Table 41A-8-001. $CsLiMoO_4$. Structure of phase I [80Kle]. Fractional coordinates and isotropic temperature parameters. *B* is defined by Eq. (e) in Introduction. Two models are proposed: oxygens on position 96(i), and oxygens on position 16(e).

Atom	Position	*x*	*y*	*z*	B [Å^2]	B' [Å^2]
Cs	4(a)	0	0	0	2.22	2.35
Mo	4(b)	0.5	0.5	0.5	1.73	1.68
Li	4(c)	0.25	0.25	0.25	2.09	2.10
O	96(i)	0.399(4)	0.352(3)	0.388(5)	2.96	–
O′	16(e)	0.3788(9)	0.3788(9)	9.3788(9)		7.29

Table 41A-8-002. $CsLiMoO_4$. Structure of phase I [80Kle]. Interatomic distances [Å] of the two models. See Table 41A-8-001.

Oxygen on position 96(i)				Oxygen on position 16(e)			
Mo–O	1.76(4)	O–O	2.51⋯3.08	Mo–O′	1.745(7)	O′–O′	2.850
Li–O	1.89(4)	O–O	2.86⋯3.38	Li–O′	1.856(7)	O′–O′	3.031
Cs–O	3.19(3); 3.55(3); 3.66(3)			Cs–O′	3.459(7)		
Cs–Cs	5.882(2)			Mo–Cs	4.159(2)		
Li⋯Li				Li–Mo	3.602(2); 6.897(2)		
Mo⋯Mo				Li–Cs			