Table 42A-1-001. $(NH_4)_3H(SO_4)_2$. Structure of phase II [78Suz]. Fractional coordinates of non-hydrogen atoms. T = RT.

	x	y	z
N (1)	0.7500	0.2692 (4)	0
N (2)	0.6528 (2)	0.7240 (3)	0.1988 (1)
S	0.4615 (1)	0.2181 (1)	0.1142 (1)
O (1)	0.3983 (2)	0.0268 (3)	0.1495 (1)
O (2)	0.4427 (2)	0.1845 (3)	0.0148 (1)
O (3)	0.6054 (1)	0.2225 (3)	0.1504 (1)
O (4)	0.3985 (2)	0.4330 (3)	0.1284 (1)

Table 42A-1-002. $(NH_4)_3H(SO_4)_2$. Structure of phase II [78Suz]. Fractional coordinates of hydrogens. T = RT.

	x	y	z	Bonded to
H (1)	0.311 (3)	0.655 (7)	0.022 (3)	N (1)
H (2)	0.226 (4)	0.797 (7)	0.046 (3)	N (1)
H (3)	0.723 (4)	0.708 (7)	0.172 (3)	N (2)
H (4)	0.660 (5)	0.720 (8)	0.258 (4)	N (2)
H (5)	0.597 (5)	0.626 (9)	0.150 (3)	N (2)
H (6)	0.617 (5)	0.860 (9)	0.163 (3)	N (2)
H (7)	0	0	0	O (2)

Table 42A-1-003. $(ND_4)_3D(SO_4)_2$. Structure of phase II [81Tan]. Fractional coordinates of non-deuterium atoms and isotropic temperature parameters. T = 287 K. B is defined by Eq. (e) in Introduction.

	x	y	z	B [Å^2]
N(1)	0.7500	0.2687(3)	0	2.22(7)
N(2)	0.6527(1)	0.7252(2)	0.1989(1)	2.73(6)
S	0.4613(0)	0.2190(1)	0.1142(0)	1.89(1)
O(1)	0.3978(1)	0.0272(2)	0.1491(1)	4.56(7)
O(2)	0.4422(1)	0.1863(2)	0.0142(1)	2.78(6)
O(3)	0.6056(1)	0.2237(2)	0.1503(1)	2.61(6)
O(4)	0.3982(1)	0.4340(2)	0.1289(1)	3.13(6)

Table 42A-1-004. $(ND_4)_3D(SO_4)_2$. Structure of phase II [81Tan]. Fractional coordinates of deuteriums and isotropic temperature parameters. T = 287 K. B is defined by Eq. (e) in Introduction.

	x	y	z	B [Å^2]
D(1)	0.304(3)	0.665(5)	0.025(2)	4.5(7)
D(2)	0.231(3)	0.785(4)	0.036(2)	4.3(7)
D(3)	0.721(4)	0.717(4)	0.186(2)	4.4(6)
D(4)	0.663(3)	0.702(5)	0.252(3)	4.6(7)
D(5)	0.610(3)	0.640(5)	0.178(2)	4.1(6)
D(6)	0.621(3)	0.840(5)	0.191(2)	3.6(6)
D(7)	0.029(4)	0.076(7)	−0.007(3)	1.8(8)

Table 42A-1-005. $(ND_4)_3D(SO_4)_2$. Deuterium bond distances and angles in phase II [81Tan]. $T = 287$ K.

N–D···O	∢ N–D···O [°]	N···O [Å]	D···O [Å]
N(1β)–D(1)···O(4)	156(3)	2.831(2)	2.16(3)
N(1)–D(2)···O(3)	149(3)	2.996(2)	2.38(3)
N(2)–D(3)···O(1)	139(2)	3.111(2)	2.50(3)
N(2)–D(3)···O(4)	160(2)	3.059(2)	2.33(4)
N(2)–D(4)···O(1)	143(3)	2.903(2)	2.21(4)
N(2)–D(4)···O(3)	120(3)	3.012(1)	2.52(3)
N(2)–D(5)···O(4)	158(3)	3.100(2)	2.45(3)
N(2)–D(5)···O(3)	141(3)	3.046(2)	2.48(3)
N(2)–D(6)···O(1)	141(3)	3.100(2)	2.48(3)
N(2)–D(6)···O(3)	157(3)	3.029(2)	2.33(3)

Table 42A-1-006. $(ND_4)_3D(SO_4)_2$. Structure of phase III′ [86Tan]. Fractional coordinates of atoms and isotropic temperature parameters. $T = 189(7)$ K. B is defined by Eq. (e) in Introduction.

	x [$\cdot 10^{-4}$]	y [$\cdot 10^{-4}$]	z [$\cdot 10^{-4}$]	B [Å^2]
S(1)	2872(1)	2836 †	3890(1)	1.3
S(2)	2121(1)	2154(1)	1110(1)	1.4
S(3)	2900(1)	−2230(3)	−1159(1)	1.4
S(4)	2109(1)	−2820(3)	−3834(1)	1.4
O(5)	3560(2)	1926(7)	1517(2)	1.9
O(6)	3363(3)	−119(7)	−1535(2)	2.0
O(7)	1303(3)	−785(6)	−3688(2)	2.1
O(8)	3673(3)	−4196(7)	−1307(2)	2.1
O(9)	3691(3)	4568(7)	3534(2)	1.8
O(10)	3558(2)	−2419(7)	−3514(2)	1.9
O(11)	1646(3)	−4900(7)	−3488(2)	1.9
O(12)	1301(3)	427(7)	1420(2)	2.0
O(13)	1428(2)	3139(8)	3495(2)	2.0
O(14)	1448(2)	−2535(7)	−1475(2)	1.9
O(15)	3359(3)	521(6)	3737(2)	1.7
O(16)	1675(3)	4476(7)	1242(2)	2.3
O(17)	1939(3)	1797(8)	137(2)	2.3
O(18)	3126(3)	−1879(8)	−159(2)	2.5
O(19)	2996(3)	3185(7)	4870(2)	2.4
O(20)	1872(3)	−3088(7)	−4838(2)	2.2
N(21)	4057(4)	2304(7)	−3005(3)	1.8
N(22)	1007(4)	−2150(9)	2991(3)	1.7
N(23)	933(3)	−7252(9)	−1990(3)	1.8
N(24)	3978(4)	7232(9)	2017(3)	1.9
N(11)	5000	−2239(11)	5000	1.7
N(12)	5000	2770(11)	0	1.5
N(13)	0	7339(12)	0	1.6
N(14)	0	2394(12)	5000	2.0

† Fixed to define the origin.

Table 42A-1-007. $(ND_4)_3D(SO_4)_2$. Interatomic distances [Å] and bond angles in deuterium bonds [86Tan]. (a) Phase III′. T = 189(7) K. (b) Phase VI. T = 233(7) K.

(a) Phase (III′)			
O(19)–O(20)	2.536(6)	O(17)–O(18)	2.544(6)
O(19)–D(54)	1.27(5)	O(18)–D(52)	0.74(5)
O(20)···D(54)	1.28(5)	O(17)···D(52)	1.84(5)
O(19)–D(54)···O(20)	169(4)°	O(18)–D(52)···O(17)	159(5)°
(b) Phase (VI)			
O(9)–O(18)	2.563(8)	O(12)–O(13)	2.564(8)
O(9)–D(54)	0.62(8)	O(12)–D(55)	0.87(7)
O(18)···D(54)	2.04(8)	O(13)···D(55)	1.70(7)
O(9)–D(54)···O(18)	145(9)°	O(12)–D(55)···O(13)	174(6)°
O(11)–O(35)	2.528(8)	O(16)–O(19)	2.547(8)
O(35)–D(53)	1.02(6)	O(16)–D(56)	0.81(7)
O(11)···D(53)	1.51(6)	O(19)···D(56)	1.74(7)
O(35)–D(53)···O(11)	174(6)°	O(16)–D(56)···O(19)	171(6)°

Table 42A-1-008. $(ND_4)_3D(SO_4)_2$. Structure of phase VI [86Tan]. Fractional coordinates of atoms and isotropic temperature parameters. $T = 233(7)$ K. B is defined by Eq. (e) in Introduction.

	$x[\cdot 10^{-4}]$	$y[\cdot 10^{-4}]$	$z[\cdot 10^{-4}]$	B[Å^2]
S(1)	367†	7189†	3862†	1.4
S(2)	381(2)	12181(3)	−1105(1)	1.7
S(3)	−377(2)	2831(3)	6136(1)	1.5
S(4)	5385(2)	7772(3)	−1144(1)	1.5
S(5)	4597(2)	7178(3)	6173(1)	1.8
S(6)	−4633(2)	2830(3)	3902(1)	1.7
S(7)	4608(2)	12172(3)	1141(1)	1.5
S(8)	9578(1)	7789(2)	1178(1)	1.9
O(9)	639(5)	6909(10)	4857(3)	2.6
O(10)	1146(5)	10320(8)	−1419(3)	2.2
O(11)	559(6)	11817(10)	−131(3)	2.9
O(12)	−4440(5)	3067(9)	4870(3)	2.5
O(13)	4398(5)	6794(9)	5171(3)	2.6
O(14)	5876(6)	9827(9)	−1496(3)	2.7
O(15)	845(5)	5044(7)	3485(3)	1.9
O(16)	5625(6)	8009(10)	−141(3)	2.8
O(17)	−1054(5)	7470(9)	3540(3)	2.5
O(18)	−525(6)	3166(10)	5136(3)	2.7
O(19)	4474(6)	11733(10)	137(3)	2.9
O(20)	852(5)	14453(8)	−1251(3)	2.2
O(21)	1118(6)	9245(9)	3701(3)	2.8
O(22)	3809(5)	10394(8)	1465(3)	2.2
O(23)	6155(5)	5734(7)	−1307(3)	2.1
O(24)	11050(5)	7453(9)	1509(3)	2.3
O(25)	−1079(4)	11922(9)	−1498(3)	2.3
O(26)	6050(4)	7429(9)	6521(3)	2.3
O(27)	−898(6)	533(8)	6279(4)	3.0
O(28)	4110(5)	5113(8)	6541(3)	2.4
O(29)	3838(6)	9178(10)	6301(4)	3.1
O(30)	3948(5)	7410(9)	−1450(3)	2.4
O(31)	−3857(6)	4575(8)	3555(3)	2.7
O(32)	−4131(5)	521(7)	3721(3)	2.1
O(33)	4127(6)	14443(9)	1242(3)	2.9
O(34)	9069(6)	9743(8)	1517(4)	2.9
O(35)	9416(6)	8140(10)	168(3)	2.8
O(36)	−6057(5)	3057(9)	3530(3)	2.4
O(37)	8809(5)	5796(8)	1315(4)	2.3
O(38)	−1186(5)	4506(8)	6489(3)	2.5
O(39)	6058(4)	11966(9)	1550(3)	2.3
O(40)	1046(5)	3014(8)	6522(3)	2.4
N(41)	−1564(5)	2277(10)	3035(4)	2.2
N(42)	−1527(6)	7236(10)	−11982(4)	2.0
N(43)	−2495(6)	12671(10)	6(4)	1.9
N(44)	2503(7)	2304(11)	5002(4)	2.2
N(45)	−3444(7)	12234(11)	−2995(5)	2.6
N(46)	6475(7)	7163(12)	2023(4)	2.4
N(47)	2522(6)	7288(10)	7(4)	2.1
N(48)	11536(7)	12736(11)	2009(4)	2.3
N(49)	−6519(6)	17768(10)	−6981(4)	2.1
N(50)	3448(5)	12693(10)	−1968(3)	1.8
N(51)	1470(7)	7819(11)	7025(5)	2.6
N(52)	−2479(6)	7712(11)	5009(4)	1.9

† Fixed to define the origin.

Table 42A-1-009. $(NH_4)_3H(SO_4)_2$. Transition heats and transition entropies.

Transition	ΔQ_m [J mol^{-1}]	ΔS_m [J K^{-1} mol^{-1}]	Ref.
I–II	4290(340)	10.5(8)	79Suz1
II–III	2120(80)	8.9(3)	
III–IV	265(16)	2.1(1)	
IV–V	301(16)	2.2(1)	
V–VII	444	5.5	88Kam1

Table 42A-1-010. $(NH_4)_3H(SO_4)_2$. Frequencies of phonon modes, A_g and B_g [cm^{-1}], with relative intensities [88Raj]. vs: very strong, s: strong, m: medium, br: broad, w: weak, vw: very weak, sh: shoulder.

A_g				B_g	
c(*aa*)*b*	*c*(*bb*)*a*	*b*(*cc*)*a*	*b*(*ab*)*c*	*c*(*ac*)*b*	*c*(*bc*)*a*
72 w	76 s	76 s	72 s	72 s	72 s
122 w			122 w	122 w	122 w
145 w	145 w	145 w	145 w	145 w	145 w
				164 w	164 m
183 m	183 s	183 s	183 m	185 s	185 s
219 m			211 m	211 m	
260 m	260 w	260 m	258 m	263 m	263 w
		300 mbr	330 mbr		
357 wbr	357 wbr	357 wbr	357 wbr	357 wbr	357 wbr
376 w	376 wbr		376 w	376 w	380 w
413 m	411 vw	411 vw	407 wbr	420 w	424 w
452 vs	452 vs	452 vs	452 vs	456 vs	456 vs
480 w	480 w		480 m	480 w	480 w
496 m	496 m	499 w	496 m	499 m	499 w
532 m	532 m	531 w	532 m	541 m	539 m
616 vs	616 vs	616 vs	616 vs	616 vs	619 vs
627 sh	627 sh	627 sh	627 sh	631 sh	631 sh
669 m	669 m	669 w	669 m	669 m	669 w
691 w			693 w	688 w	688 w
709 m	709 w	710 w	709 w	756 w	754 w
	745 w				
828 m	828 m	828 m	822 w	824 w	822 m
846 wbr	855 wbr	855 wbr	846 wbr	856 m	855 m
966 sh			966 sh	961 w	961 w
978 vs	978 vs	978 vs	978 vs	970 vs	978 vs
				1025 wbr	1025 m
1046 m	1046 m	1046 w	1046 w	1046 m	1046 w
1070 mbr	1070 s	1070 s	1070 m	1070 w	1070 w
1108 s	1103 w	1103 s	1108 m	1108 s	1108 s
1126 vs	1126 w	1126 m	1126 m	1126 m	1126 w
1162 m	1162 m	1162 w	1162 w	1162 m	1162 w
1250 w	1250 w	1250 vw	1250 m	1250 wbr	1250 m
	1300 vw		1295 w	1290 w	1300 wbr
1421 sbr	1419 sbr	1419 sbr	1421 sbr	1421 mbr	1421 sbr
1449 w	1449 w	1446 mbr	1449 sbr	1450 wbr	1454 wbr
1538 w			1551 sbr	1562 mbr	1559 wbr
1623 wbr	1626 wbr	1626 wbr	1626 wbr	1626 wbr	1626 wbr
1680 mbr	1680 mbr			1682 wbr	
1722 m	1722 w	1722 w	1722 mbr		1695 mbr
1763 vw	1763 w	1763 w	1764 wbr	1760 w	
1782 w	1785 wbr	1785 wbr	1785 mbr		
2030 w	2029 w	2023 wbr		2030 w	2029 w
	2047 w	2045 w			
2063 w	2065 wbr	2063 wbr	2065 wbr	2065 w	2065 w
2859 m	2859 mbr	2859 mbr	2859 mbr	2859 mbr	2859 mbr
				2896 w	2904 w
2986 m	2986 m	2986 mbr	2986 m	2986 wbr	2986 wbr
3010 wbr		3011 w		3007 wbr	3013 w
			3115 mbr	3109 w	3110 vw
3132 mbr	3132 mbr	3132 sbr	3132 mbr	3144 wbr	3132 w
3176 mbr	3176 w	3176 m	3176 m	3183 mbr	3176 wbr

Table 42A-1-011. $(NH_4)_3H(SO_4)_2$. ΔU and A [95Sin]. Electrical conductivity σ is given by $\sigma T = A \exp(-\Delta U/kT)$.

Phase	$E \parallel a$		$E \parallel c$	
	ΔU [eV]	A [Ω^{-1} m^{-1} K]	ΔU [eV]	A [Ω^{-1} m^{-1} K]
I	0.10(4)	$3(1) \cdot 10^3$	0.48(5)	$1.3(5) \cdot 10^7$
II	1.00(4)	$1.17(50) \cdot 10^{14}$	1.03(5)	$1.1(5) \cdot 10^{13}$

Table 42A-1-012. $(NH_4)_3H(SO_4)_2$. ^{51}V hyperfine tensors in VO^{2+} ESR spectra at different temperatures [83Fuj]. Direction cosines are given with respect to $x \parallel a$, $y \parallel b$, $z \perp (001)$. Two specta $(VO^{2+})_1$ and $(VO^{2+})_2$ are unresolved at 100 °C.

	$(VO^{2+})_1$		$(VO^{2+})_2$	
T [°C]	Principal values [$\cdot 10^2$ Am^{-1}]	Direction cosines	Principal values [$\cdot 10^2$ Am^{-1}]	Direction cosines
31.5	186.2(4)	$-0.472, \pm 0.811, 0.346$	186.2(4)	$-0.483, \pm 0.802, 0.351$
	69.2(4)	$-0.880, \mp 0.549, -0.123$	68.4(4)	$-0.860, \mp 0.357, -0.366$
	66.8(4)	$0.058, \mp 0.363, 0.930$	66.0(4)	$-0.168, \mp 0.487, 0.862$
49.5	186.2(4)	$-0.472, \pm 0.812, 0.345$	186.2(4)	$-0.480, \pm 0.805, 0.349$
	69.2(4)	$-0.880, \mp 0.406, -0.247$	68.4(4)	$-0.870, \mp 0.384, -0.310$
	66.8(4)	$-0.061, \mp 0.420, 0.906$	66.0(4)	$-0.115, \mp 0.452, 0.885$
63.0	186.2(4)	$-0.471, \pm 0.813, 0.342$	186.2(4)	$-0.476, \pm 0.849, 0.348$
	69.2(4)	$-0.877, \mp 0.391, -0.280$	68.4(4)	$-0.849, \mp 0.318, -0.422$
	66.8(4)	$-0.094, \mp 0.432, 0.897$	66.0(4)	$-0.230, \mp 0.497, 0.837$
100.0	186.2(4)	$-0.473, \pm 0.816, 0.332$		
	68.4(4)	$-0.881, \mp 0.452, -0.144$		
	66.8(4)	$0.034, \mp 0.360, 0.932$		

Table 42A-1-013. $(NH_4)_3H(SO_4)_2$. Spin Hamiltonian parameters for Cu^{2+} and Mn^{2+} centers [85Bab]. T = RT.

Cu^{2+}				Mn^{2+}				
$g_\parallel$	$g_\perp$	$\lvert A_\parallel \rvert$ [m^{-1}]	$\lvert A_\perp \rvert$ [m^{-1}]	g	$\lvert D \rvert$ [m^{-1}]	$\lvert E \rvert$ [m^{-1}]	$\lvert a \rvert$ [m^{-1}]	A [m^{-1}]
2.320(2)	2.080(2)	1.04(2)	0.19(2)	2.004(2)	4.24(2)	0.55(2)	0.15(3)	−0.86(2)