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Hexaaquamagnesium(II) bis[4-(2-hydroxybenzylideneamino)benzenesulfonate]

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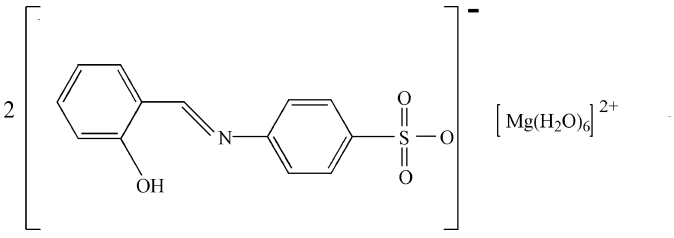
Key indicators: single-crystal X-ray study; T = 291 K; mean σ(C–C) = 0.006 Å; R factor = 0.064; wR factor = 0.146; data-to-parameter ratio = 14.8.

In the crystal structure of the title compound, $[Mg(H_2O)_6](C_{13}H_{10}NO_4S)_2$, the packing is stabilized by $O_{water}—H\cdots O_{anion}$ hydrogen bonds. An intramolecular O—H···N bond occurs in the anion. The Mg atom has site symmetry $\overline{1}$.

Related literature

For related literature, see: Tai *et al.* (2003).



Experimental

Crystal data

$[Mg(H_2O)_6](C_{13}H_{10}NO_4S)_2$
M_r = 684.97
Monoclinic, $P2_1/n$
a = 6.2997 (17) Å
b = 35.313 (9) Å
c = 6.9561 (19) Å
β = 90.75 (1)°
V = 1547.3 (7) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.26 mm^{-1}
T = 291 (2) K
0.30 × 0.24 × 0.22 mm

Data collection

Bruker SMART APEX CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
T_{min} = 0.93, T_{max} = 0.94
8390 measured reflections
3041 independent reflections
2173 reflections with $I > 2\sigma(I)$
R_{int} = 0.044

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.064
$wR(F^2)$ = 0.146
S = 1.00
3041 reflections
205 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.25 e Å^{-3}
$\Delta\rho_{min}$ = −0.46 e Å^{-3}

Table 1
Selected bond lengths (Å).

Mg1—O5	2.031 (2)	Mg1—O7	2.071 (2)
Mg1—O6	2.055 (2)		

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1*C*···N1	0.85	1.78	2.574 (5)	154
O5—H5*A*···O4^{i}	0.96	2.03	2.732 (3)	129
O5—H5*B*···O3	0.96	1.87	2.768 (3)	154
O6—H6*B*···O3^{ii}	0.96	2.19	2.749 (3)	116
O6—H6*C*···O2	0.97	1.86	2.783 (3)	160
O7—H7*B*···O4^{iii}	0.96	2.25	2.770 (3)	113
O7—H7*C*···O2^{iv}	0.95	1.85	2.760 (3)	159

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

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

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB2398).

References

Bruker (2000). *SADABS*, *SMART*, *SAINT* and *SHELXTL*. Bruker AXS Inc., Madison, Wisconsin, USA.
Tai, X.-S., Yin, X.-H., Tan, M.-Y. & Li, Y.-Z. (2003). *Acta Cryst.* E**59**, o681–o682.

  doi:10.1107/S160053680702274X

supplementary materials

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Hexaaquamagnesium(II) bis[4-(2-hydroxybenzylideneamino)benzenesulfonate]

L.-H. Wang, J. Yin and X.-S. Tai

Comment

As part of our ongoing studies of the coordination chemistry of Schiff base ligands (Tai *et al.*, 2003), we now report the synthesis and structure of the title compound, (I), (Fig. 1). Here, however, the ligand is not coordinated to the metal, but instead, a molecular salt arises.

In the crystal of (I), the Mg(II) center (site symmetry $\bar{1}$) is six-coordinate to water molecules. The C7—N1 distance [1.251 (5) Å] in the anion is close to a double-bond value. Otherwise, the geometrical parameters for (I) are normal. The dihedral angle between the two benzene ring is 32.6 (2)°, indicating that the molecule is non-planar, which perhaps correlates with the intramolecular hydrogen bond (Table 1).

Experimental

1 mmol of magnesium perchlorate was added to a solution of salicylaldehyde-4-aminobenzene sulfonic acid (1 mmol) in 10 ml of 95% ethanol. The mixture was stirred for 3 h at refluxing temperature. Evaporating some ethanol, clear blocks of (I) were obtained after two weeks.

Refinement

The O-bound H atoms were located in difference maps and refined as riding in their as-found relative positions with U_{iso}(H) = 1.2U_{eq}(O).

The other H atoms were placed geometrically (C—H = 0.93–0.96 Å, and refined as riding with U_{iso}(H) = 1.2U_{eq}(carrier) or 1.5U_{eq}(methyl C).

Figures

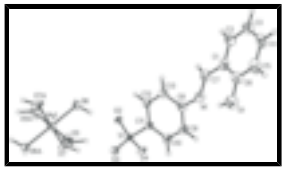

Fig. 1. The molecular structure of (I) showing 30% displacement ellipsoids (arbitrary spheres for the H atoms). Atoms with the suffix A are generated by the symmetry operator (2 − *x*, −*y*, −*z*).

Hexaaquamagnesium(II) bis[4-(2-hydroxybenzylideneamino)benzenesulfonate]

Crystal data

$[Mg(H_2O)_6](C_{13}H_{10}NO_4S)_2$	F_{000} = 716
M_r = 684.97	D_x = 1.470 Mg m^{-3}

Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
Hall symbol: -P 2yn	Cell parameters from 3237 reflections
$a = 6.2997$ (17) Å	$\theta = 2.3$–26.9°
$b = 35.313$ (9) Å	$\mu = 0.26$ mm^{-1}
$c = 6.9561$ (19) Å	$T = 291$ (2) K
$\beta = 90.75$ (1)°	Block, brown
$V = 1547.3$ (7) Å^3	0.30 × 0.24 × 0.22 mm
$Z = 2$	

Data collection

Bruker SMART APEX CCD diffractometer	3041 independent reflections
Radiation source: sealed tube	2173 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.044$
$T = 291(2)$ K	$\theta_{max} = 26.0^\circ$
phi and ω scans	$\theta_{min} = 3.0^\circ$
Absorption correction: multi-scan (SADABS; Bruker, 2000)	$h = -7\rightarrow7$
$T_{min} = 0.93$, $T_{max} = 0.94$	$k = -22\rightarrow43$
8390 measured reflections	$l = -8\rightarrow8$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.064$	H-atom parameters constrained
$wR(F^2) = 0.146$	$w = 1/[\sigma^2(F_o^2) + (0.0657P)^2 + 0.77P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.00$	$(\Delta/\sigma)_{max} < 0.001$
3041 reflections	$\Delta\rho_{max} = 0.25$ e Å^{-3}
205 parameters	$\Delta\rho_{min} = -0.46$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	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 $F^2 > 2\text{sigma}(F^2)$ 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}
C1	0.5147 (7)	0.29797 (12)	0.5190 (6)	0.0540 (10)
C2	0.6701 (8)	0.32508 (13)	0.5548 (6)	0.0647 (12)
H2	0.8064	0.3173	0.5893	0.078*
C3	0.6272 (9)	0.36279 (14)	0.5404 (7)	0.0724 (13)
H3	0.7326	0.3806	0.5663	0.087*
C4	0.4255 (9)	0.37428 (13)	0.4871 (7)	0.0712 (14)
H4	0.3957	0.4000	0.4748	0.085*
C5	0.2695 (9)	0.34828 (14)	0.4524 (6)	0.0696 (13)
H5	0.1344	0.3564	0.4158	0.083*
C6	0.3106 (8)	0.31045 (12)	0.4710 (6)	0.0575 (11)
C7	0.5634 (7)	0.25773 (12)	0.5315 (5)	0.0532 (10)
H7	0.7020	0.2506	0.5614	0.064*
C8	0.4826 (6)	0.19365 (11)	0.5055 (5)	0.0466 (9)
C9	0.3252 (6)	0.16787 (12)	0.5564 (6)	0.0556 (10)
H9	0.1914	0.1765	0.5901	0.067*
C10	0.3670 (6)	0.13009 (12)	0.5569 (6)	0.0495 (9)
H10	0.2622	0.1130	0.5925	0.059*
C11	0.5665 (5)	0.11689 (10)	0.5043 (4)	0.0349 (7)
C12	0.7255 (6)	0.14225 (11)	0.4507 (5)	0.0455 (9)
H12	0.8588	0.1336	0.4155	0.055*
C13	0.6805 (6)	0.18019 (12)	0.4514 (6)	0.0525 (10)
H13	0.7845	0.1973	0.4148	0.063*
Mg1	1.0000	0.0000	0.0000	0.0385 (4)
N1	0.4280 (5)	0.23230 (10)	0.5038 (5)	0.0536 (8)
O1	0.1544 (5)	0.28509 (10)	0.4396 (5)	0.0771 (10)
H1C	0.2119	0.2635	0.4541	0.092*
O2	0.8439 (3)	0.06285 (7)	0.4953 (3)	0.0406 (6)
O3	0.5166 (4)	0.05345 (7)	0.3242 (3)	0.0465 (6)
O4	0.5167 (4)	0.05225 (7)	0.6716 (3)	0.0452 (6)
O5	0.7139 (3)	0.02654 (7)	−0.0016 (3)	0.0421 (6)
H5A	0.7144	0.0460	−0.0981	0.063*
H5B	0.6887	0.0377	0.1221	0.063*
O6	1.1087 (4)	0.03733 (8)	0.2055 (4)	0.0536 (7)
H6B	1.2111	0.0247	0.2852	0.080*
H6C	0.9918	0.0457	0.2832	0.080*
O7	0.8927 (4)	−0.03449 (8)	0.2191 (4)	0.0519 (7)
H7B	0.7912	−0.0209	0.2956	0.078*
H7C	1.0104	−0.0419	0.2983	0.078*
S1	0.61427 (12)	0.06773 (2)	0.49840 (11)	0.0325 (2)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.067 (3)	0.050 (2)	0.046 (2)	0.0107 (19)	0.0090 (19)	0.0048 (17)

C2	0.070 (3)	0.053 (3)	0.071 (3)	0.002 (2)	0.002 (2)	0.005 (2)
C3	0.086 (4)	0.057 (3)	0.075 (3)	−0.008 (3)	0.014 (3)	0.003 (2)
C4	0.107 (4)	0.044 (2)	0.063 (3)	0.018 (3)	0.012 (3)	0.002 (2)
C5	0.098 (4)	0.059 (3)	0.052 (3)	0.028 (3)	−0.008 (2)	0.010 (2)
C6	0.072 (3)	0.052 (2)	0.048 (2)	0.003 (2)	−0.004 (2)	0.0087 (18)
C7	0.057 (3)	0.052 (2)	0.050 (2)	0.015 (2)	−0.0015 (18)	0.0063 (18)
C8	0.049 (2)	0.041 (2)	0.049 (2)	0.0062 (17)	−0.0054 (16)	0.0030 (16)
C9	0.036 (2)	0.059 (3)	0.072 (3)	0.0088 (18)	0.0053 (18)	−0.002 (2)
C10	0.0361 (19)	0.053 (2)	0.059 (2)	0.0043 (17)	0.0096 (16)	−0.0018 (18)
C11	0.0269 (16)	0.0469 (19)	0.0309 (15)	−0.0006 (13)	−0.0022 (12)	0.0033 (14)
C12	0.0388 (19)	0.047 (2)	0.051 (2)	0.0036 (16)	0.0147 (16)	0.0013 (16)
C13	0.051 (2)	0.049 (2)	0.058 (2)	−0.0100 (18)	0.0121 (18)	−0.0013 (18)
Mg1	0.0372 (9)	0.0385 (9)	0.0398 (9)	−0.0013 (7)	−0.0019 (6)	−0.0002 (7)
N1	0.057 (2)	0.052 (2)	0.0507 (19)	0.0073 (17)	−0.0018 (15)	0.0017 (15)
O1	0.069 (2)	0.066 (2)	0.096 (3)	0.0148 (17)	−0.0236 (18)	0.0034 (17)
O2	0.0178 (10)	0.0545 (15)	0.0494 (13)	0.0060 (9)	−0.0004 (9)	−0.0018 (11)
O3	0.0340 (12)	0.0584 (16)	0.0470 (14)	0.0014 (11)	−0.0062 (10)	−0.0143 (12)
O4	0.0306 (12)	0.0580 (16)	0.0471 (14)	0.0023 (11)	0.0035 (10)	0.0138 (12)
O5	0.0310 (12)	0.0564 (15)	0.0388 (12)	0.0093 (11)	0.0012 (9)	−0.0032 (11)
O6	0.0300 (13)	0.077 (2)	0.0534 (16)	0.0003 (12)	−0.0036 (11)	−0.0246 (14)
O7	0.0286 (12)	0.0743 (19)	0.0528 (15)	−0.0006 (11)	0.0012 (10)	0.0264 (13)
S1	0.0202 (4)	0.0428 (5)	0.0345 (4)	0.0020 (3)	−0.0012 (3)	−0.0007 (3)

Geometric parameters (Å, °)

C1—C2	1.389 (6)	C11—C12	1.398 (5)
C1—C6	1.396 (6)	C11—S1	1.762 (4)
C1—C7	1.456 (6)	C12—C13	1.369 (5)
C2—C3	1.362 (7)	C12—H12	0.9300
C2—H2	0.9300	C13—H13	0.9300
C3—C4	1.380 (7)	Mg1—O5	2.031 (2)
C3—H3	0.9300	Mg1—O5^{i}	2.031 (2)
C4—C5	1.364 (7)	Mg1—O6	2.055 (2)
C4—H4	0.9300	Mg1—O6^{i}	2.055 (2)
C5—C6	1.366 (6)	Mg1—O7^{i}	2.071 (2)
C5—H5	0.9300	Mg1—O7	2.071 (2)
C6—O1	1.346 (5)	O1—H1C	0.8500
C7—N1	1.251 (5)	O2—S1	1.457 (2)
C7—H7	0.9300	O3—S1	1.443 (2)
C8—C13	1.391 (5)	O4—S1	1.465 (2)
C8—C9	1.395 (6)	O5—H5A	0.9599
C8—N1	1.408 (5)	O5—H5B	0.9618
C9—C10	1.360 (6)	O6—H6B	0.9551
C9—H9	0.9300	O6—H6C	0.9653
C10—C11	1.394 (5)	O7—H7B	0.9645
C10—H10	0.9300	O7—H7C	0.9544
C2—C1—C6	118.0 (4)	C12—C13—C8	121.4 (4)
C2—C1—C7	121.0 (4)	C12—C13—H13	119.3

C6—C1—C7	121.0 (4)	C8—C13—H13	119.3
C3—C2—C1	121.5 (5)	O5—Mg1—O5^{i}	180.0
C3—C2—H2	119.3	O5—Mg1—O6	89.73 (10)
C1—C2—H2	119.3	O5^{i}—Mg1—O6	90.27 (10)
C2—C3—C4	119.2 (5)	O5—Mg1—O6^{i}	90.27 (10)
C2—C3—H3	120.4	O5^{i}—Mg1—O6^{i}	89.73 (10)
C4—C3—H3	120.4	O6—Mg1—O6^{i}	180.0
C5—C4—C3	120.6 (4)	O5—Mg1—O7^{i}	91.30 (10)
C5—C4—H4	119.7	O5^{i}—Mg1—O7^{i}	88.70 (10)
C3—C4—H4	119.7	O6—Mg1—O7^{i}	91.47 (11)
C4—C5—C6	120.4 (5)	O6^{i}—Mg1—O7^{i}	88.53 (11)
C4—C5—H5	119.8	O5—Mg1—O7	88.70 (10)
C6—C5—H5	119.8	O5^{i}—Mg1—O7	91.30 (10)
O1—C6—C5	119.9 (4)	O6—Mg1—O7	88.53 (11)
O1—C6—C1	119.9 (4)	O6^{i}—Mg1—O7	91.47 (11)
C5—C6—C1	120.2 (5)	O7^{i}—Mg1—O7	180.0
N1—C7—C1	123.3 (4)	C7—N1—C8	121.9 (4)
N1—C7—H7	118.4	C6—O1—H1C	105.6
C1—C7—H7	118.4	Mg1—O5—H5A	108.8
C13—C8—C9	119.2 (4)	Mg1—O5—H5B	110.0
C13—C8—N1	123.3 (4)	H5A—O5—H5B	109.5
C9—C8—N1	117.4 (4)	Mg1—O6—H6B	108.7
C10—C9—C8	120.2 (4)	Mg1—O6—H6C	109.7
C10—C9—H9	119.9	H6B—O6—H6C	109.4
C8—C9—H9	119.9	Mg1—O7—H7B	109.8
C9—C10—C11	120.2 (4)	Mg1—O7—H7C	109.1
C9—C10—H10	119.9	H7B—O7—H7C	109.5
C11—C10—H10	119.9	O3—S1—O2	111.04 (14)
C10—C11—C12	120.5 (3)	O3—S1—O4	112.40 (15)
C10—C11—S1	119.4 (3)	O2—S1—O4	113.27 (14)
C12—C11—S1	120.1 (3)	O3—S1—C11	107.02 (15)
C13—C12—C11	118.5 (3)	O2—S1—C11	106.65 (14)
C13—C12—H12	120.8	O4—S1—C11	105.96 (15)
C11—C12—H12	120.8		

Symmetry codes: (i) −*x*+2, −*y*, −*z*.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1C···N1	0.85	1.78	2.574 (5)	154
O5—H5A···O4^{ii}	0.96	2.03	2.732 (3)	129
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O6—H6C···O2	0.97	1.86	2.783 (3)	160
O7—H7B···O4^{iv}	0.96	2.25	2.770 (3)	113
O7—H7C···O2^{v}	0.95	1.85	2.760 (3)	159

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

Fig. 1