Table 46A-9-001. $(CH_3)_2NH_2Ga(SO_4)_2 \cdot 6H_2O$. Fractional coordinates and mean square displacements in phase I [93Pie]. T = 295 K. $\overline{u^2}$ is estimated by one third of the trace of the orthogonalized U_{ij} tensor. U_{ij} is defined by Eq. (d) in Introduction. OCP: occupancy parameter.

Atom	x	y	z	OCP	$\overline{u^2}$ [Å^2]
S	0.0694(1)	0.1829(1)	0.2397(1)		0.028
Ga	0.5	0	0		0.022
O(11)	0.2880(4)	0.0780(2)	–0.1268(2)		0.036
O(12)	0.7396(3)	0.0663(2)	–0.0639(2)		0.028
O(13)	0.5070(3)	0.1548(2)	0.0895(2)		0.036
O(21)	0.0595(3)	0.0475(2)	0.2197(2)		0.037
O(22)	–0.1476(3)	0.2326(2)	0.2352(2)		0.042
O(23)	0.1991(4)	0.2073(2)	0.3578(2)		0.049
O(24)	0.1629(4)	0.2433(2)	0.1471(3)		0.052
C(l)	0.3599(8)	–0.0243(5)	0.5586(5)		0.077
N(1)	0.4376(14)	–0.0137(7)	0.4556(7)	0.38	0.051
N(2)	0.5329(26)	–0.0628(19)	0.4931(18)	0.12	0.039
H(11)	0.313(3)	0.146(3)	–0.171(2)		0.064
H(12)	0.184(3)	0.047(3)	–0.160(2)		0.036
H(21)	0.780(3)	0.023(3)	–0.126(2)		0.054
H(22)	0.732(3)	0.129(3)	–0.088(2)		0.051
H(31)	0.396(3)	0.186(3)	0.103(2)		0.051
H(32)	0.621(3)	0.179(3)	0.136(2)		0.051

Table 46A-9-002. $(CH_3)_2NH_2Ga(SO_4)_2 \cdot 6H_2O$. Hydrogen bond distances and angles in phase I [93Pie]. T = 295 K. Hydrogen bonds are those between oxygens O^{Al} in water molecules coordinated by Al^{3+} ions and oxygen atoms O^S in sulphate ions.

Bond	Distance [Å]			Angle [°]
O^{Ga}–H...O^S	O^{Ga}–O^S	O^{Al}–H	H...O^S	O^{Ga}–H...O^S
O(11)–H(11)...O(22)	2.645(3)	0.92(3)	1.73(3)	175(2)
O(11)–H(12)...O(21)	2.636(3)	0.77(2)	1.87(2)	170(3)
O(12)–H(21)...O(21)	2.668(3)	0.92(3)	1.78(3)	162(2)
O(12)–H(22)...O(23)	2.582(3)	0.72(3)	1.86(3)	176(3)
O(13)–H(31)...O(24)	2.584(4)	0.82(2)	1.77(2)	174(3)
O(13)–H(32)...O(22)	2.629(3)	0.85(2)	1.77(2)	178(3)

Table 46A-9-003. $(CH_3)_2NH_2Ga(SO_4)_2 \cdot 6H_2O$. Fractional coordinates and mean square displacements in phase II [95Pie]. T = 125 K. $\overline{u^2}$ is estimated by one third of the trace of the orthogonalized U_{ij} tensor. U_{ij} is defined by Eq. (d) in Introduction.

Atom	x	y	z	$\overline{u^2}$
	[10^{-4}]			[10^{-3} Å^2]
Ga	5000	2517(1)	0	11(1)
S(1)	5659(2)	5702(1)	7401(1)	15(1)
S(2)	4358(2)	9338(1)	2629(1)	14(1)
O(1)	2938(6)	3310(3)	–1229(3)	21(1)
O(2)	7136(6)	1731(3)	1259(4)	18(1)
O(3)	7368(5)	3190(3)	–649(3)	17(1)
O(4)	2621(6)	1818(3)	631(3)	15(1)
O(5)	5047(6)	4089(3)	920(3)	17(1)
O(6)	4959(5)	991(4)	–894(4)	22(1)
O(11)	5555(5)	7081(3)	7135(3)	19(1)
O(12)	6878(6)	5488(3)	8575(4)	22(1)
O(13)	3443(5)	5201(3)	7366(4)	22(1)
O(14)	6541(6)	5097(3)	6444(4)	24(1)
O(21)	4452(6)	7983(4)	2829(3)	17(1)
O(22)	3026(7)	9575(4)	1422(4)	27(1)
O(23)	6471(6)	9822(4)	2653(4)	23(1)
O(24)	3314(7)	9998(4)	3511(4)	23(1)
C(1)	3744(10)	2246(7)	5693(6)	39(2)
C(2)	6462(11)	2750(5)	4455(7)	33(2)
N	4236(7)	2382(4)	4526(4)	25(1)
H(1)	2749(57)	2035(53)	6183(43)	
H(2)	4527(101)	2945(51)	5943(91)	
H(3)	4805(72)	1616(54)	5915(81)	
H(4)	6703(107)	3476(33)	4806(49)	
H(5)	7429(79)	2160(42)	4905(45)	
H(6)	6299(84)	2262(39)	3820(31)	
H(7)	3285(90)	3165(49)	3893(50)	
H(8)	3317(88)	1508(46)	4492(59)	
H(11)	1845(84)	2808(71)	–1311(15)	
H(12)	2963(69)	4055(30)	–1574(37)	
H(21)	8227(54)	2120(39)	1633(39)	
H(22)	6463(73)	1643(61)	1850(37)	
H(31)	7790(65)	2737(37)	–1233(32)	
H(32)	6993(129)	3974(38)	–828(79)	
H(41)	1523(56)	2106(50)	810(49)	
H(42)	2592(79)	1080(30)	914(42)	
H(51)	3813(69)	4447(80)	924(105)	
H(52)	6073(81)	4525(59)	1357(62)	
H(61)	5990(52)	759(43)	–1223(38)	
H(62)	3783(60)	987(56)	–1398(44)	

Table 46A-9-004. $(CH_3)_2NH_2Ga(SO_4)_2 \cdot 6H_2O$. Bond distances and bond angles in phases II and III [95Pie].

Phase II, T = 125 K		Phase III, T = 100 K	
Distance [Å]			
Ga–O(6)	1.916(4)	Ga–O(5)	1.925(4)
Ga–O(1)	1.940(3)	Ga–O(3)	1.941(4)
Ga–O(3)	1.942(4)	Ga–O(1)	1.944(4)
Ga–O(4)	1.948(4)	Ga–O(6)	1.961(3)
Ga–O(5)	1.973(3)	Ga–O(2)	1.967(3)
Ga–O(2)	1.984(4)	Ga–O(4)	1.967(4)
S(1)–O(12)	1.442(4)	S(1)–O(12)	1.447(4)
S(1)–O(14)	1.465(4)	S(1)–O(14)	1.468(4)
S(1)–O(11)	1.499(3)	S(1)–O(11)	1.473(3)
S(1)–O(13)	1.512(3)	S(1)–O(13)	1.479(3)
S(2)–O(23)	1.445(5)	S(2)–O(24)	1.461(5)
S(2)–O(21)	1.462(4)	S(2)–O(23)	1.499(4)
S(2)–O(24)	1.481(5)	S(2)–O(23)	1.499(4)
S(2)–O(22)	1.505(4)	S(2)–O(21)	1.519(4)
O(11)–O(14)	2.381(5)	O(11)–O(12)	2.380(5)
O(11)–O(12)	2.407(5)	O(11)–O(13)	2.393(4)
O(11)–O(13)	2.458(5)	O(11)–O(14)	2.406(5)
O(12)–O(13)	2.400(5)	O(12)–O(14)	2.406(5)
O(12)–O(14)	2.436(6)	O(12)–O(13)	2.419(4)
O(13)–O(14)	2.411(5)	O(13)–O(14)	2.366(5)
O(21)–O(23)	2.377(6)	O(21)–O(24)	2.415(5)
O(21)–O(22)	2.401(6)	O(21)–O(22)	2.417(5)
O(21)–O(24)	2.439(6)	O(21)–O(23)	2.469(5)
O(22)–O(24)	2.397(6)	O(22)–O(23)	2.402(5)
O(22)–O(23)	2.410(6)	O(22)–O(24)	2.438(6)
O(23)–O(24)	2.407(6)	O(23)–O(24)	2.455(5)
N–C(1)	1.429(8)	N–C(1)	1.460(6)
N–C(2)	1.496(9)	N–C(2)	1.512(6)
Angle [°]			
C(1)–N–C(2)	116.7(5)	C(1)–N–C(2)	114.8(3)

Table 46A-9-005. $(CH_3)_2NH_2Ga(SO_4)_2 \cdot 6H_2O$. Hydrogen bond distances and angles in phase II [95Pie]. T = 125 K.

Bond	Distance [Å]			Angles [°]
D–H...*A*	*D*–*A*	*D*–H	H...*A*	*D*–H...*A*
N–H(7)...O(12)	2.834(6)	1.20(5)	1.70(5)	156(5)
N–H(8)...O(24)	2.811(6)	1.00(4)	1.81(4)	170(4)
O(1)–H(11)...O(21)	2.682(5)	0.87(4)	1.87(8)	154(10)
O(1)–H(12)...O(13)	2.630(5)	0.89(3)	1.78(4)	159(4)
O(2)–H(21)...O(11)	2.574(5)	0.86(3)	1.73(3)	170(5)
O(2)–H(22)...O(23)	2.662(6)	0.87(4)	2.15(4)	118(5)
O(3)–H(31)...O(21)	2.680(5)	0.90(3)	1.81(3)	162(4)
O(3)–H(32)...O(12)	2.604(5)	0.88(4)	1.75(5)	163(9)
O(4)–H(41)...O(11)	2.624(5)	0.83(4)	1.94(5)	140(5)
O(4)–H(42)...O(22)	2.551(6)	0.85(4)	1.71(3)	169(5)
O(5)–H(51)...O(14)	2.578(5)	0.88(4)	1.74(6)	159(10)
O(5)–H(52)...O(13)	2.598(5)	0.88(4)	1.76(4)	158(4)
O(6)–H(61)...O(24)	2.593(6)	0.85(3)	1.77(5)	162(4)
O(6)–H(62)...O(23)	2.678(5)	0.86(3)	1.88(4)	153(6)

Table 46A-9-006. $(CH_3)_2NH_2Ga(SO_4)_2 \cdot 6H_2O$. Fractional coordinates and mean square displacements in phase III [95Pie]. T = 100 K. $\overline{u^2}$ is estimated by one third of the trace of the orthogonalized U_{ij} tensor. U_{ij} is defined by Eq (d) in Introduction. Unit cell is chosen with 2_1 axis at 1/4, y, 1/4.

Atom	x	y	z	$\overline{u^2}$
	[10^{-4}]			[10^{-3} Å^2]
Ga	4997(2)	0	0(1)	9(1)
S(1)	5866(2)	3218(1)	7505(1)	11(1)
S(2)	4116(2)	6794(1)	2487(1)	11(1)
O(1)	2928(6)	703(3)	–1425(4)	24(1)
O(2)	7108(5)	–715(3)	1433(3)	11(1)
O(3)	7509(5)	602(3)	–573(3)	12(1)
O(4)	2464(5)	–629(3)	582(3)	13(1)
O(5)	5045(5)	1560(3)	820(3)	19(1)
O(6)	4959(5)	–1580(3)	–851(3)	10(1)
O(11)	5810(5)	4564(3)	7368(3)	11(1)
O(12)	7377(6)	2896(3)	8667(4)	24(1)
O(13)	3598(5)	2786(3)	7460(3)	12(1)
O(14)	6530(6)	2653(3)	6452(3)	21(1)
O(21)	4038(6)	5408(3)	2617(3)	17(1)
O(22)	2578(6)	7124(3)	1294(4)	17(1)
O(23)	6386(6)	7184(3)	2412(4)	19(1)
O(24)	3463(6)	7349(4)	3542(4)	22(1)
C(1)	3717(6)	9(5)	5716(4)	20(1)
C(2)	6638(8)	447(4)	4574(4)	21(1)
N	4585(6)	–263(3)	4637(3)	17(1)
H(1)	4544(117)	–473(57)	6371(42)	
H(2)	3895(154)	839(31)	5893(69)	
H(3)	2249(50)	–289(49)	5485(47)	
H(4)	6297(71)	1263(27)	4645(41)	
H(5)	7758(71)	308(43)	5354(32)	
H(6)	6915(75)	–5(39)	3959(32)	
H(7)	3240(100)	368(55)	3784(53)	
H(8)	4813(155)	–1437(48)	4609(91)	
H(11)	2082(72)	674(67)	–912(43)	
H(12)	3213(66)	1362(29)	–1677(38)	
H(21)	8272(53)	–287(34)	1734(38)	
H(22)	6298(97)	–277(74)	1816(74)	
H(31)	7894(65)	241(35)	–1208(30)	
H(32)	8279(92)	1260(42)	–592(80)	
H(41)	2960(353)	–206(88)	1249(68)	
H(42)	2430(77)	–1384(27)	777(41)	
H(51)	3755(55)	1482(61)	807(64)	
H(52)	6172(69)	2048(46)	1074(61)	
H(61)	6078(52)	–1872(40)	–1015(40)	
H(62)	3779(55)	–1629(43)	–1333(37)	

Table 46A-9-007. $(CH_3)_2NH_2Ga(SO_4)_2 \cdot 6H_2O$. Hydrogen bond distances and angles in phase III [95Pie]. T = 100 K.

	Distance [Å]			Angle [°]
D–H...*A*	*D*–*A*	*D*–H	H...*A*	*D*–H...*A*
N–H(7)...O(21)	3.032(5)	1.30(5)	1.84(5)	150(5)
N–H(7)...O(22)	2.996(5)	1.30(5)	1.98(6)	131(4)
N–H(8)...O(24)	2.886(5)	1.29(5)	1.84(8)	134(6)
N–H(8)...O(12)	3.074(5)	1.29(5)	2.38(9)	110(5)
O(1)–H(11)...O(11)	2.626(5)	0.87(4)	2.44(6)	93(4)
O(1)–H(11)...O(4)	2.734(5)	0.87(4)	2.15(6)	144(5)
O(1)–H(12)...O(13)	2.665(5)	0.81(3)	1.87(3)	170(4)
O(2)–H(21)...O(21)	2.677(5)	0.86(3)	1.82(5)	172(4)
O(2)–H(22)...O(5)	2.799(5)	0.88(5)	2.33(9)	114(7)
O(2)–H(22)...O(4)	2.823(5)	0.88(5)	2.48(7)	104(5)
O(3)–H(31)...O(11)	2.712(5)	0.89(3)	1.83(4)	170(4)
O(3)–H(32)...O(12)	2.632(5)	0.87(4)	1.99(5)	130(5)
O(4)–H(41)...O(21)	2.657(5)	0.86(5)	2.08(19)	123(10)
O(4)–H(41)...O(5)	2.853(5)	0.86(5)	2.43(15)	111(10)
O(4)–H(42)...O(22)	2.567(5)	0.85(3)	1.72(3)	174(4)
O(5)–H(51)...O(24)	2.601(6)	0.81(3)	1.95(6)	137(6)
O(5)–H(52)...O(23)	2.679(5)	0.87(4)	1.99(5)	136(6)
O(6)–H(61)...O(14)	2.576(5)	0.83(3)	1.75(3)	174(5)