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# Hexaaquamagnesium bis(3-carboxy-4-hydroxybenzenesulfonate) dihydrate

**Graham Smith,[a]* Urs D. Wermuth[a] and Michael L. Williams[b]**

[a]Faculty of Science and Technology, Queensland University of Technology, GPO Box 2434, Brisbane, Queensland 4001, Australia, and [b]School of Biomolecular and Physical Sciences, Griffith University, Nathan, Queensland 4111, Australia
Correspondence e-mail: g.smith@qut.edu.au

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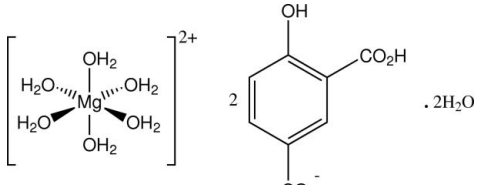
Key indicators: single-crystal X-ray study; $T$ = 200 K; mean $\sigma$(C–C) = 0.002 Å; $R$ factor = 0.032; $wR$ factor = 0.086; data-to-parameter ratio = 13.9.

In the crystal structure of the title compound, $[Mg(H_2O)_6](C_7H_5O_6S)_2\cdot 2H_2O$, the octahedral complex cation lies on an inversion centre and is hydrogen bonded through the coordinated water molecules to the substituted benzenesulfonate monoanions and the water molecules of solvation. These interactions together with a carboxylic acid O—H···O(sulfonate) association give a three-dimensional structure.

## Related literature

For the structure of the isotypic $Mn^{II}$, $Cu^{II}$ and $Co^{II}$ dihydrate complexes, see: Ma *et al.* (2003*a*,*d*); Abdelhak *et al.* (2005). For the structures of the analogous $Co^{II}$, $Ni^{II}$ and $Zn^{II}$ tetrahydrate complexes, see: Ma *et al.* (2003*b*,*c*,*e*).




## Experimental

### Crystal data

$[Mg(H_2O)_6](C_7H_5O_6S)_2\cdot 2H_2O$
$M_r$ = 602.78
Triclinic, $P\overline{1}$
$a$ = 6.8694 (4) Å
$b$ = 6.9069 (4) Å
$c$ = 14.3950 (8) Å
$\alpha$ = 77.472 (5)°
$\beta$ = 78.120 (4)°
$\gamma$ = 70.131 (5)°
$V$ = 620.51 (6) Å$^3$
$Z$ = 1
Mo $K\alpha$ radiation
$\mu$ = 0.33 mm$^{-1}$
$T$ = 200 K
0.40 × 0.12 × 0.10 mm

### Data collection

Oxford Diffraction Gemini-S CCD-detector diffractometer
Absorption correction: multi-scan (*CrysAlis PRO*; Oxford Diffraction, 2010)
$T_{min}$ = 0.96, $T_{max}$ = 0.99
8134 measured reflections
2899 independent reflections
2553 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.023

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.032
$wR(F^2)$ = 0.086
$S$ = 1.14
2899 reflections
209 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.34 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.43 e Å$^{-3}$

**Table 1**
Hydrogen-bond geometry (Å, °).

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| O2—H2···O12 | 0.85 (2) | 1.87 (2) | 2.632 (2) | 149 (2) |
| O11—H11···O53$^{i}$ | 0.79 (3) | 1.92 (3) | 2.678 (2) | 161 (3) |
| O1$W$—H11$W$···O12$^{ii}$ | 0.85 (2) | 1.93 (2) | 2.779 (2) | 175 (2) |
| O1$W$—H12$W$···O51 | 0.82 (3) | 2.00 (3) | 2.824 (2) | 175 (2) |
| O2$W$—H21$W$···O4$W^{iii}$ | 0.82 (3) | 1.91 (3) | 2.728 (3) | 173 (3) |
| O3$W$—H31$W$···O51$^{iv}$ | 0.75 (3) | 2.10 (3) | 2.850 (2) | 171 (3) |
| O3$W$—H32$W$···O4$W^{v}$ | 0.89 (3) | 1.87 (3) | 2.748 (3) | 167 (2) |
| O4$W$—H41$W$···O53$^{vi}$ | 0.79 (3) | 2.04 (3) | 2.803 (2) | 162 (3) |
| O4$W$—H42$W$···O52 | 0.84 (3) | 1.88 (3) | 2.717 (2) | 178 (3) |

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

Data collection: *CrysAlis PRO* (Oxford Diffraction, 2010); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis PRO*; program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1994); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008) within *WinGX* (Farrugia, 1999); molecular graphics: *PLATON* (Spek, 2009); software used to prepare material for publication: *PLATON*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: TK2770).

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# supporting information

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## Hexaaquamagnesium bis(3-carboxy-4-hydroxybenzenesulfonate) dihydrate

**Graham Smith, Urs D. Wermuth and Michael L. Williams**

### S1. Comment

The title compound, $[Mg(H_2O)_6]^{2+}$ $2(C_7H_5O_6S^-)$. $2(H_2O)$ was obtained from the reaction of 3-carboxy-4-hydroxybenzenesulfonic acid (5-sulfosalicylic acid, 5-SSA) with $MgCO_3$ and the structure is reported here In the structure of this compound (Fig. 1), the octahedral cationic Mg complex cations lie on crystallographic inversion centres [Mg—O, 2.0396 (17)–2.0664 (19) Å]. This complex is isomorphous with other divalent first transition metal–5-SSA complexes with the same basic dihydrate formula $[M(H_2O)_6]$ 2(5-SSA$^-$). $2(H_2O)$, [*M* = Mn (Ma *et al.*, 2003*a*); Co (Abdelhak *et al.*, 2005); Cu (Ma *et al.*, 2003*d*)]. These complexes are also similar to the tetrahydrate analogues $\{[M(H_2O)_6]$ 2(5-SSA$^-$). $4(H_2O)\}$, having triclinic unit cells with comparable cell parameters *e.g.* $Co^{II}$ (Ma *et al.*, 2003*b*) and Ni (Ma *et al.*, 2003*c*) and Zn (Ma *et al.*, 2003*e*).

The coordinated water molecules are involved in a number of O—H···O hydrogen-bonding interactions with sulfonate and carboxylate O acceptors of the uncoordinated 5-SSA monoanions and the water molecules of solvation (Table 1) and together with a carboxylic acid *O*—*H*···$O_{sulfonate}$ hydrogen bond form a three-dimensional structure (Fig. 2). In the anion there is the intramolecular cyclic phenol *O*—*H*···$O_{carboxyl}$ hydrogen bond which is invariably present in this monoanion (Ma *et al.*, 2003*a*). One H of one of the coordinated water molecules (H22W) has no reasonable acceptor in the structure.

### S2. Experimental

The title compound was synthesized by heating 218 mg (1 mmol) of 3-carboxy-4-hydroxybenzenesulfonic acid (5-sulfosalicylic acid) with an excess of $MgCO_3$ in 50 ml of 1:1 ethanol–water under reflux for 10 min. After completion of the reaction, the unreacted $MgCO_3$ was removed by filtration and the solution was allowed evaporate to incipient dryness at room temperature, giving small colourless prisms of the title compound from which a specimen was cleaved for the X-ray analysis.

### S3. Refinement

Hydrogen atoms involved in hydrogen-bonding interactions were located by difference methods and their positional and isotropic displacement parameters were refined. Other H-atoms were included in the refinement at calculated positions [C–H = 0.93 Å and with $U_{iso}$(H) = 1.2$U_{eq}$(C), using a riding-model approximation.

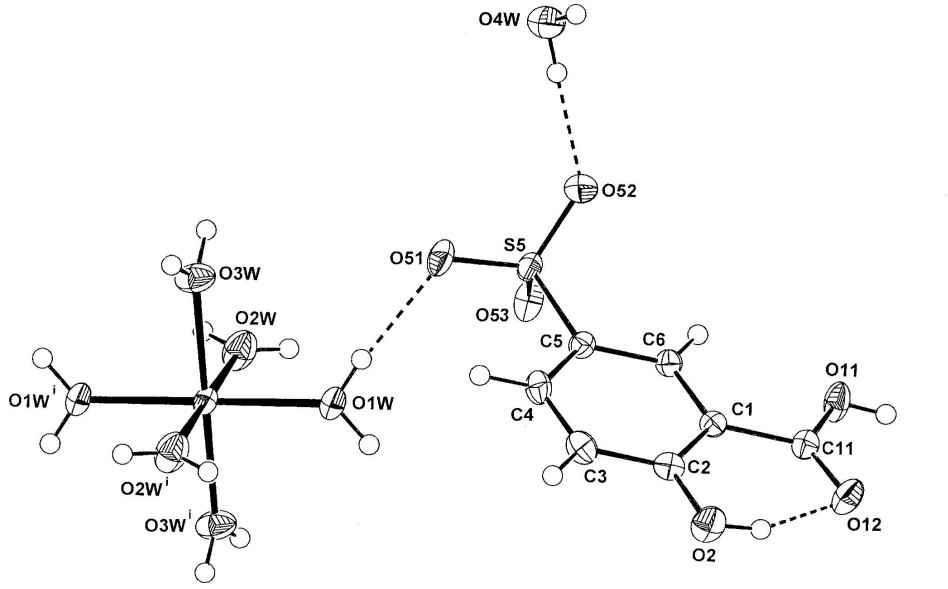


**Figure 1**

Molecular configuration and atom naming scheme for the cation, anion and water species in the asymmetric unit of the title compound. Inter-species hydrogen bonds are shown as dashed lines and displacement ellipsoids are drawn at the 50% probability level. For symmetry code (i): -*x*, -*y*, -*z*.

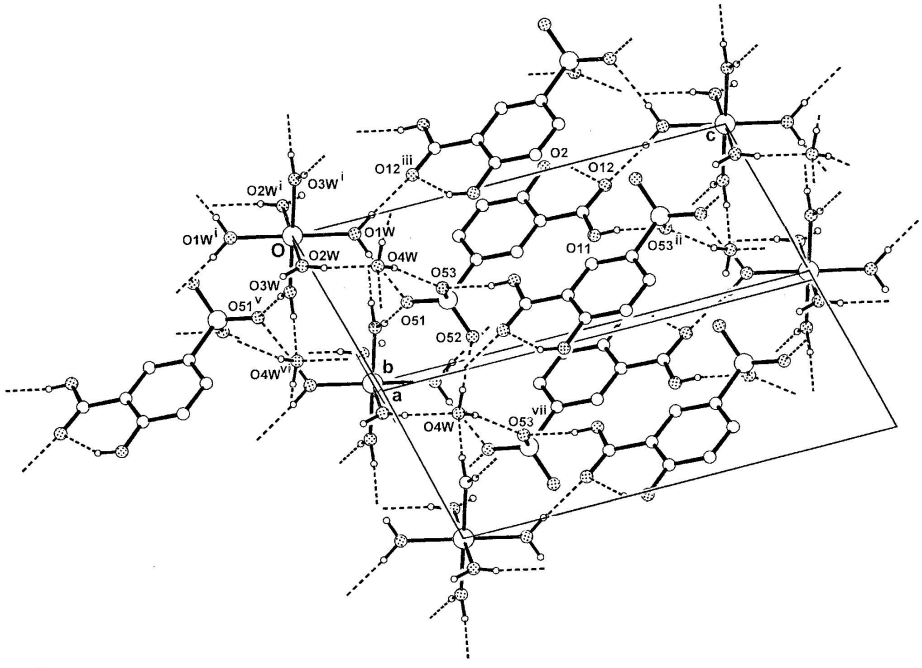


**Figure 2**

The hydrogen-bonding interactions in the title compound viewed down *a*. For symmetry codes, see Table 1.

**Hexaaquamagnesium bis(3-carboxy-4-hydroxybenzenesulfonate) dihydrate**

*Crystal data*

$[Mg(H_2O)_6](C_7H_5O_6S)_2\cdot 2H_2O$
$M_r = 602.78$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 6.8694$ (4) Å
$b = 6.9069$ (4) Å
$c = 14.3950$ (8) Å
$\alpha = 77.472$ (5)°
$\beta = 78.120$ (4)°
$\gamma = 70.131$ (5)°
$V = 620.51$ (6) Å$^3$
$Z = 1$
$F(000) = 314$
$D_x = 1.613$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 4714 reflections
$\theta = 3.2$–$28.9°$
$\mu = 0.33$ mm$^{-1}$
$T = 200$ K
Prism, colourless
0.40 × 0.12 × 0.10 mm

*Data collection*

Oxford Diffraction Gemini-S CCD-detector diffractometer
Radiation source: Enhance (Mo) X-ray source
Graphite monochromator
$\omega$ scans
Absorption correction: multi-scan (*CrysAlis PRO*; Oxford Diffraction, 2010)
$T_{min} = 0.96$, $T_{max} = 0.99$
8134 measured reflections
2899 independent reflections
2553 reflections with $I > 2\sigma(I)$
$R_{int} = 0.023$
$\theta_{max} = 28.8°$, $\theta_{min} = 3.2°$
$h = -9\rightarrow 9$
$k = -9\rightarrow 8$
$l = -19\rightarrow 18$

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.032$
$wR(F^2) = 0.086$
$S = 1.14$
2899 reflections
209 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0388P)^2 + 0.10P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.34$ e Å$^{-3}$
$\Delta\rho_{min} = -0.43$ e Å$^{-3}$

*Special details*

**Geometry**. Bond distances, angles *etc*. have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell e.s.d.'s are taken into account in the estimation of distances, angles and torsion angles

**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* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| S5 | 0.32291 (6) | 0.27288 (6) | 0.24107 (3) | 0.0205 (1) |
| O2 | −0.30636 (17) | 0.30257 (19) | 0.58938 (9) | 0.0293 (4) |
| O11 | 0.33290 (17) | 0.10533 (19) | 0.60809 (9) | 0.0282 (4) |

| | | | | |
|---|---|---|---|---|
| O12 | 0.00797 (17) | 0.16915 (18) | 0.68922 (8) | 0.0285 (3) |
| O51 | 0.21125 (18) | 0.34405 (17) | 0.15798 (8) | 0.0282 (3) |
| O52 | 0.4428 (2) | 0.4036 (2) | 0.24880 (9) | 0.0358 (4) |
| O53 | 0.45513 (17) | 0.05481 (18) | 0.24189 (8) | 0.0288 (3) |
| C1 | 0.0565 (2) | 0.2280 (2) | 0.51806 (10) | 0.0168 (4) |
| C2 | −0.1584 (2) | 0.2911 (2) | 0.51141 (11) | 0.0198 (4) |
| C3 | −0.2240 (2) | 0.3455 (2) | 0.42131 (12) | 0.0235 (5) |
| C4 | −0.0799 (2) | 0.3391 (2) | 0.33881 (11) | 0.0223 (4) |
| C5 | 0.1338 (2) | 0.2784 (2) | 0.34503 (11) | 0.0182 (4) |
| C6 | 0.2005 (2) | 0.2238 (2) | 0.43408 (11) | 0.0176 (4) |
| C11 | 0.1284 (2) | 0.1655 (2) | 0.61309 (11) | 0.0193 (4) |
| Mg1 | 0.00000 | 0.00000 | 0.00000 | 0.0200 (2) |
| O1W | 0.0127 (2) | 0.0693 (2) | 0.12890 (9) | 0.0323 (4) |
| O2W | 0.3193 (2) | −0.1459 (2) | −0.01676 (11) | 0.0338 (4) |
| O3W | 0.0515 (2) | 0.27534 (19) | −0.06749 (9) | 0.0307 (4) |
| O4W | 0.5409 (2) | 0.7353 (2) | 0.13401 (10) | 0.0313 (4) |
| H2 | −0.244 (3) | 0.264 (3) | 0.6383 (17) | 0.045 (6)* |
| H3 | −0.36580 | 0.38640 | 0.41680 | 0.0280* |
| H4 | −0.12490 | 0.37510 | 0.27890 | 0.0270* |
| H6 | 0.34260 | 0.18390 | 0.43800 | 0.0210* |
| H11 | 0.369 (4) | 0.070 (3) | 0.6595 (18) | 0.049 (7)* |
| H11W | −0.002 (3) | −0.002 (3) | 0.1845 (18) | 0.049 (6)* |
| H12W | 0.067 (4) | 0.155 (4) | 0.1343 (17) | 0.050 (7)* |
| H21W | 0.395 (4) | −0.180 (4) | 0.025 (2) | 0.061 (8)* |
| H22W | 0.383 (5) | −0.180 (4) | −0.068 (2) | 0.083 (10)* |
| H31W | −0.028 (4) | 0.370 (4) | −0.0898 (17) | 0.044 (7)* |
| H32W | 0.177 (4) | 0.293 (4) | −0.0885 (17) | 0.055 (7)* |
| H41W | 0.490 (4) | 0.826 (4) | 0.1655 (18) | 0.058 (8)* |
| H42W | 0.514 (4) | 0.631 (4) | 0.1686 (18) | 0.055 (7)* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| S5 | 0.0224 (2) | 0.0251 (2) | 0.0139 (2) | −0.0083 (2) | −0.0034 (1) | −0.0009 (1) |
| O2 | 0.0175 (6) | 0.0402 (7) | 0.0254 (7) | −0.0054 (5) | 0.0016 (5) | −0.0055 (5) |
| O11 | 0.0199 (6) | 0.0418 (7) | 0.0185 (6) | −0.0022 (5) | −0.0075 (5) | −0.0035 (5) |
| O12 | 0.0263 (6) | 0.0358 (6) | 0.0176 (6) | −0.0060 (5) | −0.0002 (5) | −0.0007 (5) |
| O51 | 0.0354 (6) | 0.0288 (6) | 0.0177 (6) | −0.0063 (5) | −0.0106 (5) | 0.0022 (4) |
| O52 | 0.0433 (7) | 0.0494 (8) | 0.0254 (6) | −0.0322 (6) | −0.0010 (6) | −0.0027 (5) |
| O53 | 0.0267 (6) | 0.0321 (6) | 0.0212 (6) | 0.0025 (5) | −0.0061 (5) | −0.0074 (5) |
| C1 | 0.0171 (7) | 0.0134 (6) | 0.0189 (7) | −0.0034 (5) | −0.0042 (6) | −0.0014 (5) |
| C2 | 0.0177 (7) | 0.0166 (7) | 0.0237 (8) | −0.0040 (6) | −0.0007 (6) | −0.0048 (6) |
| C3 | 0.0154 (7) | 0.0246 (8) | 0.0301 (9) | −0.0028 (6) | −0.0067 (6) | −0.0058 (6) |
| C4 | 0.0218 (7) | 0.0224 (7) | 0.0223 (8) | −0.0029 (6) | −0.0105 (6) | −0.0025 (6) |
| C5 | 0.0192 (7) | 0.0174 (7) | 0.0173 (7) | −0.0052 (6) | −0.0030 (6) | −0.0017 (5) |
| C6 | 0.0152 (7) | 0.0177 (7) | 0.0192 (7) | −0.0038 (5) | −0.0044 (6) | −0.0016 (5) |
| C11 | 0.0206 (7) | 0.0168 (7) | 0.0190 (7) | −0.0033 (6) | −0.0036 (6) | −0.0029 (6) |
| Mg1 | 0.0227 (4) | 0.0233 (4) | 0.0142 (4) | −0.0084 (3) | −0.0045 (3) | 0.0007 (3) |

| | | | | | | |
|---|---|---|---|---|---|---|
| O1W | 0.0492 (8) | 0.0395 (7) | 0.0156 (6) | −0.0245 (6) | −0.0067 (5) | −0.0005 (5) |
| O2W | 0.0254 (6) | 0.0455 (8) | 0.0245 (7) | −0.0053 (6) | −0.0017 (6) | −0.0042 (6) |
| O3W | 0.0247 (6) | 0.0250 (6) | 0.0371 (7) | −0.0078 (5) | −0.0063 (6) | 0.0079 (5) |
| O4W | 0.0300 (7) | 0.0287 (7) | 0.0357 (7) | −0.0114 (6) | −0.0048 (6) | −0.0022 (6) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| S5—O51 | 1.4584 (15) | O2W—H21W | 0.82 (3) |
| S5—O52 | 1.4466 (17) | O2W—H22W | 0.82 (3) |
| S5—O53 | 1.4699 (15) | O3W—H32W | 0.89 (3) |
| S5—C5 | 1.7661 (19) | O3W—H31W | 0.75 (3) |
| Mg1—O1W | 2.0396 (17) | O4W—H42W | 0.84 (3) |
| Mg1—O2W | 2.0664 (19) | O4W—H41W | 0.79 (3) |
| Mg1—O3W | 2.0494 (17) | C1—C11 | 1.476 (2) |
| Mg1—O1W$^{i}$ | 2.0396 (17) | C1—C6 | 1.394 (2) |
| Mg1—O2W$^{i}$ | 2.0664 (19) | C1—C2 | 1.408 (2) |
| Mg1—O3W$^{i}$ | 2.0494 (17) | C2—C3 | 1.393 (2) |
| O2—C2 | 1.347 (2) | C3—C4 | 1.379 (2) |
| O11—C11 | 1.314 (2) | C4—C5 | 1.399 (2) |
| O12—C11 | 1.229 (2) | C5—C6 | 1.382 (2) |
| O2—H2 | 0.85 (2) | C3—H3 | 0.9300 |
| O11—H11 | 0.79 (3) | C4—H4 | 0.9300 |
| O1W—H11W | 0.85 (2) | C6—H6 | 0.9300 |
| O1W—H12W | 0.82 (3) | | |
| | | | |
| S5···H12W | 2.96 (3) | O1W···H22W$^{i}$ | 2.83 (4) |
| S5···H42W | 3.08 (3) | O2···H3$^{v}$ | 2.5300 |
| S5···H11$^{ii}$ | 2.92 (2) | O2W···H32W | 2.87 (3) |
| S5···H22W$^{iii}$ | 2.91 (3) | O3W···H12W | 2.86 (2) |
| O1W···O2W | 2.907 (3) | O4W···H32W$^{x}$ | 1.87 (3) |
| O1W···O3W | 2.879 (2) | O4W···H21W$^{xi}$ | 1.91 (3) |
| O1W···O51 | 2.824 (2) | O11···H6 | 2.3800 |
| O1W···O12$^{iv}$ | 2.779 (2) | O11···H6$^{ii}$ | 2.5200 |
| O1W···O2W$^{i}$ | 2.900 (3) | O12···H11W$^{iv}$ | 1.93 (2) |
| O1W···O3W$^{i}$ | 2.903 (2) | O12···H2 | 1.87 (2) |
| O2···C3$^{v}$ | 3.324 (3) | O51···H4 | 2.5600 |
| O2···O11$^{vi}$ | 3.151 (3) | O51···H31W$^{ix}$ | 2.10 (3) |
| O2···O12 | 2.632 (2) | O51···H22W$^{iii}$ | 2.78 (3) |
| O2···O52$^{vii}$ | 3.207 (3) | O51···H12W | 2.00 (3) |
| O2W···O3W$^{i}$ | 2.926 (3) | O52···H6 | 2.8900 |
| O2W···O1W | 2.907 (3) | O52···H2$^{vii}$ | 2.89 (2) |
| O2W···O3W | 2.894 (2) | O52···H42W | 1.88 (3) |
| O2W···O1W$^{i}$ | 2.900 (3) | O53···H11$^{ii}$ | 1.92 (3) |
| O2W···O4W$^{viii}$ | 2.728 (3) | O53···H22W$^{iii}$ | 2.61 (3) |
| O3W···O2W | 2.894 (2) | O53···H41W$^{viii}$ | 2.04 (3) |
| O3W···O1W | 2.879 (2) | C1···C2$^{iv}$ | 3.515 (3) |
| O3W···O51$^{ix}$ | 2.850 (2) | C1···C1$^{vii}$ | 3.511 (3) |
| O3W···O1W$^{i}$ | 2.903 (2) | C1···C2$^{vii}$ | 3.543 (3) |

| | | | |
|---|---|---|---|
| O3W···O2W$^{i}$ | 2.926 (3) | C2···C1$^{vii}$ | 3.543 (3) |
| O3W···O4W$^{x}$ | 2.748 (3) | C2···C6$^{iv}$ | 3.570 (3) |
| O4W···O2W$^{xi}$ | 2.728 (3) | C2···C6$^{vii}$ | 3.509 (3) |
| O4W···O53$^{xi}$ | 2.803 (2) | C2···C1$^{iv}$ | 3.515 (3) |
| O4W···O52 | 2.717 (2) | C3···C11$^{vii}$ | 3.568 (3) |
| O4W···O3W$^{x}$ | 2.748 (3) | C3···C11$^{iv}$ | 3.490 (3) |
| O11···O2$^{xii}$ | 3.151 (3) | C3···O2$^{v}$ | 3.324 (3) |
| O11···O53$^{ii}$ | 2.678 (2) | C4···C11$^{vii}$ | 3.529 (3) |
| O11···C6$^{ii}$ | 3.264 (3) | C4···C11$^{iv}$ | 3.519 (3) |
| O12···O1W$^{iv}$ | 2.779 (2) | C6···C2$^{iv}$ | 3.570 (3) |
| O12···O2 | 2.632 (2) | C6···C2$^{vii}$ | 3.509 (3) |
| O51···O1W | 2.824 (2) | C6···O11$^{ii}$ | 3.264 (3) |
| O51···O3W$^{ix}$ | 2.850 (2) | C11···C4$^{vii}$ | 3.529 (3) |
| O52···O4W | 2.717 (2) | C11···C3$^{iv}$ | 3.490 (3) |
| O52···O2$^{vii}$ | 3.207 (3) | C11···C3$^{vii}$ | 3.568 (3) |
| O53···O4W$^{viii}$ | 2.803 (2) | C11···C4$^{iv}$ | 3.519 (3) |
| O53···O11$^{ii}$ | 2.678 (2) | C11···H2 | 2.38 (2) |
| O1W···H21W | 2.92 (3) | | |

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|---|---|---|---|
| O51—S5—O52 | 114.10 (7) | Mg1—O2W—H21W | 126.5 (19) |
| O51—S5—O53 | 110.20 (7) | H21W—O2W—H22W | 113 (3) |
| O51—S5—C5 | 107.36 (7) | Mg1—O3W—H32W | 125.3 (17) |
| O52—S5—O53 | 111.08 (8) | Mg1—O3W—H31W | 126 (2) |
| O52—S5—C5 | 106.81 (7) | H31W—O3W—H32W | 107 (3) |
| O53—S5—C5 | 106.91 (7) | H41W—O4W—H42W | 105 (3) |
| O2W—Mg1—O3W$^{i}$ | 90.64 (6) | C2—C1—C11 | 120.22 (13) |
| O1W$^{i}$—Mg1—O3W | 90.48 (5) | C6—C1—C11 | 120.43 (13) |
| O2W$^{i}$—Mg1—O3W | 90.64 (6) | C2—C1—C6 | 119.35 (13) |
| O3W—Mg1—O3W$^{i}$ | 180.00 | O2—C2—C1 | 122.58 (14) |
| O1W$^{i}$—Mg1—O2W$^{i}$ | 90.12 (6) | C1—C2—C3 | 119.67 (14) |
| O1W$^{i}$—Mg1—O3W$^{i}$ | 89.53 (5) | O2—C2—C3 | 117.75 (13) |
| O2W$^{i}$—Mg1—O3W$^{i}$ | 89.36 (6) | C2—C3—C4 | 120.41 (14) |
| O1W$^{i}$—Mg1—O2W | 89.88 (6) | C3—C4—C5 | 120.14 (14) |
| O1W—Mg1—O2W | 90.12 (6) | C4—C5—C6 | 119.90 (14) |
| O1W—Mg1—O3W | 89.53 (5) | S5—C5—C6 | 118.58 (11) |
| O1W—Mg1—O1W$^{i}$ | 180.00 | S5—C5—C4 | 121.52 (12) |
| O1W—Mg1—O2W$^{i}$ | 89.88 (6) | C1—C6—C5 | 120.53 (14) |
| O1W—Mg1—O3W$^{i}$ | 90.48 (5) | O11—C11—O12 | 123.56 (14) |
| O2W—Mg1—O3W | 89.36 (6) | O11—C11—C1 | 113.42 (13) |
| O2W—Mg1—O2W$^{i}$ | 180.00 | O12—C11—C1 | 123.02 (14) |
| C2—O2—H2 | 107.2 (15) | C2—C3—H3 | 120.00 |
| C11—O11—H11 | 112 (2) | C4—C3—H3 | 120.00 |
| Mg1—O1W—H11W | 128.1 (14) | C3—C4—H4 | 120.00 |
| Mg1—O1W—H12W | 123.6 (17) | C5—C4—H4 | 120.00 |
| H11W—O1W—H12W | 106 (2) | C1—C6—H6 | 120.00 |
| Mg1—O2W—H22W | 121 (2) | C5—C6—H6 | 120.00 |

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|---|---|---|---|
| O51—S5—C5—C4 | 1.22 (13) | C2—C1—C11—O11 | 178.30 (13) |

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|---|---|---|---|
| O51—S5—C5—C6 | −177.90 (11) | C2—C1—C11—O12 | −1.5 (2) |
| O52—S5—C5—C4 | 124.00 (12) | C6—C1—C11—O11 | −1.25 (19) |
| O52—S5—C5—C6 | −55.12 (13) | C6—C1—C11—O12 | 178.95 (13) |
| O53—S5—C5—C4 | −117.02 (12) | O2—C2—C3—C4 | 179.28 (13) |
| O53—S5—C5—C6 | 63.86 (13) | C1—C2—C3—C4 | −0.4 (2) |
| C6—C1—C2—O2 | −178.76 (13) | C2—C3—C4—C5 | −0.2 (2) |
| C6—C1—C2—C3 | 0.9 (2) | C3—C4—C5—S5 | −178.80 (11) |
| C11—C1—C2—O2 | 1.7 (2) | C3—C4—C5—C6 | 0.3 (2) |
| C11—C1—C2—C3 | −178.65 (12) | S5—C5—C6—C1 | 179.34 (10) |
| C2—C1—C6—C5 | −0.8 (2) | C4—C5—C6—C1 | 0.2 (2) |
| C11—C1—C6—C5 | 178.75 (12) | | |

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

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| O2—H2···O12 | 0.85 (2) | 1.87 (2) | 2.632 (2) | 149 (2) |
| O11—H11···O53$^{ii}$ | 0.79 (3) | 1.92 (3) | 2.678 (2) | 161 (3) |
| O1*W*—H11*W*···O12$^{iv}$ | 0.85 (2) | 1.93 (2) | 2.779 (2) | 175 (2) |
| O1*W*—H12*W*···O51 | 0.82 (3) | 2.00 (3) | 2.824 (2) | 175 (2) |
| O2*W*—H21*W*···O4*W*$^{viii}$ | 0.82 (3) | 1.91 (3) | 2.728 (3) | 173 (3) |
| O3*W*—H31*W*···O51$^{ix}$ | 0.75 (3) | 2.10 (3) | 2.850 (2) | 171 (3) |
| O3*W*—H32*W*···O4*W*$^{x}$ | 0.89 (3) | 1.87 (3) | 2.748 (3) | 167 (2) |
| O4*W*—H41*W*···O53$^{xi}$ | 0.79 (3) | 2.04 (3) | 2.803 (2) | 162 (3) |
| O4*W*—H42*W*···O52 | 0.84 (3) | 1.88 (3) | 2.717 (2) | 178 (3) |
| C3—H3···O2$^{v}$ | 0.93 | 2.53 | 3.324 (3) | 144 |
| C4—H4···O51 | 0.93 | 2.56 | 2.940 (3) | 105 |
| C6—H6···O11 | 0.93 | 2.38 | 2.705 (2) | 100 |
| C6—H6···O11$^{ii}$ | 0.93 | 2.52 | 3.264 (3) | 137 |

Symmetry codes: (ii) −*x*+1, −*y*, −*z*+1; (iv) −*x*, −*y*, −*z*+1; (v) −*x*−1, −*y*+1, −*z*+1; (viii) *x*, *y*−1, *z*; (ix) −*x*, −*y*+1, −*z*; (x) −*x*+1, −*y*+1, −*z*; (xi) *x*, *y*+1, *z*.