Table 40A-9-001. NH_4HSeO_4. Unit cell parameters of phase III [80Kru]. T = 223 K. It is convenient to choose B1 cell for comparison with phase I. The relation between the cell axes of P1 and B1 cells: $\boldsymbol{a}_{B1} = 2\boldsymbol{a}_{P1} + \boldsymbol{b}_{P1}$, $\boldsymbol{b}_{B1} = \boldsymbol{b}_{P1}$, $\boldsymbol{c}_{B1} = \boldsymbol{c}_{P1}$.

	Space group	
Parameters	P1	B1
a [Å]	10.487(4)	19.593(7)
b [Å]	4.598(2)	4.598(2)
c [Å]	7.507(4)	7.507(4)
α [°]	90.02(4)	90.02(4)
β [°]	110.91(4)	89.03(5)
γ [°]	101.67 (4)	102.13(7)

Table 40A-9-002. NH_4HSeO_4. Structure of phase I [80Ale]. T = 293 K. Fractional coordinates and anisotropic temperature parameters. B_{ij} is defined by Eq. (a) in Introduction.

Atom	x	y	z	B_{11}	B_{22}	B_{33}	B_{12}	B_{23}	B_{13}
Se(1)	0	0	0	0.00097(2)	0.0192(3)	0.0082(1)	0.0031(1)	0	0
Se(2)	0.1675(1)	0.6990(1)	0.5794(1)	0.00119(1)	0.01721(1)	0.00958(9)	0.00052(8)	–0.0025(3)	0.00106(8)
O(1)	0.0299(2)	0.2847(7)	–0.1347(5)	0.0014(1)	0.017(2)	0.0140(8)	0.0013(6)	0.006(2)	0.0020(5)
O(2)	0.0639(2)	–0.0558(8)	0.1195(5)	0.0015(1)	0.042(2)	0.013(1)	0.0078(7)	0.000(2)	–0.0027(5)
O(3)	0.1933(2)	0.4680(7)	0.7138(6)	0.0019(1)	0.023(2)	0.0139(8)	0.0066(7)	–0.001(2)	–0.0005(5)
O(4)	0.2310(2)	0.9052(8)	0.4736(7)	0.0021(1)	0.037(2)	0.0169(9)	–0.0041(8)	–0.006(2)	0.0060(6)
O(5)	0.1311(2)	0.9184(7)	0.7158(6)	0.0018(1)	0.022(2)	0.0169(9)	0.0036(5)	–0.004(2)	0.0047(5)
O(6)	0.1051(2)	0.5330(9)	0.4529(6)	0.0021(1)	0.043(2)	0.014(1)	–0.0048(9)	–0.006(2)	–0.0027(6)
$NH_4(1)$	0.1654(2)	0.5671(9)	0.0879(9)	0.0014(1)	0.037(2)	0.0137(9)	0.0040(8)	–0.014(4)	–0.0002(8)
$NH_4(2)$	0	0	0.4814(10)	0.0019(2)	0.035(3)	0.009(1)	0.0000(1)	0	0
H(1)	0.022(5)	0.492(29)	0.859(15)						
H(2)	0.165(8)	0.252(37)	0.681(15)						
H(2)'	0.151(5)	0.036(24)	0.714(23)						

Table 40A-9-003. NH_4HSeO_4. Structure of phase I [80Ale]. T = 293 K. Interatomic distances [Å] and bond angles [°].

Se(1)–O(1)	1.664(4) Å	NH_4(1)–O(3)'	2.933(7) Å
–O(2)	1.617(5) Å	–O(2)'	2.935(7) Å
mean	1.641 Å	–O(4)'	2.946(6) Å
		–O(3)''	2.986(7) Å
O(1)–Se(1)–O(2)	108°10(19)'	–O(6)	2.994(6) Å
O(1)–Se(1)–O(1)'	104°37(20)'	–O(2)	3.133(7) Å
O(1)–Se(1)–O(2)'	111°45(21)'	–O(1)	3.188(7) Å
O(1)'–Se(1)–O(2)'	108°10(17)'	–O(5)'	3.385(7) Å
O(2)'–Se(1)–O(2)'	112°10(20)'	–O(4)'	3.407(7) Å
O(1)'–Se(1)–O(2)	111°45(19)'	–O(4)	3.422(6) Å
Se(2)–O(3)	1.630(5) Å	NH_4(2)–O(6)	2.858(6) Å
–O(4)	1.611(6) Å	–O(6)'	2.858(6) Å
–O(5)	1.709(6) Å	–O(2)	3.045(7) Å
–O(6)	1.615(5) Å	–O(2)''	3.045(7) Å
mean	1.641 Å	–O(1)'	3.184(7) Å
		–O(1)''	3.184(7) Å
O(3)–Se(2)–O(4)	112°25(20)'	–O(5)	3.225(6) Å
O(3)–Se(2)–O(5)	104°04(20)'	–O(5)''	3.225(7) Å
O(3)–Se(2)–O(6)	111°55(19)'	–O(6)''	3.307(7) Å
O(4)–Se(2)–O(5)	108°53(17)'	–O(6)'''	3.307(7) Å
O(4)–Se(2)–O(6)	113°42(21)'		
O(5)–Se(2)–O(6)	105°05(21)'		

Table 40A-9-004. NH_4HSeO_4. Structure of phase I [90Mak2]. T = 293 and 400 K. Interatomic distances [Å] and bond angles [°].

Atom	NH_4HSeO_4	
	293 K	400 K
O(1)–O(1″)	2.531(9)	2.483(16)
O(1)–H(1)*	1.03(1)	1.04(6)
O(1″)...H(1)*	1.51(1)	1.46(5)
O(1)H(1)O(1″)*	172(2)	170(3)
H(1)–H(1′)*	0.49(2)	0.46(6)
O(3′)–O(5)	2.565(6)	2.568(9)
O(5)–H(2)	1.011(9)	0.997(12)
H(3′)...H(2)	1.556(9)	1.572(12)
O(3′)H(2)O(5)	176(1)	177(1)
Se(1)–O(1) × 2	1.670(5)	1.677(7)
–O(2) × 2	1.607(5)	1.608(8)
Se(2)–O(3)	1.636(5)	1.623(8)
–O(4)	1.606(5)	1.603(8)
–O(5)	1.709(5)	1.712(8)
–O(6)	1.616(6)	1.599(8)
O(1)–O(1′)	2.628(9)	2.653(13)
O(1)–O(2) × 2	2.658(7)	2.664(10)
O(1)–O(2′) × 2	2.708(6)	2.706(9)
O(2)–O(2′)	2.680(9)	2.688(18)
O(3)–O(4)	2.684(8)	2.688(11)
O(3)–O(5)	2.634(6)	2.627(9)
O(3)–O(6)	2.698(7)	2.668(11)
O(4)–O(5)	2.698(7)	2.685(10)
O(4)–O(6)	2.709(7)	2.677(11)
O(5)–O(6)	2.638(8)	2.645(10)
N(1)–H(3) × 2	0.97(2)	0.94(3)
–H(4) × 2	0.92(2)	0.89(2)
N(2)–H(5)	0.99(2)	0.90(2)
–H(6)	0.91(3)	0.91(3)
–H(7)	0.93(2)	0.71(3)
–H(8)	0.92(2)	0.87(3)

* Geometry of α-bond is given for the two-position model.

Table 40A-9-005. NH_4HSeO_4. Structure of phase III [80Kru]. T = 223 K. Fractional coordinates and anisotropic temperature parameters (isotropic temperature parameters for hydrogens). B and B_{ij} are defined by Eq. (e) and Eq. (a) in Introduction, respectively.

Atom	x	y	z	B [Å^2]	B_{11}	B_{22}	B_{33}	B_{12}	B_{13}	B_{23}
Se(1)	0	0	0		0.0034(1)	0.0161(2)	0.0066(1)	0.0054(2)	0.0031(1)	0.0028(2)
Se(2)	0.3347(1)	0.7003(2)	0.7464(1)		0.0043(1)	0.0143(3)	0.0094(1)	0.0011(2)	0.0055(1)	–0.0009(3)
Se(3)	0.6649(1)	0.2997(1)	0.4117(1)		0.0043(1)	0.0162(2)	0.0071(1)	0.0018(2)	0.0022(1)	0.0018(2)
O(1)	0.0606(5)	0.2862(10)	–0.1037(7)		0.0051(5)	0.0192(12)	0.0115(11)	0.0057(17)	0.0059(13)	0.0025(25)
O(2)	–0.0613(5)	–0.2870(19)	–0.1668(7)		0.0063(6)	0.0160(20)	0.0096(10)	0.0068(17)	0.0032(12)	–0.0033(23)
O(3)	0.1278(5)	–0.0607(12)	0.1833(7)		0.0052(6)	0.0341(27)	0.0073(9)	0.0140(20)	0.0002(12)	0.0035(26)
O(4)	–0.1278(6)	0.0607(12)	0.0571(8)		0.0052(6)	0.0369(29)	0.0144(12)	0.0127(21)	0.0073(13)	0.0063(30)
O(5)	0.3876(5)	0.4692(10)	0.9082(7)		0.0058(6)	0.0207(22)	0.0120(11)	0.0098(18)	0.0052(13)	0.0031(25)
O(6)	0.4630(6)	0.9053(11)	0.7052(9)		0.0072(7)	0.0292(26)	0.0199(15)	–0.0061(20)	0.0161(16)	–0.0040(32)
O(7)	0.2593(6)	0.9191(11)	0.8448(8)		0.0068(7)	0.0183(23)	0.0169(12)	0.0054(19)	0.0134(15)	0.0008(27)
O(8)	0.2075(6)	0.5342(12)	0.5559(7)		0.0077(7)	0.0357(29)	0.0086(10)	–0.0040(22)	0.0008(13)	–0.0045(28)
O(9)	0.6122(5)	0.5319(9)	0.5218(6)		0.0058(5)	0.0204(20)	0.0122(9)	0.0097(16)	0.0055(11)	0.0029(22)
O(10)	0.5360(5)	0.0929(11)	0.2406(7)		0.0079(6)	0.0306(27)	0.0109(11)	–0.0029(20)	–0.0038(13)	–0.0036(28)
O(11)	0.7401(5)	0.0831(9)	0.5849(6)		0.0069(5)	0.0180(21)	0.0101(9)	0.0057(16)	–0.0002(11)	0.0071(22)
O(12)	0.7912(5)	0.4667(7)	0.3467(7)		0.0077(6)	0.0341(26)	0.0144(11)	–0.0024(20)	0.0113(13)	0.0010(27)
NH_4(1)	0.3293(6)	0.5609(13)	0.2518(8)		0.0057(7)	0.0323(29)	0.0097(12)	0.0072(22)	0.0044(14)	–0.0029(31)
NH_4(2)	–0.0006(7)	0.0014(15)	0.4808(9)		0.0068(6)	0.0292(24)	0.0082(11)	0.0018(19)	0.0058(13)	0.0007(29)
NH_4(3)	0.6700(6)	0.4369(13)	0.9226(8)		0.0036(6)	0.0304(28)	0.0126(12)	0.0044(22)	0.0050(14)	0.0068(30)
H(1)	–0.009(7)	0.541(13)	0.877(9)	3.0(14)						
H(2)	0.308(9)	0.067(21)	0.829(14)	8.6(27)						
H(3)	0.727(9)	0.916(18)	0.573(12)	5.2(21)						

Table 40A-9-006. NH_4HSeO_4. Structure of phase III [80Kru]. T = 223 K. Interatomic distances [Å] and bond angles [°].

Selenate ions					
Se(1)–O(1)	1.661(3) Å	Se(2)–O(5)	1.638(3) Å	Se(3)–O(9)	1.639(3) Å
–O(2)	1.677(3)	–O(6)	1.604(4)	–O(10)	1.616(4)
–O(3)	1.613(4)	–O(7)	1.719(4)	–O(11)	1.714(4)
–O(4)	1.614(4)	–O(8)	1.625(3)	–O(12)	1.618(3)
Average	1.642(4)		1.646(4)		1.644(4)
O(1)Se(1)O(2)	104°50′(13)	O(5)Se(2)O(6)	111°52′(13)	O(9)Se(3)O(10)	111°34′(12)
O(1)Se(1)O(3)	108°45′(12)	O(5)Se(2)O(7)	104°01′(13)	O(9)Se(3)O(11)	104°13′(13)
O(1)Se(1)O(4)	111°18′(14)	O(5)Se(2)O(8)	112°20′(12)	O(9)Se(3)O(12)	112°15′(12)
O(2)Se(1)O(3)	111°16′(12)	O(6)Se(2)O(7)	109°07′(10)	O(10)Se(3)O(11)	109°12′(11)
O(2)Se(1)O(4)	108°42′(10)	O(6)Se(2)O(8)	114°07′(14)	O(10)Se(3)O(12)	113°56′(13)
O(3)Se(1)O(4)	111°46′(13)	O(7)Se(2)O(8)	104°35′(14)	O(11)Se(3)O(12)	104°57′(13)
Ammonium polyhedra					
NH_4(1)–O(5)′	2.890(5) Å	NH_4(2)–O(8)	2.839(4) Å	NH_4(3)–O(9)	2.894(4) Å
–O(3)′	2.916(5)	–O(12)′	2.843(5)	–O(4)′	2.919(5)
–O(10)′	2.943(4)	–O(4)	3.032(5)	–O(6)′	2.946(5)
–O(9)	2.964(5)	–O(3)	3.039(5)	–O(5)	2.961(4)
–O(8)	2.981(4)	–O(2)′	3.145(5)	–O(12)′	2.975(5)
–O(3)	3.113(5)	–O(1)′	2.154(5)	–O(4)′	3.119(5)
–O(1)	3.137(5)	–O(11)′	3.167(4)	–O(2)′	3.147(4)
–O(10)	3.369(4)	–O(7)′	3.184(5)	–O(6)	3.368(4)
–O(7)′	3.378(5)	–O(12)′	3.275(5)	–O(11)	3.375(5)
–O(6)	3.432(4)	–O(8)′	3.280(5)	–O(10)	3.432(5)
Hydrogen bonds					
H(1)–O(2)	1.04(3) Å	H(2)–O(7)	0.80(3) Å	H(3)–O(11)	0.75(3) Å
–O(1)	1.48(3)	–O(5)	1.87(4)	–O(9)	1.88(4)
O(1)–O(2)	2.508(6)	O(5)–O(7)	2.561(5)	O(11)–O(9)	2.572(5)
O(1)···H(1)–O(2)	168°(1)	O(5)···H(2)–O(7)	144°(1)	O(9)···H(3)–O(11)	153°(1)

Table 40A-9-007. ND_4DSeO_4. Crystal structure at RT [82Was]. Interatomic distances [Å] and angles [°] in SeO_4 tetrahedra.

Se–O(1)	1.606(4)
–O(2)	1.626(3)
–O(3)	1.629(3)
–O(4)	1.714(3)
mean	1.644(7)
O(1)–Se–O(2)	112.7(2)
O(1)– –O(3)	113.3(2)
O(1)– –O(4)	108.9(2)
O(2)– –O(3)	112.7(2)
O(2)– –O(4)	104.6(2)
O(3)– –O(4)	103.8(2)

Table 40A-9-008. $(NH_4H)_x(ND_4D)_{1-x}SeO_4$ (x = 0.4). EFG tensor parameter of hydrogen bonded deuterons [84Mos].

Hydrogen bond	Principal values of the EFG tensor Φ_{ii} [kHz]	Direction cosines relative to the crystallographic axes			$\frac{e^2qQ}{h}$ [kHz]	$\eta = \frac{\Phi_{xx} - \Phi_{yy}}{\Phi_{zz}}$	∢ ($\Phi_{zz'}$ O...O)	∢ ($\Phi_{yy'}$ n(Se–O...O))
		a	*b*	*c*				
O(4′)–D(1)...O(3)–Se(1)	Φ_{xx} = 131(1) Φ_{yy} = 99(1) Φ_{zz} = 221(1)	0.550 0.661 –0.510	0.311 0.404 0.860	0.775 –0.632 0.017	147.3(10)	0.14(1)	2.3°	3.5°