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Poly[diaqua-μ_4-biphenyl-4,4′-dicarboxylato-magnesium(II)]

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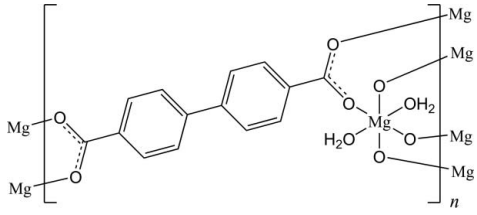
Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.003 Å; R factor = 0.041; wR factor = 0.106; data-to-parameter ratio = 16.4.

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
μ = 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*.

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

References

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Kitagawa, S., Kitaura, R. & Noro, S. (2004). *Angew. Chem. Int. Ed.* **43**, 2334–2375.
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supplementary materials

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

Poly[diaqua-μ_4-biphenyl-4,4'-dicarboxylato-magnesium(II)]

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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).

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.

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) = 1.2U_{eq}(C). The H atoms at the water molecule were found in difference map and were refined with varying coordinates isotropic.

Figures

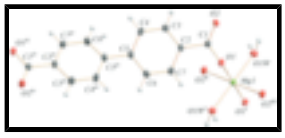

Fig. 1. Crystal structure of the title compound with labeling and displacement ellipsoids drawn at the 50% probability level. [symmetry codes: (i) -*x* + 2,-*y* + 1,-*z*; (ii) -*x* + 3/2,*y* - 1/2,*z*; (iii) *x* + 1/2,-*y* + 3/2,-*z*; (iv) -*x* + 2,*y*,-*z* + 1/2.].

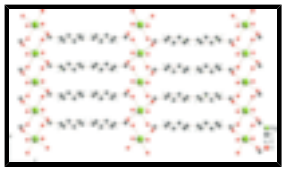

Fig. 2. Crystal structure of the title compound with view along the *a* axis.

Poly[diaqua-μ4-biphenyl-4,4'-dicarboxylato-magnesium(II)]

Crystal data

$[Mg(C_{14}H_8O_4)(H_2O)_2]$	$D_x = 1.553$ Mg m^{-3}
$M_r = 150.27$	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
Orthorhombic, *Pbcn*	Cell parameters from 1007 reflections
$a = 6.5913$ (10) Å	$\theta = 3.1$–$25.2°$
$b = 7.2900$ (9) Å	$\mu = 0.16$ mm^{-1}
$c = 26.759$ (4) Å	$T = 295$ (2) K
$V = 1285.8$ (3) Å^3	Lamellar, colorless
$Z = 8$	0.15 × 0.10 × 0.05 mm
$F_{000} = 624$	

Data collection

Bruker APEXII CCD diffractometer	1589 independent reflections
Radiation source: fine-focus sealed tube	1048 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.048$
$T = 295(2)$ K	$\theta_{max} = 28.4°$
φ and ω scans	$\theta_{min} = 1.5°$
Absorption correction: multi-scan (SADABS; Bruker, 2007)	$h = -7 \rightarrow 8$
$T_{min} = 0.976$, $T_{max} = 0.995$	$k = -9 \rightarrow 9$
5950 measured reflections	$l = -22 \rightarrow 35$

Refinement

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

	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, °)

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*.

Fig. 1

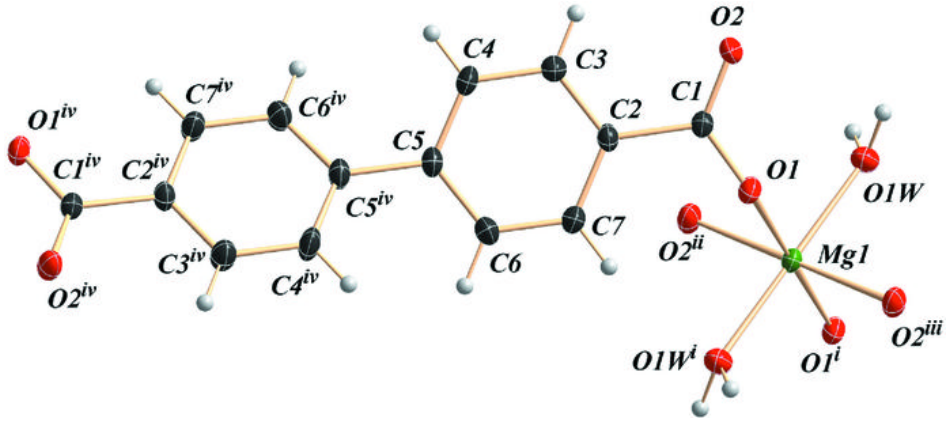
O2
C4
C3
C1
C2
C7iv
C6iv
O1iv
C5
O1
O1W
C1iv
C2iv
C5iv
C7
O2ii
Mg1
C3iv
C6
C4iv
O2iv
O2iii
O1Wi
O1i

Fig. 2