

Electronic Supplementary Information

Table S1. Spin population obtained using a Mulliken approach for the iron and oxygen bridging atoms in the highest (HS) and lowest spin (LS) configuration.

	HS	LS
Fe1	4.3129	4.3035
Fe2	4.3129	4.3035
Fe3	4.1933	-4.1848
Fe4	4.1933	-4.1848
O1 [Fe1, Fe2, Fe4, Y6]	0.3989	0.1720
O2 [Fe1, Fe2, Fe3, Y5]	0.3989	0.1720
O3 [Fe3, Y5]	0.1847	-0.1816
O4 [Fe4, Y6]	0.1847	-0.1816
O5 [Fe1, Fe3]	0.2420	-0.0594
O6 [Fe2, Fe4]	0.2420	-0.0594
O7 [Fe2, Fe3]	0.2267	-0.0196
O8 [Fe1, Fe4]	0.2267	-0.0196

