

Table 41A-7-001. RbLiMoO_4 . Structure of phase IV [83Kru]. $T = \text{RT}$. Fractional coordinates and temperature parameters. B_{ij} is defined by Eq. (a) in Introduction.

Atom	x	y	z	B_{11}	B_{22}	B_{33}	B_{12}	B_{13}	B_{23}
Mo	0.5000	0.2500	0.0006(6)	0.0050(5)	0.0034(4)	0.0079(7)	0.0044(5)	-0.0004(6)	-0.0005(5)
Rb	0.4969(6)	0.5009(6)	0.5244(2)	0.0090(7)	0.0071(7)	0.0152(6)	0.0089(10)	-0.0034(8)	-0.0054(9)
O(1)	0.665(2)	0.235(2)	0.039(3)	0.0100(20)	0.0070(15)	0.0035(12)	0.0100(32)	0.0030(28)	0.0030(27)
O(2)	0.569(2)	0.430(1)	0.066(20)	0.0102(20)	0.0029(12)	0.0233(21)	0.0050(20)	-0.0081(30)	0.0000(25)
O(3)	0.346(2)	0.125(2)	0.195(2)	0.0051(16)	0.0070(15)	0.0142(18)	0.0040(28)	0.0073(30)	0.0040(27)
O(4)	0.426(2)	0.203(2)	-0.291(2)	0.0121(21)	0.0059(15)	0.0157(18)	0.0081(31)	0.0119(32)	0.0048(27)
Li	0.757(5)	0.631(5)	-0.008(6)	0.0033(15)	0.0097(30)	0.0252(41)	0.0070(39)	0.0034(19)	0.0081(39)

Table 41A-7-002. RbLiMoO₄. Structure of phase IV [83Kru]. *T* = RT. Interatomic distances [Å] and bond angles [°].

Mo–O(1)	1.768(24)	Li–O(1)′	1.87(4)	Rb–O(1)′	2.915(14)
–O(2)	1.761(15)	–O(2)	1.96(4)	–O(2)	2.947(15)
–O(3)	1.749(11)	–O(3)′	1.86(4)	–O(3)′	3.035(18)
–O(4)	1.775(12)	–O(4)′	1.94(4)	–O(4)′	3.063(20)
Average	1.763	Average	1.907	–O(3)″	3.080(21)
				–O(4)	3.172(19)
				–O(1)″	3.289(19)
				–O(2)″	3.370(21)
O(1)–Mo–O(2)	108.8(8)	O(1)′–Li–O(2)	105(1)		
O(1)–Mo–O(3)	106.0(8)	O(1)′–Li–O(3)′	116(1)		
O(1)–Mo–O(4)	109.9(9)	O(1)′–Li–O(4)′	110(1)		
O(2)–Mo–O(3)	111.4(8)	O(2)–Li–O(3)′	112(1)		
O(2)–Mo–O(4)	110.8(8)	O(2)–Li–O(4)′	107(1)		
O(3)–Mo–O(4)	109.7(6)	O(3)′–Li–O(4)′	105(1)		