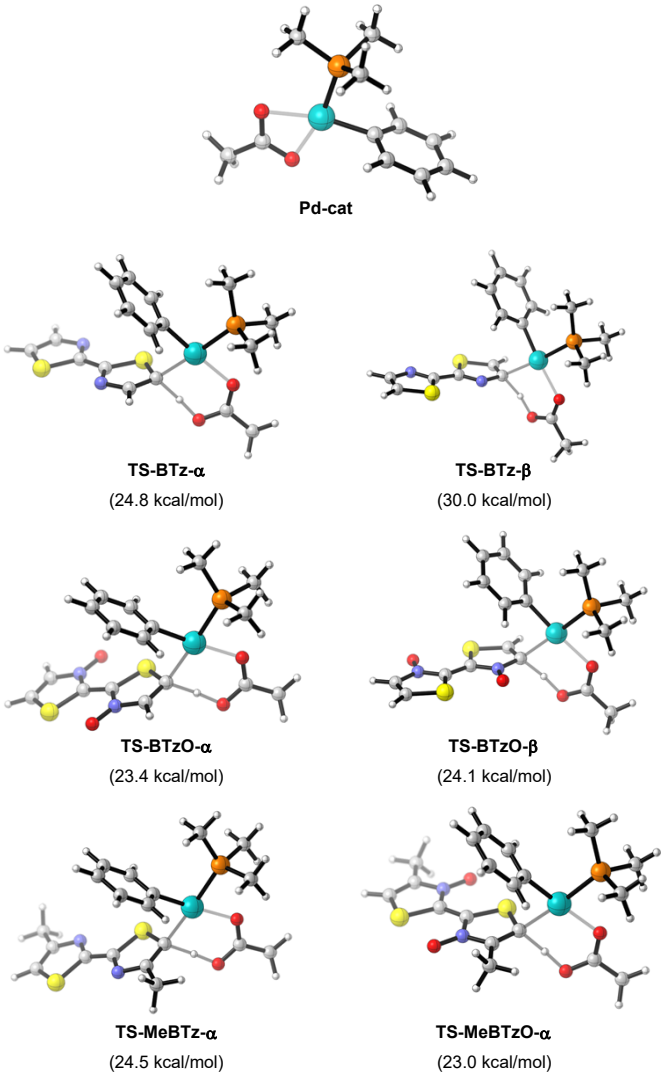


Fig. S2 Optimized geometries of the C-H bond activation transition states via CMD mechanism. The Gibbs free energies were computed with B3LYP/TZVP (DZVP for palladium) level.

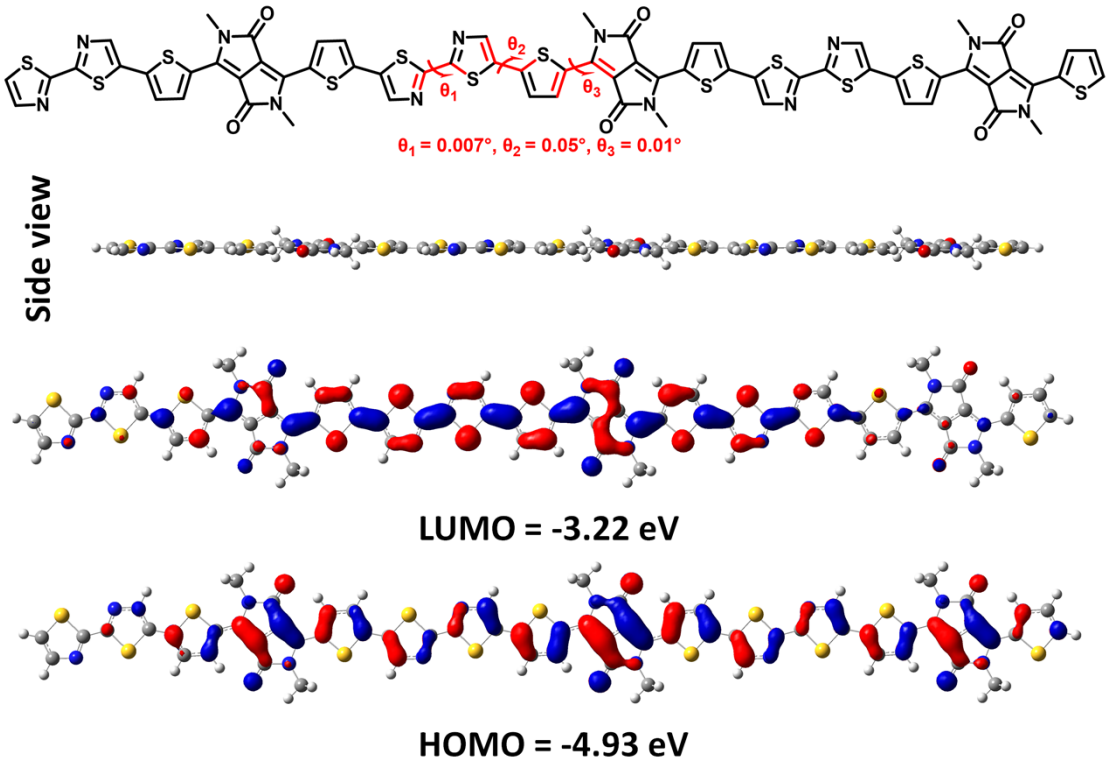


Fig. S3 DFT-derived (B3LYP/6-31G*) HOMO/LUMO energy levels and side view representations of polymer PDPPBTz.

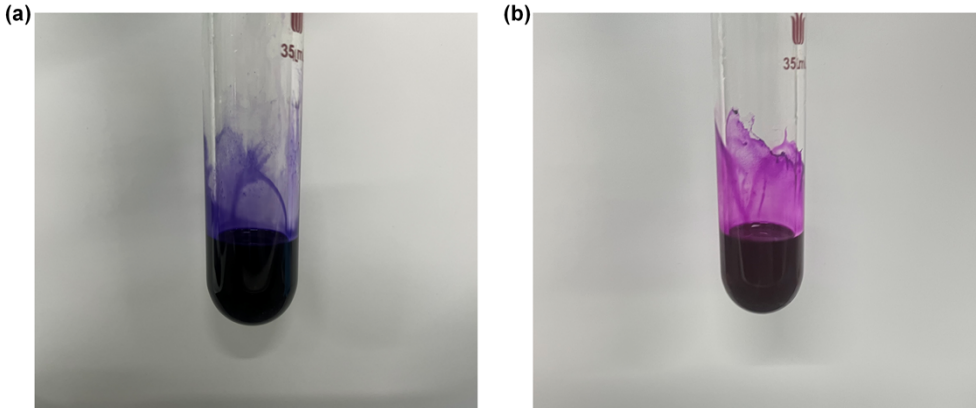


Fig. S4 Color changes of the (a) PDPPMeBTzO and (b) PDPPMeBTz within 30 mins after polymerization.

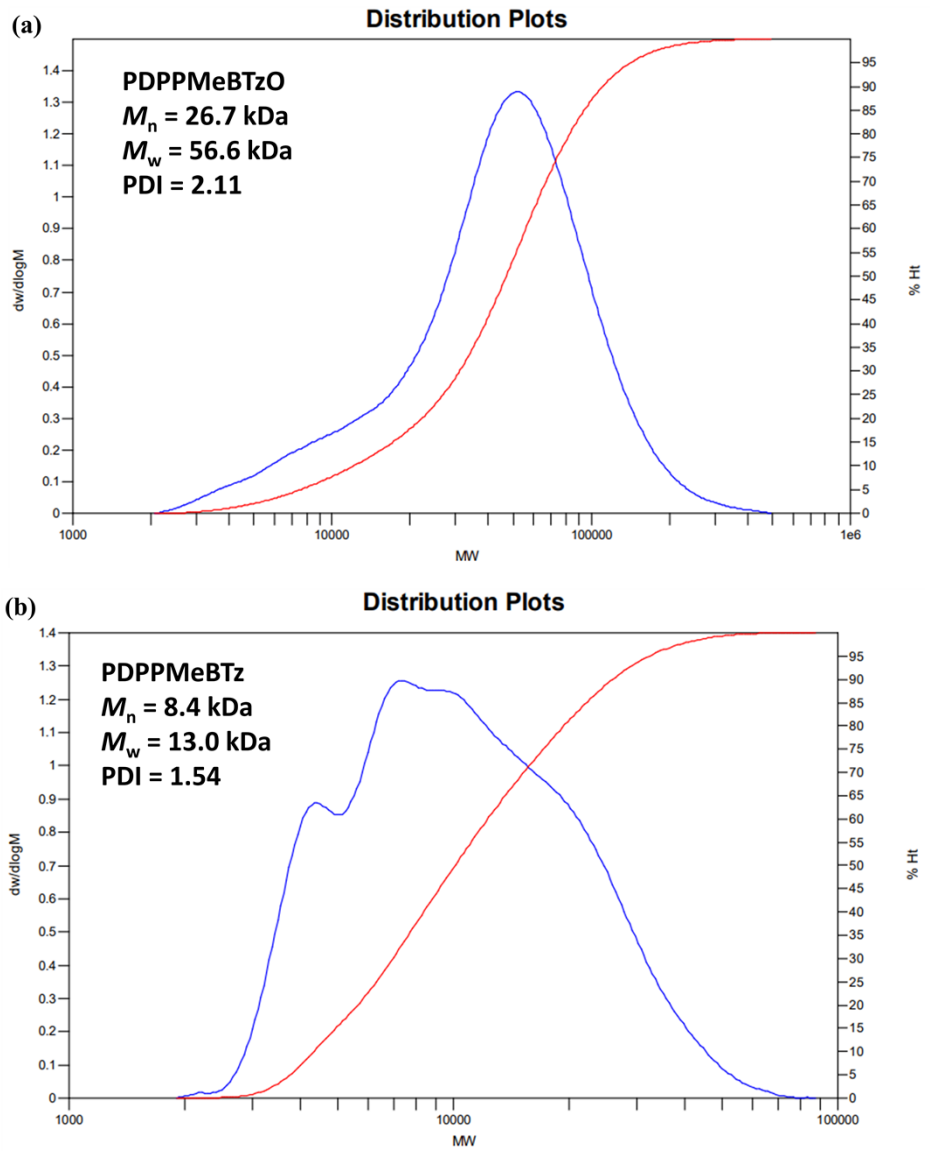


Fig. S5 Molecular weights and polymer dispersity index (PDI) of (a) PDPPMeBTzO and (b) PDPPMeBTz measured by high-temperature GPC at 150 °C.

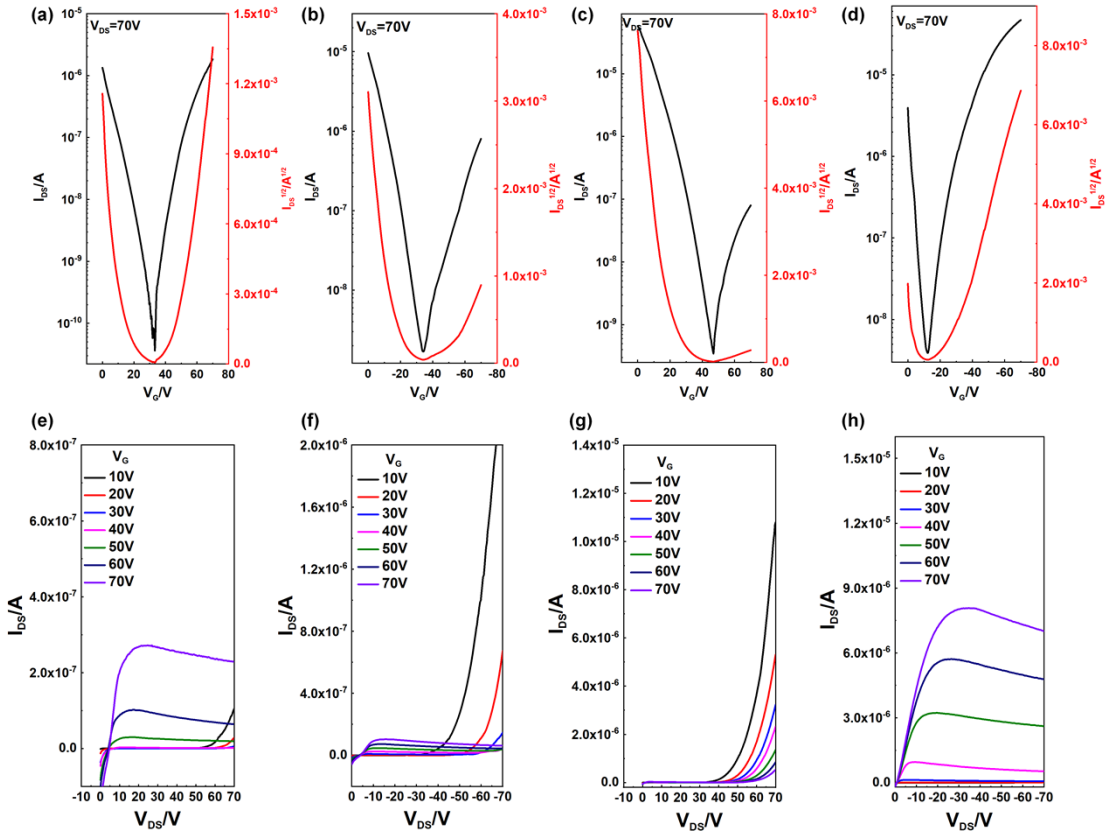


Fig. S6 n-Type (a, c) transfer and (e, g) output characteristics of (a, e) PDPPMeBTzO and (c, g) PDPPMeBTz at 150 °C. p-type (b, d) transfer and (f, h) output characteristics of (b, f) PDPPMeBTzO and (d, h) PDPPMeBTz at 150 °C.

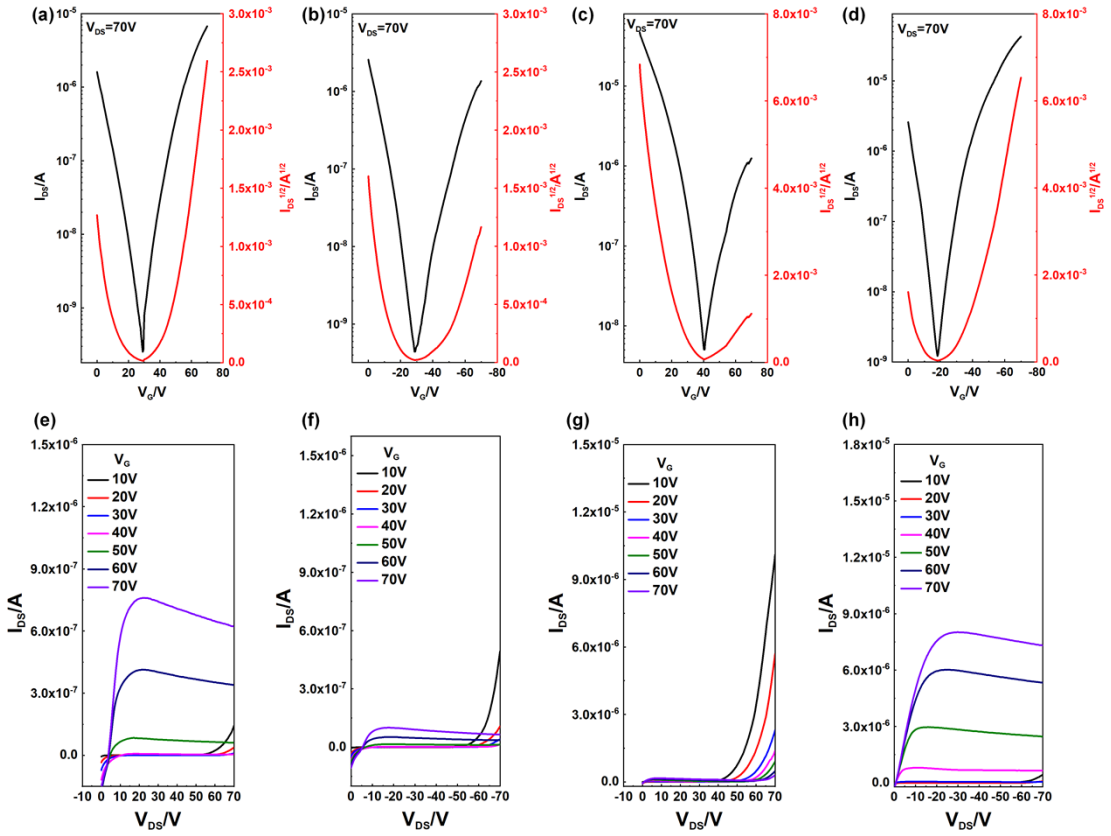


Fig. S7 n-Type (a, c) transfer and (e, g) output characteristics of (a, e) PDPPMeBTzO and (c, g) PDPPMeBTz at 200 ℃. p-type (b, d) transfer and (f, h) output characteristics of (b, f) PDPPMeBTzO and (d, h) PDPPMeBTz at 200 ℃.

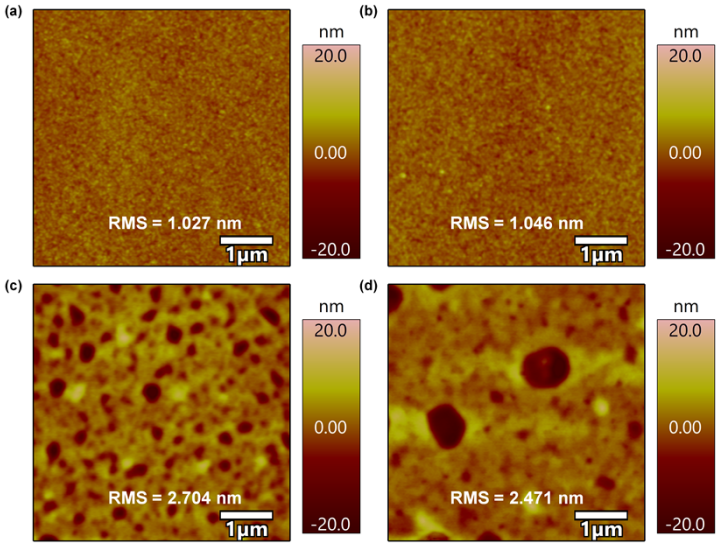


Fig. S8 AFM height images of the (a, c) 150 ℃ and (b, d) 200 ℃ annealed polymer thin films of

(a, b) PDPPMeBTzO and (c, d) PDPPMeBTz.

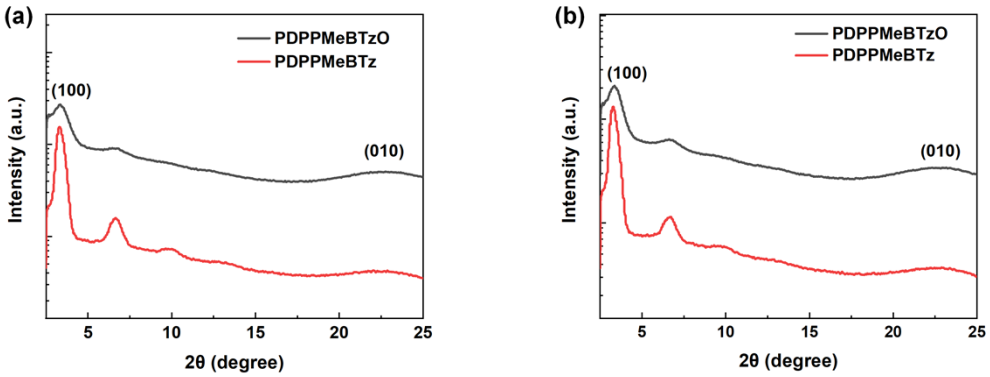


Fig. S9 1D-GIWAXS in-plane line-cut profiles of the (a) 150 ℃ and (b) 200 ℃ annealed polymer thin films of both polymers.

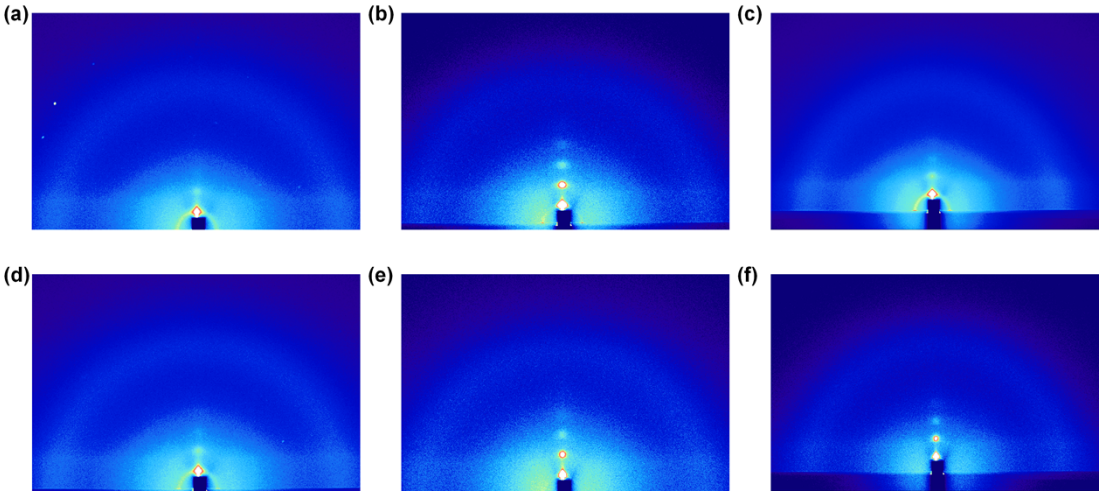
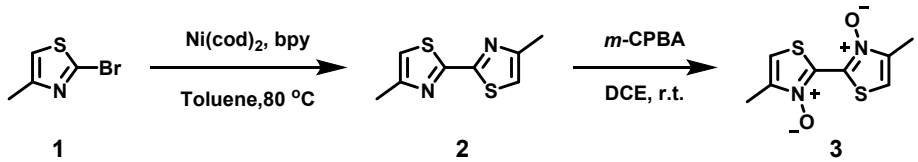


Fig. S10 2D-GIWAXS images of the 150 ℃, 200 ℃ and 250 ℃ annealed films of (a, b, c) PDPPMeBTzO and (d, e, f) PDPPMeBTz, respectively.

3. Synthesis of Monomers and Polymers

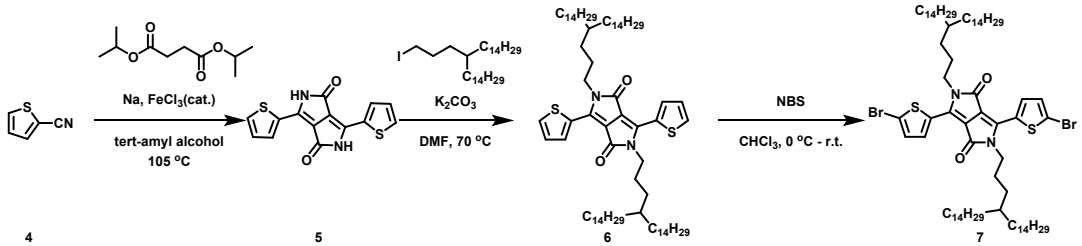
3.1 Synthesis of monomers



1 2-bromo-4-methylthiazole | 2 4,4'-dimethyl-2,2'-bithiazole | 3 4,4'-dimethyl-[2,2'-bithiazole] 3,3'-dioxide

4,4'-dimethyl-2,2'-bithiazole (2): In the argon-filled glove box, a dried Schlenk tube was added with 2-bromo-4-methylthiazole (1.0 equiv., 708 mg, 4.0 mmol), $Ni(cod)_2$ (0.5 equiv., 550 mg, 2.0 mmol), 2,2'-bipyridine (0.6 equiv., 374 mg, 2.4 mmol) and toluene (30 mL). The mixture was sealed and stirred at 80 °C. After the reaction mixture was cooled to room temperature, the reaction was evaporated to remove solvent under reduced pressure. The crude product was purified by silica gel chromatography (petroleum ether/ethyl acetate = 100:0 ~ 4:1). The white solid was obtained after recrystallization in petroleum ether (280 mg, 71%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 6.96 (s, 2H), 2.50 (s, 6H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 160.98, 154.31, 115.58, 17.30.

4,4'-dimethyl-[2,2'-bithiazole] 3,3'-dioxide (3): Synthesized according to the first report by Schipper and co-workers.[5] The orange solid was obtained after recrystallization in dichloromethane/petroleum ether (53 mg, 54%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.17 (s, 2H), 2.47 (s, 6H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 144.40, 134.70, 113.95, 12.40. Data consistent with previously reported literature.

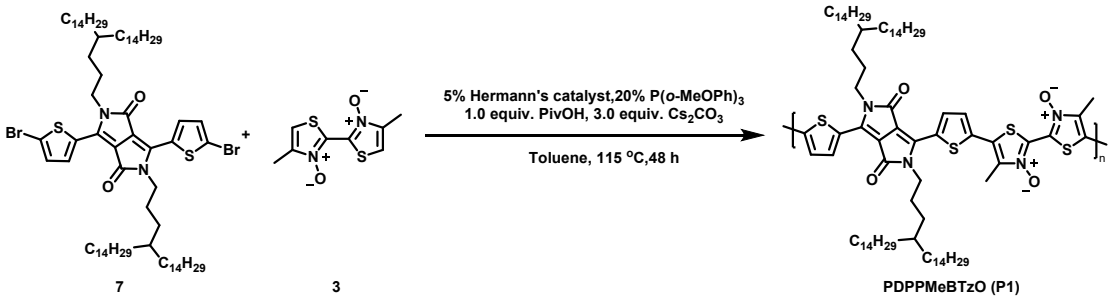


4 thiophene-2-carbonitrile | 5 ThDPP | 6 C_{14}ThDPP | 7 C_{14}ThDPP-2Br

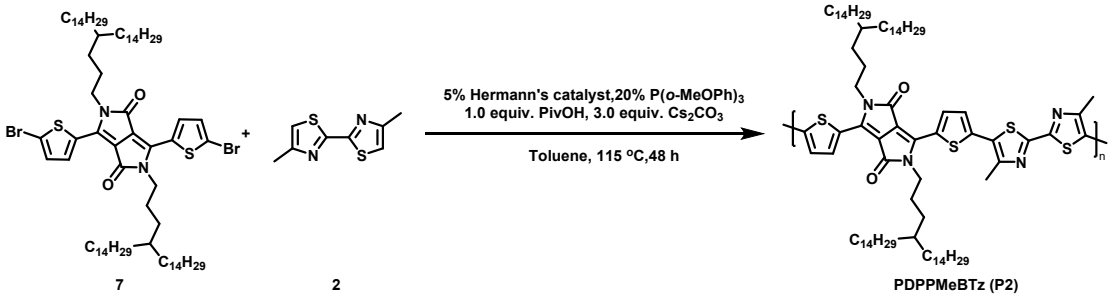
C_{14}ThDPP-2Br (7): Synthesized according to the report by Lei and co-workers.[6] The purple solid was obtained after recrystallization in methanol (313 mg). ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.69 (d, J = 4.2 Hz, 2H), 7.24 (d, J = 4.3 Hz, 2H), 3.98 – 3.92 (m, 4H), 1.72 – 1.62 (m, 4H), 1.39 – 1.18 (m, 110H), 0.88 (t, J = 6.9 Hz, 12H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 161.16, 139.16, 135.55, 131.80, 131.28, 119.29, 107.96, 42.76, 37.22, 33.66, 32.08, 30.54, 30.25, 29.87, 29.82, 29.52, 27.18, 26.85, 22.84,

14.27. MALDI-TOF HRMS calcd. for (M+): 1352.8253, Found: 1353.1820. Data consistent with previously reported literature.

3.2 Synthesis of polymers



PDPPMeBTzO (P1): A dried Schlenk tube was added **C_{14}ThDPP-2Br** (1.0 equiv., 54.1 mg, 0.04 mmol), compound **3** (1.0 equiv., 9.1 mg, 0.04 mmol), Hermann's catalyst (0.05 equiv., 1.88 mg, 0.002 mmol), P(*o*-MeOPh)$_3$ (0.20 equiv., 2.82 mg, 0.008 mmol), PivOH (1.0 equiv., 4.09 mg, 0.04 mmol), Cs_2CO_3 (3.0 equiv., 39.1 mg, 0.12 mmol) and anhydrous toluene (5 mL). The tube was placed in liquid nitrogen to freeze the solution and evacuation for three times. Then the reaction mixture was heated to 115 °C and stirred for 48 h. The reaction mixture was poured into methanol to precipitate the polymer. The solid was filtered and then purified by Soxhlet extraction by extracting sequentially with methanol, acetone, hexane and chloroform. The chloroform solution was concentrated under reduced pressure and the concentrated solution was poured into methanol to precipitate the polymer. The product was filtered and dried in vacuum to afford a dark green solid. $CHCl_3$ fraction: 52 mg, yield: 91%. ^{1}H NMR (400 MHz, $CDCl_3$) δ. GPC (TCB, 150 °C): M_n = 26.7 kDa, M_w = 56.6 kDa, PDI = 2.11.



PDPPMeBTz (P2): A dried Schlenk tube was added **C_{14}ThDPP-2Br** (1.0 equiv., 54.1 mg, 0.04 mmol), compound **2** (1.0 equiv., 7.8 mg, 0.04 mmol), Hermann's catalyst (0.05 equiv., 1.88 mg,

0.002 mmol), P(*o*-MeOPh)$_3$ (0.20 equiv., 2.82 mg, 0.008 mmol), PivOH (1.0 equiv., 4.09 mg, 0.04 mmol), Cs_2CO_3 (3.0 equiv., 39.1 mg, 0.12 mmol) and anhydrous toluene (5 mL). The tube was placed in liquid nitrogen to freeze the solution and evacuation for three times. Then the reaction mixture was heated to 115 °C and stirred for 48 h. The reaction mixture was poured into methanol to precipitate the polymer. The solid was filtered and then purified by Soxhlet extraction by extracting sequentially with methanol, acetone, hexane. The hexane solution was concentrated under reduced pressure and the concentrated solution was poured into methanol to precipitate the polymer. The product was filtered and dried in vacuum to afford a dark green solid. Hexane fraction: 53 mg, yield: 95%. ^{1}H NMR (500 MHz, $CDCl_3$) δ GPC (TCB, 150 °C): M_n = 8.4 kDa , M_w = 13.0 kDa, PDI = 1.54.

3.3 NMR spectra of compounds

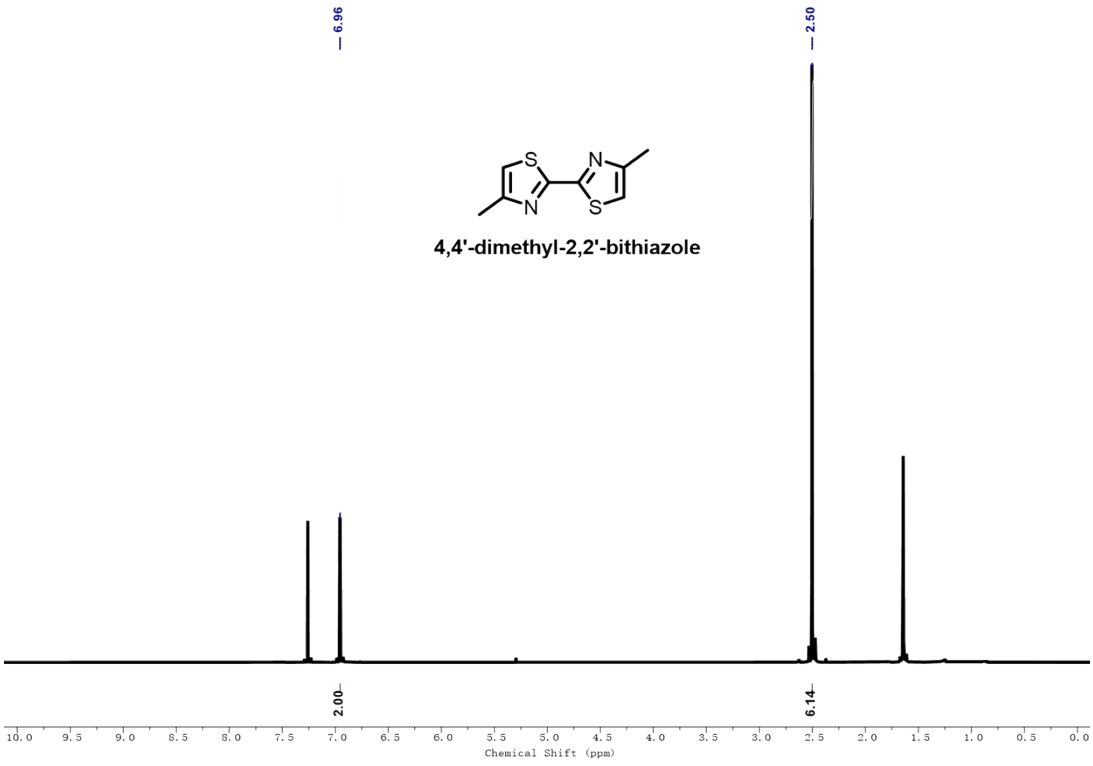


Figure S11 ^{1}H NMR spectrum of 4,4'-dimethyl-2,2'-bithiazole

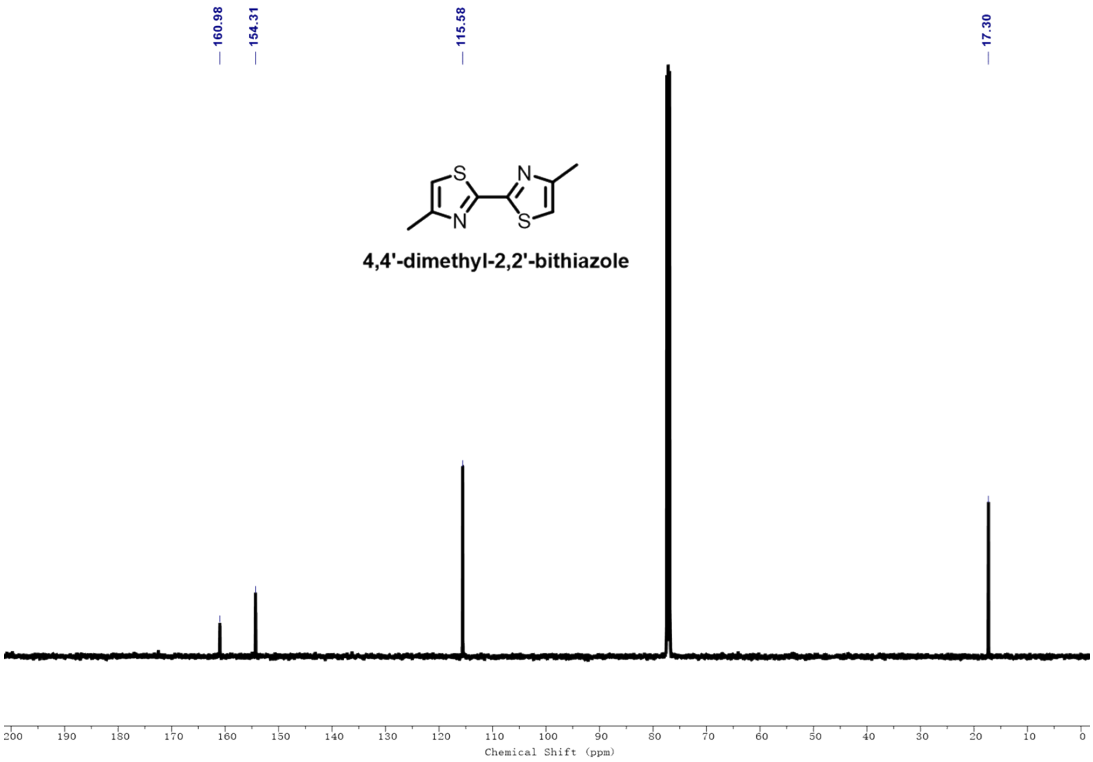


Figure S12 ^{13}C NMR spectrum of 4,4'-dimethyl-2,2'-bithiazole

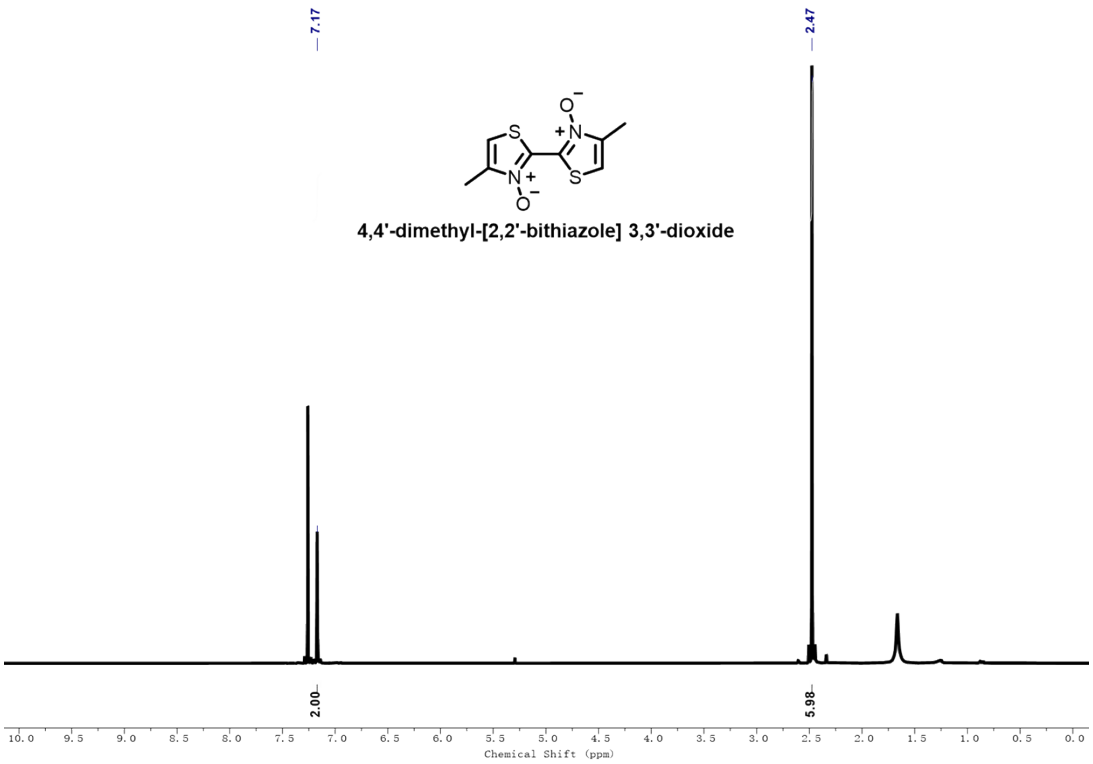


Figure S13 ^{1}H NMR spectrum of 4,4'-dimethyl-[2,2'-bithiazole] 3,3'-dioxide

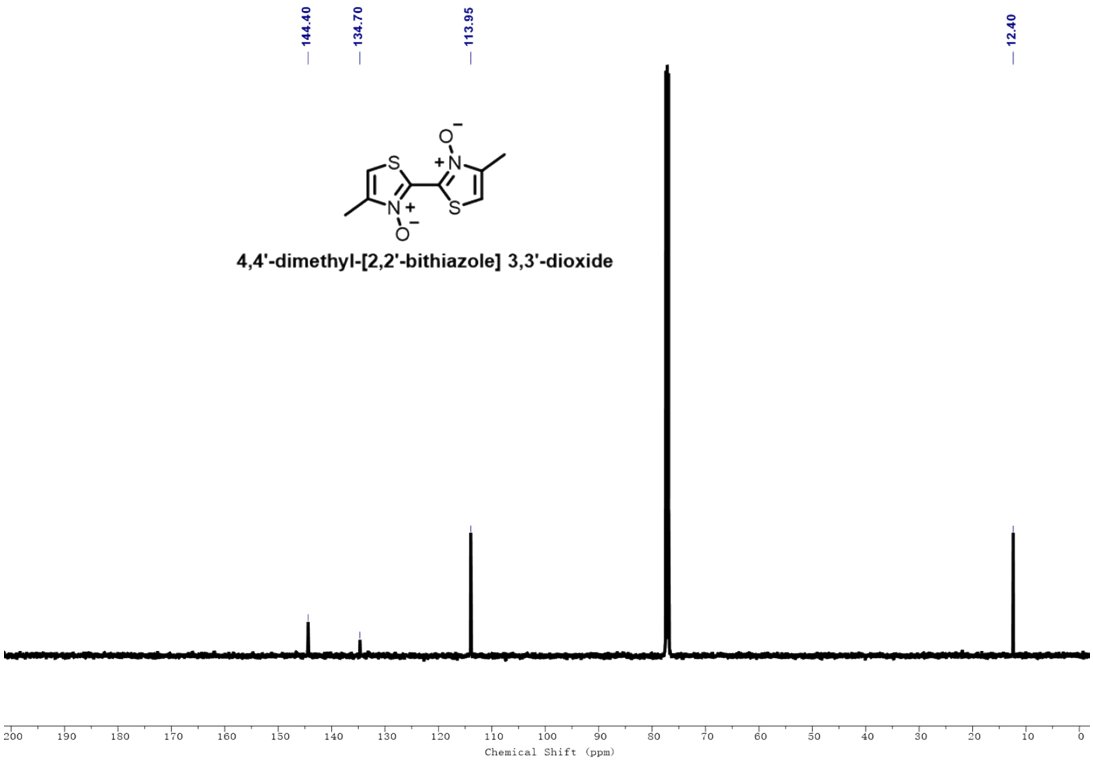


Figure S14 ^{13}C NMR spectrum of 4,4'-dimethyl-[2,2'-bithiazole] 3,3'-dioxide

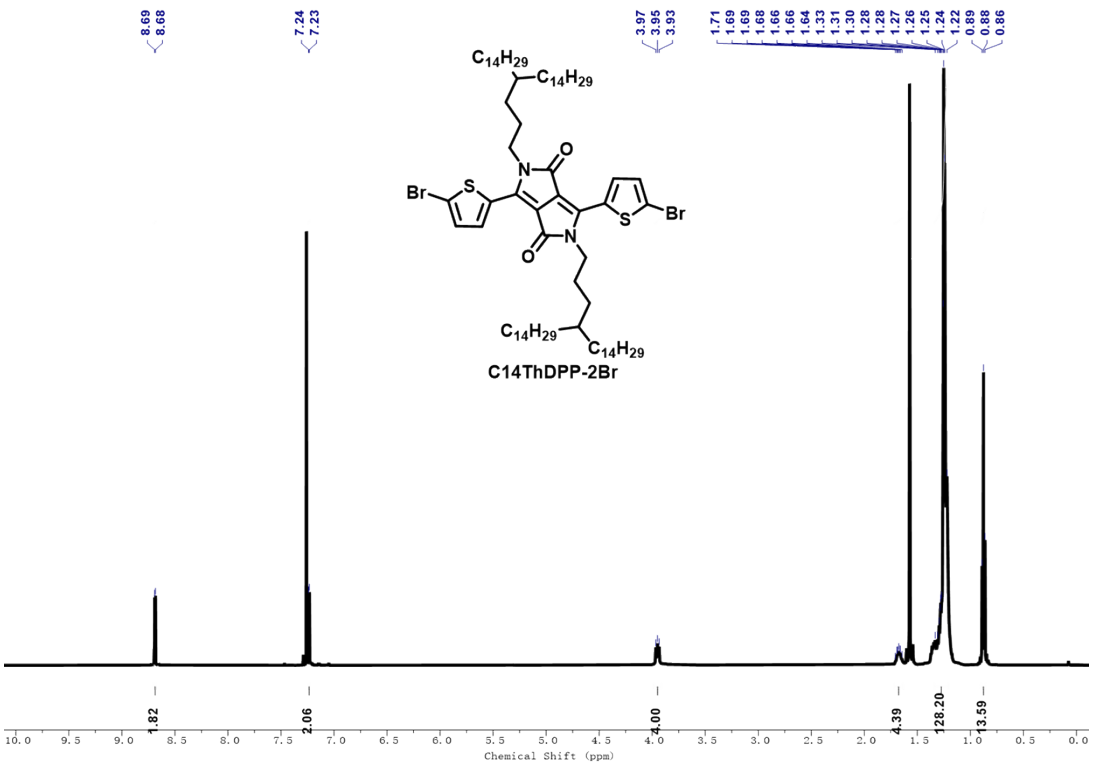


Figure S15 ^{1}H NMR spectrum of C_{14}ThDPP-2Br

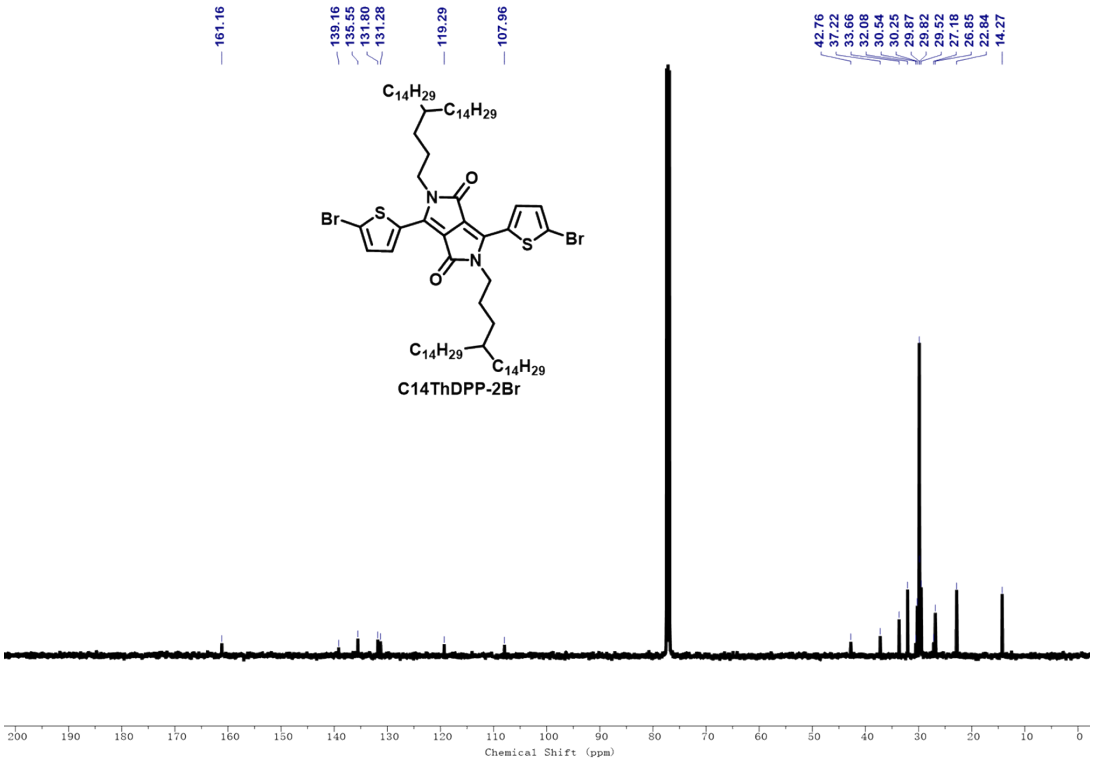


Figure S16 ^{13}C NMR spectrum of C_{14}ThDPP-2Br

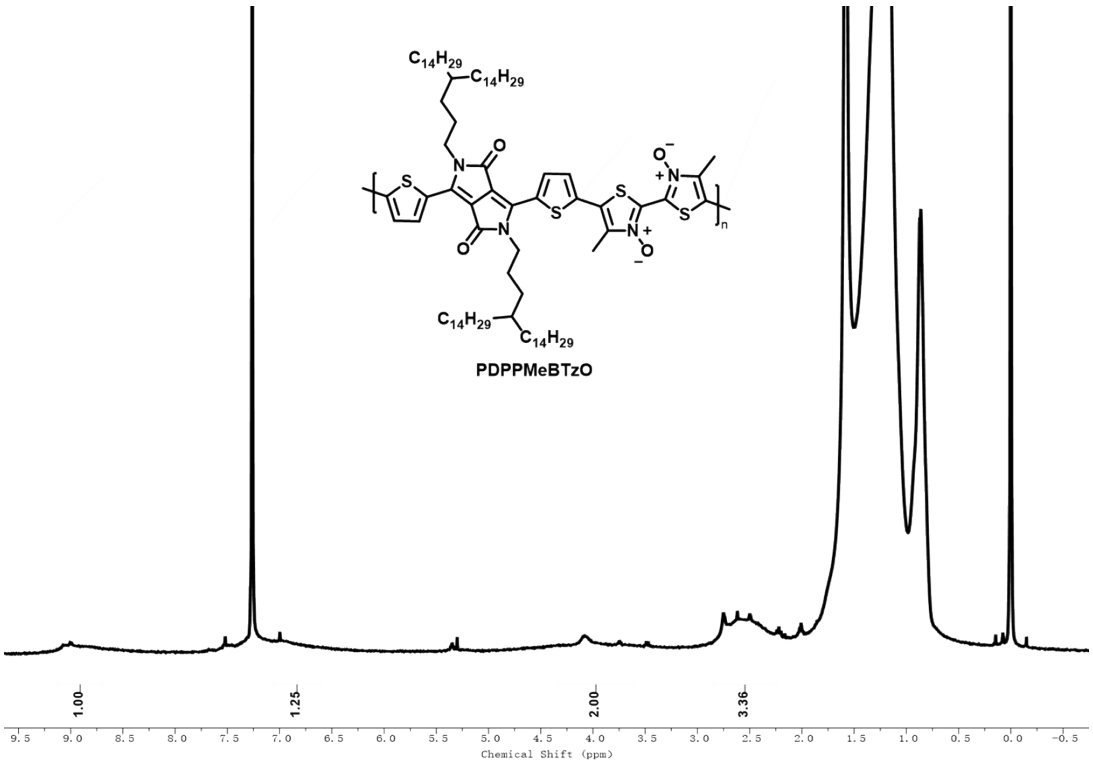


Figure S17 ^{1}H NMR spectrum of PDPPMeBTzO (P1)

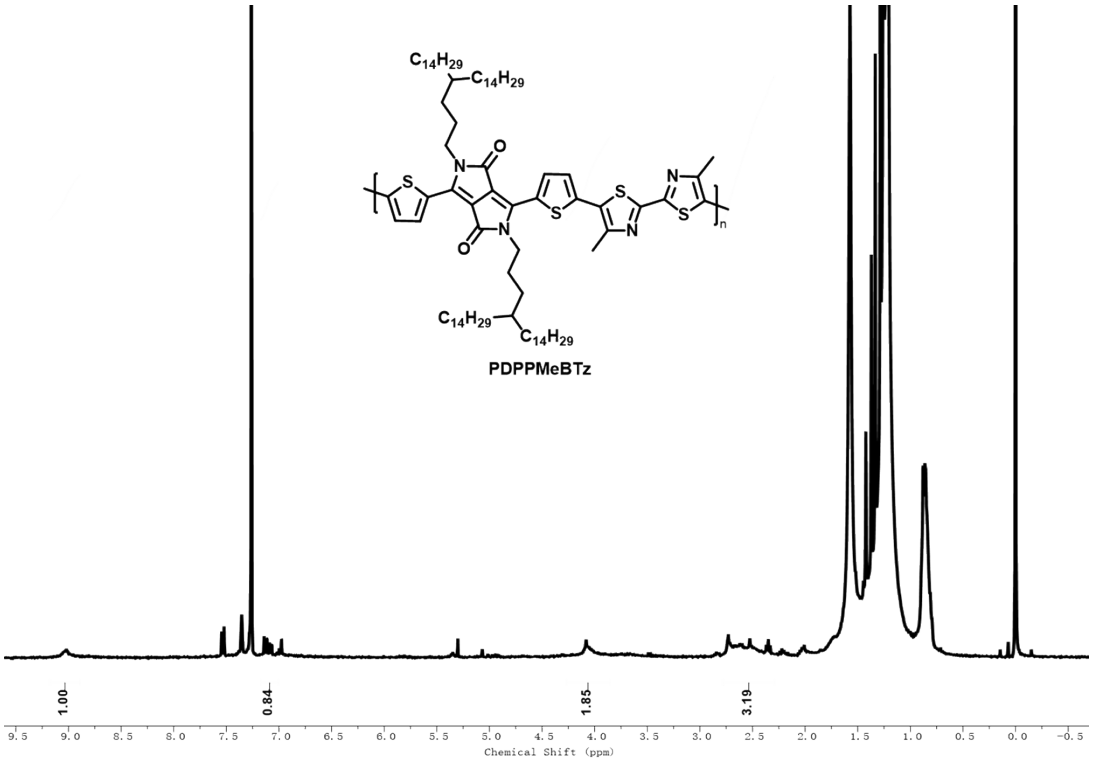


Figure S18 ^{1}H NMR spectrum of PDPPMeBTz (P2)

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Energies and Cartesian Coordinates

Pd-cat

G = -5861.008908 Hartree

Pd	2.435601	3.306022	17.788889
P	0.835323	4.698419	18.660132
C	2.270025	4.332494	16.048947
C	3.142328	5.991323	14.515932
H	3.823604	6.810739	14.316172
C	1.414641	3.878678	15.044468
H	0.745357	3.045716	15.227333
C	3.129011	5.398022	15.778248
H	3.808129	5.762416	16.540576
C	1.429214	4.473591	13.782772
H	0.767708	4.102624	13.007988
C	2.290381	5.533034	13.516042
H	2.301291	5.994104	12.535845
O	3.002365	1.873985	19.396785
O	3.963521	1.728247	17.416649
C	3.824952	1.313094	18.605818
C	4.659462	0.152997	19.086251
H	4.299355	-0.209868	20.046974
H	4.641834	-0.647834	18.346510
H	5.696538	0.479600	19.191098
C	1.187394	6.507913	18.686818
H	1.286160	6.871336	17.664990
H	0.385220	7.049059	19.192419
H	2.126997	6.686296	19.209745
C	-0.846743	4.595323	17.912436
H	-1.547570	5.241554	18.444588
H	-0.795660	4.894891	16.866412
H	-1.199455	3.565104	17.961168
C	0.555842	4.277865	20.434660
H	-0.214920	4.915449	20.872538
H	0.259052	3.232451	20.513726
H	1.489276	4.399747	20.983476

BTz

G = -1137.008408 Hartree

H	-1.168073	0.521194	1.143653
C	-0.283672	1.094809	0.919157
C	1.020817	0.746806	1.101720
S	-0.393481	2.684212	0.232953
H	1.360303	-0.192258	1.514191
C	1.368205	2.748825	0.249137
C	2.076641	3.914965	-0.234829
S	3.838327	3.979578	-0.218645
C	2.424028	5.916984	-1.087412
C	3.728518	5.568981	-0.904848
H	2.084543	6.856048	-1.499882
H	4.612918	6.142596	-1.129345
N	1.944088	1.680781	0.722944
N	1.500758	4.983009	-0.708636

TS-BTz-α

G = -6997.977818 Hartree

Pd	-1.616841	-0.595482	-0.249144
C	0.860053	-0.151698	-3.752368
C	-0.118596	0.026123	-2.774267
C	-0.197170	-0.841288	-1.684821
C	0.720213	-1.889331	-1.592343
C	1.699605	-2.065435	-2.570015
C	1.770936	-1.198518	-3.655513
O	-3.227657	-0.501787	1.300785
C	-3.029769	0.055230	2.407312
P	-2.950814	-2.202553	-1.355371
O	-1.956795	0.670223	2.719627
H	-0.808635	0.856225	-2.866244
H	2.409868	-2.879332	-2.476067
H	2.532635	-1.333015	-4.413908
H	0.910369	0.536485	-4.588697
H	0.692450	-2.572041	-0.750228
C	-4.118169	0.031384	3.455145
H	-3.695878	-0.238530	4.423056
H	-4.536674	1.035626	3.550457
H	-4.907789	-0.662871	3.177494
H	-1.192156	0.732653	1.747177
C	-2.683480	-2.586279	-3.138097
H	-3.394618	-3.341594	-3.478082
H	-2.809441	-1.678443	-3.727513
H	-1.666083	-2.944974	-3.286855
C	-2.856123	-3.859661	-0.544130
H	-3.547041	-4.566323	-1.008624
H	-1.839913	-4.245196	-0.627067
H	-3.101683	-3.753317	0.512221

C	-4.746001	-1.784041	-1.266202
H	-5.360371	-2.606316	-1.638491
H	-4.998709	-1.562977	-0.230303
H	-4.937755	-0.892613	-1.863881
C	-0.302970	0.953641	0.714344
C	1.036063	0.720109	0.984507
S	-0.388889	2.564717	0.013483
H	1.398803	-0.189479	1.445267
C	1.347574	2.726049	0.147520
C	2.059109	3.909458	-0.281994
S	3.810415	4.027017	-0.086490
C	2.438660	5.912999	-1.119160
C	3.727650	5.604881	-0.799956
H	2.117950	6.838408	-1.575668
H	4.613012	6.203229	-0.940786
N	1.941196	1.682442	0.677479
N	1.507329	4.957896	-0.826225

TS-BTz-β

G = -6997.969462 Hartree

Pd	1.862923	0.530036	0.254059
C	3.374442	-1.276702	-3.358450
C	3.210384	-0.851986	-2.039515
C	2.101801	-0.087824	-1.669981
C	1.160942	0.244342	-2.644820
C	1.326880	-0.177965	-3.963899
C	2.434627	-0.937876	-4.326473
O	1.752838	1.277289	2.360730
C	1.249522	0.539979	3.240710
P	3.330840	2.332311	-0.167219
O	0.730729	-0.602181	3.004910
H	3.953019	-1.135302	-1.301531
H	0.582035	0.084352	-4.706934
H	2.560230	-1.268399	-5.350435
H	4.238086	-1.875931	-3.625219
H	0.282612	0.821399	-2.380494
C	1.221107	1.006712	4.676642
H	1.516177	0.193764	5.339689
H	1.870544	1.867831	4.815684
H	0.196294	1.283553	4.933785
H	0.671765	-0.798567	1.794047
C	2.752991	3.874280	0.665328
H	3.502490	4.665308	0.596635
H	1.828864	4.210660	0.194719
H	2.541469	3.644425	1.708539
C	5.013687	2.065494	0.547961
H	5.636739	2.955054	0.433227
H	4.914306	1.826048	1.606418
H	5.492692	1.225041	0.045639
C	3.680488	2.876046	-1.893146
H	4.365807	3.725814	-1.898177
H	4.112081	2.050018	-2.456550
H	2.746466	3.159622	-2.377616
C	0.342058	-1.124006	0.469239
C	0.593735	-2.421349	0.086240
S	-0.740344	-3.139981	-0.749920
C	-1.601909	-1.608972	-0.538278
C	-2.951103	-1.434773	-1.037466
S	-3.809139	0.089264	-0.796243
C	-4.873427	-1.878073	-2.022571
C	-5.159424	-0.603035	-1.640094
H	-5.546014	-2.529374	-2.562001
N	-3.631504	-2.339258	-1.681391
N	-0.929752	-0.700347	0.097188
H	-6.066376	-0.043067	-1.799626
H	1.493696	-2.992542	0.253406

BTzO

G = -1287.374001 Hartree

H	-1.161996	0.511547	1.148183
C	-0.276715	1.083253	0.924310
C	1.003461	0.704391	1.119410
S	-0.404950	2.679440	0.234288
H	1.397811	-0.212585	1.523992
C	1.338911	2.785451	0.232633
C	2.105935	3.878339	-0.218325
S	3.849796	3.984351	-0.219979
C	2.441384	5.959399	-1.105102
C	3.721561	5.580537	-0.910001
H	2.047035	6.876374	-1.509684
H	4.606842	6.152243	-1.133875
N	1.922962	1.672260	0.725968
N	1.521883	4.991530	-0.711660
O	0.245120	5.134955	-0.805119
O	3.199726	1.528835	0.819427

TS-BTzO-α

G = -7148.34568 Hartree

Pd	-1.620335	-0.601770	-0.209442
C	0.887131	-0.091837	-3.680456
C	-0.110449	0.059423	-2.716797
C	-0.195770	-0.827702	-1.644240
C	0.727635	-1.870061	-1.554104
C	1.725429	-2.018768	-2.517688
C	1.806454	-1.131329	-3.585640
O	-3.239063	-0.536086	1.328386
C	-3.058924	0.011007	2.443781
P	-2.941333	-2.174747	-1.363244
O	-1.996033	0.633391	2.773432
H	-0.807250	0.884024	-2.806617
H	2.442770	-2.826380	-2.425446
H	2.583002	-1.244335	-4.332260
H	0.944705	0.611521	-4.503451
H	0.692102	-2.568026	-0.724909
C	-4.158704	-0.036050	3.478240
H	-3.743399	-0.301993	4.450179
H	-4.595711	0.960494	3.571681
H	-4.933009	-0.742476	3.188515
H	-1.215557	0.711736	1.809367
C	-2.661070	-2.514313	-3.152084
H	-3.371359	-3.260260	-3.513823
H	-2.782788	-1.592538	-3.720315
H	-1.643239	-2.870763	-3.302798
C	-2.853200	-3.848166	-0.587506
H	-3.540802	-4.542878	-1.074331
H	-1.836750	-4.232823	-0.670633
H	-3.108480	-3.765291	0.468611
C	-4.733800	-1.748704	-1.273568
H	-5.348720	-2.560204	-1.667876
H	-4.991118	-1.550213	-0.234310
H	-4.918189	-0.843503	-1.852446
C	-0.302273	0.950770	0.812186
C	1.015414	0.674081	1.057950
S	-0.411817	2.546670	0.072865
H	1.438869	-0.204040	1.519347
C	1.314073	2.732852	0.120972
C	2.080359	3.827515	-0.322525
S	3.822962	3.961936	-0.219175
C	2.444602	5.887354	-1.250603
C	3.715085	5.534738	-0.963854
H	2.063394	6.785803	-1.706168
H	4.603531	6.115238	-1.149982
N	1.916307	1.649579	0.677505
N	1.513260	4.919094	-0.886533
O	3.195190	1.565257	0.833731
O	0.246837	5.049238	-1.067639

TS-BTzO-β

G = -7148.344535 Hartree

Pd	1.946378	0.497923	0.335201
C	2.793703	-1.150659	-3.560296
C	2.853271	-0.820416	-2.206155
C	1.898103	0.025462	-1.641850
C	0.884243	0.539305	-2.449944
C	0.829532	0.210371	-3.805175
C	1.784937	-0.631476	-4.365395
O	2.109813	1.159086	2.460187
C	1.414312	0.610323	3.351196
P	3.455098	2.235283	-0.123072
O	0.613502	-0.356432	3.141833
H	3.646370	-1.239671	-1.597050
H	0.031712	0.611626	-4.420070
H	1.738506	-0.888291	-5.416753
H	3.537607	-1.817051	-3.982640
H	0.117494	1.175927	-2.023174
C	1.498826	1.123084	4.770087
H	1.507533	0.289229	5.471125
H	2.380499	1.745718	4.904332
H	0.606408	1.718121	4.977381
H	0.557319	-0.642431	1.918228
C	2.734958	3.842035	0.426754
H	3.465609	4.649534	0.345247
H	1.864720	4.077426	-0.185815
H	2.411869	3.736954	1.461673
C	4.998629	2.091536	0.878056
H	5.614032	2.988441	0.781359
H	4.719325	1.945648	1.920769
H	5.570667	1.225408	0.545169
C	4.060069	2.581958	-1.827345
H	4.719439	3.451998	-1.829308
H	4.596748	1.714841	-2.209965
H	3.209895	2.764289	-2.483617

C	0.351431	-1.110347	0.659249
C	0.596313	-2.430909	0.410365
S	-0.633289	-3.244962	-0.503595
C	-1.531035	-1.746995	-0.552943
C	-2.776572	-1.541337	-1.182271
S	-3.662391	-0.034425	-1.221835
C	-4.640812	-2.128018	-2.370683
C	-4.916586	-0.828001	-2.139201
H	-5.213296	-2.871256	-2.899813
N	-3.425738	-2.534870	-1.826818
N	-0.889547	-0.750978	0.087581
H	-5.791316	-0.285378	-2.457104
H	1.456994	-2.986896	0.747418
O	-2.967746	-3.735751	-1.926310
O	-1.375922	0.442336	0.146602

MeBTz

G = -1215.625886 Hartree

H	-1.174639	0.534641	1.140963
C	-0.285542	1.102101	0.917977
C	1.016459	0.735396	1.106612
S	-0.394639	2.692734	0.231334
C	1.365185	2.750282	0.248757
C	2.079661	3.913509	-0.234449
S	3.839484	3.971057	-0.217025
C	2.428387	5.928394	-1.092304
C	3.730388	5.561690	-0.903669
H	4.619485	6.129149	-1.126654
N	1.935640	1.680505	0.722186
N	1.509206	4.983285	-0.707877
C	1.495272	-0.562447	1.676400
H	2.136017	-1.082439	0.960897
H	2.086900	-0.390728	2.578351
H	0.659332	-1.214140	1.929847
C	1.949574	7.226238	-1.662091
H	1.357946	7.054518	-2.564043
H	1.308829	7.746229	-0.946589
H	2.785514	7.877930	-1.915538

TS-MeBTz-α

G = -7076.595698 Hartree

Pd	1.725357	-0.216949	-0.038428
C	-0.205296	3.589381	-0.666707
C	0.264532	2.285338	-0.822519
C	1.015122	1.675913	0.183476
C	1.287222	2.397813	1.347045
C	0.814553	3.701170	1.503819
C	0.069120	4.303084	0.495481
O	2.664747	-2.242224	-0.252717
C	2.109666	-3.264850	0.212814
P	3.806556	0.651909	-0.762474
O	0.959577	-3.268615	0.768338
H	0.023579	1.744853	-1.729785
H	1.029488	4.242724	2.418442
H	-0.299302	5.314541	0.616812
H	-0.793517	4.043092	-1.456512
H	1.862754	1.949651	2.149336
C	2.806689	-4.601374	0.111501
H	2.731819	-5.133731	1.059494
H	2.298978	-5.205501	-0.643642
H	3.848429	-4.472848	-0.173017
H	0.434753	-2.163668	0.681975
C	3.989596	2.427959	-1.219901
H	5.013526	2.642523	-1.531832
H	3.304064	2.664803	-2.033066
H	3.725252	3.053569	-0.368341
C	5.147287	0.388874	0.481597
H	6.116718	0.706992	0.092171
H	4.920270	0.955303	1.384899
H	5.187531	-0.669711	0.737047
C	4.428626	-0.246773	-2.249869
H	5.448213	0.055787	-2.497273
H	4.394883	-1.316097	-2.045710
H	3.775379	-0.036707	-3.097045
C	-0.286821	-0.976728	0.557280
C	-0.963315	-0.589160	1.710854
S	-1.473461	-1.018897	-0.743867
C	-2.719671	-0.508692	0.370447
C	-4.093870	-0.305070	-0.033737
S	-5.314456	0.188627	1.139468
C	-5.889673	-0.199266	-1.330975
C	-6.474160	0.164434	-0.150486
H	-7.507276	0.415739	0.028294
N	-2.298614	-0.336566	1.598562
N	-4.545405	-0.459810	-1.245790
C	-0.333868	-0.460432	3.062119

H	-0.327314	0.586082	3.377780
H	-0.906118	-1.022311	3.803299
H	0.692997	-0.823973	3.052196
C	-6.578040	-0.329525	-2.653394
H	-6.131088	0.345193	-3.387018
H	-6.475160	-1.345701	-3.040597
H	-7.639615	-0.096502	-2.570148

MeBTzO

G = -1365.99655 Hartree

H	-1.157827	0.512644	1.150005
C	-0.269761	1.080709	0.926869
C	1.009107	0.685982	1.127613
S	-0.401550	2.676737	0.236383
C	1.339268	2.784770	0.233111
C	2.105579	3.879020	-0.218804
S	3.846396	3.987053	-0.222076
C	2.435739	5.977808	-1.113305
C	3.714607	5.583081	-0.912561
H	4.602673	6.151147	-1.135696
N	1.921117	1.671700	0.725642
N	1.523729	4.992090	-0.711334
O	0.245039	5.137422	-0.804612
O	3.199807	1.526367	0.818920
C	1.894723	7.243825	-1.671556
H	1.241374	7.732864	-0.946307
H	2.707324	7.918318	-1.936928
H	1.288568	7.043052	-2.557234
C	1.550123	-0.580034	1.685864
H	2.203471	-1.069074	0.960615
H	2.156278	-0.379261	2.571542
H	0.737521	-1.254527	1.951237

TS-MeBTzO-α

G = -7226.968761 Hartree

Pd	1.917404	-0.217651	-0.033371
C	-0.136049	3.518949	-0.699733
C	0.356893	2.221229	-0.836916
C	1.195426	1.676682	0.135882
C	1.536630	2.455406	1.243039
C	1.041615	3.752873	1.379589
C	0.205197	4.289888	0.406814
O	2.872526	-2.237763	-0.174259
C	2.373490	-3.233858	0.400975
P	3.917860	0.667562	-0.923930
O	1.259899	-3.218708	1.026107
H	0.064591	1.636374	-1.700515
H	1.309609	4.339598	2.251157
H	-0.181722	5.295997	0.513177
H	-0.794096	3.922626	-1.460955
H	2.183119	2.057405	2.017423
C	3.096985	-4.558814	0.355313
H	3.086859	-5.023488	1.340988
H	2.563713	-5.225508	-0.326002
H	4.118075	-4.429856	0.004076
H	0.697337	-2.136545	0.877274
C	3.946112	2.351698	-1.670945
H	4.942233	2.584858	-2.051826
H	3.225239	2.398265	-2.486603
H	3.655796	3.088327	-0.923360
C	5.290974	0.724519	0.310680
H	6.223911	1.049900	-0.154507
H	5.029946	1.416195	1.111721
H	5.426806	-0.268125	0.739370
C	4.585367	-0.414749	-2.260627
H	5.578333	-0.086503	-2.574300
H	4.626232	-1.437650	-1.889450
H	3.909771	-0.387084	-3.115842
C	-0.073540	-0.996561	0.689420
C	-0.707071	-0.494579	1.802256
S	-1.236610	-1.133340	-0.630735
C	-2.502992	-0.490437	0.363719
C	-3.847417	-0.258699	0.011941
S	-5.083565	0.380125	1.069253
C	-5.679719	-0.213390	-1.388731
C	-6.221326	0.272051	-0.247312
H	-7.245464	0.576307	-0.105646
N	-2.057345	-0.214017	1.614881
N	-4.319847	-0.513559	-1.229135
O	-2.826157	0.257510	2.541481
O	-3.595811	-0.987917	-2.182779
C	-0.150542	-0.245604	3.156377
H	-0.745650	-0.763102	3.911960
H	0.882866	-0.583774	3.203780
H	-0.194114	0.819717	3.395554
C	-6.296332	-0.460487	-2.717861

H	-5.786754	0.119294	-3.490219
H	-6.196598	-1.511644	-2.995959
H	-7.351261	-0.190269	-2.701456
