

Supplementary information

Charge-transfer Complexes from Decamethylferrocene and 1,4-Quinone Derivatives — Neutral–ionic Phase Diagrams for Metallocene Complexes

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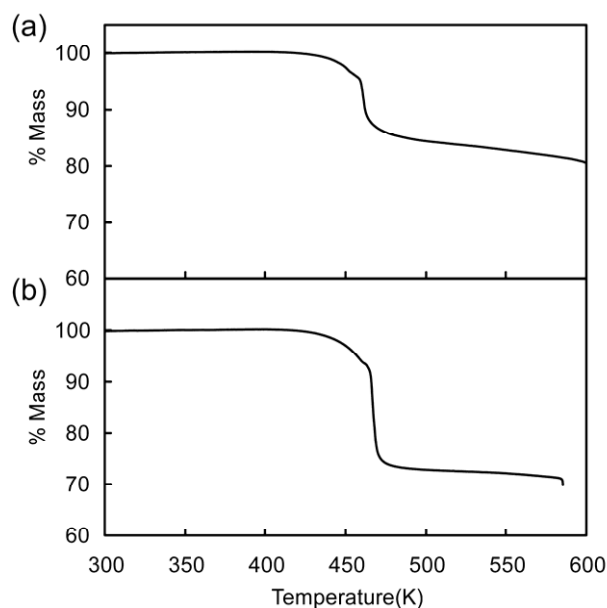


Fig. S1. TG traces of (a) **1** and (b) **2**.

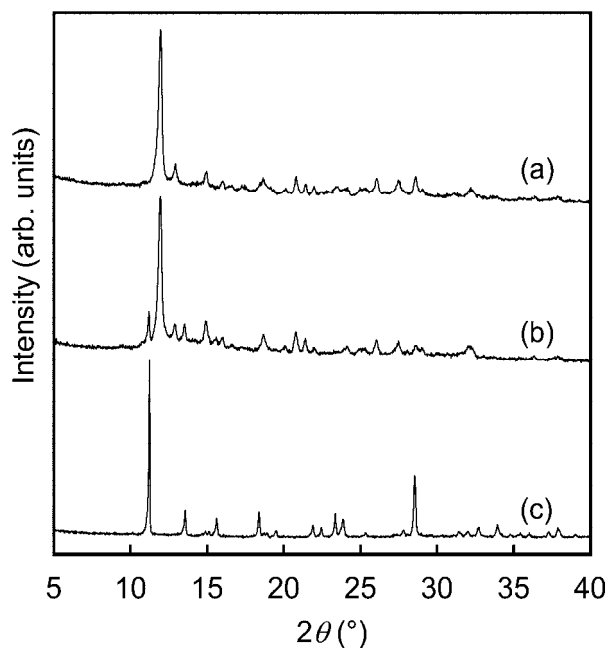


Fig. S2. XRD patterns of powders obtained by ball-milling of $[\text{Fe}(\text{C}_5\text{HMe}_4)_2]$ and Cl_2BQ in the presence of a drop of dichloromethane in DA ratios of (a) 1:2 and (b) 1:1. (c) XRD pattern of a mixture of $[\text{Fe}(\text{C}_5\text{HMe}_4)_2]$ and Cl_2BQ .

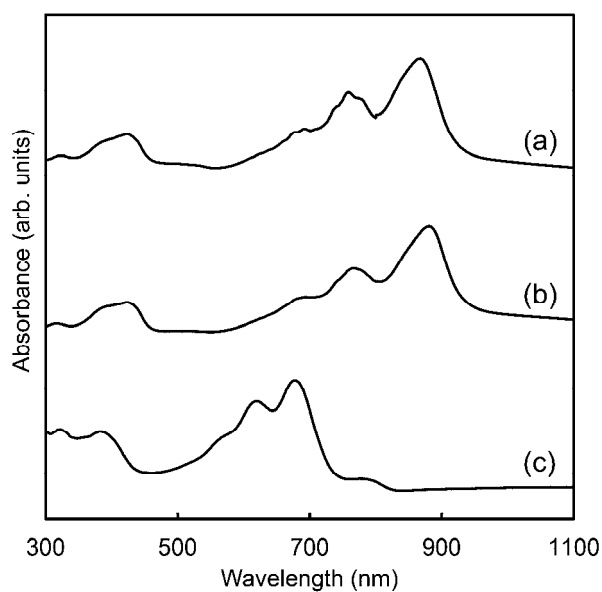


Fig. S3. Solid-state electronic spectra of (a) $[\text{Fe}(\text{Cp}^*)_2][\text{TCNQ}]$, (b) $[\text{Fe}(\text{C}_5\text{HMe}_4)_2][\text{TCNQ}]$, and (c) $[\text{Fe}(\text{Cp}^*)_2][\text{DMDCNQI}]$.

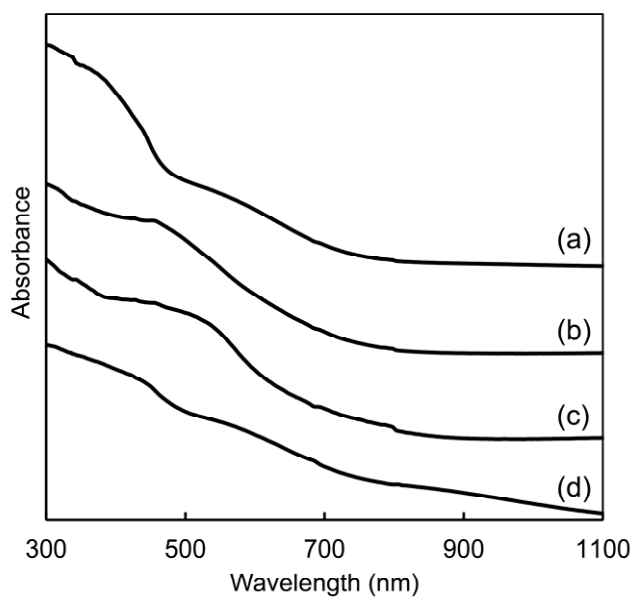


Fig. S4. Solid-state electronic spectra of the reaction products of $[\text{Co}(\text{Cp}^*)_2]$ and (a) F_4BQ , (b) Cl_4BQ , (c) Br_4BQ , and (d) Cl_2BQ .

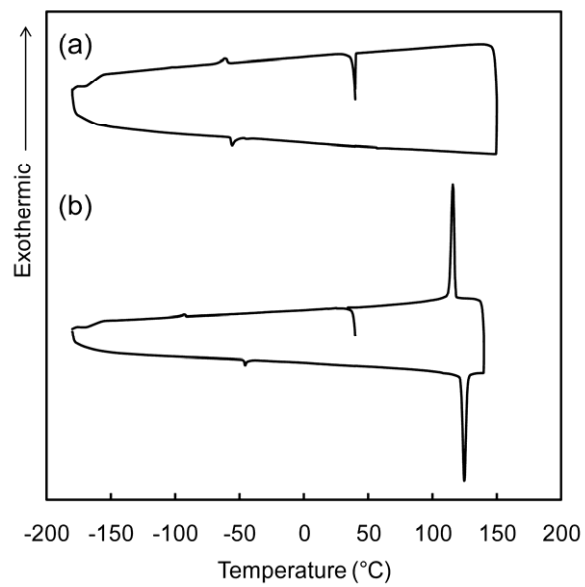


Fig. S5. DSC traces for (a) $[\text{Fe}(\text{Cp}^*)_2][\text{TCNQ}]$ (1-D phase) and (b) $[\text{Fe}(\text{C}_5\text{HMe}_4)_2][\text{TCNQ}]$.