Table 41A-9-001. $CsLiWO_4$. Structure of phase I [80Oka]. T = 298 K. Fractional coordinates and isotropic temperature parameters. B is defined by Eq. (e) in Introduction.

	x	y	z	B [Å^2]
Cs	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$	2.55(3)
Li	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$	2.2(13)
W	$\frac{1}{2}$	$\frac{1}{2}$	0	1.37(2)
O	0.390(3)	0.390	0.147(4)	3.7(8)

Table 41A-9-002. $CsLiWO_4$. Structure of phase I [87Pet]. Fractional coordinates and isotropic temperature parameters. B is defined by Eq. (e) in Introduction.

Atom	Position	Occupancy	x	y	z	B [Å^2]
Cs	4*a*	1	0	0	0	2.83(1)
W	4*b*	1	1/2	1/2	1/2	1.74(1)
Li	4*c*	1	3/4	3/4	3/4	2.5(4)
O	96*i*	1/6	0.590(1)	0.627(1)	0.649(1)	2.7(2)

Table 41A-9-003. $CsLiWO_4$. Structure of phase I [80Oka]. T = 298 K. Interatomic distances [Å].

W–O	1.78(3)	Li–O	1.87(3)
Cs–O	3.22(3)	Cs–O	3.60(3)

Table 41A-9-004. $CsLiWO_4$. Structure of phase I [87Pet]. Interatomic distances [Å].

$[WO_4]$ polyhedron		Between cations	
W–O	1.775(8)	W–W	5.887(2)
O–O	2.51–3.22(1)	Cs–Cs	5.887(2)
$[LiO_4]$ polyhedron		Li–Li	5.887(2)
Li–O	1.897(8)	Cs–W	4.163(2)
O–O	2.68–3.38(1)	Cs–Li	3.605(2)
$[CsO_{12}]$ polyhedron		Cs–Li	6.904(2)
Cs–O	3.286(8)	W–Li	3.605(2)
Cs–O	3.457(8)	W–Li	6.904(2)
Cs–O	3.774(8)		