

# Poly[diaqua( $\mu_3$ -1*H*-benzimidazole-5,6-dicarboxylato- $\kappa^4$ N<sup>3</sup>:O<sup>5</sup>,O<sup>6</sup>:O<sup>6'</sup>)-magnesium(II)]

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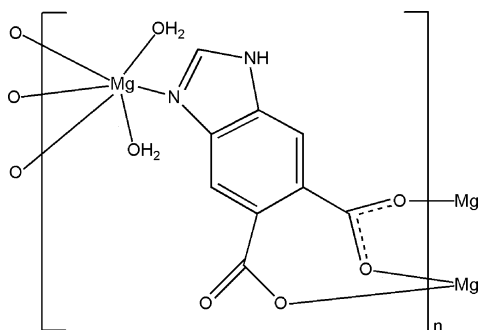
Received 28 December 2009; accepted 8 January 2010

Key indicators: single-crystal X-ray study;  $T = 293$  K; mean  $\sigma(\text{C}-\text{C}) = 0.005$  Å;  $R$  factor = 0.036;  $wR$  factor = 0.090; data-to-parameter ratio = 7.0.

In the title complex,  $[\text{Mg}(\text{C}_9\text{H}_4\text{N}_2\text{O}_4)(\text{H}_2\text{O})_2]_n$ , the  $\text{Mg}^{\text{II}}$  atom is six-coordinated by one N and three O atoms from three different 1*H*-benzimidazole-5,6-dicarboxylate ligands and two O atoms from two water molecules, forming a slightly distorted octahedral geometry. The ligand links the  $\text{Mg}^{\text{II}}$  centres into a three-dimensional network. Extensive N—H...O and O—H...O hydrogen bonds exist between the ligands and water molecules, stabilizing the crystal structure.

## Related literature

For related structures of 1*H*-benzimidazole-5,6-dicarboxylate complexes, see: Song, Wang, Hu *et al.* (2009); Song, Wang, Li *et al.* (2009); Song, Wang, Qin *et al.* (2009); Wang *et al.* (2009).



## Experimental

### Crystal data

$[\text{Mg}(\text{C}_9\text{H}_4\text{N}_2\text{O}_4)(\text{H}_2\text{O})_2]$

$M_r = 264.48$

Monoclinic,  $Cc$

$a = 7.4793$  (15) Å

$b = 18.958$  (4) Å

$c = 7.3132$  (15) Å

$\beta = 99.38$  (3)°

$V = 1023.1$  (4) Å<sup>3</sup>

$Z = 4$

Mo  $K\alpha$  radiation

$\mu = 0.20$  mm<sup>-1</sup>

$T = 293$  K

$0.30 \times 0.25 \times 0.21$  mm

### Data collection

Rigaku/MSM Mercury CCD

diffractometer

Absorption correction: multi-scan

(*REQAB*; Jacobson, 1998)

$T_{\text{min}} = 0.943$ ,  $T_{\text{max}} = 0.960$

4611 measured reflections

1143 independent reflections

1096 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.031$

### Refinement

$R[F^2 > 2\sigma(F^2)] = 0.036$

$wR(F^2) = 0.090$

$S = 1.06$

1143 reflections

163 parameters

2 restraints

H-atom parameters constrained

$\Delta\rho_{\text{max}} = 0.38$  e Å<sup>-3</sup>

$\Delta\rho_{\text{min}} = -0.25$  e Å<sup>-3</sup>

**Table 1**

Selected bond lengths (Å).

Mg1—N1	2.195 (3)	Mg1—O4 <sup>ii</sup>	2.113 (3)
Mg1—O1 <sup>i</sup>	2.051 (3)	Mg1—O1W	2.063 (3)
Mg1—O3 <sup>i</sup>	2.106 (3)	Mg1—O2W	2.074 (3)

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

**Table 2**

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
N3—H3 $\cdots$ O1 <sup>iii</sup>	0.86	2.29	2.992 (4)	138
O1W—H1W $\cdots$ O2 <sup>iv</sup>	0.84	1.84	2.651 (4)	163
O1W—H2W $\cdots$ O3 <sup>ii</sup>	0.84	1.92	2.734 (4)	164
O2W—H3W $\cdots$ O4 <sup>iv</sup>	0.84	2.27	3.068 (4)	160
O2W—H4W $\cdots$ O2 <sup>v</sup>	0.84	1.87	2.685 (4)	164

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

Data collection: *CrystalStructure* (Rigaku/MSM, 2002); cell refinement: *CrystalStructure*; data reduction: *CrystalStructure*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEPII* (Johnson, 1976) and *DIAMOND* (Brandenburg, 1999); software used to prepare material for publication: *SHELXL97*.

The authors acknowledge Guang Dong Ocean University for supporting this work.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HY2269).

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**supplementary materials**

*Acta Cryst.* (2010). E66, m151 [ doi:10.1107/S1600536810001029 ]

## Poly[*diaqua*( $\mu_3$ -1*H*-benzimidazole-5,6-dicarboxylato- $\kappa^4N^3:O^5,O^6:O^6'$ )magnesium(II)]

H. Wang, X.-F. Li, W.-D. Song, X.-T. Ma and J.-H. Liu

### Comment

1*H*-Benzimidazole-5,6-dicarboxylic acid ( $H_2L$ ) can function as a multidentate ligand and several complexes formed from this ligand have been reported recently, including *catena*-poly[[*diaqua*(1,10-phenanthroline- $\kappa^2N,N'$ ) nickel(II)]- $\mu$ - $L$ - $\kappa^2N^3:O^6$ ] (Song, Wang, Hu *et al.*, 2009), pentaqua( $L$ - $\kappa N^3$ )cobalt(II) pentahydrate (Song, Wang, Li *et al.*, 2009), pentaqua( $L$ - $\kappa N^3$ )nickel(II) pentahydrate (Song, Wang, Qin *et al.*, 2009) and tetraaquabis( $L$ - $\kappa N^3$ )cobalt(II) dimethylformamide disolvate dihydrate (Wang *et al.*, 2009). However, the Mg complex of the  $H_2L$  ligand has not been reported up to now.

As shown in Fig. 1, the  $Mg^{II}$  atom is six-coordinated by one N and three O atoms from three different  $L$  ligands, and two O atoms from two water molecules (Table 1), showing a slightly distorted octahedral geometry. The equatorial plane is defined by O1W, O2W, O1<sup>i</sup> and O3<sup>i</sup> atoms, while N1 and O4<sup>ii</sup> occupy the axial positions [symmetry codes: (i)  $x, 1 - y, -1/2 + z$ ; (ii)  $1/2 + x, 1/2 + y, z$ ]. Intermolecular O—H $\cdots$ O and N—H $\cdots$ O hydrogen bonds between the ligand and the coordinated water molecules stabilize the structure (Table 2 and Fig 2).

### Experimental

A mixture of  $MgCl_2$  (1.0 mmol),  $H_2L$  (0.6 mmol),  $CH_3CN$  (6 ml) and water (4 ml) was added to a 20 ml Teflon-lined stainless container, which was heated to 150°C and held at that temperature for 5 d. After cooling to room temperature, colourless crystals were recovered by filtration.

### Refinement

C- and N-bound H atoms were placed at calculated positions and treated as riding on the parent C or N atoms, with C—H = 0.93 and N—H = 0.86 Å, and with  $U_{iso}(H) = 1.2U_{eq}(C, N)$ . The water H atoms were located in a difference Fourier map and refined as riding with a distance restraint of O—H = 0.84 Å and with  $U_{iso}(H) = 1.5U_{eq}(O)$ .

### Figures

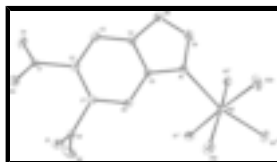


Fig. 1. The structure of the title compound, showing the 30% probability displacement ellipsoids. [Symmetry codes: (i)  $x, 1 - y, -1/2 + z$ ; (ii)  $1/2 + x, 1/2 + y, z$ .]

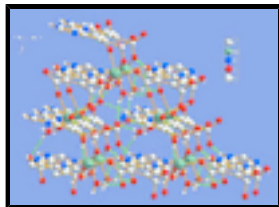


Fig. 2. A view of the three-dimensional network structure of the title compound. Hydrogen bonds are shown as dashed lines.

## Poly[*diaqua*( $\mu_3$ -1*H*-benzimidazole-5,6-dicarboxylato- $\kappa^4N^3:O^5,O^6:O^{6'}$ )magnesium(II)]

### Crystal data

[Mg(C<sub>9</sub>H<sub>4</sub>N<sub>2</sub>O<sub>4</sub>)(H<sub>2</sub>O)<sub>2</sub>]

$M_r = 264.48$

Monoclinic, *Cc*

Hall symbol: C -2yc

$a = 7.4793$  (15) Å

$b = 18.958$  (4) Å

$c = 7.3132$  (15) Å

$\beta = 99.38$  (3)°

$V = 1023.1$  (4) Å<sup>3</sup>

$Z = 4$

$F(000) = 544$

$D_x = 1.717$  Mg m<sup>-3</sup>

Mo  $K\alpha$  radiation,  $\lambda = 0.71073$  Å

Cell parameters from 4114 reflections

$\theta = 3.6$ – $27.5$ °

$\mu = 0.20$  mm<sup>-1</sup>

$T = 293$  K

Block, colourless

$0.30 \times 0.25 \times 0.21$  mm

### Data collection

Rigaku/MSM Mercury CCD diffractometer

Radiation source: fine-focus sealed tube graphite

$\omega$  scans

Absorption correction: multi-scan (REQAB; Jacobson, 1998)

$T_{\min} = 0.943$ ,  $T_{\max} = 0.960$

4611 measured reflections

1143 independent reflections

1096 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.031$

$\theta_{\max} = 27.5$ °,  $\theta_{\min} = 3.6$ °

$h = -9 \rightarrow 9$

$k = -24 \rightarrow 24$

$l = -8 \rightarrow 9$

### Refinement

Refinement on  $F^2$

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.036$

$wR(F^2) = 0.090$

$S = 1.06$

1143 reflections

163 parameters

2 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

$w = 1/[\sigma^2(F_o^2) + (0.04P)^2 + 2P]$

where  $P = (F_o^2 + 2F_c^2)/3$

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

$\Delta\rho_{\max} = 0.38$  e Å<sup>-3</sup>

$\Delta\rho_{\min} = -0.25$  e Å<sup>-3</sup>

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ( $\text{\AA}^2$ )

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Mg1	0.27807 (16)	0.68928 (5)	0.63241 (16)	0.0172 (3)
O1	0.4349 (4)	0.37147 (14)	0.9888 (4)	0.0234 (5)
O2	0.5047 (4)	0.37926 (16)	0.7087 (4)	0.0317 (7)
O3	0.1320 (4)	0.28489 (12)	0.8699 (4)	0.0237 (6)
O4	-0.0733 (4)	0.28304 (12)	0.6132 (3)	0.0236 (6)
N1	0.0678 (5)	0.61142 (15)	0.6633 (5)	0.0214 (6)
N3	-0.2035 (5)	0.56134 (16)	0.6122 (5)	0.0271 (7)
H3	-0.3196	0.5577	0.5874	0.033*
C1	0.0380 (5)	0.31481 (16)	0.7326 (5)	0.0173 (6)
C2	0.0549 (5)	0.39389 (16)	0.7123 (5)	0.0182 (7)
C3	-0.1002 (5)	0.43318 (18)	0.6560 (5)	0.0223 (7)
H2	-0.2127	0.4116	0.6240	0.027*
C4	-0.0816 (5)	0.50629 (18)	0.6490 (5)	0.0206 (7)
C5	0.0876 (5)	0.53907 (17)	0.6828 (5)	0.0184 (7)
C6	0.2438 (5)	0.49930 (18)	0.7332 (5)	0.0185 (7)
H1	0.3574	0.5206	0.7531	0.022*
C7	0.2259 (4)	0.42738 (16)	0.7529 (4)	0.0154 (6)
C8	0.3985 (5)	0.38839 (17)	0.8204 (5)	0.0173 (7)
C9	-0.1073 (6)	0.62155 (18)	0.6224 (6)	0.0262 (8)
H9	-0.1599	0.6659	0.6023	0.031*
O1W	0.4663 (4)	0.65596 (14)	0.8537 (4)	0.0289 (6)
H1W	0.4573	0.6408	0.9598	0.043*
H2W	0.5355	0.6911	0.8601	0.043*
O2W	0.1388 (5)	0.75021 (15)	0.7982 (5)	0.0374 (8)
H3W	0.0660	0.7342	0.8639	0.056*
H4W	0.1176	0.7927	0.7704	0.056*

Atomic displacement parameters ( $\text{\AA}^2$ )

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
Mg1	0.0191 (6)	0.0134 (4)	0.0184 (5)	-0.0004 (4)	0.0009 (4)	0.0004 (4)
O1	0.0186 (13)	0.0310 (13)	0.0202 (12)	0.0004 (10)	0.0019 (11)	0.0074 (10)
O2	0.0247 (16)	0.0462 (17)	0.0253 (14)	0.0133 (12)	0.0075 (12)	0.0005 (12)
O3	0.0274 (14)	0.0165 (11)	0.0235 (12)	-0.0008 (10)	-0.0074 (11)	0.0006 (9)
O4	0.0281 (15)	0.0195 (12)	0.0203 (13)	-0.0067 (10)	-0.0045 (11)	0.0014 (9)
N1	0.0215 (16)	0.0167 (13)	0.0265 (15)	0.0018 (11)	0.0058 (12)	0.0039 (11)
N3	0.0147 (16)	0.0249 (14)	0.0400 (19)	0.0032 (12)	-0.0009 (14)	0.0065 (13)
C1	0.0195 (17)	0.0151 (13)	0.0175 (16)	-0.0016 (12)	0.0043 (14)	-0.0002 (11)
C2	0.0197 (18)	0.0150 (14)	0.0192 (16)	-0.0024 (12)	0.0008 (14)	0.0015 (12)
C3	0.0184 (18)	0.0204 (16)	0.0274 (19)	-0.0040 (13)	0.0011 (15)	0.0023 (13)
C4	0.0151 (19)	0.0216 (16)	0.0244 (18)	0.0023 (12)	0.0011 (14)	0.0045 (13)
C5	0.0191 (17)	0.0160 (14)	0.0203 (16)	-0.0019 (12)	0.0035 (14)	0.0016 (12)
C6	0.0129 (16)	0.0198 (15)	0.0224 (17)	-0.0022 (11)	0.0018 (14)	0.0008 (12)
C7	0.0151 (16)	0.0178 (14)	0.0134 (14)	0.0002 (12)	0.0027 (13)	-0.0002 (11)

## supplementary materials

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C8	0.0154 (17)	0.0154 (14)	0.0204 (17)	-0.0024 (11)	0.0007 (14)	-0.0011 (11)
C9	0.024 (2)	0.0208 (16)	0.034 (2)	0.0068 (14)	0.0050 (17)	0.0067 (14)
O1W	0.0340 (15)	0.0271 (13)	0.0225 (12)	-0.0071 (11)	-0.0043 (12)	0.0052 (10)
O2W	0.0486 (19)	0.0219 (12)	0.0476 (19)	0.0063 (12)	0.0251 (16)	-0.0022 (12)

### *Geometric parameters (Å, °)*

Mg1—N1	2.195 (3)	C1—C2	1.514 (4)
Mg1—O1 <sup>i</sup>	2.051 (3)	C2—C3	1.384 (5)
Mg1—O3 <sup>i</sup>	2.106 (3)	C2—C7	1.416 (5)
Mg1—O4 <sup>ii</sup>	2.113 (3)	C3—C4	1.395 (5)
Mg1—O1W	2.063 (3)	C3—H2	0.9300
Mg1—O2W	2.074 (3)	C4—C5	1.395 (5)
O1—C8	1.259 (4)	C5—C6	1.388 (5)
O2—C8	1.241 (4)	C6—C7	1.380 (5)
O3—C1	1.263 (4)	C6—H1	0.9300
O4—C1	1.257 (4)	C7—C8	1.499 (5)
N1—C9	1.310 (5)	C9—H9	0.9300
N1—C5	1.384 (4)	O1W—H1W	0.8401
N3—C9	1.345 (5)	O1W—H2W	0.8400
N3—C4	1.383 (5)	O2W—H3W	0.8399
N3—H3	0.8600	O2W—H4W	0.8400
O1 <sup>i</sup> —Mg1—O1W	81.69 (12)	C7—C2—C1	120.7 (3)
O1 <sup>i</sup> —Mg1—O2W	174.71 (15)	C2—C3—C4	117.5 (3)
O1W—Mg1—O2W	93.18 (14)	C2—C3—H2	121.2
O1 <sup>i</sup> —Mg1—O3 <sup>i</sup>	85.34 (12)	C4—C3—H2	121.3
O1W—Mg1—O3 <sup>i</sup>	166.51 (13)	N3—C4—C3	133.6 (3)
O2W—Mg1—O3 <sup>i</sup>	99.68 (13)	N3—C4—C5	104.4 (3)
O1 <sup>i</sup> —Mg1—O4 <sup>ii</sup>	95.02 (12)	C3—C4—C5	122.0 (3)
O1W—Mg1—O4 <sup>ii</sup>	90.61 (11)	N1—C5—C6	129.5 (3)
O2W—Mg1—O4 <sup>ii</sup>	83.68 (12)	N1—C5—C4	110.1 (3)
O3 <sup>i</sup> —Mg1—O4 <sup>ii</sup>	86.80 (11)	C6—C5—C4	120.3 (3)
O1 <sup>i</sup> —Mg1—N1	98.87 (12)	C7—C6—C5	118.2 (3)
O1W—Mg1—N1	97.00 (12)	C7—C6—H1	120.9
O2W—Mg1—N1	82.98 (13)	C5—C6—H1	120.9
O3 <sup>i</sup> —Mg1—N1	88.65 (12)	C6—C7—C2	121.4 (3)
O4 <sup>ii</sup> —Mg1—N1	164.98 (12)	C6—C7—C8	115.4 (3)
C8—O1—Mg1 <sup>iii</sup>	126.4 (2)	C2—C7—C8	123.2 (3)
C1—O3—Mg1 <sup>iii</sup>	139.4 (2)	O2—C8—O1	123.3 (3)
C1—O4—Mg1 <sup>iv</sup>	130.8 (2)	O2—C8—C7	117.5 (3)
C9—N1—C5	104.8 (3)	O1—C8—C7	119.0 (3)
C9—N1—Mg1	125.8 (2)	N1—C9—N3	113.2 (3)
C5—N1—Mg1	127.6 (3)	N1—C9—H9	123.4
C9—N3—C4	107.4 (3)	N3—C9—H9	123.4
C9—N3—H3	126.3	Mg1—O1W—H1W	133.0

C4—N3—H3	126.3	Mg1—O1W—H2W	97.9
O4—C1—O3	123.8 (3)	H1W—O1W—H2W	111.1
O4—C1—C2	117.6 (3)	Mg1—O2W—H3W	124.6
O3—C1—C2	118.6 (3)	Mg1—O2W—H4W	119.1
C3—C2—C7	120.4 (3)	H3W—O2W—H4W	111.8
C3—C2—C1	118.9 (3)		

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

*Hydrogen-bond geometry (Å, °)*

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
N3—H3 $\cdots$ O1 <sup>v</sup>	0.86	2.29	2.992 (4)	138.
O1W—H1W $\cdots$ O2 <sup>iii</sup>	0.84	1.84	2.651 (4)	163.
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O2W—H3W $\cdots$ O4 <sup>iii</sup>	0.84	2.27	3.068 (4)	160.
O2W—H4W $\cdots$ O2 <sup>vi</sup>	0.84	1.87	2.685 (4)	164.

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

Fig. 1

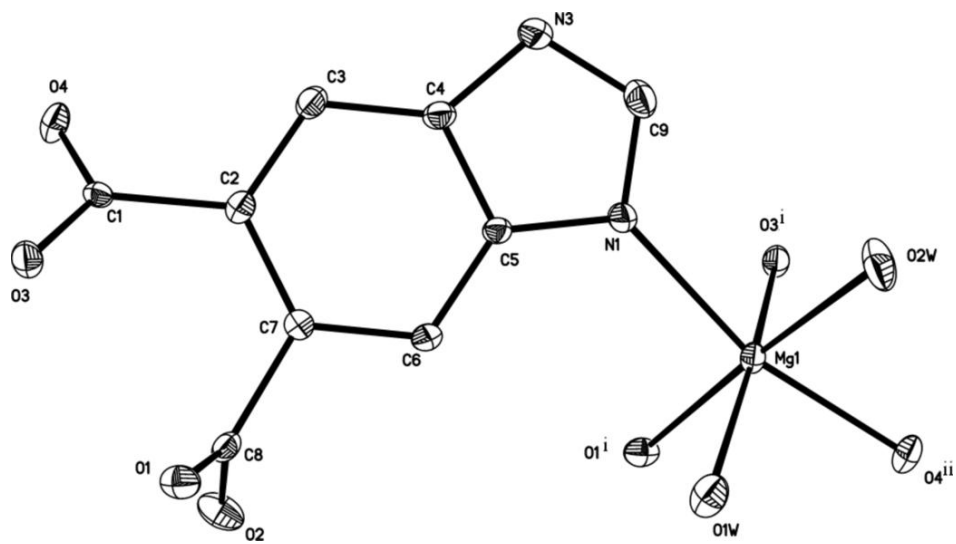




Fig. 2

