No. 40A-9 NH_4HSeO_4, Ammonium hydrogen selenate

(M = 162.00; [D:167.01])

1a Ferroelectricity in NH_4HSeO_4 below –22 °C was discovered by Czapla et al. in 1979. 79Cza

b

phase	IV	III	II	I	I′
state		F	P		superionic
crystal system		triclinic [a])	monoclinic [b])	monoclinic [c])	monoclinic [d])
space group		P1–C_1^{1} [e])	B2–C_2^{3} [a]) [b])	$P2_1/b$–C_{2h}^{5} [c])	
Θ [K]		100	251.3	285	417

87Roz

[a]) 80Ges

[b]) 79Cza

[c]) 80Ale

[d]) 88Ono

[e]) 79Kra

The crystal in phase III can be looked upon pseudoorthorhombic, where the unit cell vectors are denoted as $\boldsymbol{a}'$, $\boldsymbol{b}'$ and $\boldsymbol{c}'$. 80Kru

ND_4DSeO_4 does not show any ferroelectricity in a temperature range between 73 K and 313 K; see 80Cza

The space group of highly deuterated ammonium biselenate crystal is reported to be orthorhombic $P2_12_12_1$ at RT. 82Was

Phases II, III, IV are pyroelectric and polar along the a-axis. 79Kra, 79Cza, 80Ges

T_{melt} = 427 K. 88Ono

Superstructure is observed in phase III. 79Kra

Cleavage plane: (001). 80Ale

Transition temperature of NH_4HSeO_4–ND_4DSeO_4: Fig. 40A-9-001, Fig. 40A-9-002.

Transition temperature of NH_4HSeO_4–NH_4HSO_4: Fig. 40A-9-003.

2a Crystal growth: slow evaporation of aqueous solution. 79Cza

b Crystal form: Fig. 40A-9-004.

3a Unit cell parameters of phase I′: a = 7.79(4) Å, b = 7.71(3) Å, c = 7.92(3) Å, γ = 112.5(4)°at 423 K. 88Ono

Unit cell parameters of phase I: a = 19.745(8) Å, b = 4.611(9) Å, c = 7.552(4) Å, γ = 102°36′ at 20 °C. 80Ale

Unit cell parameters of phase II for monoclinic system: a = 19.75(8) Å, b = 4.611(9) Å, c = 7.552(4) Å, γ = 102° 4(1)′ at 20 °C. 79Cza

Unit cell parameters for pseudoorthorhombic system: a' = 19.27(8) Å, b' = 4.611(9) Å, c' = 7.55(4) Å, γ' = 89° 5(2)′, where $\boldsymbol{a}' = \boldsymbol{a} + \boldsymbol{b}$, $\boldsymbol{b}' = \boldsymbol{b}$, $\boldsymbol{c}' = \boldsymbol{c}$. 80Kru

Unit cell parameters of phase III: a = 4.562 Å, b = 7.486 Å, c = 19.050 Å, $\alpha = \gamma$ = 90°, β = 91.02° in P1 cell at –50 °C. 79Kra

Unit cell parameters of phase III in B1 cell: Table 40A-9-001.

The unit cell vectors of the pseudoorthorhombic cell in phase III are given by $\boldsymbol{a}' = \boldsymbol{a}$, $\boldsymbol{b}' = \boldsymbol{b}$, $\boldsymbol{c}' = \boldsymbol{c} - \boldsymbol{a}$. 79Kra

b Structure of phase I:

Z = 4. 80Kru

Table 40A-9-002; Fig. 40A-9-005.

Interatomic distances and bond angles at 293 K and 400 K: Table 40A-9-003, Table 40A-9-004.

Distribution of nuclear density of protons observed by neutron diffraction at 400 K: Fig. 40A-9-006.

Distribution of nuclear density of protons observed by neutron diffraction at 293 K: Fig. 40A-9-007, Fig. 40A-9-008, Fig. 40A-9-009.

	The axial system ($\boldsymbol{a}$, $\boldsymbol{b}$, $\boldsymbol{c}$, α, β, γ) in phase I cited by Czapla et al. is related to the axial system ($\boldsymbol{a}'$, $\boldsymbol{b}'$, $\boldsymbol{c}'$, α', β', γ') by Kruglik et al. as follows: $\boldsymbol{a} = -\boldsymbol{b}'$, $\boldsymbol{b} = \boldsymbol{c}'$, $\boldsymbol{c} = \boldsymbol{a}'$, $\alpha = \beta'$, $\beta = \pi - \gamma'$, $\gamma = \alpha'$. Structure of phase III: Table 40A-9-005; Fig. 40A-9-010. Interatomic distances and bond angles at 223 K: Table 40A-9-006. Crystal structure of deuterated crystal at RT: Fig. 40A-9-011, Fig. 40A-9-012. Interatomic distances and bond angles of SeO_4 tetrahedra in ND_4DSeO_4: Table 40A-9-007.	79Cza, 80Kru
4	Linear thermal expansion: Fig. 40A-9-013, Fig. 40A-9-014, Fig. 40A-9-015. Linear thermal expansion coefficient α_{ii} (i = 1, 2, 3): see	83Pop
5a	Dielectric constants: temperature dependence at $8 \cdot 10^2$ Hz, $1 \cdot 10^7$ Hz: Fig. 40A-9-016; temperature dependence at $1 \cdot 10^3$ Hz: Fig. 40A-9-017; temperature dependence at $1 \cdot 10^3$ Hz, $1 \cdot 10^6$ Hz: Fig. 40A-9-018, Fig. 40A-9-019, Fig. 40A-9-020; temperature dependence at 10^9 Hz region: Fig. 40A-9-021. Relaxation frequency: Fig. 40A-9-022. Cole-Cole diagram: Fig. 40A-9-023. Curie-Weiss law constant: $C = 5.453 \cdot 10^3$ K; $\Theta_p = 248$ K.	79Cza, 81Cza
	Dielectric constant κ'' in the far infrared region: Fig. 40A-9-024. Dielectric constant of partially deuterated crystals: Fig. 40A-9-025, Fig. 40A-9-026. See also:	80Cza, 80Pop, 81Cza, 85Pyk1, 86Cza
	Pressure dependence of κ_b and κ_a: Fig. 40A-9-027, Fig. 40A-9-028. Phase diagram in regard to p: Fig. 40A-9-029, Fig. 40A-9-030. Effect of uniaxial stress on κ_b: Fig. 40A-9-031, Fig. 40A-9-032, Fig. 40A-9-033, Fig. 40A-9-034. Effect of uniaxial stress on Θ: Fig. 40A-9-035.	
b	Effect of E_{bias} on κ_b: Fig. 40A-9-036, Fig. 40A-9-037. Effect of E_{bias} on Θ (phase diagram in regard to E_{bias}): Fig. 40A-9-038. See also	81Cza, 84Pop1, 85Pyk2
	Nonlinear dielectric properties: $\xi = -2.64 \cdot 10^{12}$ V C^{-3} m^5, $\zeta = 5.3 \cdot 10^{16}$ V C^{-5} m^9.	80Pop
c	Spontaneous polarization and coercive field: Fig. 40A-9-039, Fig. 40A-9-040, Fig. 40A-9-041. Spontaneous polarization under uniaxial stress: Fig. 40A-9-042. Spontaneous polarization of partially deuterated crystal: see Polarization change along the b axis: see	85Pop 86Pyk1
d	Pyroelectricity: Fig. 40A-9-043. Pyroelectric coefficient: Fig. 40A-9-044, Fig. 40A-9-045, Fig. 40A-9-046.	
6a	Specific heat capacity at constant pressure: Fig. 40A-9-047. Specific heat capacity for deuterated crystal: see Transition heat ΔQ_m and transition entropy ΔS_m at $\Theta_{IV-III} = 105.3$ K: $\Delta Q_m = 150$ J mol^{-1}, $\Delta S_m = 1.4$ J mol^{-1} K^{-1}. For deuterated crystal, see	84Pop2 84Pop2 84Pop2

8a	Ultrasonic velocity and attenuation coefficient at $5 \cdot 10^6$ Hz and $1 \cdot 10^7$ Hz: Fig. 40A-9-048. Elastic stiffness constants measured by ultrasonic method at $1 \cdot 10^7$ Hz: Fig. 40A-9-049, Fig. 40A-9-050.	
9a	Birefringence: Fig. 40A-9-051. For electric field dependence: see Infrared reflection spectra: see	 82Mar 81Kro
b	Electrooptic constant: Fig. 40A-9-052.	
10a	Raman scattering spectra in 300...1000 cm^{-1} at RT: Fig. 40A-9-053, Fig. 40A-9-054. Temperature dependence: Fig. 40A-9-055, Fig. 40A-9-056. Raman scattering spectra of deuterated crystal: Fig. 40A-9-057. For low-frequency (0...250 cm^{-1}) region: see	 83Smo
13a	Second moment of proton NMR lines: Fig. 40A-9-058. For correlation time τ_c: see Deuteron NMR determined EFG tensor parameters of 60% deuterated crystal: Table 40A-9-008. Chemical shift of ^{77}Se line: Fig. 40A-9-059. See Table 40A-7-009 in No. 40A-7.	 84Mos
14	Temperature dependence of incommensurate wave vector in phase II: Fig. 40A-9-060. Integrated intensity of the satellite reflection: Fig. 40A-9-061. For deuterated crystal: see Integrated intensity of neutron scattering: Fig. 40A-9-062.	 89Den
15	Domain structure: For deuterated crystal, see	81Pyk, 81Mro 85Pyk2
16	Effect of X-ray irradiation on κ: see	86Pyk2