Table 42A-2-001. $(NH_4)_3H(SeO_4)_2$. Structure of phases I and II [93Luk]. Fractional coordicates and temperature parameters. U_{eq} for non-hydrogen atoms: 1/3 of the trace of the orthogonalized U_{ij}. U_{ij} is defined by Eq. (d) in Introduction. $\overline{u^2}$ for hydrogens: mean square displacement.

	x	y	z	Occup.	$U_{eq}/\overline{u^2}$
Phase II (310 K)					
Se	0	0	0.40906(3)	1	39
O(1)	0.2918(6)	0.1634(8)	0.4301(2)	1	79
O(2)	0.0408(23)	0.0773(16)	0.3376(3)	1/3	61
N(1)	0	0	0	1	46
N(2)	0	0	0.1974(3)	1	53
H(1)	0.123(3)	0.226(7)	0.326(3)	1/6	19
H(2)	0	0	0.037(3)	1/2	66
H(3)	0.062(6)	0.112(3)	0.018(2)	1/2	71
H(4)	0	0	0.149(5)	1	131
H(5)	0.062(3)	0.141(3)	0.223(2)	1	135
Phase I (355 K)					
Se	0	0	0.40876(3)	1	46
O(1)	0.2893(7)	0.1748(16)	0.4301(2)	1/2	74
O(2)	0.0639(22)	0.0817(15)	0.3365(3)	1/6	65
N(1)	0	0	0	1	56
N(2)	0	0	0.1981(6)	1	65
H(1)	0.103(3)	0.205(6)	0.323(3)	1/6	48
H(2)	0	0	0.043(3)	1/2	57
H(3)	0.080(3)	0.160(5)	0.006(2)	1/2	72
H(4)	0	0	0.171(2)	1	86
H(5)	0.081(2)	0.162(5)	0.219(2)	1	137

Table 42A-2-002. $(NH_4)_3H(SeO_4)_2$. Structure of phases I at 355 K and II at 310 K [93Luk]. Interatomic distances [Å].

	Phase II	Phase I
Se–O(1)	1.610(3)	1.611(3)
Se–O(2)	1.687(8)	1.705(6)
O(1)–O(1^{i})	2.660(6)	2.661(8)
O(2)–O(1)	2.507(10)	2.441(9)
O(2)–O(1^{i})	2.550(10)	2.641(10)
O(2)–O(1^{ii})	2.873(8)	2.892(8)
N(1)–H(2)	0.84(6)	0.99(3)
N(1)–H(3)	0.71(3)	0.85(3)
N(2)–H(4)	1.10(6)	0.62(5)
N(2)–H(5)	0.94(3)	0.98(3)
O(2)...O(2^{iii})	2.696(16)	2.674(17)
O(2)–H(1)	0.82(3)	0.73(4)
H(1)...O(2^{iii})	1.91(2)	2.01(3)
∠O(1)–H(1)...O(2′)	159(6)	150(6)

Symmetry code: (i) $-y, x-y, z$; (ii) $y-x, -x, z$; (iii) $\frac{1}{3}-x, \frac{2}{3}-y, \frac{2}{3}-z$.

Table 42A-2-003. $(NH_4)_3H(SeO_4)_2$. Structure of phase III [92Pie]. Fractional coordinates in the pseudo-monoclinic lattice cell and equivalent isotropic temperature parameters [Å^2]. T = 296 K. U_{eq}: 1/3 of the trace of the orthogonalized U_{ij}. U_{ij} is defined by Eq. (d) in Introduction.

Atom	x	y	z	U_{eq}
Se(1)	0.11382(2)	0.22378(5)	0.45950(3)	0.025
Se(2)	–0.11459(2)	0.22804(5)	0.04056(3)	0.026
O(1)	0.0078(2)	0.1778(5)	0.4418(3)	0.052
O(2)	0.1563(2)	0.1914(4)	0.6140(3)	0.043
O(3)	0.1258(2)	0.4727(4)	0.4114(3)	0.043
O(4)	0.1498(2)	0.0404(4)	0.3686(3)	0.041
O(5)	–0.0080(2)	0.1774(5)	0.0629(3)	0.054
O(6)	–0.1481(2)	0.2793(4)	–0.1138(3)	0.041
O(7)	–0.1294(2)	0.4380(4)	0.1313(3)	0.041
O(8)	–0.1564(2)	0.0043(4)	0.0829(3)	0.044
N(1)	0.5000(2)	0.2396(5)	0.2500(3)	0.032
N(2)	0.2024(2)	0.2634(5)	0.1531(3)	0.037
N(3)	0.7998(2)	0.2728(5)	0.3492(3)	0.040
H(1)	0.470(3)	0.161(7)	0.212(4)	0.048
H(2)	0.468(3)	0.346(7)	0.256(4)	0.066
H(3)	0.536(3)	0.173(7)	0.300(4)	0.046
H(4)	0.525(3)	0.350(7)	0.245(4)	0.051
H(5)	0.192(3)	0.220(7)	0.242(4)	0.055
H(6)	0.187(3)	0.150(7)	0.069(4)	0.046
H(7)	0.262(3)	0.258(7)	0.188(4)	0.048
H(8)	0.169(3)	0.384(7)	0.101(4)	0.062
H(9)	0.810(3)	0.275(7)	0.258(4)	0.061
H(10)	0.817(3)	0.122(7)	0.383(4)	0.048
H(11)	0.746(3)	0.266(7)	0.311(4)	0.055
H(12)	0.826(3)	0.368(7)	0.432(4)	0.041
H(13)	0.000(3)	0.052(7)	0.468(4)	0.029
H(14)	0.000(3)	0.026(7)	0.030(4)	0.037

Table 42A-2-004. $(NH_4)_3H(SeO_4)_2$. Structure of phase III [92Pie]. Interatomic distances [Å] and angles [°]. T = 296 K.

Se(1)–O(1)	1.674(3)	Se(2)–O(5)	1.676(3)
Se(1)–O(2)	1.629(3)	Se(2)–O(6)	1.625(3)
Se(1)–O(3)	1.622(3)	Se(2)–O(7)	1.621(3)
Se(1)–O(4)	1.626(3)	Se(2)–O(8)	1.624(3)
O(1)–O(2)	2.641(4)	O(5)–O(6)	2.638(4)
O(1)–O(3)	2.672(4)	O(5)–O(7)	2.674(4)
O(1)–O(4)	2.642(5)	O(5)–O(8)	2.635(4)
O(2)–O(3)	2.698(4)	O(6)–O(7)	2.689(4)
O(2)–O(4)	2.699(4)	O(6)–O(8)	2.694(4)
O(2)–O(4)	2.683(3)	O(7)–O(8)	2.690(4)
O(1)–Se(1)–O(2)	106.15(16)	O(5)–Se(2)–O(6)	106.14(17)
O(1)–Se(1)–O(3)	108.32(16)	O(5)–Se(2)–O(7)	108.42(16)
O(1)–Se(1)–O(4)	106.35(15)	O(5)–Se(2)–O(8)	105.93(15)
O(2)–Se(1)–O(3)	112.20(14)	O(6)–Se(2)–O(7)	111.88(14)
O(2)–Se(1)–O(4)	112.04(14)	O(6)–Se(2)–O(8)	112.05(14)
O(3)–Se(1)–O(4)	111.39(16)	O(7)–Se(2)–O(8)	111.99(16)
N(1)–H(1)	0.73(4)	N(3)–H(9)	1.01(4)
N(1)–H(1)	0.83(4)	N(3)–H(10)	0.99(2)
N(1)–H(3)	0.79(4)	N(3)–H(11)	0.86(4)
N(1)–H(4)	0.79(3)	N(3)–H(12)	1.05(3)
N(2)–H(5)	1.02(4)		
N(2)–H(6)	1.10(3)		
N(2)–H(7)	0.93(4)		
N(2)–H(8)	1.00(3)		

Table 42A-2-005. $(NH_4)_3H(SeO_4)_2$. Structure of phase III [92Pie]. Hydrogen bond distances [Å] and angles [°]. $T = 296$ K.

D–H...*A*	*D*–*A* [Å]	*D*–H [Å]	H...*A* [Å]	*D*–H...*A* [°]
O(1)–H(13)...O(1^{ix})	2.529(6)	0.83(3)	1.72(3)	166(3)
O(5)–H(14)...O(5^{iv})	2.541(6)	1.00(3)	1.57(3)	163(3)
N(1)–H(1)...O(7^{i})	2.833(4)	0.73(4)	2.11(4)	169(4)
N(1)–H(3)...O(3^{i})	2.824(4)	0.79(4)	2.03(4)	173(3)
N(2)–H(5)...O(4)	2.921(5)	1.02(4)	1.96(4)	157(2)
N(2)–H(6)...O(8^{iv})	2.903(4)	1.10(3)	1.81(3)	172(2)
N(2)–H(7)...O(2^{iii})	2.950(4)	0.93(4)	2.22(4)	135(3)
N(2)–H(7)...O(8^{ii})	2.911(5)	0.93(4)	2.41(4)	113(2)
N(2)–H(8)...O(6^{v})	2.893(4)	1.00(3)	2.07(2)	139(3)
N(3)–H(9)...O(7^{vi})	2.942(5)	1.01(4)	2.06(4)	145(3)
N(3)–H(10)...O(2^{vii})	2.895(4)	0.99(2)	1.94(2)	161(3)
N(3)–H(11)...O(4^{ii})	2.893(5)	0.86(4)	2.40(4)	117(2)
N(3)–H(12)...O(3^{viii})	2.957(4)	1.05(3)	1.91(3)	177(3)

Symmetry codes:

(i) $x + \frac{1}{2}, y - \frac{1}{2}, z$
(ii) $x + \frac{1}{2}, y + \frac{1}{2}, z$
(iii) $-x + \frac{1}{2}, -y + \frac{1}{2}, -z + 1$
(iv) $-x, -y, -z$
(v) $-x, -y + 1, -z$
(vi) $x + 1, y, z$
(vii) $-x + 1, -y, -z + 1$
(viii) $-x + 1, -y + 1, -z + 1$
(ix) $-x, -y, -z + 1$

Table 42A-2-006. $(NH_4)_3H(SeO_4)_2$. Structure of phase IV [93Pie]. Fractional coordicates and temperature parameters [$Å^2$]. $T = 200$ K. U_{eq}: 1/3 of the trace of the orthogonalized U_{ij}. U_{ij} is defined by Eq. (d) in Introduction.

Atom	*x*	*y*	*z*	U_{eq}
Se1	0.3048(1)	0.2421(1)	0.1350(1)	0.018(1)
O1	0.1482(2)	0.2868(4)	0.1219(2)	0.027(1)
O2	0.3759(4)	0.2671(4)	0.2417(2)	0.036(1)
O3	0.3353(2)	–0.0117(3)	0.1084(1)	0.025(1)
O4	0.3721(2)	0.4245(3)	0.0839(1)	0.028(1)
N1	0.3982(4)	0.7698(5)	0.9541(2)	0.024(1)
N2	0.5000	0.2582(6)	0.7500	0.023(1)
H1	0.567(8)	0.258(11)	0.268(7)	0.017(30)
H11	0.339(4)	0.687(6)	0.936(2)	0.019(90)
H12	0.391(4)	0.887(6)	0.930(2)	0.025(90)
H13	0.402(5)	0.788(7)	0.007(4)	0.048(15)
H14	0.457(5)	0.704(7)	0.944(3)	0.038(13)
H21	0.553(5)	0.184(8)	0.782(3)	0.060(14)
H22	0.466(7)	0.330(9)	0.769(4)	0.085(20)

Table 42A-2-007. $(NH_4)_3H(SeO_4)_2$. Structure of phase IV [93Pie]. Interatomic distances [Å] and angles [°]. T = 200 K.

Se1–O1	1.620(3)
Se1–O2	1.679(3)
Se1–O3	1.634(2)
Se1–O4	1.620(2)
O1–O2	2.661(4)
O1–O3	2.699(3)
O1–O4	2.682(4)
O2–O3	2.647(3)
O2–O4	2.662(4)
O3–O4	2.691(3)
N1–H11	0.79(4)
N1–H12	0.79(4)
N1–H13	0.84(6)
N1–H14	0.78(5)
N2–H21	0.79(5)
N2–H22	0.67(6)
O4–Se1–O1	111.74(11)
O4–Se1–O3	111.62(11)
O1–Se1–O3	112.05(11)
O4–Se1–O2	107.6(2)
O1–Se1–O2	107.5(2)
O3–Se1–O2	106.00(11)

Table 42A-2-008. $(NH_4)_3H(SeO_4)_2$. Structure of phase IV [93Pie]. Hydrogen bond distances [Å] and angles [°]. T = 200 K.

D–H...*A*	*D*–*A* [Å]	*D*–H [Å]	H...*A* [Å]	∠*D*–H...*A* [°]
O2–H1...O2 [i]	2.541(9)	0.65(10)	1.94(9)	154(10)
N1–H11...O3 [ii]	2.857(4)	0.79(4)	2.08(4)	171(4)
N1–H12...O1 [iii]	2.916(4)	0.79(4)	2.13(4)	171(4)
N1–H13...O3 [iv]	2.982(5)	0.84(6)	2.43(6)	147(4)
N1–H14...O4 [v]	2.859(5)	0.78(5)	2.09(6)	171(6)
N2–H21...O3 [vi]	2.883(3)	0.79(5)	2.11(5)	165(6)
N2–H22...O1 [ii]	2.845(3)	0.67(6)	2.43(6)	122(6)

Symmetry codes:

(i) $-x+1, y, -z+\frac{1}{2}$ (iv) $x, y+1, z+1$

(ii) $-x+\frac{1}{2}, -y+\frac{1}{2}, -z+1$ (v) $-x+1, -y+1, -z+1$

(iii) $-x+\frac{1}{2}, -y+\frac{3}{2}, -z+1$ (vi) $-x+1, -y, -z+1$

Table 42A-2-009. $(NH_4)_3H(SeO_4)_2$. Transition heats and transition entropies [84Osa].

Phase transition	ΔQ [$\cdot 10^4$ J mol^{-1}]	ΔS [J K^{-1} mol^{-1}]
II–I	3.299	10.5
III–II	2.782	9.2
IV–III	1.075	7.5
V–IV	0.635	5.0

Table 42A-2-010. $(NH_4)_3H(SeO_4)_2$. ΔU, A [90Paw]. Electrical conductivity σ is given by $\sigma T = A \exp(-\Delta U/kT)$.

Phase	$\boldsymbol{E} \parallel \boldsymbol{a}$		$\boldsymbol{E} \parallel \boldsymbol{c}$	
	ΔU [eV]	A [Ω^{-1} m^{-1} K]	ΔU [eV]	A [Ω^{-1} m^{-1} K]
I	0.27	$2.8 \cdot 10^6$	0.40	$5.4 \cdot 10^6$
II	0.32	$1.9 \cdot 10^7$	0.48	$9.5 \cdot 10^7$
III	0.83	$9.6 \cdot 10^4$	0.81	$3.3 \cdot 10^{13}$

Table 42A-2-011. $(NH_4)_3H(SeO_4)_2$. Principal g-values and hyperfine constants for Cu^{2+} and VO^{2+} [91Chi]. The spin Hamiltonian is given by Eq. (3) in Table IC-4 in Introduction.

Ion	$g_\parallel$	$g_\perp$	$A_\parallel$ [MHz]	$A_\perp$ [MHz]	T [K]
Cu^{2+}	2.438	2.091	317	17	309
Cu^{2+}	2.423	2.075	377	11	290
VO^{2+}	1.912	1.970	535	199	290
VO^{2+}	1.912	1.970	535	199	260