Supplementary Information

New Members of Layered Oxychloride Perovskites with Square Planar Coordination: $Sr_2MO_2Cl_2$ (M = Mn, Ni) and $Ba_2PdO_2Cl_2$

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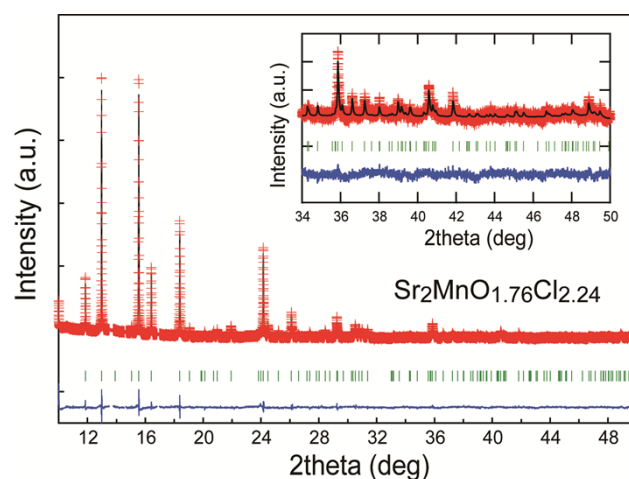
● Reinvestigation of the structural model for $Sr_2MnO_2Cl_2$.

Fig. S1 Rietveld refinement against the synchrotron X-ray diffraction data collected from $Sr_2MnO_2Cl_2$ on the basis of a model with mixed anion at the equatorial sites.

Table. S1. Crystallographic data for $Sr_2MnO_2Cl_2$ from Rietveld refinement of synchrotron X-ray diffraction data on the assumption of mixed anions at the equatorial sites.

Atom	Site	Occupancy	z	B_{iso} (Å)
Sr	(0,0,z) 4e	1	0.38711(10)	1.64(3)
Mn	(0,0,0) 2a	1	—	1.88(8)
O	(0,1/2,0) 4c	0.88(1)[a]	—	1.5(2)[b]
Cl1	(0,1/2,0) 4c	0.12[a]	—	1.5[b]
Cl2	(0,0,z) 4e	1	0.1848(2)	0.80(6)

a (Å)	4.10225(3)
c (Å)	15.01160(11)
R_{wp} (%)	1.49
R_B (%)	7.84
S	2.01
Mn–O (Å)	2.05113(1)
Mn–Cl (Å)	2.775(4)
Sr–O (Å)	2.6606(10)
Sr–Cl×2 (Å)	3.0953(14), 3.036(4)

[a] Occupancies of O and Cl1 was constrained to one in total. [b] The values of B_{iso} for O and Cl1 were constrained to the same one.

● Reinvestigation of the magnetic susceptibility (χ) of the Mn phase. The magnetization data is normalized using the formula weight of the chemical composition determined by the Rietveld refinement shown in Fig. S1 and Table S1.
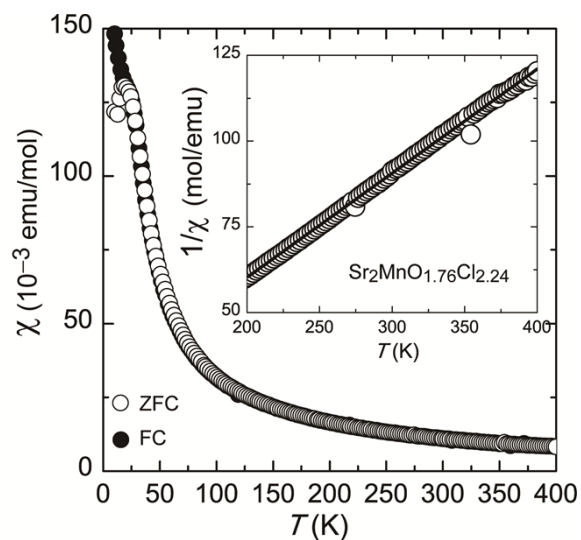

Fig. S2 Magnetic susceptibility of 'Sr$_2$MnO$_{1.76}$Cl$_{2.24}$'. Open and solid circles represent the data measured under zero-field cooled (ZFC) and field cooled (FC) conditions. The inset shows the inverse susceptibility (open circles) and Curie-Weiss fit (solid line). The estimated Curie constant and Weiss temperature are $C = 3.29(1)$ emu K/mol and $\theta = 1.5(11)$ K, respectively.