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Supplementary Information

Synthesis and properties of indigo based donor-acceptor conjugated polymers

Chang Guo, Bin Sun, Jesse Quinn, Zhuangqing Yan and Yuning Li*

Department of Chemical Engineering/Waterloo Institute for Nanotechnology (WIN), University of Waterloo, 200 University Avenue West, Waterloo, Ontario, Canada N2L 3G1; Fax: +1 519-888-4347; Tel: +1 519-888-4567 ext. 31105; Email: yuning.li@uwaterloo.ca.

Supplementary Information

1. Computer simulations of model compounds

Geometry optimization of model compounds (see Table S1 and Figures 2, S1-S4) was performed based on the density functional theory (DFT) using the B3LYP hybrid function[1] and the 6-31G* basis set. GaussView 5.0 software[2] was used to draw the Lowest Unoccupied Molecular Orbitals (LUMO) and the Highest Occupied Molecular Orbitals (HOMO). Calculations were performed on the Shared Hierarchical Academic Research Computer Network (SHARCNET) of Canada using the Gaussian 09W package[3].

2. Additional data

Table S1. Summary of computer simulation results of model compounds.

Entry	Model compounds [a]	$\varphi_{1,}$ °	$\varphi_{2,}$ °	$\varphi_{3,}$ °	E_{HOMO}, eV	E_{LUMO}, eV	E_g, eV
1	IDH-BT-IDH-BT	0	24	16	-5.28	-2.92	2.37
2	IDMe-BT-IDMe-BT	29	24	1	-5.13	-2.80	2.33
3	IDCOMe-BT-IDCOMe-BT	23	24	15	-5.60	-3.00	2.60
4	IIDH-BT-IIDH-BT	11	19	16	-5.09	-2.95	2.14
5	IIDMe-BT-IIDMe-BT	11	20	5	-5.03	-2.89	2.14
6	IIDCOMe-BT-IIDCOMe-BT	17	22	14	-5.32	-3.30	2.02

[a] Structures of IDCOMe-BT-IDCOMe-BT and IIDMe-BT-IIDMe-BT are shown in Figure 2 in the main text, while the structures of other model compounds are shown Figures S1-S4.

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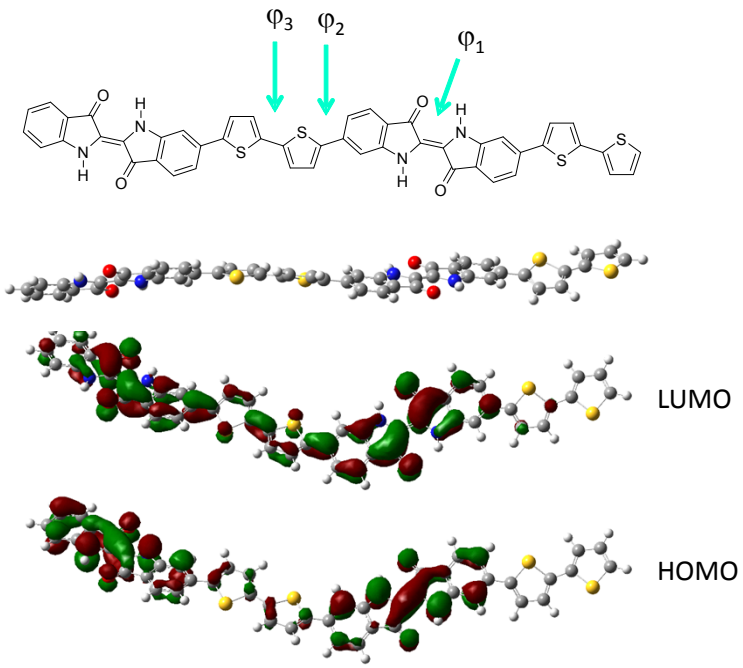

Figure S1. The chemical structure, geometry, LUMO orbital, and HOMO orbital of a model dimer IDH-BT-IDH-BT obtained by performing density functional theory (DFT) calculations with B3LYP 6-31G*.

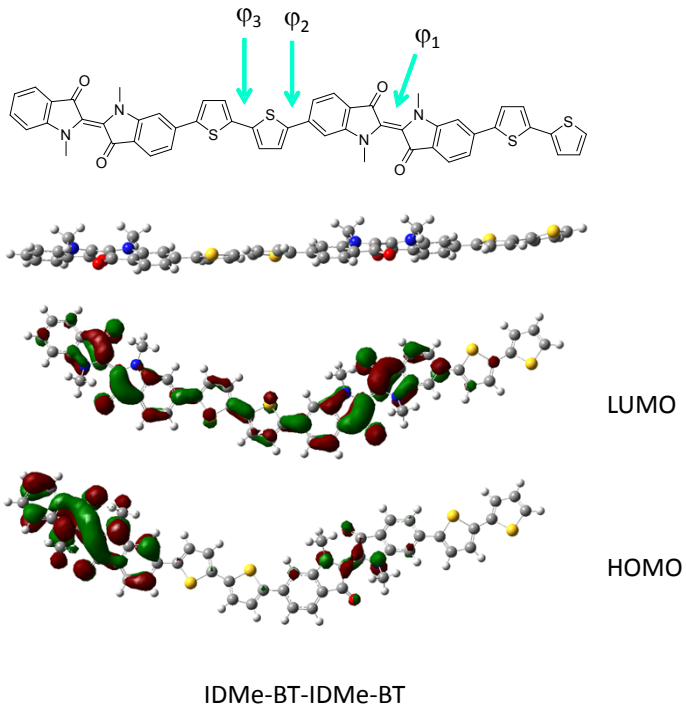

Figure S2. The chemical structure, geometry, LUMO orbital, and HOMO orbital of a model dimer IDMe-BT-IDMe-BT obtained by performing density functional theory (DFT) calculations with B3LYP 6-31G*.

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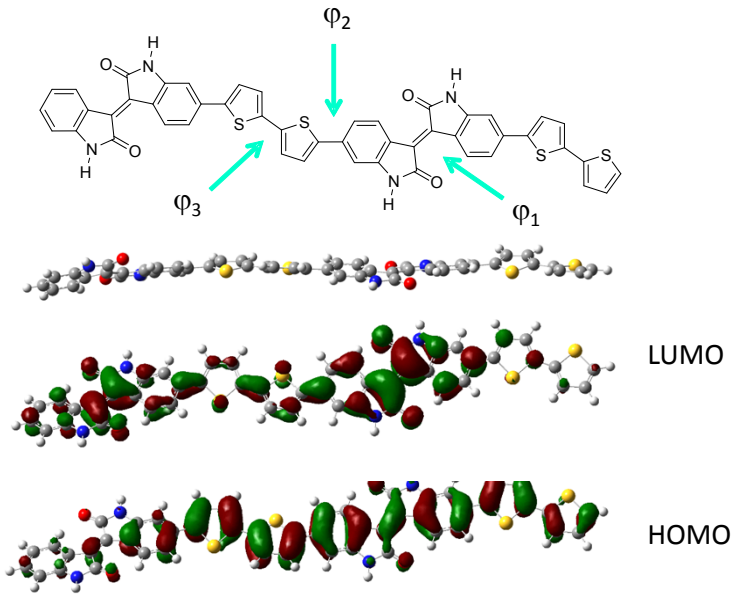

Figure S3. The chemical structure, geometry, LUMO orbital, and HOMO orbital of a model dimer IIDH-BT-IIDH-BT obtained by performing density functional theory (DFT) calculations with B3LYP 6-31G*.

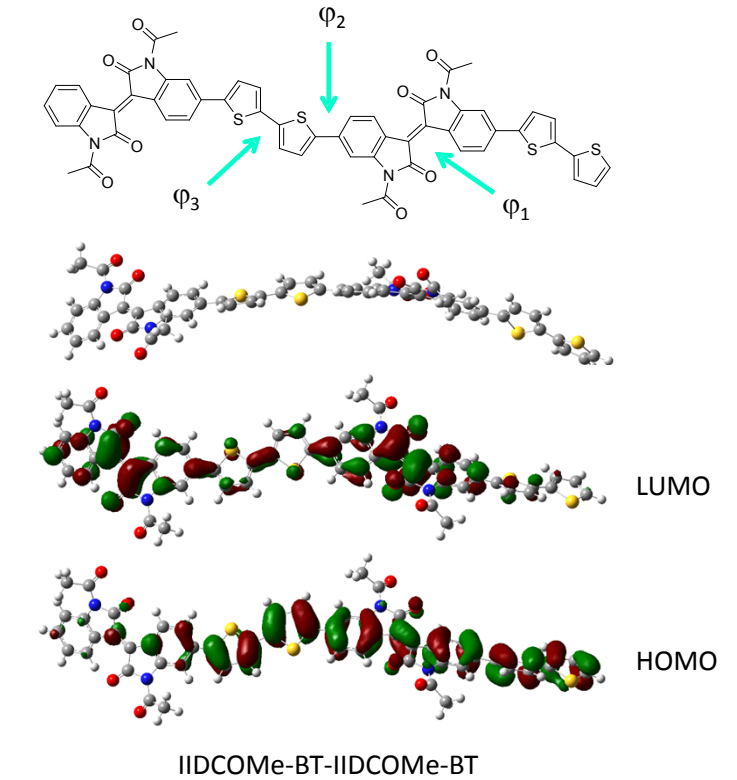

Figure S4. The chemical structure, geometry, LUMO orbital, and HOMO orbital of a model dimer IIDCOMe-BT-IDCOMe-BT obtained by performing density functional theory (DFT) calculations with B3LYP 6-31G*.

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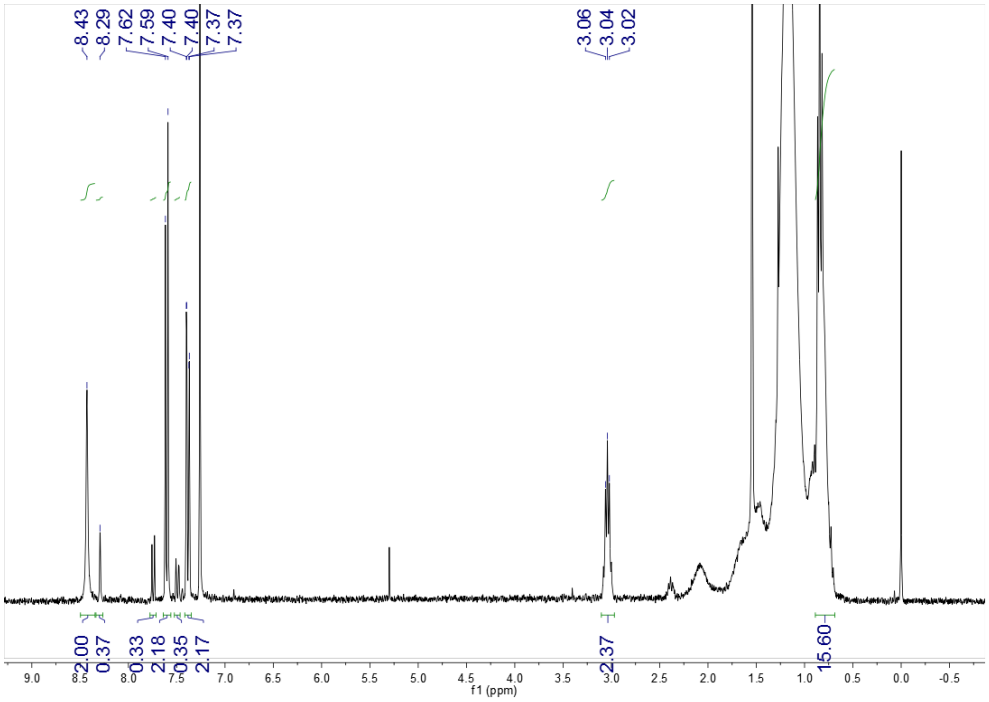

Figure S5 The 300 MHz ^{1}H NMR spectrum of 6,6'-dibromo-1,1'-bis(2-hexyldecanoyl)-[2,2'-biindolinylidene]-3,3'-dione (compound **2a**) measured in $CDCl_3$.

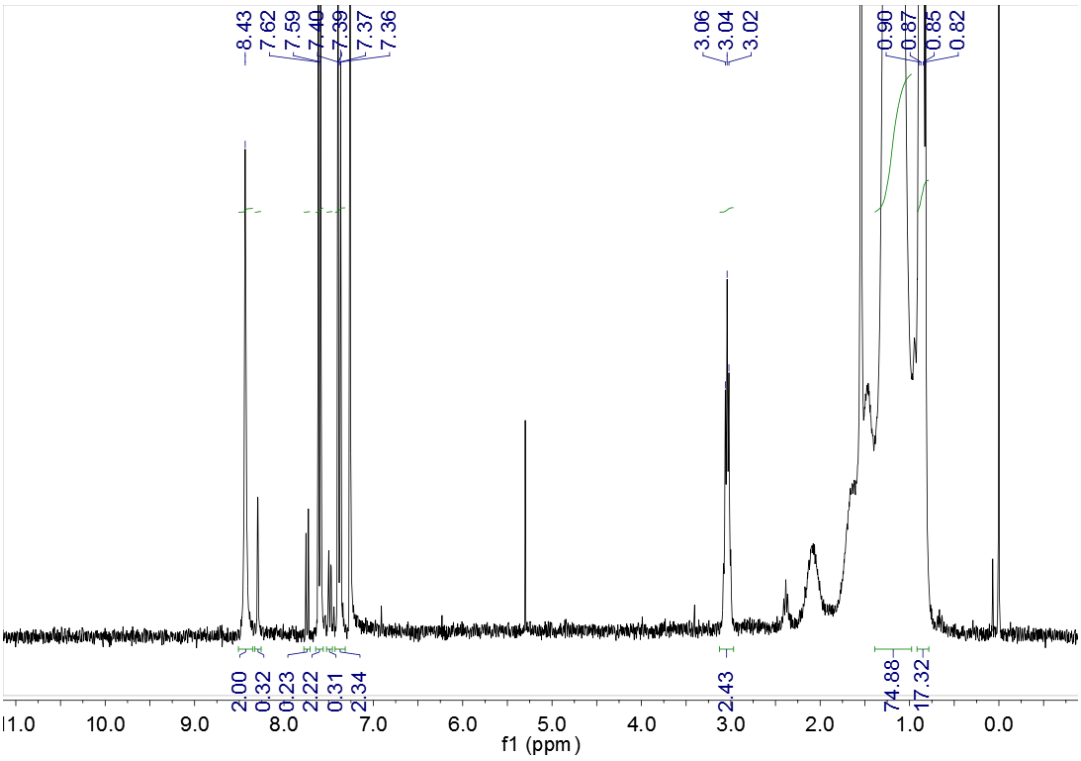

Figure S6 The 300 MHz ^{1}H NMR spectrum of 6,6'-dibromo-1,1'-bis(2-octyldodecanoyl)-[2,2'-biindolinylidene]-3,3'-dione (compound **2b**) measured in $CDCl_3$.

Supplementary Information

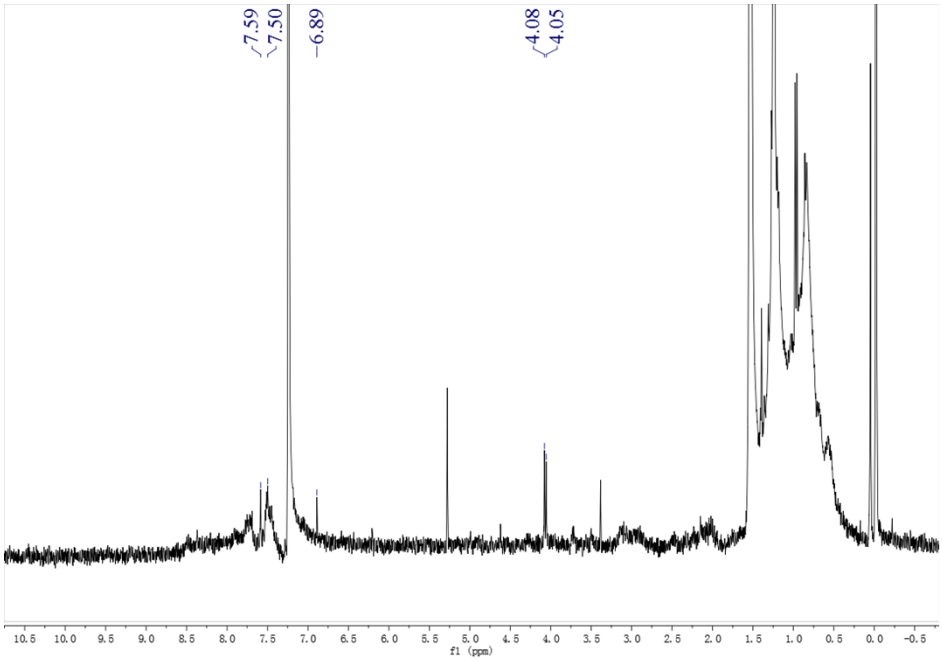

Figure S7. The 300 MHz ^{1}H NMR spectrum of **P1** measured in $CDCl_3$.

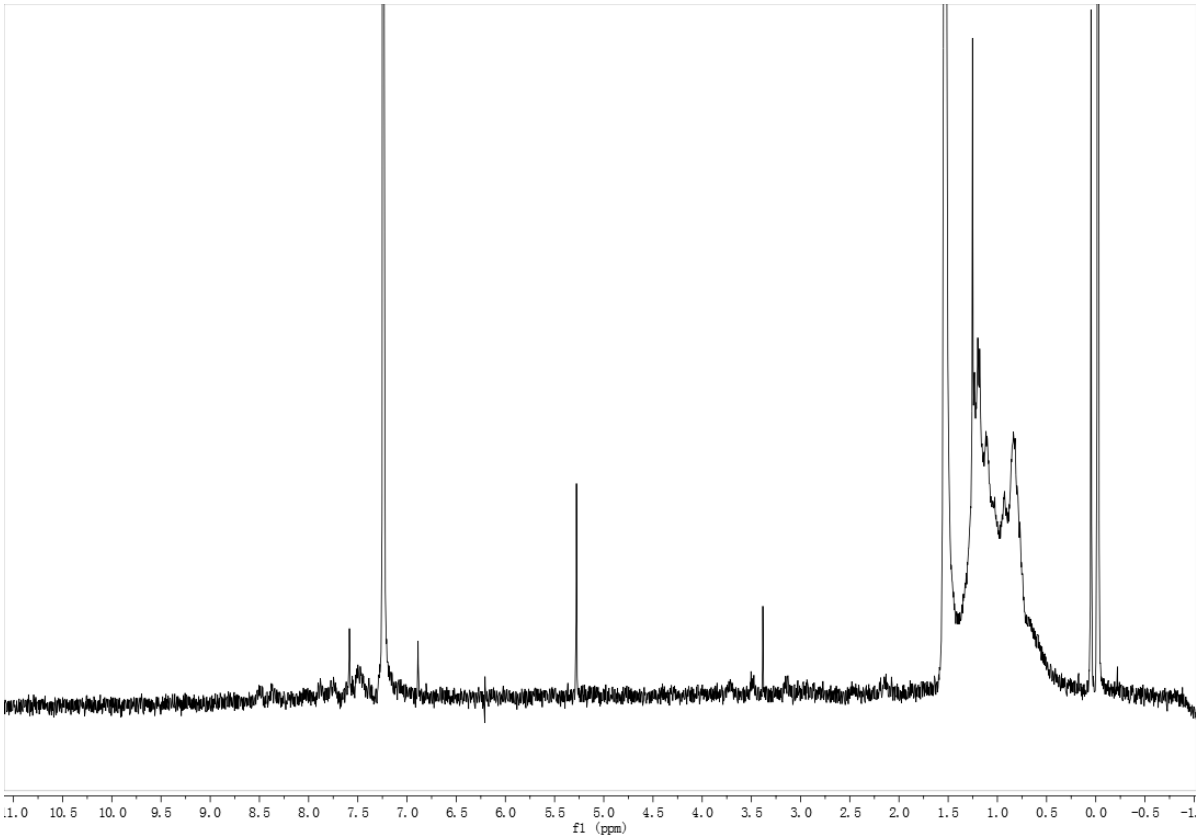

Figure S8. The 300 MHz ^{1}H NMR spectrum of **P2** measured in $CDCl_3$.

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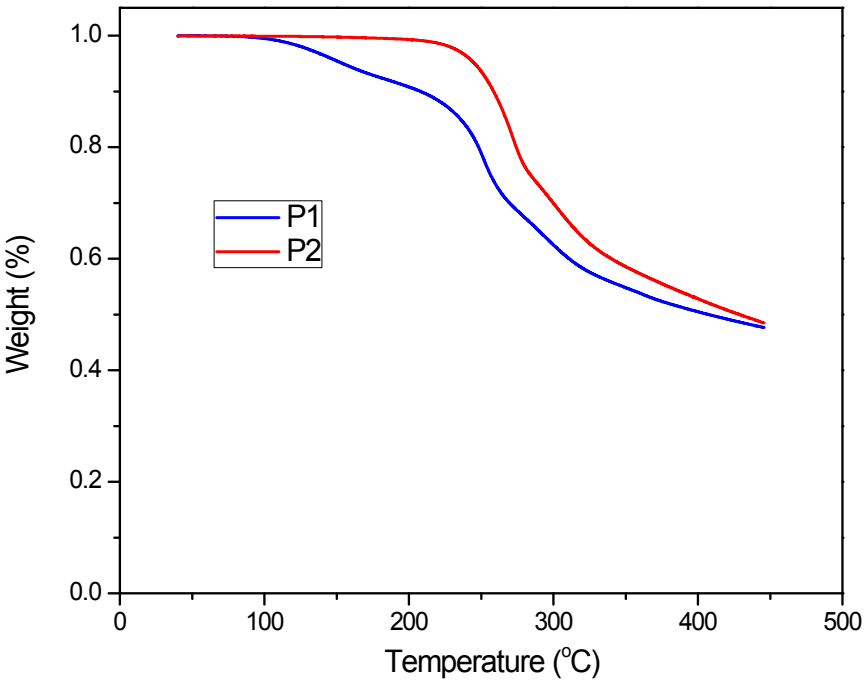

Figure S9. TGA curves of **P1** and **P2** with a heating rate of 10 °C·min^{-1} under N_2.

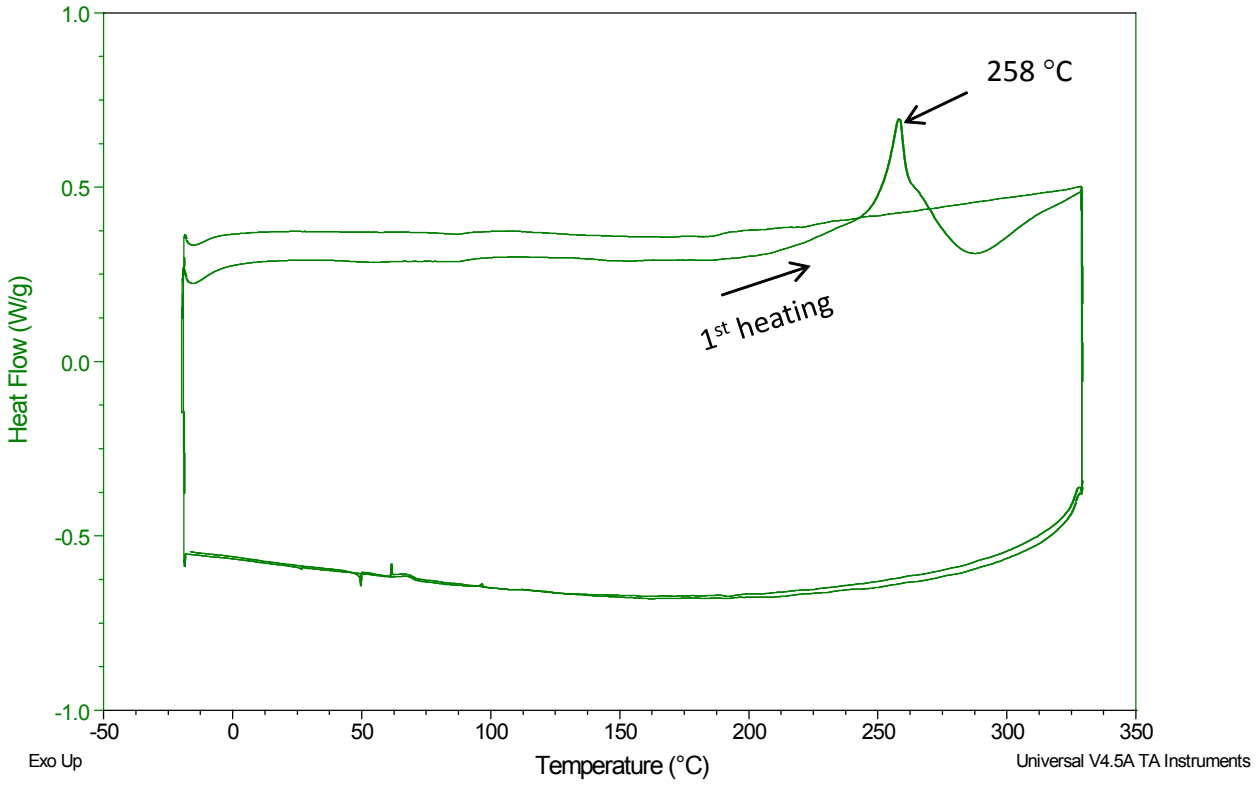

Figure S10. DSC curves of **P1** with a heating rate of 10 °C·min^{-1} under N_2.

Supplementary Information

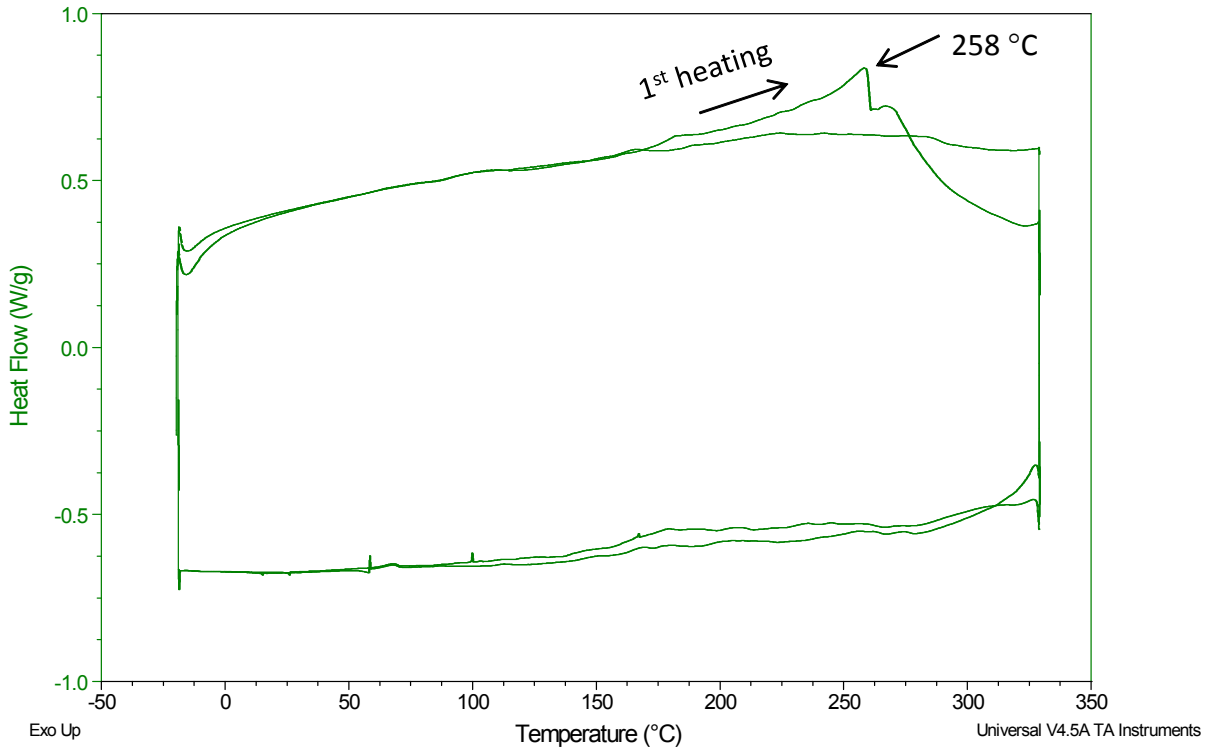

Figure S11. DSC curves of **P2** with a heating rate of 10 °C·min^{-1} under N_2.

3. References

1. (a) A. D. Becke, *Phys. Rev. A*, 1988, **38**, 3098. (b) C. Lee, W. Yang and G. G. Parr, *Phys. Rev. B*, 1988, **37**, 785.
2. Æ. Frisch, H. P. Hratchian, R. D. Dennington II, T. A. Keith, J. Millam, A. B. Nielsen, A. J. Holder and J. Hiscocks, *GaussView 5 Reference,* Gaussian, Inc., Wallingford, CT, 2009.
3. (a) Æ. Frisch, *Gaussian 09W Reference*, Gaussian, Inc., Wallingford, CT, 2009. (b) *Gaussian 09, Revision B.01*, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken,

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