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mer-Triaqua(1,10-phenanthroline- κ^2N,N')(sulfato- κO)magnesium(II)

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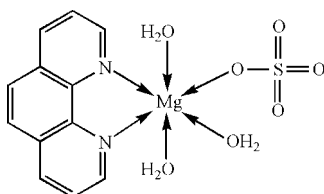
Received 15 March 2008; accepted 11 April 2008

 Key indicators: single-crystal X-ray study; $T = 295$ K; mean $\sigma(C-C) = 0.003$ Å; R factor = 0.034; wR factor = 0.098; data-to-parameter ratio = 15.3.

In the title compound, $[Mg(SO_4)(C_{12}H_8N_2)(H_2O)_3]$, the Mg^{II} centre exhibits a slightly distorted octahedral coordination environment defined by two N atoms from a 1,10-phenanthroline molecule, one O atom from a sulfate dianion and three meridionally arranged O atoms from coordinated water molecules. The crystal structure involves intra- and intermolecular $O-H\cdots O$ hydrogen bonds.

Related literature

For copper(II), zinc(II) and cadmium(II) complexes of phenanthroline, see: Xu *et al.* (2003); Zhang *et al.* (1999).



Experimental

Crystal data

 $[Mg(SO_4)(C_{12}H_8N_2)(H_2O)_3]$
 $M_r = 354.62$

 Monoclinic, $P2_1/c$
 $a = 11.968$ (2) Å

 $b = 10.025$ (2) Å

 $c = 13.798$ (3) Å

 $\beta = 113.53$ (3)°

 $V = 1517.8$ (6) Å³
 $Z = 4$

 Mo $K\alpha$ radiation

 $\mu = 0.29$ mm⁻¹
 $T = 295$ (2) K

 $0.36 \times 0.28 \times 0.20$ mm

Data collection

 Rigaku R-AXIS RAPID diffractometer
 Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
 $T_{\min} = 0.902$, $T_{\max} = 0.944$

 14532 measured reflections
 3454 independent reflections
 2941 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.023$

Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.033$
 $wR(F^2) = 0.098$
 $S = 1.07$

3454 reflections

226 parameters

9 restraints

H atoms treated by a mixture of independent and constrained refinement

 $\Delta\rho_{\max} = 0.39$ e Å⁻³
 $\Delta\rho_{\min} = -0.30$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$O2W-H2W1\cdots O3^i$	0.850 (9)	1.891 (11)	2.7170 (17)	163.8 (16)
$O3W-H3W1\cdots O2^{ii}$	0.848 (9)	1.906 (10)	2.7375 (17)	166.2 (17)
$O1W-H1W1\cdots O1^{ii}$	0.864 (9)	1.862 (10)	2.7235 (17)	174.8 (17)
$O2W-H2W2\cdots O2^{iii}$	0.852 (9)	1.873 (10)	2.7232 (17)	175.4 (19)
$O1W-H1W2\cdots O2$	0.859 (19)	1.862 (19)	2.7030 (17)	166.0 (19)
$O3W-H3W2\cdots O3^{iii}$	0.843 (9)	1.965 (10)	2.7961 (19)	168.5 (17)

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

Data collection: *RAPID-AUTO* (Rigaku, 1998); cell refinement: *RAPID-AUTO*; data reduction: *CrystalStructure* (Rigaku/MS, 2002); 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: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: IM2060).

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supplementary materials

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mer-Triaqua(1,10-phenanthroline- κ^2N,N')(sulfato- κO)magnesium(II)

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Comment

1,10-Phenanthroline (phen) is one of the most commonly used aromatic N,N' chelating ligands and has in form of several functionalized derivatives been widely used in the construction of supramolecular architectures.

Copper(II), zinc(II) and cadmium(II) derivatives of phen have been reported (Xu *et al.*, 2003; Zhang *et al.* 1999).

As a continuation of these studies, we now report the crystal structure of the title complex, (I).

As illustrated in Fig. 1, the Mg(II) ion is surrounded by two N atoms from the phen ligand and four O atoms from three meridionally arranged H₂O molecules and one sulfato group to form distorted MgN₂O₄ octahedron. The Mg—O and Mg—N bond lengths are in the normal range of 2.033 (1)–2.086 (1) and 2.210 (1)–2.234 (2) Å, respectively. The units are connected by O—H...O hydrogen bonds to produce a complex three dimensional supramolecular network, shown in figure 2.

Experimental

1,10-phenanthroline (0.05 g, 0.25 mmol) was dissolved in a water-DMF mixture (1:1 v/v, 50 ml), and MgSO₄ × 7 H₂O (0.06 g, 0.25 mmol) was added to the solution. The resulting mixture was stirred at room temperature for 12 h and filtered. Colorless single crystals of (I) were obtained from the solution after several weeks.

Refinement

The carbon-bound H atoms were positioned geometrically (C—H = 0.93–0.97 Å) and refined as riding with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$. The O-bound H atoms were located in a difference map and refined with a distance restraint of 0.85 (1) Å and the constraint $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{O})$.

Figures

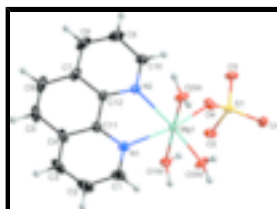


Fig. 1. Molecular structure of (I), showing 30% displacement ellipsoids level.

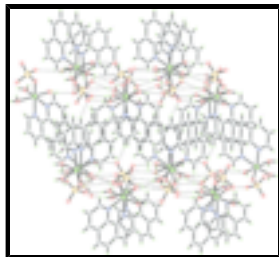


Fig. 2. Packing diagram of (I).

***mer*-Triaqua(1,10-phenanthroline- κ^2 N,N')(sulfato- κ -O)magnesium(II)**

Crystal data

[Mg(SO₄)(C₁₂H₈N₂)(H₂O)₃]

$M_r = 354.62$

Monoclinic, $P2_1/c$

Hall symbol: -P 2ybc

$a = 11.968 (2) \text{ \AA}$

$b = 10.025 (2) \text{ \AA}$

$c = 13.798 (3) \text{ \AA}$

$\beta = 113.53 (3)^\circ$

$V = 1517.8 (6) \text{ \AA}^3$

$Z = 4$

$F_{000} = 736$

$D_x = 1.552 \text{ Mg m}^{-3}$

Mo $K\alpha$ radiation

$\lambda = 0.71073 \text{ \AA}$

Cell parameters from 11791 reflections

$\theta = 3.0\text{--}27.5^\circ$

$\mu = 0.29 \text{ mm}^{-1}$

$T = 295 (2) \text{ K}$

Prism, colorless

$0.36 \times 0.28 \times 0.20 \text{ mm}$

Data collection

Rigaku R-Axis RAPID
diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

Detector resolution: $10.000 \text{ pixels mm}^{-1}$

$T = 295(2) \text{ K}$

ω scans

Absorption correction: multi-scan
(ABSCOR; Higashi, 1995)

$T_{\min} = 0.902$, $T_{\max} = 0.944$

14532 measured reflections

3454 independent reflections

2941 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.023$

$\theta_{\max} = 27.5^\circ$

$\theta_{\min} = 3.0^\circ$

$h = -15 \rightarrow 15$

$k = -12 \rightarrow 13$

$l = -17 \rightarrow 17$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.033$

$wR(F^2) = 0.098$

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

$w = 1/[\sigma^2(F_o^2) + (0.059P)^2 + 0.2998P]$
where $P = (F_o^2 + 2F_c^2)/3$

$S = 1.07$ $(\Delta/\sigma)_{\max} = 0.001$
 3454 reflections $\Delta\rho_{\max} = 0.39 \text{ e } \text{Å}^{-3}$
 226 parameters $\Delta\rho_{\min} = -0.30 \text{ e } \text{Å}^{-3}$
 9 restraints Extinction correction: none
 Primary atom site location: structure-invariant direct methods

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	$U_{\text{iso}}^*/U_{\text{eq}}$
Mg1	0.13726 (4)	0.25963 (5)	0.47420 (4)	0.02612 (13)
S1	-0.06777 (3)	0.22093 (3)	0.57725 (3)	0.02562 (11)
O1	-0.17699 (10)	0.15328 (13)	0.50549 (11)	0.0455 (3)
O1W	0.19239 (10)	0.09656 (11)	0.57638 (9)	0.0334 (2)
O2	0.01644 (11)	0.12166 (11)	0.65134 (9)	0.0366 (3)
O2W	0.08603 (12)	0.40809 (11)	0.36365 (9)	0.0391 (3)
O3	-0.09964 (11)	0.32153 (11)	0.63949 (9)	0.0384 (3)
O3W	0.06431 (12)	0.13366 (12)	0.34794 (9)	0.0446 (3)
O4	-0.00451 (10)	0.28537 (12)	0.51813 (9)	0.0382 (3)
N1	0.32491 (12)	0.24769 (13)	0.47706 (11)	0.0356 (3)
N2	0.24343 (11)	0.41322 (12)	0.58883 (10)	0.0298 (3)
C1	0.36509 (19)	0.1648 (2)	0.42311 (17)	0.0524 (5)
H1	0.3098	0.1075	0.3744	0.063*
C2	0.4875 (2)	0.1602 (2)	0.4366 (2)	0.0659 (6)
H2	0.5124	0.0993	0.3983	0.079*
C3	0.56924 (19)	0.2443 (2)	0.5052 (2)	0.0598 (6)
H3	0.6504	0.2424	0.5138	0.072*
C4	0.53087 (15)	0.3344 (2)	0.56323 (15)	0.0440 (4)
C5	0.61079 (16)	0.4266 (2)	0.63750 (18)	0.0583 (6)
H5	0.6930	0.4274	0.6495	0.070*
C6	0.56954 (18)	0.5119 (2)	0.69028 (16)	0.0587 (6)
H6	0.6237	0.5711	0.7381	0.070*
C7	0.44359 (16)	0.51409 (19)	0.67458 (13)	0.0443 (4)
C8	0.3943 (2)	0.6039 (2)	0.72430 (16)	0.0599 (6)
H8	0.4441	0.6679	0.7702	0.072*
C9	0.2739 (2)	0.5983 (2)	0.70592 (16)	0.0574 (5)

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H9	0.2405	0.6589	0.7379	0.069*
C10	0.20141 (16)	0.50001 (17)	0.63810 (13)	0.0407 (4)
H10	0.1196	0.4955	0.6271	0.049*
C11	0.40669 (13)	0.33127 (16)	0.54670 (12)	0.0324 (3)
C12	0.36302 (13)	0.42130 (15)	0.60482 (11)	0.0311 (3)
H2W1	0.0974 (17)	0.4912 (10)	0.3757 (13)	0.047*
H3W1	0.0497 (17)	0.0531 (11)	0.3577 (14)	0.047*
H1W1	0.1920 (16)	0.0180 (12)	0.5506 (14)	0.047*
H2W2	0.0668 (18)	0.3949 (17)	0.2979 (8)	0.047*
H1W2	0.1422 (15)	0.0933 (18)	0.6067 (14)	0.047*
H3W2	0.0186 (15)	0.1583 (17)	0.2863 (9)	0.047*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Mg1	0.0285 (3)	0.0215 (2)	0.0276 (3)	-0.00238 (18)	0.0104 (2)	-0.00030 (17)
S1	0.03023 (19)	0.01845 (18)	0.03043 (19)	-0.00086 (12)	0.01448 (15)	-0.00115 (12)
O1	0.0335 (6)	0.0388 (7)	0.0627 (8)	-0.0073 (5)	0.0177 (6)	-0.0200 (6)
O1W	0.0371 (6)	0.0265 (5)	0.0364 (6)	0.0044 (4)	0.0145 (5)	0.0030 (4)
O2	0.0492 (6)	0.0277 (6)	0.0367 (6)	0.0085 (5)	0.0212 (5)	0.0088 (4)
O2W	0.0656 (8)	0.0205 (5)	0.0299 (5)	-0.0014 (5)	0.0177 (5)	0.0015 (4)
O3	0.0519 (7)	0.0244 (5)	0.0410 (6)	0.0034 (5)	0.0206 (5)	-0.0070 (4)
O3W	0.0656 (8)	0.0230 (6)	0.0317 (6)	-0.0114 (5)	0.0054 (6)	-0.0001 (4)
O4	0.0349 (5)	0.0378 (6)	0.0470 (7)	0.0080 (5)	0.0216 (5)	0.0181 (5)
N1	0.0396 (7)	0.0303 (7)	0.0425 (8)	0.0008 (5)	0.0223 (7)	-0.0016 (5)
N2	0.0311 (6)	0.0278 (6)	0.0303 (6)	-0.0003 (5)	0.0121 (5)	-0.0022 (5)
C1	0.0600 (12)	0.0448 (11)	0.0648 (12)	0.0045 (9)	0.0380 (10)	-0.0088 (9)
C2	0.0752 (15)	0.0628 (14)	0.0839 (16)	0.0239 (12)	0.0573 (14)	0.0053 (12)
C3	0.0444 (11)	0.0698 (14)	0.0799 (16)	0.0211 (10)	0.0403 (12)	0.0285 (12)
C4	0.0306 (8)	0.0519 (11)	0.0512 (10)	0.0054 (7)	0.0182 (8)	0.0233 (8)
C5	0.0272 (8)	0.0749 (15)	0.0629 (12)	-0.0076 (9)	0.0076 (9)	0.0273 (11)
C6	0.0416 (9)	0.0677 (14)	0.0484 (10)	-0.0247 (10)	-0.0015 (9)	0.0075 (10)
C7	0.0443 (9)	0.0438 (10)	0.0339 (8)	-0.0147 (8)	0.0041 (7)	0.0006 (7)
C8	0.0755 (14)	0.0480 (12)	0.0442 (10)	-0.0217 (10)	0.0114 (10)	-0.0191 (9)
C9	0.0798 (15)	0.0431 (11)	0.0507 (11)	-0.0004 (10)	0.0276 (11)	-0.0178 (9)
C10	0.0481 (9)	0.0356 (9)	0.0394 (8)	0.0042 (7)	0.0186 (7)	-0.0049 (7)
C11	0.0291 (7)	0.0323 (8)	0.0364 (8)	0.0009 (6)	0.0137 (6)	0.0103 (6)
C12	0.0313 (7)	0.0298 (7)	0.0283 (7)	-0.0041 (6)	0.0078 (6)	0.0036 (6)

Geometric parameters (\AA , $^\circ$)

Mg1—O4	2.0333 (13)	C1—C2	1.403 (3)
Mg1—O2W	2.0423 (12)	C1—H1	0.9300
Mg1—O3W	2.0439 (13)	C2—C3	1.350 (3)
Mg1—O1W	2.0864 (12)	C2—H2	0.9300
Mg1—N2	2.2096 (14)	C3—C4	1.401 (3)
Mg1—N1	2.2335 (15)	C3—H3	0.9300
S1—O1	1.4545 (12)	C4—C11	1.411 (2)
S1—O4	1.4659 (11)	C4—C5	1.427 (3)

S1—O3	1.4702 (11)	C5—C6	1.339 (3)
S1—O2	1.4929 (12)	C5—H5	0.9300
O1W—H1W1	0.864 (9)	C6—C7	1.435 (3)
O1W—H1W2	0.859 (19)	C6—H6	0.9300
O2W—H2W1	0.850 (9)	C7—C8	1.397 (3)
O2W—H2W2	0.852 (9)	C7—C12	1.407 (2)
O3W—H3W1	0.848 (9)	C8—C9	1.361 (3)
O3W—H3W2	0.843 (9)	C8—H8	0.9300
N1—C1	1.327 (2)	C9—C10	1.397 (3)
N1—C11	1.354 (2)	C9—H9	0.9300
N2—C10	1.321 (2)	C10—H10	0.9300
N2—C12	1.3607 (19)	C11—C12	1.437 (2)
O4—Mg1—O2W	95.32 (5)	N1—C1—C2	122.7 (2)
O4—Mg1—O3W	102.08 (6)	N1—C1—H1	118.7
O2W—Mg1—O3W	85.12 (5)	C2—C1—H1	118.7
O4—Mg1—O1W	88.53 (5)	C3—C2—C1	119.86 (19)
O2W—Mg1—O1W	174.49 (5)	C3—C2—H2	120.1
O3W—Mg1—O1W	90.23 (5)	C1—C2—H2	120.1
O4—Mg1—N2	90.46 (5)	C2—C3—C4	119.51 (17)
O2W—Mg1—N2	86.69 (5)	C2—C3—H3	120.2
O3W—Mg1—N2	165.60 (6)	C4—C3—H3	120.2
O1W—Mg1—N2	97.24 (5)	C3—C4—C11	117.25 (18)
O4—Mg1—N1	162.63 (6)	C3—C4—C5	123.33 (18)
O2W—Mg1—N1	92.99 (6)	C11—C4—C5	119.42 (19)
O3W—Mg1—N1	93.80 (6)	C6—C5—C4	121.16 (17)
O1W—Mg1—N1	84.35 (5)	C6—C5—H5	119.4
N2—Mg1—N1	74.81 (5)	C4—C5—H5	119.4
O1—S1—O4	110.49 (8)	C5—C6—C7	121.38 (18)
O1—S1—O3	110.20 (7)	C5—C6—H6	119.3
O4—S1—O3	109.56 (7)	C7—C6—H6	119.3
O1—S1—O2	109.44 (8)	C8—C7—C12	116.99 (17)
O4—S1—O2	108.51 (6)	C8—C7—C6	124.00 (18)
O3—S1—O2	108.60 (7)	C12—C7—C6	119.01 (18)
Mg1—O1W—H1W1	119.2 (13)	C9—C8—C7	120.31 (17)
Mg1—O1W—H1W2	105.4 (13)	C9—C8—H8	119.8
H1W1—O1W—H1W2	106.0 (12)	C7—C8—H8	119.8
Mg1—O2W—H2W1	126.3 (12)	C8—C9—C10	118.85 (18)
Mg1—O2W—H2W2	123.7 (12)	C8—C9—H9	120.6
H2W1—O2W—H2W2	108.3 (13)	C10—C9—H9	120.6
Mg1—O3W—H3W1	119.9 (12)	N2—C10—C9	123.16 (17)
Mg1—O3W—H3W2	124.3 (13)	N2—C10—H10	118.4
H3W1—O3W—H3W2	110.3 (13)	C9—C10—H10	118.4
S1—O4—Mg1	141.98 (7)	N1—C11—C4	123.02 (16)
C1—N1—C11	117.67 (15)	N1—C11—C12	117.63 (13)
C1—N1—Mg1	127.63 (13)	C4—C11—C12	119.34 (16)
C11—N1—Mg1	114.61 (10)	N2—C12—C7	122.64 (15)
C10—N2—C12	117.98 (14)	N2—C12—C11	117.74 (13)
C10—N2—Mg1	126.81 (11)	C7—C12—C11	119.62 (15)
C12—N2—Mg1	115.12 (10)		

supplementary materials

O1—S1—O4—Mg1	-99.19 (14)	C2—C3—C4—C5	179.9 (2)
O3—S1—O4—Mg1	139.21 (13)	C3—C4—C5—C6	179.20 (19)
O2—S1—O4—Mg1	20.79 (15)	C11—C4—C5—C6	-1.3 (3)
O2W—Mg1—O4—S1	166.33 (13)	C4—C5—C6—C7	0.1 (3)
O3W—Mg1—O4—S1	80.20 (14)	C5—C6—C7—C8	-177.5 (2)
O1W—Mg1—O4—S1	-9.73 (14)	C5—C6—C7—C12	2.2 (3)
N2—Mg1—O4—S1	-106.96 (14)	C12—C7—C8—C9	1.0 (3)
N1—Mg1—O4—S1	-75.4 (2)	C6—C7—C8—C9	-179.3 (2)
O4—Mg1—N1—C1	146.11 (19)	C7—C8—C9—C10	1.1 (3)
O2W—Mg1—N1—C1	-95.33 (16)	C12—N2—C10—C9	-0.5 (2)
O3W—Mg1—N1—C1	-10.02 (16)	Mg1—N2—C10—C9	-176.88 (14)
O1W—Mg1—N1—C1	79.84 (16)	C8—C9—C10—N2	-1.4 (3)
N2—Mg1—N1—C1	178.93 (17)	C1—N1—C11—C4	0.5 (2)
O4—Mg1—N1—C11	-30.2 (2)	Mg1—N1—C11—C4	177.26 (12)
O2W—Mg1—N1—C11	88.34 (11)	C1—N1—C11—C12	179.79 (16)
O3W—Mg1—N1—C11	173.64 (11)	Mg1—N1—C11—C12	-3.49 (17)
O1W—Mg1—N1—C11	-96.50 (11)	C3—C4—C11—N1	-1.1 (2)
N2—Mg1—N1—C11	2.60 (10)	C5—C4—C11—N1	179.40 (15)
O4—Mg1—N2—C10	-14.19 (14)	C3—C4—C11—C12	179.68 (15)
O2W—Mg1—N2—C10	81.12 (14)	C5—C4—C11—C12	0.2 (2)
O3W—Mg1—N2—C10	136.5 (2)	C10—N2—C12—C7	2.7 (2)
O1W—Mg1—N2—C10	-102.77 (13)	Mg1—N2—C12—C7	179.56 (12)
N1—Mg1—N2—C10	175.12 (14)	C10—N2—C12—C11	-176.75 (14)
O4—Mg1—N2—C12	169.30 (10)	Mg1—N2—C12—C11	0.08 (17)
O2W—Mg1—N2—C12	-95.39 (11)	C8—C7—C12—N2	-3.0 (2)
O3W—Mg1—N2—C12	-40.0 (3)	C6—C7—C12—N2	177.28 (15)
O1W—Mg1—N2—C12	80.72 (11)	C8—C7—C12—C11	176.47 (16)
N1—Mg1—N2—C12	-1.39 (10)	C6—C7—C12—C11	-3.3 (2)
C11—N1—C1—C2	0.7 (3)	N1—C11—C12—N2	2.3 (2)
Mg1—N1—C1—C2	-175.54 (16)	C4—C11—C12—N2	-178.38 (14)
N1—C1—C2—C3	-1.4 (3)	N1—C11—C12—C7	-177.16 (14)
C1—C2—C3—C4	0.8 (3)	C4—C11—C12—C7	2.1 (2)
C2—C3—C4—C11	0.4 (3)		

Hydrogen-bond geometry (\AA , $^\circ$)

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O2W—H2W1 \cdots O3 ⁱ	0.850 (9)	1.891 (11)	2.7170 (17)	163.8 (16)
O3W—H3W1 \cdots O2 ⁱⁱ	0.848 (9)	1.906 (10)	2.7375 (17)	166.2 (17)
O1W—H1W1 \cdots O1 ⁱⁱ	0.864 (9)	1.862 (10)	2.7235 (17)	174.8 (17)
O2W—H2W2 \cdots O2 ⁱⁱⁱ	0.852 (9)	1.873 (10)	2.7232 (17)	175.4 (19)
O1W—H1W2 \cdots O2	0.859 (19)	1.862 (19)	2.7030 (17)	166.0 (19)
O3W—H3W2 \cdots O3 ⁱⁱⁱ	0.843 (9)	1.965 (10)	2.7961 (19)	168.5 (17)

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

Fig. 1

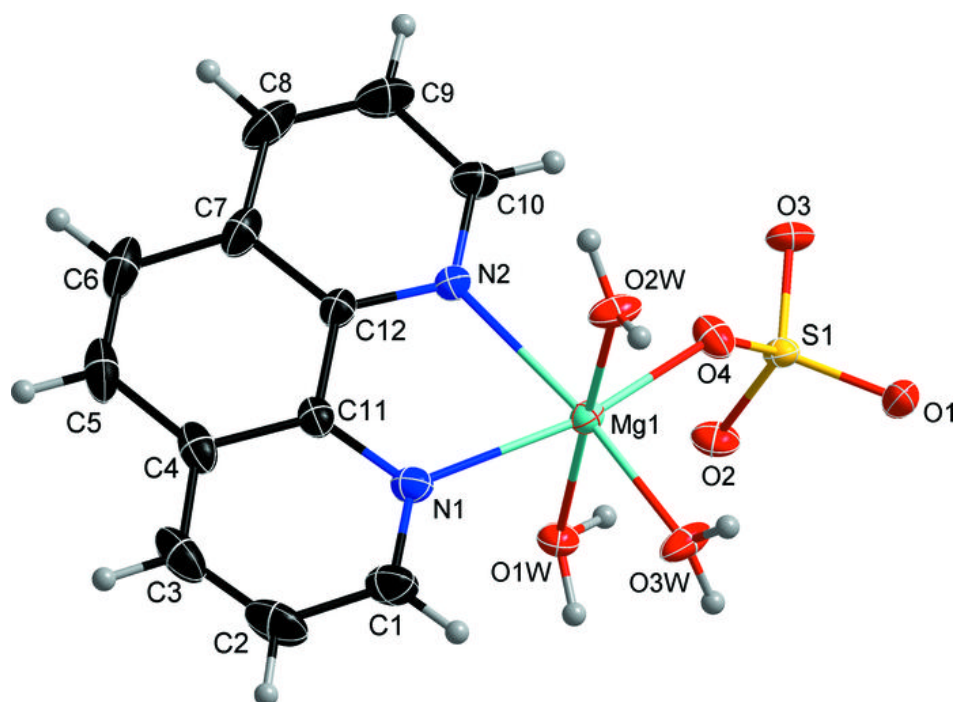


Fig. 2

