Table 40A-5-001. NH_4HSO_4. Structure of phase I [71Nel]. Pseudoorthorhombic cell. Fractional coordinates and temperature factors b_{ij}. b_{ij} is defined by Eq. (b) in Introduction.

	x	y	z
S (1)	0.06208 (2)	0.71422 (9)	0.11079 (3)
S (2)	0.31343 (1)	0.76186 (9)	0.10707 (2)
O (1)	0.01521 (5)	0.61791 (36)	0.15926 (9)
O (2)	0.10986 (6)	0.70472 (51)	0.16386 (11)
O (3)	0.05250 (9)	0.98660 (39)	0.06552 (15)
O (4)	0.07093 (8)	0.51118 (40)	0.02896 (11)
O (5)	0.26636 (5)	0.68751 (34)	0.15988 (9)
O (6)	0.35675 (5)	0.88429 (30)	0.15996 (8)
O (7)	0.29432 (6)	0.99568 (32)	0.03814 (10)
O (8)	0.33160 (5)	0.52234 (27)	0.05042 (9)
N (1)	0.06223 (5)	0.63909 (38)	0.35245 (10)
N (2)	0.31258 (5)	0.79758 (38)	0.34988 (10)
H (9)	0.0691 (140)	0.3614 (890)	0.0502 (240)
H (10)	0.3057 (100)	0.1299 (650)	0.0449 (190)

	b_{11}	b_{22}	b_{33}	b_{23}	b_{31}	b_{12}
S (1)	0.00107 (1)	0.02160 (19)	0.00355 (2)	−0.00098 (5)	0.00031 (1)	−0.00054 (3)
S (2)	0.00084 (1)	0.02100 (16)	0.00237 (1)	0.00048 (5)	−0.00008 (1)	−0.00051 (3)
O (1)	0.00134 (2)	0.05505 (94)	0.00445 (7)	−0.00231 (23)	0.00079 (3)	−0.00255 (12)
O (2)	0.00137 (3)	0.1112 (170)	0.00582 (9)	−0.00586 (34)	−0.00049 (4)	−0.00134 (17)
O (3)	0.00411 (6)	0.03212 (87)	0.00981 (14)	0.00605 (30)	0.00238 (7)	0.00353 (17)
O (4)	0.00300 (4)	0.03886 (87)	0.00350 (7)	−0.00233 (22)	0.00124 (4)	−0.00190 (16)
O (5)	0.00116 (2)	0.05329 (91)	0.00372 (6)	0.00044 (20)	0.00057 (3)	−0.00204 (11)
O (6)	0.00121 (2)	0.03728 (69)	0.00316 (6)	0.00064 (17)	−0.00062 (3)	−0.00190 (10)
O (7)	0.00162 (3)	0.02373 (60)	0.00403 (7)	0.00185 (18)	−0.00089 (3)	−0.00061 (10)
O (8)	0.00144 (2)	0.02413 (59)	0.00385 (6)	−0.00102 (16)	0.00009 (3)	0.00061 (9)
N (1)	0.00097 (2)	0.03649 (77)	0.00347 (7)	−0.00007 (20)	−0.00005 (3)	−0.00024 (11)
N (2)	0.00118 (2)	0.04439 (96)	0.00282 (6)	0.00007 (21)	0.00007 (3)	−0.00065 (13)
H (9)	$B = 3.5$ (10) Å^2 [a])					
H (10)	$B = 3.0$ (10) Å^2 [a])					

[a]) Isotropic temperature factors for the hydrogen atoms of the HSO_4^- groups. B is defined by Eq. (e) in Introduction.

Table 40A-5-002. NH_4HSO_4. Structure of phase I [71Nel]. Interatomic distances and angles. See Fig. 40A-5-001 and Fig. 40A-5-003 about the method of labelling symmetry related atoms.

Bond lengths	[Å]	Bond lengths	[Å]
S (1) – O (1)	1.430 (2)	S (2) – O (5)	1.440 (2)
O (2)	1.419 (2)	O (6)	1.441 (2)
O (3)	1.441 (3)	O (7)	1.557 (2)
O (4)	1.546 (3)	O (8)	1.455 (2)
N (1) – O (6b)	3.134 (5)	N (2) – O (5b)	2.965 (4)
O (6b″)	2.972 (4)	O (5b″)	3.070 (5)
O (1h′)	3.070 (5)	O (2d)	3.006 (5)
[O (1h′)]″	2.921 (4)	O (2d″)	2.990 (5)
O (4i)	3.079 (4)	O (7k)	3.131 (4)
O (3i)	3.219 (5)	O (8k)	3.122 (4)
O (1)	3.093 (4)	O (5)	3.082 (4)
O (2)	3.044 (4)	O (6)	3.042 (4)
O (8b)	3.081 (3)	O (7b″)	3.254 (3)
O (3h′)	3.156 (3)		
O (3) – H (9″)	1.790 (40)	O (7) – H (10″)	0.690 (30)
H (9″) – O (4″)	0.760 (40)	H (10″) – O (8″)	1.920 (30)
O (3) – O (4″)	2.514 (6)	O (7) – O (8″)	2.598 (5)

Bond angles	[deg]	Bond angles	[deg]
O (1) – S (1) – O (2)	112.5 (1)	O (5) – S (2) – O (6)	113.3 (1)
O (1) – S (1) – O (3)	111.7 (1)	O (5) – S (2) – O (7)	106.0 (1)
O (1) – S (1) – O (4)	108.6 (1)	O (5) – S (2) – O (8)	112.4 (1)
O (2) – S (1) – O (3)	115.0 (1)	O (6) – S (2) – O (7)	108.2 (1)
O (2) – S (1) – O (4)	107.5 (1)	O (6) – S (2) – O (8)	112.5 (1)
O (3) – S (1) – O (4)	100.5 (1)	O (7) – S (2) – O (8)	103.8 (1)
O (3)···H (9″) – O (4″)	160 (4)	O (7) – H (10″)···O (8″)	172 (6)

Table 40A-5-003. NH_4HSO_4. Structure of phase II [72Nel]. Pseudoorthorhombic cell. Coordinates and temperature factors. X, Z: coordinates along a', b'^*, respectively. B is defined by Eq. (e) in Introduction. These parameters correspond to the atoms of the subcells labelled as a, b, c and d in Fig. 40A-5-003. a' and b' are pseudoorthorhombic lattice parameters. b'^* is perpendicular to the a' c' plane.

Atom	X [Å]	Z [Å]	B [Å^2]	Atom	X [Å]	Z [Å]	B [Å^2]
S(1)	1.52	1.61	0.9(1)	S(1′)	10.73(6)	5.74(7)	1.5(2)
O(1)	0.46(2)	2.44(2)	2.0(4)	O(1′)	11.98(2)	5.16(2)	2.2(4)
O(2)	2.70(2)	2.40(2)	1.7(4)	O(2′)	9.59(2)	4.96(2)	1.8(4)
O(3)	1.11(2)	0.76(2)	1.8(4)	O(3′)	10.76(3)	6.25(3)	3.1(5)
O(4)	1.98(2)	0.56(2)	1.5(3)	O(4′)	10.75(2)	7.08(2)	1.4(3)
N(1)	1.50(2)	5.23(2)	0.6(3)	N(1′)	10.71(3)	2.24(3)	2.3(6)
S(2)	7.70(1)	1.62(1)	0.8(1)	S(2′)	4.60(6)	5.82(6)	0.7(1)
O(5)	6.53(2)	2.45(2)	1.4(3)	O(5′)	5.77(1)	5.09(2)	0.2(3)
O(6)	8.76(2)	2.33(2)	2.0(4)	O(6′)	3.57(1)	4.96(2)	1.0(4)
O(7)	7.23(2)	0.52(2)	1.8(4)	O(7′)	5.14(2)	6.78(2)	2.0(4)
O(8)	8.20(2)	0.82(2)	0.9(3)	O(8′)	4.16(2)	6.68(2)	2.1(4)
N(2)	7.65(2)	5.18(2)	0.2(3)	N(2′)	4.61(3)	2.29(3)	2.1(6)