Supplementary Material (ESI) for *PCCP*

Electronic Supplementary Information (ESI) Available:

Reference of Gaussian 03; QM Computed Mulliken Charge of Neutral and Cationic States of Eight Molecules in Scheme **1** (Figure S1); Computation details of cation internal reorganization energy λ (Table S1). HOMO and LUMO of the molecules in Scheme **1** (Figure S2).

Revealing quantitative structure-activity relationships of transport properties in acene and acene derivative organic materials

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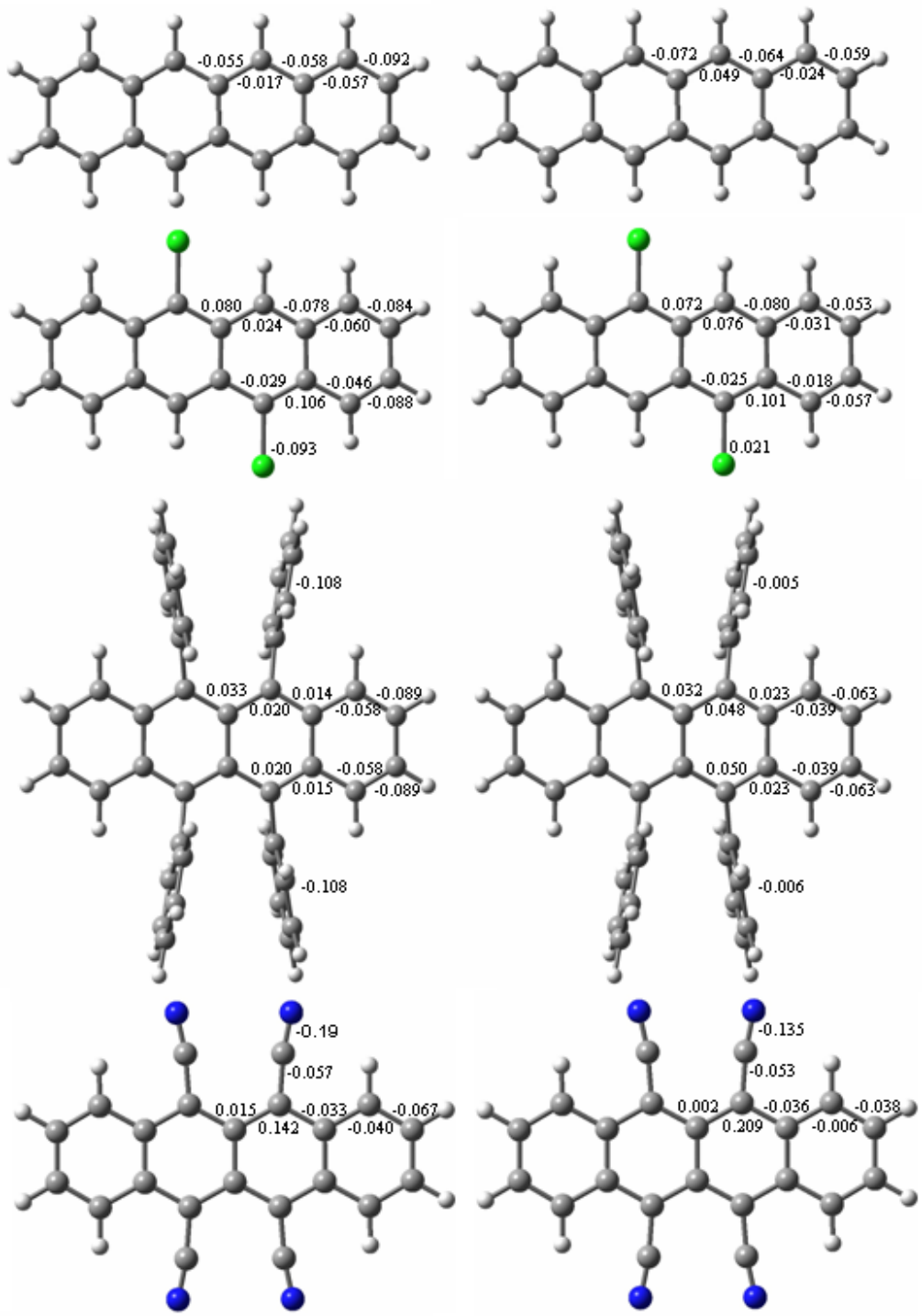
Gaussian 03, Revision C.02:
M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, J. A. Montgomery, Jr., T. Vreven, K. N. Kudin, J. C. Burant, J. M. Millam, S. S. Iyengar, J. Tomasi, V. Barone, B. Mennucci, M. Cossi, G. Scalmani, N. Rega, G. A. Petersson, H. Nakatsuji, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, M. Klene, X. Li, J. E. Knox, H. P. Hratchian, J. B. Cross, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, P. Y. Ayala, K. Morokuma, G. A. Voth, P. Salvador, J. J. Dannenberg, V. G. Zakrzewski, S. Dapprich, A. D. Daniels, M. C. Strain, O. Farkas, D. K. Malick, A. D. Rabuck, K. Raghavachari, J. B. Foresman, J. V. Ortiz, Q. Cui, A. G. Baboul, S. Clifford, J. Cioslowski, B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I. Komaromi, R. L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham, C. Y. Peng, A. Nanayakkara, M. Challacombe, P. M. W. Gill, B. Johnson, W. Chen, M. W. Wong, C. Gonzalez, and J. A. Pople, Gaussian, Inc., 2004.

Fig. S1. QM Computed Mulliken Charge of Neutral and Cationic States of Eight Molecules in Scheme **1.**



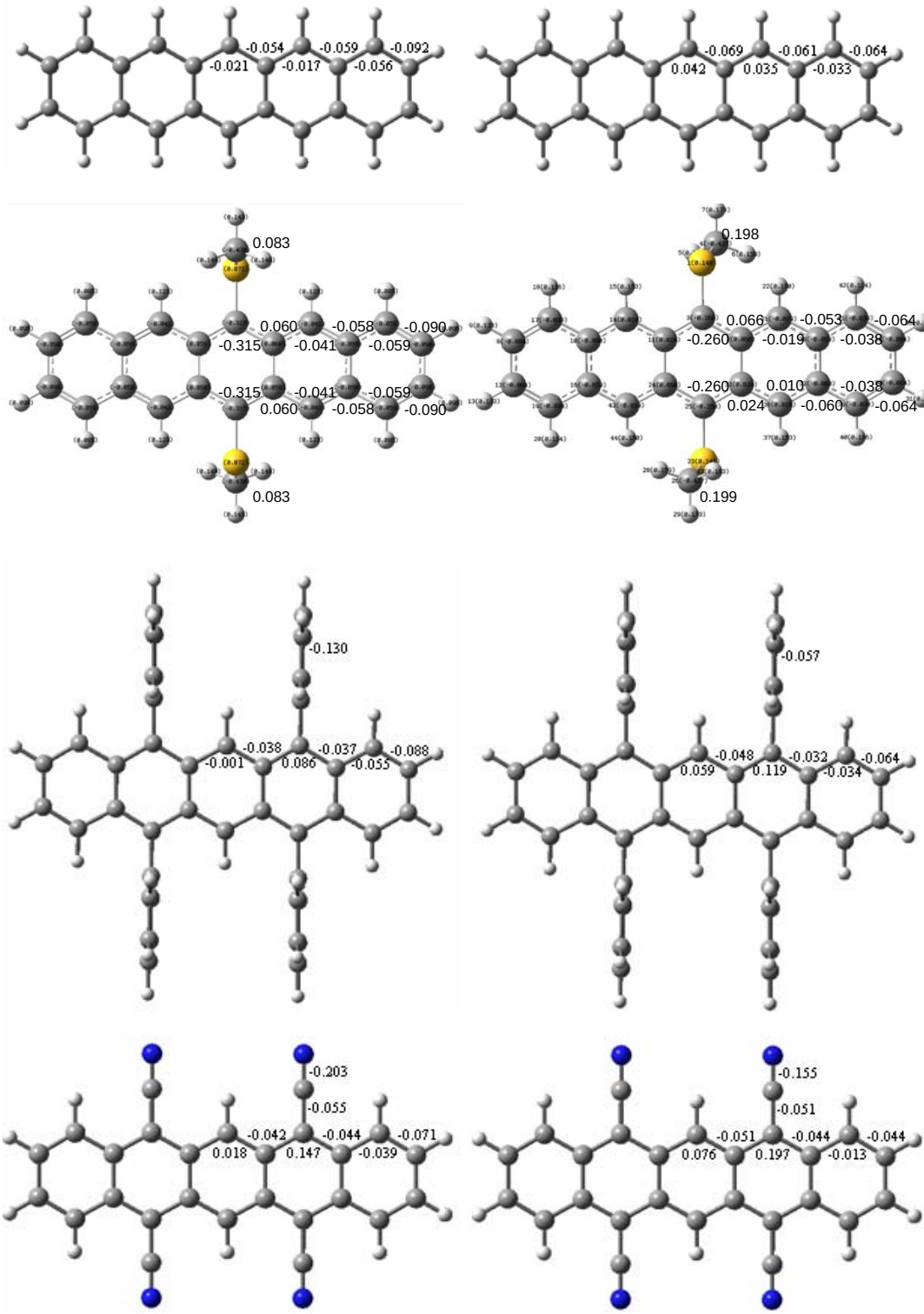


Table S1. Computation details of cation internal reorganization energy λ. E (neutral in neutral geometry), E^*(neutral in cation geometry), E_+(cation in cation geometry) and E_+^* (cation in neutral geometry) are in Hartree, and the IP(ionization potential) and λ are in eV.

	TETR	DCT	RUBR	TCT	PENT	BMP	TPP	TCP
E (hartree)	-693.32294	-1612.55922	-1617.69733	-1062.34506	-846.98952	-1722.05239	-1771.40103	-1216.03824
E^* (hartree)	-693.32083	-1612.55654	-1617.69449	-1062.34365	-846.98775	-1722.05006	-1771.39892	-1216.03691
E_+ (hartree)	-693.08380	-1612.31177	-1617.47588	-1062.05731	-846.76436	-1721.82566	-1771.19019	-1215.76728
E_+^* (hartree)	-693.08164	-1612.30905	-1617.47309	-1062.05586	-846.76255	-1721.82368	-1771.18805	-1215.76593
IP (eV)	6.5662	6.8075	6.1019	7.8696	6.1762	6.1697	5.7955	7.4100
	6.97[a]		6.41[a]		6.63[a]			7.148[b]
λ (eV)	0.1160	0.1468	0.1531	0.0778	0.0976	0.1172	0.1248	0.0730
	0.1130[c]	0.1410[b]	0.1590[d]		0.0970[c]			0.0690[b]

[a] Reference 66. [b] Reference 11. [c] Reference 62. [d] Reference 64.

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Fig. S2. HOMO and LUMO of the molecules in Scheme **1.**