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Article

Effects of Chemically-Modified Polypyridyl Ligands on the Structural and Redox Properties of Tricarbonylmanganese(I) Complexes

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Table S1. Hydrogen-bond geometry (Å, °) for **Mn-dpq** and **Mn-dpc**.

<Mn-dpq>

***D*–H···A**	***D*–H**	**H···A**	***D*···A**	***D*–H···A**
C5–H2···Br1^{i}	0.95	2.93	3.681(5)	137
C13–H4···Br1^{ii}	0.95	2.85	3.536(5)	130
C18–H10···O4^{iii}	0.98	2.60	3.399(7)	139
C18–H12···O4^{iv}	0.98	2.38	3.333(7)	163

Symmetry codes: (i) $x, 1+y, z$; (ii) $x, -\frac{1}{2}-y, -\frac{1}{2}+z$; (iii) $2-x, -y, 1-z$; (iv) $x, \frac{1}{2}-y, \frac{1}{2}+z$

<Mn-dpc>

***D*–H···A**	***D*–H**	**H···A**	***D*···A**	***D*–H···A**
O4–H1···O5	0.84	2.56	2.949(2)	110
O4–H1···Br1^{i}	0.84	2.46	3.2601(19)	159
O5–H2···O4	0.84	2.56	2.949(2)	110
O5–H2···Br1^{i}	0.84	2.50	3.304(2)	162
C6–H5···O2^{ii}	0.95	2.36	3.080(3)	132

Symmetry codes: (i) $1-x, -y, 2-z$; (ii) $-1+x, -1+y, z$

Table S2. Hydrogen-bond geometry (Å, °) for **Mn-qpy** and **Mn-dmqpy**

<Mn-qpy>

***D*–H···A**	***D*–H**	**H···A**	***D*···A**	***D*–H···A**
C16–H8···O1^{i}	0.95	2.60	3.399(3)	142
C18–H10···Br1^{ii}	0.95	2.92	3.7693(19)	149
C21–H12···O2^{iii}	0.95	2.53	3.461(3)	168

Symmetry codes: (i) $1-x, -\frac{1}{2}+y, \frac{1}{2}-z$; (ii) $2-x, 2-y, 1-z$; (iii) $2-x, -\frac{1}{2}+y, \frac{3}{2}-z$

<Mn-dmqpy>

D–H···A	*D*–H	H···A	*D*···A	*D*–H···A
C7–H3···Br2	0.95	2.86	3.810(8)	175
C10–H4···Br2	0.95	2.89	3.843(7)	177
C13–H6···Br1^{i}	0.95	2.92	3.573(7)	127
C15–H7···F5^{ii}	0.95	2.54	3.181(16)	125
C18–H10···Br2	0.95	2.64	3.492(11)	150
C19–H12···F4^{iii}	0.98	2.51	3.278(13)	135
C19–H13···F1^{iv}	0.98	2.51	3.259(14)	133
C21–H14···Br2	0.95	2.68	3.567(9)	156
C25–H20···O1^{v}	0.98	2.21	3.088(12)	148

Symmetry codes: (i) $-1+x, y, z$; (ii) $1+x, y, z$; (iii) $2-x, 1-y, -z$; (iv) $3-x, 1-y, -z$; (v) $x, -1+y, z$

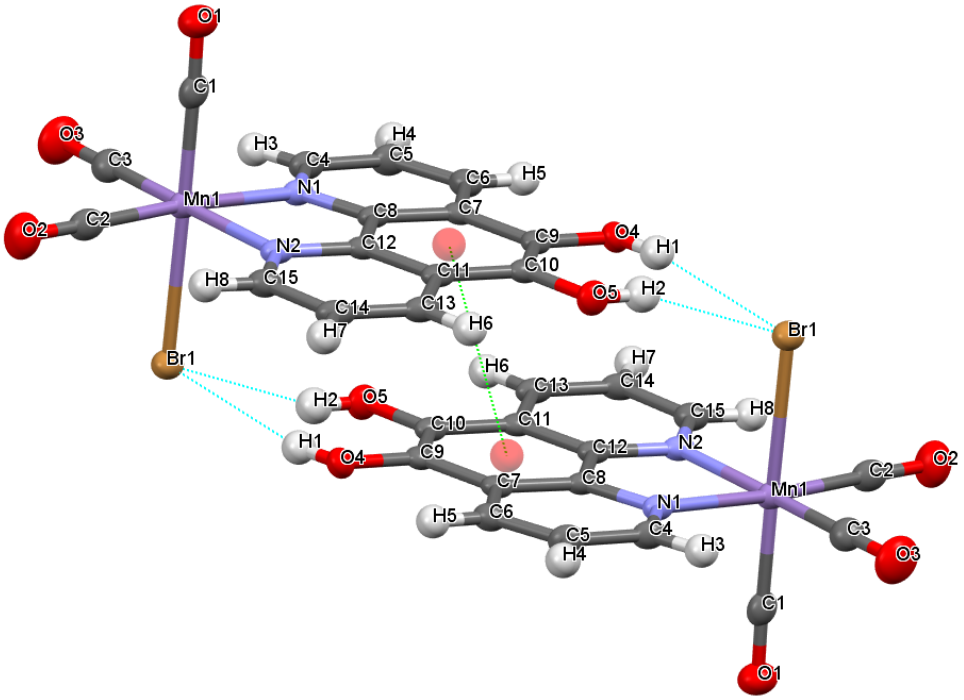

Figure S1. A dimer formation caused by intermolecular hydrogen bonds and π-π stacking in the crystal packing of **Mn-dpc**.

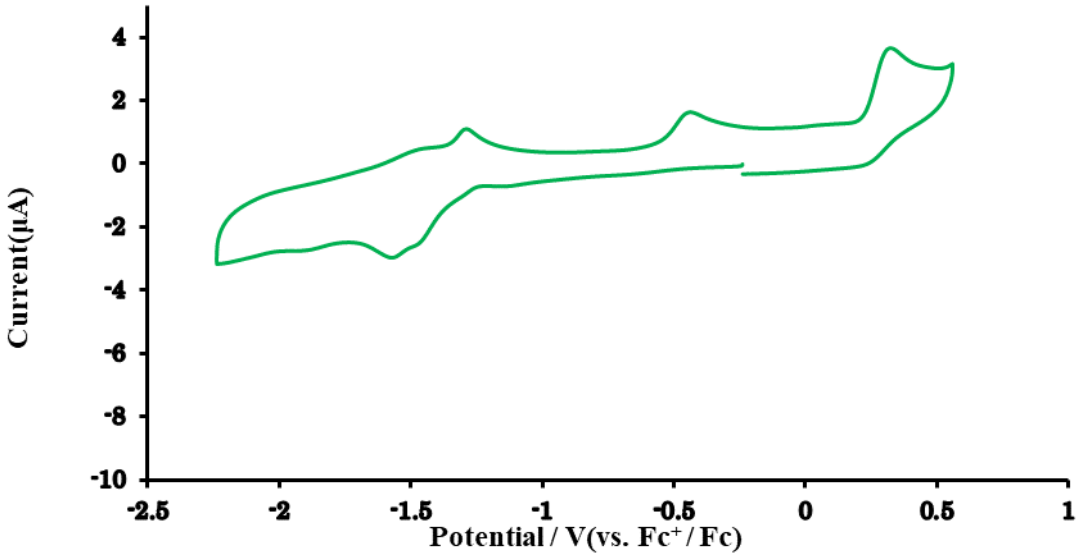

Figure S2. Cyclic voltammogram of **Mn-qpy** in DMF (v = 0.1 V s^{-1}, c = 0.5 mM).

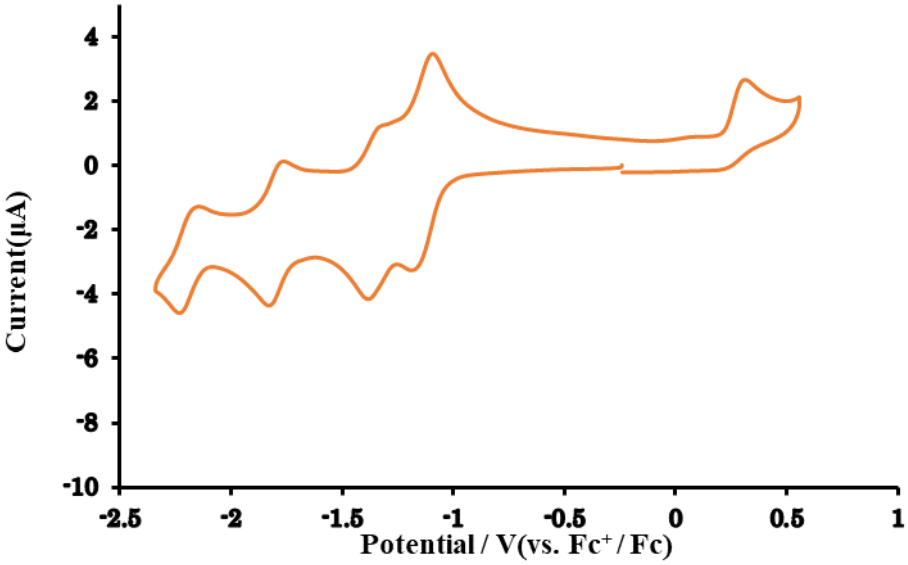

Figure S3. Cyclic voltammogram of **Mn-dmqpy** in DMF (v = 0.1 V s^{-1}, c = 1 mM).