Table 39A-1-001. $(NH_4)_2SO_4$. Unit cell parameters [81Has].

	−140 °C	−90 °C	−64 °C	−53.5 °C	−48.5 °C	−40 °C
a [Å]	7.924	7.882	7.867	7.830	7.747	7.762
b [Å]	10.526	10.560	10.579	10.569	10.593	10.612
c [Å]	5.953	5.951	5.953	5.956	5.977	5.979

Table 39A-1-002. $(NH_4)_2SO_4$. Structure of phase I [66Sch]. Fractional coordinates of the heavy atoms at RT by various authors.

		X-ray	Electron diffraction	Neutron diffraction	
S	*x*	0.2441(4)	0.255	0.238(2)	0.2440(9)
	y	0.4110(3)	0.420	0.422(2)	0.4192(6)
	z	0.250	0.250		0.250
O(1)	*x*	0.060(2)	0.046	0.055(2)	0.0612(6)
	y	0.394(2)	0.412	0.395(2)	0.3887(60)
	z	0.250	0.250		0.250
O(2)	*x*	0.273(2)	0.309	0.269(3)	0.2701(7)
	y	0.554(2)	0.542	0.558(3)	0.5559(4)
	z	0.250	0.250		0.250
O(3)	*x*	0.320(1)	0.317	0.325(2)	0.3239(5)
	y	0.364(1)	0.352	0.367(2)	0.3665(3)
	z	0.052(2)	0.041		0.0488(5)
N(1)	*x*	0.687(2)	0.690	0.688(1)	0.6895(3)
	y	0.403(2)	0.405	0.402(1)	0.4025(2)
	z	0.250	0.250		0.250
N(2)	*x*	0.966(2)	0.985	0.968(1)	0.9677(4)
	y	0.703(2)	0.692	0.704(1)	0.7050(2)
	z	0.250	0.250		0.250
Ref.		[62Sin] [1])	[63Uda]	[62Sin] [1])	[66Sch]

[1]) hk0 data only.

Table 39A-1-003. $(NH_4)_2SO_4$. Structure of phase I [66Sch]. Fractional coordinates of H atoms at RT by various authors.

		Electron diffraction	Neutron diffraction and X-ray	Neutron diffraction
H(1)	*x*	0.652	0.813	0.810(2)
	y	0.304	0.372	0.372(1)
	z	0.250	0.250	0.250
H(2)	*x*	0.545	0.597	0.600(2)
	y	0.435	0.341	0.343(1)
	z	0.250	0.250	0.250
H(3)	*x*	0.758	0.683	0.676(1)
	y	0.437	0.468	0.457(1)
	z	0.111	0.100	0.122(2)
H(4)	*x*	0.882	1.016	0.991(2)
	y	0.780	0.777	0.792(1)
	z	0.250	0.250	0.250
H(5)	*x*	1.143	1.069	1.069(1)
	y	0.700	0.634	0.649(1)
	z	0.250	0.250	0.250
H(6)	*x*	0.957	0.883	0.893(1)
	y	0.639	0.686	0.682(1)
	z	0.111	0.100	0.124(2)
Ref.		[63Uda]	[62Sin] [1])	[66Sch]

[1]) Based on average coordinates for pairs of H atoms from a twofold disorder model.

Table 39A-1-004. $(NH_4)_2SO_4$. Structure of phases I and II [66Sch]. Fractional coordinates above and below Θ_t. RT ≈ 298 K, LT ≈ 180 K. Neutron diffraction.

	T	*x*	*y*	*z*
S	RT	0.244(1)	0.419(1)	0.250
	LT	0.243(2)	0.421(1)	0.250
	LT [62Sin]	0.2421(4)	0.4230(3)	0.250
O (1)	RT	0.0612(6)	0.3887(6)	0.250
	LT	0.061(1)	0.402(1)	0.212(4)
	LT [62Sin]	0.0602(13)	0.4024(90)	0.2127(16)
O (2)	RT	0.2701(7)	0.5559(4)	0.250
	LT	0.284(1)	0.557(1)	0.222(4)
	LT [62Sin]	0.2873(15)	0.5565(11)	0.2255(18)
O (3)	RT	0.3239(5)	0.3665(3)	0.0488(5)
	LT	0.339(1)	0.346(1)	0.083(4)
	LT [62Sin]	0.3375(11)	0.3462(8)	0.0872(14)
O (4)	RT	0.3239(5)	0.3665(3)	0.4512(5)
	LT	0.294(1)	0.382(1)	0.477(4)
	LT [62Sin]	0.2885(12)	0.3849(9)	0.4795(15)
N (1)	RT	0.6895(3)	0.4025(2)	0.250
	LT	0.6808(7)	0.3958(5)	0.245(4)
	LT [62Sin]	0.6789(15)	0.3966(11)	0.2533(18)
N (2)	RT	0.9677(4)	0.7050(2)	0.250
	LT	0.9796(6)	0.6999(5)	0.256(4)
	LT [62Sin]	0.9786(14)	0.7007(10)	0.2656(16)
H (1)	RT	0.810(2)	0.372(1)	0.250
	LT	0.771(3)	0.336(2)	0.202(5)
H (2)	RT	0.600(2)	0.343(1)	0.250
	LT	0.564(3)	0.360(2)	0.206(5)
H (3)	RT	0.676(1)	0.457(1)	0.122(2)
	LT	0.691(2)	0.480(1)	0.157(5)
H (4)	RT	0.676(1)	0.457(1)	0.378(2)
	LT	0.682(2)	0.412(2)	0.408(5)
H (5)	RT	1.069(1)	0.649(1)	0.250
	LT	1.092(2)	0.658(2)	0.222(5)
H (6)	RT	0.991(2)	0.792(1)	0.250
	LT	0.990(3)	0.793(2)	0.265(8)
H (7)	RT	0.893(1)	0.682(1)	0.124(2)
	LT	0.896(3)	0.670(2)	0.142(5)
H (8)	RT	0.893(1)	0.682(1)	0.376(2)
	LT	0.945(3)	0.672(2)	0.412(5)

Table 39A-1-005. $(NH_4)_2SO_4$. Structure of phase I [66Sch]. Anisotropic temperature parameters at RT. Neutron diffraction. The second row for each atom gives the standard deviations from the least-squares variance-covariance matrix. U_{ij} [Å^2] is defined by Eq. (d) in Introduction.

	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
S	0.0243	0.0292	0.0231	0.0025	0	0
	0.0028	0.0034	0.0025	0.0025	0	0
O (1)	0.0221	0.0802	0.0632	−0.0130	0	0
	0.0021	0.0040	0.0031	0.0025	0	0
O (2)	0.0519	0.0229	0.0519	0.0008	0	0
	0.0028	0.0017	0.0025	0.0017	0	0
O (3)	0.0522	0.0476	0.0306	0.0092	0.0090	−0.0129
	0.0018	0.0017	0.0013	0.0013	0.0012	0.0010
N (1)	0.0261	0.0309	0.0284	0.0025	0	0
	0.0012	0.0011	0.0009	0.0013	0	0
N (2)	0.0322	0.0287	0.0335	−0.0013	0	0
	0.0012	0.0011	0.0013	0.0008	0	0
H (1)	0.0663	0.1129	0.1043	0.0486	0	0
	0.0068	0.0109	0.0093	0.0071	0	0
H (2)	0.0985	0.0945	0.0950	−0.0453	0	0
	0.0092	0.0097	0.0087	0.0084	0	0
H (3)	0.0758	0.1559	0.1096	−0.0050	−0.0111	0.0824
	0.0049	0.0103	0.0071	0.0059	0.0050	0.0074
H (4)	0.0556	0.0865	0.0905	0.0193	0	0
	0.0055	0.0074	0.0073	0.0054	0	0
H (5)	0.1458	0.0470	0.1421	−0.0281	0	0
	0.0147	0.0057	0.0135	0.0075	0	0
H (6)	0.1108	0.0785	0.1065	−0.0059	−0.0526	0.0039
	0.0071	0.0052	0.0066	0.0050	0.0059	0.0048

Table 39A-1-006. $(NH_4)_2SO_4$. Structure of phase II [66Sch]. Anisotropic temperature parameters at about 180 K. Neutron diffraction. The second row for each atom gives the standard deviations from the least-squares variance-covariance matrix. U_{ij} [Å^2] is defined by Eq. (d) in Introduction.

	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
S	0.0221	0.0091	0.0307	0.0004	−0.0021	−0.0019
	0.0072	0.0063	0.0078	0.0051	0.0034	0.0024
O (1)	0.0165	0.0280	0.0265	−0.0046	−0.0054	−0.0006
	0.0037	0.0040	0.0047	0.0029	0.0033	0.0035
O (2)	0.0265	0.0080	0.0245	−0.0059	0.0033	−0.0029
	0.0044	0.0034	0.0047	0.0025	0.0033	0.0035
O (3)	0.0286	0.0137	0.0231	0.0021	0.0090	0.0013
	0.0050	0.0040	0.0038	0.0034	0.0036	0.0035
O (4)	0.0277	0.0131	0.0177	0.0004	−0.0021	0.0019
	0.0050	0.0046	0.0038	0.0034	0.0033	0.0035
N (1)	0.0293	0.0080	0.0224	−0.0046	−0.0036	0.0067
	0.0034	0.0029	0.0034	0.0021	0.0028	0.0032
N (2)	0.0246	0.0057	0.0256	0.0004	−0.0088	0.0048
	0.0037	0.0034	0.0029	0.0021	0.0031	0.0032
H (1)	0.1030	0.0365	0.0732	0.0375	0.0479	0.0045
	0.0177	0.0103	0.0166	0.0118	0.0147	0.0099
H (2)	0.0429	0.0462	0.0586	−0.0110	−0.0073	0.0071
	0.0109	0.0091	0.0128	0.0076	0.0090	0.0093
H (3)*	0.0498	0.0154	0.0310	0.0093	0.0190	0.0298
	0.0103	0.0080	0.0083	0.0059	0.0064	0.0074
H (4)	0.0342	0.0536	0.0483	0.0042	0.0102	−0.0157
	0.0103	0.0120	0.0123	0.0072	0.0081	0.0093
H (5)	0.0461	0.0708	0.0256	0.0253	0.0092	0.0241
	0.0103	0.0103	0.0088	0.0088	0.0078	0.0090
H (6)	0.0921	0.0086	0.0761	0.0067	−0.0301	−0.0225
	0.0156	0.0086	0.0117	0.0080	0.0149	0.0103
H (7)	0.0654	0.0360	0.0561	−0.0139	−0.0308	0.0170
	0.0149	0.0103	0.0110	0.0088	0.0104	0.0090
H (8)	0.0261	0.0639	0.0458	−0.0046	−0.0040	0.0109
	0.0096	0.0126	0.0128	0.0072	0.0078	0.0106

*) These parameters do not describe a real ellipsoid since $U_{23}^2 > U_{22} \cdot U_{33}$.

Table 39A-1-007. $(NH_4)_2SO_4$. Structures of phases I and II [66Sch]. Interatomic distances and angles in ammonium ions. Neutron diffraction. RT ≈ 298 K, LT ≈ 180 K.

	RT	LT
	Distances in [Å]	
N (1)–H (1)	1.08 (1)	1.07 (2)
N (1)–H (2)	1.04 (2)	1.06 (2)
N (1)–H (3)	1.09 (1)	1.06 (2)
N (1)–H (4)	1.09 (1)	1.02 (3)
N (2)–H (5)	1.05 (1)	1.04 (2)
N (2)–H (6)	1.06 (2)	1.06 (2)
N (2)–H (7)	1.07 (1)	1.04 (3)
N (2)–H (8)	1.07 (1)	1.05 (2)
Average N–H	1.08 (1)	1.05 (1)
	Bond angles in [°]	
H (1)–N (1)–H (2)	118.5 (15)	109. 9 (21)
H (1)–N (1)–H (3)	107.6 (9)	111.6 (16)
H (1)–N (1)–H (4)	107.6 (9)	111.3 (20)
H (2)–N (1)–H (3)	108.8 (9)	106.1 (16)
H (2)–N (1)–H (4)	108.8 (9)	107.4 (17)
H (3)–N (1)–H (4)	104.7 (9)	110.4 (19)
H (5)–N (2)–H (6)	116.2 (14)	112.2 (18)
H (5)–N (2)–H (7)	108.4 (8)	107.6 (20)
H (5)–N (2)–H (8)	108.4 (8)	107.1 (16)
H (6)–N (2)–H (7)	111.2 (8)	114.1 (18)
H (6)–N (2)–H (8)	111.2 (8)	104.7 (24)
H (7)–N (2)–H (8)	100.2 (8)	111.0 (17)

Table 39A-1-008. $(NH_4)_2SO_4$. Structures of phases I and II [66Sch]. Interatomic distances and angles in sulfate ion. Neutron diffraction. RT ≈ 298 K, LT ≈ 180 K.

	RT	LT
	Distances in [Å]	
S–O (1)	1.49 (1)	1.47 (1)
S–O (2)	1.49 (1)	1.50 (1)
S–O (3)	1.49 (1)	1.48 (1)
S–O (4)	1.49 (1)	1.47 (1)
	Bond angles in [°]	
O (1)–S–O (2)	110.8 (5)	108.8 (10)
O (1)–S–O (3)	109.1 (4)	108.9 (12)
O (1)–S–O (4)	109.1 (4)	111.6 (14)
O (2)–S–O (3)	108.7 (4)	109.4 (13)
O (2)–S–O (4)	108.7 (4)	108.5 (12)
O (3)–S–O (4)	110.5 (4)	109.6 (10)

Table 39A-1-009. $(NH_4)_2SO_4$. Structures of phases I and II [66Sch]. O–H distances and O...H–N bond angles. Neutron diffraction. RT ≈ 298 K, LT ≈ 180 K.

	RT	LT
	Distances in [Å]	
O (1)–H (1)	1.97	2.38
O (1)–H (2)	2.48	2.78
O (1)–H (7)	2.39	2.70
O (1)–H (8)	2.39	1.96
O (2)–H (5)	1.85	1.85
O (2)–H (3)	2.27	2.63
O (2)–H (4)	2.27	1.92
O (2)–H (6)	2.36	2.28
O (3)–H (8)	2.05	2.46
O (3)–H (6)	2.43	2.39
O (3)–H (2)	2.48	1.91
O (3)–H (4)	2.14	2.78
O (4)–H (7)	2.05	1.87
O (4)–H (6)	2.43	2.59
O (4)–H (2)	2.48	2.68
O (4)–H (3)	2.14	1.82
	Bond angles in [°]	
O (1)···H (1)–N (1)	155.7	119.2
O (1)···H (2)–N (1)	139.3	—
O (1)···H (7)–N (2)	135.4	—
O (1)···H (8)–N (2)	135.4	164.3
O (2)···H (5)–N (2)	174.9	165.5
O (2)···H (3)–N (1)	136.0	—
O (2)···H (4)–N (1)	136.0	172.7
O (2)···H (6)–N (2)	122.2	129.0
O (3)···H (8)–N (2)	159.7	130.4
O (3)···H (6)–N (2)	115.7	108.9
O (3)···H (2)–N (1)	124.9	160.2
O (3)···H (4)–N (1)	155.0	—
O (4)···H (7)–N (2)	159.7	168.2
O (4)···H (6)–N (2)	115.7	111.9
O (4)···H (2)–N (1)	124.9	—
O (4)···H (3)–N (1)	155.0	174.3

Table 39A-1-010. $(NH_4)_2SO_4$. Structures of phases I and II [66Sch]. Root mean square thermal displacements in [Å] in directions of principal axes of the thermal ellipsoid. Neutron diffraction. RT ≈ 298 K, LT ≈ 180 K.

Atom	*T*	Axis 1	Axis 2	Axis 3
S	RT	0.152 (9)	0.152 (8)	0.175 (10)
	LT	0.09 (3)	0.15 (3)	0.18 (2)
O (1)	RT	0.139 (8)	0.251 (6)	0.288 (7)
	LT	0.11 (2)	0.17 (1)	0.17 (1)
O (2)	RT	0.150 (6)	0.228 (5)	0.228 (6)
	LT	0.08 (2)	0.15 (1)	0.18 (1)
O (3)	RT	0.138 (4)	0.228 (4)	0.244 (4)
	LT	0.12 (2)	0.13 (1)	0.19 (1)
O (4)	RT	0.138 (4)	0.228 (4)	0.244 (4)
	LT	0.10 (2)	0.14 (2)	0.17 (1)
N (1)	RT	0.158 (4)	0.168 (3)	0.180 (4)
	LT	0.07 (3)	0.15 (1)	0.18 (1)
N (2)	RT	0.169 (4)	0.181 (4)	0.183 (3)
	LT	0.07 (3)	0.13 (1)	0.19 (1)
H (1)	RT	0.19 (1)	0.32 (1)	0.38 (2)
	LT	0.12 (4)	0.23 (3)	0.38 (4)
H (2)	RT	0.23 (1)	0.31 (1)	0.38 (2)
	LT	0.18 (3)	0.22 (2)	0.26 (3)
H (3)	RT	0.21 (1)	0.28 (1)	0.47 (1)
	LT		0.18 (2)	0.27 (2)
H (4)	RT	0.21 (1)	0.28 (1)	0.47 (1)
	LT	0.16 (3)	0.21 (2)	0.26 (2)
H (5)	RT	0.21 (1)	0.30 (1)	0.31 (1)
	LT	0.12 (3)	0.18 (3)	0.31 (2)
H (6)	RT	0.20 (1)	0.38 (2)	0.39 (2)
	LT	0.04 (11)	0.24 (3)	0.34 (3)
H (7)	RT	0.24 (1)	0.28 (1)	0.40 (1)
	LT	0.16 (3)	0.18 (3)	0.32 (2)
H (8)	RT	0.24 (1)	0.28 (1)	0.40 (1)
	LT	0.16 (3)	0.20 (3)	0.26 (3)

Table 39A-1-011. $(NH_4)_2SO_4$. Fractional coordinates and anisotropic temperature parameters [81Has]. X-ray diffraction. b_{ij} [$\cdot 10^{-4}$] is defined by Eq. (b) in Introduction.

(**a**) $T = -40$°C ($R = 0.039$)

	x	y	z	b_{11}	b_{22}	b_{33}	b_{12}	b_{13}	b_{23}
S	0.2455(1)	0.4195(0)	0.25	47(0)	27(0)	85(1)	0	0	0
O(1)	0.0618(2)	0.3878(2)	0.25	58(2)	100(2)	287(7)	–30(2)	0	0
O(2)	0.2692(3)	0.5572(1)	0.25	137(3)	25(1)	256(5)	–6(2)	0	0
O(3)	0.3265(2)	0.3670(1)	0.0487(2)	133(2)	79(1)	145(3)	16(2)	37(2)	–43(2)
O(4)	0.3265(2)	0.3670(1)	0.4513(2)	133(2)	79(1)	145(3)	16(2)	–37(2)	43(2)
N(1)	0.6901(2)	0.4019(2)	0.2466(2)	70(2)	36(1)	106(4)	0(1)	11(15)	–15(11)
N(2)	0.9655(3)	0.7040(2)	0.2579(3)	81(2)	37(1)	104(4)	–5(1)	–8(10)	4(7)

(**b**) $T = -48.5$°C ($R = 0.041$)

	x	y	z	b_{11}	b_{22}	b_{33}	b_{12}	b_{13}	b_{23}
S	0.2455(0)	0.4196(0)	0.25	47(0)	26(0)	82(1)	–1	0	0
O(1)	0.0620(2)	0.3878(2)	0.25	57(2)	100(2)	279(7)	–30(2)	0	0
O(2)	0.2692(3)	0.5573(2)	0.25	138(3)	25(1)	253(6)	–6(2)	0	0
O(3)	0.3267(2)	0.3670(1)	0.0486(2)	134(2)	79(1)	141(3)	15(2)	37(2)	–43(2)
O(4)	0.3267(2)	0.3670(1)	0.4514(2)	134(2)	79(1)	141(3)	15(2)	–37(2)	43(2)
N(1)	0.6901(3)	0.4018(2)	0.2466(4)	70(2)	37(1)	104(4)	0(2)	–18(13)	–21(10)
N(2)	0.9655(3)	0.7038(2)	0.2579(3)	80(2)	35(1)	101(4)	–6(2)	–4(11)	4(8)

Table 39A-1-012. $(NH_4)_2SO_4$. Fractional coordinates and anisotropic temperature parameters [81Has]. X-ray diffraction. b_{ij} [$\cdot 10^{-4}$] and B [Å^2] are defined by Eq. (b) and Eq. (e) in Introduction, respectively. A bar is attached to the identification number of ammonium ions with small occupation probabilities, for example N($\bar{1}$). For occupation probability, see Table 39A-1-013.

(**a**) $T = -53.5$°C ($R = 0.039$)

Atom	x	y	z	B	b_{11}	b_{22}	b_{33}	b_{12}	b_{13}	b_{23}
S	0.2429(0)	0.4208(0)	0.25		47(0)	23(0)	75(1)	–2(0)	1(1)	–1(1)
O(1)	0.0596(2)	0.3987(2)	0.2272(6)		51(2)	75(2)	229(8)	–15(1)	–6(4)	–14(4)
O(2)	0.2809(2)	0.5570(1)	0.2226(4)		102(2)	23(1)	129(5)	–5(1)	1(3)	5(2)
O(3)	0.3343(3)	0.3487(2)	0.0773(4)		113(3)	44(1)	121(4)	4(2)	36(3)	–25(2)
O(4)	0.3020(3)	0.3798(2)	0.4754(3)		116(3)	41(1)	94(4)	6(2)	–21(3)	14(2)
N(1)	0.6821(3)	0.3970(2)	0.2466(7)		69(2)	29(1)	99(4)	–2(1)	15(6)	–5(4)
H(1)	0.769(7)	0.324(5)	0.214(14)	3.2(14)						
H(2)	0.587(6)	0.349(4)	0.210(11)	1.9(11)						
H(3)	0.682(7)	0.485(5)	0.172(10)	2.6(13)						
H(4)	0.689(7)	0.419(5)	0.373(11)	2.5(13)						
N($\bar{1}$)	0.6833	0.3987	0.2544		67	32	102	–1	–19	1
H($\bar{1}$)	0.759	0.327	0.283	2.9						
H($\bar{2}$)	0.583	0.361	0.285	2.0						
H($\bar{3}$)	0.689	0.503	0.354	2.8						
H($\bar{4}$)	0.698	0.421	0.092	2.6						
N(2)	0.9766(3)	0.7006(2)	0.2579(8)		74(3)	34(1)	101(5)	–2(2)	–5(6)	–8(4)
H(5)	1.083(7)	0.659(5)	0.250(19)	2.7(12)						
H(6)	0.994(7)	0.780(5)	0.256(20)	3.5(14)						
H(7)	0.894(7)	0.671(5)	0.149(10)	1.9(13)						
H(8)	0.942(8)	0.680(5)	0.387(11)	2.3(14)						
N($\bar{2}$)	0.9758	0.7007	0.2425		71	33	105	–1	3	10
H($\bar{5}$)	1.087	0.652	0.252	2.6						
H($\bar{6}$)	0.996	0.776	0.241	3.3						
H($\bar{7}$)	0.897	0.672	0.351	2.4						
H($\bar{8}$)	0.931	0.687	0.102	2.6						

(**b**) $T = -64$°C ($R = 0.037$)

Atom	x	y	z	B	b_{11}	b_{22}	b_{33}	b_{12}	b_{13}	b_{23}
S	0.2426(1)	0.4213(0)	0.25		43(0)	21(0)	70(1)	–2(0)	2(1)	–1(1)
O(1)	0.0597(2)	0.4003(2)	0.2224(4)		48(2)	64(1)	196(7)	–13(1)	–7(3)	–12(3)
O(2)	0.2831(2)	0.5574(1)	0.2215(3)		88(2)	22(1)	119(5)	–4(1)	2(2)	3(1)
O(3)	0.3361(2)	0.3477(2)	0.0793(3)		95(2)	39(1)	115(4)	6(1)	34(3)	–21(2)
O(4)	0.2975(2)	0.3810(2)	0.4774(3)		98(2)	37(1)	84(3)	2(1)	–16(2)	13(2)
N(1)	0.6815(2)	0.3969(2)	0.2465(5)		62(2)	30(1)	92(3)	–2(1)	5(5)	–2(3)
H(1)	0.766(6)	0.323(4)	0.203(11)	2.9(13)						
H(2)	0.590(6)	0.353(4)	0.216(11)	2.2(11)						
H(3)	0.689(7)	0.482(5)	0.165(10)	3.7(14)						
H(4)	0.692(6)	0.422(5)	0.388(10)	3.0(12)						
N($\bar{1}$)	0.6824	0.3987	0.2563		60	32	95	–3	–5	2
H($\bar{1}$)	0.767	0.324	0.295	2.7						
H($\bar{2}$)	0.588	0.324	0.286	2.4						
H($\bar{3}$)	0.686	0.486	0.341	3.4						
H($\bar{4}$)	0.693	0.419	0.099	2.8						
N(2)	0.9787(3)	0.7002(2)	0.2579(7)		62(2)	30(1)	110(5)	–1(1)	–14(5)	–8(3)
H(5)	1.081(6)	0.659(4)	0.241(16)	2.4(11)						
H(6)	0.992(7)	0.784(5)	0.265(17)	3.6(14)						
H(7)	0.893(7)	0.672(5)	0.159(10)	2.3(13)						
H(8)	0.946(7)	0.672(5)	0.384(10)	1.9(12)						
N($\bar{2}$)	0.9778	0.7008	0.2418		61	29	113	–2	12	6
H($\bar{5}$)	1.083	0.654	0.263	2.5						
H($\bar{6}$)	0.996	0.777	0.223	3.4						
H($\bar{7}$)	0.896	0.676	0.345	2.4						
H($\bar{8}$)	0.940	0.675	0.103	2.0						

(c) $T = -90$°C ($R = 0.031$)

Atom	x	y	z	B	b_{11}	b_{22}	b_{33}	b_{12}	b_{13}	b_{23}
S	0.2424(0)	0.4223(0)	0.25		35(0)	18(0)	59(0)	–2(0)	3(1)	–2(1)
O(1)	0.0603(1)	0.4026(1)	0.2152(3)		39(1)	52(1)	152(4)	–8(1)	–6(2)	–11(2)
O(2)	0.2857(1)	0.5581(1)	0.2208(2)		69(1)	20(1)	98(3)	–4(1)	3(2)	3(1)
O(3)	0.3389(2)	0.3464(1)	0.0853(2)		69(1)	31(1)	95(2)	4(1)	20(2)	–19(1)
O(4)	0.2912(2)	0.3824(1)	0.4801(2)		77(1)	31(1)	75(2)	1(1)	–4(1)	9(2)
N(1)	0.6813(1)	0.3962(1)	0.2472(3)		55(1)	28(1)	88(2)	0(1)	3(3)	–1(2)
H(1)	0.768(4)	0.337(3)	0.205(6)	1.0(6)						
H(2)	0.584(4)	0.361(3)	0.208(6)	1.1(6)						
H(3)	0.695(4)	0.464(3)	0.158(6)	1.2(7)						
H(4)	0.679(4)	0.416(3)	0.386(6)	1.0(6)						
N($\bar{1}$)	0.6830	0.3985	0.2551		57	28	86	0	–4	1
H($\bar{1}$)	0.768	0.337	0.298	1.0						
H($\bar{2}$)	0.584	0.362	0.295	1.0						
H($\bar{3}$)	0.695	0.464	0.341	1.2						
H($\bar{4}$)	0.679	0.417	0.113	1.0						
N(2)	0.9800(2)	0.6997(1)	0.2578(4)		56(1)	29(1)	97(3)	–1(1)	–5(3)	–6(2)
H(5)	1.088(4)	0.667(3)	0.235(8)	1.3(6)						
H(6)	0.991(4)	0.779(3)	0.275(8)	2.1(8)						
H(7)	0.902(4)	0.679(3)	0.144(6)	1.4(7)						
H(8)	0.938(4)	0.676(3)	0.374(6)	1.3(7)						
N($\bar{2}$)	0.9798	0.6977	0.2410		58	28	95	–1	4	6
H($\bar{5}$)	1.088	0.668	0.267	1.3						
H($\bar{6}$)	0.992	0.777	0.222	2.0						
H($\bar{7}$)	0.904	0.679	0.355	1.5						
H($\bar{8}$)	0.937	0.677	0.125	1.3						

(d) $T = -140$°C ($R = 0.028$)

Atom	x	y	z	B	b_{11}	b_{22}	b_{33}	b_{12}	b_{13}	b_{23}
S	0.2424(0)	0.4236(0)	0.25		23(0)	12(0)	39(0)	–1(0)	2(0)	–2(0)
O(1)	0.0608(1)	0.4055(1)	0.2095(2)		24(1)	33(1)	96(2)	–5(1)	–4(1)	–10(1)
O(2)	0.2887(1)	0.5595(1)	0.2205(2)		45(1)	14(0)	68(2)	–3(1)	1(1)	3(1)
O(3)	0.3407(1)	0.3460(1)	0.0894(2)		42(1)	21(1)	65(2)	3(1)	12(1)	–12(1)
O(4)	0.2861(1)	0.3839(1)	0.4826(2)		49(1)	22(1)	47(2)	0(1)	–1(1)	6(1)
N(1)	0.6805(1)	0.3944(1)	0.2463(3)		39(1)	20(0)	63(2)	–1(1)	3(2)	1(2)
H(1)	0.762(3)	0.329(3)	0.205(6)	0.9(6)						
H(2)	0.578(3)	0.365(3)	0.209(5)	0.7(5)						
H(3)	0.687(4)	0.467(3)	0.164(6)	1.4(7)						
H(4)	0.693(4)	0.420(3)	0.389(6)	1.0(6)						
N($\bar{1}$)	0.6804	0.3946	0.2540		38	19	61	0	–2	–2
H($\bar{1}$)	0.762	0.323	0.301	1.0						
H($\bar{2}$)	0.579	0.365	0.295	0.9						
H($\bar{3}$)	0.687	0.470	0.335	1.3						
H($\bar{4}$)	0.692	0.424	0.113	1.0						
N(2)	0.9817(1)	0.6991(1)	0.2614(3)		40(1)	18(1)	62(2)	–1(1)	–5(2)	–4(1)
H(5)	1.095(4)	0.674(3)	0.250(9)	1.2(6)						
H(6)	0.987(4)	0.783(3)	0.280(7)	1.8(8)						
H(7)	0.888(4)	0.680(3)	0.146(6)	0.9(6)						
H(8)	0.943(4)	0.673(3)	0.379(6)	0.8(6)						
N($\bar{2}$)	0.9816	0.6991	0.2387		39	19	60	–1	6	5
H($\bar{5}$)	1.095	0.677	0.250	1.3						
H($\bar{6}$)	0.988	0.780	0.215	1.6						
H($\bar{7}$)	0.886	0.684	0.355	1.0						
H($\bar{8}$)	0.943	0.677	0.121	0.8						

Table 39A-1-013. $(NH_4)_2SO_4$. Occupation probabilities of two kinds of ammonium ions [81Has].

	–140 °C	–90 °C	–64 °C	–53.5 °C
Ammonium ion I	0.996(4)	0.987(24)	0.886(10)	0.832(11)
Ammonium ion II	0.935(12)	0.972(19)	0.767(23)	0.746(29)

Table 39A-1-014. $(NH_4)_2SO_4$. Elastic stiffness [78Yos]. c_{ij} [$\cdot 10^9$ N m^{-2}] determined by Brillouin scattering.

c_{ij}	[72Lus]	[65Hau]	[78Yos]
c_{11}	35.2(3)	36.1	35.6(5)
c_{22}	29.7(3)	29.8	28.1(5)
c_{33}	36.0(3)	35.3	36.3(5)
c_{44}	9.5(3)	10.3	9.3(5)
c_{55}	7.0(3)	7.2	7.5(5)
c_{66}	10.3(3)	9.7	9.9(5)
c_{12}	14.1(2)	16.5	
c_{23}	17.3(2)	14.6	
c_{13}	15.7(2)	15.8	

Table 39A-1-015. $(NH_4)_2SO_4$. Refractive indices and optical axial angle [03Tut].

	RT					T = 80°C			
λ [nm]	n_α	n_β	n_γ	$2V$	λ [nm]	n_α	n_β	n_γ	$2V$
431	1.5318	1.5340	1.5445	–	431	1.5287	1.5315	1.5406	–
486	1.5270	1.5291	1.5394	+52°00'	486	1.5239	1.5266	1.5355	–
535	1.5237	1.5288	1.5359	+52°07'	535	1.5206	1.5233	1.5320	–
589	1.5209	1.5230	1.5330	+52°12'	589	1.5178	1.5205	1.5291	–
656	1.5182	1.5204	1.5302	+52°17'	656	1.5151	1.5179	1.5263	–
671	1.5177	1.5199	1.5297	+52°18'	671	1.5146	1.5174	1.5258	–

Table 39A-1-016. $(NH_4)_2SO_4$. Piezooptic constants at RT [72Lus]. λ = 633 nm.

$\lvert p_{12}\rvert = 0.270$	$\lvert p_{21}\rvert = 0.230$	$\lvert p_{13}\rvert = 0.260$	$\lvert p_{31}\rvert = 0.234$
$\lvert p_{23}\rvert = 0.254$	$\lvert p_{32}\rvert = 0.130$	$\lvert p_{12} - p_{21}\rvert = 0.130$	$\lvert p_{11} - p_{31}\rvert = 0.120$
$p_{22} \cong p_{32} \cong p_{12}$	$p_{33} \cong p_{13} \cong p_{23}$	$p_{44} = +0.015$	$\lvert p_{55}\rvert \leq 0.0015$
$p_{66} \cong 0.012$			

Table 39A-1-017. $(NH_4)_2SO_4$. Piezooptic constants [73Mar]. T = 22 °C. λ = 632.8 nm.

Crystal	p_{11}	p_{12}	p_{31}
$(NH_4)_2SO_4$	0.261(11)	0.191(11)	0.197(11)

Table 39A-1-018. $(NH_4)_2SO_4$. Nonlinear optical susceptibilities [77Suz]. T = –100 °C. l_c: coherence length. A Q-switched Nd–YAG laser was used.

d_{ij}	Relative to $d_{11}(SiO_2)$	l_c μm	Relative sign
d_{31}	0.56 (6)	10.0 (5)	$d_{31} \cdot d_{33} < 0$
d_{32}	0.59 (6)	11 (1)	$d_{32} \cdot d_{33} < 0$
d_{33}	1.3 (1)	18 (1)	

Table 39A-1-019. $(NH_4)_2SO_4$. ESR of $(SeO_3)^-$ [77Owe]. Spin Hamiltonian parameters of $(SeO_3)^-$ radical.

T [K]	$g_{\|\|}$	$g_\perp$	$A_{\|\|}$	$A_\perp$
246	2.006	2.027	541.8	389.6
206	2.006	2.027	549.2	389.6

Table 39A-1-020. $(NH_4)_2SO_4$. $\boldsymbol{g}$ and $\boldsymbol{A}_H$ tensor and their direction cosines for $(CrO_4)^{3-}$ [82Bha]. Error in $\boldsymbol{g}$ is ±0.001. $\boldsymbol{A}_H$: proton super-hyperfine constant.

$T = 300$ K				$T = 220$ K			
Principal values	Direction cosines			Principal values	Direction cosines		
	a	*b*	*c*		*a*	*b*	*c*
1.983	0	0	1	1.971	0	0	0.9986
1.986	0.891	0.454	0	1.988	0.9003	0.435	±0.0523
1.947	0.454	0.891	0	1.946	0.435	0.9003	±0.0523
A_H: $9.03 \cdot 10^2$ A m^{-1}		isotropic		A_H: $11.45 \cdot 10^2$ A m^{-1}		isotropic	

Table 39A-1-021. $(NH_4)_2SO_4$. ESR of V–O [75Pan]. Spin Hamiltonian parameters and direction cosines at 25 °C for site I. (The VO^{2+} occupy four type of sites in the lattice. Only the spectra corresponding to V–O sites I...III have been analyzed. See also Fig. 39A-1-002, Fig. 39A-1-003. Direction cosines relating the crystal axes (*a*, *b*, *c*) to the principal axes of $\boldsymbol{g}$ and $\boldsymbol{A}$ tensors.1', 2', 3': principal axes of $\boldsymbol{g}$ tensor. 1, 2, 3: principal axes of $\boldsymbol{A}$ tensor [$\cdot 10^{-2}$ m^{-1}]; see also [77Kaw].

Spin Hamiltonian parameters:

$\lvert g_1 \rvert = 1.976$	$\lvert A_1 \rvert = 68.2$
$\lvert g_2 \rvert = 1.982$	$\lvert A_2 \rvert = 73.7$
$\lvert g_3 \rvert = 1.930$	$\lvert A_3 \rvert = 180.2$

Direction cosines:

For **g**	*a*	*b*	*c*
1′	0.976	−0.212	−0.046
2′	0.172	0.887	−0.428
3′	0.132	0.410	0.902
For A	*a*	*b*	*c*
1	0.813	−0.570	0.117
2	0.561	0.714	−0.419
3	0.156	0.406	0.900

Table 39A-1-022. $(NH_4)_2SO_4$. ESR of V–O [75Pan]. Spin Hamiltonian parameters and direction cosines at 25 °C for site II. For explanations, see Table 39A-1-021.

Spin Hamiltonian parameters:

$\lvert g_1 \rvert = 1.981$	$\lvert A_1 \rvert = 67.4$
$\lvert g_2 \rvert = 1.934$	$\lvert A_2 \rvert = 178.9$
$\lvert g_3 \rvert = 1.979$	$\lvert A_3 \rvert = 72.5$

Direction cosines:

For **g**	*a*	*b*	*c*
1′	0.797	−0.384	0.466
2′	0.338	0.923	0.182
3′	−0.500	0.012	0.866
For A	*a*	*b*	*c*
1	0.807	−0.141	−0.574
2	0.300	0.934	0.192
3	0.509	−0.327	0.796

Table 39A-1-023. $(NH_4)_2SO_4$. ESR of V–O [75Pan]. Spin Hamiltonian parameters and direction cosines at 25 °C for site III. For explanations, see Table 39A-1-021.

Spin Hamiltonian parameters:

$\|g_{1'}\| = 1.984$	$\|A_1\| = 69.3$
$\|g_{2'}\| = 1.978$	$\|A_2\| = 70.5$
$\|g_{3'}\| = 1.928$	$\|A_3\| = 180.2$

Direction cosines:

For **g** or **A**	*a*	*b*	*c*
1′ or 1	0.000	1.000	0.000
2′ or 2	−0.647	0.000	0.763
3′ or 3	0.763	0.000	0.647

Table 39A-1-024. $(NH_4)_2SO_4$. ESR of Cu^{2+} [77Man]. Spin Hamiltonian parameters and direction cosines of the principal axes (*x*, *y*, *z*), relative to the crystalline axes (*a*, *b*, *c*). See also [68Cha].

Direction cosines:

	x	*y*	*z*
a	0.2940	0.1101	0.9241
b	0.3007	0.9272	0.1435
c	0.9463	0.1732	0.9255

Spin Hamiltonian parameters:

T	g_x	g_y	g_z	A_x	A_y	A_z
K				$\cdot 10^{-2}\,m^{-1}$		
300	2.2890 (20)	2.2821 (20)	2.0446 (20)	79.3 (9)	56.27 (90)	189.09 (80)
77	2.2519 (20)	2.2779 (20)	2.0253 (20)	85.03 (9)	57.74 (90)	168.57 (90)