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# Tetraaquadiglycinemagnesium(II) hexaaquamagnesium(II) bis(sulfate)

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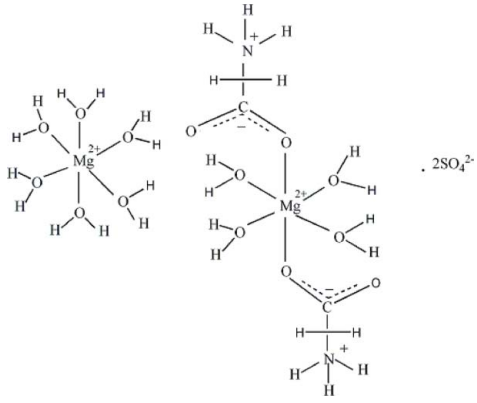
Key indicators: single-crystal X-ray study; $T$ = 293 K; mean $\sigma$(C–C) = 0.004 Å; $R$ factor = 0.066; $wR$ factor = 0.171; data-to-parameter ratio = 9.9.

In the title compound, $[Mg(C_2H_5NO_2)_2(H_2O)_4][Mg(H_2O)_6](SO_4)_2$, the $Mg^{II}$ atoms of both dications lie on inversion centres, and each of them is in an octahedral coordination environment. The glycine molecule exists in the zwitterionic form. The $[Mg(H_2O)_6]^{2+}$ and $[Mg(C_2H_5NO_2)_2(H_2O)_4]^{2+}$ dications pack as alternate layers parallel to the *ab* plane, with the sulfate anions lying between them. The ions are linked to form a three-dimensional network by O—H···O and N—H···O hydrogen bonds.

## Related literature

For related literature, see: Baur (1964); Fleck & Bohatý (2005); Muller *et al.* (1994); Peterková *et al.* (1991).



## Experimental

### Crystal data

$[Mg(C_2H_5NO_2)_2(H_2O)_4][Mg(H_2O)_6](SO_4)_2$
$M_r$ = 571.04
Triclinic, $P\overline{1}$
$a$ = 5.988 (3) Å
$b$ = 6.783 (2) Å
$c$ = 13.391 (2) Å
$\alpha$ = 85.39 (2)°
$\beta$ = 82.87 (2)°
$\gamma$ = 82.88 (2)°
$V$ = 534.4 (3) Å$^3$
$Z$ = 1
Mo $K\alpha$ radiation
$\mu$ = 0.41 mm$^{-1}$
$T$ = 293 (2) K
0.21 × 0.19 × 0.16 mm

### Data collection

Siemens AED diffractometer
Absorption correction: none
1998 measured reflections
1998 independent reflections
1992 reflections with $I > 2\sigma(I)$
1 standard reflection
every 50 reflections
intensity decay: none

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.066
$wR(F^2)$ = 0.171
$S$ = 1.16
1998 reflections
201 parameters
18 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.94 e Å$^{-3}$
$\Delta\rho_{min}$ = −1.07 e Å$^{-3}$

**Table 1**
Selected bond lengths (Å).

| | | | |
|---|---|---|---|
| Mg1—O5 | 2.031 (2) | Mg2—O11 | 2.048 (2) |
| Mg1—O6 | 2.085 (2) | Mg2—O10 | 2.057 (2) |
| Mg1—O7 | 2.128 (2) | Mg2—O9 | 2.105 (2) |

**Table 2**
Hydrogen-bond geometry (Å, °).

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| N1—H1$N$···O7$^{i}$ | 0.87 (3) | 2.08 (5) | 2.939 (4) | 168 (4) |
| N1—H2$N$···O4 | 0.87 (3) | 2.12 (4) | 2.877 (4) | 145 (4) |
| N1—H3$N$···O6 | 0.87 (3) | 2.48 (4) | 3.195 (5) | 140 (5) |
| N1—H3$N$···O8$^{ii}$ | 0.87 (3) | 2.21 (6) | 2.865 (4) | 131 (4) |
| O5—H5$A$···O4$^{iii}$ | 0.84 (1) | 1.92 (3) | 2.765 (4) | 178 (6) |
| O5—H5$B$···O8$^{ii}$ | 0.85 (1) | 1.83 (3) | 2.673 (4) | 175 (3) |
| O6—H6$A$···O3$^{iv}$ | 0.84 (1) | 1.87 (3) | 2.710 (4) | 176 (3) |
| O6—H6$B$···O4$^{v}$ | 0.84 (1) | 1.95 (3) | 2.755 (4) | 163 (4) |
| O9—H9$A$···O1$^{v}$ | 0.83 (1) | 1.90 (2) | 2.730 (3) | 178 (5) |
| O9—H9$B$···O2 | 0.84 (1) | 2.01 (3) | 2.808 (3) | 160 (3) |
| O10—H10$A$···O3$^{iv}$ | 0.84 (1) | 1.92 (4) | 2.755 (4) | 174 (5) |
| O10—H10$B$···O2$^{vi}$ | 0.84 (1) | 2.02 (3) | 2.800 (4) | 153 (3) |
| O11—H11$A$···O2$^{vii}$ | 0.84 (1) | 1.91 (3) | 2.747 (4) | 175 (4) |
| O11—H11$B$···O1 | 0.84 (1) | 1.98 (3) | 2.786 (4) | 162 (3) |

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

Data collection: AED software (Belletti, 2004); cell refinement: AED software; data reduction: AED software; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CI2471).

  

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# supplementary materials

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# Tetraaquadiglycinemagnesium(II) hexaaquamagnesium(II) bis(sulfate)

**K. Elayaraja, S. P. Parthiban, S. Ramalingom, G. Bocelli and S. N. Kalkura**

## Comment

The glycine molecule is found to form many compounds with metal sulfates, metal halogenides and acids. There are many examples in the literature on glycine metallic sulfates (Peterková *et al.*, 1991; Fleck & Bohatý, 2005). We report here the crystal structure of the title magnesium sulfate complex, with glycine.

The asymmetric unit of the title compound consists of one-half each of $[Mg(H_2O)_6]^{2+}$ and $[Mg(C_2H_5NO_2)_2(H_2O)_4]^{2+}$ dications, and one $SO_4^{2-}$ anion (Fig. 1). The $Mg^{II}$ atoms of both dications lie on inversion centres, and they are in an octahedral coordination environment. The Mg—O distances of the $[Mg(H_2O)_6]^{2+}$ dication lie in the range 2.048 (2) Å-2.105 (2) Å (Table 1), which is in good agreement with the literature value [2.045 (4)–2.099 (4) Å; Baur, 1964]. In the $[Mg(C_2H_5NO_2)_2(H_2O)_4]^{2+}$ dication, the $Mg^{II}$ atom is coordinated by two O atoms from two glycine ligands, and four water molecules. The Mg—O distance [2.128 (2) Å] involving the glycine molecule is longer than that involving the water molecule (Table 1).

The $[Mg(H_2O)_6]^{2+}$ and $[Mg(C_2H_5NO_2)_2(H_2O)_4]^{2+}$ dications pack as alternate layers parallel to the *ab* plane, with the sulfate anions lying between them. The complex cations and sulfate anions are linked to form a three-dimensional network by O—H···O and N—H···O hydrogen bonds (Table 2).

In the crystal structure, the glycine molecule exists in the zwitterionic form, which is normal for compounds of amino acids with inorganic salts. There are also many examples in the literature of glycinum and glycinate compounds (Muller *et al.*, 1994). The non-hydrogen atoms of the glycine molecule are coplanar, with the caboxylate C—O distances being 1.269 (4) Å [C1—O7] and 1.239 (4) Å [C1—O8].

## Experimental

Colourless single crystals of the title compound were grown from a saturated aqueous solution. Glycine (3 g, 1.6 mol) was added to 25 ml of magnesium sulfate heptahydrate (40 g, 6.5 mol) solution at 313 K using a constant temperature water both. The solution was continuously stirred upto complete dissolution of glycine and the temperature was raised to 318 K to avoid nucleation during the filtration of the solution. This solution was subjected to solvent evaporation at room temperature and after 10 days, white tabular form of crystals were collected.

## Refinement

C-bound H atoms were positioned geometrically (C—H = 0.97 Å) and allowed to ride on their parent atoms, with $U_{iso}$(H) = 1.2$U_{eq}$(C). The water H atoms were located and refined with distance restraints [O—H = 0.84 (1) Å and H···H = 1.37 (2) Å]. The three N—H distances were restrained to be equal.

## Figures

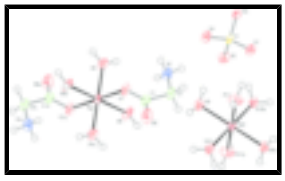

Fig. 1. The asymmetric unit of the title compound. Displacement ellipsoids are drawn at the 50% probability level. Atoms labelled with the suffixes a and b are generated by the symmetry operations (1 − *x*, −*y*, 1 − *z*) and (1 − *x*, 1 − *y*, −*z*), respectively. Only one sulfate anion is shown.

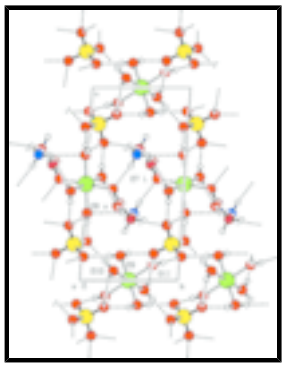

Fig. 2. View of the crystal structure of the title compound.

## Tetraaquadiglycinemagnesium(II) hexaaquamagnesium(II) bis(sulfate)

*Crystal data*

| | |
|---|---|
| $[Mg(C_2H_5NO_2)_2(H_2O)_4][Mg(H_2O)_6](SO_4)_2$ | $Z = 1$ |
| $M_r = 571.04$ | $F_{000} = 300$ |
| Triclinic, $P\overline{1}$ | $D_x = 1.775$ Mg m$^{-3}$ |
| Hall symbol: -P 1 | Mo $K\alpha$ radiation<br>$\lambda = 0.71073$ Å |
| $a = 5.988$ (3) Å | Cell parameters from 36 reflections |
| $b = 6.783$ (2) Å | $\theta = 7.9$–$17.5$º |
| $c = 13.391$ (2) Å | $\mu = 0.41$ mm$^{-1}$ |
| $\alpha = 85.39$ (2)º | $T = 293$ (2) K |
| $\beta = 82.87$ (2)º | Block, colourless |
| $\gamma = 82.88$ (2)º | 0.21 × 0.19 × 0.16 mm |
| $V = 534.4$ (3) Å$^3$ | |

*Data collection*

| | |
|---|---|
| Siemens AED diffractometer | $R_{int} = 0.0000$ |
| Radiation source: fine-focus sealed tube | $\theta_{max} = 25.5$º |
| Monochromator: graphite | $\theta_{min} = 1.5$º |
| $T = 293(2)$ K | $h = -7 \rightarrow 6$ |
| ω–2θ scans | $k = -6 \rightarrow 8$ |
| Absorption correction: none | $l = -12 \rightarrow 16$ |
| 1998 measured reflections | 1 standard reflections |
| 1998 independent reflections | every 50 reflections |
| 1992 reflections with $I > 2\sigma(I)$ | intensity decay: none |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Secondary atom site location: difference Fourier map |
| Least-squares matrix: full | Hydrogen site location: inferred from neighbouring sites |
| $R[F^2 > 2\sigma(F^2)] = 0.066$ | H atoms treated by a mixture of independent and constrained refinement |
| $wR(F^2) = 0.171$ | $w = 1/[\sigma^2(F_o^2) + (0.1149P)^2 + 0.6843P]$ where $P = (F_o^2 + 2F_c^2)/3$ |
| $S = 1.16$ | $(\Delta/\sigma)_{max} = 0.007$ |
| 1998 reflections | $\Delta\rho_{max} = 0.94$ e Å$^{-3}$ |
| 201 parameters | $\Delta\rho_{min} = -1.07$ e Å$^{-3}$ |
| 18 restraints | Extinction correction: SHELXL97 (Sheldrick, 1997), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$ |
| Primary atom site location: structure-invariant direct methods | Extinction coefficient: 0.37 (3) |

*Special details*

**Geometry**. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

**Refinement**. Refinement of $F^2$ against ALL reflections. The weighted *R*-factor *wR* and goodness of fit S are based on $F^2$, conventional *R*-factors *R* are based on F, with F set to zero for negative $F^2$. The threshold expression of $F^2 > 2\text{sigma}(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on $F^2$ are statistically about twice as large as those based on F, and R– factors based on ALL data will be even larger.

*Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å$^2$)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| S1 | 0.01345 (11) | 0.91384 (10) | 0.18807 (5) | 0.0170 (3) |
| O1 | 0.1835 (4) | 1.0199 (3) | 0.12319 (18) | 0.0300 (6) |
| O2 | −0.0271 (4) | 0.7357 (3) | 0.13906 (17) | 0.0279 (6) |
| O3 | −0.2019 (4) | 1.0445 (3) | 0.20413 (17) | 0.0282 (6) |
| O4 | 0.0986 (4) | 0.8490 (4) | 0.28613 (17) | 0.0294 (6) |
| Mg1 | 0.5000 | 0.0000 | 0.5000 | 0.0184 (4) |
| O5 | 0.1910 (4) | 0.1538 (4) | 0.53615 (18) | 0.0318 (6) |
| H5B | 0.116 (6) | 0.206 (6) | 0.489 (2) | 0.044 (12)* |
| H5A | 0.101 (6) | 0.150 (7) | 0.5897 (17) | 0.046 (13)* |
| O6 | 0.4411 (4) | 0.0276 (4) | 0.34899 (15) | 0.0289 (6) |
| H6B | 0.326 (4) | −0.002 (6) | 0.327 (3) | 0.040 (12)* |
| H6A | 0.547 (4) | 0.032 (6) | 0.302 (2) | 0.033 (11)* |
| O7 | 0.6414 (4) | 0.2747 (3) | 0.47278 (16) | 0.0271 (6) |
| O8 | 0.9719 (4) | 0.3338 (5) | 0.3855 (2) | 0.0440 (8) |
| N1 | 0.3922 (5) | 0.5024 (5) | 0.3456 (2) | 0.0317 (7) |

| | | | | |
|---|---|---|---|---|
| H2N | 0.314 (7) | 0.580 (6) | 0.304 (3) | 0.039 (11)* |
| H1N | 0.369 (10) | 0.555 (8) | 0.404 (3) | 0.069 (17)* |
| H3N | 0.330 (10) | 0.392 (6) | 0.351 (5) | 0.073 (18)* |
| C1 | 0.7621 (5) | 0.3521 (5) | 0.3988 (2) | 0.0238 (7) |
| C2 | 0.6414 (6) | 0.4810 (5) | 0.3195 (2) | 0.0285 (7) |
| H2A | 0.6936 | 0.6117 | 0.3127 | 0.034* |
| H2B | 0.6794 | 0.4221 | 0.2550 | 0.034* |
| Mg2 | 0.5000 | 0.5000 | 0.0000 | 0.0186 (4) |
| O9 | 0.2942 (4) | 0.3973 (3) | 0.12778 (17) | 0.0273 (6) |
| H9B | 0.178 (4) | 0.478 (4) | 0.139 (3) | 0.026 (10)* |
| H9A | 0.264 (6) | 0.281 (2) | 0.126 (4) | 0.055 (14)* |
| O10 | 0.7834 (4) | 0.3371 (4) | 0.04927 (17) | 0.0283 (6) |
| H10B | 0.885 (6) | 0.292 (6) | 0.005 (2) | 0.041 (12)* |
| H10A | 0.777 (9) | 0.249 (6) | 0.097 (3) | 0.067 (17)* |
| O11 | 0.5499 (4) | 0.7319 (4) | 0.0805 (2) | 0.0351 (6) |
| H11B | 0.462 (5) | 0.835 (4) | 0.092 (3) | 0.040 (12)* |
| H11A | 0.678 (4) | 0.740 (6) | 0.098 (4) | 0.054 (14)* |

*Atomic displacement parameters (Å$^2$)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| S1 | 0.0201 (5) | 0.0216 (5) | 0.0101 (5) | −0.0058 (3) | −0.0018 (3) | −0.0006 (3) |
| O1 | 0.0306 (13) | 0.0290 (12) | 0.0293 (13) | −0.0113 (10) | 0.0076 (10) | 0.0004 (10) |
| O2 | 0.0299 (12) | 0.0317 (12) | 0.0255 (12) | −0.0102 (9) | −0.0044 (9) | −0.0095 (9) |
| O3 | 0.0299 (13) | 0.0316 (12) | 0.0204 (11) | 0.0002 (9) | 0.0013 (9) | 0.0032 (9) |
| O4 | 0.0335 (13) | 0.0385 (13) | 0.0173 (11) | −0.0045 (10) | −0.0091 (9) | 0.0022 (9) |
| Mg1 | 0.0209 (7) | 0.0262 (8) | 0.0090 (7) | −0.0065 (5) | −0.0031 (5) | 0.0016 (5) |
| O5 | 0.0248 (12) | 0.0476 (14) | 0.0208 (12) | 0.0000 (10) | −0.0015 (9) | 0.0021 (10) |
| O6 | 0.0265 (12) | 0.0520 (15) | 0.0109 (10) | −0.0142 (10) | −0.0034 (9) | −0.0020 (9) |
| O7 | 0.0350 (13) | 0.0319 (12) | 0.0158 (11) | −0.0122 (10) | −0.0032 (9) | 0.0034 (9) |
| O8 | 0.0279 (13) | 0.0605 (18) | 0.0419 (16) | −0.0090 (12) | −0.0067 (11) | 0.0176 (13) |
| N1 | 0.0319 (16) | 0.0396 (17) | 0.0240 (14) | −0.0035 (13) | −0.0102 (12) | 0.0045 (12) |
| C1 | 0.0296 (16) | 0.0278 (15) | 0.0160 (14) | −0.0101 (12) | −0.0050 (12) | 0.0009 (11) |
| C2 | 0.0323 (17) | 0.0359 (17) | 0.0172 (15) | −0.0078 (14) | −0.0018 (12) | 0.0034 (13) |
| Mg2 | 0.0230 (8) | 0.0219 (7) | 0.0124 (7) | −0.0054 (5) | −0.0050 (5) | −0.0015 (5) |
| O9 | 0.0310 (12) | 0.0282 (12) | 0.0227 (12) | −0.0086 (10) | −0.0001 (9) | 0.0011 (9) |
| O10 | 0.0315 (13) | 0.0344 (13) | 0.0171 (11) | 0.0021 (10) | −0.0032 (9) | 0.0016 (9) |
| O11 | 0.0277 (13) | 0.0348 (13) | 0.0475 (15) | −0.0036 (10) | −0.0113 (11) | −0.0199 (12) |

*Geometric parameters (Å, °)*

| | | | |
|---|---|---|---|
| S1—O1 | 1.473 (2) | N1—H1N | 0.87 (3) |
| S1—O3 | 1.474 (2) | N1—H3N | 0.87 (3) |
| S1—O2 | 1.480 (2) | C1—C2 | 1.517 (4) |
| S1—O4 | 1.482 (2) | C2—H2A | 0.97 |
| Mg1—O5$^{i}$ | 2.031 (2) | C2—H2B | 0.97 |
| Mg1—O5 | 2.031 (2) | Mg2—O11$^{ii}$ | 2.048 (2) |
| Mg1—O6$^{i}$ | 2.085 (2) | Mg2—O11 | 2.048 (2) |

| | | | |
|---|---|---|---|
| Mg1—O6 | 2.085 (2) | Mg2—O10$^{ii}$ | 2.057 (2) |
| Mg1—O7 | 2.128 (2) | Mg2—O10 | 2.057 (2) |
| Mg1—O7$^{i}$ | 2.128 (2) | Mg2—O9 | 2.105 (2) |
| O5—H5B | 0.846 (10) | Mg2—O9$^{ii}$ | 2.105 (2) |
| O5—H5A | 0.842 (10) | O9—H9B | 0.835 (10) |
| O6—H6B | 0.838 (10) | O9—H9A | 0.834 (10) |
| O6—H6A | 0.838 (10) | O10—H10B | 0.844 (10) |
| O7—C1 | 1.269 (4) | O10—H10A | 0.842 (10) |
| O8—C1 | 1.239 (4) | O11—H11B | 0.837 (10) |
| N1—C2 | 1.481 (5) | O11—H11A | 0.836 (10) |
| N1—H2N | 0.87 (3) | | |
| O1—S1—O3 | 110.14 (14) | O8—C1—O7 | 125.9 (3) |
| O1—S1—O2 | 109.60 (14) | O8—C1—C2 | 116.3 (3) |
| O3—S1—O2 | 108.77 (14) | O7—C1—C2 | 117.8 (3) |
| O1—S1—O4 | 109.55 (15) | N1—C2—C1 | 111.9 (3) |
| O3—S1—O4 | 110.07 (14) | N1—C2—H2A | 109.2 |
| O2—S1—O4 | 108.69 (14) | C1—C2—H2A | 109.2 |
| O5$^{i}$—Mg1—O5 | 180.00 (13) | N1—C2—H2B | 109.2 |
| O5$^{i}$—Mg1—O6$^{i}$ | 89.18 (10) | C1—C2—H2B | 109.2 |
| O5—Mg1—O6$^{i}$ | 90.82 (10) | H2A—C2—H2B | 107.9 |
| O5$^{i}$—Mg1—O6 | 90.82 (10) | O11$^{ii}$—Mg2—O11 | 180.00 (13) |
| O5—Mg1—O6 | 89.18 (10) | O11$^{ii}$—Mg2—O10$^{ii}$ | 89.87 (10) |
| O6$^{i}$—Mg1—O6 | 180.0 | O11—Mg2—O10$^{ii}$ | 90.13 (10) |
| O5$^{i}$—Mg1—O7 | 90.78 (10) | O11$^{ii}$—Mg2—O10 | 90.13 (10) |
| O5—Mg1—O7 | 89.22 (10) | O11—Mg2—O10 | 89.87 (10) |
| O6$^{i}$—Mg1—O7 | 92.84 (9) | O10$^{ii}$—Mg2—O10 | 180.00 (12) |
| O6—Mg1—O7 | 87.16 (9) | O11$^{ii}$—Mg2—O9 | 92.24 (11) |
| O5$^{i}$—Mg1—O7$^{i}$ | 89.22 (10) | O11—Mg2—O9 | 87.76 (11) |
| O5—Mg1—O7$^{i}$ | 90.78 (10) | O10$^{ii}$—Mg2—O9 | 88.69 (10) |
| O6$^{i}$—Mg1—O7$^{i}$ | 87.16 (9) | O10—Mg2—O9 | 91.31 (10) |
| O6—Mg1—O7$^{i}$ | 92.84 (9) | O11$^{ii}$—Mg2—O9$^{ii}$ | 87.76 (11) |
| O7—Mg1—O7$^{i}$ | 180.0 | O11—Mg2—O9$^{ii}$ | 92.24 (11) |
| Mg1—O5—H5B | 119 (3) | O10$^{ii}$—Mg2—O9$^{ii}$ | 91.31 (10) |
| Mg1—O5—H5A | 131 (3) | O10—Mg2—O9$^{ii}$ | 88.69 (10) |
| H5B—O5—H5A | 108 (2) | O9—Mg2—O9$^{ii}$ | 180.00 (15) |
| Mg1—O6—H6B | 125 (3) | Mg2—O9—H9B | 110 (3) |
| Mg1—O6—H6A | 122 (2) | Mg2—O9—H9A | 115 (3) |
| H6B—O6—H6A | 110 (2) | H9B—O9—H9A | 112 (3) |
| C1—O7—Mg1 | 133.9 (2) | Mg2—O10—H10B | 117 (3) |
| C2—N1—H2N | 116 (3) | Mg2—O10—H10A | 123 (3) |
| C2—N1—H1N | 105 (4) | H10B—O10—H10A | 106 (2) |
| H2N—N1—H1N | 107 (5) | Mg2—O11—H11B | 128 (3) |
| C2—N1—H3N | 115 (4) | Mg2—O11—H11A | 120 (3) |
| H2N—N1—H3N | 104 (5) | H11B—O11—H11A | 111 (2) |
| H1N—N1—H3N | 109 (6) | | |

| | | | |
|---|---|---|---|
| O5$^{i}$—Mg1—O7—C1 | 53.2 (3) | Mg1—O7—C1—O8 | −90.2 (4) |
| O5—Mg1—O7—C1 | −126.8 (3) | Mg1—O7—C1—C2 | 90.6 (4) |
| O6$^{i}$—Mg1—O7—C1 | 142.4 (3) | O8—C1—C2—N1 | −176.7 (3) |
| O6—Mg1—O7—C1 | −37.6 (3) | O7—C1—C2—N1 | 2.6 (4) |

Symmetry codes: (i) −*x*+1, −*y*, −*z*+1; (ii) −*x*+1, −*y*+1, −*z*.

*Hydrogen-bond geometry (Å, °)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N1—H1N···O7$^{iii}$ | 0.87 (3) | 2.08 (5) | 2.939 (4) | 168 (4) |
| N1—H2N···O4 | 0.87 (3) | 2.12 (4) | 2.877 (4) | 145 (4) |
| N1—H3N···O6 | 0.87 (3) | 2.48 (4) | 3.195 (5) | 140 (5) |
| N1—H3N···O8$^{iv}$ | 0.87 (3) | 2.21 (6) | 2.865 (4) | 131 (4) |
| O5—H5A···O4$^{v}$ | 0.84 (1) | 1.92 (3) | 2.765 (4) | 178 (6) |
| O5—H5B···O8$^{iv}$ | 0.85 (1) | 1.83 (3) | 2.673 (4) | 175 (3) |
| O6—H6A···O3$^{vi}$ | 0.84 (1) | 1.87 (3) | 2.710 (4) | 176 (3) |
| O6—H6B···O4$^{vii}$ | 0.84 (1) | 1.95 (3) | 2.755 (4) | 163 (4) |
| O9—H9A···O1$^{vii}$ | 0.83 (1) | 1.90 (2) | 2.730 (3) | 178 (5) |
| O9—H9B···O2 | 0.84 (1) | 2.01 (3) | 2.808 (3) | 160 (3) |
| O10—H10A···O3$^{vi}$ | 0.84 (1) | 1.92 (4) | 2.755 (4) | 174 (5) |
| O10—H10B···O2$^{ii}$ | 0.84 (1) | 2.02 (3) | 2.800 (4) | 153 (3) |
| O11—H11A···O2$^{viii}$ | 0.84 (1) | 1.91 (3) | 2.747 (4) | 175 (4) |
| O11—H11B···O1 | 0.84 (1) | 1.98 (3) | 2.786 (4) | 162 (3) |

Symmetry codes: (iii) −*x*+1, −*y*+1, −*z*+1; (iv) *x*−1, *y*, *z*; (v) −*x*, −*y*+1, −*z*+1; (vi) *x*+1, *y*−1, *z*; (vii) *x*, *y*−1, *z*; (ii) −*x*+1, −*y*+1, −*z*; (viii) *x*+1, *y*, *z*.

**Fig. 1**

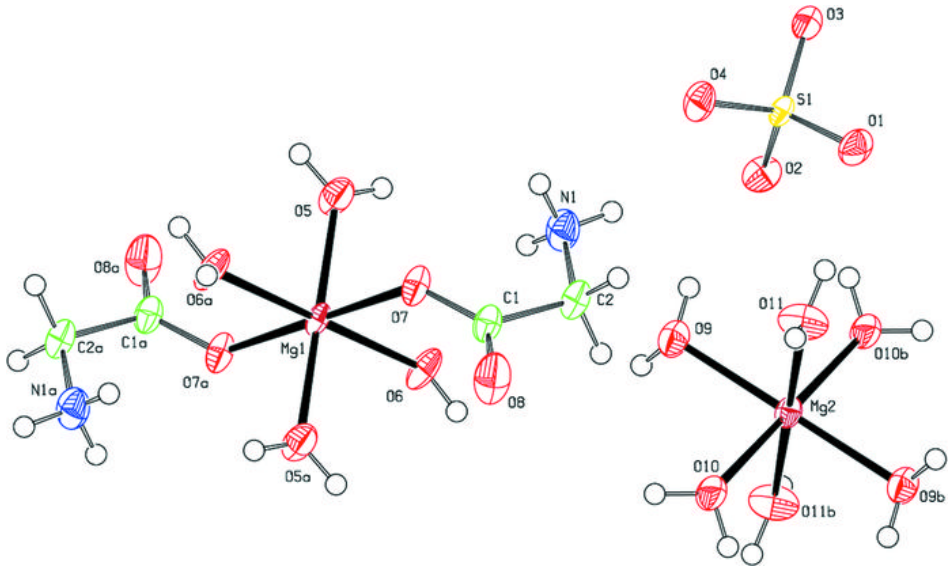
O3
O4
S1
O1
O2
N1
O5
O8a
O6a
C1
C2
O7
C2a
C1a
Mg1
O7a
O6
O8
N1a
O5a
O11
O9
O10b
Mg2
O10
O11b
O9b

**Fig. 2**