Supplementary Information

From kröhnkite- to alluaudite-type of structure: novel method of synthesis of sodium manganese sulfates with electrochemical properties in alkaline ion batteries

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Table 1. Fractional atomic coordinates, occupancies and isotropic displacement parameters for the *P21/c* model of $Na_{2+\delta}Mn_{2-\delta/2}(SO_4)_3$.

Atom	x	y	z	Occ.	B / Å^2
Na1	0.2393(17)	0.5216(6)	0.4912(30)	1	1.81(33)
Na2	0.7651(26)	0.2518(25)	0.2967(35)	0.853(13)	17.94(78)
Na3	0.2340(17)	0.2297(11)	0.4471(26)	0.887(11)	10.07(56)
Mn1	0.4719(5)	0.0949(4)	0.3290(9)	0.908(8)	4.42(16)
Mn2	0.0190(5)	0.4073(4)	0.1564(9)	0.954(8)	4.42(16)
S1	0.0273(11)	0.1335(8)	0.1151(16)	1	2.06(16)
O11	0.9129(21)	0.1795(17)	0.100(4)	1	1.517(16)
O12	0.0892(23)	0.0940(17)	0.9417(34)	1	=O11
O13	0.0201(22)	0.0908(21)	0.3473(32)	1	=O11
O14	0.0570(19)	0.2436(21)	0.1989(30)	1	=O11
S2	0.4983(11)	0.3505(10)	0.3304(18)	1	=S1
O21	0.4765(20)	0.4239(22)	0.185(4)	1	=O11
O22	0.4189(20)	0.2522(22)	0.3056(34)	1	=O11
O23	0.4192(22)	0.4127(18)	0.4481(32)	1	=O11
O24	0.6072(20)	0.3476(15)	0.4804(34	1	=O11
S3	0.2461(16)	0.5310(7)	1.0007(24)	1	=S1
O31	0.1583(18)	0.6074(23)	0.8785(33)	1	=O11
O32	0.1873(20)	0.4539(16)	0.1162(35)	1	=O11
O33	0.2957(21)	0.4715(17)	0.8141(33)	1	=O11
O34	0.3145(17)	0.5893(21)	0.124(4)	1	=O11

Table 2. Selected interatomic distances (Å) for the coordination polyhedra in the *P21/c* model of $Na_{2+\delta}Mn_{2-\delta/2}(SO_4)_3$.

S1 – O11	1.444(24)	S2 – O21	1.357(30)	S3 – O31	1.584(22)
– O12	1.490(22)	– O22	1.568(23)	– O32	1.458(23)
– O13	1.636(23)	– O23	1.487(24)	– O33	1.599(26)
– O14	1.556(26)	– O24	1.528(21)	– O34	1.320(20)
Na1 – O11	2.727(20)	Na2– O11	2.421(24)	Na3– O13	3.077(25)
– O12	2.290(24)	– O11	2.660(26)	– O14	2.506(22)
– O23	2.546(25)	– O24	2.592(24)	– O14	2.766(21)
– O24	2.445(21)	– O24	2.939(20)	– O22	2.422(21)
– O31	3.008(22)	– O31	2.918(26)	– O22	3.046(23)
– O32	2.639(22)	– O31	2.370(28)	– O32	2.700(21)
– O33	2.263(20)	– O34	2.372(25)	– O33	2.858(22)
– O34	2.782(23)				
Mn1 – O21	2.296(28)	Mn2 – O12	1.978(23)		
– O21	2.353(25)	– O13	2.417(26)		
– O22	2.127(29)	– O13	2.038(21)		
– O23	2.530(20)	– O14	2.177(29)		
– O33	2.202(25)	– O31	2.048(21)		
– O34	2.457(20)	– O32	2.073(23)		