

SUPPORTING INFORMATION

A New Rod-Shaped BODIPY-Acetylene Molecule for Solution-Processed Semiconducting Microribbons in N-Channel Organic Field-Effect Transistors

Mehmet Ozdemir,¹ Donghee Choi,² Y. Zorlu,³ B. Cosut,³ Hyungsug Kim,²

Choongik Kim*,² and Hakan Usta*¹

¹ Department of Materials Science and Nanotechnology Engineering, Abdullah Gül University, Kayseri, Turkey

² Department of Chemical and Biomolecular Engineering, Sogang University, Mapo-gu, Seoul, Korea

³ Department of Chemistry, Gebze Technical University, Gebze, Kocaeli, Turkey

*Correspondence to: Prof. Hakan Usta (E-mail:hakan.usta@agu.edu.tr), Prof. Choongik Kim (E-mail: choongik@sogang.ac.kr).

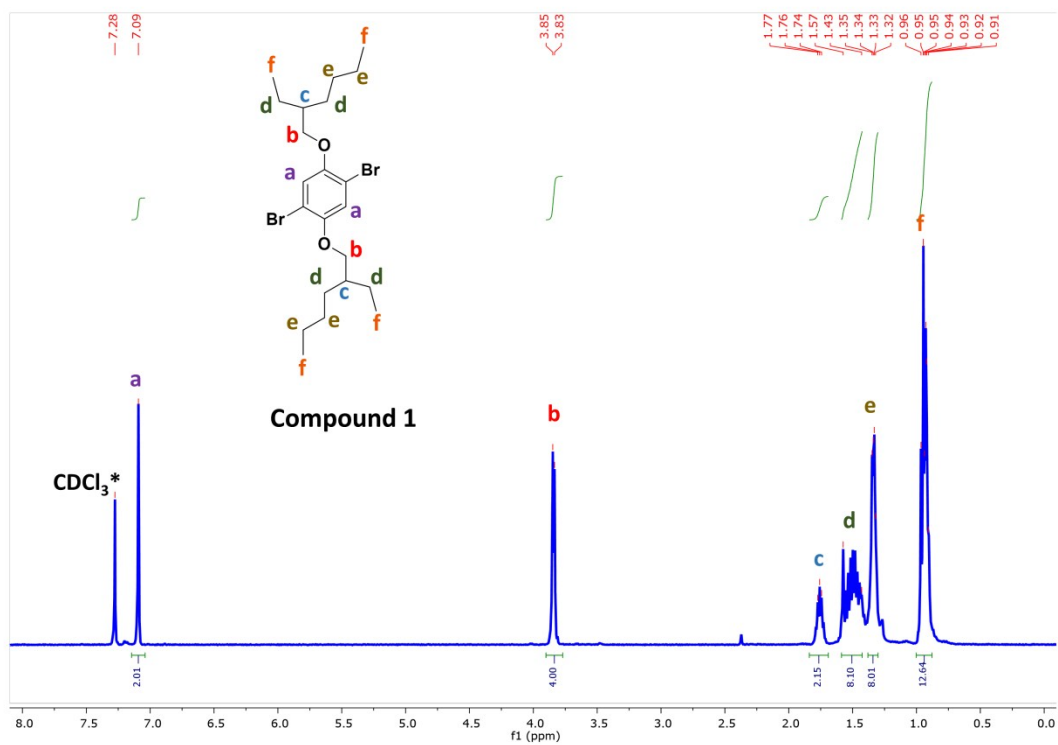


Figure S1. ^1H NMR spectra of compound **1** in CDCl_3 at room temperature.

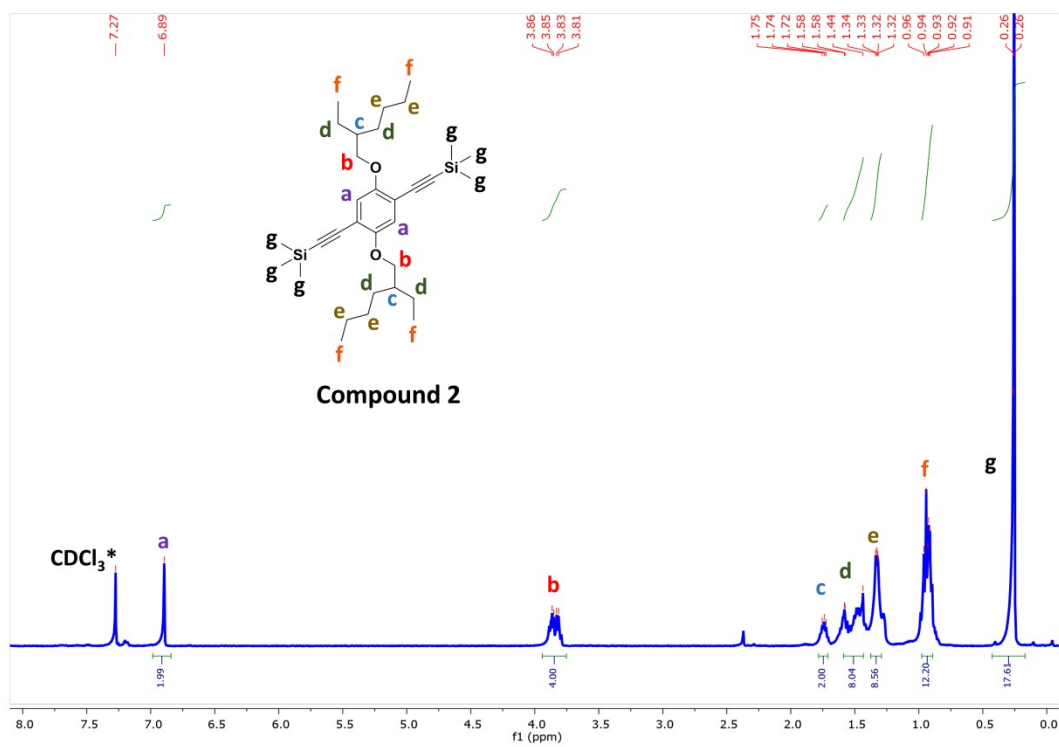


Figure S2. ^1H NMR spectra of compound **2** in CDCl_3 at room temperature.

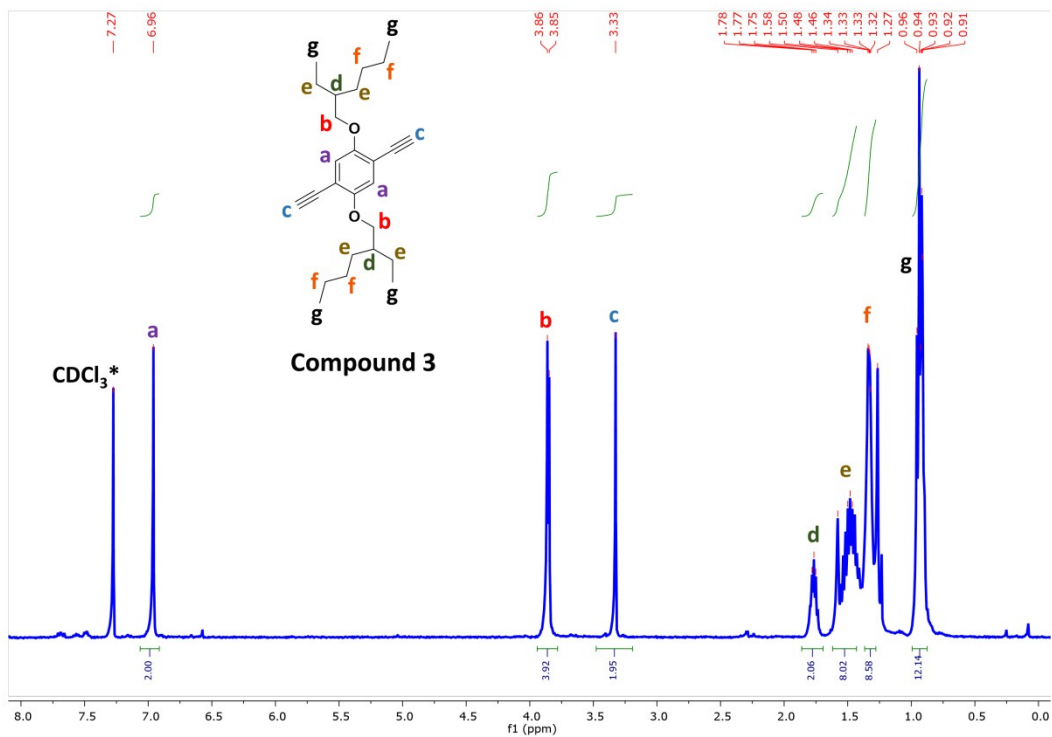


Figure S3. ¹H NMR spectra of compound **3** in CDCl₃ at room temperature.

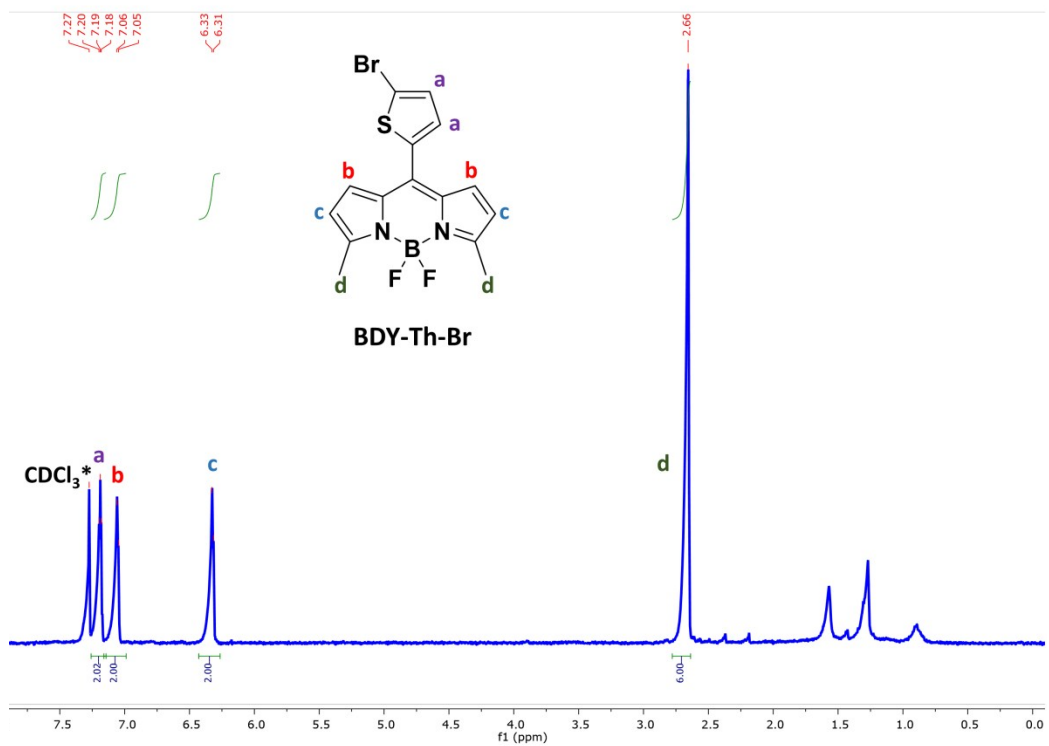


Figure S4. ¹H NMR spectra of compound **BDY-Th-Br** in CDCl₃ at room temperature.

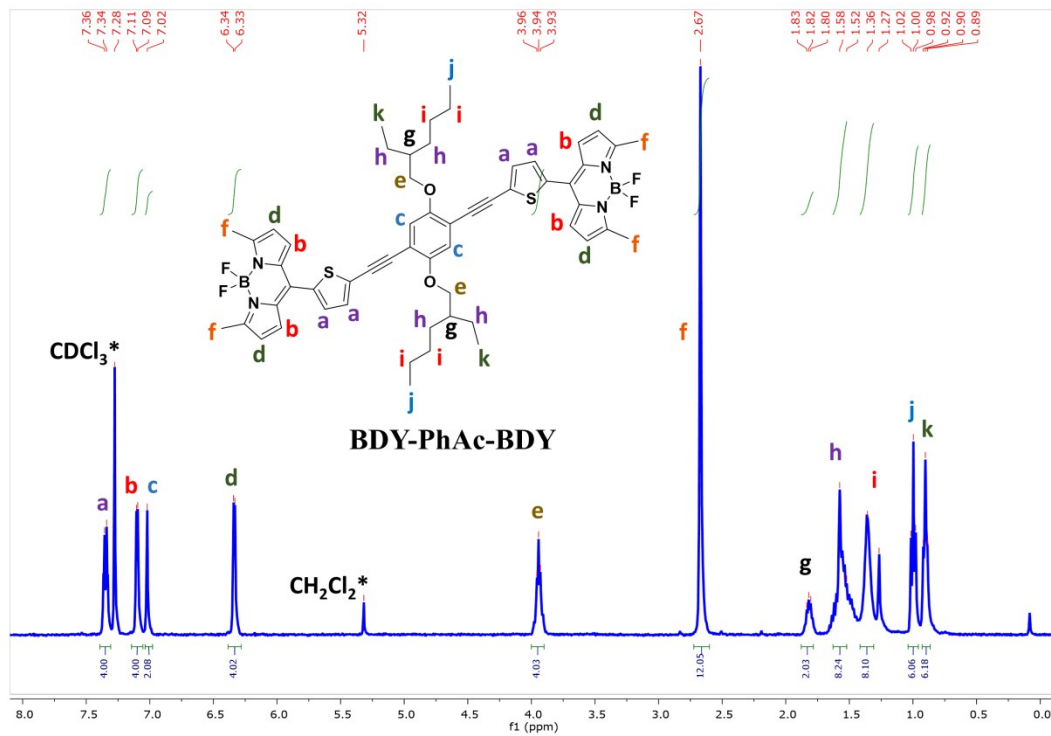


Figure S5. ¹H NMR spectra of compound **BDY-PhAc-BDY** in CDCl₃ at room temperature.

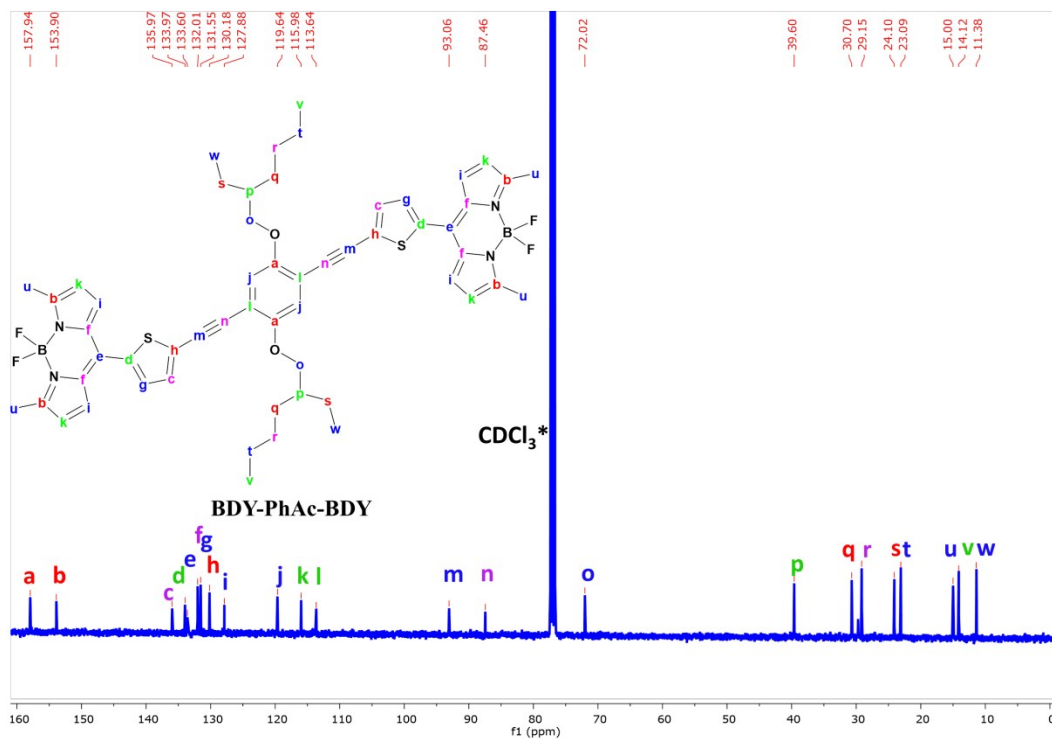


Figure S6. ¹³C NMR spectra of compound **BDY-PhAc-BDY** in CDCl₃ at room temperature.

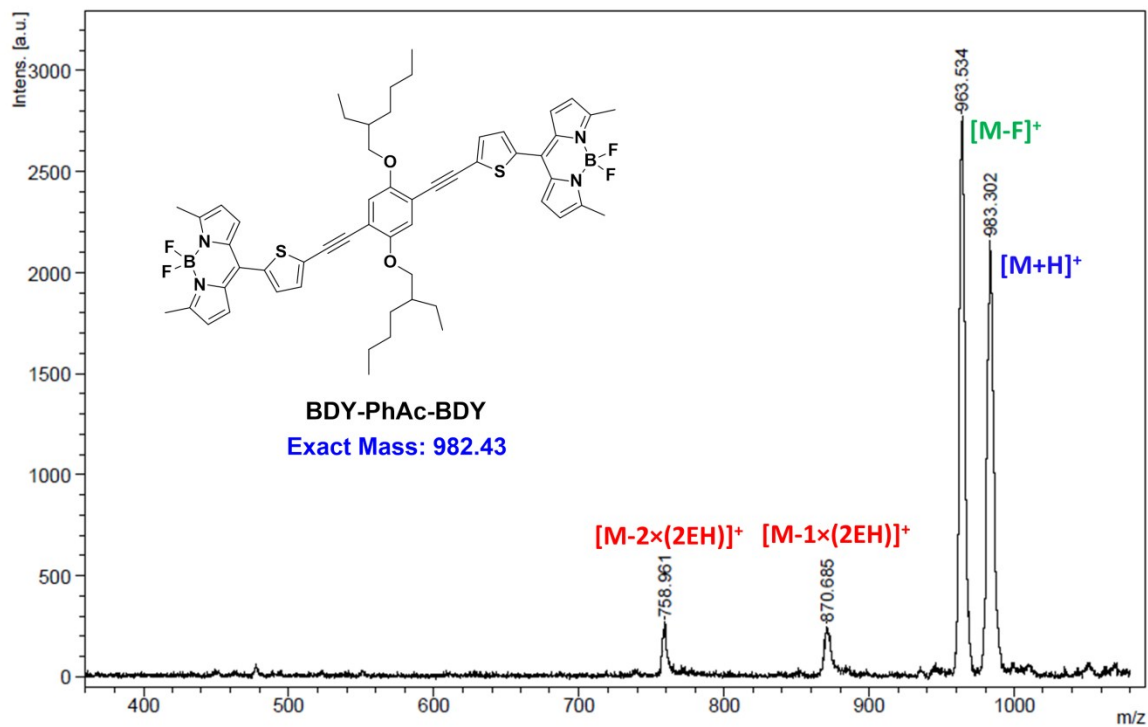


Figure S7. Positive ion and linear mode MALDI TOF-MS spectrum of **BDY-PhAc-BDY**.

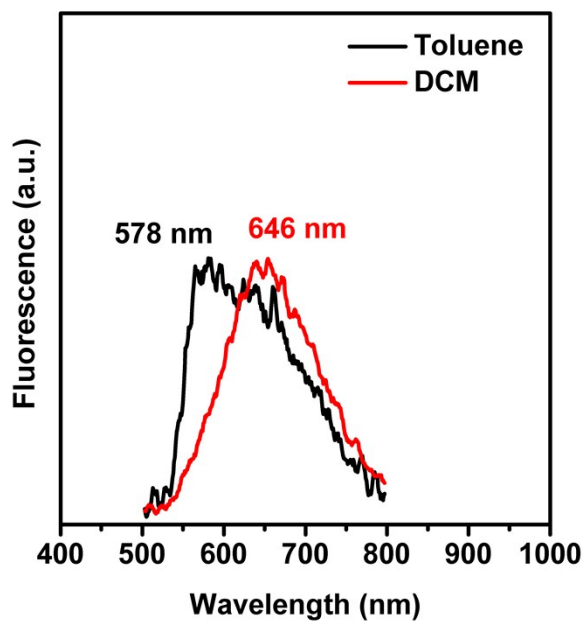


Figure S8. Fluorescence emission spectra of **BDY-PhAc-BDY** in dichloromethane (DCM) and toluene solutions (1×10^{-5} M) (Excitation wavelength= 510 nm).

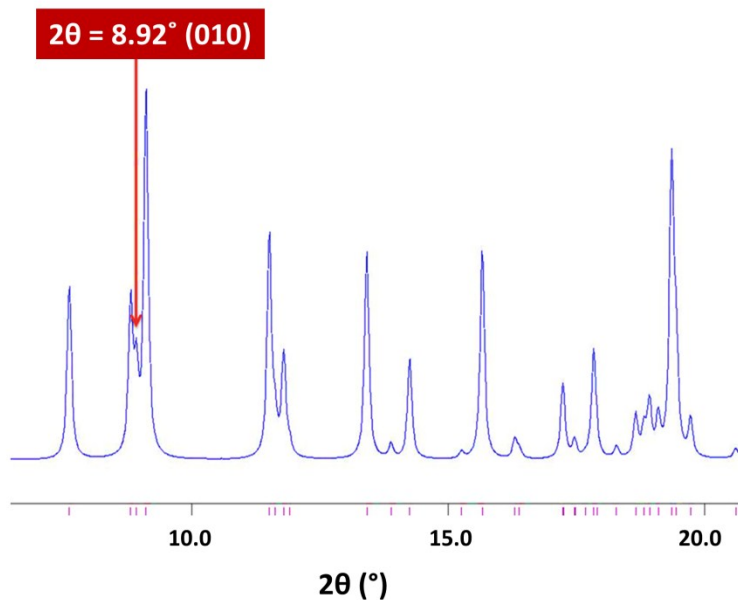


Figure S9. Simulated XRD powder pattern of **BDY-PhAc-BDY** with the selected matching peak at $2\theta = 8.92^\circ$ corresponding to (010) diffraction plane.

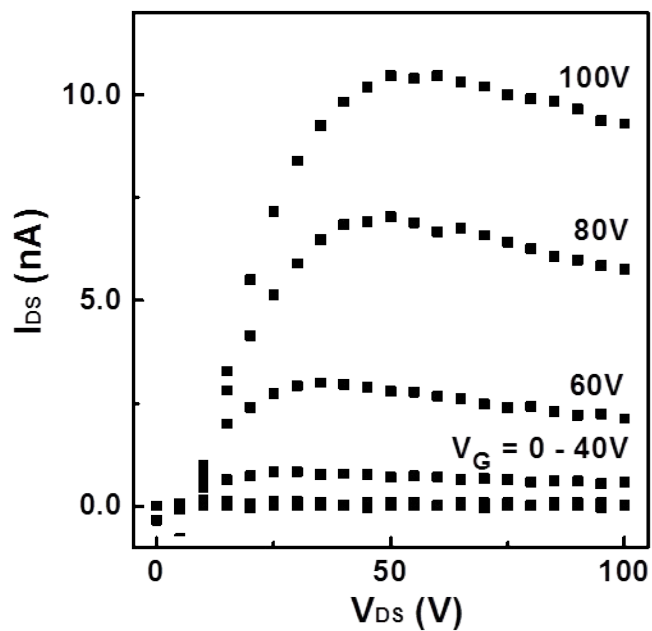


Figure S10. Representative output plot for the OFET devices fabricated with solution-sheared **BDY-PhAc-BDY** thin-film.

X-ray data collection and structure refinement

Single crystal x-ray diffraction analysis was carried out on an Bruker APEX II QUAZAR three-circle diffractometer using monochromatized Mo K α X-radiation ($\lambda = 0.71073 \text{ \AA}$) using φ and ω technique at 173(2) K. Indexing was performed using APEX2.¹ Data integration and reduction were carried out with SAINT V8.34A.² Absorption correction was performed by multi-scan method implemented in SADABS V2014/5.³ Space groups were determined using XPREP implemented in APEX2. The structure was solved using SIR-92.⁴ The least-square refinement on F^2 was achieved with the CRYSTALS software.⁵ All non-hydrogen atoms were refined anisotropically. The hydrogen atoms were all located in a difference map, but those attached to carbon atoms were repositioned geometrically. The H atoms were initially refined with soft restraints on the bond lengths and angles to regularize their geometry (C---H in the range 0.93--0.98 \AA) and Uiso(H) (in the range 1.2-1.5 times Ueq of the parent atom), after which the positions were refined with riding constraints. The crystals available for X-ray structural analysis were of quite poor quality and weak scatterers at high resolution ($\approx 1.00 \text{ \AA}$), thus resulting in comparatively high R/wR values. A crystallographic data and refinement detail of the data collection for BDY-PhAc-BDY is given in Table 1. The final geometrical calculations and the molecular drawings were carried out with PLATON program.⁶

Table S1. Crystal data and refinement parameters for **BDY-PhAc-BDY**.

Crystal parameters	BDY-PhAc-BDY
CCDC	1482958
Empirical Formula	C ₅₆ H ₆₀ B ₂ F ₄ N ₄ O ₂ S ₂
Formula weight (g. mol⁻¹)	982.86
Temperature (K)	173(2)
Wavelength (\AA)	0.71073
Crystal system	Triclinic
Space group	<i>P</i> -1

<i>a</i> (Å)	10.1366 (12)
<i>b</i> (Å)	10.9280 (12)
<i>c</i> (Å)	12.6758 (14)
α (°)	66.265 (7)
β (°)	87.951 (7)
γ (°)	81.738 (7)
Crystal size (mm)	0.46 × 0.44 × 0.08
<i>V</i> (Å ³)	1271.65 (14)
<i>Z</i>	1
ρ_{calcd} (Mg. cm ⁻³)	1.283
μ (mm ⁻¹)	0.17
<i>F</i>(000)	518
θ range for data collection (°)	1.755 - 25.027
<i>h/k/l</i>	-11/12, -11/13, 0/15
Measured Reflections	11886
Independent reflections (<i>R</i>_{int})	4418 (0.103)
Data/restraints/parameters	2591/36/316
Goodness-of-fit on <i>F</i>² (<i>S</i>)	0.95
<i>R</i>[<i>F</i>² > 2<i>s</i>(<i>F</i>²)]	0.0860
<i>wR</i>₂ (all data)	0.2139
Largest diff. peak and hole (e.Å⁻³)	1.00 and -0.37

REFERENCES

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