

*Supporting Information*

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**Axle charge effects on photoinduced electron transfer  
processes in rotaxanes containing porphyrin and [60]fullerene**

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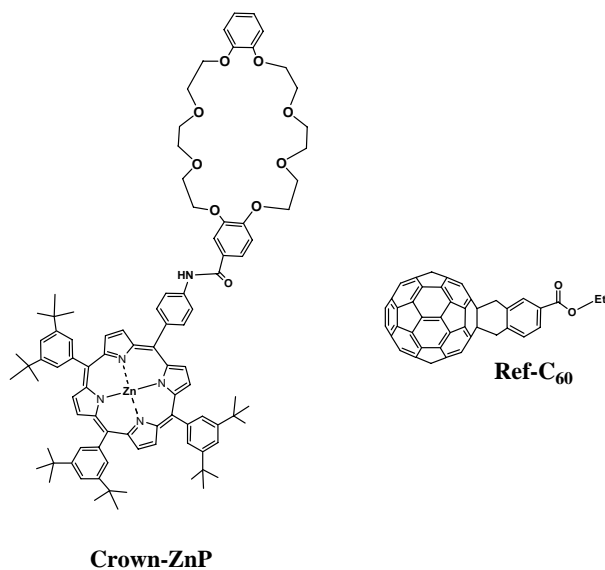
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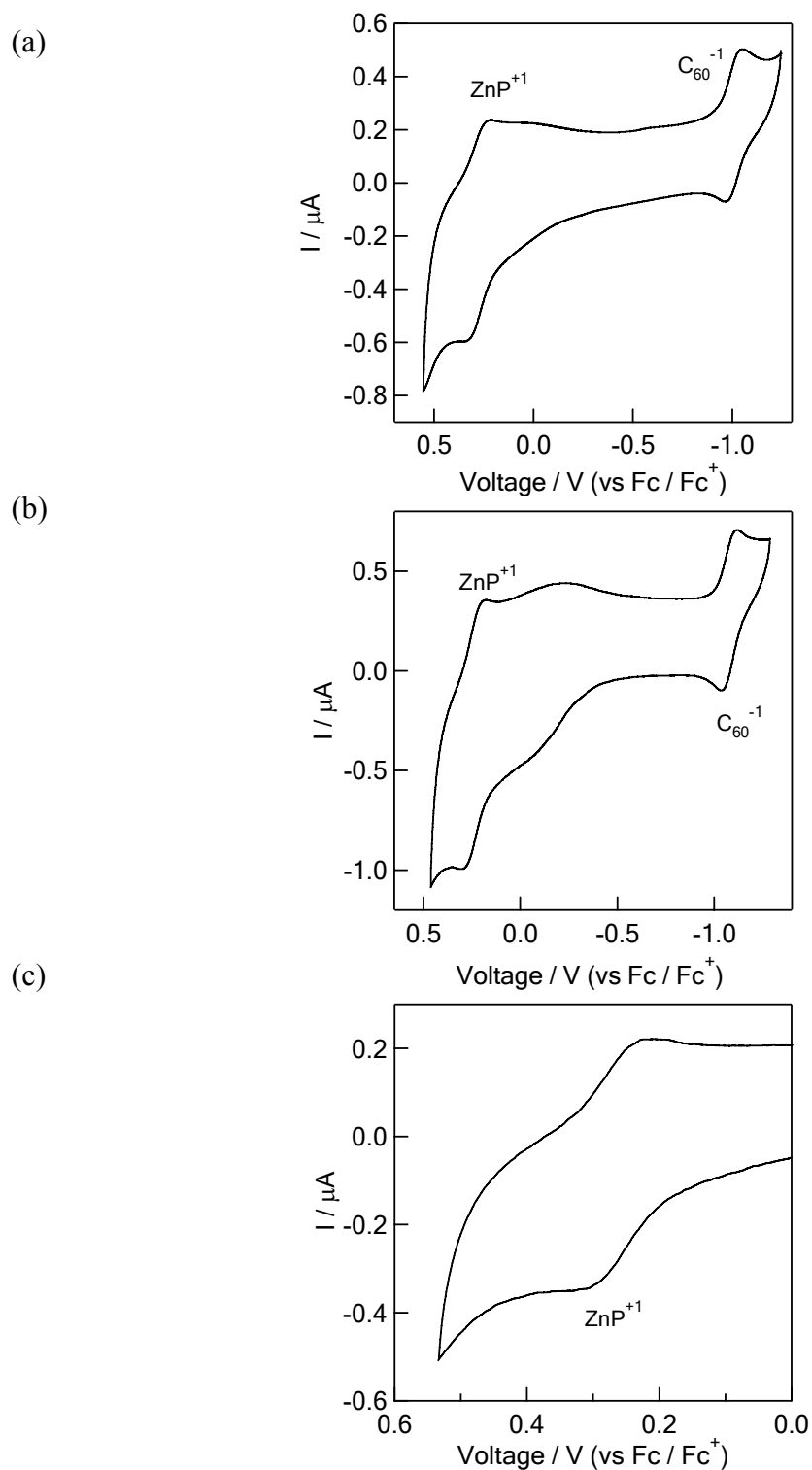
**Scheme S1.** Molecular structures of references Crown-**ZnP**<sup>ref-1</sup> and Ref-**C<sub>60</sub>**.<sup>ref-2</sup>

<sup>ref-1</sup> H. Sasabe, Y. Furusho, A.S. D. Sandanayaka, Y. Araki, N. Kihara, K. Mizuno, A. Ogawa, T. Takata, O. Ito, *J. Porphyrins Phthalocyanines* **2006**, *10*, 1346-1359

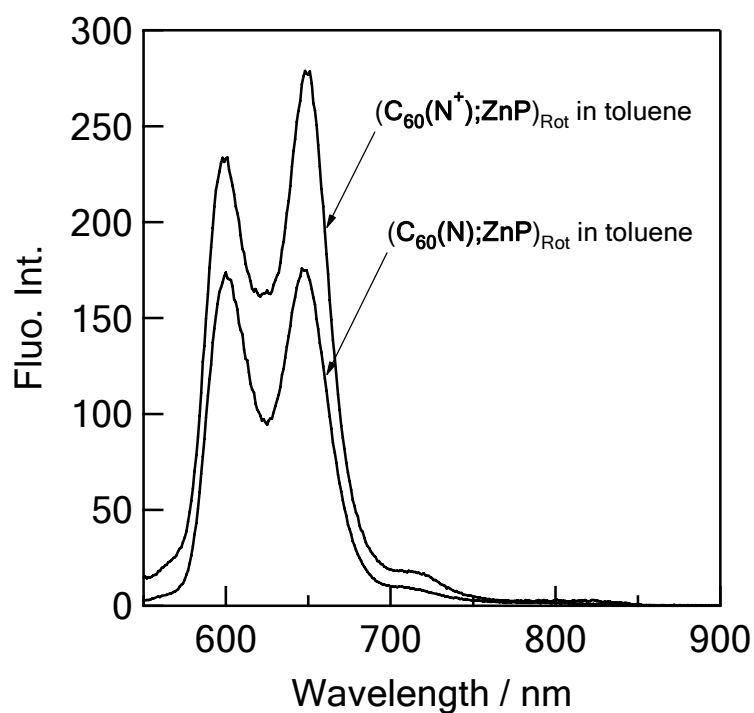
<sup>ref-2</sup> A. S. D. Sandanayaka, K. Ikeshita, G. A. Rajkumar, Y. Furusho, Y. Araki, T. Takata, O. Ito, *J. Phys. Chem. A* **2005**, *109*, 8088-8095.

**Table S1.** Free-energy changes of charge-recombination ( $\Delta G_{CR}$ ) of  $(C_{60}(N);ZnP)_{Rot}$  and  $(C_{60}(N^+);ZnP)_{Rot}$  in DMF, PhCN, THF, and toluene

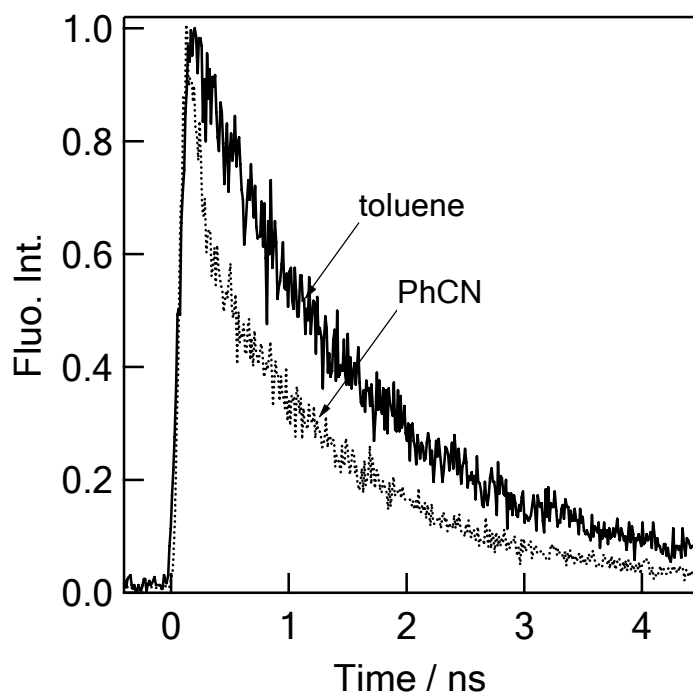
Rotaxanes	Solvs.	$-\Delta G_{CR}^a$ ( $C_{60};ZnP$ )
$(C_{60}(N);ZnP)_{Rot}$	DMF	1.22
	PhCN	1.24
	THF	1.37
	TN	1.79
$(C_{60}(N^+);ZnP)_{Rot}$	DMF	1.17
	PhCN	1.19
	THF	1.25
	toluene	1.45



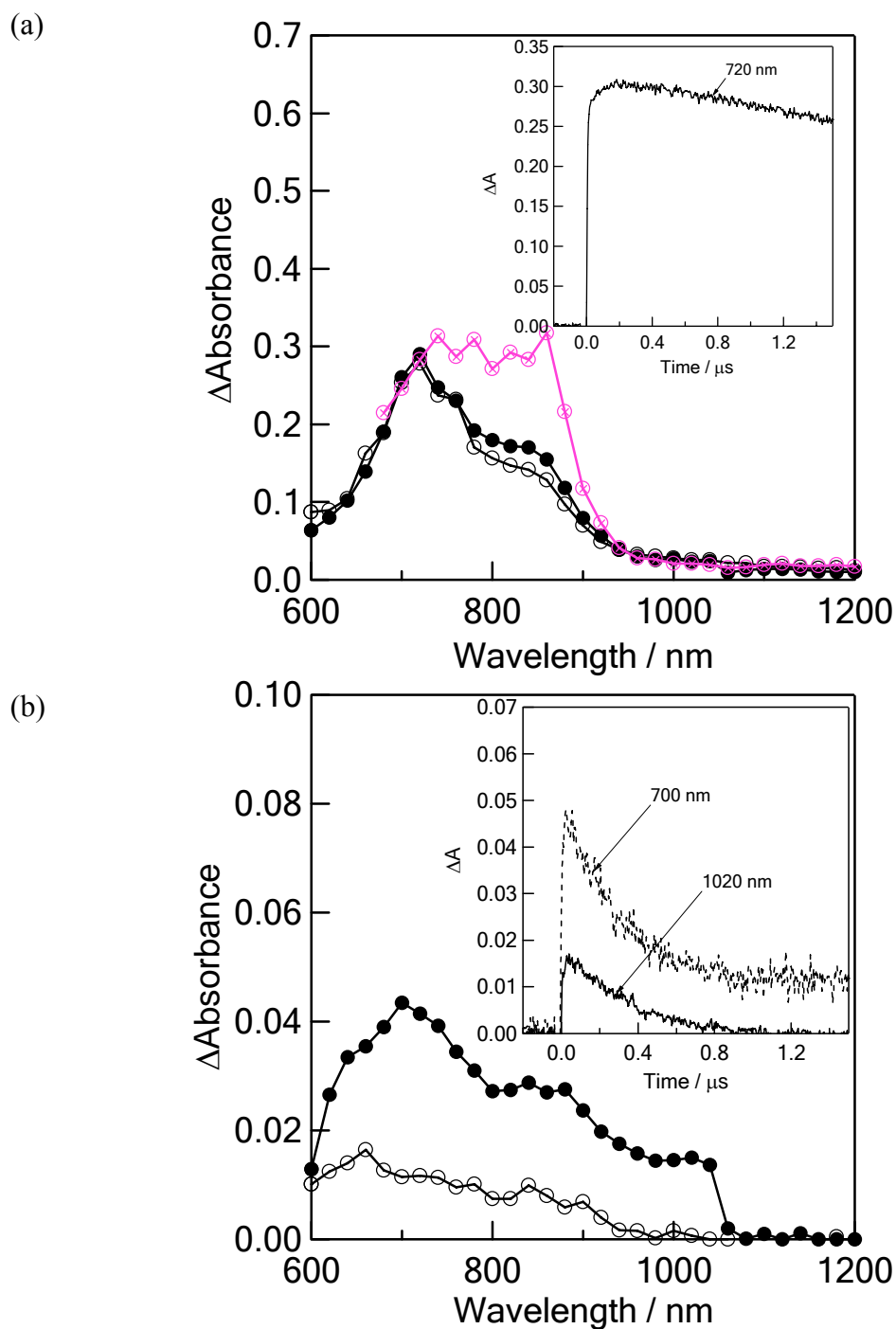
**Fig. S1.** Cyclic voltammograms in PhCN at scan rate of 100 mV/s at room temperature; (a)  $(\text{C}_{60}(\text{N});\text{ZnP})_{\text{Rot}}$  (b)  $(\text{C}_{60}(\text{N}^+);\text{ZnP})_{\text{Rot}}$  (c) Crown-ZnP.



**Fig. S2.** Steady-state fluorescence spectra of  $(C_{60}(N);ZnP)_{Rot}$  and  $(C_{60}(N^+);ZnP)_{Rot}$  (0.1 mM) in toluene  $\lambda_{ex} = 550$  nm.



**Fig. S3.** Time profiles of the fluorescence at 720-800 nm of  $(C_{60}(N);ZnP)_{Rot}$  in PhCN and toluene. Excitation wavelength was 410 nm.



**Fig. S4.** Nanosecond transient absorption spectra of (a)  $(C_{60}(N);ZnP)_{Rot}$  and Crown-ZnP (pink) at 0.1  $\mu s$  (b)  $(C_{60}(N^+);ZnP)_{Rot}$  (0.1mM) observed by 550 nm laser light irradiation in at 0.1  $\mu s$  (●) and 1.0  $\mu s$  (○) in toluene. Inset: Absorption-time profiles in toluene.

Reference 14 A. *Gaussian 03*, Revision A.7; Gaussian, Inc.: Pittsburgh, PA, 2003 (ESI)

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, V. Bakken, 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., Wallingford CT, 2004.