Table 41A-2-001. $KLiSO_4$. Structure of phases III and IV [85Sch]. Fractional coordinates and isotropic temperature parameters. *B* is defined by Eq. (e) in Introduction. The Wyckoff notation is in square brackets after the atomic designation.

	293 K	398 K	568 K
K [2(*a*)]			
z	0	0	0
B [Å^2]	1.8	2.3	3.2
Li [2(*b*)]			
z	0.815(1)	0.822(2)	0.818(2)
B [Å^2]	1.4	2.0	2.6
S [2(*b*)]			
z	0.20626(8)	0.20683(9)	0.2081(2)
B [Å^2]	1.0	1.3	1.6
O(1) [2(*b*)]			
z	0.0367(7)	0.0398(9)	0.0462(7)
B [Å^2]	3.6	4.5	6.1
O(2) [6(*c*)]			
x	0.3474(4)	0.3494(5)	0.3547(8)
y	0.9399(4)	0.9395(5)	0.9367(8)
z	0.2634(5)	0.2638(6)	0.2667(7)
B [Å^2]	2.5	3.2	4.4

Table 41A-2-002. $KLiSO_4$. Structure of phases III and IV [85Sch]. Interatomic distances [Å] corrected and uncorrected for the harmonic part of temperature parameters.

	No. of	293 K		398 K		568 K	
	bonds	Uncorrected	Corrected	Uncorrected	Corrected	Uncorrected	Corrected
K–O(1)	3	2.988(2)	3.009(2)	2.999(2)	3.024(2)	3.023(2)	3.057(2)
–O(2)	3	2.832(4)	2.851(4)	2.841(4)	2.865(4)	2.857(5)	2.891(6)
–O(2)	3	3.003(4)	3.021(4)	3.016(4)	3.040(4)	3.067(6)	3.094(6)
mean		2.941(3)	2.960(3)	2.952(3)	2.976(4)	2.982(5)	3.014(5)
Li–O(1)	1	1.91(1)	1.96(1)	1.88(2)	1.93(2)	1.97(1)	2.04(1)
–O(2)	3	1.916(2)	1.946(3)	1.933(5)	1.973(5)	1.929(5)	1.982(5)
mean		1.915(5)	1.950(6)	1.920(11)	1.962(11)	1.939(7)	1.997(7)
S–O(1)	1	1.464(6)	1.497(6)	1.442(8)	1.484(8)	1.398(6)	1.458(7)
–O(2)	3	1.458(2)	1.477(3)	1.454(2)	1.478(3)	1.441(3)	1.478(5)
mean		1.460(3)	1.482(4)	1.451(4)	1.480(5)	1.430(4)	1.473(6)

Table 41A-2-003. $KLiSO_4$. Structure of phase IV [84Cha]. Fractional coordinates at 300 K.

Atom	Molecule number	Fractional coordinates		
		x	*y*	*z*
Li	1	1/3	2/3	0.8147
Li	2	2/3	1/3	0.3147
K	3	0	0	0
K	4	0	0	0.5
S	5	1/2	2/3	0.2066
O(1)		1/3	2/3	0.0357
O(2)		0.3417	0.9397	0.2587
O(2)		0.0603	0.4020	0.2587
O(2)		0.5980	0.6583	0.2587
S	6	2/3	1/3	0.7066
O(1)		2/3	1/3	0.5357
O(2)		0.6583	0.0603	0.7587
O(2)		0.9397	0.5980	0.7587
O(2)		0.4020	0.3417	0.7587

Table 41A-2-004. $KLiSO_4$. Structure of phase V [88Zha]. $T = 200$ K. Fractional coordinates and isotropic temperature parameters. B is defined by Eq. (e) in Introduction.

	x	*y*	*z*	B [Å^2]
Ordered structure				
K	0	0	0	1.27(5)
Li	$\frac{1}{3}$	$\frac{2}{3}$	0.8156(6)	0.89(10)
S	$\frac{1}{3}$	$\frac{2}{3}$	0.2049(3)	0.74(7)
O(1)	$\frac{1}{3}$	$\frac{2}{3}$	0.0350(3)	2.44(5)
O(2)	0.0591(2)	0.6589(2)	0.2595(3)	1.65(3)
Disordered structure				
K	0	0	0	1.27(3)
Li	$\frac{1}{3}$	$\frac{2}{3}$	0.8162(5)	1.05(5)
S	$\frac{1}{3}$	$\frac{2}{3}$	0.2052(3)	0.70(4)
O(1)	0.2824(7)	0.6571(14)	0.0369(5)	0.82(4)
O(21)	0.0603(10)	0.6811(10)	0.2595(11)	0.65(12)
O(22)	0.0715(7)	0.6502(11)	0.2844(7)	1.11(10)
O(23)	0.0461(8)	0.6433(10)	0.2414(6)	0.44(11)

Table 41A-2-005. $KLiSO_4$. Structure of phase V [88Zha]. T = 200 K. Interatomic distances [Å] and bond angles [°].

Ordered structure		Disordered structure	
S–O(1)	1.47	S–O(1)	1.47
S–O(2)	1.46	S–O(21)	1.51
		S–O(22)	1.47
		S–O(23)	1.45
O(1)–S–O(2)	109	O(1)–S–O(21^{i})	111
		O(1)–S–O(22)	108
		O(1)–S–O(23^{ii})	108
O(2)–S–O(2^{i})	110	O(21^{i})–S–O(22)	102
		O(21^{i})–S–O(23^{ii})	119
		O(22)–S–O(23^{ii})	109
Li–O(1^{iii})	1.90	Li–O(1^{iii})	1.92
Li–O(2^{iv})	1.93	Li–O(21^{v})	1.97
		Li–O(22^{iv})	1.91
		Li–O(23^{vi})	1.91

Labeling of positions: (i) $1-y, 1+x-y, z$; (ii) $-x+y, 1-x, z$; (iii) $x, y, 1+z$; (iv) $-x, -x+y, z+0.5$; (v) $1+x-y, 1-y, z+0.5$; (vi) $y, 1+x, z+0.5$.

Table 41A-2-006. $KLiSO_4$. Structure of phase V [88Zha]. T = 200 K. r.m.s. displacements of oxygens along the principal directions of vibration and the corresponding direction cosines in a Cartesian system. The Cartesian coordinates: x axis is perpendicular to the crystallographic bc plane, y and z axes are parallel to b and c axes, respectively. r.m.s. amplitude $\sqrt{\overline{u^2}}$ is measured along each principal axis.

	$\sqrt{\overline{u^2}}$ [Å]	cos α	cos β	cos γ
O(1)	0.205	1.000	0.0000	0.0000
	0.205	0.0000	1.0000	0.0000
	0.093	0.0000	0.0000	1.0000
O(2)	0.098	0.8755	–1.3662	–0.3153
	0.125	0.4080	1.9098	1.0760
	0.193	0.2590	–1.1952	1.9460

Table 41A-2-007. $KLiSO_4$. c_{ij} obtained by Brillouin scattering [89Mro]. T = 200 K. c_{ij} in units of [$\cdot 10^{10}$ N m^{-2}].

c_{11}	c_{33}	c_{44}	c_{66}	c_{12}	c_{13}
5.67	6.71(8)	2.14	1.42(5)	2.83(15)	2.35

Table 41A-2-008. $KLiSO_4$. c_{ij} obtained by ultrasonic measurements [88Kab] and Brillouin scattering [86Pim]. c_{ij} in units of [$\cdot 10^{10}$ N m^{-2}].

c_{11}^E	c_{12}^E	c_{33}^E	c_{44}^E	c_{66}^E	Ref.
5.50(11)	2.64(14)	6.53(13)	2.05(4)	1.43(3)	88Kab
5.74	2.92	6.73	2.11	1.42	86Pop

Table 41A-2-009. $KLiSO_4$. Elastooptic constants at RT [90Cza].

p_{12}	p_{13}	p_{16}	p_{31}	p_{45}
0.239	0.194	0.176	0.227	0.125

Table 41A-2-010. $KLiSO_4$. ρ vs. λ. ρ: optical rotatory power [86Sor].

λ [nm]	ϱ [$\cdot 10^3$ °m^{-1}]
657	2.75
589	3.25
551	4.25
485	4.50
441.6	5.00(6)

Table 41A-2-011. $KLiSO_4$. Raman frequencies at 234K in $Z(YZ)X$, $Z(YY)X$, $Z(XY)X$ geometries [87Kih]. The frequencies with an asterisk correspond to lines 15% in intensity of the main YYA_1 vibration. Subscripts ext, tr, r indicate the external vibration, torsional oscillation and rotation, respectively. ν_1 ... ν_4 corresponds to the internal vibration modes.

ν/c [cm^{-1}]			
$Z(YZ)X$	$Z(YY)X$	$Z(XY)X$	
62	61	61	ν_{ext}
134	134	134	ν_{tr}
208*	208	209*	ν_r
–	405	403	
411	411	411	ν_{tr}
–	442	443	
467	467	467	ν_2
626	625	626	
636	636	635	ν_4
643	643	–	
1014*	1014	1014*	ν_1
1121	1121	1120	ν_3
1202	1202	1202	

Table 41A-2-012. $KLiSO_4$. External-mode frequencies in units of [cm^{-1}] [82Tee]. Frequencies for isotopically substituted $KLiSO_4$ are shown with calculated frequency ratios.

Symmetry of mode	ν/c [cm^{-1}]		
	$^7LiKSO_4$	$^6LiKSO_4$	$\nu(^6Li)/\nu(^7Li)$
A	128	128	
	202	202	
	370	395	1.07
E_1	43	43	
	410	429	1.05
	445(LO)	449	1.01
E_2	53	53	
	103	103	
	130	130	
	404	421	1.04

Table 41A-2-013. $KLiSO_4$. Principal values of a tensor of SO_4-radicals [83Fon]. g_c: principal axis is parallel to the c axis. ϕ: angles between the principal axis g_1 and the c axis.

T [° C]	Center	g_c	g_1	g_2	ϕ
26	A	2.0198	2.0294	2.0044	0°
	B				60°
	C				120°
− 95.5	A_1	2.0093	2.0407	2.0033	− 6.2°
	A_2		2.0398	2.0033	− 1.4°
	A_3		2.0399	2.0034	2.4°
	A_4		2.0412	2.0032	6.2°
	B_1		2.0410	2.0036	53.8°
	B_2		2.0395	2.0036	58.6°
	B_3		2.0391	2.0032	62.4°
	B_4		2.0408	2.0035	66.2°
	C_1		2.0410	2.0036	113.8°
	C_2		2.0395	2.0035	118.6°
	C_3		2.0399	2.0036	122.4°
	C_4		2.0409	2.0036	126.2°
−190	A	2.0083	2.0399	2.0020	0°
	B				60°
	C				120°

Table 41A-2-014. $KLiSO_4$. Principal values and direction cosines of g-tensor of Cu^{2+} [88Aly]. T = 77 K.

Principal g-values	Principal A-values	Direction cosines of g-tensor, principal directions with respect to axes		
		a	b^*	c
g_y = 2.044(5)	A_y = 8.2(2)	± 0.1857	–0.9217	∓ 0.3403
g_x = 2.181(5)	A_x = 2.4(3)	± 0.2425	0.3792	∓ 0.8929
g_z = 2.400(5)	A_z = 9.4(2)	± 0.9496	0.0162	∓ 0.3148