Supplementary Material (ESI) for Dalton Transactions

Curly-curly, loop-loop: homoleptic metal(II) complexes of pyridinecarbaldehyde 4'-(2,2':6',2''-terpyridyl)hydrazones and their coordination polymers

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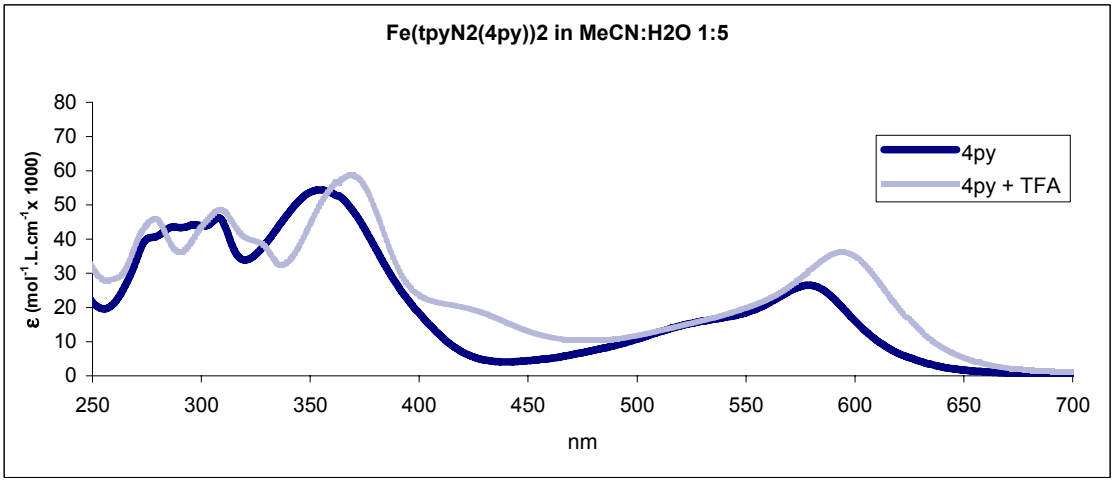
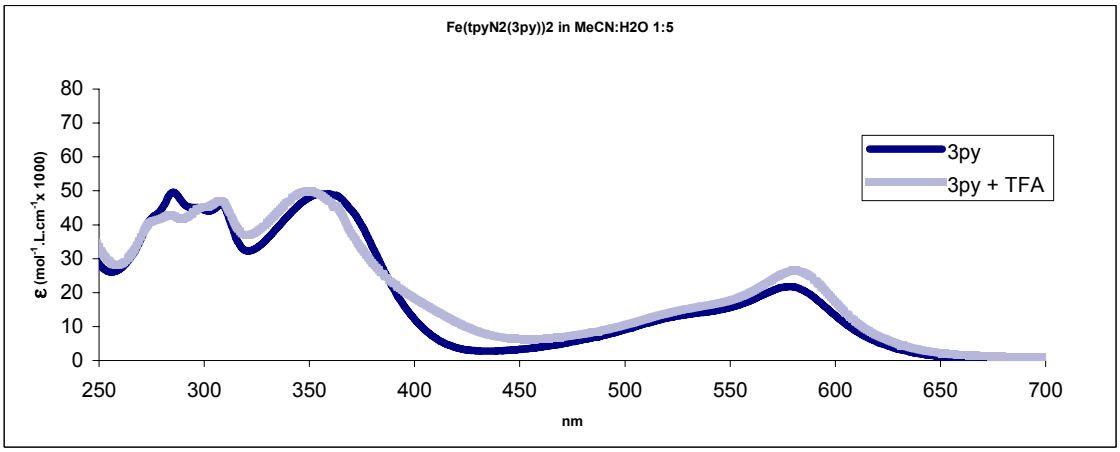
Electronic absorption spectra for $[Fe(\mathbf{1})_2][PF_6]_2$, $[Fe(\mathbf{2})_2][PF_6]_2$ and $[Fe(\mathbf{3})_2][PF_6]_2$ and their protonated analogues.

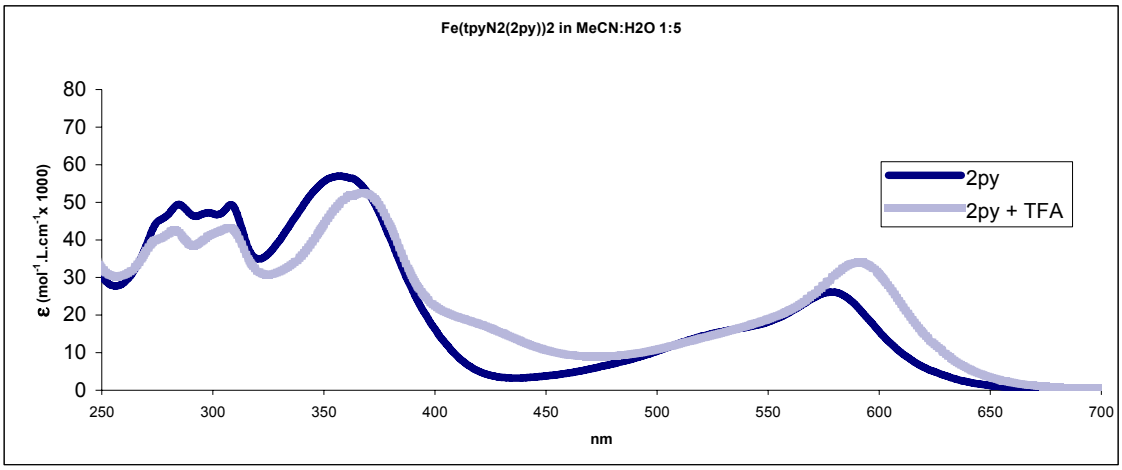
$[Fe(\mathbf{1})_2][PF_6]_2$



$[Fe(\mathbf{2})_2][PF_6]_2$



$[Fe(\mathbf{3})_2][PF_6]_2$



500 MHz ^{1}H NMR and 125 MHz ^{13}C{^{1}H} NMR spectrosocpic data for $[Fe(H\mathbf{1})_2]^{4+}$, $[Fe(H\mathbf{2})_2]^{4+}$ and $[Fe(H\mathbf{3})_2]^{4+}$.

$[Fe(H\mathbf{1})_2]^{4+}$: $[Fe(\mathbf{1})_2][PF_6]_2$ in MeCN-d_3 + TFA-d_1

^{1}H δ / ppm: 11.14 (s, 2H, NH), 8.73 (d, J 6.9 Hz, 4H, H^{C2}), 8.66 (s, 4H, H^{B3}), 8.50 (d, J 8.0 Hz, 4H, H^{A3}), 8.48 (d, J 6.9 Hz, 4H, H^{C3}), 8.35 (s, 2H, N=CH), 7.89 (td, J 1.2, 7.8 Hz, 4H, H^{A4}), 7.24 (d, J 5.5 Hz, 4H, H^{A6}), 7.09 (ddd, J 1.0, 5.7, 7.1 Hz, 4H, H^{A5}). ^{13}C{^{1}H} δ / ppm: 159.0 ($C^{A2/B2}$), 158.7 ($C^{A2/B2}$), 154.4 (C^{A6}), 153.0 (C^{C4}), 142.5 (C^{C2}), 139.4 (CA4), 138.3 ($C^{CH=N}$), 128.2 (C^{A5}), 124.6 (C^{A3}), 124.5 (C^{C3}), 109.3 (C^{B3}).

$[Fe(H\mathbf{2})_2]^{4+}$: $[Fe(\mathbf{2})_2][PF_6]_2$ in MeCN-d_3 + TFA-d_1

^{1}H δ / ppm: 10.75 (s, 2H, NH), 9.24 (s, 4H, H^{C2}), 9.14 (d, J 8.2 Hz, 2H, H^{C4}), 8.73 (d, J 5.7, 2H, H^{C6}), 8.60 (br s, 4H, H^{B3}), 8.48 (d, J 7.6 Hz, 4H, H^{A3}), 8.36 (s, 2H, N=CH), 8.16 (dd, J 5.8, 8.0 Hz, 2H, H^{C5}), 7.88 (t, J 7.6, 4H, H^{A4}), 7.25 (d, J 5.2 Hz, 4H, H^{A6}), 7.09 (dd, J = 5.8, 6.9 Hz, 4H, H^{A5}). ^{13}C{^{1}H} δ / ppm: 159.2 ($C^{A2/B2}$), 154.5 (C^{A6}), 153.4 (C^{B4}), 144.7 (C^{C4}), 141.9 (C^{C6}), 140.7

(C^{C2}), 139.4 (C^{A4}), 137.4 ($C^{CH=N}$), 136.2 (C^{C3}), 128.8 (C^{C5}), 128.1 (C^{A5}), 124.4 (C^{A3}), 108.8 C^{B3}).

$[Fe(H\mathbf{3})_2]^{4+}$: $[Fe(\mathbf{3})_2][PF_6]_2$ in MeCN-d_3 + TFA-d_1

^{1}H δ / ppm: 11.12 (s, 2H, NH), 8.82 (d, J 5.5 Hz, 2H, C^{C6}), 8.70 (br s, 4H, H^{B3}), 8.68 (td, J 1.2, 8.1 Hz, 2H, H^{C4}), 8.48 (d, J 8.0 Hz, 4H, H^{A3}), 8.35 (s, 2H, $H^{CH=N}$), 8.32 (d, J 8.2 Hz, 2H, H^{C3}), 8.02 (t, J 6.5 Hz, 2H, H^{C5}), 7.91 (t, J 7.3 Hz, 4H, H^{A4}), 7.25 (d, J 5.2 Hz, 4H, H^{A6}), 7.10 (t, J 6.1 Hz, 4H, H^{A5}). $^{13}C\{^1H\}$ δ / ppm: 159.1 ($C^{A2/B2}$), 154.5 (C^{A6}), 149.1 (C^{C4}), 142.9 (C^{C6}), 139.6 (C^{A4}), 133.0 ($C^{CH=N}$), 128.3 (C^{A5}), 127.7 ($C^{C3/C5}$), 127.6 ($C^{C3/C5}$), 124.5 (C^{A3}), 109.5 (C^{B3}).