Table 41A-4-001. $CsLiSO_4$. Unit cell parameters [88Asa].

	–100 °C	–78 °C	–71 °C	–20 °C	25 °C
a [Å]	9.410(3)	9.415(3)	9.421(2)	9.441(1)	9.454(3)
b [Å]	5.434(2)	5.430(2)	5.433(1)	5.443(1)	5.456(2)
c [Å]	8.819(2)	8.787(3)	8.780(2)	8.786(1)	8.823(3)
γ[°]	90.25(2)	90.20(2)	90.14(2)		

Table 41A-4-002. $CsLiSO_4$. Crystal structure of phase I [88Asa]. T = –20 °C. Fractional coordinates [$\cdot 10^{-4}$] and isotropic temperature parameters [$\cdot 10^{-4}$ Å^2]. U_{ij} and u^2 are defined by Eqs. (d) and (e) in Introduction, respectively.

Atom	x	y	z	U_{11}, $\overline{u^2}$	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Cs	7500	2163(1)	4983(1)	185(1)	193(1)	172(1)	0	0	1(1)
S	2500	827(1)	2044(2)	80(4)	101(4)	111(4)	0	0	–6(2)
O(1)	2416(32)	854(9)	402(7)	230(26)	503(38)	123(17)	–17(56)	–16(36)	35(12)
O(2)	2097(30)	2255(7)	2627(11)	464(117)	150(26)	562(50)	30(17)	3(25)	–74(15)
O(3)	455(14)	–83(8)	2570(8)	213(30)	225(28)	243(28)	–70(14)	–23(12)	38(12)
O(4)	4766(12)	284(8)	2641(8)	111(25)	314(34)	221(28)	22(12)	–30(11)	–32(13)
Li	2500	4155(21)	3301(22)	252(33)					

Table 41A-4-003. $CsLiSO_4$. Crystal structure of phase I (T = 293K) and II (T = 163K) [79Kru]. Fractional coordinates and isotropic temperature parameters [Å^2]. Values of phase I are above the line, of phase II below the line. O(4) is related to O(2) by mirror operation on phase I. β_{ij} and B are defined by Eqs. (c) and (e) in Introduction, respectively.

	x	y	z	β_{11}	β_{22}	β_{33}	β_{12}	β_{13}	β_{23}	B
Cs	0.28432(5)	0.75	0.99848(7)	1.82(2)	1.79(2)	1.61(1)	0	–0.04(2)	0	1.73(1)
	0.28113(3)	0.75382(5)	0.99917(5)	1.11(1)	1.05(1)	0.96(1)	–0.03(1)	–0.02(1)	0.00(1)	1.04(1)
S	0.0831(2)	0.25	0.2040(2)	0.90(6)	0.83(5)	0.96(5)	0	–0.13(5)	0	0.87(3)
	0.0818(1)	0.2470(2)	0.2030(1)	0.51(3)	0.48(3)	0.57(3)	–0.06(2)	–0.05(3)	0.03(3)	0.52(1)
O_1	0.0840(9)	0.25	0.0412(7)	4.3(4)	2.7(3)	0.8(2)	0	0.4(2)	0	2.4(1)
	0.0851(5)	0.2491(8)	0.0379(4)	2.6(2)	1.6(1)	0.5(9)	0.0(1)	0.1(1)	0.2(1)	1.47(6)
O_2	0.0101(5)	0.0325(8)	0.2609(6)	5.0(2)	1.6(2)	2.6(2)	2.1(2)	0.2(2)	0.1(1)	3.2(1)
	0.9809(5)	0.0552(8)	0.2555(5)	1.8(2)	1.2(1)	1.5(2)	–0.6(1)	0.7(1)	–0.4(1)	1.33(7)
O_3	0.2260(6)	0.25	0.2632(9)	0.5(2)	9.7(7)	5.6(5)	0	–1.1(3)	0	4.3(3)
	0.2239(5)	0.1886(9)	0.2632(6)	0.9(1)	2.2(2)	2.0(2)	0.2(1)	–0.5(1)	0.3(2)	1.57(8)
O_4	0.0101(5)	0.4675(8)	0.2609(6)	5.0(2)	1.6(2)	2.6(2)	–2.1(2)	0.2(2)	–0.1(1)	3.2(1)
	0.0348(5)	0.4867(8)	0.2612(5)	2.1(2)	1.0(1)	1.0(1)	1.1(1)	–0.3(1)	–0.2(1)	1.35(8)
Li	0.416(2)	0.25	0.331(2)	3.1(7)	3.0(7)	1.3(5)	0	–0.7(6)	0	2.5(4)
	0.416(1)	0.238(2)	0.327(1)	1.6(4)	1.2(4)	0.8(4)	0.2(3)	–0.1(3)	–0.5(3)	1.3(2)

Table 41A-4-004. $CsLiSO_4$. Crystal structure of phase I (T = 293 K) and II (T = 163 K) [79Kru]. Interatomic distance [Å] and angles.

Phase I					
S–O_1	1.436(6)	O_1SO_2	110°16'(19')	Cs – O'_2	3.235(5)
O_2	1.482(5)	O_1SO_3	110°50'(21')	O'_4	3.235(5)
O_3	1.446(7)	O_1SO_4	110°16'(19')	O''_2	3.247(5)
O_4	1.462(5)	O_2SO_3	108°25'(20')	O''_4	3.247(5)
		O_2SO_4	108°32'(17')	O'_1	3.347(5)
		O_2SO_4	108°25'(20')	O''_1	3.343(5)
Li–O_1	1.849(17)	O_1LiO_2	114°45'(46')	O'_3	3.429(6)
O_2	1.954(12)	O_1LiO_3	108°15'(46')	O''_3	3.429(6)
O_3	1.904(21)	O_1LiO_4	114°45'(46')	O'''_1	3.500(8)
O_4	1.954(12)	O_2LiO_3	107°15'(45')	O'''_3	3.633(6)
		O_2LiO_4	104°06'(42')	O'''_3	3.633(6)
		O_3LiO_4	107°15'(45')		
Phase II					
S–O_1	1.458(4)	O_1SO_2	109°22'(16')	Cs – O'_2	3.429(5)
O_2	1.484(5)	O_1SO_3	110°10'(17')	O'_4	3.058(5)
O_3	1.468(5)	O_1SO_4	110°32'(16')	O''_2	3.066(5)
O_4	1.464(5)	O_2SO_3	108°27'(17')	O''_4	3.520(5)
		O_2SO_2	108°46'(17')	O'_1	3.266(5)
		O_3SO_4	109°30'(17')	O'_1	3.322(5)
Li–O_1	1.858(12)	O_1LiO_2	110°05'(38')	O'_3	3.197(5)
O_2	1.967(13)	O_1LiO_3	107°22'(38')	O'''_1	3.451(5)
O_3	1.910(14)	O_1LiO_4	115°53'(39')	O''_3	3.358(5)
O_4	1.926(13)	O_2LiO_3	107°56'(37')	O'''_2	3.486(5)
		O_2LiO_4	106°38'(36')	O'''_4	3.581(5)
		O_2LiO_4	108°43'(37')		

Table 41A-4-005. $CsLiSO_4$. Crystal structure of phase II [88Asa]. T = –78 °C. Fractional coordinates [$\cdot 10^{-4}$] and isotropic temperature parameters [$\cdot 10^{-4}$ Å^2]. U_{ij} and u^2 are defined by Eqs. (d) and (e) in Introduction, respectively. Parameters of SO_4 with larger occupancy 0.95(1) are listed, which are assumed to relate to those with smaller occupancy by a hypothetical mirror reflection at x = 1/4 or 3/4.

Atom	x	y	z	U_{11}, $\overline{u^2}$	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Cs	7550(1)	2174(1)	4986(1)	136(1)	137(1)	120(1)	–6(1)	3(2)	2(4)
S	2491(7)	823(1)	2046(1)	60(4)	70(4)	73(4)	4(6)	12(6)	–5(2)
O(1)	2455(24)	841(9)	399(5)	190(11)	400(32)	51(13)	42(30)	–9(20)	27(9)
O(2)	2059(14)	2247(7)	2615(9)	311(47)	122(23)	355(37)	37(12)	6(14)	–41(24)
O(3)	514(13)	–107(9)	2606(8)	191(26)	245(31)	176(27)	–36(13)	–61(10)	42(12)
O(4)	4848(14)	300(10)	2619(9)	167(26)	323(37)	210(30)	72(13)	–53(11)	6(14)
Li	2271(48)	4137(20)	3340(20)	252(36)					

Table 41A-4-006. $CsLiSO_4$. Elastic stiffness constants obtained by Brillouin scattering at RT [87Dro].

c_{11}	c_{22}	c_{33}	c_{44}	c_{55}	c_{66}	c_{23}	c_{13}	c_{12}
[$\cdot 10^{10}$ N m^{-2}]								
5.64	6.20	3.51	1.09	1.56	1.67	3.21	1.36	2.70

Table 41A-4-007. $CsLiSO_4$. Elastic stiffness constants at RT [87Mro]. a) Tortion pendurum method [83Pak]. b) Ultrasonic method [82Ale]. c) Brillouin scattering [87Mro].

	c_{11}	c_{22}	c_{33}	c_{44}	c_{55}	c_{66}	c_{12}	c_{23}	c_{13}
	[$\cdot 10^{10}$ N m^{-2}]								
a)				1.4	1.0	1.6			
b)	5.8	6.3	3.6	1.1	1.6	1.9		2.9	
c)	5.89	6.37(8)	3.57	1.15	1.61(5)	2.03	2.54	1.73(15)	2.47

Table 41A-4-008. $CsLiSO_4$. ^{7}Li EFG principal values and orientations (θ, ϕ of the spherical coordinates in the crystallographic system) of the principal values [82Roz].

T [°C]	$\lvert eQ\phi_{xx}/h\rvert$ [kHz]	$\lvert eQ\phi_{yy}/h\rvert$ [kHz]	$\lvert eQ\phi_{zz}/h\rvert$ [kHz]
20	1.8(0°, 70°)	19.0(90°, 90°)	20.8(180°, 20°)
–113	3.0(2°, 85°)	21.9(91°, 86°)	24.8(202°, 9°)

Table 41A-4-009. $CsLiSO_4$. Electric field gradient tensor of ^{133}Cs site at T = 300 K [86Hol]. Principal values are in the last row. X, Y, Z correspond to a, b, c respectively.

Axis	X	Y	Z
X	–1.29	0	±3.69
Y		24.33	0
Z			–23.03
	24.330	–0.681	–23.640

Table 41A-4-010. $CsLiSO_4$. Spin Hamiltonian parameters g and A at 143 K [93Ana].

Principal values	Principal values	Direction cosines		
g	A	a	b	c
$g_{XX} = 1.987$	$A_{XX} = 7.8 \pm 0.2$ mT	0.7452	–0.5085	0.4313
$g_{YY} = 1.983$	$A_{YY} = 7.4 \pm 0.2$ mT	–0.5595	–0.1250	0.8193
$g_{ZZ} = 1.932$	$A_{ZZ} = 19.8 \pm 0.2$ mT	0.3627	0.8518	0.3777

Site I $g_{\parallel} = 1.935$, $g_{\perp} = 1.991$; $A_{\parallel} = 19.68$ mT, $A_{\perp} = 7.41$ mT.