Supporting Information

Influencing Electronic Interaction in Diferrocenyl-1-Phenyl-1H-Pyrroles

Alexander Hildebrandt and Heinrich Lang*

Table of Contents

Figure SI1 $^1$H NMR and simulated spectrum of 3e 2
Figure SI2 $^1$H-$^1$H-COSY NMR spectrum of 3e 2
Figure SI3 $^1$H-$^{13}$C-HSQC NMR spectrum of 3e 3
Figure SI4 NIR spectra of 3a. 3
Figure SI5 NIR spectra of 3b. 4
Figure SI6 NIR spectra of 3e. 4
Figure SI7 NIR spectra of 3f. 5
**Figure SI1** Top: $^1$H NMR spectrum of 3e in the range between 6.9 and 7.5 ppm in CDCl$_3$ (7.26 ppm) at 25 °C; bottom: simulated spectrum of 3e for a frequency of 500.13 MHz and a line width of 0.5 Hz.

**Figure SI2** Top: $^1$H-$^1$H-COSY NMR spectrum of 3e in the range between 6.9 and 7.5 ppm in CDCl$_3$ (7.26 ppm) at 25 °C.
**Figure S13** Top: $^1$H-$^{13}$C-HSQC NMR spectrum of 3e (range: $^1$H 6.9 to 7.5 ppm; $^{13}$C 110 to 145 ppm) in CDCl$_3$ at 25 °C.

**Figure S14** NIR spectrum of 3a. Arrows indicate increasing, decreasing or shifting of the absorptions; dichloromethane solutions (1.0 mmol·L$^{-1}$) at 25 °C, supporting electrolyte [N$^n$Bu$_4$][B(C$_6$F$_5$)$_4$] (0.1 mol·L$^{-1}$); bottom: oxidation of 3a to 3a$^+$ at potentials from -400 to 350 mV; middle: oxidation of 3a$^+$ to 3a$^{2+}$ (375 - 600 mV); top: oxidation of 3a$^{2+}$ to 3a$^{3+}$ (600 – 1500 mV).
Figure SI5 NIR spectrum of 3b. Arrows indicate increasing, decreasing or shifting of the absorptions; dichloromethane solutions (1.0 mmol·L⁻¹) at 25 °C, supporting electrolyte [NºBu₄][B(C₆F₅)₄] (0.1 mol·L⁻¹); bottom: oxidation of 3b to 3b⁺ at potentials from -200 to 325 mV; top: oxidation of 3b⁺ to 3b²⁺ (350 - 1000 mV).

Figure SI6 NIR spectrum of 3e. Arrows indicate increasing, decreasing or shifting of the absorptions; dichloromethane solutions (1.0 mmol·L⁻¹) at 25 °C, supporting electrolyte [NºBu₄][B(C₆F₅)₄] (0.1 mol·L⁻¹); bottom: oxidation of 3e to 3e⁺ at potentials from -200 to 350 mV; top: oxidation of 3e⁺ to 3e²⁺ (350 - 1000 mV).
Figure SI7 NIR spectrum of 3f. Arrows indicate increasing, decreasing or shifting of the absorptions; dichloromethane solutions (1.0 mmol·L⁻¹) at 25 °C, supporting electrolyte [N⁺Bu₄][B(C₆F₅)₄] (0.1 mol·L⁻¹); bottom: oxidation of 3f to 3f⁺ at potentials from -200 to 350mV; top: oxidation of 3f⁺ to 3f²⁺ (350 - 1000 mV).