Table 41A-5-001. NH_4LiSO_4. Structure of phase I [81Ito]. Fractional coordinates and isotropic temperature parameters. $T = 478$ K. Except for Li, the temperature parameters are reduced by $(U_{11} + U_{22} + U_{33})/3$. U_{ij} is defined by Eq. (d) in Introduction.

	x	y	z	$\overline{u^2}$ [$\cdot 10^{-2}$ Å^2]
S	0.25	0.08639(6)	0.20494(6)	3.37(1)
NH_4	0.75	0.2058(3)	0.5004(3)	5.39(7)
O(1)′	0.2706(36)	0.0959(6)	0.0429(3)	12.6(3)
O(2)′	0.0661(7)	−0.0225(4)	0.2546(5)	7.6(1)
O(3)′	0.4972(6)	0.0479(4)	0.2588(5)	6.7(1)
O(4)′	0.1741(8)	0.2214(3)	0.2712(6)	11.1(2)
Li	0.25	0.4168(5)	0.3273(5)	4.4(1)

Table 41A-5-002. NH_4LiSO_4. Structure of phase I [81Ito]. Interatomic distances [Å] and bond angles [°]. $T = 478$ K.

S–O(1)′	1.423(3)	NH_4–O(1^{iv+a})′	3.328(16)
–O(2)′	1.463(4)	–O(2^{+a})′	3.440(4)
–O(3)′	1.436(3)	–O(2^{ii+c})′	2.895(5)
–O(4)′	1.428(4)	–O(2^{iii})′	3.487(4)
Li–O(1^{iv})′	1.892(5)	–O(3)′	2.892(4)
–O(2^{iii})′	1.905(4)	–O(3^{ii+c})′	3.404(5)
–O(3^{iii-a})′	1.953(5)	–O(3^{iv})′	3.469(4)
–O(4)′	1.906(4)	–O(4^{+a})′	3.014(5)
NH_4–O(1^{iv})′	3.150(16)	–O(4^{iv+a})′	3.332(5)
O(1)′–S–O(2)′	112.8(6)	O(1^{iv})′–Li–O(2^{iii})′	110.0(6)
O(1)′–S–O(3)′	105.8(8)	O(1^{iv})′–Li–O(3^{iii-a})′	117.5(5)
O(1)′–S–O(4)′	111.8(4)	O(1^{iv})′–Li–O(4)′	102.2(3)
O(2)′–S–O(3)′	109.9(2)	O(2^{iii})′–Li–O(3^{iii-a})′	106.1(3)
O(2)′–S–O(4)′	106.7(2)	O(2^{iii})′–Li–O(4)′	111.4(2)
O(3)′–S–O(4)′	109.8(2)	O(3^{iii-a})′–Li–O(4)′	109.8(2)

Symmetry code: (+a) $1+x, y, z$; (ii) $\frac{1}{2}+x, \bar{y}, \bar{z}$; (ii+c) $\frac{1}{2}+x, \bar{y}, 1+\bar{z}$; (iii) $\frac{1}{2}+x, \frac{1}{2}+y, \frac{1}{2}-z$; (iii−a) $-\frac{1}{2}+x, \frac{1}{2}+y, \frac{1}{2}-z$; (iv) $x, \frac{1}{2}-y, \frac{1}{2}+z$; (iv+a) $1+x, \frac{1}{2}-y, \frac{1}{2}+z$.

Table 41A-5-003. NH_4LiSO_4. Structure of phase II [69Dol]. Fractional coordinates and temperature parameters at RT. Root-mean-square amplitude of thermal vibrations for oxygens are also shown. b_{ij} is defined by Eq. (b), B is defined by Eq. (e) in Introduction. φ's are the angles between the ellipsoid axes and the unit cell axes.

	x	y	z	B		
NH_4	0.4912 (25)	0.2137 (7)	0.4999 (7)	1.8 (1) Å^2		
Li	0.0084 (73)	0.4117 (14)	0.3234 (15)	1.5 (2)		
S	0*)	0.0836 (2)	0.2030 (2)	0.90 (4)		
O (1)	0.0003 (33)	0.0961 (10)	0.0384 (7)			
O (2)	0.3323 (15)	0.4631 (7)	0.2496 (9)			
O (3)	0.2585 (15)	0.0537 (7)	0.2565 (9)			
O (4)	0.9059 (16)	0.2191 (7)	0.2705 (11)			
	b_{11}	b_{22}	b_{33}	$2b_{12}$	$2b_{13}$	$2b_{23}$
O (1)	0.028 (3)	0.030 (2)	0.003 (1)	−0.004 (4)	0.001 (3)	0.003 (1)
O (2)	0.016 (3)	0.006 (1)	0.011 (1)	−0.005 (1)	0.006 (2)	−0.004 (1)
O (3)	0.009 (2)	0.007 (1)	0.009 (1)	0.002 (1)	−0.004 (1)	−0.004 (1)
O (4)	0.019 (3)	0.004 (1)	0.021 (2)	0.001 (1)	0.002 (2)	−0.004 (1)
	Ellipsoid axis	r.m.s. amplitude	φa	φb	φc	
O (1)	1	0.20 (1) Å	9 (12)°	86 (6)°	82 (13)°	
	2	0.36 (1)	95 (7)	8 (4)	84 (2)	
	3	0.09 (2)	97 (13)	97 (2)	10 (9)	
O (2)	1	0.11 (2)	44 (21)	46 (20)	88 (20)	
	2	0.13 (2)	122 (24)	59 (24)	48 (4)	
	3	0.25 (1)	64 (4)	120 (4)	42 (4)	
O (3)	1	0.10 (2)	23 (15)	87 (19)	67 (13)	
	2	0.13 (2)	105 (21)	35 (6)	60 (11)	
	3	0.23 (1)	107 (5)	125 (5)	40 (5)	
O (4)	1	0.17 (1)	16 (10)	74 (10)	90 (4)	
	2	0.10 (2)	106 (10)	21 (8)	77 (3)	
	3	0.29 (1)	86 (4)	103 (3)	13 (3)	

*) Fixed, to define x as origin.

Table 41A-5-004. NH_4LiSO_4. Structure of phase II [69Dol]. Interatomic distances and angles at RT. See also Fig. 41A-5-003.

Bonds	Uncorrected length	Corrected *) length	Bonds	Angle
S–O (1)	1.450 (7) Å	1.496 Å	O (1)–S–O (2)	110.0 (7)°
–O (2)	1.474 (8)	1.493	O (1)–S–O (3)	109.4 (8)
–O (3)	1.469 (8)	1.490	O (1)–S–O (4)	109.8 (6)
–O (4)	1.460 (7)	1.489	O (2)–S–O (3)	109.2 (5)
Li–O (1)	1.891 (105)		O (2)–S–O (4)	108.3 (5)
–O (2)	1.889 (36)		O (3)–S–O (4)	110.1 (5)
–O (3)	1.979 (28)		O (1)–Li–O (2)	111.9 (20)
–O (4)	1.899 (18)		O (1)–Li–O (3)	111.3 (20)
NH_4–O (1)	3.139 (19)		O (1)–Li–O (4)	101.7 (13)
–O (1′)	3.219 (19)		O (2)–Li–O (3)	108.6 (19)
–O (2)	3.277 (10)		O (2)–Li–O (4)	113.9 (20)
–O (2′)	2.851 (11)		O (3)–Li–O (4)	109.4 (13)
–O (3)	2.867 (11)		S–O (1)–Li	173.2 (17)
–O (3′)	3.333 (11)		S–O (2)–Li	129.3 (7)
–O (4)	2.976 (14)		S–O (3)–Li	128.9 (7)
–O (4′)	3.290 (13)		S–O (4)–Li	142.0 (13)

*) Assuming oxygen atoms "riding" on sulfur atoms.

Table 41A-5-005. NH_4LiSO_4. Structure of phase III [93Mas]. T = 190 K. Fractional coordinates and isotropic temperature parameters. B [Å^2] and U_{ij} [$\cdot 10^{-4}$ Å^2] are defined by Eqs. (e) and (d) in Introduction, respectively.

Atom	x	y	z	B
Li1	0.2668(6)	0.0900(4)	0.1612(2)	1.00(5)
Li2	0.2270(6)	0.4097(4)	0.4140(2)	1.19(5)
S1	0.23742(6)	0.41488(4)	0.10258(2)	0.678(5)
S2	0.26928(6)	0.07681(4)	0.35221(2)	0.657(4)
O1	0.2806(3)	0.3703(2)	0.0228(1)	1.79(3)
O2	0.3213(3)	0.2960(2)	0.1538(1)	1.78(2)
O3	–0.0340(2)	0.4415(2)	0.1162(1)	1.56(2)
O4	0.3838(2)	0.5494(1)	0.1201(1)	1.15(2)
O5	0.2654(3)	0.0610(2)	0.2685(1)	1.55(2)
O6	0.3426(3)	0.2264(1)	0.3741(1)	1.49(2)
O7	0.0161(2)	0.0407(2)	0.3835(1)	1.20(2)
O8	0.4543(2)	–0.0281(1)	0.3847(1)	1.22(2)
N1	0.7689(3)	0.2789(2)	0.2479(1)	1.22(2)
N2	0.7445(3)	0.2011(2)	0.4952(1)	1.24(2)
H1	0.809(9)	0.170(5)	0.259(3)	3.2(4)
H2	0.621(12)	0.287(6)	0.226(3)	5.7(6)
H3	0.861(9)	0.338(5)	0.209(3)	2.6(4)
H4	0.799(8)	0.332(4)	0.299(2)	1.4(3)
H5	0.839(8)	0.269(4)	0.515(2)	1.5(3)
H6	0.600(10)	0.254(5)	0.461(3)	3.1(4)
H7	0.834(8)	0.143(4)	0.459(2)	1.7(3)
H8	0.691(8)	0.156(5)	0.540(3)	2.0(4)

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Li1	127(10)	113(10)	140(11)	1(10)	–4(9)	5(10)
Li2	137(11)	136(11)	180(12)	6(11)	–19(11)	11(10)
S1	83(1)	77(1)	97(1)	6(1)	5(1)	14(1)
S2	74(1)	89(1)	86(1)	1(1)	6(1)	0(1)
O1	267(6)	284(6)	128(5)	–51(6)	53(5)	–54(5)
O2	259(6)	120(4)	299(6)	–17(4)	–135(5)	84(5)
O3	92(4)	161(5)	341(6)	12(4)	53(4)	16(5)
O4	135(4)	98(4)	204(5)	–36(3)	39(4)	–13(4)
O5	199(5)	305(7)	84(4)	1(5)	1(4)	0(5)
O6	173(5)	95(4)	299(6)	–19(4)	19(5)	–47(4)
O7	83(4)	210(5)	163(4)	–32(4)	30(4)	–40(4)
O8	121(4)	165(4)	176(4)	48(4)	31(4)	63(4)
N1	167(5)	159(5)	139(5)	–19(5)	–3(5)	6(4)
N2	171(5)	157(5)	144(5)	4(5)	15(5)	19(4)

Table 41A-5-006. NH_4LiSO_4. Structure of phase III [93Mas]. T = 190 K. Interatomic distances [Å] and bond angles [°] of SO_4 and NH_4 tetrahedra.

S1–O1	1.468(14)	S2–O5	1.468(5)
–O2	1.473(24)	–O6	1.469(13)
–O3	1.475(2)	–O7	1.481(5)
–O4	1.482(9)	–O8	1.481(13)
mean	1.474	mean	1.475
N1–H1	1.04(5)	N2–H5	0.87(4)
–H2	0.87(6)	–H6	1.08(5)
–H3	0.99(5)	–H7	0.95(4)
–H4	1.02(4)	–H8	0.92(5)
mean	0.98	mean	0.96
O1–S1–O2	108.9(10)	O5–S2–O6	110.7(18)
O1–S1–O3	110.5(2)	O5–S2–O7	109.4(4)
O1–S1–O4	110.1(15)	O5–S2–O8	109.0(12)
O2–S1–O3	108.4(3)	O6–S2–O7	110.4(7)
O2–S1–O4	109.1(6)	O6–S2–O8	109.1(4)
O3–S1–O4	109.7(5)	O7–S2–O8	108.1(9)
H1–N1–H2	110(3)	H5–N2–H6	108(2)
H1–N1–H3	123(3)	H5–N2–H7	112(3)
H1–N1–H4	105(2)	H5–N2–H8	99(2)
H2–N1–H3	95(3)	H6–N2–H7	103(2)
H2–N1–H4	119(2)	H6–N2–H8	117(3)
H3–N1–H4	105(2)	H7–N2–H8	118(2)

Table 41A-5-007. NH_4LiSO_4. Structure of phase III [93Mas]. T = 190 K. Interatomic distances [Å] of the nearest Li–O pairs and O–H–N angles [°].

Li1–O2	1.906	Li2–O1(iii)	1.933
–O5	1.890	–O3(ii″)	1.926
–O7(ii)	1.940	–O4(ii‴)	1.944
–O8(ii′)	1.919	–O6	1.911
mean	1.914	mean	1.929
H1–O5(ii)	2.17	H5–O1(iii′)	2.21
H2–O2	2.02	H6–O6	2.05
H3–O3(i)	1.96	H7–O7(i)	1.88
H4–O4(ii″)	1.84	H8–O8(iv)	1.92
mean	1.99	mean	2.01
N1–H1–O5	150.4	N2–H5–O1	147.6
N1–H2–O2	167.6	N2–H6–O6	145.5
N1–H3–O3	165.3	N2–H7–O7	166.3
N1–H4–O4	170.1	N1–H8–O8	176.3

Symmetry code:

(i) $1+x, y, z$	(ii‴) $-\frac{1}{2}+x, 1-y, \frac{1}{2}-z$
(ii) $\frac{1}{2}+x, -y, \frac{1}{2}-z$	(iii) $\frac{1}{2}-x, y, \frac{1}{2}+z$
(ii′) $-\frac{1}{2}+x, -y, \frac{1}{2}-z$	(iii′) $\frac{3}{2}-x, y, \frac{1}{2}+z$
(ii″) $\frac{1}{2}-x, 1-y, \frac{1}{2}-z$	(iv) $1-x, -y, 1-z$

Table 41A-5-008. NH_4LiSO_4. Structure of phase VI [94Has]. Fractional coordinates [$\cdot 10^{-4}$] and isotropic temperature parameters [$\cdot 10^{-4}$ Å^2]. $\overline{u^2}$ is defined by Eq. (e) in Introduction.

Atom	x	y	z	$\overline{u^2}$
S(1)	2500	891(3)	2015(4)	109(5)
O(11)	2582(29)	1358(10)	406(13)	333(25)
O(12)	3466(21)	2099(10)	3027(13)	253(24)
O(13)	3978(20)	–473(10)	2315(12)	233(23)
O(14)	–186(20)	622(10)	2423(12)	226(23)
S(2)	2779(7)	4212(3)	7034(4)	111(5)
O(21)	2546(26)	4472(9)	5363(11)	286(23)
O(22)	3481(22)	2677(10)	7306(13)	279(25)
O(23)	4723(19)	5215(10)	7736(12)	203(22)
O(24)	308(20)	4571(9)	7743(11)	190(22)
N(1)	7787(28)	2194(10)	5037(13)	168(23)
N(2)	7422(28)	2971(12)	–44(14)	228(25)
Li(1)	2775(57)	4115(24)	3202(26)	199(47)
Li(2)	2411(49)	783(22)	8241(25)	166(47)

Table 41A-5-009. ND_4LiSO_4. Structure at T = 323 K [89Fis]. Fractional coordinates and isotropic temperature parameters. B is defined by Eq. (e) in Introduction.

Atom	x	y	z	B [Å^2]
S	0.082(5)	0.0000	0.196(1)	1.3(8)
O1	0.087(2)	0.074(7)	0.038(2)	3.2(2)
O2	0.961(4)	–0.062(1)	0.257(4)	3.2(2)
O3	0.037(3)	0.330(9)	0.256(3)	3.2(2)
O4	0.233(3)	–0.011(8)	0.238(3)	3.2(2)
D1	0.374(3)	0.588(9)	0.124(4)	9.9(6)
D2	0.346(3)	0.841(8)	–0.008(5)	9.9(6)
D3	0.185(5)	0.502(8)	0.000(5)	9.9(6)
D4	0.311(4)	0.545(1)	–0.087(4)	9.9(6)
N	0.274(2)	0.629(7)	–0.002(3)	4.0(3)
Li	0.561(6)	0.156(2)	0.235(9)	3(1)

Table 41A-5-010. NH_4LiSO_4. Elastic stiffness [$\cdot 10^{10}$ N m^{-2}] [75Ale]. Ultrasonic method. f = 10 MHz.

T [°C]	c_{11}	c_{22}	c_{23}	c_{44}	c_{55}	c_{66}	c_{12}	c_{13}	c_{23}
32.0	4.150	4.399	4.958	1.538	0.987	1.558	1.97	2.61	2.28
27.0	4.159	4.410	4.973	1.540	0.988	1.573	1.97	2.61	2.28
22.0	4.165	4.422	4.984	1.543	0.990	1.586	1.97	2.62	2.29
17.0	4.170	4.434	4.996	1.545	0.993	1.598	1.97	2.62	2.30
14.0	4.169	4.439	4.999	1.546	0.993	1.602	1.97	2.62	2.30
12.0	4.161	4.431	5.001	1.547	0.994	1.600	1.97	2.61	2.30