Acta Crystallographica Section E
**Structure Reports Online**
ISSN 1600-5368

# Bis(1-acetyl-2-naphtholato)diaqua-magnesium(II)

**Li-Hua Wang,[a] Jie Yin[b] and Xi-Shi Tai[c]***

[a]College of Information and Autocontrol Engineering, Weifang University, Weifang 261061, People's Republic of China, [b]Department of Chemistry and Chemical Engineering, Ningxia University, Yinchuan 750021, People's Republic of China, and [c]Department of Chemistry and Chemical Engineering, Weifang University, Weifang 261061, People's Republic of China
Correspondence e-mail: taixishi@lzu.edu.cn

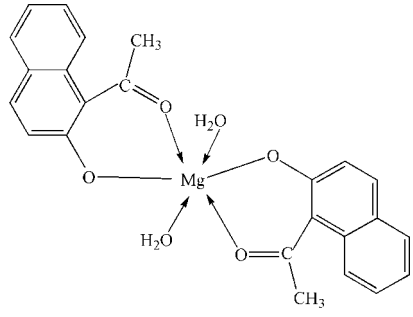
Received 29 April 2007; accepted 14 May 2007

Key indicators: single-crystal X-ray study; $T$ = 291 K; mean $\sigma$(C–C) = 0.003 Å; $R$ factor = 0.052; $wR$ factor = 0.115; data-to-parameter ratio = 13.6.

In the title compound, $[Mg(C_{12}H_9O_2)_2(H_2O)_2]$, the magnesium cation (site symmetry $\overline{1}$) is octahedrally coordinated by two $O,O'$-bidentate 1-acetyl-2-naphtholate anions and two water molecules. Intermolecular O—H···O hydrogen bonds help to consolidate the crystal packing.

## Related literature

For background information on magnesium coordination chemistry, see: Erxleben *et al.* (2001).




## Experimental

### Crystal data

$[Mg(C_{12}H_9O_2)_2(H_2O)_2]$
$M_r$ = 430.73
Orthorhombic, *Pbca*
$a$ = 33.261 (19) Å
$b$ = 7.951 (5) Å
$c$ = 7.461 (5) Å
$V$ = 1973 (2) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.13 mm$^{-1}$
$T$ = 291 (2) K
0.30 × 0.22 × 0.20 mm

### Data collection

Bruker SMART APEX CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
$T_{min}$ = 0.97, $T_{max}$ = 0.98
9925 measured reflections
1940 independent reflections
1486 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.055

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.052
$wR(F^2)$ = 0.115
$S$ = 1.06
1940 reflections
143 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.18 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.18 e Å$^{-3}$

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

| | | | |
|---|---|---|---|
| Mg1—O1 | 1.9940 (16) | Mg1—O2 | 2.0545 (17) |
| Mg1—O3 | 2.0283 (19) | | |

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| O3—H3$A$···O2$^{ii}$ | 0.95 | 2.00 | 2.885 (2) | 153 |
| O3—H3$B$···O1$^{iii}$ | 0.97 | 2.02 | 2.742 (3) | 130 |

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

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*.

The authors thank the National Natural Science Foundation of China (20671073), the NingXia Natural Gas Transferring Key Laboratory (2004007), the Science and Technology Foundation of Weifang and Weifang University for research grants.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB2401).

## References

Bruker (2000). *SMART*, *SAINT*, *SADABS* and *SHELXTL*. Bruker AXS Inc., Madison, Wisconsin, USA.
Erxleben, A. & Schumacher, D. (2001). *Eur. J. Inorg. Chem.* pp. 3039–3043.

# supplementary materials

*Acta Cryst.* (2007). E**63**, m1665 [ **doi:10.1107/S1600536807023677** ]

# Bis(1-acetyl-2-naphtholato)diaquamagnesium(II)

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

## Comment

The coordination chemistry of Mg(II) ion has received more and more attention over the past two decades (Erxleben *et al.*, 2001). We now report the synthesis and structure of the title compound, (I), (Fig. 1).

In the molecule of (I), The Mg (II) center (site symmetry $\bar{1}$) is six-coordinate (Table 1) with six O-atom donors of 1-acetyl-2-naphthol and $H_2O$. The C11—O2 [1.249 (2) Å] length is close to a double-bond. Otherwise, the geometrical parameters for (I) are normal. Intermolecular O—H···O hydrogen bonds occur and help to consolidate the crystal packing (Table 2).

## Experimental

1 mmol of magnesium perchlorate was added to a solution of 1-acetyl-2-naphthol (2 mmol) in 10 ml of 95% ethanol. The mixture was stirred for 3 h at refluxing temperature. After evaporating some ethanol, clear blocks of (I) were obtained after two weeks.

## Refinement

The water H atoms were located in a difference map and refined as riding with $U_{iso}(H) = 1.2U_{eq}(O)$. The C-bound H atoms were placed geometrically (C—H = 0.93–0.96 Å, and refined as riding with $U_{iso}(H) = 1.2U_{eq}(C)$ or $1.5U_{eq}$(methyl C).

## Figures

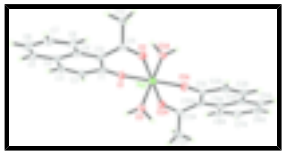


Fig. 1. The molecular structure of (I) showing 30% displacement ellipsoids (arbitrary spheres for the H atoms). Atoms with the suffix A are generated by the symmetry operation (−*x*, −*y*, −*z*).

### bis(1-acetyl-2-naphtholato)diaquamagnesium(II)

*Crystal data*

| | |
|---|---|
| $[Mg(C_{12}H_9O_2)_2(H_2O)_2]$ | $F_{000}$ = 904 |
| $M_r$ = 430.73 | $D_x$ = 1.450 Mg m$^{-3}$ |
| Orthorhombic, *Pbca* | Mo *K*α radiation<br>λ = 0.71073 Å |
| Hall symbol: -P 2ac 2ab | Cell parameters from 548 reflections |
| *a* = 33.261 (19) Å | θ = 2.1–20.2º |

| | |
|---|---|
| $b$ = 7.951 (5) Å | μ = 0.13 mm$^{-1}$ |
| $c$ = 7.461 (5) Å | $T$ = 291 (2) K |
| $V$ = 1973 (2) Å$^3$ | Block, colourless |
| $Z$ = 4 | 0.30 × 0.22 × 0.20 mm |

*Data collection*

| | |
|---|---|
| Bruker Smart Apex CCD diffractometer | 1940 independent reflections |
| Radiation source: sealed tube | 1486 reflections with $I > 2\sigma(I)$ |
| Monochromator: graphite | $R_{int}$ = 0.055 |
| $T$ = 291(2) K | $\theta_{max}$ = 26.0º |
| ω scans | $\theta_{min}$ = 2.5º |
| Absorption correction: multi-scan (SADABS; Bruker, 2000) | $h$ = −40→40 |
| $T_{min}$ = 0.97, $T_{max}$ = 0.98 | $k$ = −8→9 |
| 9925 measured reflections | $l$ = −8→9 |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Secondary atom site location: difference Fourier map |
| Least-squares matrix: full | Hydrogen site location: difmap and geom |
| $R[F^2 > 2\sigma(F^2)]$ = 0.052 | H-atom parameters constrained |
| $wR(F^2)$ = 0.115 | $w = 1/[\sigma^2(F_o^2) + (0.05P)^2 + 0.55P]$ where $P = (F_o^2 + 2F_c^2)/3$ |
| $S$ = 1.06 | $(\Delta/\sigma)_{max} < 0.001$ |
| 1940 reflections | $\Delta\rho_{max}$ = 0.18 e Å$^{-3}$ |
| 143 parameters | $\Delta\rho_{min}$ = −0.18 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 | 0.08501 (6) | 0.0828 (3) | −0.0880 (3) | 0.0288 (5) |

| | | | | |
|---|---|---|---|---|
| C2 | 0.11300 (7) | 0.2069 (3) | −0.1541 (3) | 0.0353 (5) |
| H2 | 0.1033 | 0.2962 | −0.2219 | 0.042* |
| C3 | 0.15261 (7) | 0.1974 (3) | −0.1209 (3) | 0.0390 (6) |
| H3 | 0.1694 | 0.2797 | −0.1680 | 0.047* |
| C4 | 0.16966 (7) | 0.0680 (3) | −0.0178 (3) | 0.0349 (5) |
| C5 | 0.21048 (7) | 0.0694 (3) | 0.0294 (3) | 0.0440 (6) |
| H5 | 0.2270 | 0.1553 | −0.0124 | 0.053* |
| C6 | 0.22596 (8) | −0.0506 (4) | 0.1333 (4) | 0.0515 (7) |
| H6 | 0.2532 | −0.0510 | 0.1612 | 0.062* |
| C7 | 0.20078 (8) | −0.1747 (3) | 0.1989 (3) | 0.0446 (6) |
| H7 | 0.2114 | −0.2557 | 0.2753 | 0.054* |
| C8 | 0.16091 (7) | −0.1827 (3) | 0.1556 (3) | 0.0397 (6) |
| H8 | 0.1452 | −0.2693 | 0.2013 | 0.048* |
| C9 | 0.14354 (6) | −0.0621 (3) | 0.0433 (3) | 0.0305 (5) |
| C10 | 0.10135 (7) | −0.0597 (3) | −0.0013 (3) | 0.0310 (5) |
| C11 | 0.07582 (7) | −0.2100 (2) | 0.0240 (3) | 0.0274 (5) |
| C12 | 0.09151 (8) | −0.3890 (3) | 0.0021 (3) | 0.0398 (6) |
| H12A | 0.0898 | −0.4469 | 0.1147 | 0.060* |
| H12B | 0.1190 | −0.3857 | −0.0366 | 0.060* |
| H12C | 0.0756 | −0.4470 | −0.0857 | 0.060* |
| Mg1 | 0.0000 | 0.0000 | 0.0000 | 0.0322 (3) |
| O1 | 0.04736 (4) | 0.10416 (19) | −0.1205 (2) | 0.0332 (4) |
| O2 | 0.03866 (4) | −0.19729 (18) | 0.0438 (2) | 0.0362 (4) |
| O3 | 0.01541 (5) | 0.1075 (2) | 0.2367 (2) | 0.0424 (4) |
| H3A | −0.0085 | 0.1493 | 0.2911 | 0.051* |
| H3B | 0.0338 | 0.2002 | 0.2188 | 0.051* |

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

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| C1 | 0.0347 (12) | 0.0239 (11) | 0.0277 (11) | −0.0001 (9) | 0.0053 (9) | −0.0074 (9) |
| C2 | 0.0465 (14) | 0.0251 (11) | 0.0344 (12) | −0.0073 (10) | 0.0049 (10) | 0.0058 (9) |
| C3 | 0.0452 (13) | 0.0337 (13) | 0.0381 (13) | −0.0123 (10) | 0.0075 (11) | 0.0001 (10) |
| C4 | 0.0415 (14) | 0.0367 (12) | 0.0266 (12) | −0.0006 (10) | 0.0055 (9) | −0.0063 (10) |
| C5 | 0.0318 (13) | 0.0524 (15) | 0.0478 (16) | −0.0090 (11) | 0.0031 (11) | −0.0110 (13) |
| C6 | 0.0376 (14) | 0.0677 (19) | 0.0492 (16) | 0.0067 (13) | −0.0056 (12) | −0.0071 (14) |
| C7 | 0.0464 (15) | 0.0465 (14) | 0.0409 (14) | 0.0144 (12) | −0.0089 (11) | 0.0019 (12) |
| C8 | 0.0377 (13) | 0.0457 (14) | 0.0356 (13) | 0.0073 (11) | −0.0006 (10) | 0.0071 (11) |
| C9 | 0.0333 (12) | 0.0360 (12) | 0.0223 (11) | 0.0037 (9) | 0.0018 (8) | −0.0011 (9) |
| C10 | 0.0376 (12) | 0.0294 (11) | 0.0261 (11) | 0.0055 (9) | 0.0092 (9) | 0.0014 (9) |
| C11 | 0.0391 (12) | 0.0222 (11) | 0.0209 (11) | 0.0051 (9) | 0.0030 (8) | −0.0020 (8) |
| C12 | 0.0532 (15) | 0.0199 (11) | 0.0462 (14) | 0.0007 (10) | 0.0033 (12) | 0.0018 (10) |
| Mg1 | 0.0347 (6) | 0.0268 (5) | 0.0351 (6) | −0.0003 (4) | −0.0014 (4) | 0.0002 (5) |
| O1 | 0.0309 (8) | 0.0266 (8) | 0.0422 (9) | 0.0022 (6) | 0.0003 (7) | 0.0081 (7) |
| O2 | 0.0338 (9) | 0.0279 (9) | 0.0469 (10) | 0.0027 (6) | 0.0026 (7) | 0.0030 (7) |
| O3 | 0.0429 (10) | 0.0408 (9) | 0.0435 (10) | −0.0023 (7) | 0.0074 (8) | −0.0149 (8) |

*Geometric parameters (Å, °)*

| | | | |
|---|---|---|---|
| C1—O1 | 1.287 (3) | C8—H8 | 0.9300 |
| C1—C10 | 1.414 (3) | C9—C10 | 1.442 (3) |
| C1—C2 | 1.443 (3) | C10—C11 | 1.478 (3) |
| C2—C3 | 1.343 (3) | C11—O2 | 1.249 (3) |
| C2—H2 | 0.9300 | C11—C12 | 1.525 (3) |
| C3—C4 | 1.404 (3) | C12—H12A | 0.9600 |
| C3—H3 | 0.9300 | C12—H12B | 0.9600 |
| C4—C5 | 1.403 (3) | C12—H12C | 0.9600 |
| C4—C9 | 1.425 (3) | Mg1—O1 | 1.9940 (16) |
| C5—C6 | 1.333 (4) | Mg1—O1$^{i}$ | 1.9940 (16) |
| C5—H5 | 0.9300 | Mg1—O3$^{i}$ | 2.0283 (19) |
| C6—C7 | 1.384 (4) | Mg1—O3 | 2.0283 (19) |
| C6—H6 | 0.9300 | Mg1—O2$^{i}$ | 2.0545 (17) |
| C7—C8 | 1.366 (3) | Mg1—O2 | 2.0545 (17) |
| C7—H7 | 0.9300 | O3—H3A | 0.9522 |
| C8—C9 | 1.398 (3) | O3—H3B | 0.9661 |
| O1—C1—C10 | 124.47 (19) | O2—C11—C10 | 121.23 (18) |
| O1—C1—C2 | 118.3 (2) | O2—C11—C12 | 115.27 (19) |
| C10—C1—C2 | 117.1 (2) | C10—C11—C12 | 122.96 (19) |
| C3—C2—C1 | 122.1 (2) | C11—C12—H12A | 109.5 |
| C3—C2—H2 | 119.0 | C11—C12—H12B | 109.5 |
| C1—C2—H2 | 119.0 | H12A—C12—H12B | 109.5 |
| C2—C3—C4 | 122.6 (2) | C11—C12—H12C | 109.5 |
| C2—C3—H3 | 118.7 | H12A—C12—H12C | 109.5 |
| C4—C3—H3 | 118.7 | H12B—C12—H12C | 109.5 |
| C5—C4—C3 | 121.5 (2) | O1—Mg1—O1$^{i}$ | 180.0 |
| C5—C4—C9 | 121.1 (2) | O1—Mg1—O3$^{i}$ | 88.96 (7) |
| C3—C4—C9 | 117.4 (2) | O1$^{i}$—Mg1—O3$^{i}$ | 91.04 (7) |
| C6—C5—C4 | 120.9 (2) | O1—Mg1—O3 | 91.04 (7) |
| C6—C5—H5 | 119.5 | O1$^{i}$—Mg1—O3 | 88.96 (7) |
| C4—C5—H5 | 119.5 | O3$^{i}$—Mg1—O3 | 180.0 |
| C5—C6—C7 | 118.8 (2) | O1—Mg1—O2$^{i}$ | 96.05 (7) |
| C5—C6—H6 | 120.6 | O1$^{i}$—Mg1—O2$^{i}$ | 83.95 (7) |
| C7—C6—H6 | 120.6 | O3$^{i}$—Mg1—O2$^{i}$ | 91.44 (7) |
| C8—C7—C6 | 122.5 (2) | O3—Mg1—O2$^{i}$ | 88.56 (7) |
| C8—C7—H7 | 118.8 | O1—Mg1—O2 | 83.95 (7) |
| C6—C7—H7 | 118.8 | O1$^{i}$—Mg1—O2 | 96.05 (7) |
| C7—C8—C9 | 120.7 (2) | O3$^{i}$—Mg1—O2 | 88.56 (7) |
| C7—C8—H8 | 119.6 | O3—Mg1—O2 | 91.44 (7) |
| C9—C8—H8 | 119.6 | O2$^{i}$—Mg1—O2 | 180.0 |
| C8—C9—C4 | 115.9 (2) | C1—O1—Mg1 | 128.98 (14) |
| C8—C9—C10 | 123.3 (2) | C11—O2—Mg1 | 131.47 (14) |
| C4—C9—C10 | 120.7 (2) | Mg1—O3—H3A | 107.9 |

| | | | |
|---|---|---|---|
| C1—C10—C9 | 119.3 (2) | Mg1—O3—H3B | 111.1 |
| C1—C10—C11 | 119.1 (2) | H3A—O3—H3B | 108.7 |
| C9—C10—C11 | 121.27 (19) | | |

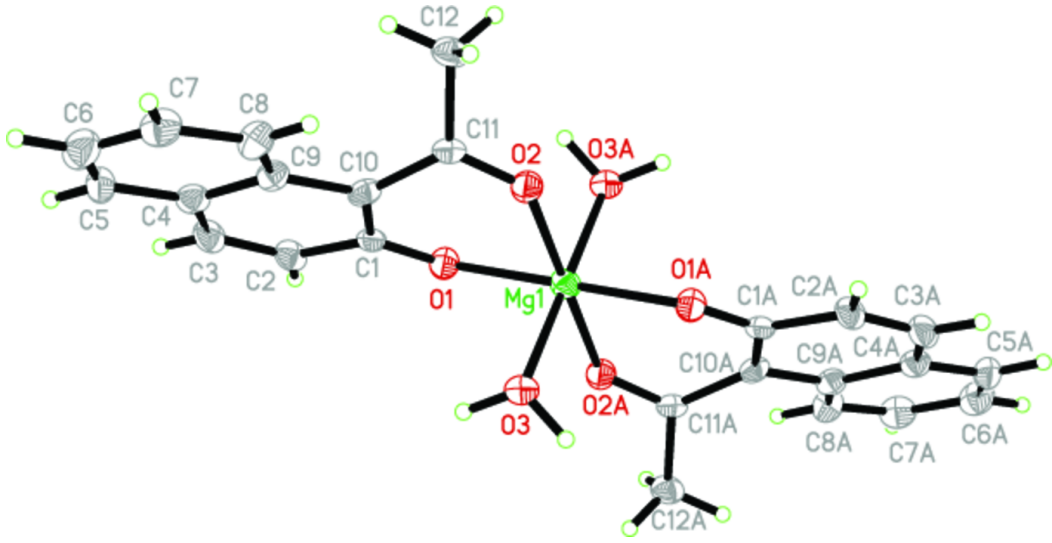
Symmetry codes: (i) −*x*, −*y*, −*z*.

*Hydrogen-bond geometry (Å, °)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| O3—H3A···O2$^{ii}$ | 0.95 | 2.00 | 2.885 (2) | 153 |
| O3—H3B···O1$^{iii}$ | 0.97 | 2.02 | 2.742 (3) | 130 |

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

**Fig. 1**


C12
C7
C8
C6
C11
C9
C10
O2
O3A
C5
C4
C3
C2
C1
O1
Mg1
O1A
C1A
C2A
C3A
C5A
C10A
C9A
C4A
O2A
C11A
O3
C8A
C7A
C6A
C12A