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Supporting information for article:

Crystal chemistry of lamprophyllite-group minerals from the Murun alkaline complex (Russia) and pegmatites of Rocky Boy and Gordon Butte (USA): Single crystal X-ray diffraction and Raman spectroscopy study

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Supporting Information

Table S1. Fractional site coordinates. equivalent displacement parameters (U_{eq}. Å^2). site multiplicities (Mult.). and site composition for the sample 184/11.

Site	*x*	*y*	*z*	U_{eq}	Mult.	Site occupancy
A	0.2841(1)	0	0.2622(1)	0.0141(2)	4	$Sr_{0.725}K_{0.18}Na_{0.055}Ba_{0.04}$
L	0.3500(1)	0.5	0.2928(2)	0.0064(3)	4	Ti
*M*1	0.5	0.5	0	0.0167(12)	2	Na
*M*2	0	0.2606(3)	0.5	0.0074(6)	4	$Na_{0.83}Mn_{0.09}Ca_{0.08}$
*M*3	0	0.5	0	0.0274(6)	2	$Ti_{0.52}Fe^{3+}_{0.38}Mg_{0.10}$
Si	0.3572(1)	0.7844(2)	0.7959(2)	0.0067(3)	8	Si
O1	0.3260(2)	0.6888(5)	0.5341(5)	0.0134(9)	8	O
O2	0.4371(3)	0.5	0.3317(8)	0.0177(15)	4	O
O3	0.3250(2)	0.6873(5)	1.0283(5)	0.0116(9)	8	O
O4	0.3240(2)	0	0.7798(7)	0.0082(12)	4	O
O5	0.4408(2)	0.7952(5)	0.8281(6)	0.0120(9)	8	O
X	-0.0589(3)	0.5	0.2722(9)	0.0201(16)	4	$((OH)_{0.58}F_{0.275}O_{0.145}$

Table S2. Fractional site coordinates. equivalent displacement parameters (U_{eq}. Å^2). site multiplicities (Mult.). and site composition for the sample Cha–192

Site	*x*	*y*	*z*	U_{eq}	Mult.	Site occupancy
A	0.2829(2)	0	0.2630(1)	0.0090(1)	4	$Ba_{0.435}Sr_{0.255}K_{0.225}Ca_{0.085}$
L	0.3530(1)	0.5	0.2945(1)	0.0070(2)	4	Ti
*M*1	0.5	0.5	0	0.0185(7)	2	Na
*M*2	0	0.2605(2)	0.5	0.0155(3)	4	$Na_{0.73}Fe^{2+}_{0.15}Mn_{0.12}$
*M*3	0	0.5	0	0.0207(3)	2	$Ti_{0.86}Mg_{0.08}Fe^{3+}_{0.06}$
Si	0.3597(1)	0.7841(1)	0.7978(1)	0.0069(2)	8	Si
O1	0.3287(1)	0.6889(3)	0.5357(3)	0.0114(5)	8	O
O2	0.4387(2)	0.5	0.3298(5)	0.0153(8)	4	O
O3	0.3280(1)	0.6874(3)	1.0300(3)	0.0111(5)	8	O
O4	0.3273(1)	1	0.7834(5)	0.0088(6)	4	O
O5	0.4416(1)	0.7953(3)	0.8313(4)	0.0112(5)	8	O
X	-0.0564(2)	0.5	0.2714(6)	0.0173(8)	4	$O_{0.435}(OH)_{0.315}F_{0.25}$

Table S3. Fractional site coordinates. equivalent displacement parameters (U_{eq}. Å^2). site multiplicities (Mult.). and site composition for the sample Cha–195.

Site	*x*	*y*	*z*	U_{eq}	Mult.	Site occupancy
A	0.284871(17)	0	0.26231(6)	0.01008(10)	4	$Sr_{0.75}Na_{0.15}K_{0.045}\square_{0.055}$
L	0.34900(2)	0.5	0.29200(8)	0.00601(13)	4	Ti
*M*1	0.5	0.5	0	0.0167(5)	2	Na
*M*2	0	0.25975(13)	0.5	0.0113(2)	4	$Na_{0.75}Mn_{0.175}Ca_{0.075}$
*M*3	0	0.5	0	0.0267(3)	2	$Ti_{0.82}Fe^{3+}_{0.13}Mg_{0.05}$
Si	0.35625(3)	0.78444(8)	0.79566(9)	0.00586(14)	8	Si
O1	0.32473(8)	0.6896(2)	0.5327(3)	0.0117(4)	8	O
O2	0.43680(12)	0.5	0.3291(4)	0.0144(6)	4	O
O3	0.32372(8)	0.6877(2)	1.0273(3)	0.0108(4)	8	O
O4	0.32213(11)	1	0.7802(4)	0.0088(5)	4	O
O5	0.44034(8)	0.7960(2)	0.8291(3)	0.0102(4)	8	O
X	-0.06001(12)	0.5	0.2699(4)	0.0151(6)	4	$(OH)_{0.43}F_{0.24}O_{0.33}$

Table S4. Fractional site coordinates. equivalent displacement parameters (U_{eq}. Å^2). site multiplicities (Mult.). and site composition for the sample 17/11.

Site	*x*	*y*	*z*	U_{eq}	Mult.	Site occupancy
A	0.2826(1)	0	0.2628(1)	0.0086(2)	4	$Ba_{0.575}K_{0.205}Sr_{0.135}Na_{0.085}$
L	0.3538(1)	0.5	0.2947(1)	0.0059(2)	4	Ti
*M*1	0.5	0.5	0	0.0160(7)	2	Na
*M*2	0	0.2605(2)	0.5	0.0066(3)	4	$Na_{0.765}Fe^{2+}_{0.09}Ca_{0.085}Mn_{0.06}$
*M*3	0	0.5	0	0.0207(3)	2	$Ti_{0.53}Fe^{3+}_{0.35}Mg_{0.12}$
Si	0.36051(4)	0.7837(1)	0.7969(1)	0.0055(2)	8	Si
O1	0.3291(1)	0.6883(3)	0.5357(4)	0.0098(5)	8	O
O2	0.4394(2)	0.5	0.3332(7)	0.0157(9)	4	O
O3	0.3292(1)	0.6868(3)	1.0304(4)	0.0096(5)	8	O
O4	0.3281(2)	0	0.7820(5)	0.0080(7)	4	O
O5	0.4418(1)	0.7935(3)	0.8278(4)	0.0117(5)	8	O
X	-0.0564(2)	0.5	0.2734(7)	0.0172(9)	4	$(OH)_{0.56}F_{0.29}O_{0.15}$

Table S5. Fractional site coordinates. equivalent displacement parameters (U_{eq}. Å^2). site multiplicities (Mult.). and site composition for the sample 25/40.

Site	*x*	*y*	*z*	U_{eq}	Mult.	Site occupancy
A	0.28435(3)	0	0.26189(12)	0.01428(18)	4	$Sr_{0.7}Na_{0.21}K_{0.05}Ba_{0.025}\square_{0.015}$
L	0.34989(4)	0.5	0.29239(15)	0.0061(2)	4	Ti
*M*1	0.5	0.5	0	0.0180(9)	2	Na
*M*2	0	0.25981(19)	0.5	0.0034(4)	4	$Na_{0.84}Mn_{0.085}Ca_{0.045}Fe^{2+}_{0.03}$
*M*3	0	0.5	0	0.0219(4)	2	$Ti_{0.43}Fe^{3+}_{0.4}Mg_{0.17}$
Si	0.35669(5)	0.78440(12)	0.79471(17)	0.0059(2)	8	Si
O1	0.32534(14)	0.6894(3)	0.5329(5)	0.0127(7)	8	O
O2	0.4376(2)	0.5	0.3321(8)	0.0205(12)	4	O
O3	0.32503(13)	0.6874(3)	1.0279(5)	0.0114(7)	8	O
O4	0.32289(19)	1	0.7813(7)	0.0090(9)	4	O
O5	0.44059(13)	0.7957(3)	0.8260(5)	0.0113(7)	8	O
X	-0.0583(2)	0.5	0.2733(8)	0.0181(11)	4	$(OH)_{0.775}F_{0.225}$

Table S6. Anisotropic atomic displacement parameters for 184/11

Site	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
A	0.0221(4)	0.0120(4)	0.0082(3)	0	0.0015(3)	0
L	0.0111(6)	0.0066(5)	0.0015(5)	0	0.0007(4)	0
*M*1	0.019(2)	0.020(2)	0.0122(17)	0	0.0060(15)	0
*M*2	0.0142(11)	0.0058(10)	0.0032(8)	0	0.0053(7)	0
*M*3	0.0332(12)	0.0106(9)	0.0318(10)	0	-0.0236(9)	0
Si	0.0124(6)	0.0058(6)	0.0018(5)	0.0002(4)	0.0001(4)	0.0001(4)
O1	0.0242(19)	0.0079(15)	0.0074(13)	0.0024(13)	-0.0010(12)	-0.0027(11)
O2	0.010(2)	0.029(3)	0.012(2)	0	-0.0016(18)	0
O3	0.0166(17)	0.0096(15)	0.0090(13)	0.0023(12)	0.0036(12)	0.0047(11)
O4	0.014(2)	0.0011(19)	0.0094(18)	0	0.0004(16)	0
O5	0.0112(16)	0.0141(16)	0.0098(14)	0.0029(13)	-0.0029(12)	-0.0014(12)
X	0.023(3)	0.020(3)	0.017(2)	0	0.004(2)	0

Table S7. Anisotropic atomic displacement parameters for Cha–192.

Site	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
A	0.0132(2)	0.0056(2)	0.0083(2)	0	0.0018(1)	0
L	0.0099(3)	0.0044(3)	0.0070(3)	0	0.0021(2)	0
*M*1	0.0211(12)	0.0180(11)	0.0181(12)	0	0.0088(9)	0
*M*2	0.0221(6)	0.0113(5)	0.0139(5)	0	0.0057(4)	0
*M*3	0.0248(5)	0.0030(4)	0.0290(6)	0	-0.0190(5)	0
Si	0.0101(3)	0.0031(3)	0.0076(3)	-0.0001(2)	0.0017(2)	-0.0001(2)
O1	0.0161(9)	0.0094(8)	0.0088(8)	0.0003(6)	0.0020(7)	-0.0022(6)
O2	0.0118(12)	0.0229(14)	0.0115(13)	0	0.0032(10)	0
O3	0.0159(9)	0.0083(8)	0.0094(8)	-0.0001(6)	0.0024(7)	0.0026(6)
O4	0.0123(11)	0.0035(10)	0.0108(12)	0	0.0027(9)	0
O5	0.0096(8)	0.0078(7)	0.0160(9)	0.0003(6)	0.0005(7)	-0.0011(7)
X	0.0181(13)	0.0179(14)	0.0170(14)	0	0.0071(11)	0

Table S8. Anisotropic atomic displacement parameters for Cha–195.

Site	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
A	0.0134(2)	0.0097(2)	0.0072(2)	0	0.0014(1)	0
L	0.0066(2)	0.0075(2)	0.0039(2)	0	0.0008(2)	0
*M*1	0.0170(9)	0.0192(10)	0.0150(8)	0	0.0067(7)	0
*M*2	0.0146(4)	0.0115(4)	0.0087(4)	0	0.0048(3)	0
*M*3	0.0287(5)	0.0070(4)	0.0372(5)	0	-0.0259(4)	0
Si	0.0068(2)	0.0058(3)	0.0050(2)	0.0001(2)	0.0008(2)	-0.0003(3)
O1	0.0133(6)	0.0125(7)	0.0087(6)	0.0019(5)	-0.0005(5)	-0.0045(5)
O2	0.0084(9)	0.0253(12)	0.0099(9)	0	0.0023(7)	0
O3	0.0117(6)	0.0120(7)	0.0091(6)	0.0005(5)	0.0023(5)	0.0043(5)
O4	0.0086(8)	0.0065(9)	0.0115(8)	0	0.0012(7)	0
O5	0.0070(6)	0.0118(7)	0.0116(6)	-0.0005(5)	0.0008(5)	-0.0005(5)
X	0.0170(10)	0.0168(11)	0.0124(9)	0	0.0055(8)	0

Table S9. Anisotropic atomic displacement parameters for 17/11.

Site	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
A	0.0119(3)	0.0067(2)	0.0073(2)	0	0.00142(15)	0
L	0.0080(4)	0.0056(4)	0.0043(3)	0	0.0012(2)	0
*M*1	0.0167(12)	0.0170(12)	0.0156(12)	0	0.0066(10)	0
*M*2	0.0105(5)	0.0058(5)	0.0043(5)	0	0.0038(4)	0
*M*3	0.0223(6)	0.0054(5)	0.0294(7)	0	-0.0183(5)	0
Si	0.0074(4)	0.0038(4)	0.0054(4)	0.0000(2)	0.0010(3)	-0.0006(2)
O1	0.0145(10)	0.0077(9)	0.0075(8)	0.0003(7)	0.0019(7)	-0.0028(7)
O2	0.0065(12)	0.0275(18)	0.0135(13)	0	0.0027(11)	0
O3	0.0134(10)	0.0082(9)	0.0073(8)	0.0004(7)	0.0013(7)	0.0018(7)
O4	0.0091(12)	0.0047(11)	0.0101(12)	0	0.0006(10)	0
O5	0.0072(9)	0.0095(9)	0.0177(10)	0.0009(7)	-0.0009(7)	0.0040(8)
X	0.0144(14)	0.0178(16)	0.0209(15)	0	0.0085(12)	0

Table S10. Anisotropic atomic displacement parameters for 25/40.

Site	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
A	0.0193(3)	0.0124(3)	0.0112(3)	0	0.0018(2)	0
L	0.0075(4)	0.0072(3)	0.0036(4)	0	0.0004(3)	0
*M*1	0.0183(16)	0.0179(14)	0.0188(17)	0	0.0066(13)	0
*M*2	0.0061(7)	0.0032(5)	0.0015(7)	0	0.0026(5)	0
*M*3	0.0243(8)	0.0058(5)	0.0298(8)	0	-0.0215(6)	0
Si	0.0076(4)	0.0049(3)	0.0053(4)	-0.0003(3)	0.0008(3)	-0.0003(3)
O1	0.0145(12)	0.0119(11)	0.0110(12)	0.0019(9)	-0.0009(10)	-0.0057(9)
O2	0.0083(17)	0.041(2)	0.012(2)	0	0.0000(15)	0
O3	0.0126(12)	0.0119(11)	0.0101(12)	0.0002(9)	0.0030(10)	0.0052(9)
O4	0.0098(16)	0.0048(13)	0.0121(17)	0	0.0003(13)	0
O5	0.0078(11)	0.0100(10)	0.0157(13)	-0.0003(9)	0.0005(10)	0.0002(9)
X	0.0170(19)	0.0206(18)	0.018(2)	0	0.0082(16)	0

Table S11. Bond valence balance in 184/11

Site	*A*	*L*	*M*1	*M*2	*M*3	Si	V_a
O1	$(0.20+0.14)_{\times 2\downarrow}$	$0.67_{\times 2\downarrow}$				1.01	2.02
O2		1.44	$0.27_{\times 2\downarrow}$	$0.25_{\times 2\downarrow}{}^{\times 2\rightarrow}$			2.21
O3	$(0.20+0.15)_{\times 2\downarrow}$	$0.66_{\times 2\downarrow}$				1.01	2.02
O4	0.16+0.15					$0.91^{\times 2\rightarrow}$	2.13
O5			$0.15_{\times 4\downarrow}$	$0.32_{\times 2\downarrow}$	$0.54_{\times 4\downarrow}$	1.03	2.04
X				$0.26_{\times 2\downarrow}{}^{\times 2\rightarrow}$	$0.61_{\times 2\downarrow}$		1.13
V_c	1.69	4.10	1.14	1.66	3.38	3.96	

Hereinafter: BVS is obtained by multiplying on site occupancy factor (taking into account site multiplicity). In mixed sites. bond-valence contribution of each cation has been weighted according to its occupancy. The ×2↓ sign indicates the doubling of the corresponding valence contributions in columns due to symmetry.

Table S12. Bond valence balance in Cha–192.

Site	*A*	*L*	*M*1	*M*2	*M*3	Si	V_a
O1	$(0.21+0.14)_{\times 2\downarrow}$	$0.66_{\times 2\downarrow}$				1.00	2.01
O2		1.44	$0.28_{\times 2\downarrow}$	$0.23_{\times 2\downarrow}{}^{\times 2\rightarrow}$			2.18
O3	$(0.21+0.15)_{\times 2\downarrow}$	$0.65_{\times 2\downarrow}$				1.01	2.02
O4	0.17+0.16					$0.90^{\times 2\rightarrow}$	2.13
O5			$0.15_{\times 4\downarrow}$	$0.29_{\times 2\downarrow}$	$0.57_{\times 4\downarrow}$	1.04	2.05
X				$0.25_{\times 2\downarrow}{}^{\times 2\rightarrow}$	$0.68_{\times 2\downarrow}$		1.18
V_c	1.75	4.06	1.16	1.54	3.64	3.95	

Table S13. Bond valence balance in Cha–195.

Site	*A*	*L*	*M*1	*M*2	*M*3	Si	V_a
O1	(0.18+0.13)$_{\times 2\downarrow}$	0.67$_{\times 2\downarrow}$				1.01	1.99
O2		1.46	0.29$_{\times 2\downarrow}$	0.25$_{\times 2\downarrow}^{\times 2\rightarrow}$			2.25
O3	(0.18+0.14)$_{\times 2\downarrow}$	0.66$_{\times 2\downarrow}$				1.03	2.01
O4	0.15+0.14					0.91$^{\times 2\rightarrow}$	2.11
O5			0.15$_{\times 4\downarrow}$	0.32$_{\times 2\downarrow}$	0.59$_{\times 4\downarrow}$	1.05	2.11
X				0.25$_{\times 2\downarrow}^{\times 2\rightarrow}$	0.65$_{\times 2\downarrow}$		1.15
V_c	1.55	4.12	1.18	1.64	3.66	4.00	

Table S14. Bond valence balance in 17/11.

Site	*A*	*L*	*M*1	*M*2	*M*3	Si	V_a
O1	(0.23+0.15)$_{\times 2\downarrow}$	0.66$_{\times 2\downarrow}$				1.00	2.04
O2		1.41	0.28$_{\times 2\downarrow}$	0.25$_{\times 2\downarrow}^{\times 2\rightarrow}$			2.19
O3	(0.22+0.16)$_{\times 2\downarrow}$	0.66$_{\times 2\downarrow}$				1.00	2.04
O4	0.18+0.18					0.90$^{\times 2\rightarrow}$	2.16
O5			0.15$_{\times 4\downarrow}$	0.32$_{\times 2\downarrow}$	0.52$_{\times 4\downarrow}$	1.06	2.05
X				0.26$_{\times 2\downarrow}^{\times 2\rightarrow}$	0.63$_{\times 2\downarrow}$		1.15
V_c	1.88	4.05	1.16	1.66	3.34	3.96	

Table S15. Bond valence balance in 25/40.

Site	*A*	*L*	*M*1	*M*2	*M*3	Si	V_a
O1	(0.18+0.13)$_{\times 2\downarrow}$	0.68$_{\times 2\downarrow}$				1.03	2.02
O2		1.45	0.29$_{\times 2\downarrow}$	0.25$_{\times 2\downarrow}^{\times 2\rightarrow}$			2.24
O3	(0.18+0.14)$_{\times 2\downarrow}$	0.67$_{\times 2\downarrow}$				1.04	2.03
O4	0.15+0.14					0.92$^{\times 2\rightarrow}$	2.13
O5			0.15$_{\times 4\downarrow}$	0.33$_{\times 2\downarrow}$	0.54$_{\times 4\downarrow}$	1.05	2.07
X				0.26$_{\times 2\downarrow}^{\times 2\rightarrow}$	0.62$_{\times 2\downarrow}$		1.14
V_c	1.55	4.15	1.18	1.68	3.40	4.04	

Table S16. Comparison of crystal structures of lamprophyllite-2*M* and ericssonite-2*M*: Atom pairing.

Wyckoff Positions		Lamprophyllite-2*M*		Ericssonite-2*M*	
		Site	Coordinates	Site	Coordinates
2b	(0.1/2.0)	Ti2	0 0.5 0	Mn2	0 0.5 0
2a	(0.0.0)	Na2	0 0 0	Mn3	0 0 0
4i	(x.0.z)	Ti1	0.1506 0 0.7078	Fe1	0.1403 0 0.7160
4i	(x.0.z)	O6	0.0623 0 0.6677	O6	0.0497 0 0.6920
4i	(x.0.z)	O4	0.1777 0.5 0.2200	O2	0.1574 0.5 0.2200
8j	(x.y.z)	O3	0.1753 0.1875 0.9712	O5	0.1690 0.1910 0.9760
8j	(x.y.z)	O2	0.1748 0.1889 0.4674	O4	0.1686 0.1910 0.4730
4i	(x.0.z)	O1	0.4425 0 0.2758	O1	0.4445 0 0.3200
8j	(x.y.z)	Si1	0.1439 0.2846 0.2049	Si1	0.1343 0.2740 0.2120
8j	(x.y.z)	O5	0.0595 0.2965 0.1725	O3	0.0547 0.2540 0.1850
4h	(0.y.1/2)	Na1	0 0.2590 0.5	Mn1	0 0.2380 0.5
4i	(x.0.z)	Sr1	0.2842 0 0.2621	Ba1	0.2750 0 0.2590

Table S17. Comparison of crystal structures of lamprophyllite-2*M* (S_1) and ericssonite-2*M* (S_2): Atom displacements.

Wyckoff Position		Site S_1	Site S_2	Atomic Displacements			
				u_x	u_y	u_z	|u|
2b	(0.1/2.0)	Ti2	Mn2	0	0	0	0
2a	(0.0.0)	Na2	Mn3	0	0	0	0
4i	(x.0.z)	Ti1	Fe1	-0.0103	0	0.0082	0.2078
4i	(x.0.z)	O6	O6	-0.0126	0	0.0243	0.2883
4i	(x.0.z)	O4	O2	-0.0203	0	0	0.3901
8j	(x.y.z)	O3	O5	-0.0063	0.0035	0.0048	0.1291
8j	(x.y.z)	O2	O4	-0.0062	0.0021	0.0056	0.1271
4i	(x.0.z)	O1	O1	0.0020	0	0.0442	0.2360
8j	(x.y.z)	Si1	Si1	-0.0096	-0.0106	0.0071	0.2068
8j	(x.y.z)	O5	O3	-0.0048	-0.0425	0.0125	0.3233
4h	(0.y.1/2)	Na1	Mn1	0.0000	-0.0210	0	0.1483
4i	(x.0.z)	Sr1	Ba1	-0.0092	0	-0.0031	0.1756

Note: u_x. u_y and u_z are given in relative units. |u| is the absolute distance given in Å.

Table S18. Comparison of crystal structures of lamprophyllite-2*O* and ericssonite-2*O*: Atom pairing.

Wyckoff Positions		Lamprophyllite-2*O*		Ericssonite-2*O*	
		Site	Coordinates	Site	Coordinates
2a	(0,0,0)	Ti2	0 0 0	Mn2	0 0 0
8h	(x,y,z)	Si1	0.1440 0.1441 0.2161	Si1	0.1644 0.1364 0.2262
4g	(x,y,0)	Sr1	0.6453 0.2158 0	Ba1	0.6644 0.2248 0
4g	(x,y,0)	O1	0.7020 0.0570 0	O1	0.6657 0.0507 0
8h	(x,y,z)	O5	0.1478 0.0593 0.2044	O3	0.1617 0.0567 0.2465
4g	(x,y,0)	O4	0.1448 0.1777 0	O2	0.1624 0.1582 0
8h	(x,y,z)	O3	0.8900 0.3250 0.1867	O4	0.9137 0.3292 0.1913
8h	(x,y,z)	O2	0.3952 0.3239 0.1864	O5	0.4180 0.3278 0.1914
4g	(x,y,0)	Ti1	0.1442 0.3491 0	Fe31	0.1663 0.3571 0
4g	(x,y,0)	O6	0.1410 0.4376 0	O6	0.1730 0.4477 0
4f	(0,1/2,z)	Na1	0 0.5 0.2588	Mn1	0 0.5 0.2404
2b	(0,0,1/2)	Na2	0.5 0.5 0	Mn3	0.5 0.5 0

Table S19. Comparison of crystal structures of lamprophyllite-2*O* (S_1) and ericssonite-2*O* (S_2): Atom displacements.

Wyckoff Position		Site S_1	Site S_2	Atomic Displacements			
				u_x	u_y	u_z	|u|
2a	(0,0,0)	Ti2	Mn2	0	0	0	0
8h	(x,y,z)	Si1	Si1	0.0204	-0.0077	0.0101	0.1971
4g	(x,y,0)	Sr1	Ba1	0.0191	0.0090	0	0.2005
4g	(x,y,0)	O1	O1	-0.0363	-0.0063	0	0.2296
8h	(x,y,z)	O5	O3	0.0139	-0.0026	0.0421	0.3113
4g	(x,y,0)	O4	O2	0.0176	-0.0195	0	0.3848
8h	(x,y,z)	O3	O4	0.0237	0.0042	0.0046	0.1542
8h	(x,y,z)	O2	O5	0.0228	0.0039	0.0050	0.1479
4g	(x,y,0)	Ti1	Fe31	0.0221	0.0080	0	0.1938
4g	(x,y,0)	O6	O6	0.0320	0.0101	0	0.2588
4f	(0,1/2,z)	Na1	Mn1	0	0	-0.0184	0.1303
2b	(0,0,1/2)	Na2	Mn3	0	0	0	0