

Table 39A-2-001. K₂SeO₄. Structure of phase I [84Iwa]. Fractional coordinates and anisotropic temperature parameters at 500.0(5) °C. b_{ij} is defined by Eq. (b) in Introduction.

	x	y	z	b_{11}	b_{22}	b_{33}	b_{12}	b_{23}	b_{13}
K(1)	0.038(8)	−0.002(7)	−0.009(5)	0.05(3)	0.07(3)	0.027(4)	0.03(3)	−0.01(3)	0.04(2)
K(2)	1/3	2/3	0.798(2)	0.048(6)	0.048(6)	0.020(3)	—	—	—
Se	1/3	2/3	0.276(1)	0.031(1)	0.031(1)	0.014(2)	—	—	—
O(1)	0.424(28)	0.678(29)	0.443(2)	0.14(5)	0.19(9)	0.02(2)	0.10(9)	0.01(1)	−0.02(1)
O(2)	0.155(3)	0.386(2)	0.216(3)	0.053(6)	0.054(3)	0.086(6)	0.021(3)	−0.045(4)	−0.010(4)

Table 39A-2-002. K₂SeO₄. Structure of phase II [70Kal]. Fractional coordinates.

	x	y	z
Se	0.2242 (2)	0.4200 (1)	$\frac{1}{4}$
K (1)	0.1705 (5)	0.0843 (3)	$\frac{1}{4}$
K (2)	−0.0057 (4)	−0.2905 (3)	$\frac{1}{4}$
O (1)	0.2931 (10)	0.3471 (6)	0.0271 (10)
O (2)	0.3024 (16)	−0.4356 (8)	$\frac{1}{4}$
O (3)	0.0126 (21)	0.4251 (10)	$\frac{1}{4}$

Table 39A-2-003. K₂SeO₄. Structure of phase II [70Kal]. Temperature parameters U_{ij} are defined by Eq. (d) in Introduction.

	U_{11} [Å ²]	U_{22} [Å ²]	U_{33} [Å ²]	U_{12} [Å ²]	U_{13} [Å ²]	U_{23} [Å ²]
Se	0.0125 (11)	0.0160 (10)	0.0172 (10)	−0.0006 (4)	0	0
K (1)	0.0164 (19)	0.0295 (17)	0.0283 (16)	0.0032 (11)	0	0
K (2)	0.0135 (15)	0.0198 (15)	0.0264 (16)	0.0002 (11)	0	0
O (1)	0.0474 (43)	0.0417 (36)	0.0239 (35)	0.0132 (31)	0.0060 (31)	−0.0107 (31)
O (2)	0.0373 (70)	0.0213 (49)	0.0465 (60)	−0.0090 (41)	0	0
O (3)	0.0389 (83)	0.0583 (75)	0.0584 (72)	−0.0088 (52)	0	0

Table 39A-2-004. K₂SeO₄. Structure of phase II [70Kal]. Interatomic distances and bond angles for the SeO₄ group. Corrections were made for thermal vibrations. O(1') is mirror-symmetric related mate of O(1).

Distance	Å	Angle	deg
Se-O (1)	1.649 (6)		
Se-O (1')	1.649 (6)		
Se-O (2)	1.644 (9)		
Se-O (3)	1.648 (16)		
O (1) ... O (1')	2.676 (9)	O (1) -Se-O (1')	110.50 (37)
O (1) ... O (2)	2.640 (10)	O (1) -Se-O (2)	108.43 (33)
O (1) ... O (3)	2.660 (15)	O (1) -Se-O (3)	109.84 (34)
O (1') ... O (2)	2.640 (10)	O (1') -Se-O (2)	108.43 (33)
O (1') ... O (3)	2.660 (15)	O (1') -Se-O (3)	109.84 (34)
O (2) ... O (3)	2.656 (19)	O (2) -Se-O (3)	109.76 (59)

Table 39A-2-005. K₂SeO₄. Structure of phase II [70Kal]. Potassium oxygen interatomic distances. The coordinates x, y, z of O(1), O(2), O(3) are given in Table 39A-2-002. Coordinates of O[I], O[II], etc. are given in the third column of this table, and numbers of these oxygen atoms can be identified in Fig. 39A-2-001 and 39A-2-002. The fourth column gives interatomic distances between K(1) and O[I], etc.

K (1) (x, y, z)		Coordinates of O [I],...	K (1)-O [I],...[Å]
O [I]	O (1)	(x, y, z)	3.20
O [II]	O (1)	($x, y, \frac{1}{2}-z$)	3.20
O [III]	O (1)	($-\frac{1}{2}+x, \frac{1}{2}-y, \frac{1}{2}-z$)	3.26
O [IV]	O (1)	($-\frac{1}{2}+x, \frac{1}{2}-y, z$)	3.26
O [V]	O (1)	($\frac{1}{2}-x, -\frac{1}{2}+y, \frac{1}{2}+z$)	3.00
O [VI]	O (1)	($\frac{1}{2}-x, -\frac{1}{2}+y, -z$)	3.00
O [VII]	O (2)	($-\frac{1}{2}+x, -\frac{1}{2}-y, \frac{1}{2}-z$)	3.23
O [VIII]	O (2)	($\frac{1}{2}-x, \frac{1}{2}+y, \frac{1}{2}+z$)	3.02
O [IX]	O (2)	($\frac{1}{2}-x, \frac{1}{2}+y, -z$)	3.02
O [X]	O (3)	($\frac{1}{2}+x, \frac{1}{2}-y, \frac{1}{2}-z$)	2.64
O [XI]	O (3)	(x, y, z)	3.76
K (2) ($x, 1+y, z$)		Coordinates of O [I],...	K (2)-O [XII]...
O [XII]	O (1)	($-x, -y, -z$)	2.83
O [XIII]	O (1)	($-x, -y, \frac{1}{2}+z$)	2.83
O [V']	O (1)	($\frac{1}{2}-x, \frac{1}{2}+y, \frac{1}{2}+z$)	2.73
O [VI']	O (1)	($\frac{1}{2}-x, \frac{1}{2}+y, -z$)	2.73
O [XIV]	O (2)	($x, 1+y, z$)	2.80
O [VII']	O (2)	($-\frac{1}{2}+x, \frac{1}{2}-y, \frac{1}{2}-z$)	2.79
O [XI]	O (3)	(x, y, z)	2.98
O [XV]	O (3)	($-x, -y, -z$)	3.32
O [XVI]	O (3)	($-x, -y, \frac{1}{2}+z$)	3.32

Table 39A-2-006. K₂SeO₄. Transition temperatures, transition heats (ΔQ) and transition entropies (ΔS) [81Cha].

	II-III	III-IV
Θ [K]	127.6(1)	95.1(1)
T -range of anomalous region [K]	85...132	94.4...96.4
ΔQ [J mol ⁻¹]	110(3)	1.1(2)
ΔS [J K ⁻¹ mol ⁻¹]	0.88(3)	0.012(2)

Table 39A-2-007. K₂SeO₄. Piezooptic constants [$\cdot 10^{-12}$ m² N⁻¹] [81Kud2].

$n_2^3 \Pi_{22} - n_3^3 \Pi_{32}$	1.48(15)
$n_2^3 \Pi_{23} - n_3^3 \Pi_{33}$	-5.38(54)
$n_3^3 \Pi_{33} - n_1^3 \Pi_{13}$	-0.86(9)
$n_3^3 \Pi_{31} - n_1^3 \Pi_{11}$	7.08(71)
$n_1^3 \Pi_{11} - n_2^3 \Pi_{21}$	1.50(15)
$n_1^3 \Pi_{12} - n_2^3 \Pi_{22}$	-1.90(19)

Table 39A-2-008. K₂SeO₄. Nonlinear optical properties [84Bee]. l_{ij} : coherence length. $\lambda = 1.06 \text{ } \mu\text{m}$. $T = 88 \text{ K}$.

	l_{ij} [μm]	d_{ik} [$\cdot 10^{-15} \text{ m V}^{-1}$]
d_{33}	17	9.1(11)
d_{32}	17.7	1.6(3)
d_{31}	38	5.3(9)
d_{24}		1.6(5)
d_{15}		5.8(17)