Table 44A-2-001. $NaNH_4SeO_4 \cdot 2H_2O$. Crystal structure of phase I [73Kru]. Fractional coordinates and temperature parameters at RT. The temperature parameters are defined by Eq. (e) in Introduction.

Atom	x	y	z	B [Å^2]
Se	0.0935	0.1284	0.3828	0.11
Na	0.2606	0.4894	0.9049	0.14
O1	0.0783	0.2064	0.1873	1.75
O2	0.0747	0.1907	0.6096	1.76
O3	0.2642	0.0744	0.3730	1.98
O4	0.0415	0.5410	0.1364	0.93
O5	0.2050	0.6321	0.6749	0.53
O6	0.0886	0.4042	0.6532	1.11
N	0.1596	0.8558	0.3772	0.91
H1	0.382	0.200	0.867	
H2	0.397	0.059	0.871	
H3	0.217	0.160	1.024	
H4	0.226	0.160	0.792	
H5	0.027	0.922	0.858	
H6	0.094	0.330	0.642	
H7	0.281	0.688	0.679	
H8	0.109	0.651	0.750	

Table 44A-2-002. $NaNH_4SeO_4 \cdot 2H_2O$. Crystal structure of phase I [73Kru]. Anisotropic temperature parameters for non-hydrogen atoms at RT. The temperature parameters are defined by Eq. (a) in Introduction.

Atom	B_{11}	B_{22}	B_{33}	B_{12}	B_{13}	B_{23}
Se	0.009	0.0036	0.017	–0.0014	–0.0002	0.0011
Na	0.009	0.0039	0.011	–0.0008	0.0019	0.0006
O1	0.018	0.005	0.025	–0.001	0.008	–0.003
O2	0.020	0.006	0.024	–0.005	–0.013	0.015
O3	0.011	0.007	0.056	–0.004	–0.005	–0.005
O4	0.121	0.006	0.015	0.001	0.000	0.000
O5	0.129	0.005	0.014	0.002	–0.004	0.003
O6	0.111	0.005	0.023	0.001	0.000	–0.002
N	0.015	0.005	0.021	0.000	0.002	0.004

Table 44A-2-003. $NaNH_4SeO_4 \cdot 2H_2O$. Crystal structure of phase I [73Kru]. Interatomic distances and angles at RT. See also Fig. 44A-2-001. Primed atoms are connected with basis atoms by symmetry operations.

Na–O5′	2.23 Å	Se–O1	1.629 Å	O1′–NH_4–O2	117°
Na–O4	2.37	Se–O2	1.643	O1–NH_4–O4′	66
Na–O5	2.41	Se–O3	1.591	O1–NH_4–O1	115
Na–O6	2.43	Se–O4	1.636	O1′–NH_4–O3′	104
Na–O4′	2.44			O1′–NH_4–O3	91
Na–O6′	2.46	O1–Se–O2	110°09′	O1′–NH_4–O3″	98
		O1–Se–O3	110°00′	O2–NH_4–O4′	115
O5′–Na–O4	101°	O1–Se–O4	108°53′	O2–NH_4–O1	78
O5′–Na–O5	157	O2–Se–O3	109°59′	O2–NH_4–O3′	73
O5′–Na–O6	103	O2–Se–O4	110°49′	O2–NH_4–O3	115
O5′–Na–O4′	99	O3–Se–O4	108°10′	O2–NH_4–O3″	53
O5′–Na–O6′	83			O4′–NH_4–O_1	118
O4–Na–O5	81	NH_4–O1′	2.80 Å	O4–NH_4–O3′	95
O4–Na–O6	83	NH_4–O2	2.87	O4–NH_4–O3	97
O4–Na–O4′	170	NH_4–O4′	2.99	O4′–NH_4–O3″	93
O4–Na–O6′	101	NH_4–O1	3.03	O1–NH_4–O3′	98
O5–Na–O6	82	NH_4–O3′	3.04	O1–NH_4–O3	49
O5–Na–O4	90	NH_4–O3	3.29	O1–NH_4–O3″	122
O5–Na–O6′	90	NH_4–O3″	3.38	O3′–NH_4–O3	100
O6–Na–O4′	86			O3′–NH_4–O3″	63
O6–Na–O6′	172			O3–NH_4–O3″	153
O4′–Na–O6′	81				

Table 44A-2-004. $NaNH_4SeO_4 \cdot 2H_2O$. Crystal structure of phase II [76Kru]. Fractional coordinates and isotropic temperature parameters at 148 K. The temperature parameters are defined by Eq. (e) in Introduction.

Atom	*x*	*y*	*z*	*B* [Å^2]
Se(I)	0.34510(13)	0.12812(8)	0.38443(59)	0.47
Se(II)	0.83987(13)	0.37056(8)	0.60884(59)	0.47
Na(I)	0.5139(6)	0.4913(4)	0.8988(11)	0.60
Na(II)	0.0089(6)	0.0111(4)	0.1002(12)	0.63
O1	0.3428(11)	0.1835(9)	0.6188(22)	1.60
O2	0.3159(11)	0.2108(8)	0.1931(20)	1.31
O3	0.2063(9)	0.0369(6)	0.3677(19)	1.09
O4	0.5157(9)	0.0753(8)	0.3291(22)	2.49
O5	0.8452(11)	0.3002(8)	0.8208(21)	1.58
O6	0.7997(11)	0.3000(9)	0.3942(26)	2.27
O7	0.7052(8)	0.4582(6)	0.6235(18)	0.87
O8	1.0129(9)	0.4224(7)	0.5659(22)	1.64
O9	0.4589(10)	0.6313(7)	0.6617(15)	0.94
O10	0.0504(11)	0.1343(7)	0.8258(19)	1.07
O11	0.1600(8)	0.9062(7)	0.8575(20)	1.07
O12	0.3324(9)	0.4013(7)	0.6532(19)	1.63
NH_4(I)	0.0924(11)	0.3582(9)	0.1237(22)	1.35
NH_4(II)	0.3956(11)	0.8563(9)	0.3938(22)	1.12

Table 44A-2-005. $NaNH_4SeO_4 \cdot 2H_2O$. Crystal structure of phase II [76Kru]. Interatomic distances and angles at 148 K. Primed atoms are connected with basis atoms by symmetry operations.

Distance [Å]		Angle [deg]		Distance [Å]		Angle [deg]	
Se(I)–O1	1.625	O1–Se(I)–O2	110°38′	Na(I)–O9′	2.30	NH_4(I)–O2	2.75
–O2	1.628	O1–Se(I)–O3	111°19′	–O7	2.39	–O5	2.89
–O3	1.656	O1–Se(I)–O4	113°09′	–O9	2.40	–O7′	2.92
–O4	1.639	O2–Se(I)–O3	108°43′	–O7′	2.41	–O8	2.95
		O2–Se(I)–O4	105°45′	–O12	2.44	–O8′	3.04
		O3–Se(I)–O4	107°00′	–O12′	2.46	–O6	3.07
		O5–Se(II)–O6	110°15′	Na(II)–O3	2.37	NH_4(II)–O1′	2.84
Se(II)–O5	1.607	O5–Se(II)–O7	112°38′	–O10	2.37	–O3	2.88
–O6	1.655	O5–Se(II)–O8	109°58′	–O3′	2.39	–O5′	2.89
–O7	1.629	O6–Se(II)–O7	107°05′	–O11′	2.41	–O4′	2.93
–O8	1.614	O6–Se(II)–O8	106°28′	–O10′	2.41	–O4	3.05
		O7–Se(II)–O8	110°12′	–O11	2.41	–O2′	3.19

Table 44A-2-006. $NaNH_4SeO_4 \cdot 2H_2O$. Principal components of quadrupole coupling tensor $|eQ\phi_{ii}/h|$ of ^{23}Na and their orientations (shown in parentheses) [71Ale]. Angles α, β, γ are angles between each principal component of nuclear quadrupole coupling tensors and the crystallographic *a*, *b*, *c* axes, respectively.

	$\lvert eQ\phi_{xx}/h \rvert$ [kHz]	(α, β, γ) [deg]	$\lvert eQ\phi_{yy}/h \rvert$ [kHz]	(α, β, γ) [deg]	$\lvert eQ\phi_{zz}/h \rvert$ [kHz]	(α, β, γ) [deg]	T [°C]
Na	190	(–17, –89, 73)	930	(90, –8, –97)	1120	(73, –97, 162)	–15
Na(I)	232	(–13, –90, 77)	752	(88, –8, –99)	984	(77, –99, 164)	–120
Na(II)	228	(–37, –96, 54)	980	(98, –172, 95)	1208	(54, –95, 144)	–120

Table 44A-2-007. $NaND_4SeO_4 \cdot 2D_2O$. Deuteron quadrupole coupling constants $|eQ\phi_{ii}/h|$ and their orientations (shown in parentheses) [71Ale]. Angles α, β, γ are angles between each principal component of nuclear quadrupole coupling tensors and the crystallographic *a*, *b*, *c* axes, respectively.

	$\lvert eQ\phi_{xx}/h \rvert$ [kHz]	(α, β, γ) [deg]	$\lvert eQ\phi_{yy}/h \rvert$ [kHz]	(α, β, γ) [deg]	$\lvert eQ\phi_{zz}/h \rvert$ [kHz]	(α, β, γ) [deg]	T [°C]
ND_4	0.4	(90, 0, –90)	3.8	(–155, 90, –65)	4.2	(–65, 90, 25)	–15
ND_4(I)	0.0	(2, ..., ...)	4.3	(–53, –135, 68)	4.3	(53, –45, –68)	–120
ND_4(II)	2.1	(99, –32, –121)	5.7	(139, 76, –52)	7.8	(51, –58, –54)	–120

Table 44A-2-008. $NaND_4SeO_4 \cdot 2D_2O$. **g** and **A** tensors for SeO_2^- and SeO_3^- radicals in γ-irradiated sample [81Ram].

Radical	T	*g* tensor			*A* tensor [mT]		
	[K]	g_{xx}	g_{yy}	g_{zz}	A_{xx}	A_{yy}	A_{zz}
SeO_2^-	300	1.9996	2.0313	2.0080	24.598	9.696	9.654
	77	1.9995	2.0327	2.0075	26.671	9.442	9.421
SeO_3^-	300	2.0156	2.0156	2.0042	55.501	50.269	75.288
	77	2.0158	2.0158	2.0035	58.946	50.627	80.636