Supplementary Information

Impact of N-substitution of carbazole unit on molecular packing and charge transport of DPP-carbazole copolymers

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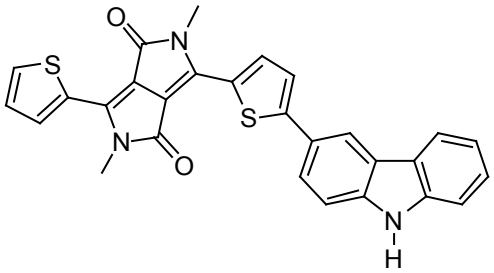
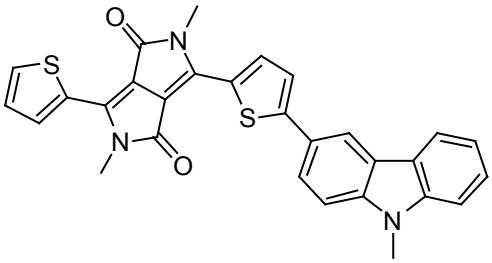
3. References

Supplementary Information

1. Computer simulations of model compounds, DBTCz-H and DBTCz-Me



DBTCz-H

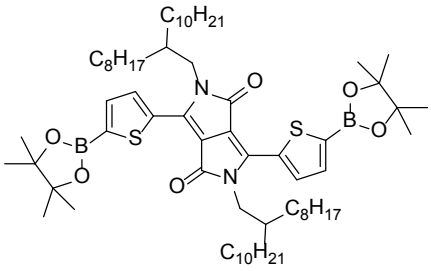


DBTCz-Me

Geometry optimization of DBTCz-H and DBTCz-Me were performed with the density functional theory (DFT) calculation using the B3LYP hybrid functional[1] with the 6-31G* basis set. Orbital shapes were prepared with the GaussView 5.0 software.[2] Calculations were performed using the Gaussian 09W package[3] on the Shared Hierarchical Academic Research Computer Network (SHARCNET) of Canada.

Supplementary Information

2. Additional data:



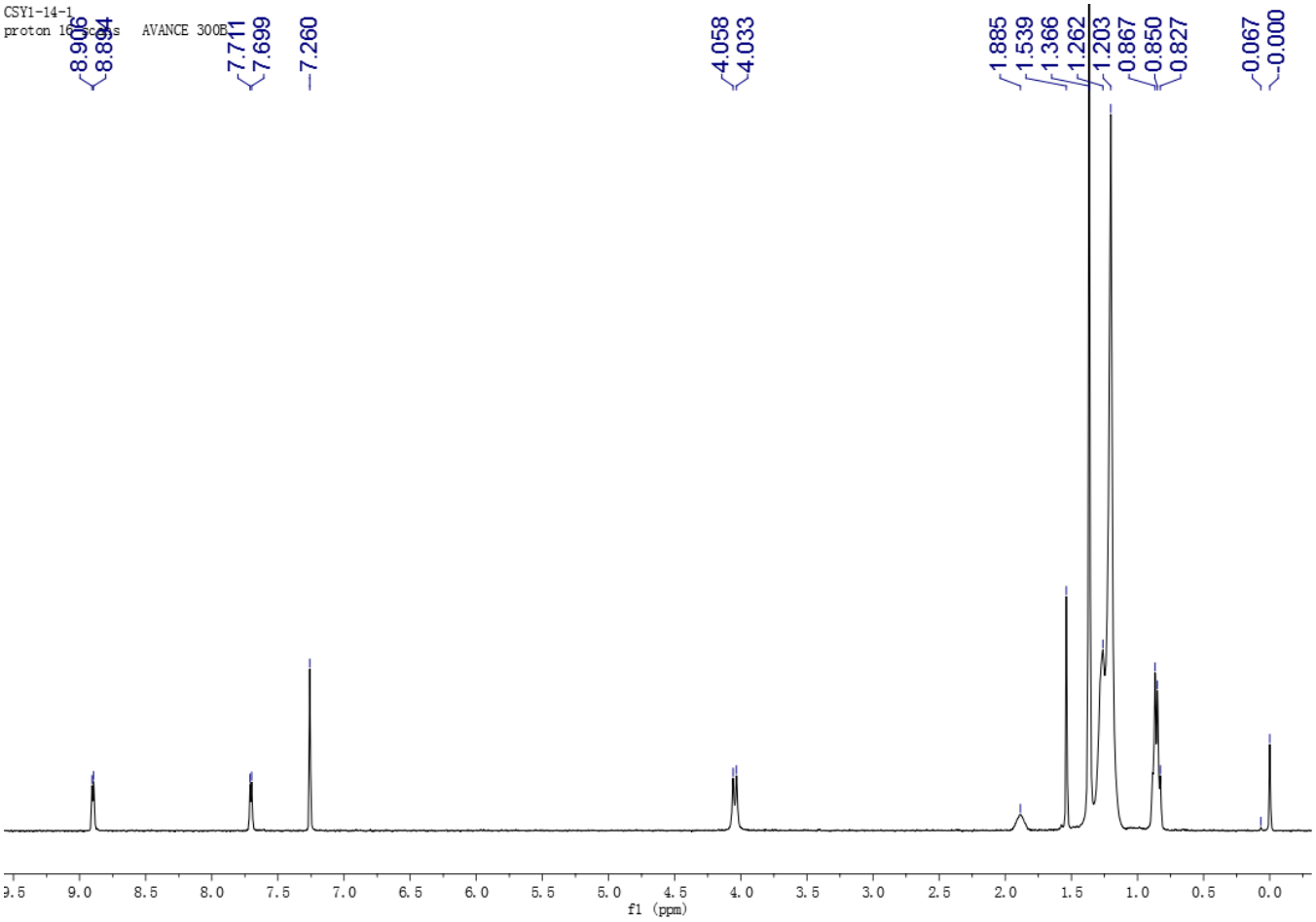


Figure S1 The 300 MHz ^{1}H NMR spectrum of 2,5-bis(2-octyldodecyl)-3,6-bis(5-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)thiophen-2-yl)pyrrolo[3,4-c]pyrrole-1,4(2*H*,5*H*)-dione (Compound **1)** measured in $CDCl_3$.

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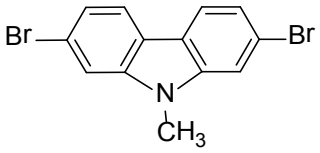

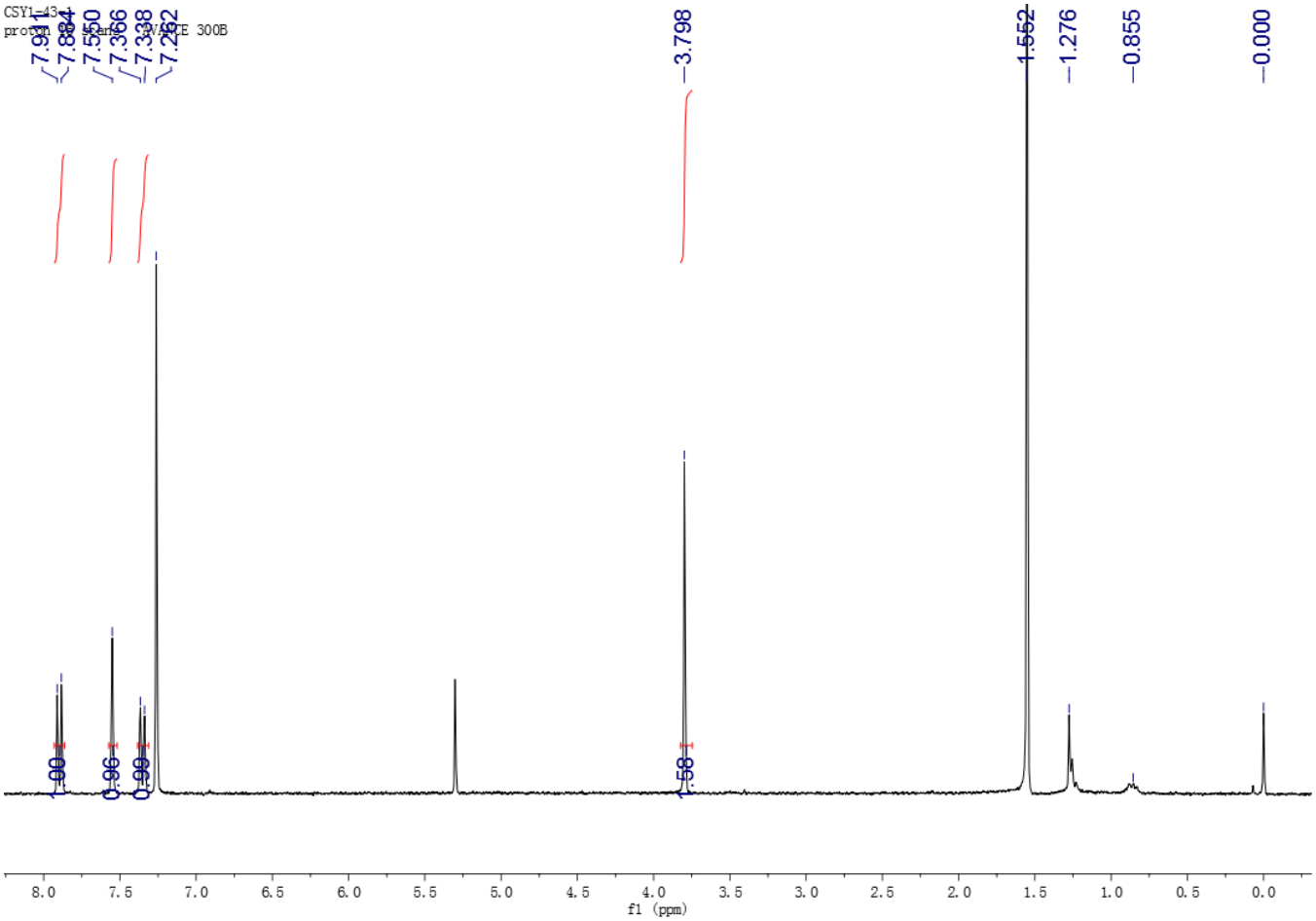

Figure S2 The 300 MHz ^{1}H NMR spectrum of 2,7-dibromo-9-methyl-9*H*-carbazole (Compound **2**) measured in $CDCl_3$.

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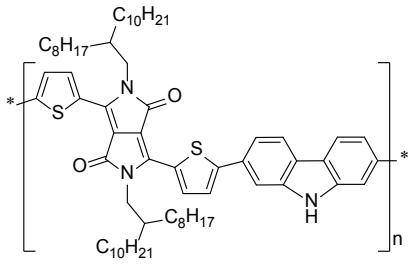

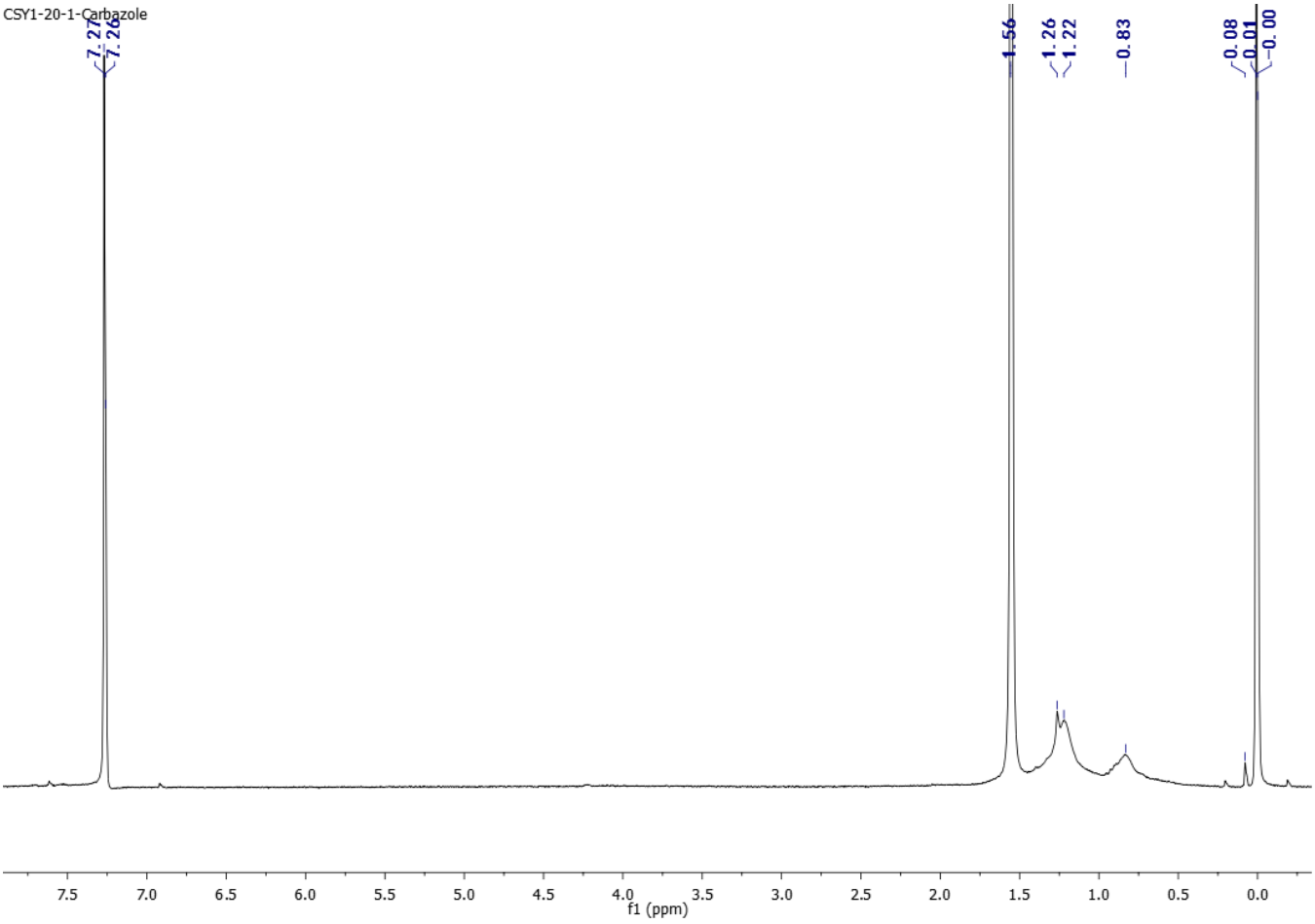

Figure S3. The 300 MHz ^{1}H NMR spectrum of **P1** measured in $CDCl_3$.

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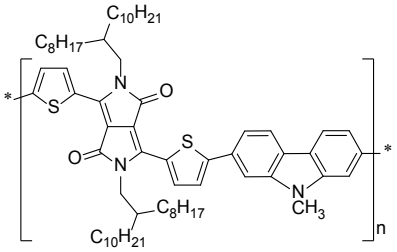

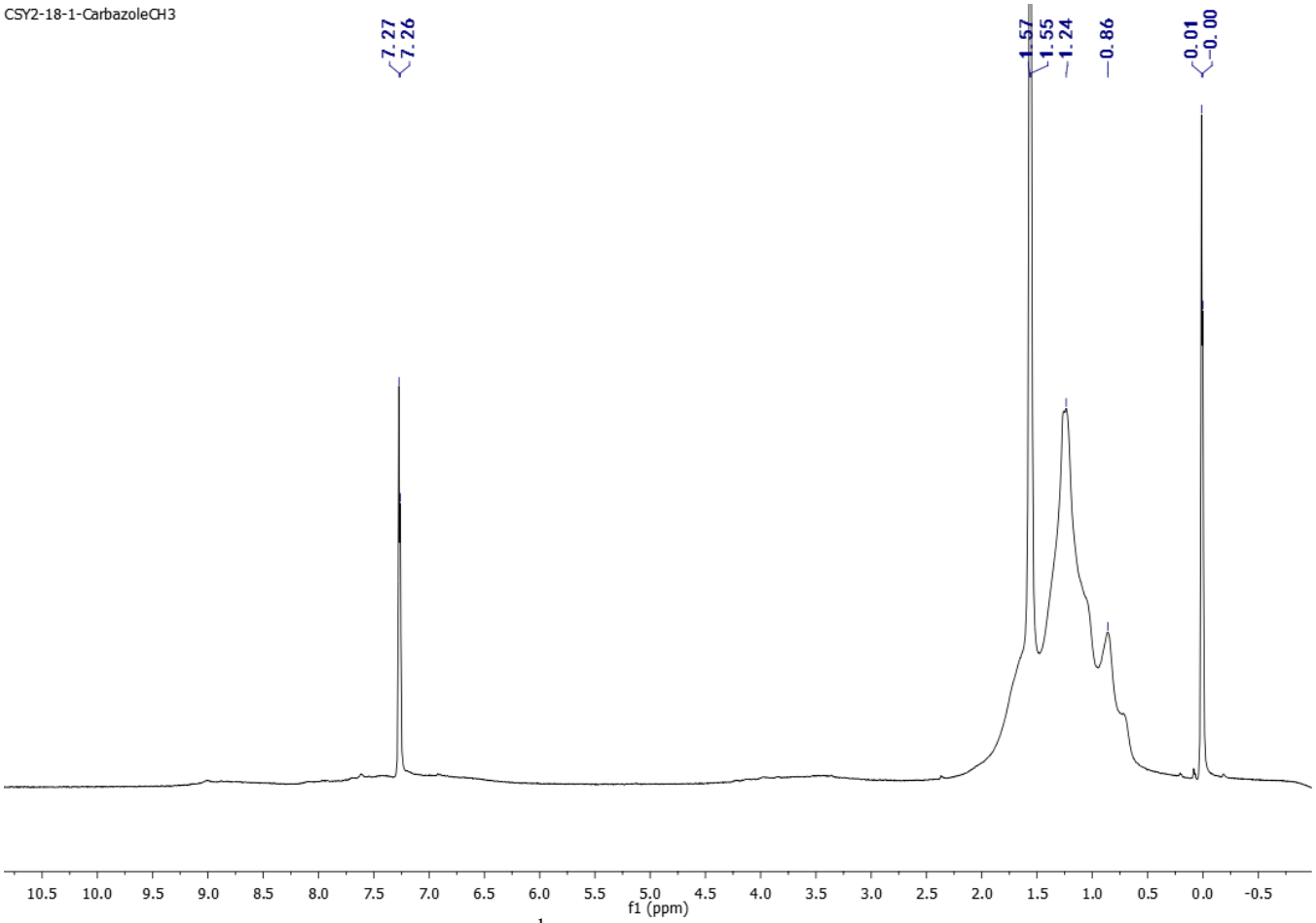

Figure S4. The 300 MHz ^{1}H NMR spectrum of **P2** measured in $CDCl_3$.

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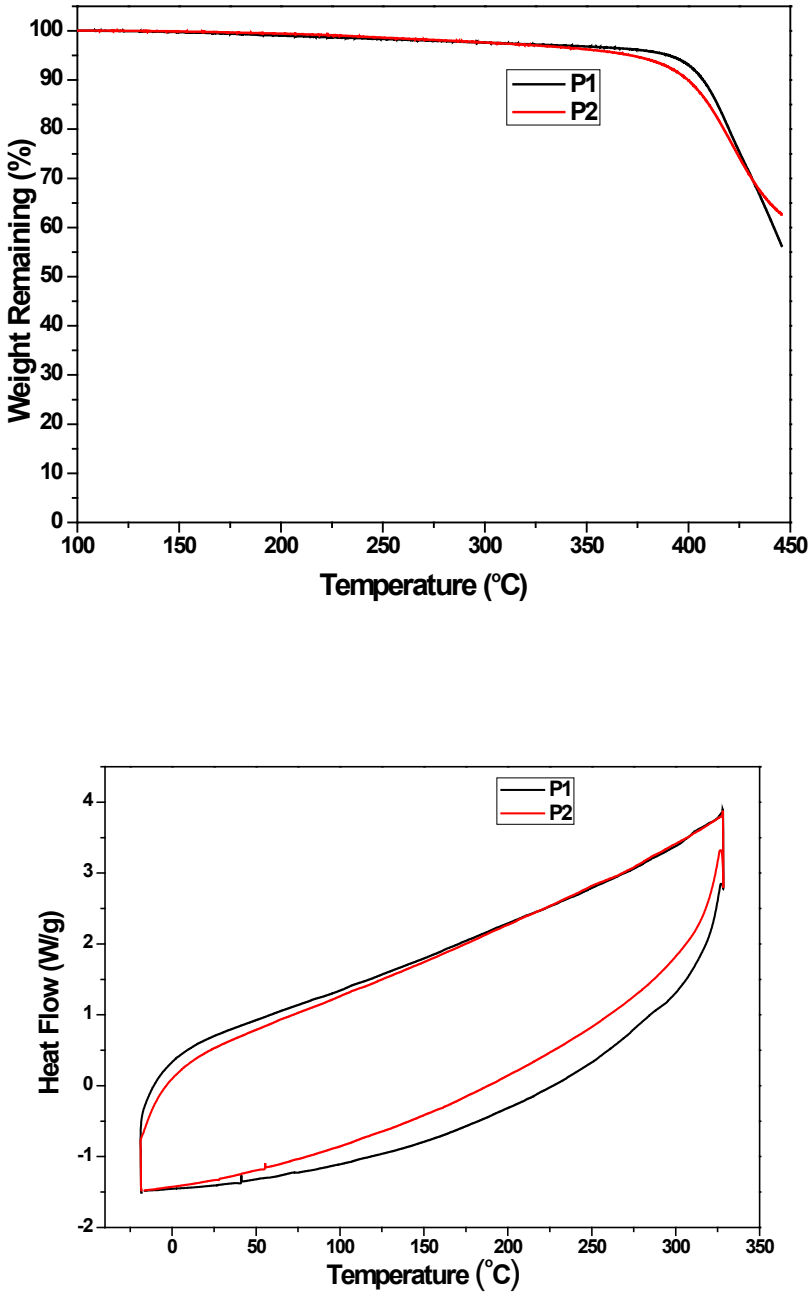

Figure S5. Diagrams of thermal analysis of **P1** and **P2**. Top: TGA curves with a heating rate of 10 °C·min^{-1} under N_2. Bottom: DSC curves with a heating/cooling rate of 10 °C·min^{-1} under nitrogen.

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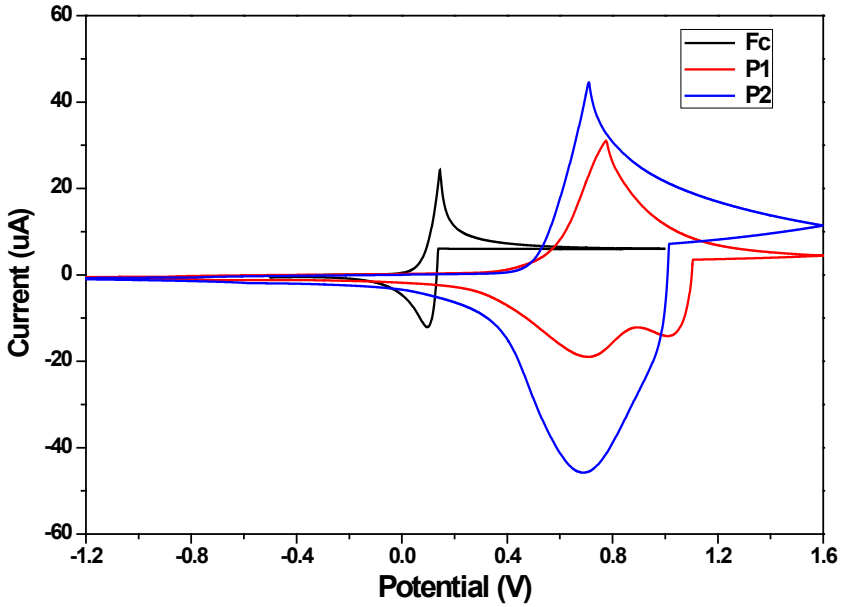

Figure S6. Cyclic voltammograms of films of **P1** and **P2** in 0.1 M tetrabutylammonium hexafluorophosphate in dry acetonitrile at a sweeping rate of 50 mV s^{-1} under nitrogen, using ferrocene (Fc) as a standard.

Supplementary Information

3. References

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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, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, Ö. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski and D. J. Fox, Gaussian, Inc., Wallingford CT, 2009.