

Supporting Information

Synthesis, Crystal Structure and MMCT of New Cyanide-bridged Complexes *cis*-M^{II}(dppm)₂(CN)₂(Fe^{III}X₃)₂ (M = Ru, Os)

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Table S1. Calculated Geometries of Compounds 1-6.

	1	2	3	4	5	6
M1-C51	2.025	2.016	1.989	1.992	1.983	1.989
M1-C52	2.024	2.003	1.991	1.993	1.988	1.988
M1-P1	2.388	2.369	2.420	2.419	2.429	2.416
M1-P2	2.387	2.365	2.501	2.500	2.492	2.482
M1-P3	2.483	2.405	2.421	2.418	2.417	2.419
M1-P4	2.486	2.397	2.502	2.499	2.487	2.478
C51≡N1	1.173	1.130	1.174	1.174	1.177	1.176
C52≡N2	1.173	1.145	1.174	1.174	1.177	1.176
C51-M1-C52	86.2	87.4	88.2	87.8	87.4	88.1
N1≡C51-M1	175.1	175.3	175.2	175.3	175.0	175.8
N2≡C52-M1	175.2	177.5	175.1	175.2	175.8	175.1
C51≡N1-Fe1			174.8	176.4	179.2	176.1
C52≡N2-Fe2			175.2	176.5	172.1	178.5
Fe1-N1			1.995	2.003	1.987	1.996
Fe2-N2			1.996	2.003	1.986	1.996
Fe1-X1			2.223	2.367	2.240	2.370
Fe1-X2			2.236	2.354	2.226	2.356
Fe1-X3			2.215	2.345	2.214	2.347
Fe2-X4			2.236	2.367	2.215	2.357
Fe2-X5			2.215	2.345	2.209	2.347
Fe2-X6			2.223	2.354	2.259	2.369