Supplementary Data:

One-pot Syntheses of 4,8-Dialkylbenzo[1,2-b:4,5-b′]dithiophenes

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Single-Crystal X-ray Analysis of DM-BDT. A pale yellow, block-like crystal of dimensions 0.25 x 0.15 x 0.10 mm^3 was secured to a cryoloop using Paratone Oil and placed into the liquid nitrogen stream of a Bruker SMART 1K diffractometer. Data were collected using graphite monochromated Mo-K_α radiation (λ = 0.71073 Å) at 203 K in four independent wedges of 606 frames each at phi angles of 0, 90, 180 and 270°. A final set of 50 frames at φ = 0° was collected to evaluate the single crystal for indications of decay. No appreciable decay was found to have occurred after comparison of measured intensities. All 2474 frames were collected at a width of 0.3°. Data collection and initial indexing were handled using SMART.[1] Frame integration, Lorentz-polarization corrections, and final cell parameter calculations were carried out using SAINT.[2] Multi-scan absorption corrections were performed using SADABS.[3] Space groups were unambiguously assigned by analysis of symmetry and systematic absences determined by XPREP and further verified by PLATON.[4,5] The structure was solved using direct methods and difference Fourier techniques. All hydrogen atoms were attached via the riding model at calculated positions. The final structural refinement included anisotropic temperature factors on all non-hydrogen atoms. Structure solution, refinement, graphics, and creation of publication material were performed using SHELXS, SHELXL and XSEED.[6-8]

References

1) *SMART*, *Software for the CCD Detector System*, version 5.050 (NT); Bruker Analytical X-ray Systems: Madison, WI, 1998.

2) *SAINT*, *Software for the CCD Detector System*, version 5.01 (NT); Bruker Analytical X-ray Systems: Madison, WI, 1998.

3) Blessing RH *SADABS*, *Program for absorption corrections using Siemens CCD based on the method of Robert Blessing*: *Acta Cryst.* **1995**, A51, 33.

4) G.M. Sheldrick, XPREP, *Program for Space Group Determination*; University of Göttingen: Germany, 1996.

5) A.L. Speck, PLATON, *A Multipurpose Crystallographic Tool*; Utrecht University: The Netherlands, 2001.

6) G.M. Sheldrick, SHELXS-97, *Program for Crystal Structure Determination*; University of Göttingen: Germany, 1997.

7) Sheldrick, G. M. *SHELXL-97*, *Program for the Refinement of Crystal Structure*; University of Göttingen: Germany, 1997.

8) Barbour, L.J. *J. Supramol. Chem.* **2001**, 1, 189.

Table S1. X-ray crystallographic and refinement data for **DM-BDT**.

Formula	$C_{12}H_{10}S_2$
Formula weight	218.32
CCDC code	832357
Temperature (K)	203(2)
Crystal System	Monoclinic
Space group	$P2_1/c$
a, Å	7.757(14)
b, Å	5.558(8)
c, Å	12.121(19)
α, deg	90.00
β, deg	102.14(5)
γ, deg	90.00
volume, Å^3	510.9(14)
Z	2
Density (calculated), mg/m^3	1.419
μ, mm^{-1}	0.473
***θ* range for data collection, deg**	2.69-28.26
Final *R* Indices [*I*>2σ]	R_1[a] = 0.0509, $wR2$[b] = 0.1442
***R* Indices (all data)**	R_1[a] = 0.0558, $wR2$[b] = 0.1491
Goodness-of-fit (*F*^{2}) [c]	1.064

[a] $R_1 = \sum||F_o| - |F_c||/\sum|F_o|$.

[b] $wR_2 = [\sum [w(F_o^2-F_c^2)^2]/ \sum [w(F_o^2)^2]^{1/2}$

[c] Goodness-of-fit = $[\sum w(|F_o|-|F_c|)^2/(N_{obs}-N_{parameter})]^{1/2}$

Table S2. Bond distances for **DM-BDT** in Å.

S(1)-C(3)	1.748(3)
S(1)-C(6)	1.739(4)
C(1)-C(2)	1.510(4)
C(2)-C(3)	1.395(4)
C(2)-C(4)	1.400(4)
C(3)-C(4)	1.424(4)
C(4)-C(5)	1.449(4)
C(5)-C(6)	1.340(5)

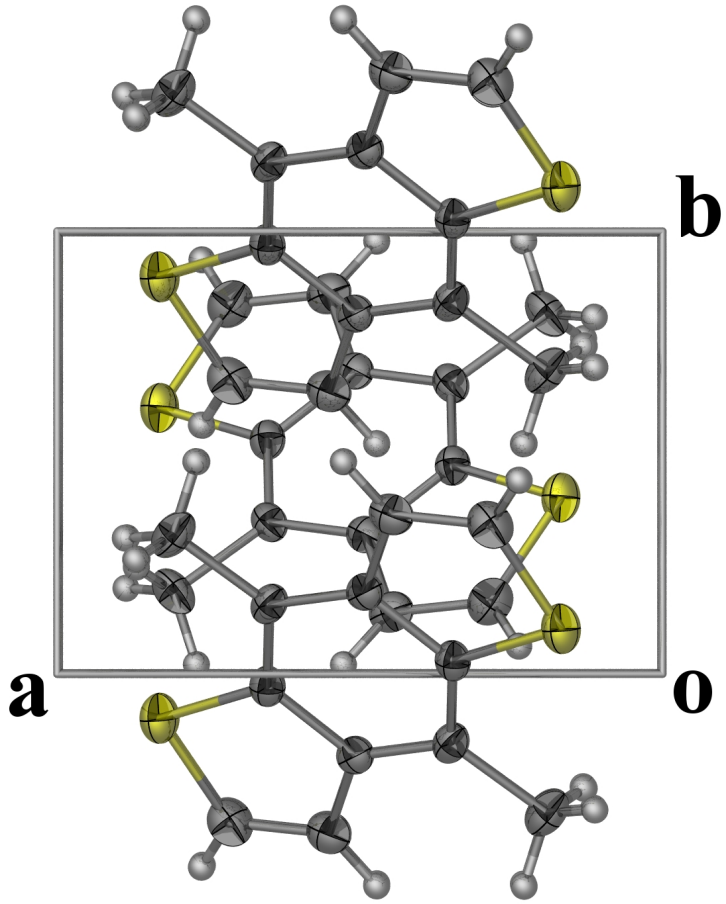

Figure S1. View of the ab plane in the crystal packing of **DM-BDT**.

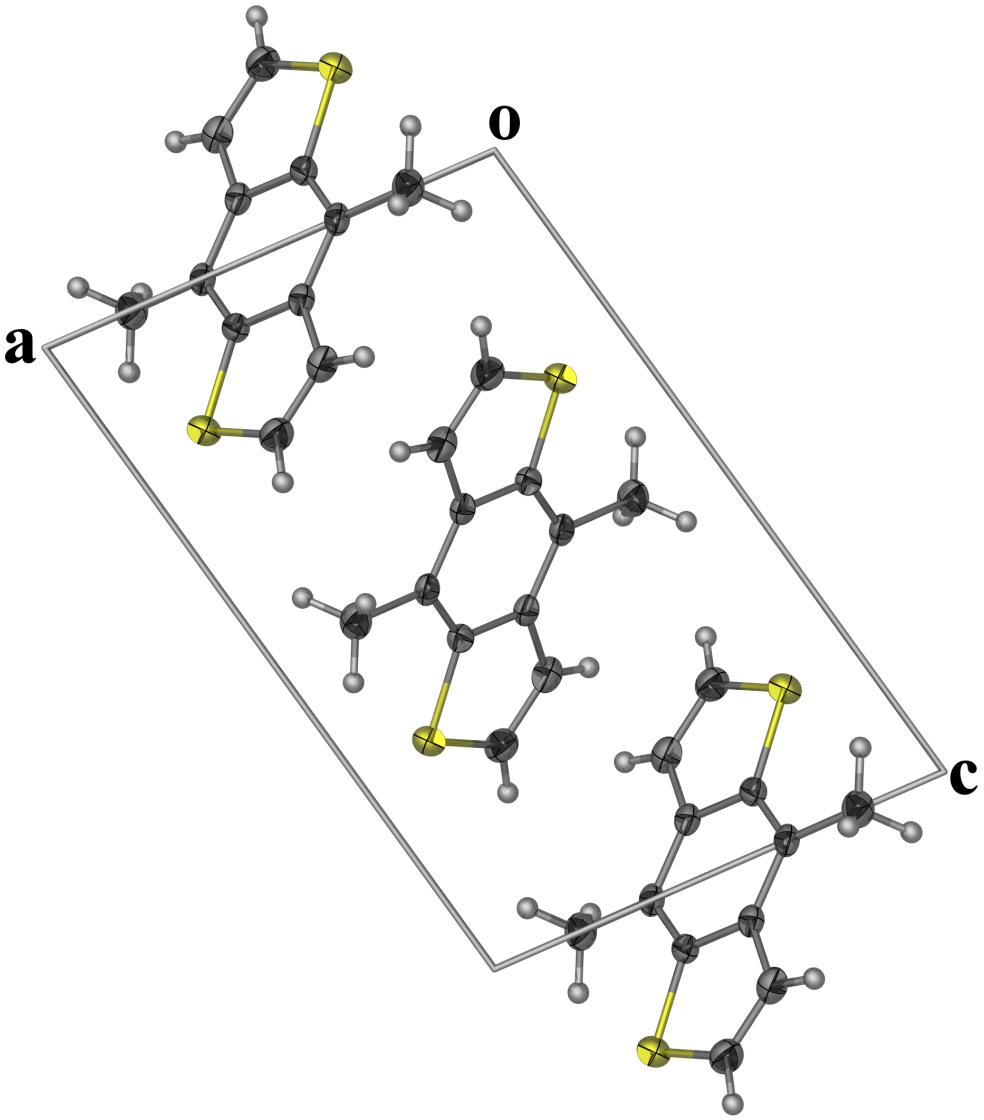

Figure S2. View of the ac plane in the crystal packing of **DM-BDT**.

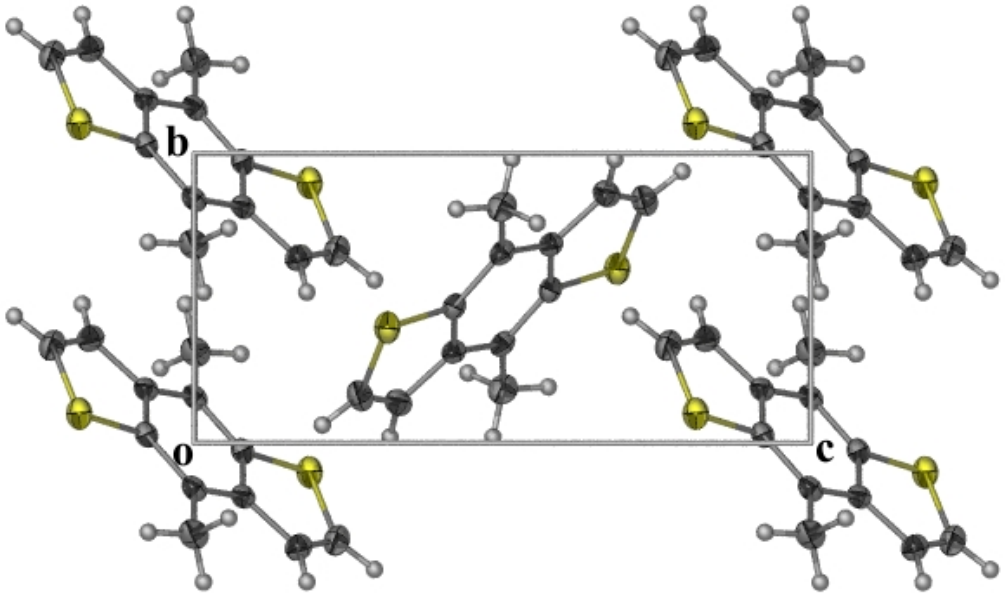

Figure S3. View of the bc plane in the crystal packing of **DM-BDT**.

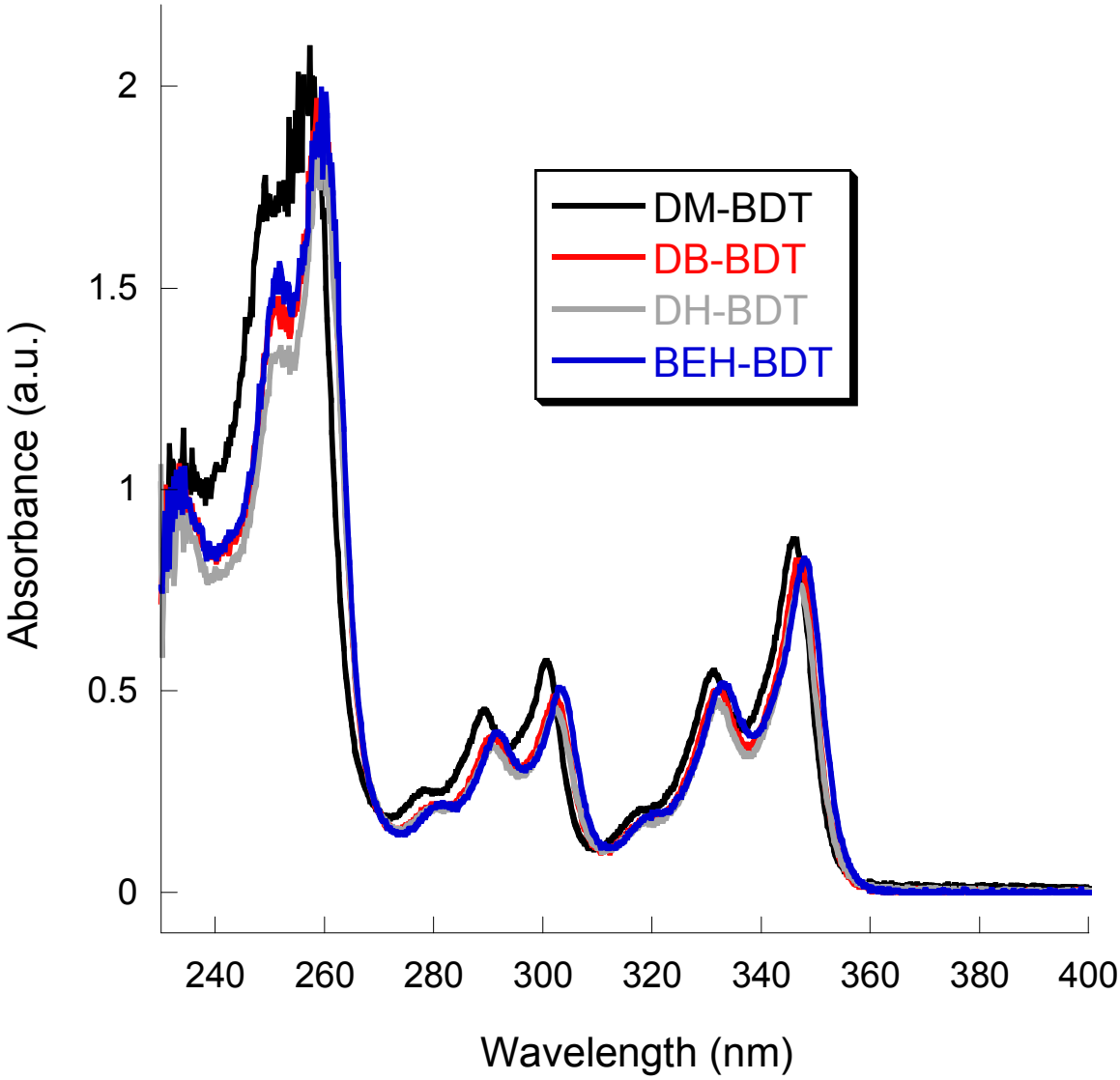

Figure S4. Solution absorption spectra for 4,8-dialkyl-BDTs in dichloromethane.

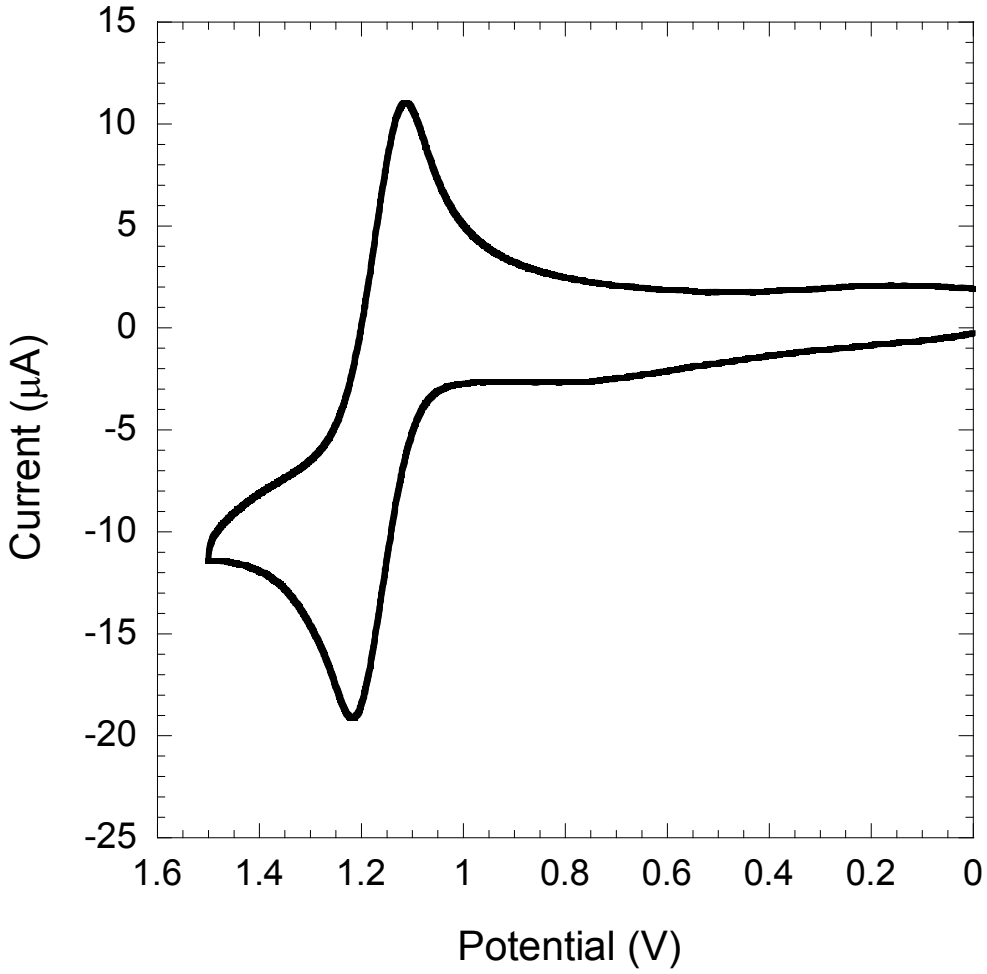

Figure S5. Cyclic voltammogram for **BEH-BDT** in 0.1 M $TBAPF_6/CH_2Cl_2$ solution at a carbon electrode, ν = 100 mV/s.