# Hexaaquamagnesium bis(4-amino-3-methylbenzenesulfonate)

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In the title molecular salt, $[Mg(H_2O)_6](C_7H_8NO_3S)_2$, the $Mg^{2+}$ cation lies on an inversion centre. In the crystal, the components are linked by N—H···O and O—H···O hydrogen bonds, thereby generating sheets parallel to (001).

## Related literature

For the isostructural cobalt-containing compound, see: Zhang & Chen (2009).
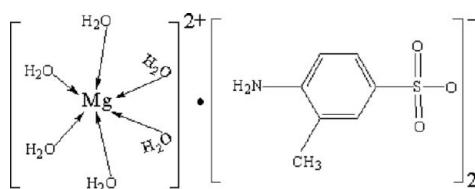


## Experimental

### Crystal data

$[Mg(H_2O)_6](C_7H_8NO_3S)_2$
$M_r = 504.81$
Monoclinic, $P2_1/n$
$a = 6.3048\ (13)$ Å
$b = 7.0395\ (15)$ Å
$c = 24.356\ (5)$ Å
$\beta = 93.921\ (3)°$

$V = 1078.5\ (4)$ Å$^3$
$Z = 2$
Mo $K\alpha$ radiation
$\mu = 0.34$ mm$^{-1}$
$T = 273$ K
$0.23 \times 0.16 \times 0.12$ mm

### Data collection

Bruker SMART CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
$T_{min} = 0.926$, $T_{max} = 0.960$

5398 measured reflections
1918 independent reflections
1779 reflections with $I > 2\sigma(I)$
$R_{int} = 0.020$

### Refinement

$R[F^2 > 2\sigma(F^2)] = 0.054$
$wR(F^2) = 0.138$
$S = 1.27$
1918 reflections
144 parameters

9 restraints
H-atom parameters constrained
$\Delta\rho_{max} = 0.37$ e Å$^{-3}$
$\Delta\rho_{min} = -0.42$ e Å$^{-3}$

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

| | | | |
|---|---|---|---|
| Mg1—O4 | 2.029 (3) | Mg1—O5 | 2.075 (3) |
| Mg1—O6 | 2.071 (3) | | |

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| N1—H1$A$···O3$^i$ | 0.86 | 2.48 | 3.208 (5) | 143 |
| N1—H1$B$···O6$^{ii}$ | 0.86 | 2.54 | 3.133 (5) | 127 |
| O4—H7···O3 | 0.85 | 1.90 | 2.748 (4) | 178 |
| O4—H8···O1$^{iii}$ | 0.85 | 1.94 | 2.778 (4) | 169 |
| O5—H9···O2$^{iii}$ | 0.85 | 1.97 | 2.810 (4) | 168 |
| O5—H10···O1$^{iv}$ | 0.85 | 1.95 | 2.790 (4) | 170 |
| O6—H11···O2 | 0.85 | 1.94 | 2.776 (4) | 169 |
| O6—H12···O3$^v$ | 0.85 | 2.01 | 2.835 (4) | 163 |

Symmetry codes: (i) $-x + \frac{3}{2}, y + \frac{1}{2}, -z + \frac{1}{2}$; (ii) $-x + \frac{1}{2}, y + \frac{1}{2}, -z + \frac{1}{2}$; (iii) $x, y - 1, z$; (iv) $x - 1, y - 1, z$; (v) $x - 1, y, z$.

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

## References

Bruker (2000). *SMART*, *SAINT* and *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Zhang, W. & Chen, Y.-T. (2009). *Acta Cryst.* E**65**, m1548.

**supplementary materials**

# Hexaaquamagnesium bis(4-amino-3-methylbenzenesulfonate)

**W. Zhang and Y.-T. Chen**

## Experimental

A solution of 1.0 mmol 4-amino-3-methyl-benzenesulfonic acid and 1.0 mmol NaOH in 10 ml ethanol was added to a solution of 0.5 mmol $MgCl_26H_2O$ in 5 ml ethanol at room temperature. The mixture was refluxed for 3 h with stirring, then the resulting precipitate was filtered, washed, and dried *in vacuo* over $P_4O_{10}$ for 48 h. Colourless blocks of (I) were obtained by slowly evaporating from ethanol at room temperature.

## Refinement

The H atoms were positioned geometrically (C—H = 0.93–0.96, N—H = 0.86, O—H = 0.85Å) and refined as riding with $U_{iso}(H)= 1.2\ U_{eq}(C,N)$ or $1.5\ U_{eq}(O)$.

## Figures
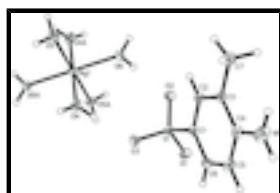


Fig. 1. The molecular structure of (I) showing 30% displacement ellipsoids. Atoms with the suffix A are generated by (−x, −y, −z).

**Hexaaquamagnesium bis(4-amino-3-methylbenzenesulfonate)**

*Crystal data*

| | |
|---|---|
| $[Mg(H_2O)_6](C_7H_8NO_3S)_2$ | $F_{000} = 532$ |
| $M_r = 504.81$ | $D_x = 1.555$ Mg m$^{-3}$ |
| Monoclinic, $P2_1/n$ | Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å |
| Hall symbol: -P 2yn | Cell parameters from 3577 reflections |
| $a = 6.3048\ (13)$ Å | $\theta = 3.0–28.6°$ |
| $b = 7.0395\ (15)$ Å | $\mu = 0.34$ mm$^{-1}$ |
| $c = 24.356\ (5)$ Å | $T = 273$ K |
| $\beta = 93.921\ (3)°$ | Block, colourless |
| $V = 1078.5\ (4)$ Å$^3$ | $0.23 \times 0.16 \times 0.12$ mm |
| $Z = 2$ | |

*Data collection*

| | |
|---|---|
| Bruker SMART CCD diffractometer | 1918 independent reflections |

# supplementary materials

Radiation source: fine-focus sealed tube

Monochromator: graphite

$T = 273$ K

$\omega$ scans

Absorption correction: multi-scan (SADABS; Bruker, 2000)

$T_{min} = 0.926$, $T_{max} = 0.960$

5398 measured reflections

1779 reflections with $I > 2\sigma(I)$

$R_{int} = 0.020$

$\theta_{max} = 25.1°$

$\theta_{min} = 1.7°$

$h = -6 \rightarrow 7$

$k = -8 \rightarrow 8$

$l = -28 \rightarrow 25$

*Refinement*

Refinement on $F^2$

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.054$

$wR(F^2) = 0.138$

$S = 1.27$

1918 reflections

144 parameters

9 restraints

Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0175P)^2 + 3.9593P]$
where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} < 0.001$

$\Delta\rho_{max} = 0.37$ e Å$^{-3}$

$\Delta\rho_{min} = -0.42$ e Å$^{-3}$

Extinction correction: none

*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 $F^2 > \sigma(F^2)$ 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 ($Å^2$)*

|      | $x$          | $y$          | $z$          | $U_{iso}*/U_{eq}$ |
|------|--------------|--------------|--------------|-------------------|
| Mg1  | 0.0000       | 0.0000       | 0.0000       | 0.0216 (4)        |
| S1   | 0.40358 (14) | 0.50773 (14) | 0.09733 (4)  | 0.0218 (3)        |
| O1   | 0.4934 (5)   | 0.6661 (4)   | 0.06800 (11) | 0.0317 (7)        |
| O2   | 0.1712 (4)   | 0.5034 (4)   | 0.09088 (12) | 0.0297 (7)        |
| O3   | 0.4968 (4)   | 0.3258 (4)   | 0.08251 (12) | 0.0304 (7)        |
| O4   | 0.2913 (5)   | 0.0074 (4)   | 0.04083 (13) | 0.0375 (8)        |
| H7   | 0.3575       | 0.1051       | 0.0533       | 0.056*            |
| H8   | 0.3647       | −0.0883      | 0.0519       | 0.056*            |
| O5   | −0.0976 (5)  | −0.1937 (4)  | 0.05737 (13) | 0.0366 (8)        |

| | | | | |
|---|---|---|---|---|
| H9 | −0.0146 | −0.2881 | 0.0624 | 0.055* |
| H10 | −0.2222 | −0.2401 | 0.0564 | 0.055* |
| O6 | −0.1022 (5) | 0.2297 (4) | 0.04427 (13) | 0.0340 (7) |
| H12 | −0.2251 | 0.2721 | 0.0498 | 0.052 (16)* |
| H11 | −0.0147 | 0.3033 | 0.0618 | 0.11 (3)* |
| N1 | 0.6584 (7) | 0.6327 (6) | 0.33201 (15) | 0.0465 (11) |
| H1A | 0.7828 | 0.6779 | 0.3408 | 0.056* |
| H1B | 0.5739 | 0.6070 | 0.3573 | 0.056* |
| C1 | 0.4753 (6) | 0.5435 (5) | 0.16775 (16) | 0.0217 (8) |
| C2 | 0.3351 (6) | 0.5006 (6) | 0.20762 (16) | 0.0248 (8) |
| H2 | 0.2013 | 0.4519 | 0.1971 | 0.030* |
| C3 | 0.3929 (6) | 0.5297 (5) | 0.26277 (16) | 0.0254 (9) |
| C4 | 0.5949 (7) | 0.6021 (6) | 0.27807 (16) | 0.0280 (9) |
| C5 | 0.7335 (7) | 0.6445 (6) | 0.23738 (17) | 0.0305 (9) |
| H5 | 0.8675 | 0.6936 | 0.2474 | 0.037* |
| C6 | 0.6748 (6) | 0.6147 (6) | 0.18287 (17) | 0.0276 (9) |
| H6 | 0.7689 | 0.6424 | 0.1562 | 0.033* |
| C7 | 0.2434 (7) | 0.4831 (7) | 0.30672 (18) | 0.0363 (10) |
| H7A | 0.1193 | 0.4209 | 0.2903 | 0.054* |
| H7B | 0.2022 | 0.5982 | 0.3243 | 0.054* |
| H7C | 0.3136 | 0.4006 | 0.3336 | 0.054* |

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

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Mg1 | 0.0199 (9) | 0.0211 (9) | 0.0240 (9) | −0.0004 (8) | 0.0032 (7) | 0.0008 (8) |
| S1 | 0.0198 (5) | 0.0208 (5) | 0.0249 (5) | −0.0004 (4) | 0.0011 (3) | −0.0008 (4) |
| O1 | 0.0331 (16) | 0.0318 (16) | 0.0304 (15) | −0.0064 (13) | 0.0045 (12) | 0.0080 (13) |
| O2 | 0.0208 (14) | 0.0326 (16) | 0.0351 (16) | 0.0015 (13) | −0.0024 (11) | −0.0017 (13) |
| O3 | 0.0299 (16) | 0.0279 (16) | 0.0335 (16) | 0.0043 (13) | 0.0021 (12) | −0.0089 (13) |
| O4 | 0.0303 (16) | 0.0275 (16) | 0.0527 (19) | −0.0020 (13) | −0.0117 (14) | −0.0009 (15) |
| O5 | 0.0264 (16) | 0.0361 (17) | 0.0486 (19) | 0.0009 (13) | 0.0121 (14) | 0.0161 (15) |
| O6 | 0.0273 (16) | 0.0312 (16) | 0.0442 (18) | 0.0002 (14) | 0.0083 (13) | −0.0131 (14) |
| N1 | 0.051 (2) | 0.060 (3) | 0.028 (2) | −0.018 (2) | −0.0021 (17) | −0.004 (2) |
| C1 | 0.0220 (19) | 0.0166 (18) | 0.0266 (19) | 0.0008 (15) | 0.0018 (15) | −0.0004 (15) |
| C2 | 0.0227 (19) | 0.0198 (19) | 0.032 (2) | −0.0004 (16) | 0.0019 (16) | 0.0006 (17) |
| C3 | 0.032 (2) | 0.0158 (19) | 0.029 (2) | 0.0006 (16) | 0.0067 (16) | 0.0000 (16) |
| C4 | 0.034 (2) | 0.022 (2) | 0.028 (2) | −0.0019 (17) | 0.0015 (17) | −0.0017 (17) |
| C5 | 0.027 (2) | 0.029 (2) | 0.035 (2) | −0.0064 (18) | −0.0047 (18) | −0.0018 (18) |
| C6 | 0.023 (2) | 0.030 (2) | 0.031 (2) | −0.0028 (17) | 0.0046 (16) | 0.0009 (18) |
| C7 | 0.047 (3) | 0.030 (2) | 0.033 (2) | −0.006 (2) | 0.012 (2) | 0.002 (2) |

*Geometric parameters (Å, °)*

| | | | |
|---|---|---|---|
| Mg1—O4[i] | 2.029 (3) | N1—C4 | 1.364 (5) |
| Mg1—O4 | 2.029 (3) | N1—H1A | 0.8600 |
| Mg1—O6[i] | 2.071 (3) | N1—H1B | 0.8600 |
| Mg1—O6 | 2.071 (3) | C1—C6 | 1.380 (5) |

| | | | |
|---|---|---|---|
| Mg1—O5 | 2.075 (3) | C1—C2 | 1.390 (5) |
| Mg1—O5ⁱ | 2.075 (3) | C2—C3 | 1.383 (6) |
| S1—O1 | 1.459 (3) | C2—H2 | 0.9300 |
| S1—O2 | 1.463 (3) | C3—C4 | 1.399 (6) |
| S1—O3 | 1.465 (3) | C3—C7 | 1.510 (6) |
| S1—C1 | 1.762 (4) | C4—C5 | 1.398 (6) |
| O4—H7 | 0.8499 | C5—C6 | 1.370 (6) |
| O4—H8 | 0.8500 | C5—H5 | 0.9300 |
| O5—H9 | 0.8500 | C6—H6 | 0.9300 |
| O5—H10 | 0.8500 | C7—H7A | 0.9600 |
| O6—H12 | 0.8500 | C7—H7B | 0.9600 |
| O6—H11 | 0.8500 | C7—H7C | 0.9600 |
| | | | |
| O4ⁱ—Mg1—O4 | 180.0 | H12—O6—H11 | 105.9 |
| O4ⁱ—Mg1—O6ⁱ | 91.62 (13) | C4—N1—H1A | 120.0 |
| O4—Mg1—O6ⁱ | 88.38 (13) | C4—N1—H1B | 120.0 |
| O4ⁱ—Mg1—O6 | 88.38 (13) | H1A—N1—H1B | 120.0 |
| O4—Mg1—O6 | 91.62 (13) | C6—C1—C2 | 120.3 (4) |
| O6ⁱ—Mg1—O6 | 180.0 | C6—C1—S1 | 118.7 (3) |
| O4ⁱ—Mg1—O5 | 90.75 (12) | C2—C1—S1 | 121.0 (3) |
| O4—Mg1—O5 | 89.25 (12) | C3—C2—C1 | 120.6 (4) |
| O6ⁱ—Mg1—O5 | 87.41 (12) | C3—C2—H2 | 119.7 |
| O6—Mg1—O5 | 92.59 (12) | C1—C2—H2 | 119.7 |
| O4ⁱ—Mg1—O5ⁱ | 89.25 (12) | C2—C3—C4 | 119.2 (4) |
| O4—Mg1—O5ⁱ | 90.75 (12) | C2—C3—C7 | 121.4 (4) |
| O6ⁱ—Mg1—O5ⁱ | 92.59 (12) | C4—C3—C7 | 119.4 (4) |
| O6—Mg1—O5ⁱ | 87.41 (12) | N1—C4—C5 | 119.5 (4) |
| O5—Mg1—O5ⁱ | 180.0 | N1—C4—C3 | 121.1 (4) |
| O1—S1—O2 | 112.49 (18) | C5—C4—C3 | 119.4 (4) |
| O1—S1—O3 | 111.84 (17) | C6—C5—C4 | 120.9 (4) |
| O2—S1—O3 | 111.78 (17) | C6—C5—H5 | 119.5 |
| O1—S1—C1 | 106.55 (17) | C4—C5—H5 | 119.5 |
| O2—S1—C1 | 107.23 (17) | C5—C6—C1 | 119.7 (4) |
| O3—S1—C1 | 106.52 (17) | C5—C6—H6 | 120.2 |
| Mg1—O4—H7 | 127.0 | C1—C6—H6 | 120.2 |
| Mg1—O4—H8 | 126.1 | C3—C7—H7A | 109.5 |
| H7—O4—H8 | 106.5 | C3—C7—H7B | 109.5 |
| Mg1—O5—H9 | 113.8 | H7A—C7—H7B | 109.5 |
| Mg1—O5—H10 | 123.4 | C3—C7—H7C | 109.5 |
| H9—O5—H10 | 105.2 | H7A—C7—H7C | 109.5 |
| Mg1—O6—H12 | 132.6 | H7B—C7—H7C | 109.5 |
| Mg1—O6—H11 | 121.5 | | |
| | | | |
| O1—S1—C1—C6 | −38.2 (4) | C2—C3—C4—N1 | −179.9 (4) |
| O2—S1—C1—C6 | −158.9 (3) | C7—C3—C4—N1 | −0.5 (6) |
| O3—S1—C1—C6 | 81.3 (3) | C2—C3—C4—C5 | 0.4 (6) |
| O1—S1—C1—C2 | 142.0 (3) | C7—C3—C4—C5 | 179.8 (4) |
| O2—S1—C1—C2 | 21.4 (4) | N1—C4—C5—C6 | 179.8 (4) |

| O3—S1—C1—C2 | −98.4 (3) | C3—C4—C5—C6 | −0.5 (6) |
| C6—C1—C2—C3 | 0.4 (6) | C4—C5—C6—C1 | 0.6 (6) |
| S1—C1—C2—C3 | −179.8 (3) | C2—C1—C6—C5 | −0.5 (6) |
| C1—C2—C3—C4 | −0.3 (6) | S1—C1—C6—C5 | 179.7 (3) |
| C1—C2—C3—C7 | −179.7 (4) | | |

Symmetry codes: (i) −*x*, −*y*, −*z*.


*Hydrogen-bond geometry (Å, °)*

| *D*—H⋯*A* | *D*—H | H⋯*A* | *D*⋯*A* | *D*—H⋯*A* |
| --- | --- | --- | --- | --- |
| N1—H1A⋯O3[ii] | 0.86 | 2.48 | 3.208 (5) | 143 |
| N1—H1B⋯O6[iii] | 0.86 | 2.54 | 3.133 (5) | 127 |
| O4—H7⋯O3 | 0.85 | 1.90 | 2.748 (4) | 178 |
| O4—H8⋯O1[iv] | 0.85 | 1.94 | 2.778 (4) | 169 |
| O5—H9⋯O2[iv] | 0.85 | 1.97 | 2.810 (4) | 168 |
| O5—H10⋯O1[v] | 0.85 | 1.95 | 2.790 (4) | 170 |
| O6—H11⋯O2 | 0.85 | 1.94 | 2.776 (4) | 169 |
| O6—H12⋯O3[vi] | 0.85 | 2.01 | 2.835 (4) | 163 |

Symmetry codes: (ii) −*x*+3/2, *y*+1/2, −*z*+1/2; (iii) −*x*+1/2, *y*+1/2, −*z*+1/2; (iv) *x*, *y*−1, *z*; (v) *x*−1, *y*−1, *z*; (vi) *x*−1, *y*, *z*.

**Fig. 1**