Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

SUPPORTING INFORMATION

Probing the Nature of Donor-Acceptor Effects in Conjugated Materials: A Joint Experimental and Computational Study of Model Conjugated Oligomers

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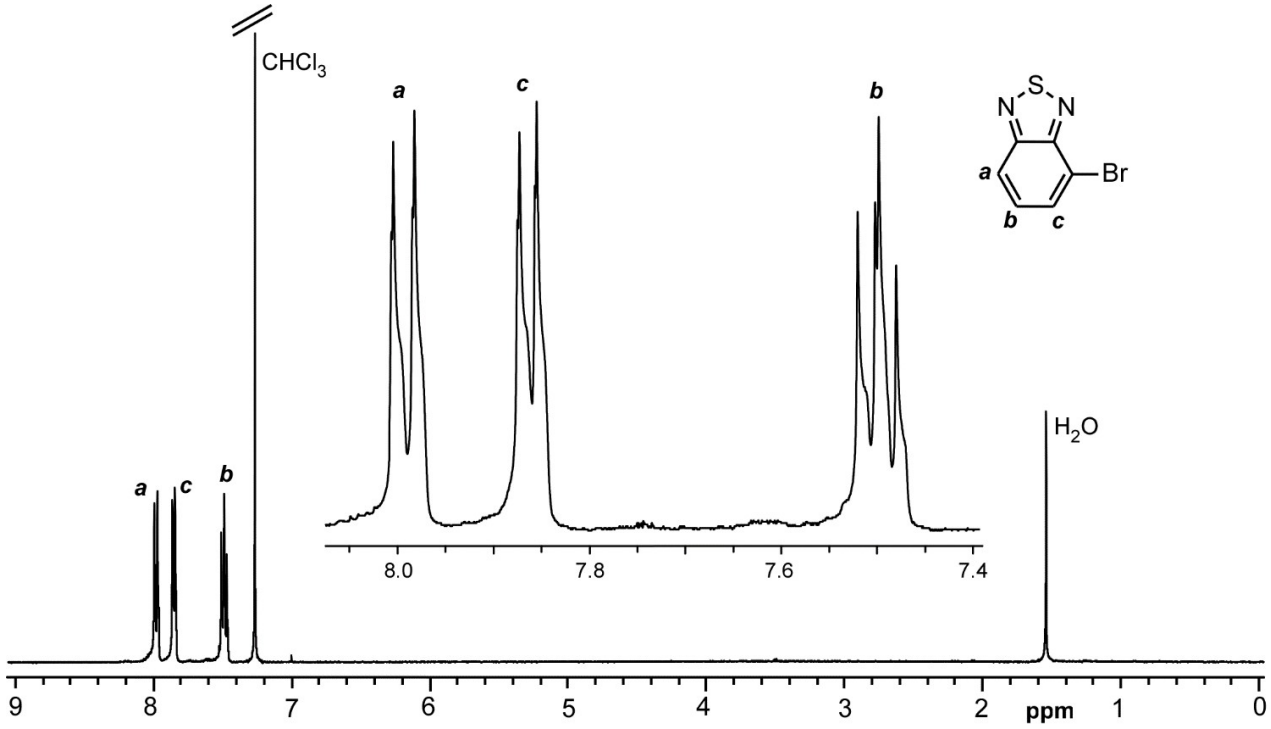


Figure S1. ^{1}H NMR spectrum of **1**

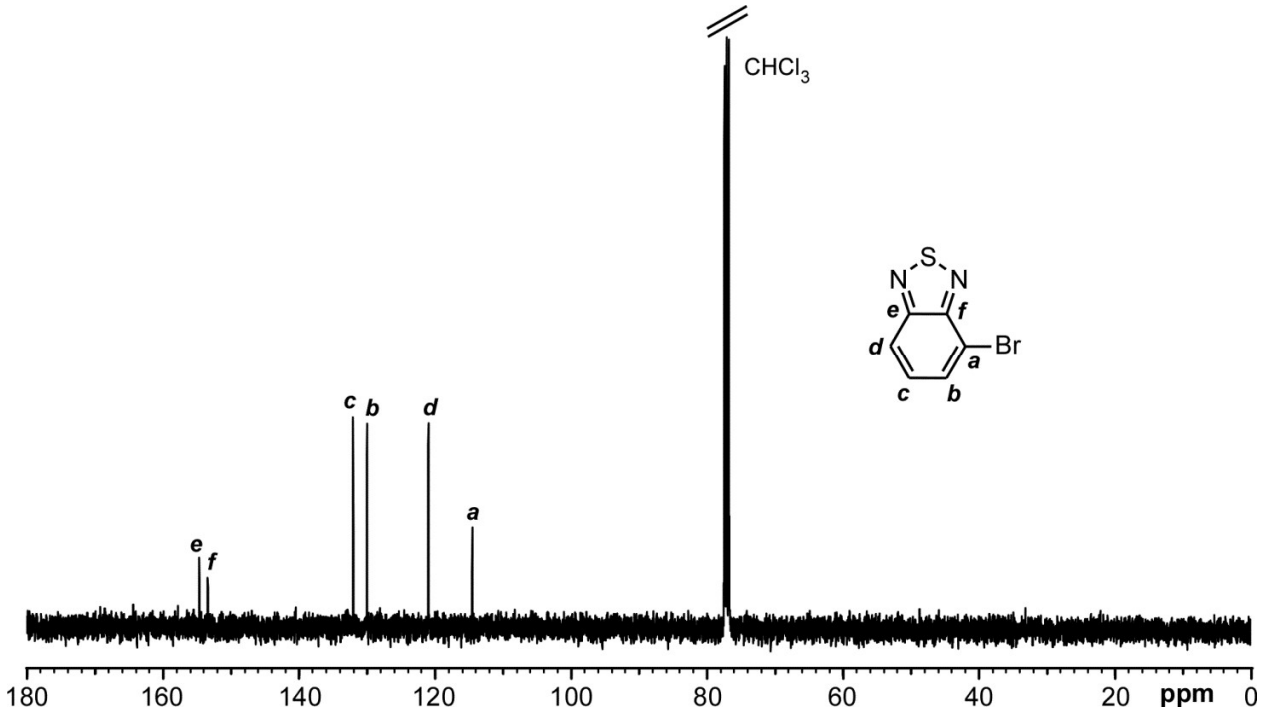


Figure S2. ^{13}C NMR spectrum of **1**

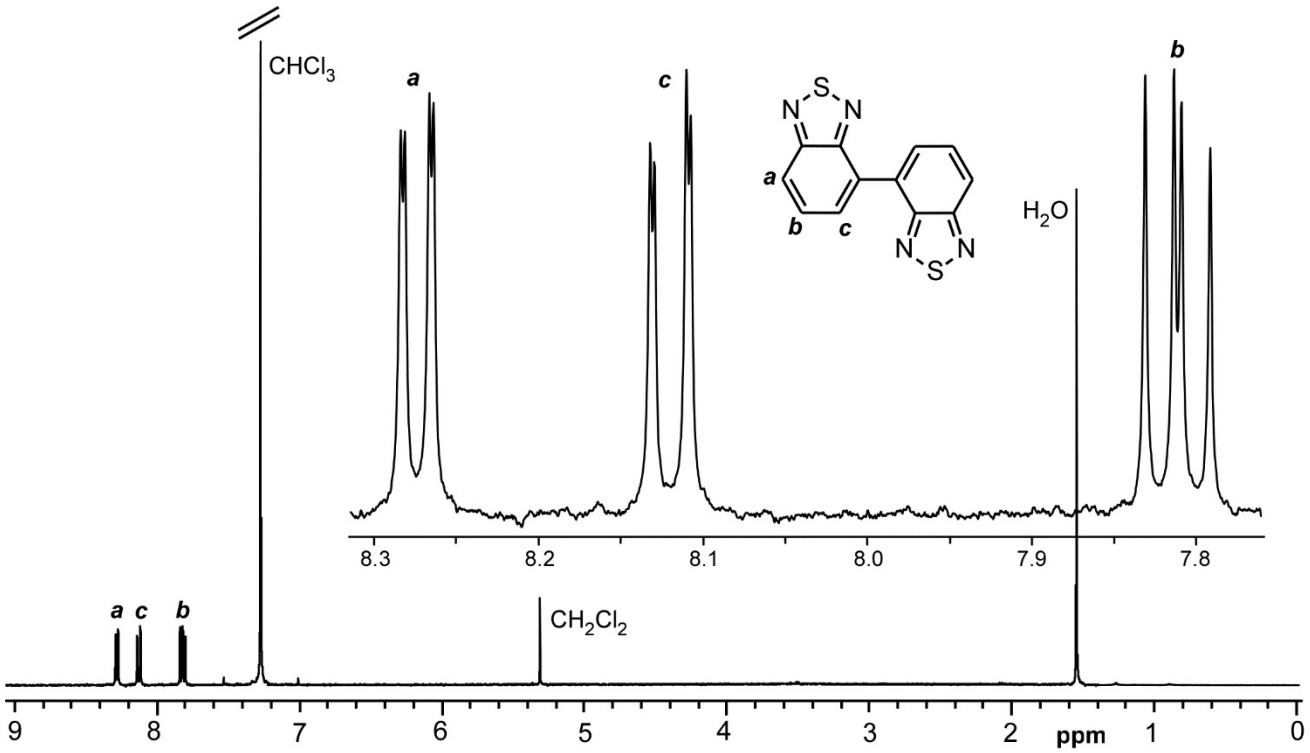


Figure S3. ^{1}H NMR spectrum of **BTD-BTD**

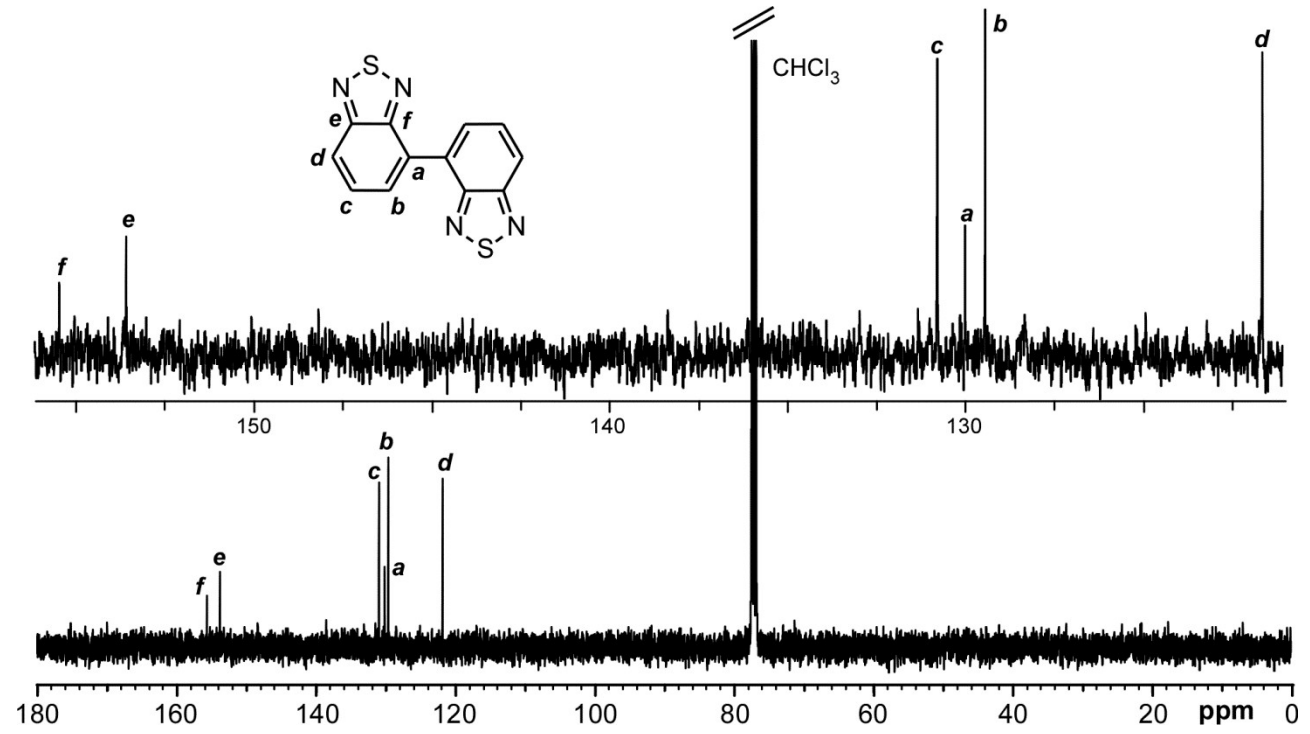


Figure S4. ^{13}C NMR spectrum of **BTD-BTD**

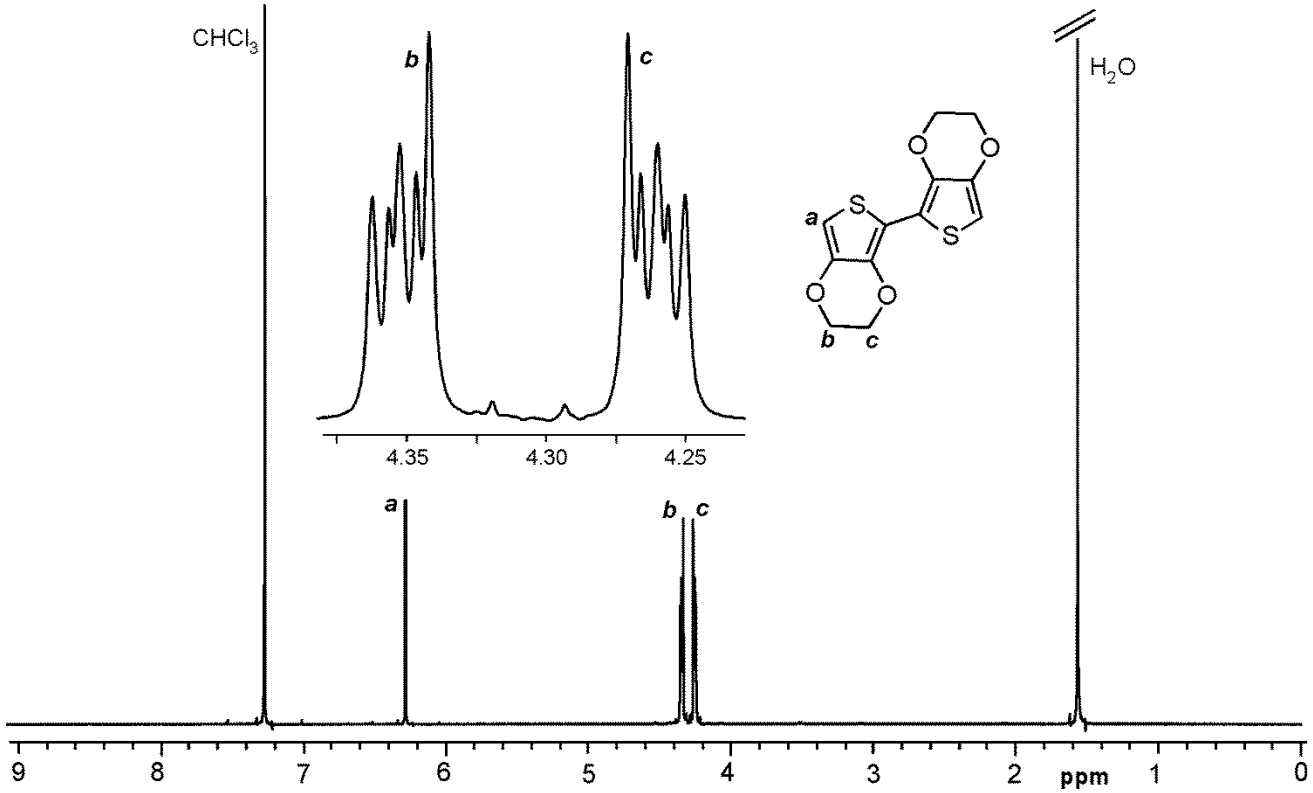


Figure S5. ^{1}H NMR spectrum of **EDOT-EDOT**

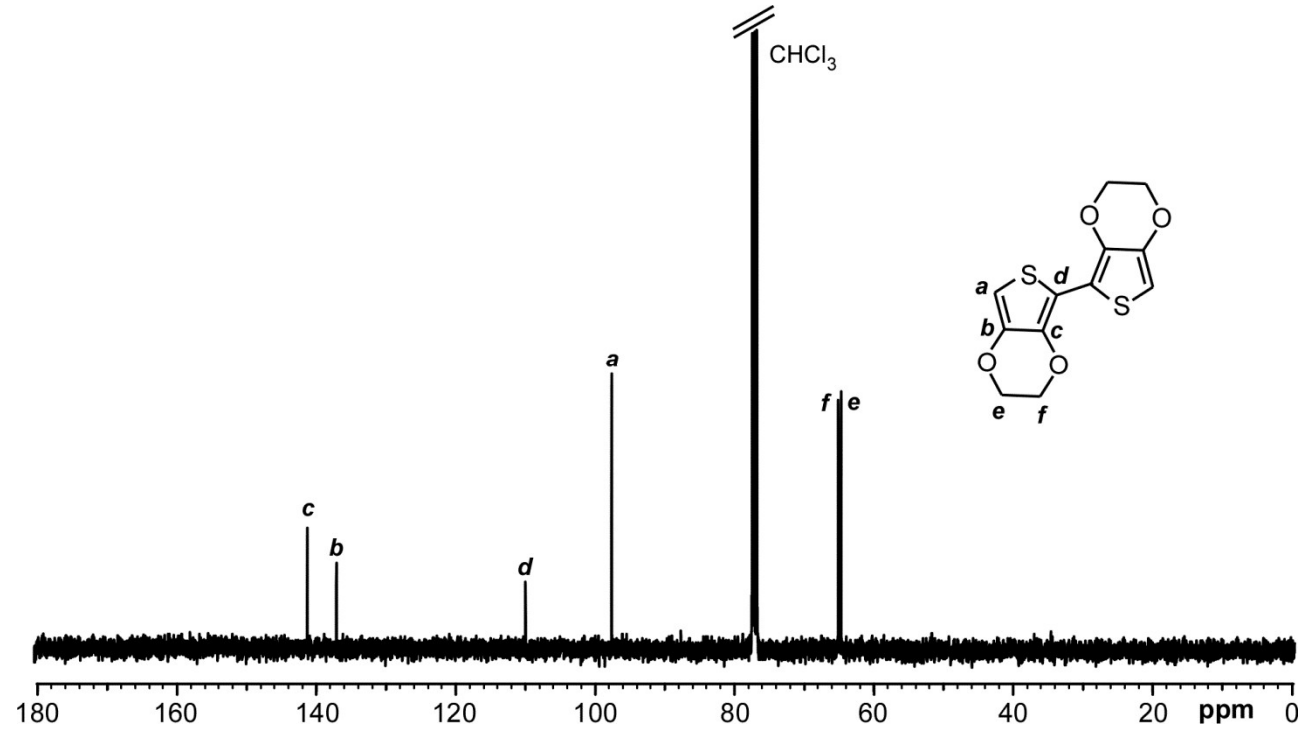


Figure S6. ^{13}C NMR spectrum of **EDOT-EDOT**

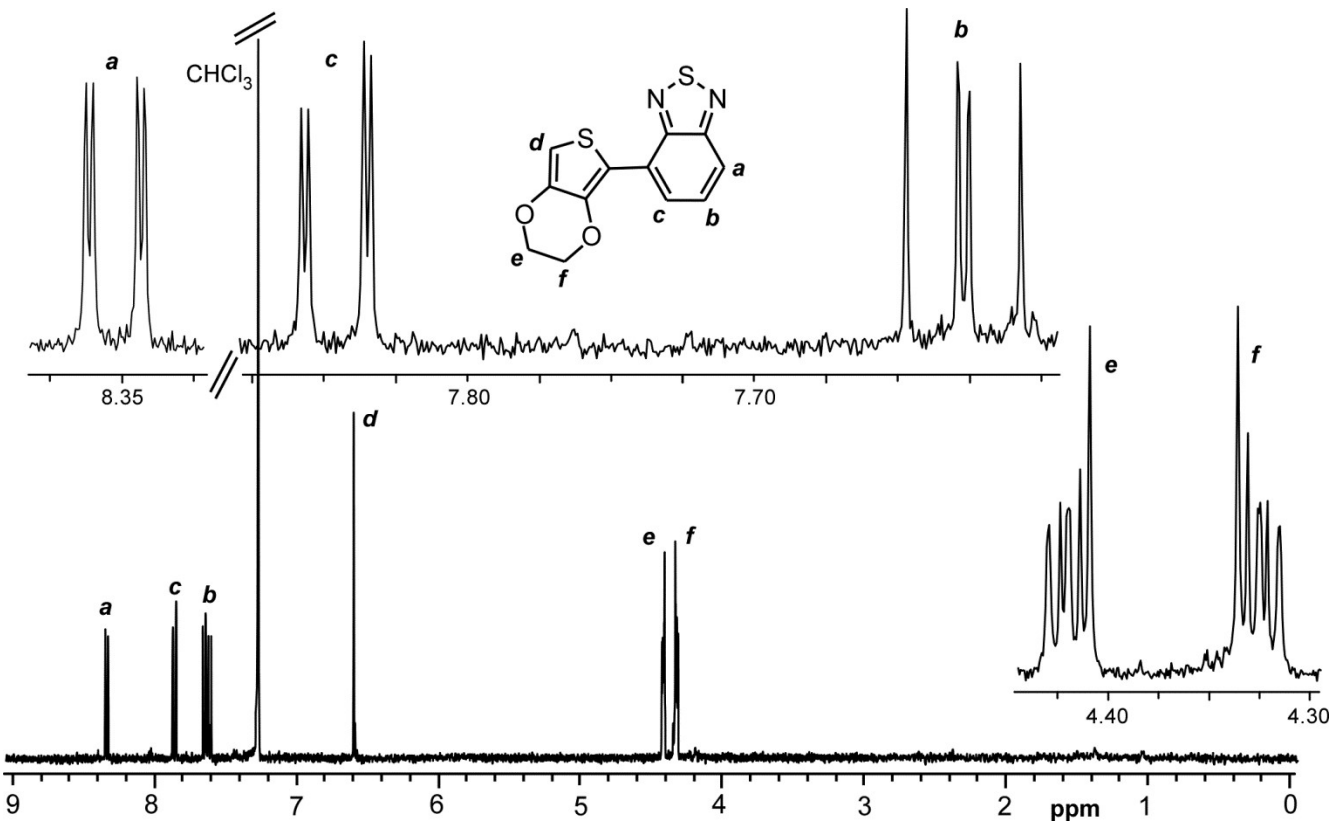


Figure S7. ^{1}H NMR spectrum of **EDOT-BTD**

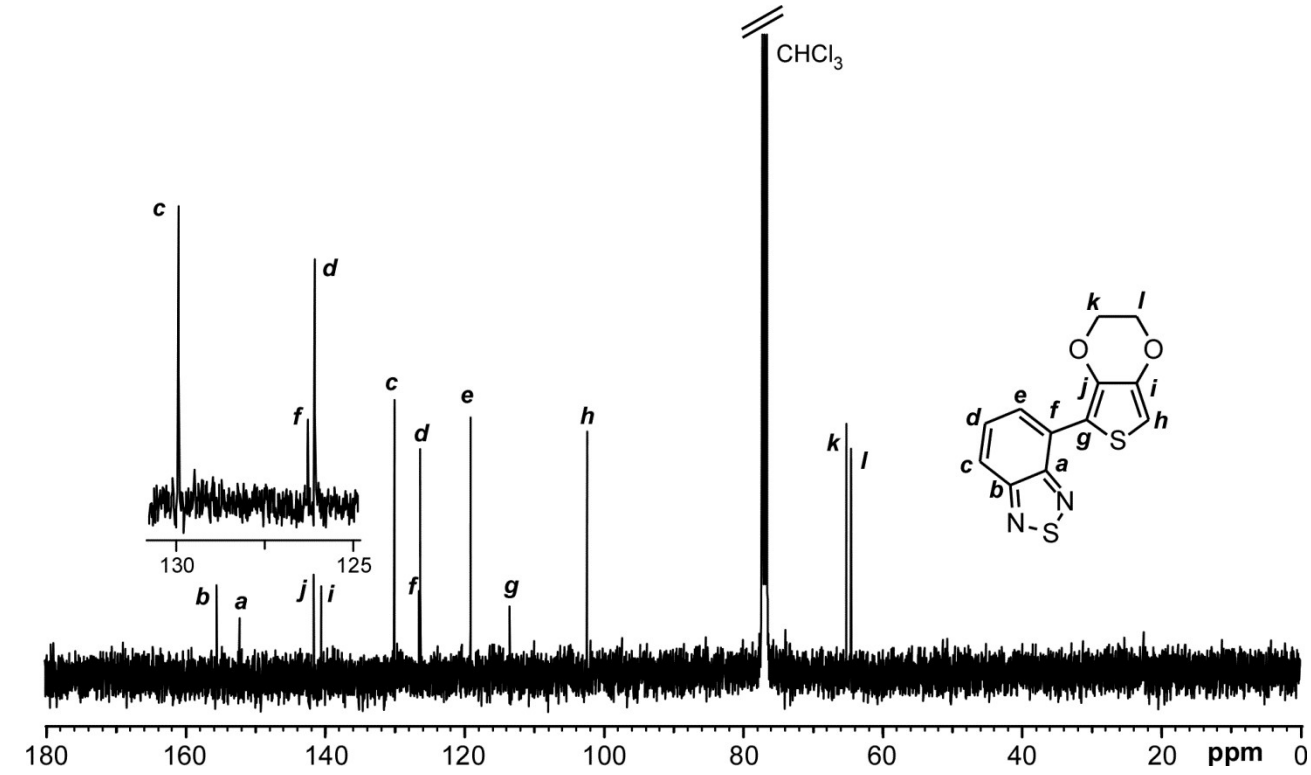


Figure S8. ^{13}C NMR spectrum of **EDOT-BTD**

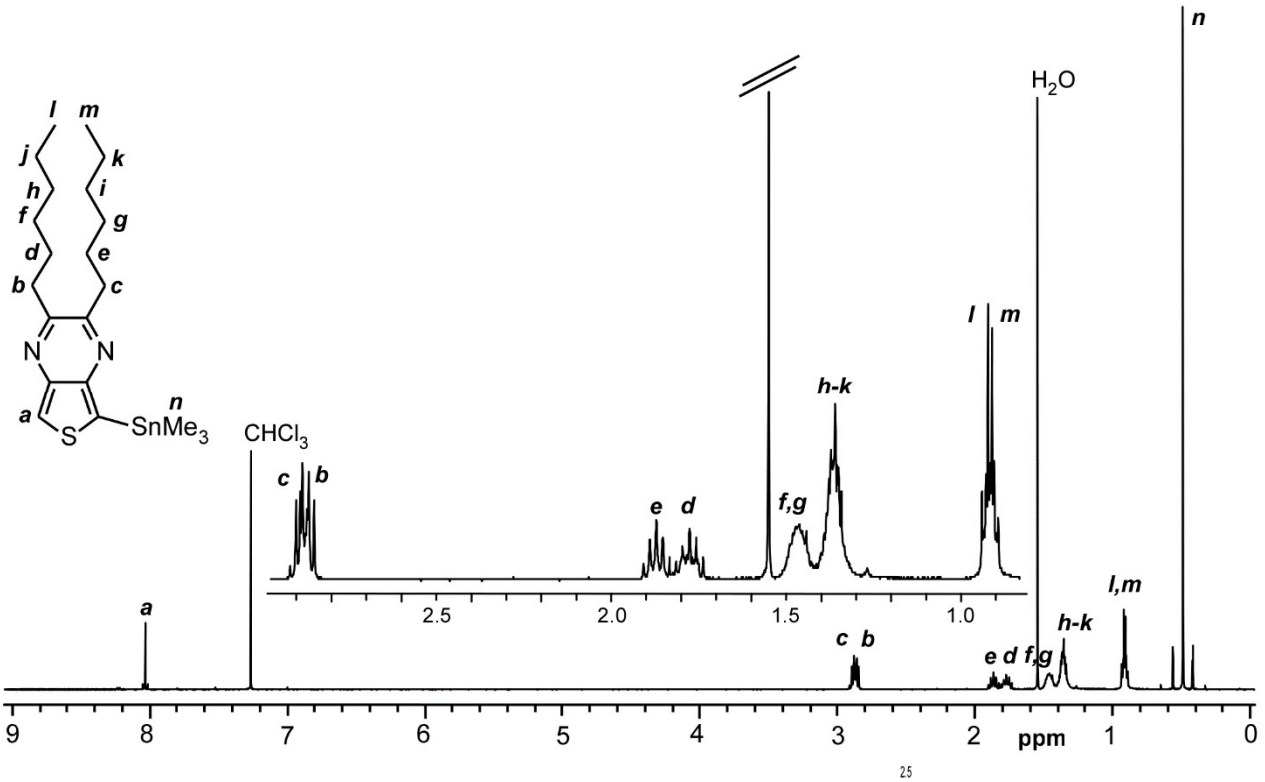


Figure S9. [1]H NMR spectrum of **4**

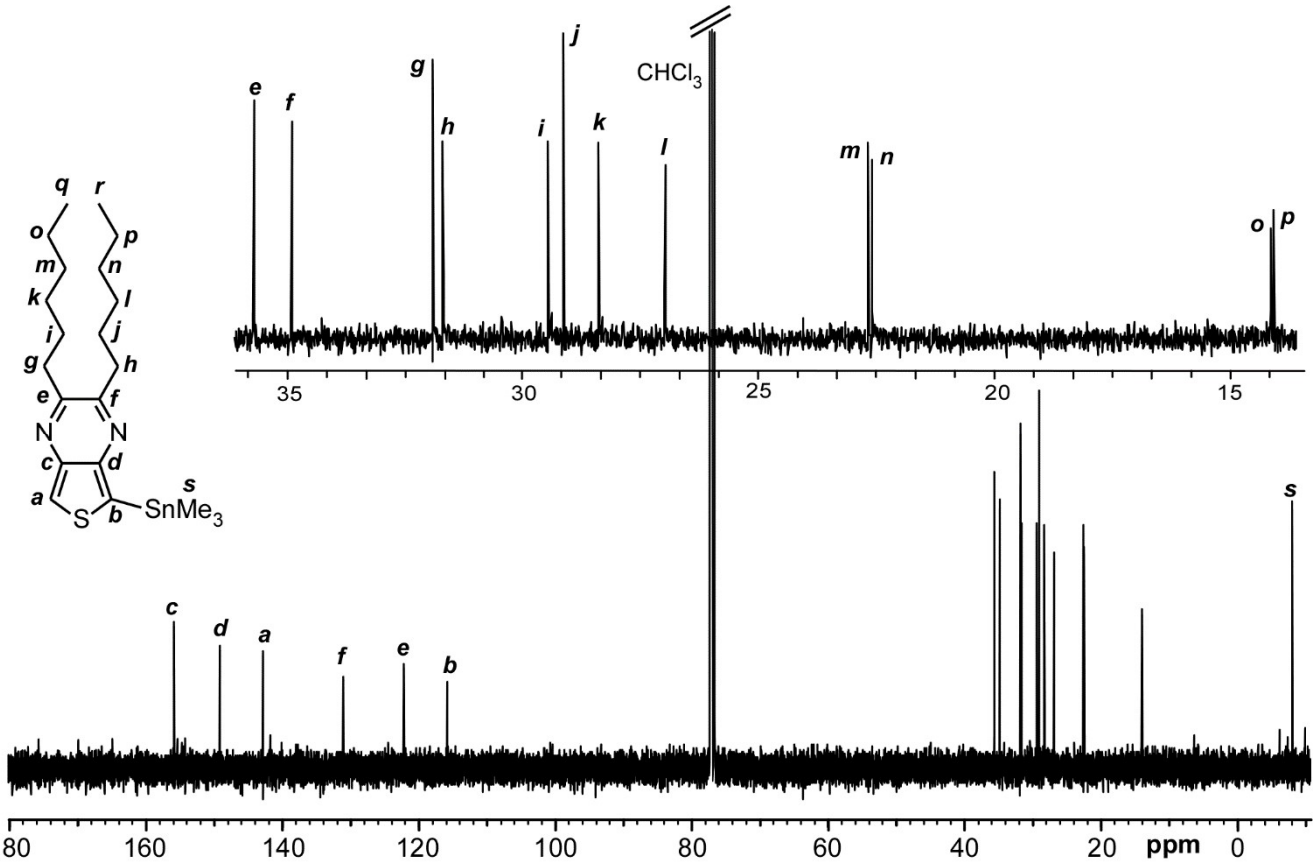


Figure S10. [13]C NMR spectrum of **4**

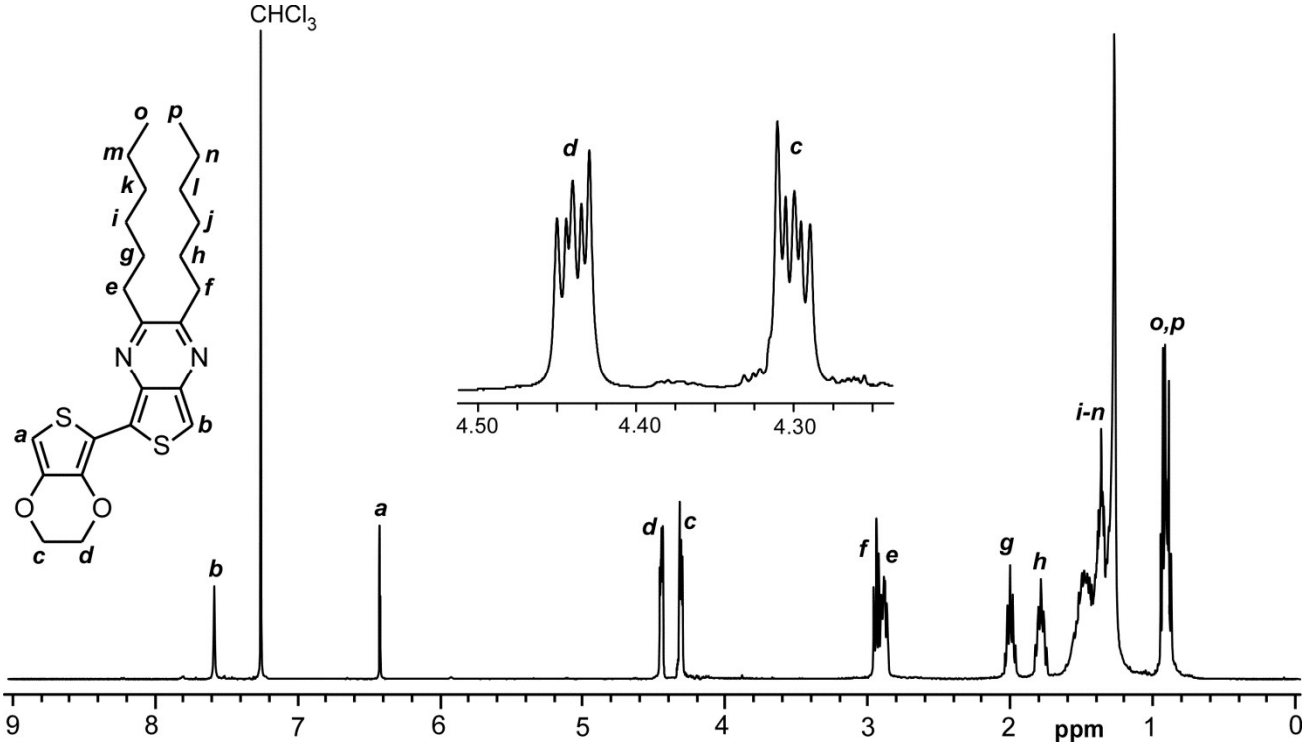


Figure S11. ^{1}H NMR spectrum of **EDOT-TP**

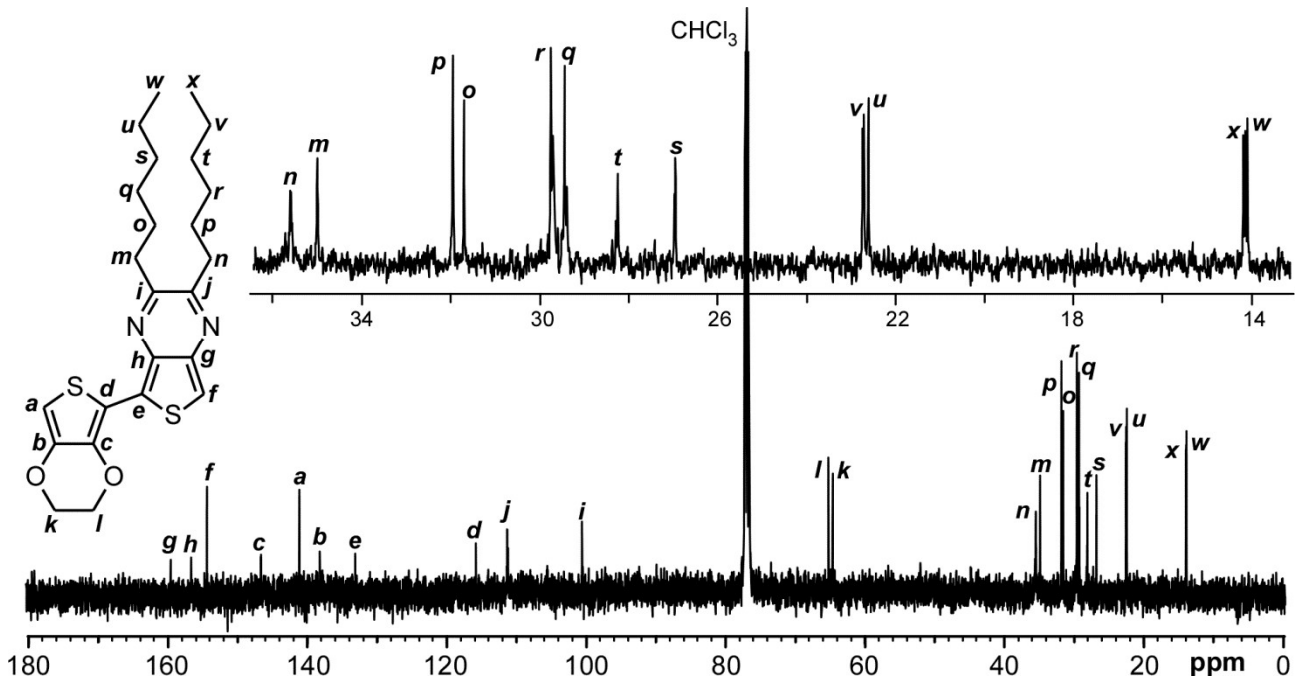


Figure S12. ^{13}C NMR spectrum of **EDOT-TP**

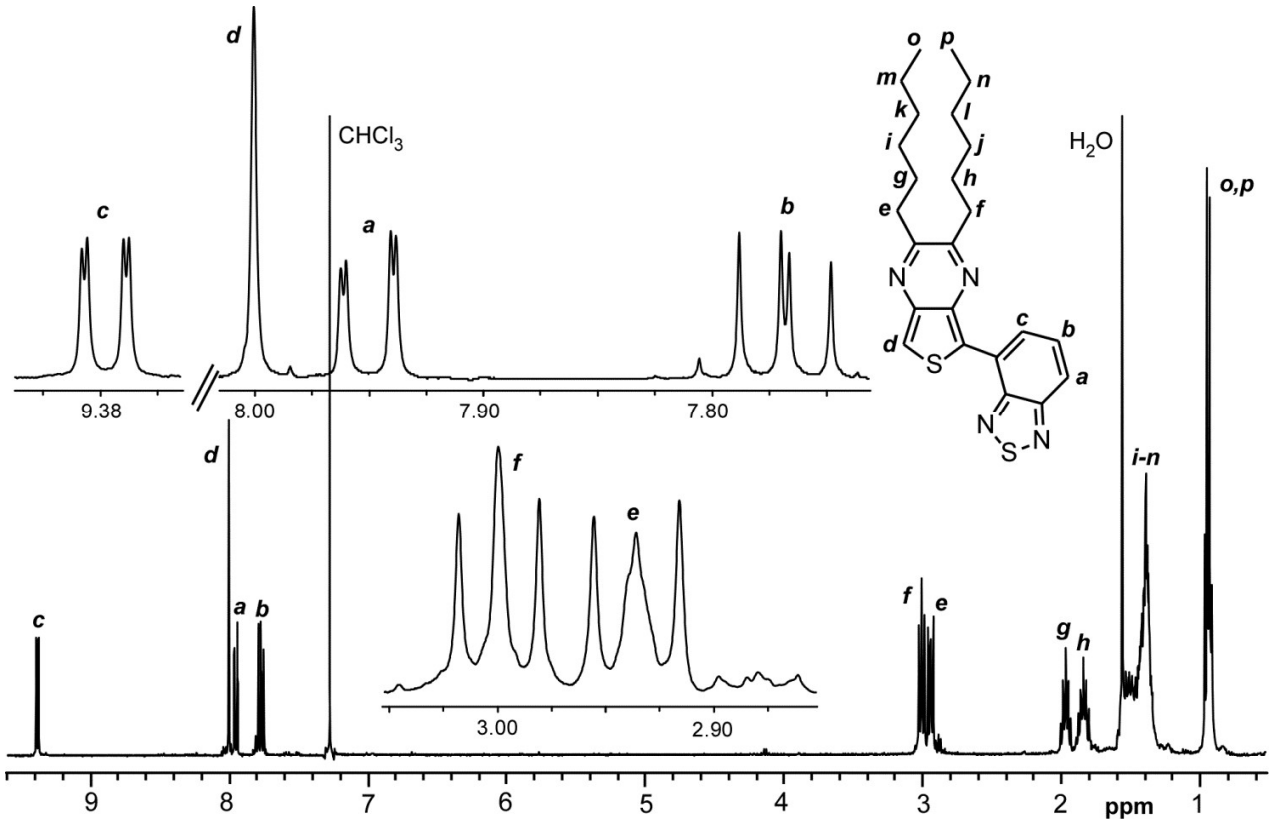


Figure S13. ^{1}H NMR spectrum of **TP-BTD**

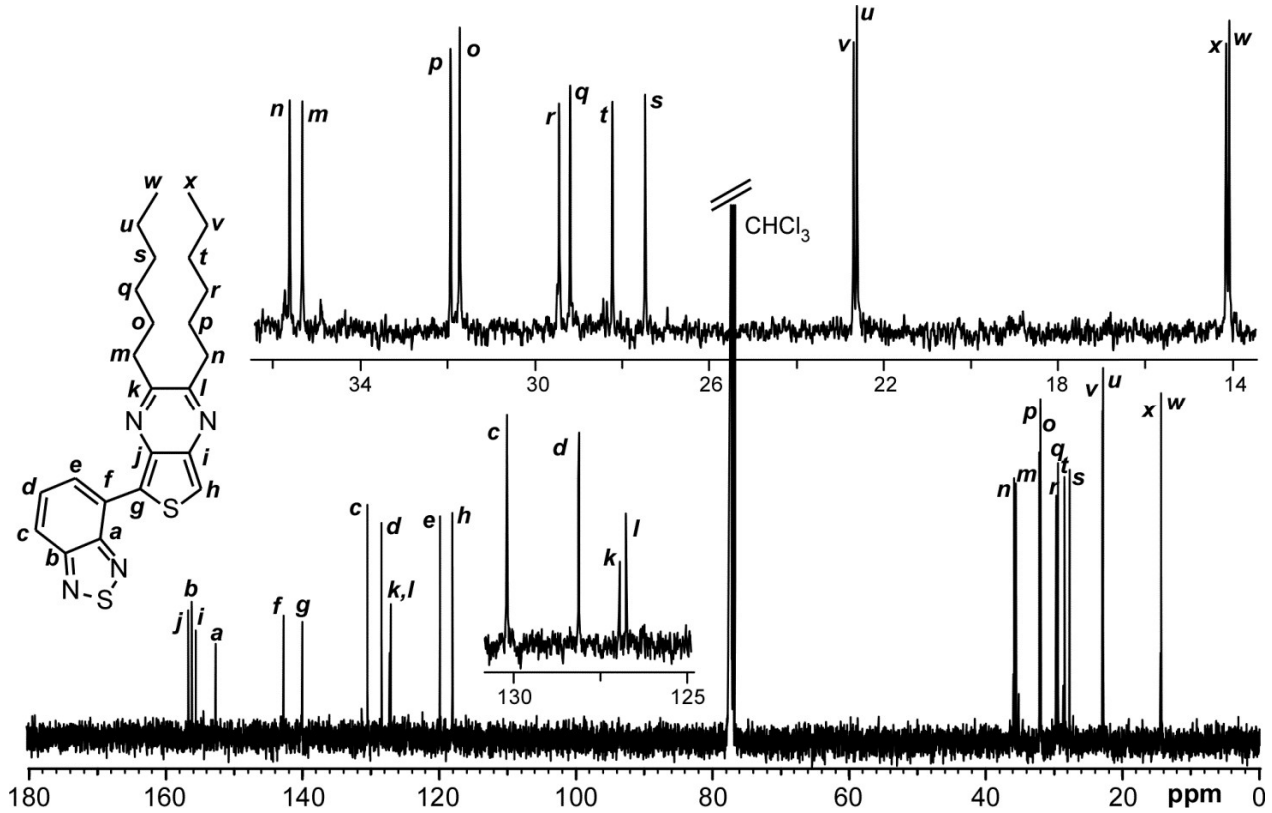


Figure S14. ^{13}C NMR spectrum of **TP-BTD**

Modeling of 2nd order coupling effects in the EDOT-containing dimers. To deconvolute the complex coupling of the ethylene bridge of the EDOT units, the experimentally determined coupling constants and chemical shifts were used to simulate the NMR spectrum. This was accomplished using a freely available NMR simulator[1] which could accurately model the 2nd order effects inherent from the close spacing of the coupled multiplets.[2] The resulting simulated spectra are directly compared to the experimental spectra in Figure S14.

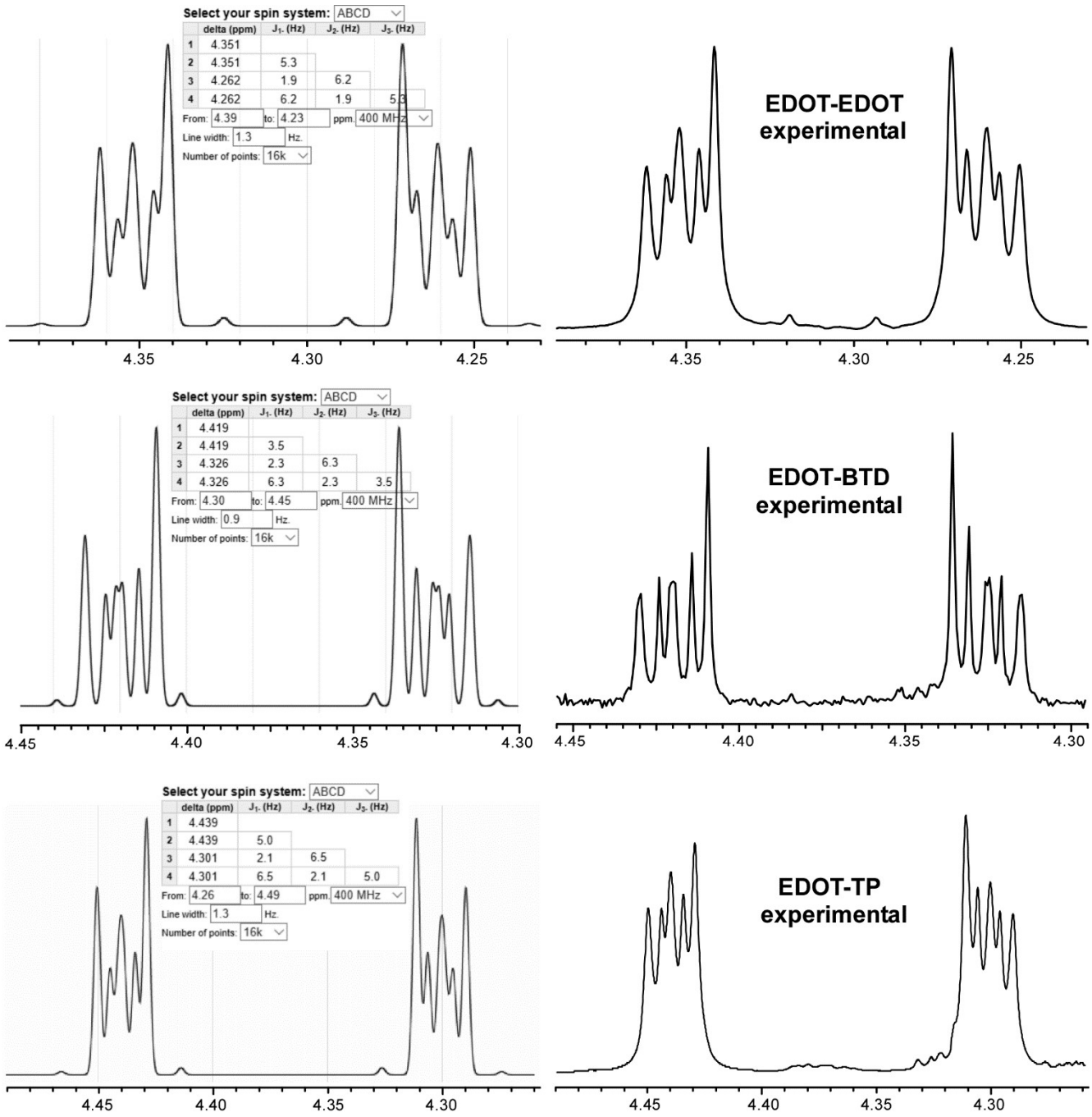


Figure S15. Comparison of results from modeling of 2nd order coupling effects in the ^{1}H NMR spectra of **EDOT-EDOT**, **EDOT-BTD**, and **EDOT-TP**.

X-ray Crystallography. X-ray quality crystals of **1** and **EDOT-BTD** were obtained by vapor diffusion with diethyl ether as the solvent and methanol as the antisolvent. The X-ray intensity data of the crystals were measured at either 273 or 100 K on a CCD-based X-ray diffractometer system equipped with a Cu X-ray tube (λ = 1.54178 Å) operated at 2000 W of power. The detector was placed at a distance of 5.047 cm from the crystal. Frames were collected with a scan width of 0.3° in ω and exposure time of 10 s/frame and then integrated with the Bruker SAINT software package using an arrow-frame integration algorithm. The unit cell was determined and refined by least-squares upon the refinement of XYZ-centeroids of reflections above 20σ(I). The structure was refined using the Bruker SHELXTL (Version 5.1) Software Package. The crystal data, data collection parameters, and refinement statistics are listed in Table S1. CCDC 2021170-2021171 contains the supplementary crystallographic data for this paper. These data can be obtained free of charge via http://www.ccdc.cam.ac.uk/conts/retrieving.html (or from the CCDC, 12 Union Road, Cambridge CB2 1EZ, UK; Fax: +44 1223 336033; E-mail: deposit@ccdc.cam.ac.uk).

Table S1. Crystallographic data for compounds **1** and **EDOT-BTD**.

	1	**EDOT-BTD**
CCDC	2021170	2021171
Chemical Formula	$C_6H_3BrN_2S$	$C_{12}H_8N_2O_2S_2$
Formula Weight	215.07	276.32
Temperature (K)	293.15	100(2)
Crystal System	triclinic	monoclinic
Space Group	P-1	P 1 21/c 1
a (Å)	7.1075(10)	3.8786(6)
b (Å)	7.1970(12)	21.357(2)
c (Å)	7.6350(10)	13.401(2)
α (º)	68.754(7)	90.00
β (º)	76.414(7)	96.283(10)
γ (º)	69.876(8)	90.00
V (Å^3)	339.06(9)	1103.4(3)
Z	2	4
D_{calc} (g cm^{-3})	2.107	1.663
μ (mm^{-1})	10.415	4.342
Final *R* indices [$I>2\sigma(I)$]	$R_1 = 0.0265$	$R_1 = 0.0817$
	$wR_2 = 0.0694$	$wR_2 = 0.1948$
R indices (all data)[a]	$R_1 = 0.0277$	$R_1 = 0.1251$
	$wR_2 = 0.0769$	$wR_2 = 0.2239$

[a] $R_1 = \Sigma(||F_o| - |F_c||) / \Sigma|F_o|$, $wR_2 = [\Sigma(w(F_o^2 - F_c^2)^2) / \Sigma(F_o^2)^2]^{1/2}$

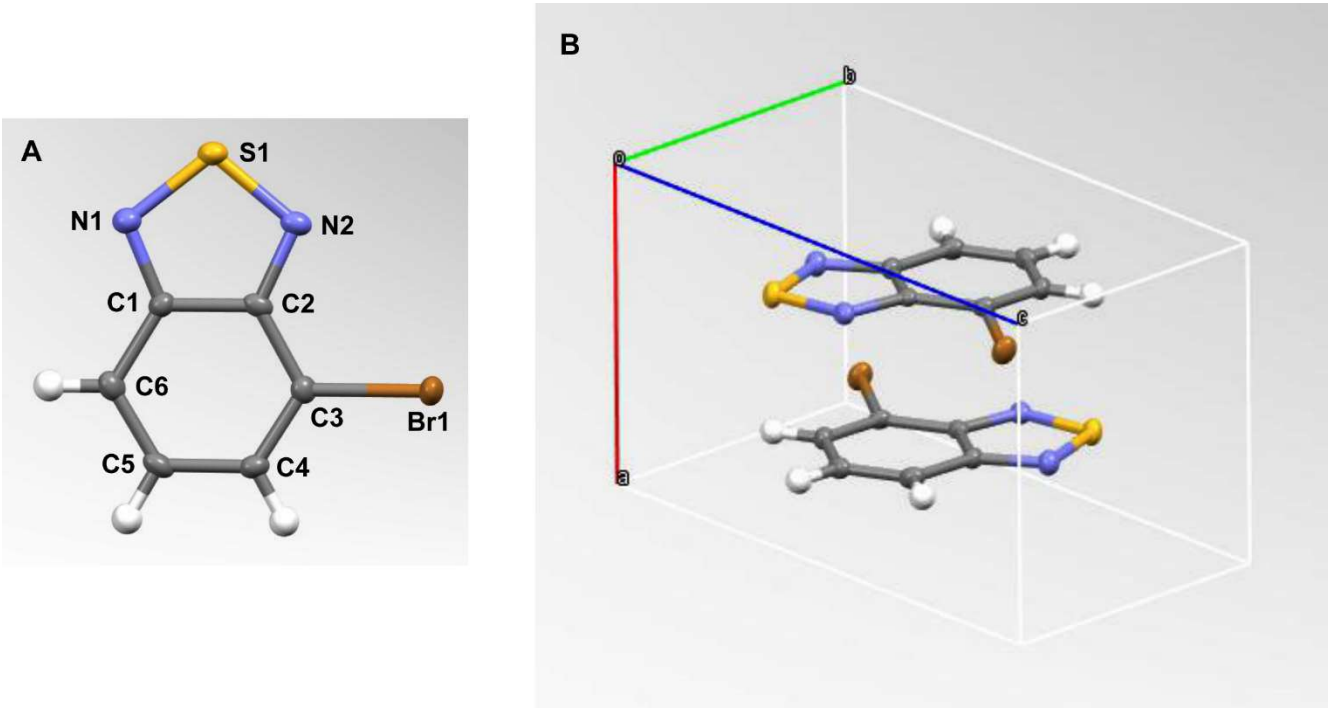


Figure S16. Thermal ellipsoid plot (50% probability level) and unit cell of **1**.

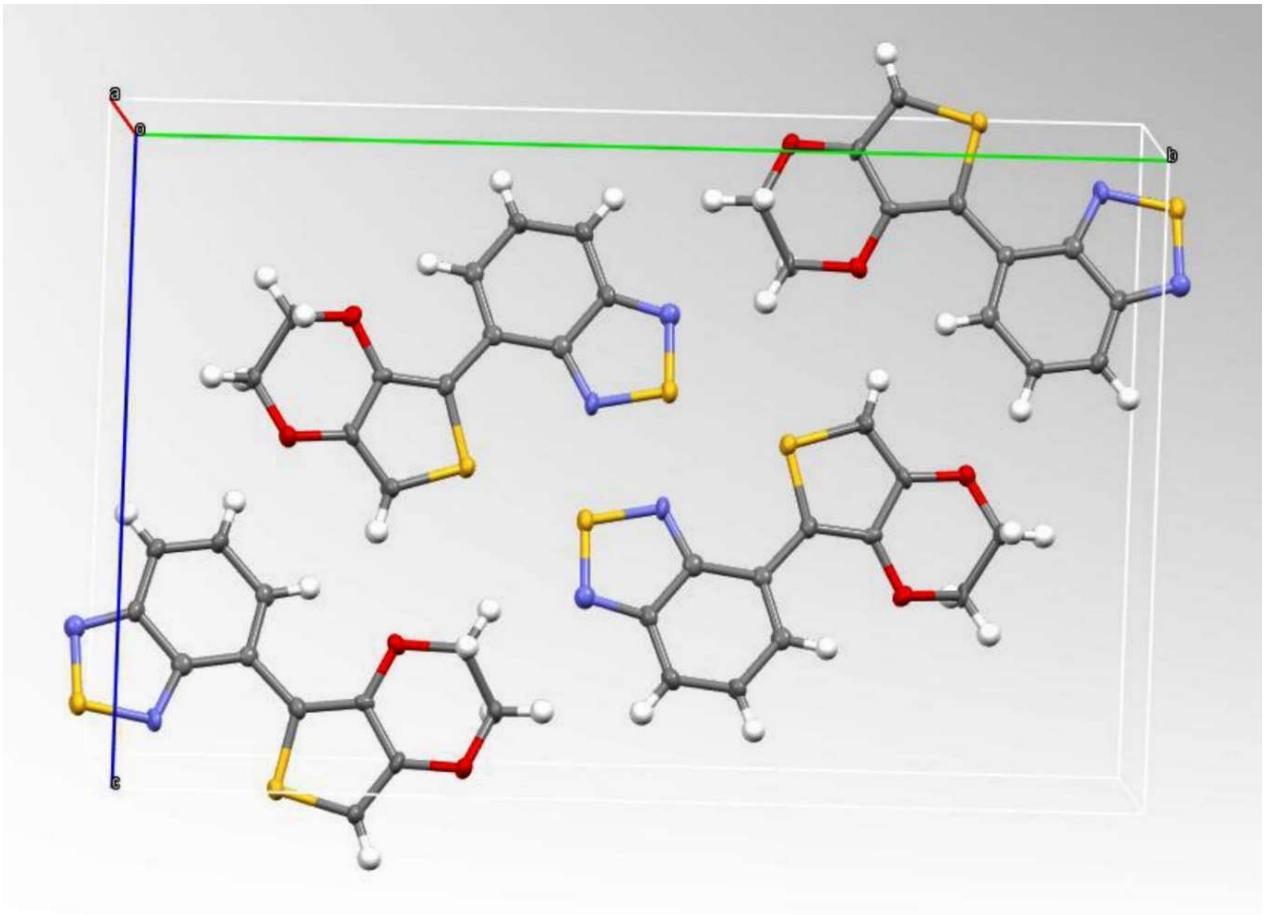


Figure S17. Unit cell of **EDOT-BTD** (thermal ellipsoids at the 50% probability level).

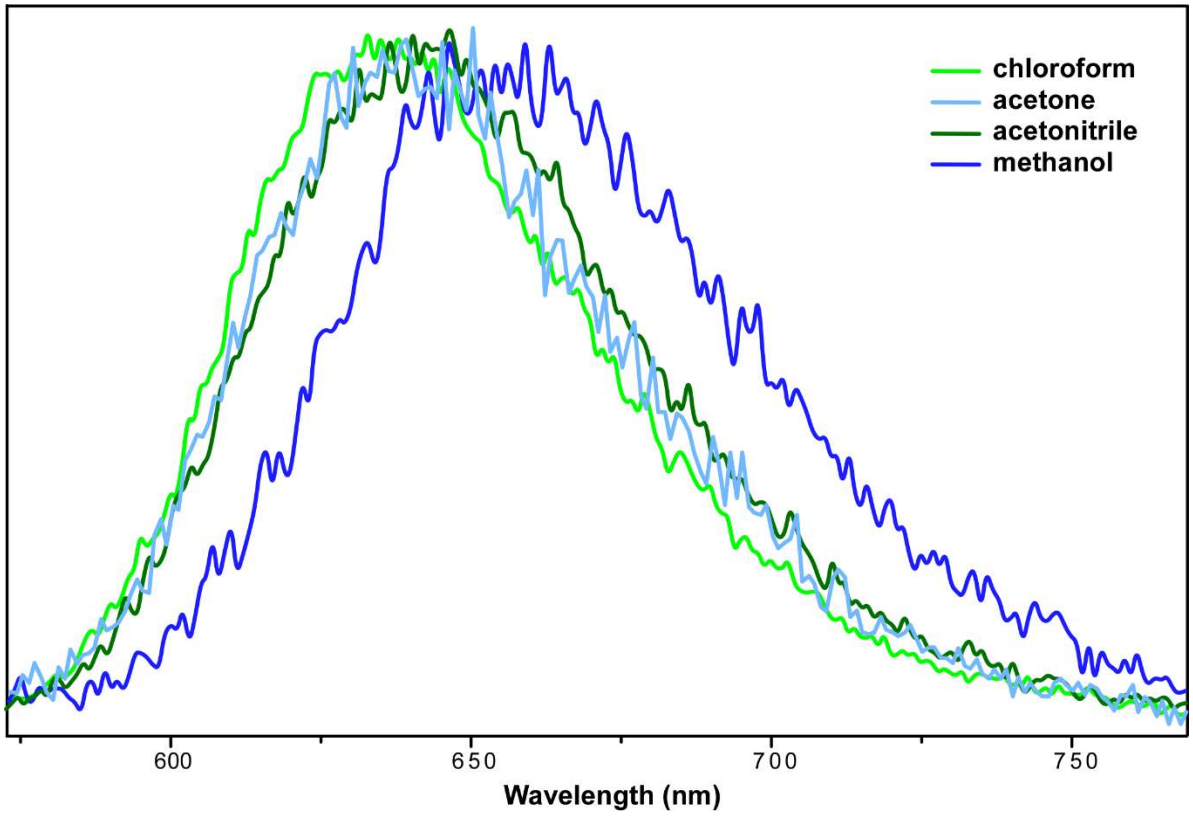


Figure S18. Solvatochromism in the emission spectra of BTD-BTD.

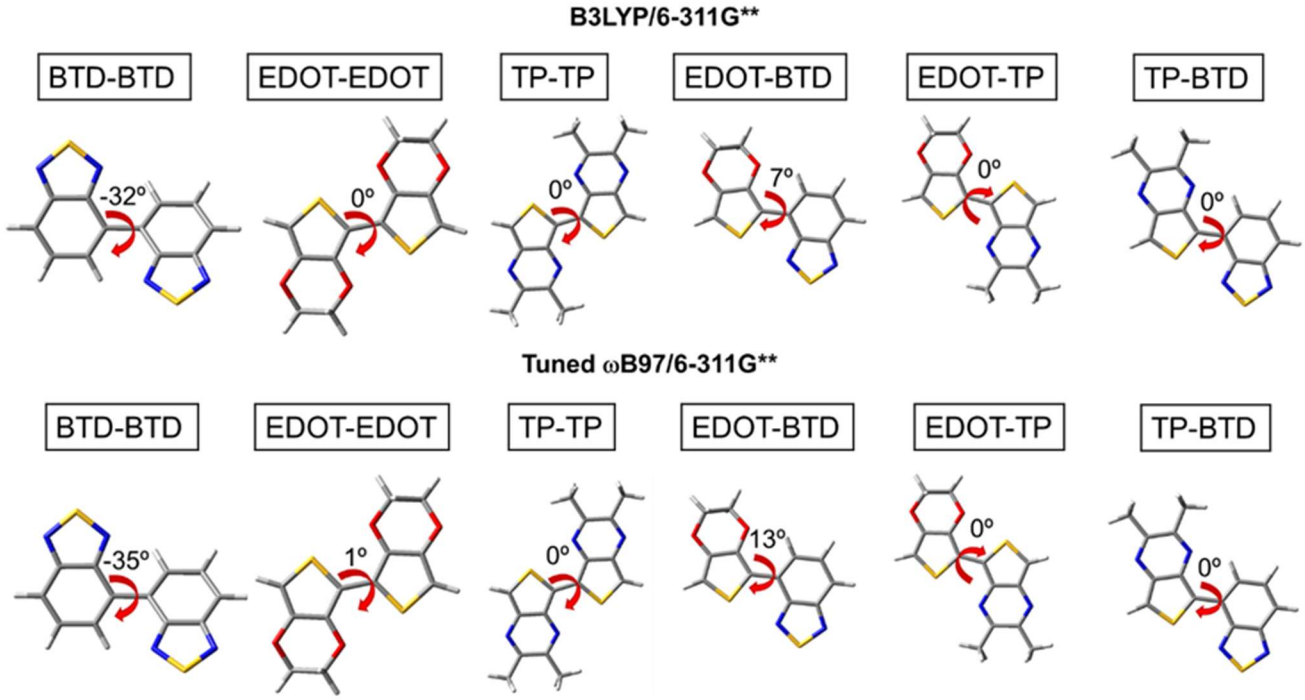
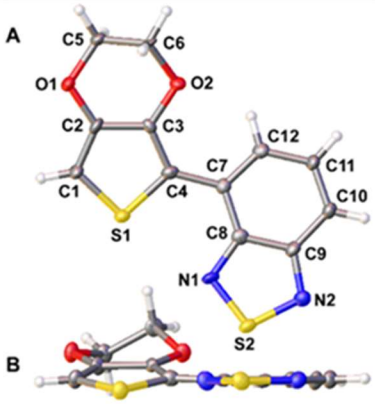


Figure S19. DFT-calculated interannular torsional angles

Table S2. Comparison of the experimental (averaged X-Ray) and DFT-calculated geometric parameters of EDOT-BTD.



Bond length (Å)	Exp.	B3LYP	ωB97
S(1)-C(1)	1.72	1.73	1.72
S(1)-C(4)	1.74	1.76	1.75
C(1)-C(2)	1.35	1.36	1.37
C(2)-C(3)	1.41	1.43	1.44
C(3)-C(4)	1.38	1.39	1.39
C(4)-C(7)	1.47	1.46	1.48
C(7)-C(8)	1.43	1.44	1.45
C(7)-C(12)	1.38	1.39	1.39
C(8)-C(9)	1.45	1.45	1.45
C(9)-C(10)	1.41	1.42	1.43
C(10)-C(11)	1.36	1.37	1.37
C(11)-C(12)	1.42	1.42	1.44
N(1)-C(8)	1.35	1.33	1.34
N(1)-S(2)	1.61	1.64	1.63
S(2)-N(2)	1.62	1.64	1.63
N(2)-C(9)	1.35	1.34	1.34

Bond angle (*)	Exp.	B3LYP	ωB97
C(1)-S(1)-C(4)	93	92	93
S(1)-C(1)-C(2)	111	112	112
C(1)-C(2)-C(3)	113	113	113
C(2)-C(3)-C(4)	114	114	114
S(1)-C(4)-C(3)	109	109	109
S(1)-C(4)-C(7)	123	123	123
C(4)-C(7)-C(8)	122	122	122
C(7)-C(8)-C(9)	121	121	121
N(1)-C(8)-C(9)	113	113	113
N(1)-S(2)-N(2)	101	100	100
S(2)-N(2)-C(9)	106	107	107
C(8)-C(9)-C(10)	121	121	121
C(9)-C(10)-C(11)	118	117	117
C(10)-C(11)-C(12)	122	123	123

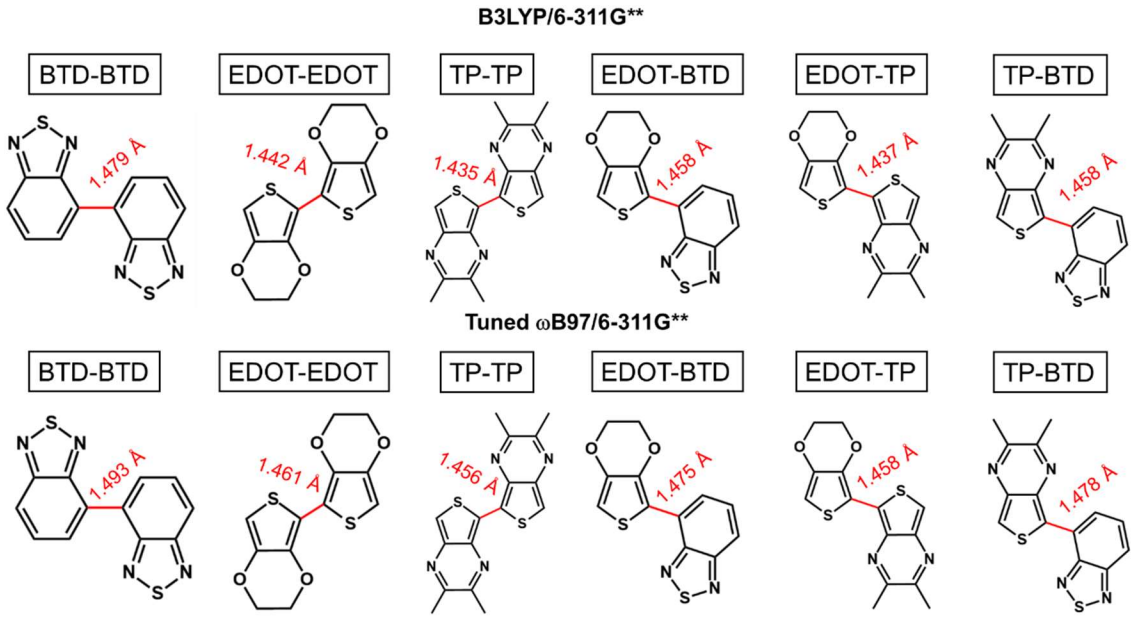


Figure S20. DFT-calculated interannular bond lengths.

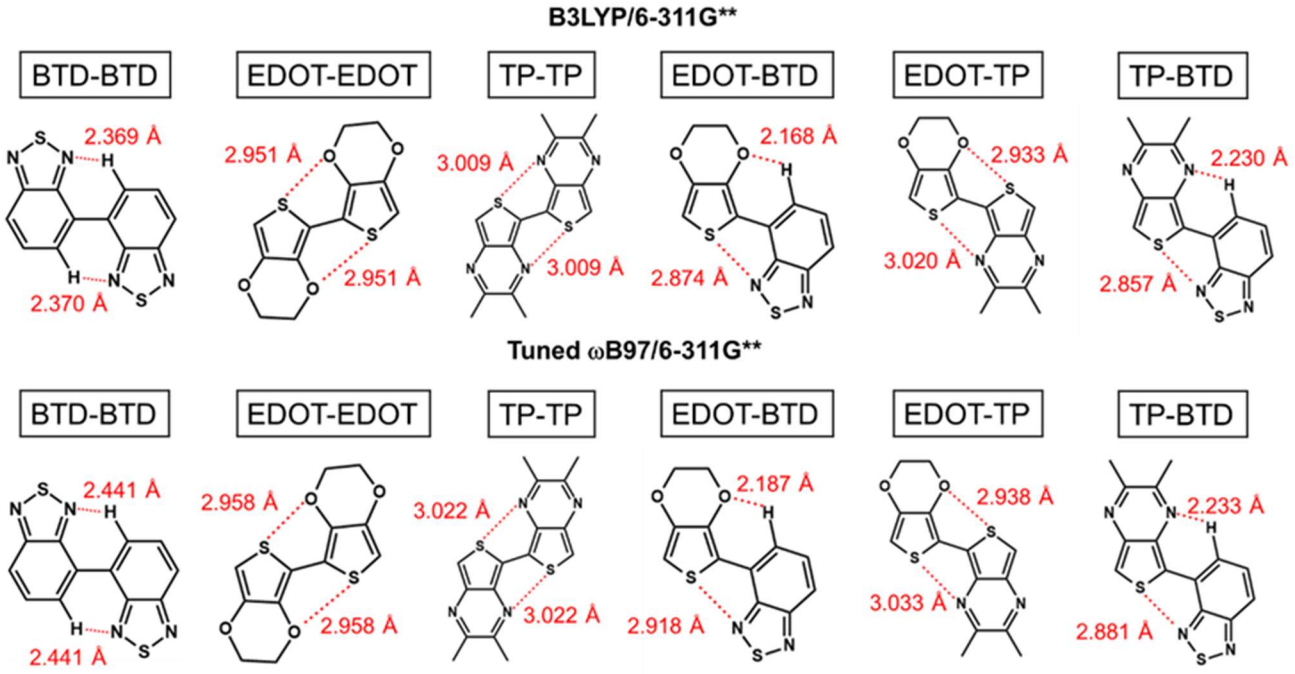


Figure S21. DFT-calculated intramolecular distances.

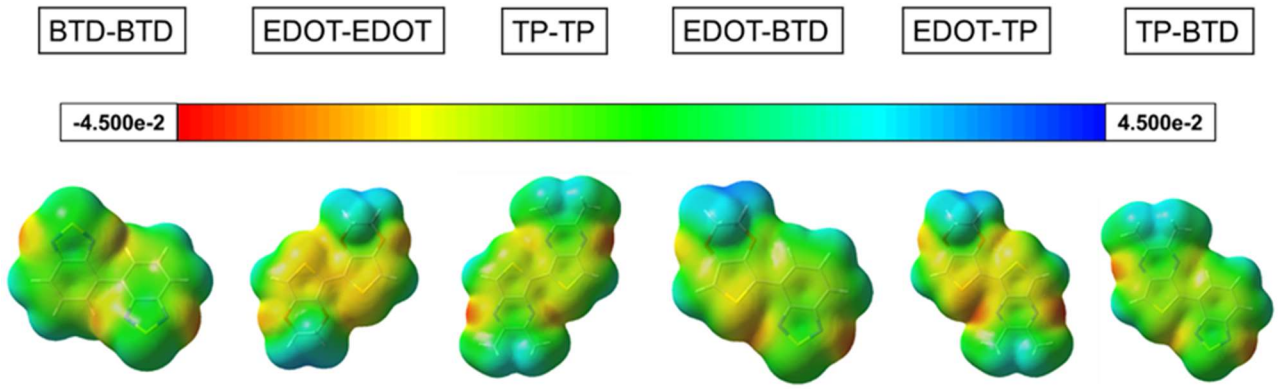


Figure S22. Electrostatic surface potentials (tuned ωB97/6-311G** level) for the dimer series of EDOT, TP and BTD units. Electrostatic potentials are scaled from negative (red) to positive (blue) values; green corresponds to neutral charge.

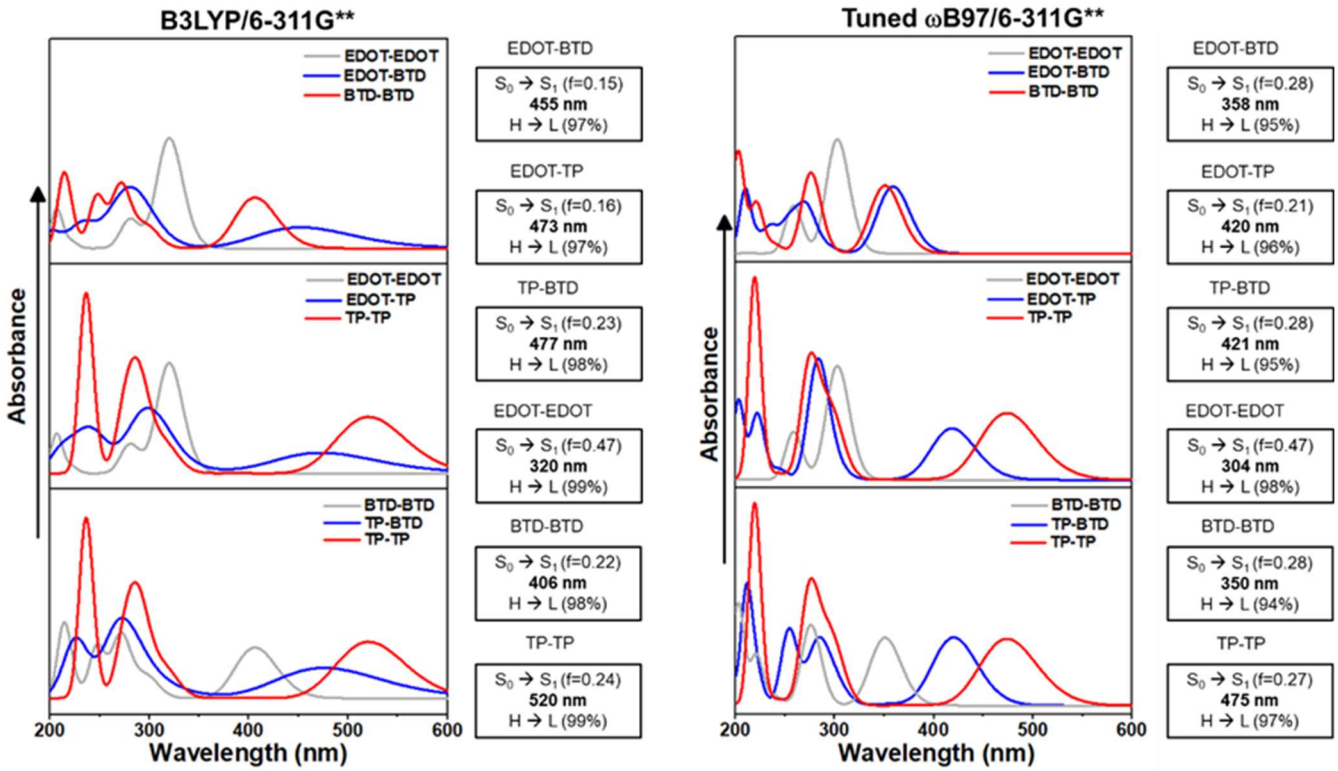


Figure S23. TD-DFT calculated absorption spectra

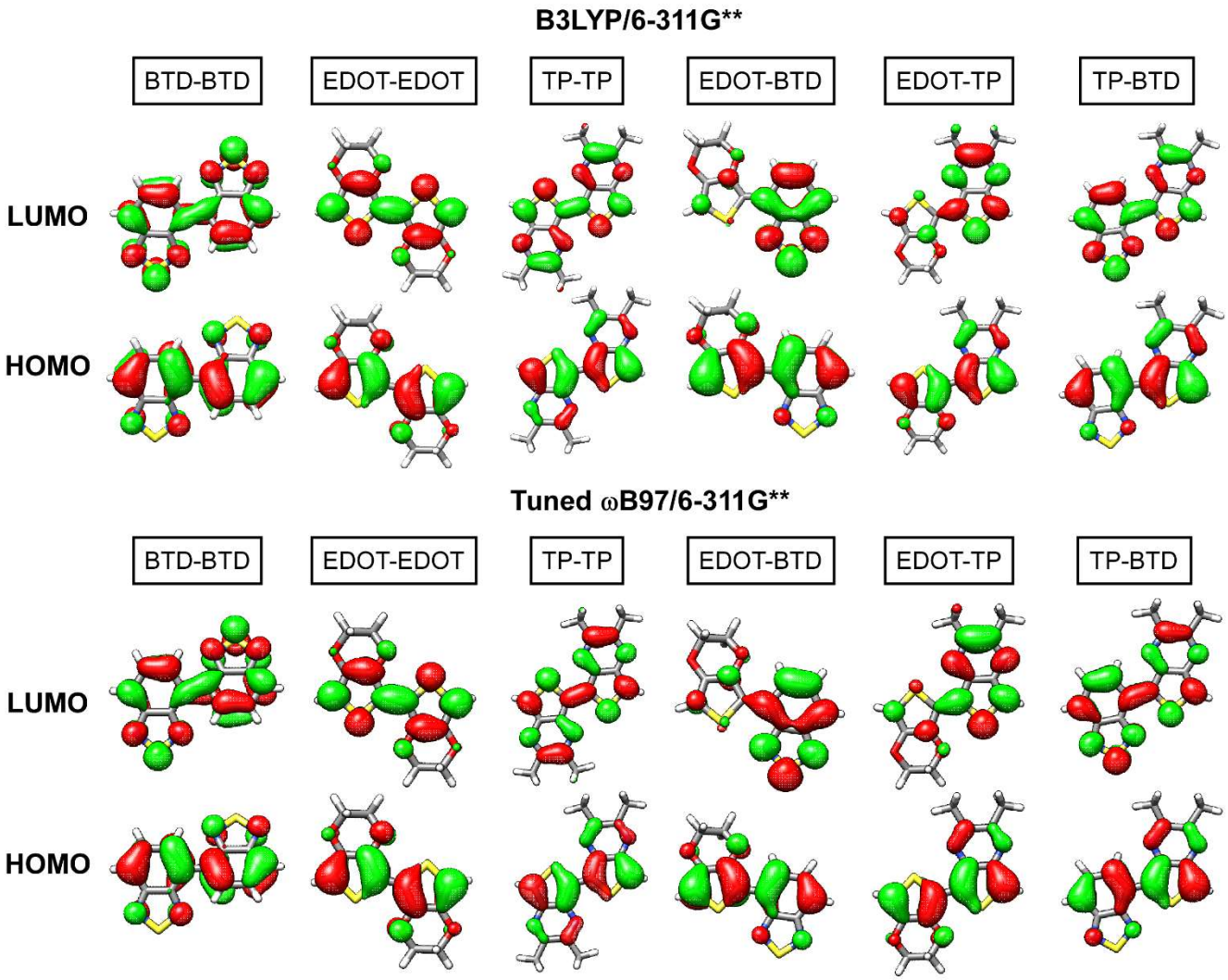


Figure S24. DFT-calculated frontier molecular orbital topologies (isovalue surface 0.03 a.u.).

Table S3. Tuned ω values ($bohr^{-1}$) for the symmetrical and asymmetrical dimers, at the ωB97/6-311G** level.

	ω values ($bohr^{-1}$)
BTD-BTD	0.2297
EDOT-EDOT	0.2339
TP-TP	0.2010
EDOT-BTD	0.2708
EDOT-TP	0.2232
TP-BTD	0.2125

Cartesian coordinates and energies of all calculated dimers at the B3LYP/6-311G level.**

BTD-BTD E_{el} (B3LYP/6-311G**) = -1476.44407570 a.u.

C	1.70441600	-2.60878800	0.69648800
C	0.55471200	-1.76696400	0.66600100
C	0.60333200	-0.42746800	0.33793600
C	1.90848400	0.09100000	0.00712000
C	3.07418800	-0.77752100	0.03085800
C	2.95264500	-2.14650300	0.38967600
N	2.20284000	1.34093400	-0.36170400
S	3.81693200	1.39222100	-0.64554000
N	4.20868800	-0.16272300	-0.31427000
C	-1.70419200	2.60867700	0.69655300
C	-0.55456800	1.76674800	0.66606200
C	-1.90851800	-0.09109300	0.00717200
C	-3.07415300	0.77755000	0.03094700
C	-2.95246400	2.14651900	0.38976800
N	-2.20300800	-1.34097500	-0.36166300
S	-3.81711300	-1.39204900	-0.64557800
N	-4.20871100	0.16291500	-0.31423100
C	-0.60330900	0.42725600	0.33805500
H	1.56788700	-3.64753100	0.97463300
H	-0.40060500	-2.20841500	0.90874500
H	3.83222200	-2.77661000	0.40717100
H	-1.56756200	3.64741900	0.97465000
H	0.40082400	2.20812000	0.90866700
H	-3.83197300	2.77672200	0.40724800

EDOT-BTD E_{el} (B3LYP/6-311G**) = -1518.59100507 a.u.

C	-0.59724100	-0.26063400	0.04978300
C	-1.91938600	0.14758000	-0.01482300
C	-2.86333700	-0.92202800	0.01139800
C	-2.27107800	-2.14602800	0.09101900
S	-0.54714900	-2.02168600	0.12600900
O	-2.32308600	1.45320600	-0.08979300
C	-3.68951300	1.60054100	-0.50750200
C	-4.58343700	0.63071300	0.24280200
O	-4.21529700	-0.71965200	-0.05588900
C	1.70584300	2.77835500	0.17868700
C	0.54608100	1.95350600	0.16750100
C	0.59946800	0.57131700	0.07197100
C	1.92691000	0.01102100	-0.00370700
C	3.10429200	0.86236600	0.01135700
C	2.97447000	2.27293300	0.10220700
N	2.22322000	-1.28538000	-0.08771400
S	3.85882200	-1.40529500	-0.14367000
N	4.25246600	0.18342100	-0.06356400
H	-2.75822300	-3.10734700	0.12030700
H	-3.96005400	2.63461300	-0.29291400
H	-3.76024400	1.42324800	-1.58652900

H	-5.62344200	0.74024400	-0.06605800
H	-4.50765100	0.80645300	1.32274600
H	1.56118000	3.85041600	0.25440800
H	-0.41734400	2.43405500	0.23842200
H	3.85782400	2.89743600	0.11242300

EDOT-EDOT E_{el} (B3LYP/6-311G**) = -1560.73527605 a.u.

C	0.60849000	-0.38678800	-0.00632900
C	1.90700100	0.07091000	-0.00477000
C	2.89257400	-0.96162500	0.00231200
C	2.35110800	-2.21123800	0.00633600
S	0.61547400	-2.14871600	0.00170800
O	2.23868500	1.39870100	-0.02396600
C	3.60207900	1.63196600	0.35604800
C	4.52671100	0.65978800	-0.35675700
O	4.23391600	-0.69119000	0.02164500
C	-1.90700400	-0.07094100	-0.00462700
C	-2.89254900	0.96163200	0.00239300
C	-2.35106800	2.21123400	0.00629400
S	-0.61545400	2.14869900	0.00167500
O	-2.23870300	-1.39870200	-0.02372100
C	-3.60220200	-1.63202600	0.35582500
C	-4.52666000	-0.65964800	-0.35692700
O	-4.23390200	0.69120000	0.02189700
C	-0.60848200	0.38675600	-0.00626500
H	2.87066100	-3.15528000	0.01246900
H	3.82361100	2.66176000	0.07509600
H	3.70289000	1.52230300	1.44210500
H	5.56596200	0.83565600	-0.07709100
H	4.42185100	0.77016300	-1.44278700
H	-2.87065700	3.15526100	0.01210300
H	-3.82369200	-2.66173500	0.07451000
H	-3.70331400	-1.52269800	1.44188800
H	-5.56595800	-0.83561400	-0.07748700
H	-4.42162700	-0.76974600	-1.44297100

EDOT-TP E_{el} (B3LYP/6-311G**) = -1597.24787072 a.u.

C	1.01360600	-0.32182400	-0.00014300
C	2.35666500	-0.00726000	0.00897800
C	3.22366700	-1.13886200	0.01797600
C	2.54498200	-2.31994600	0.02022000
S	0.82485200	-2.07370500	0.01061600
O	2.82554500	1.27628600	-0.00358900
C	4.21244900	1.36475500	0.36012300
C	5.02038700	0.29341900	-0.35237200
O	4.58649100	-1.01488500	0.03900900
C	-0.10304800	0.58313700	-0.01150000
C	-1.46747700	0.28074500	-0.00809900
C	-2.31958700	1.43982600	-0.01677600
C	-1.60928800	2.62073600	-0.02960200
S	0.08502900	2.31961100	-0.03015900

N	-1.98855300	-0.97689900	0.00233600
C	-3.29329800	-1.08132400	0.00507700
C	-4.15885300	0.09635800	-0.00243600
N	-3.68262700	1.31369100	-0.01315000
C	-5.65615000	-0.06351400	0.00176900
C	-3.88626500	-2.46448100	0.01622000
H	2.95948300	-3.31496900	0.02701500
H	4.53902300	2.36295200	0.06823600
H	4.31024100	1.25320100	1.44587700
H	6.07447800	0.35913900	-0.08117000
H	4.91994200	0.40674400	-1.43852500
H	-1.99274700	3.62825100	-0.03882700
H	-5.99859600	-0.60957700	0.88669800
H	-6.11683100	0.92312300	-0.00518900
H	-6.00211200	-0.62362800	-0.87294700
H	-3.08223800	-3.19882200	0.02033100
H	-4.51532500	-2.62367100	0.89812900
H	-4.51817400	-2.63657900	-0.86121400

TP-BTD E_{el} (B3LYP/6-311G**) = -1555.10217548 a.u.

C	1.47454400	0.18159700	0.00011300
C	2.27918500	1.37486700	0.00016500
C	1.52044700	2.52787500	0.00036600
S	-0.15013800	2.16909400	0.00052300
N	2.07462900	-1.04540700	-0.00020800
C	3.38408400	-1.07858000	-0.00036400
C	4.18930300	0.13642300	-0.00020800
N	3.64389600	1.32444400	0.00002100
C	5.69271500	0.05858200	-0.00030900
C	4.04881000	-2.42890000	-0.00056600
C	0.09163300	0.43748300	0.00031500
C	-1.88726200	-2.82066900	0.00067700
C	-0.81973100	-1.88057300	0.00068100
C	-1.01833800	-0.50825200	0.00031100
C	-2.39766100	-0.08443500	-0.00004300
C	-3.47986900	-1.05390300	-0.00003500
C	-3.20313300	-2.44608000	0.00033300
N	-2.82921600	1.17614500	-0.00035900
S	-4.47067300	1.12665100	-0.00066100
N	-4.69365200	-0.49599800	-0.00039000
H	1.87246200	3.54732100	0.00074100
H	6.06716900	-0.47541800	0.87892500
H	6.06707000	-0.47303300	-0.88104900
H	6.09859200	1.06900200	0.00096400
H	3.28734500	-3.20727200	-0.00185900
H	4.68863100	-2.55888300	-0.87934800
H	4.68666100	-2.56001400	0.87950500
H	-1.63125700	-3.87434300	0.00097500
H	0.19584600	-2.24784200	0.00095800
H	-4.01751400	-3.15832600	0.00032200

TP-TP E_{el} (B3LYP/6-311G**) = -1633.76016553 a.u.

C	-0.40677500	0.59081300	-0.00011800
C	0.00595900	1.92789000	-0.00000900
C	-1.07900100	2.87017000	-0.00004200
C	-2.31247500	2.25300100	-0.00016200
S	-2.15362600	0.54036800	-0.00016600
N	1.30102600	2.34533100	0.00011600
C	1.51013700	3.63857400	0.00019500
C	0.40677500	4.59592000	0.00011300
N	-0.84511600	4.21772400	0.00002800
C	0.68579300	6.07552400	0.00009600
C	2.93621700	4.11812100	0.00016100
H	-3.28544900	2.71804300	-0.00021400
H	1.26417500	6.37462300	-0.87997500
H	-0.26094500	6.61341900	0.00025100
H	1.26455300	6.37473000	0.87986400
H	3.60444700	3.25838200	0.00084600
H	3.15144100	4.73295400	-0.87982700
H	3.15115400	4.73423800	0.87929700
C	0.40677500	-0.59081300	-0.00011800
C	-0.00595900	-1.92789000	-0.00000900
S	2.15362600	-0.54036800	-0.00016600
C	1.07900100	-2.87017000	-0.00004200
N	-1.30102600	-2.34533100	0.00011600
C	2.31247500	-2.25300100	-0.00016200
N	0.84511600	-4.21772400	0.00002800
C	-1.51013700	-3.63857400	0.00019500
H	3.28544900	-2.71804300	-0.00021400
C	-0.40677500	-4.59592000	0.00011300
C	-2.93621700	-4.11812100	0.00016100
C	-0.68579300	-6.07552400	0.00009600
H	-3.60444700	-3.25838200	0.00084600
H	-3.15144100	-4.73295400	-0.87982700
H	-3.15115400	-4.73423800	0.87929700
H	-1.26417500	-6.37462300	-0.87997500
H	0.26094500	-6.61341900	0.00025100
H	-1.26455300	-6.37473000	0.87986400

Cartesian coordinates and energies of all calculated dimers at the optimally tuned ωB97/6-311G level.**

BTD-BTD E_{el} (tuned ωB97/6-311G**) = -1476.53989483 a.u.

C	1.74126100	-2.60647200	0.76584700
C	0.57243400	-1.76630200	0.73909300
C	0.61033400	-0.42948700	0.37657100
C	1.91254600	0.09654300	0.00740500
C	3.08716000	-0.76039700	0.02836400
C	2.98640000	-2.13591400	0.42239000
N	2.18603000	1.35499600	-0.39546400
S	3.79346100	1.40357200	-0.70698000
N	4.21992400	-0.13655200	-0.35429300
C	-1.74124300	2.60645800	0.76593100
C	-0.57241700	1.76628800	0.73913600

C	-1.91254600	-0.09654400	0.00744500
C	-3.08716000	0.76039600	0.02844500
C	-2.98639000	2.13590700	0.42249300
N	-2.18604000	-1.35498900	-0.39544000
S	-3.79347700	-1.40355800	-0.70692300
N	-4.21993200	0.13655900	-0.35419600
C	-0.61032500	0.42947900	0.37659200
H	1.61924200	-3.64876900	1.07093000
H	-0.38541800	-2.21019200	1.01298300
H	3.88024600	-2.76148500	0.43592200
H	-1.61921600	3.64875000	1.07103000
H	0.38544200	2.21017200	1.01301200
H	-3.88023500	2.76147800	0.43605700

EDOT-BTD E_{el} (tuned ωB97/6-311G**) = -1518.58894974 a.u.

C	0.60643600	-0.27141400	-0.09526900
C	1.92250900	0.15476100	0.01803300
C	2.88081700	-0.91591200	-0.02923100
C	2.28682900	-2.14080500	-0.17604700
S	0.57002200	-2.01417400	-0.24247800
O	2.30884200	1.46878600	0.15774400
C	3.66698400	1.58651700	0.63066700
C	4.58913500	0.65928900	-0.15298100
O	4.23797500	-0.71530300	0.08132700
C	-1.72461300	2.77722400	-0.28763500
C	-0.55160400	1.94377500	-0.27506700
C	-0.60635500	0.56763500	-0.12338100
C	-1.93732200	0.00315600	0.00908400
C	-3.11405600	0.85010700	-0.00944400
C	-2.99157400	2.27045500	-0.15861900
N	-2.23154500	-1.29871500	0.15174100
S	-3.85706400	-1.40570900	0.25110100
N	-4.26482600	0.16829100	0.12124100
H	2.77850100	-3.10761600	-0.23132600
H	3.94623300	2.63839400	0.48729000
H	3.70282100	1.33783500	1.70525500
H	5.63006800	0.77045100	0.17802300
H	4.52105100	0.88421000	-1.23223100
H	-1.58266500	3.85354700	-0.40941600
H	0.41891900	2.42317800	-0.39015200
H	-3.88531200	2.89449900	-0.16949800

EDOT-EDOT E_{el} (tuned ωB97/6-311G**) = -1560.77814074 a.u.

C	0.61746600	0.39086900	0.00446500
C	1.91923600	-0.08000100	0.00899000
C	2.91152200	0.96234900	-0.00522700
C	2.35539200	2.21709400	-0.02116700
S	0.62346000	2.14282300	-0.01828700
O	2.24446800	-1.41969200	0.03732400
C	3.61994500	-1.63797700	-0.34815200
C	4.54250600	-0.65954800	0.37807200

O	4.26506700	0.70061400	-0.01852500
C	-1.91923600	0.07999900	0.00903800
C	-2.91152200	-0.96234900	-0.00516400
C	-2.35539300	-2.21709400	-0.02116300
S	-0.62346000	-2.14281900	-0.01858100
O	-2.24446700	1.41968900	0.03745900
C	-3.61996400	1.63799000	-0.34793700
C	-4.54248500	0.65953300	0.37830100
O	-4.26507000	-0.70061500	-0.01836200
C	-0.61746600	-0.39087000	0.00444100
H	2.87172400	3.17274300	-0.03233800
H	3.85012700	-2.67620100	-0.07247000
H	3.72018100	-1.51434200	-1.44148500
H	5.59335600	-0.84371300	0.11454400
H	4.41403300	-0.76179300	1.47109700
H	-2.87172500	-3.17274300	-0.03231400
H	-3.85013000	2.67620400	-0.07219900
H	-3.72026000	1.51440000	-1.44126800
H	-5.59334900	0.84370900	0.11484000
H	-4.41394900	0.76173600	1.47132200

EDOT-TP E_{el} (tuned ωB97/6-311G**) = -1597.32984420 a.u.

C	1.02611100	0.32746200	0.00116700
C	2.37408400	-0.00025700	-0.00651200
C	3.24789300	1.14210200	-0.01878800
C	2.55489100	2.32791000	-0.02500900
S	0.83885600	2.07122800	-0.01449600
O	2.83834000	-1.29747200	0.00895100
C	4.23524300	-1.36824600	-0.36610800
C	5.04366600	-0.29445000	0.36273300
O	4.62270600	1.02773500	-0.03822000
C	-0.10905000	-0.58837700	0.01188500
C	-1.47931300	-0.27851100	0.00850300
C	-2.33171100	-1.44393900	0.01559200
C	-1.60716000	-2.62982700	0.02707800
S	0.08212100	-2.31571500	0.02766400
N	-1.99832300	0.99891400	-0.00066900
C	-3.31228500	1.08732300	-0.00329500
C	-4.18275100	-0.10325700	0.00301800
N	-3.71187100	-1.33240000	0.01228500
C	-5.68924200	0.06509400	-0.00085000
C	-3.92257300	2.47406200	-0.01298500
H	2.96504300	3.33419100	-0.03395600
H	4.57164600	-2.37579100	-0.08543700
H	4.32702400	-1.23761700	-1.45918100
H	6.10918400	-0.36553700	0.10300100
H	4.92320600	-0.40822200	1.45574300
H	-1.98519800	-3.64887800	0.03527800
H	-6.02767100	0.61899400	-0.89226700
H	-6.15728400	-0.92736400	0.00428000
H	-6.03105600	0.62965700	0.88255200
H	-3.11789500	3.22015700	-0.01620800
H	-4.55663000	2.62546400	-0.90244300

H	-4.55982300	2.63651100	0.87223200

TP-BTD E_{el} = -1555.23325861 a.u.

C	-1.52432100	-2.54077300	-0.00073600
C	-2.29475400	-1.38093500	-0.00011200
S	0.14358000	-2.17199200	-0.00102200
C	-1.48679800	-0.18186700	0.00001100
N	-3.67596200	-1.34365200	0.00033900
C	-0.09660300	-0.44627800	-0.00050100
N	-2.08454200	1.06545100	0.00061200
C	-4.21520200	-0.14156600	0.00090000
C	1.02992300	0.51129400	-0.00072200
C	-3.40366200	1.08514800	0.00104900
C	-5.72873200	-0.05373600	0.00139500
C	0.82731600	1.88973000	-0.00142200
C	2.41907500	0.08209600	-0.00021600
C	-4.08312800	2.44012300	0.00172400
H	-6.09837100	0.48590200	0.88936600
H	-6.09891800	0.48653900	-0.88596000
H	-6.14336700	-1.06983900	0.00116000
C	1.90653900	2.83995500	-0.00160800
H	-0.19835400	2.25995600	-0.00176400
C	3.50416900	1.05273800	-0.00042900
N	2.85321200	-1.19411800	0.00045600
H	-3.32041800	3.22932200	0.00188000
H	-4.72686800	2.56329500	-0.88525100
H	-4.72650700	2.56259600	0.88905800
C	3.23031500	2.45993300	-0.00113800
H	1.64914700	3.90267100	-0.00216500
N	4.73183100	0.49095700	0.00009200
S	4.49417600	-1.13111300	0.00078600
H	4.05452300	3.17491100	-0.00129300
H	-1.87156000	-3.57130200	-0.00092800

TP-TP E_{el} (tuned ωB97/6-311G**) = -1633.91913157 a.u.

C	0.01159900	0.72862200	-0.00001000
C	-1.08128700	1.61687700	0.00007100
C	-0.69170800	3.00815600	-0.00013100
C	0.69170800	3.16711100	-0.00039700
S	1.49268500	1.64527200	0.00014100
N	-2.40605300	1.23590900	0.00019400
C	-3.28946800	2.21764100	0.00015400
C	-2.89105900	3.63688100	-0.00002900
N	-1.62995400	4.02523600	-0.00018000
C	-3.95256300	4.72069500	-0.00017700
C	-4.75761200	1.83936600	0.00022300
H	1.25996100	4.09428000	-0.00065200
H	-4.60291100	4.64465000	0.88753100
H	-3.45944700	5.70126600	-0.00034600
H	-4.60296400	4.64437100	-0.88782500
H	-4.84859600	0.74551400	0.00031700

H	-5.27378800	2.24308600	0.88757500
H	-5.27384400	2.24293900	-0.88716400
C	-0.01159900	-0.72862200	-0.00001000
C	1.08128700	-1.61687700	0.00007100
S	-1.49268500	-1.64527200	0.00014100
C	0.69170800	-3.00815600	-0.00013100
N	2.40605300	-1.23590900	0.00019400
C	-0.69170800	-3.16711100	-0.00039700
N	1.62995400	-4.02523600	-0.00018000
C	3.28946800	-2.21764100	0.00015400
H	-1.25996100	-4.09428000	-0.00065200
C	2.89105900	-3.63688100	-0.00002900
C	4.75761200	-1.83936600	0.00022300
C	3.95256300	-4.72069500	-0.00017700
H	4.84859600	-0.74551400	0.00031700
H	5.27378800	-2.24308600	0.88757500
H	5.27384400	-2.24293900	-0.88716400
H	4.60291100	-4.64465000	0.88753100
H	3.45944700	-5.70126600	-0.00034600
H	4.60296400	-4.64437100	-0.88782500

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2. Castillo, A. M.; Patiny, L.; Wist, J. Fast and accurate algorithm for the simulation of NMR for large spin systems. *J. Mag. Res.* **2011**, *209*, 123-130. [10.1016/j.jmr.2010.12.008]