No. 31A-3 $KH_3(SeO_3)_2$, Potassium trihydrogen selenite

(M = 296.04; [D: 299.06])

1a Elastic anomaly in $KH_3(SeO_3)_2$ associated with the phase transition was found by Ivanov et al. in 1975. 75Iva

b

phase	II	I	
state		P [a])	[a]) 67Shu
crystal system	monoclinic	orthorhombic [b])	[b]) 69Han
space group	$P2_1/b-C_{2h}^5$ [c])	$Pbcn-D_{2h}^{14}$ [b])	[c]) 77Mak1
Θ [°C]	–61.6 [a])		

For $KD_3(SeO_3)_2$, Θ = +23.5 °C. 69Yag

$T_{melt} \approx 70$ °C. 67Shu

$\rho = 3.01 \cdot 10^3$ kg m^{-3}, $\rho_X = 3.08 \cdot 10^3$ kg m^{-3}. 71Gor

2a Crystal growth: cooling method from a saturated aqueous solution. 67Shu

b Crystal form: Fig. 31A-3-001.

3a Unit cell parameters: a = 16.152(5) Å, b = 6.249(2) Å, c = 6.307(2) Å at RT. 69Han
Sometimes another axial system is adopted, where $\boldsymbol{a'} = -\boldsymbol{b}$, $\boldsymbol{b'} = \boldsymbol{a}$, $\boldsymbol{c'} = \boldsymbol{c}$.
For notation of a', b', c', see Fig. 31A-3-001.
a = 16.13 Å, b = 6.206 Å, c = 6.257 Å, α = 91.2° at 144 K. 77Mak2

b Z = 4. 71Gor
Crystal structure: Table 31A-3-001, Table 31A-3-002, Table 31A-3-003, Table 31A-3-004, Table 31A-3-005; Fig. 31A-3-002, Fig. 31A-3-003, Fig. 31A-3-004; see also 71Gor
For positions of hydrogen atoms in phase I, see 72Pre

4 Thermal expansion: Fig. 31A-3-005, Fig. 31A-3-006, Fig. 31A-3-007, Fig. 31A-3-008, Fig. 31A-3-009, Fig. 31A-3-010; see also 78Pie

5a Dielectric constants: Fig. 31A-3-011, Fig. 31A-3-012.
Pressure effect: see Table 31A-2-006; Fig. 31A-2-010 in No. 31A-2.
For deuterated crystals: Fig. 31A-3-013.

6a Heat capacity: Fig. 31A-3-014.
Transition heat, transition entropy: ΔQ_m = 439(22) J · mol^{-1}, 77Mak2
ΔS_m = 2.47(13) J K^{-1} mol^{-1}.

8a Elastic compliance and stiffness: Fig. 31A-3-015, Fig. 31A-3-016, Fig. 31A-3-017, Fig. 31A-3-018, Fig. 31A-3-019;
see also 75Iva
c_{44} obtained from Brillouin scattering, see Fig. 31A-3-032, Fig. 31A-3-033 in 10b.
Relaxation and sound attenuation: Fig. 31A-3-019, Fig. 31A-3-020, Fig. 31A-3-021.

b The value of the fourth order elastic constant c_{5555} was measured to be $16.7 \cdot 10^2$ N m^{-2} from the shear stress (T_5) dependence of c_{55}. 82Sor2

9a Infrared absorption and optical indicatrix: Fig. 31A-3-022, Fig. 31A-3-023;
see also 78Iva

10a	Raman scattering: Fig. 31A-3-024, Fig. 31A-3-025, Fig. 31A-3-026, Fig. 31A-3-027, Fig. 31A-3-028.	
	Low frequency Raman spectrum and its temperature dependence at $8 \cdot 10^8$ Pa; see	80Kra
b	Brillouin scattering and Rayleigh scattering: Fig. 31A-3-029, Fig. 31A-3-030, Fig. 31A-3-031, Fig. 31A-3-032, Fig. 31A-3-033.	
	Rayleigh and Brilloun scattering for a slightly deuterated crystal, see	78Tan2
	Isotope effect on the central peak, see	78Tan1
13a	NMR: Table 31A-3-006, Table 31A-3-007; Fig. 31A-3-034, Fig. 31A-3-035, Fig. 31A-3-036, Fig. 31A-3-037, Fig. 31A-3-038, Fig. 31A-3-039, Fig. 31A-3-040;	
	see also	78Gra
b	ESR: Table 31A-3-008, Table 31A-3-009, Table 31A-3-010.	