42 $(NH_4)_3H(SO_4)_2$ family

42A Pure compounds

No. 42A-1 $(NH_4)_3H(SO_4)_2$, Triammonium hydrogen disulfate

(M = 247.25; [D: 260.33])

1a Ferroelectricity in pressure-induced phases of $(NH_4)_3H(SO_4)_2$ was discovered by Gesi in 1976. 76Ges2

b

phase	VII	V	IV	III	II	I	VI *)
state	F						F
crystal system	triclinic	triclinic		mono-clinic	mono-clinic	trigonal	triclinic
space group	P1–C_1^{1} [a])	P$\bar{1}$–C_i^{1} [a])		P2/n–C_{2h}^{4} [a])	A2/a–C_{2h}^{6} [b])	R$\bar{3}$m–D_{3d}^{5} [c])	P1–C_1^{1} [d])**)
Θ [K]	62 [e])	133 [f])	137 [f])	265 [f])	413 [f])		

[a]) 94Tam
[b]) 78Suz
[c]) 79Suz2
[d]) 86Tan
[e]) 80Ges1
[f]) 77Ges2

A phase transition was suggested at 463 K by Fukami et al. from DSC and conductivity measurements. 94Fuk

Phase diagram of $[(NH_4)_3H]_{1-x}[(ND_4)_3D]_x(SO_4)_2$: Fig. 42A-1-001.

Phase III′ of $(ND_4)_3D(SO_4)_2$ is identical with phase III from the phase diagram. However, different space group P2–C_2^1 was reported for phase III′ of $(ND_4)_3D(SO_4)_2$. 86Tan

By deuteration phase VI is stabilized at atmospheric pressure; see Fig. 42A-1-001, Fig. 42A-1-019.

P_s: perpendicular to (100). 77Ges2

$\rho = 1.831 \cdot 10^3$ kg m^{-3}. 04Gos

Transparent, colorless, deliquescent.

*) High pressure phase; see Fig. 42A-1-017.

**) Determined from corresponding phase in deuterated crystal at atmospheric pressure.

2a Crystal growth: evaporation of aqueous solution. 76Ges1

b Crystal form: Fig. 42A-1-002.

3a Unit cell parameters in phase II:

a = 10.153(3) Å, b = 5.854(2) Å, c = 15.410(6) Å, β = 101.76(2)°. T = RT. 78Suz

[D: a = 10.158(1) Å, b = 5.860(1) Å, c = 15.401(1) Å, β = 101.88(1)°. T = 287 K.] 81Tan

Unit cell parameters in phase I: a = 8.29 Å, α = 41.7 °. T = 418 K. 79Suz2

Relation between the unit cell parameters in phase I, $\boldsymbol{a}_I$, $\boldsymbol{b}_I$, $\boldsymbol{c}_I$ ($|\boldsymbol{a}_I| = |\boldsymbol{b}_I| = |\boldsymbol{c}_I| = a$), to those in phase II, $\boldsymbol{a}_{II}$, $\boldsymbol{b}_{II}$, $\boldsymbol{c}_{II}$: $\boldsymbol{a}_I = (\boldsymbol{a}_{II} + \boldsymbol{c}_{II})/2$, $\boldsymbol{b}_I = (\boldsymbol{b}_{II} + \boldsymbol{c}_{II})/2$, $\boldsymbol{c}_I = (-\boldsymbol{b}_{II} + \boldsymbol{c}_{II})/2$. 79Suz2

Unit cell parameters of $(ND_4)_3D(SO_4)_2$:

Phase III′: a = 10.087(2) Å, b = 5.835(1) Å, c = 15.542(2) Å, β = 101.71(2)°. T = 189(7) K. 86Tan

Phase VI: a = 10.123(1) Å, b = 5.846(1) Å, c = 15.476(1) Å, α = 89.98(1)°, β = 101.78(2)°, γ = 90.01(1) °. T = 233(7) K. 86Tan

b	phase	VII	V	III	II	I	[a]) 94Tam
	Z	2 [a])	4 [a])	4 [a])	4 [b])	1 [c])	[b]) 78Suz [c]) 79Suz2

For $(ND_4)_3D(SO_4)_2$: $Z = 4$ in phases VI, III′ and II. 86Tan
Crystal structure of phase II: Table 42A-1-001, Table 42A-1-002; Fig. 42A-1-003, Fig. 42A-1-004; see also 85Lec
Structure of $(ND_4)_3D(SO_4)_2$:
Phase II: Table 42A-1-003, Table 42A-1-004, Table 42A-1-005; Fig. 42A-1-005.
Phase III′:Table 42A-1-006, Table 42A-1-007; Fig. 42A-1-006.
Phase VI: Table 42A-1-007, Table 42A-1-008; Fig. 42A-1-007.

4 Thermal expansion: Fig. 42A-1-008, Fig. 42A-1-009.

5a Dielectric constant: Fig. 42A-1-010, Fig. 42A-1-011, Fig. 42A-1-012, Fig. 42A-1-013, Fig. 42A-1-014.
Dielectric constant of $[(NH_4)_3H]_{1-x}[(ND_4)_3D]_x(SO_4)_2$ system: Fig. 42A-1-015, Fig. 42A-1-016.
Phase diagram with regard to p: Fig. 42A-1-017, Fig. 42A-1-018.
Θ–p phase diagram of $(ND_4)_3D(SO_4)_2$: Fig. 42A-1-019.
Θ–p phase diagram of $[(NH_4)_3H]_{1-x}[(ND_4)_3D]_x(SO_4)_2$ system: see 80Ges1

c Spontaneous polarization: Fig. 42A-1-020.
Spontaneous polarization of $[(NH_4)_3H]_{1-x}[(ND_4)_3D]_x(SO_4)_2$ system: Fig. 42A-1-021.

6a Heat capacity: Fig. 42A-1-022, Fig. 42A-1-023.
Transition heats and transition entropies: Table 42A-1-009.

9a Birefringence: Fig. 42A-1-024, Fig. 42A-1-025.
Infrared absorption: see 73Ach, 88Kam3, 91Vid

10a Raman scattering: Table 42A-1-010; Fig. 42A-1-026, Fig. 42A-1-027;
see also 88Sri

11 Electrical conductivity: Table 42A-1-011; Fig. 42A-1-028.

13b ESR: Table: 42A-1-012, Table: 42A-1-013; Fig. 42A-1-029;
see also 83Min, 86Woj