**Table 46A-8-001**. $(CH_3)_2NH_2Al(SO_4)_2 \cdot 6H_2O$. Fractional coordinates and mean square displacements [Å$^2$] in phase I [93Pie2]. $T$ = 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 | 0.0657(1) | 0.1826(1) | 0.2381(1) | | 0.035 |
| A(1) | 0.5 | 0 | 0 | | 0.029 |
| O(11) | 0.2939(3) | 0.0754(2) | –0.1215(2) | | 0.038 |
| O(12) | 0.7246(3) | 0.0660(2) | –0.0669(2) | | 0.035 |
| O(13) | 0.5046(3) | 0.1471(2) | 0.0912(2) | | 0.039 |
| O(21) | 0.0538(3) | 0.0469(2) | 0.2165(2) | | 0.043 |
| O(22) | –0.1500(3) | 0.2329(2) | 0.2343(2) | | 0.047 |
| O(23) | 0.1947(4) | 0.2061(3) | 0.3582(3) | | 0.056 |
| O(24) | 0.1615(5) | 0.2430(3) | 0.1437(3) | | 0.057 |
| C(1) | 0.3611(10) | –0.0242(6) | 0.5631(5) | | 0.083 |
| N(1) | 0.4353(13) | –0.0151(7) | 0.4530(7) | 0.40 | 0.049 |
| N(2) | 0.5253(28) | –0.0558(21) | 0.4977(21) | 0.10 | 0.034 |
| H(11) | 0.303(4) | 0.144(3) | –0.160(3) | | 0.069 |
| H(12) | 0.198(4) | 0.037(3) | –0.157(3) | | 0.036 |
| H(21) | 0.787(4) | 0.022(3) | –0.109(3) | | 0.056 |
| H(22) | 0.716(4) | 0.133(3) | –0.082(3) | | 0.041 |
| H(31) | 0.405(4) | 0.197(3) | 0.094(3) | | 0.054 |
| H(32) | 0.614(4) | 0.183(3) | 0.129(3) | | 0.067 |

**Table 46A-8-002**. $(CH_3)_2NH_2Al(SO_4)_2 \cdot 6H_2O$, $(CH_3)_2NH_2Ga(SO_4)_2 \cdot 6H_2O$. Interatomic distances [Å] and angles [°] of non-hydrogen atoms in phase I [93Pie2]. $T$ = 295 K. Primed atoms are related by inversion.

| | $(CH_3)_2NH_2Al(SO_4)_2 \cdot 6H_2O$ | $(CH_3)_2NH_2Ga(SO_4)_2 \cdot 6H_2O$ |
|---|---|---|
| S–O(21) | 1.478(3) | 1.470(2) |
| S–O(22) | 1.477(2) | 1.474(2) |
| S–O(23) | 1.459(3) | 1.461(2) |
| S–O(24) | 1.462(3) | 1.455(3) |
| O(21)–S–O(22) | 109.7(1) | 109.8(1) |
| O(21)–S–O(23) | 108.9(1) | 108.6(1) |
| O(21)–S–O(24) | 109.7(2) | 109.8(2) |
| O(22)–S–O(23) | 109.5(2) | 109.4(1) |
| O(22)–S–O(24) | 109.2(2) | 108.9(2) |
| O(23)–S–O(24) | 109.9(2) | 110.3(2) |
| Al(Ga)–O(11) | 1.892(2) | 1.967(2) |
| Al(Ga)–O(12) | 1.874(2) | 1.945(2) |
| Al(Ga)–O(13) | 1.876(2) | 1.943(2) |
| N(1)–C | 1.395(11) | 1.359(11) |
| N(1)–C′ | 1.413(11) | 1.392(11) |
| N(2)–C | 1.424(23) | 1.500(21) |
| N(2)–C′ | 1.380(23) | 1.355(21) |

**Table 46A-8-003**. $(CH_3)_2NH_2Al(SO_4)_2 \cdot 6H_2O$. Hydrogen bond distances and angles in phase I [93Pie2]. $T$ = 295 K. Hydrogen bonds are those between oxygen atoms $O^{Al}$ in water molecules coordinated by $Al^{3+}$ ions and oxygen atoms $O^S$ in sulphate ions.

| Bond | Distance [Å] | | | Angle [°] |
|---|---|---|---|---|
| $O^{Al}$–H...$O^S$ | $O^{Al}$–$O^S$ | $O^{Al}$–H | H...$O^S$ | $O^{Al}$–H...$O^S$ |
| O(11)–H(11)…O(22) | 2.675(3) | 0.86(3) | 1.83(3) | 167(3) |
| O(11)–H(12)…O(21) | 2.636(3) | 0.78(3) | 1.86(3) | 169(3) |
| O(12)–H(21)…O(21) | 2.667(3) | 0.82(3) | 1.86(3) | 168(3) |
| O(12)–H(22)…O(23) | 2.583(4) | 0.74(3) | 1.85(3) | 172(3) |
| O(13)–H(31)…O(24) | 2.587(4) | 0.84(3) | 1.82(3) | 153(3) |
| O(13)–H(32)…O(22) | 2.645(3) | 0.84(3) | 1.82(3) | 167(3) |

**Table 46A-8-004**. $(CH_3)_2NH_2Al(SO_4)_2 \cdot 6H_2O$. Fractional coordinates and mean square displacements [Å$^2$] in phase II [93Pie1]. $T$ = 95 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 | $x$ | $y$ | $z$ | $\overline{u^2}$ [Å$^2$] |
|---|---|---|---|---|
| S(1) | 0.5626(2) | –0.4282(1) | 0.7441(1) | 0.010(1) |
| S(2) | –0.0609(2) | 0.0650(1) | –0.2303(1) | 0.010(1) |
| Al | 0.5000 | 0.2508(2) | 0.0058(2) | 0.008(1) |
| O(1) | 0.2939(5) | 0.3276(3) | –0.1136(3) | 0.011(1) |
| O(2) | 0.7037(6) | 0.1747(3) | 0.1253(3) | 0.013(1) |
| O(3) | 0.7247(5) | 0.3185(3) | –0.0619(3) | 0.011(1) |
| O(4) | 0.2788(5) | 0.1821(3) | 0.0724(3) | 0.010(1) |
| O(5) | 0.5054(5) | 0.3969(3) | 0.0996(3) | 0.012(1) |
| O(6) | 0.4965(5) | 0.1048(3) | –0.0880(3) | 0.014(1) |
| O(11) | 0.5524(5) | –0.2906(3) | 0.7219(3) | 0.010(1) |
| O(12) | 0.6938(5) | –0.4494(3) | 0.8647(3) | 0.016(1) |
| O(13) | 0.3472(5) | –0.4771(3) | 0.7449(3) | 0.013(1) |
| O(14) | 0.6549(5) | –0.4898(3) | 0.6474(3) | 0.016(1) |
| O(21) | –0.0462(5) | 0.1994(3) | –0.2031(3) | 0.014(1) |
| O(22) | 0.1535(5) | 0.0124(3) | –0.2236(3) | 0.015(1) |
| O(23) | –0.1795(6) | 0.0457(3) | –0.3540(3) | 0.019(1) |
| O(24) | –0.1671(6) | 0.0003(3) | –0.1403(3) | 0.019(1) |
| C(1) | 0.3793(8) | 0.2239(5) | 0.5851(4) | 0.023(1) |
| C(2) | –0.3574(8) | 0.2732(6) | –0.5466(5) | 0.023(1) |
| N | 0.4232(4) | 0.2379(3) | 0.4593(2) | 0.016(1) |
| H(1) | 0.241(8) | 0.185(5) | 0.592(6) | 0.070(19) |
| H(2) | 0.390(9) | 0.309(4) | 0.618(5) | 0.055(16) |
| H(3) | 0.482(6) | 0.157(4) | 0.617(4) | 0.028(11) |
| H(4) | –0.336(9) | 0.354(5) | –0.511(5) | 0.064(17) |
| H(5) | –0.282(7) | 0.205(4) | –0.517(4) | 0.041(13) |
| H(6) | –0.346(8) | 0.271(5) | –0.630(4) | 0.046(15) |
| H(7) | 0.338(6) | 0.295(4) | 0.419(3) | 0.015(9) |
| H(8) | 0.374(7) | 0.156(4) | 0.421(4) | 0.037(12) |
| H(11) | 0.185(6) | 0.291(5) | –0.138(4) | 0.010(12) |
| H(12) | 0.271(10) | 0.395(5) | –0.153(6) | 0.074(22) |
| H(21) | 0.819(9) | 0.207(7) | 0.166(6) | 0.055(23) |
| H(22) | 0.679(6) | 0.120(4) | 0.172(3) | 0.000(8) |
| H(31) | 0.801(6) | 0.268(4) | –0.106(3) | 0.005(10) |
| H(32) | 0.702(12) | 0.391(5) | –0.082(7) | 0.086(26) |
| H(41) | 0.214(11) | 0.209(7) | 0.119(6) | 0.065(24) |
| H(42) | 0.274(6) | 0.112(4) | 0.096(4) | 0.000(9) |
| H(51) | 0.394(7) | 0.426(5) | 0.109(5) | 0.022(16) |
| H(52) | 0.616(7) | 0.438(5) | 0.150(4) | 0.022(14) |
| H(61) | 0.608(9) | 0.069(6) | –0.112(6) | 0.057(22) |
| H(62) | 0.394(7) | 0.088(4) | –0.126(4) | 0.005(11) |

**Table 46A-8-005**. $(CH_3)_2NH_2Al(SO_4)_2 \cdot 6H_2O$. Interatomic distances [Å] in phase II [93Pie1]. $T = 95$ K.

| | |
|---|---|
| S(1)–O(14) | 1.469(3) |
| S(1)–O(12) | 1.476(3) |
| S(1)–O(13) | 1.485(3) |
| S(1)–O(11) | 1.491(3) |
| | |
| S(2)–O(21) | 1.468(3) |
| S(2)–O(23) | 1.471(4) |
| S(2)–O(24) | 1.476(4) |
| S(2)–O(22) | 1.482(4) |
| | |
| Al–O(4) | 1.864(4) |
| Al–O(6) | 1.874(4) |
| Al–O(5) | 1.874(4) |
| Al–O(3) | 1.885(4) |
| Al–O(2) | 1.886(4) |
| Al–O(1) | 1.898(3) |
| | |
| O(11)–O(12) | 2.396(5) |
| O(11)–O(14) | 2.417(4) |
| O(11)–O(13) | 2.430(5) |
| O(12)–O(13) | 2.418(4) |
| O(12)–O(14) | 2.424(5) |
| O(13)–O(14) | 2.418(5) |
| | |
| O(21)–O(23) | 2.401(5) |
| O(21)–O(24) | 2.409(5) |
| O(21)–O(22) | 2.409(5) |
| O(22)–O(23) | 2.405(5) |
| O(22)–O(24) | 2.406(5) |
| O(22)–O(2) | 2.665(5) |
| O(23)–O(24) | 2.411(5) |
| | |
| N–C(1) | 1.480(5) |
| N–C(2) | 1.476(6) |

**Table 46A-8-006**. $(CH_3)_2NH_2Al(SO_4)_2 \cdot 6H_2O$. Hydrogen bond distances and angles in phase II [93Pie1]. $T$ = 95 K.

| Hydrogen bond | Bond length [Å] | | | Bond angle [°] |
|---|---|---|---|---|
| *D*–H…*A* | *D*–*A* | *D*–H | H…*A* | *D*–H…*A* |
| N–H(7)...O(12)$^{ii}$ | 2.806(4) | 0.89(3) | 1.94(4) | 164(3) |
| N–H(8)...O(24)$^{v}$ | 2.798(5) | 1.00(4) | 1.81(4) | 170(4) |
| O(1)–H(11)...O(21) | 2.633(5) | 0.81(4) | 1.83(4) | 174(5) |
| O(1)–H(12)...O(13)$^{i}$ | 2.670(5) | 0.84(5) | 1.90(5) | 153(6) |
| O(2)–H(21)...O(11)$^{iii}$ | 2.631(5) | 0.87(5) | 1.77(5) | 169(7) |
| O(2)–H(22)...O(22)$^{v}$ | 2.665(5) | 0.82(4) | 1.85(4) | 173(4) |
| O(3)–H(31)...O(21)$^{iv}$ | 2.653(5) | 0.93(4) | 1.74(3) | 169(4) |
| O(3)–H(32)...O(12)$^{i}$ | 2.609(5) | 0.82(5) | 1.80(5) | 170(8) |
| O(4)–H(41)...O(11)$^{ii}$ | 2.654(5) | 0.77(5) | 1.89(5) | 174(8) |
| O(4)–H(42)...O(23)$^{v}$ | 2.567(5) | 0.79(4) | 1.79(4) | 168(4) |
| O(5)–H(51)...O(14)$^{ii}$ | 2.603(5) | 0.81(4) | 1.80(4) | 174(6) |
| O(5)–H(52)...O(13)$^{iii}$ | 2.644(5) | 0.94(4) | 1.73(4) | 166(5) |
| O(6)–H(61)...O(24)$^{iv}$ | 2.590(5) | 0.89(5) | 1.70(5) | 174(7) |
| O(6)–H(62)...O(22) | 2.648(5) | 0.74(4) | 1.92(4) | 169(5) |

Symmetry codes: (i) $x, y-1, z+1$; (ii) $x+1/2, -y, z+1/2$; (iii) $x-1/2, y, x+1/2$; (iv) $x-1/2, -y, z-1/2$; (v) $x-1, y, z$.