No. 40A-7 $RbHSeO_4$, Rubidium hydrogen selenate

(M = 229.43; [D: 230.44])

1a Ferroelectricity in $RbHSeO_4$ below 370.7 K was found by Czapla et al. in 1979. 79Cza
In addition, Suzuki et al. found a new ferroelectric phase below 446 K in 1979. 79Suz

b

phase	III	II	I	
state	F	F	P(super ionic)	
crystal system	triclinic	monoclinic	monoclinic	
space group	$P1-C_1^1$	$P2-C_2^1$		[a]) 79Cza
Θ [K]	370.7 [a])	446 [b])		[b]) 79Suz

P_s || [010]. [c]) [c]) 79Pop
$\rho_X = 3.38 \cdot 10^3$ kg m^{-3}. 78Was
The crystal system in phase III can be looked upon pseudoorthorhombic. 79Pie
Phase diagram with deuterium concentration: Fig. 40A-7-001.

2a Crystal growth: evaporation method from aqueous solution. 79Pie
Crystal form: Fig. 40A-7-002.

3a Unit cell parameters:

phase	T [K]	a [Å]	b [Å]	c [Å]	α [°]	β [°]	γ [°]	
II	423	19.464	4.626	7.599			90.74	79Suz
III	RT	19.359(3)	4.619(3)	7.572(4)	90.60(5)	89.80(5)	90.73(5)	78Was

The unit cell vectors of the pseudoorthorhombic cell in phase III are given by
$\boldsymbol{a}' = \boldsymbol{b}$, $\boldsymbol{b}' = \boldsymbol{c}$, and $\boldsymbol{c}' = \boldsymbol{a} - \boldsymbol{b}$.
Crystal system of 92 % deuterated crystal at RT; orthorhombic. Space group $P2_12_12_1$. 82Was
Unit cell parameters: a = 12.887(3) Å, b = 4.599(6) Å, c = 7.515(4) Å.

b Crystal structure of phase II: Fig. 40A-7-003.
Fractional coordinates: Table 40A-7-001.
Fractional coordinates with the origin on the c axis and anisotropic temperature parameters at 387 K: Table 40A-7-002.
Interatomic distances and bond angles at 387 K: Table 40A-7-003.
Z = 6 in phase II and phase III. 78Was
Nuclear density map of hydrogen: Fig. 40A-7-004, Fig. 40A-7-005.
Interatomic distances and bond angles in phase II: Fig. 40A-7-006.
Fractional coordinates and thermal motion parameters of phase III: Table 40A-7-004.
Crystal structure of 92% deuterated crystal at RT: Table 40A-7-005, Table 40A-7-006; Fig. 40A-7-007.
Z = 4 for 92% deuterated crystal at RT. 82Was

4 Lattice distortions with temperature: Table 40A-7-007; Fig. 40A-7-008, Fig. 40A-7-009.

5a	Dielectric constant: temperature dependence at $1.0 \cdot 10^3$ Hz: Fig. 40A-7-010, Fig. 40A-7-011, Fig. 40A-7-012. at $1.0 \cdot 10^6$ Hz: Fig. 40A-7-013. Curie-Weiss law constants: $C = 3.6 \cdot 10^5$ K, $\Theta_p = 317$ K in phase II. Temperature dependence of κ'_b, $\tan\delta$ of $RbH_{1-x}D_xSeO_4$: Fig. 40A-7-014. Temperature dependence of κ'^{-1}_a under hydrostatic pressure: Fig. 40A-7-015, Fig. 40A-7-016. Effect of hydrostatic pressure on Θ: Fig. 40A-7-017.	79Pop
b	Nonlinear dielectric properties: $\xi = -1.63 \cdot 10^{10}$ V C^{-3} m^5, $\zeta = 3.37 \cdot 10^3$ V C^{-5} m^9.	80Pop
c	Spontaneous polarization and coercive field: Fig. 40A-7-018, Fig. 40A-7-019. Spontaneous polarization of $RbH_{1-x}D_xSeO_4$: Fig. 40A-7-020.	
d	Pyroelectric coefficient: see Fig. 40A-7-019.	
9a	Far infrared reflectivity and dielectric constant along the *a*, *b*, *c* axes: Fig. 40A-7-021, Fig. 40A-7-022, Fig. 40A-7-023. Optical birefringence: Fig. 40A-7-024. Infrared absorption: see Infrared spectra at RT and 29 K: see	81Bar 86Bar
10a	Raman scattering frequency shifts at 20 K and 300 K: Table 40A-7-008. For spectra, see	81Bar, 82Car, 85Fed
13a	NMR: chemical shifts of ^{77}Se: Table 40A-7-009. Second moment of proton NMR lines: see Fig. 40A-9-058 in No. 40A-9.	
15a	Domain structure: 180° laminar domains were observed by polarized light. See Domain structure was observed in the presence of either electric field or shear stresses. Deflection of light at domain wall: see	79Pop, 80Cza 83Tsu, 84Tsu 83Tsu, 84Tsu