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

# Poly[diaqua-$\mu_4$-biphenyl-4,4′-dicarboxylato-magnesium(II)]

**Hsin-Kuan Liu, Xiang-Wen Peng and Chia-Her Lin***

Department of Chemistry, Chung-Yuan Christian University, Chung-Li 320, Taiwan
Correspondence e-mail: chiaher@cycu.edu.tw

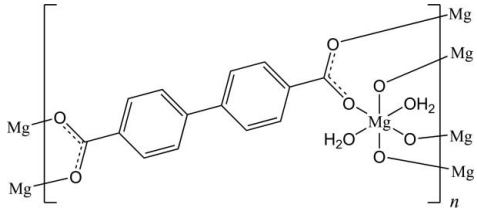
Received 21 January 2009; accepted 22 January 2009

Key indicators: single-crystal X-ray study; $T$ = 295 K; mean $\sigma$(C–C) = 0.003 Å; $R$ factor = 0.041; $wR$ factor = 0.106; data-to-parameter ratio = 16.4.

The solvothermal reaction of magnesium nitrate with biphenyl-4,4′-dicarboxylic acid in *N*,*N*-dimethylformamide and water leads to the formation of crystals of the title complex, $[Mg(C_{14}H_8O_4)(H_2O)_2]_n$. In the crystal structure, the Mg cations are coordinated by six O atoms from two water molecules and four symmetry-related biphenyl-4,4′-dicarboxylate anions within slightly distorted octahedra. The Mg cations are located on a center of inversion, the biphenyl-4,4′-dicarboxylate anions around a twofold rotation axis and the water molecule in a general position. The Mg cations are linked by the anions into a three-dimensional framework.

## Related literature

For related structures, see: Kitagawa *et al.* (2004).




## Experimental

### Crystal data

$[Mg(C_{14}H_8O_4)(H_2O)_2]$
$M_r$ = 150.27
Orthorhombic, *Pbcn*
$a$ = 6.5913 (10) Å
$b$ = 7.2900 (9) Å
$c$ = 26.759 (4) Å
$V$ = 1285.8 (3) Å$^3$
$Z$ = 8
Mo $K\alpha$ radiation
$\mu$ = 0.16 mm$^{-1}$
$T$ = 295 (2) K
0.15 × 0.10 × 0.05 mm

### Data collection

Bruker APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2007)
$T_{min}$ = 0.976, $T_{max}$ = 0.995
5950 measured reflections
1589 independent reflections
1048 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.048

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.106
$S$ = 1.02
1589 reflections
97 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.30 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.30 e Å$^{-3}$

Data collection: *APEX2* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT*; 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: *SHELXTL*.

This research was supported by the National Science Council, Taiwan (grant No. NSC97-2113-M-033–003-MY2), and Chung-Yuan Christian University, Taiwan, under grant No. CYCU-97-CR-CH.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: NC2132).

## References

Bruker (2007). *SADABS*, *SAINT* and *APEX2*. Bruker AXS Inc., Madison, Wisconsin, USA.
Kitagawa, S., Kitaura, R. & Noro, S. (2004). *Angew. Chem. Int. Ed.* **43**, 2334–2375.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.

# supporting information

*Acta Cryst.* (2009). E**65**, m237 [doi:10.1107/S1600536809002864]

## Poly[diaqua-$\mu_4$-biphenyl-4,4′-dicarboxylato-magnesium(II)]

**Hsin-Kuan Liu, Xiang-Wen Peng and Chia-Her Lin**

### S1. Comment

The synthesis of coordination polymers, or so-called metal-organic frameworks (MOF), has been a subject of intense research owing to their interesting structural chemistry and potential applications in gas storage, separation, catalysis, magnetism, luminescence. A large number of these compounds have been synthesized by solvothermal reactions with organic carboxyl acids (Kitagawa *et al.*, 2004). Here we report on the new metal organic framework bis(aqua)-biphenyl-4,4′-dicarboxylate magnesium (II). In the crystal structure the Mg cations are sorrounded by two O atoms from two symmetry related water molecules and four O atoms of four symmetry related anions (Fig. 1). The coordination polyhedron around the Mg cations can be described as a slightly distorted octahedron. The Mg cations are linked *via* the anions into a three-dimensional network (Fig. 2).

### S2. Experimental

The reaction was carried out under solvothermal conditions in a teflon-lined autoclav with an inner volume of 23 ml. A single-phase product consisting of transparent colorless crystals was obtained by heating a mixture of $Mg(NO_3)_2{\cdot}6H_2O$, (0.1281 g, 0.5 mmol), biphenyl-4,4′-dicarboxylic acid ($C_{14}H_{10}O_4$, 0.0290 g, 0.125 mmol), *N*,*N*-dimethylformamide (10.0 ml), and $H_2O$ (2.0 ml)at 423 K for 2 d followed by slow cooling at 6 K/h to room temperature.

### S3. Refinement

The C—H H atoms were positioned with idealized geometry and were refined isotropic using a riding model with C—H = 0.93 Å and $U_{iso}$(H) = 1.2$U_{eq}$(C). The H atoms at the water molecule were found in difference map and were refined with varying coordinates isotropic.

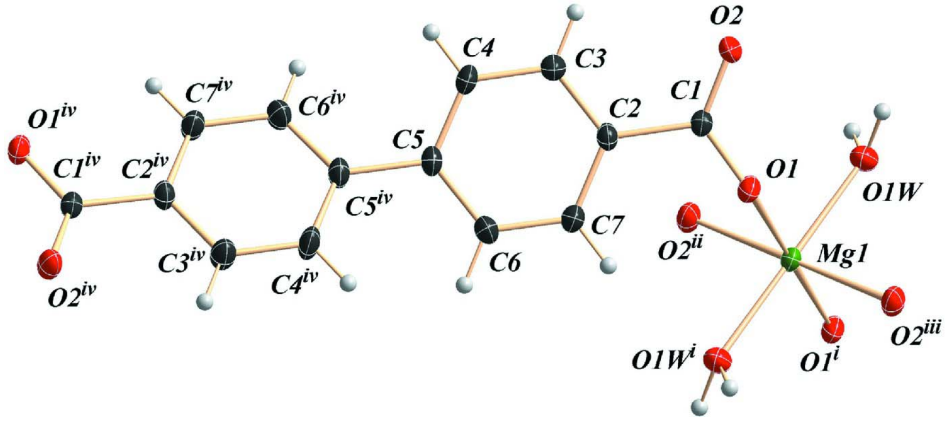



**Figure 1**

Crystal structure of the title compound with labeling and displacement ellipsoids drawn at the 50% probability level. [symmetry codes: (i) -*x* + 2,-*y* + 1,-*z*; (ii) -*x* + 3/2,*y* - 1/2,*z*; (iii) *x* + 1/2,-*y* + 3/2,-*z*; (iv) -*x* + 2,*y*,-*z* + 1/2.].

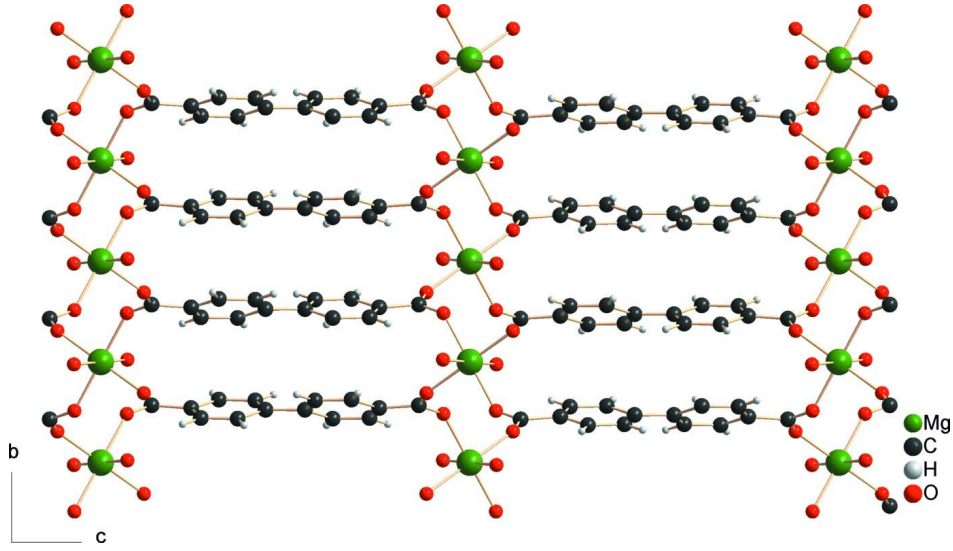



**Figure 2**

Crystal structure of the title compound with view along the *a* axis.

**Poly[diaqua-$\mu_4$-biphenyl-4,4′-dicarboxylato-magnesium(II)]**

*Crystal data*

$[Mg(C_{14}H_8O_4)(H_2O)_2]$
$M_r = 150.27$
Orthorhombic, *Pbcn*
$a = 6.5913$ (10) Å
$b = 7.2900$ (9) Å
$c = 26.759$ (4) Å
$V = 1285.8$ (3) Å$^3$
$Z = 8$
$F(000) = 624$
$D_x = 1.553$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 1007 reflections
$\theta = 3.1$–$25.2°$
$\mu = 0.16$ mm$^{-1}$
$T = 295$ K
Lamellar, colorless
0.15 × 0.10 × 0.05 mm

*Data collection*

Bruker APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\varphi$ and $\omega$ scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2007)
$T_{min} = 0.976$, $T_{max} = 0.995$
5950 measured reflections
1589 independent reflections
1048 reflections with $I > 2\sigma(I)$
$R_{int} = 0.048$
$\theta_{max} = 28.4°$, $\theta_{min} = 1.5°$
$h = -7 \rightarrow 8$
$k = -9 \rightarrow 9$
$l = -22 \rightarrow 35$

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.041$
$wR(F^2) = 0.106$
$S = 1.02$
1589 reflections
97 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-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0448P)^2 + 0.3401P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.30$ e Å$^{-3}$
$\Delta\rho_{min} = -0.30$ e Å$^{-3}$

*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 (Å²)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| Mg1 | 1.0000 | 0.5000 | 0.0000 | 0.0159 (2) |
| C1 | 0.7888 (3) | 0.7850 (2) | 0.06884 (7) | 0.0162 (4) |
| C2 | 0.8503 (3) | 0.7715 (3) | 0.12262 (7) | 0.0184 (4) |
| C3 | 0.7124 (3) | 0.8132 (3) | 0.16000 (7) | 0.0245 (5) |
| H3 | 0.5796 | 0.8440 | 0.1517 | 0.029* |
| C4 | 0.7715 (4) | 0.8092 (3) | 0.20963 (7) | 0.0259 (5) |
| H4 | 0.6775 | 0.8380 | 0.2343 | 0.031* |
| C5 | 0.9691 (3) | 0.7629 (3) | 0.22334 (7) | 0.0211 (5) |
| C6 | 1.1051 (3) | 0.7183 (3) | 0.18550 (7) | 0.0261 (5) |
| H6 | 1.2372 | 0.6854 | 0.1938 | 0.031* |
| C7 | 1.0476 (3) | 0.7220 (3) | 0.13581 (8) | 0.0242 (5) |
| H7 | 1.1409 | 0.6915 | 0.1111 | 0.029* |
| O1 | 0.9201 (2) | 0.74253 (17) | 0.03552 (5) | 0.0194 (3) |
| O1W | 0.7228 (2) | 0.48848 (18) | −0.03619 (5) | 0.0221 (3) |
| H1WA | 0.6306 | 0.5799 | −0.0412 | 0.080* |
| H1WB | 0.6335 | 0.4082 | −0.0293 | 0.080* |
| O2 | 0.6164 (2) | 0.8454 (2) | 0.05857 (5) | 0.0233 (4) |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Mg1 | 0.0166 (5) | 0.0205 (4) | 0.0107 (4) | 0.0010 (4) | 0.0010 (4) | −0.0006 (4) |
| C1 | 0.0195 (11) | 0.0161 (9) | 0.0129 (9) | 0.0000 (8) | 0.0000 (8) | 0.0002 (7) |
| C2 | 0.0214 (12) | 0.0218 (10) | 0.0121 (9) | 0.0017 (8) | −0.0020 (8) | 0.0004 (8) |
| C3 | 0.0214 (12) | 0.0352 (12) | 0.0171 (10) | 0.0075 (10) | −0.0001 (9) | 0.0004 (9) |
| C4 | 0.0271 (13) | 0.0388 (11) | 0.0116 (9) | 0.0057 (10) | 0.0022 (9) | −0.0003 (9) |
| C5 | 0.0240 (12) | 0.0272 (10) | 0.0120 (10) | 0.0006 (9) | −0.0017 (9) | −0.0002 (8) |
| C6 | 0.0202 (12) | 0.0416 (12) | 0.0166 (10) | 0.0029 (10) | −0.0037 (9) | 0.0012 (9) |
| C7 | 0.0216 (12) | 0.0369 (12) | 0.0141 (10) | 0.0042 (10) | 0.0010 (8) | −0.0005 (9) |
| O1 | 0.0221 (8) | 0.0232 (7) | 0.0129 (7) | 0.0025 (6) | 0.0012 (6) | −0.0015 (6) |
| O1W | 0.0165 (8) | 0.0279 (7) | 0.0221 (7) | 0.0001 (6) | −0.0011 (6) | 0.0012 (6) |
| O2 | 0.0200 (8) | 0.0346 (8) | 0.0152 (7) | 0.0065 (7) | −0.0015 (7) | 0.0041 (6) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| Mg1—O1W$^{i}$ | 2.0696 (14) | C3—H3 | 0.9300 |
| Mg1—O1W | 2.0696 (14) | C4—C5 | 1.395 (3) |
| Mg1—O1 | 2.0753 (12) | C4—H4 | 0.9300 |
| Mg1—O1$^{i}$ | 2.0753 (12) | C5—C6 | 1.391 (3) |
| Mg1—O2$^{ii}$ | 2.0774 (13) | C5—C5$^{iv}$ | 1.484 (4) |
| Mg1—O2$^{iii}$ | 2.0774 (13) | C6—C7 | 1.383 (3) |
| C1—O2 | 1.249 (2) | C6—H6 | 0.9300 |
| C1—O1 | 1.281 (2) | C7—H7 | 0.9300 |
| C1—C2 | 1.498 (3) | O1W—H1WA | 0.9119 |
| C2—C3 | 1.385 (3) | O1W—H1WB | 0.8502 |
| C2—C7 | 1.395 (3) | O2—Mg1$^{v}$ | 2.0774 (13) |
| C3—C4 | 1.384 (3) | | |
| | | | |
| O1W$^{i}$—Mg1—O1W | 180.00 (10) | C4—C3—C2 | 120.2 (2) |
| O1W$^{i}$—Mg1—O1 | 88.58 (5) | C4—C3—H3 | 119.9 |
| O1W—Mg1—O1 | 91.42 (5) | C2—C3—H3 | 119.9 |
| O1W$^{i}$—Mg1—O1$^{i}$ | 91.42 (5) | C3—C4—C5 | 121.3 (2) |
| O1W—Mg1—O1$^{i}$ | 88.58 (5) | C3—C4—H4 | 119.3 |
| O1—Mg1—O1$^{i}$ | 180.00 (6) | C5—C4—H4 | 119.3 |
| O1W$^{i}$—Mg1—O2$^{ii}$ | 89.72 (5) | C6—C5—C4 | 117.84 (18) |
| O1W—Mg1—O2$^{ii}$ | 90.28 (5) | C6—C5—C5$^{iv}$ | 121.5 (2) |
| O1—Mg1—O2$^{ii}$ | 91.31 (5) | C4—C5—C5$^{iv}$ | 120.6 (2) |
| O1$^{i}$—Mg1—O2$^{ii}$ | 88.69 (5) | C7—C6—C5 | 121.3 (2) |
| O1W$^{i}$—Mg1—O2$^{iii}$ | 90.28 (5) | C7—C6—H6 | 119.4 |
| O1W—Mg1—O2$^{iii}$ | 89.72 (5) | C5—C6—H6 | 119.4 |
| O1—Mg1—O2$^{iii}$ | 88.69 (5) | C6—C7—C2 | 120.2 (2) |
| O1$^{i}$—Mg1—O2$^{iii}$ | 91.31 (5) | C6—C7—H7 | 119.9 |
| O2$^{ii}$—Mg1—O2$^{iii}$ | 180.00 (8) | C2—C7—H7 | 119.9 |
| O2—C1—O1 | 123.14 (17) | C1—O1—Mg1 | 134.15 (12) |
| O2—C1—C2 | 118.73 (17) | Mg1—O1W—H1WA | 128.9 |
| O1—C1—C2 | 118.03 (17) | Mg1—O1W—H1WB | 122.5 |
| C3—C2—C7 | 119.06 (18) | H1WA—O1W—H1WB | 94.2 |
| C3—C2—C1 | 120.10 (18) | C1—O2—Mg1$^{v}$ | 133.89 (13) |
| C7—C2—C1 | 120.82 (18) | | |

Symmetry codes: (i) −*x*+2, −*y*+1, −*z*; (ii) −*x*+3/2, *y*−1/2, *z*; (iii) *x*+1/2, −*y*+3/2, −*z*; (iv) −*x*+2, *y*, −*z*+1/2; (v) *x*−1/2, −*y*+3/2, −*z*.