Supporting Information

X-Ray Absorption Spectroscopic Study of the Transition-Metal-Only Double Perovskite Oxide Mn_2CoReO_6

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Table S1. Rietveld refinement results of MCRO. Space group is $P2_1/n$ (No. 14) with lattice parameters a = 5.23506(1) Å, b = 5.35179(1) Å, c = 7.63109(2) Å, and β = 89.966(0)°. R_{wp} = 8.21%, R_p = 4.91%, and χ^2 = 18.15.

Atom	x	y	z	Site occupancy	$U_{iso} \times 100$ (Å^2)
Mn (4*e*)	0.4970(2)	0.5495(2)	0.7448(2)	1	0.84(3)
Co (2*c*)	0	0.5	0	0.978(2)	0.04(7)
Re (2*d*)	0.5	0	0	0.978(2)	0.16(1)
Co (2*d*) (anti-site)	0.5	0	0	0.022(2)	0.04(7)
Re (2*c*) (anti-site)	0	0.5	0	0.022(2)	0.16(1)
O(1) (4*e*)	0.3429(14)	0.2971(14)	0.9354(11)	1	0.99(2)
O(2) (4*e*)	0.3147(13)	0.3238(14)	0.5617(10)	1	0.17(2)
O(3) (4*e*)	0.8769(12)	0.4304(12)	0.7356(10)	1	0.20(2)

Table S2. Bond lengths of MCRO from the refinement. The BVS values (V_i) were calculated using the formula $V_i = \sum_j S_{ij}$, and $S_{ij} = exp[(r_0 - r_{ij})/0.37]$ with r_0 = 1.790 Å and 1.692 Å for Mn and Co, respectively.

Mn-O(1) (Å)	2.142(8), 2.611(7), 2.708(8)
Mn-O(2) (Å)	2.080(8), 2.627(8), 2.644(7)
Mn-O(3) (Å)	2.090(6). 2.148(7)
BVS (Mn)	**2.06**
Co-O(1) (Å) (×2)	2.155(8)
Co-O(2) (Å) (×2)	2.041(7)
Co-O(3) (Å) (×2)	2.151(7)
BVS (Co)	**1.93**
Re-O(1) (Å) (×2)	1.857(8)
Re -O(2) (Å) (×2)	1.956(7)
Re -O(3) (Å) (×2)	1.946(7)

Table S3. Bond angles of MCRO from the refinement.

∠Mn-O1-Co (°)	98.68(31)
∠Mn-O2-Co (°)	115.48(34)
∠Mn-O3-Co (°)	90.39(26)
∠Mn-O1-Re (°)	123.6(4)
∠Mn-O2-Re (°)	105.57(33)
∠Mn-O3-Re (°)	106.71(31)
∠Co-O1-Re (°)	137.7(4)
∠Co-O2-Re (°)	138.9(4)
∠Co-O3-Re (°)	137.25(33)