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Diaquabis(quinoline-2-carboxylato-κ^2N,O)magnesium(II) dihydrate methanol disolvate

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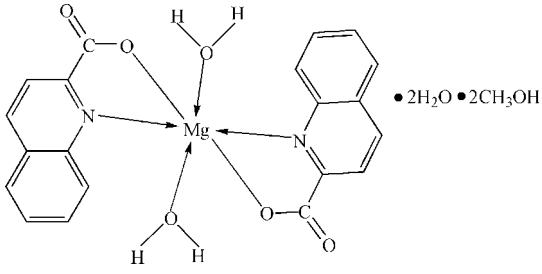
Key indicators: single-crystal X-ray study; T = 291 K; mean σ(C–C) = 0.005 Å; R factor = 0.064; wR factor = 0.129; data-to-parameter ratio = 15.2.

In the crystal structure of the title compound, $[Mg(C_{10}H_6NO_2)_2(H_2O)_2]\cdot 2H_2O\cdot 2CH_3OH$, the Mg atom (site symmetry $\bar{1}$) adopts a slightly distorted *trans*-MgN_2O_4 octahedral geometry arising from two *N*,*O*-bidentate quinaldine ligands and two water molecules. The structure is stabilized by intermolecular O—H···O hydrogen bonds.

Related literature

For a related structure, see: Wang *et al.* (2007).



Experimental

Crystal data

$[Mg(C_{10}H_6NO_2)_2(H_2O)_2]\cdot 2H_2O\cdot 2CH_4O$
M_r = 504.77
Triclinic, $P\bar{1}$
a = 7.129 (3) Å
b = 9.038 (3) Å
c = 10.846 (4) Å
α = 75.677 (5)°
β = 74.138 (5)°
γ = 70.160 (5)°
V = 623.0 (4) Å^3
Z = 1
Mo $K\alpha$ radiation
μ = 0.13 mm^{-1}
T = 291 (2) K
0.30 × 0.26 × 0.24 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
T_{min} = 0.96, T_{max} = 0.97
5796 measured reflections
2445 independent reflections
1640 reflections with $I > 2\sigma(I)$
R_{int} = 0.062

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.064
$wR(F^2)$ = 0.129
S = 1.09
2445 reflections
161 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.22 e Å^{-3}
$\Delta\rho_{min}$ = −0.23 e Å^{-3}

Table 1
Selected bond lengths (Å).

Mg1—O1	1.9913 (17)	Mg1—N1	2.267 (3)
Mg1—O3	2.081 (2)		

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

D—H···A	D—H	H···A	D···A	D—H···A
O3—H3A···O2^{i}	0.96	1.74	2.696 (3)	171
O3—H3B···O4	0.96	1.76	2.713 (3)	175
O4—H4A···O5^{ii}	0.85	1.99	2.759 (3)	149
O4—H4B···O5^{iii}	0.85	2.21	2.968 (3)	149
O5—H5C···O2^{iv}	0.96	1.77	2.665 (3)	153

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

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: HB2431).

References

Bruker (2000). *SMART*, *SAINT*, *SADABS* and *SHELXTL*. Bruker AXS Inc., Madison, Wisconsin, USA.
Wang, L.-H., Yin, J. & Tai, X.-S. (2007). *Acta Cryst.* E**63**, m1664.

  doi:10.1107/S1600536807027687

supplementary materials

Acta Cryst. (2007). E**63**, m1850 [**doi:10.1107/S1600536807027687**]

Diaquabis(quinoline-2-carboxylato-κ^2N,O)magnesium(II) dihydrate methanol disolvate

X.-S. Tai, J. Yin and M.-Y. Hao

Comment

As part of our ongoing studies of the coordination chemistry of magnesium(II) (Tai *et al.*, 2007), 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 with two O donor of H_2O, four O, N donor of two quinaldine anions (Table 1). Intermolecular O—H···O hydrogen bonds help to consolidate the crystal packing (Table 2).

Experimental

1 mmol of magnesium perchlorate was added to a solution of quinaldine acid (2 mmol) in 10 ml of 95% methanol. The mixture was stirred for 3 h at refluxing temperature and cooled. Clear blocks of (I) were obtained after one week as the solvents slowly evaporated.

Refinement

The H atoms were placed geometrically (C—H = 0.93—0.96 Å, O—H = 0.85–0.96 Å) and refined as riding with U_{iso}(H) = 1.2U_{eq}(carrier) or 1.5U_{eq}(methyl C).

Figures

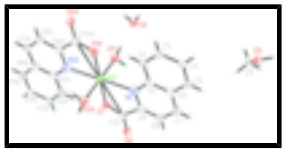


Fig. 1. The molecular structure of (I) showing 30% displacement ellipsoids (arbitrary spheres for the H atoms).

Diaquabis(quinoline-2-carboxylato-κ$^2N,O$)magnesium(II) dihydrate methanol disolvate

Crystal data

$[Mg(C_{10}H_6NO_2)_2(H_2O)_2]\cdot 2H_2O\cdot 2CH_4O$	$Z = 1$
$M_r = 504.77$	$F_{000} = 266$
Triclinic, $P\bar{1}$	$D_x = 1.344$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 7.129$ (3) Å	Cell parameters from 318 reflections
$b = 9.038$ (3) Å	$\theta = 2.4$–$19.2°$
$c = 10.846$ (4) Å	$\mu = 0.13$ mm^{-1}

α = 75.677 (5)º	T = 291 (2) K
β = 74.138 (5)º	Block, colourless
γ = 70.160 (5)º	0.30 × 0.26 × 0.24 mm
V = 623.0 (4) Å^3	

Data collection

Bruker SMART APEX CCD area-detector diffractometer	2445 independent reflections
Radiation source: sealed tube	1640 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.062
T = 291(2) K	θ_{max} = 26.0º
ω scans	θ_{min} = 2.0º
Absorption correction: multi-scan (SADABS; Bruker, 2000)	$h = -8 \rightarrow 8$
T_{min} = 0.96, T_{max} = 0.97	$k = -10 \rightarrow 11$
5796 measured reflections	$l = -13 \rightarrow 13$

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
$wR(F^2)$ = 0.129	$w = 1/[\sigma^2(F_o^2) + (0.04P)^2 + 0.11P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.09	$(\Delta/\sigma)_{max} < 0.001$
2445 reflections	$\Delta\rho_{max}$ = 0.22 e Å^{-3}
161 parameters	$\Delta\rho_{min}$ = −0.23 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}
C1	0.5400 (4)	0.3602 (3)	0.8444 (3)	0.0447 (6)

C2	0.3913 (5)	0.3680 (4)	0.7786 (3)	0.0512 (7)
H2	0.3326	0.2854	0.7970	0.061*
C3	0.3347 (4)	0.4995 (4)	0.6868 (3)	0.0482 (7)
H3	0.2357	0.5062	0.6432	0.058*
C4	0.4245 (4)	0.6259 (3)	0.6570 (3)	0.0440 (6)
H4	0.3873	0.7135	0.5931	0.053*
C5	0.5670 (4)	0.6163 (4)	0.7241 (3)	0.0470 (7)
H5	0.6230	0.7001	0.7077	0.056*
C6	0.6292 (4)	0.4820 (4)	0.8172 (3)	0.0500 (7)
C7	0.7774 (4)	0.4703 (3)	0.8849 (3)	0.0456 (6)
H7	0.8385	0.5512	0.8680	0.055*
C8	0.8292 (4)	0.3384 (4)	0.9753 (3)	0.0482 (7)
H8	0.9266	0.3279	1.0215	0.058*
C9	0.7375 (4)	0.2212 (4)	0.9980 (3)	0.0472 (7)
C10	0.7840 (5)	0.0708 (3)	1.0976 (3)	0.0484 (7)
C11	0.9682 (5)	0.7515 (4)	0.4226 (3)	0.0585 (9)
H11A	1.0915	0.7807	0.4051	0.088*
H11B	0.9838	0.6788	0.3667	0.088*
H11C	0.9400	0.7010	0.5117	0.088*
Mg1	0.5000	0.0000	1.0000	0.0406 (3)
N1	0.5957 (4)	0.2269 (3)	0.9335 (2)	0.0507 (6)
O1	0.7001 (3)	−0.0334 (2)	1.10861 (17)	0.0459 (5)
O2	0.9058 (3)	0.0623 (2)	1.16859 (17)	0.0451 (5)
O3	0.7270 (3)	−0.0998 (2)	0.85156 (18)	0.0528 (5)
H3A	0.8505	−0.0769	0.8482	0.063*
H3B	0.6846	−0.0546	0.7702	0.063*
O4	0.6256 (3)	0.0316 (2)	0.61644 (17)	0.0432 (5)
H4A	0.7206	−0.0108	0.5575	0.052*
H4B	0.5156	0.0148	0.6157	0.052*
O5	0.8078 (3)	0.8873 (2)	0.39970 (17)	0.0445 (5)
H5C	0.8589	0.9636	0.3320	0.053*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0443 (15)	0.0422 (16)	0.0441 (14)	0.0006 (13)	−0.0151 (12)	−0.0135 (11)
C2	0.0641 (19)	0.0474 (18)	0.0474 (15)	−0.0157 (15)	−0.0168 (14)	−0.0127 (13)
C3	0.0423 (15)	0.0540 (18)	0.0483 (14)	−0.0087 (14)	−0.0147 (12)	−0.0101 (13)
C4	0.0476 (15)	0.0444 (16)	0.0441 (13)	−0.0105 (13)	−0.0143 (12)	−0.0135 (12)
C5	0.0383 (14)	0.0620 (19)	0.0444 (14)	−0.0137 (14)	−0.0107 (12)	−0.0146 (13)
C6	0.0438 (15)	0.0514 (19)	0.0509 (15)	−0.0001 (14)	−0.0141 (13)	−0.0164 (13)
C7	0.0433 (15)	0.0423 (16)	0.0506 (15)	−0.0120 (13)	−0.0018 (12)	−0.0165 (12)
C8	0.0446 (15)	0.0575 (19)	0.0473 (14)	−0.0140 (14)	−0.0119 (12)	−0.0161 (13)
C9	0.0476 (15)	0.0444 (16)	0.0489 (15)	−0.0035 (13)	−0.0131 (13)	−0.0176 (12)
C10	0.0576 (17)	0.0386 (16)	0.0513 (15)	−0.0138 (14)	−0.0089 (14)	−0.0149 (12)
C11	0.0489 (17)	0.0486 (18)	0.0517 (16)	−0.0107 (14)	0.0080 (14)	0.0128 (13)
Mg1	0.0534 (8)	0.0355 (7)	0.0402 (6)	−0.0157 (6)	−0.0123 (6)	−0.0125 (5)
N1	0.0550 (14)	0.0517 (15)	0.0441 (12)	−0.0065 (12)	−0.0148 (11)	−0.0133 (11)

O1	0.0380 (10)	0.0565 (13)	0.0477 (10)	−0.0136 (9)	−0.0126 (8)	−0.0129 (9)
O2	0.0419 (10)	0.0483 (11)	0.0493 (10)	−0.0215 (9)	0.0089 (9)	−0.0242 (8)
O3	0.0614 (13)	0.0532 (13)	0.0464 (10)	−0.0149 (11)	−0.0122 (9)	−0.0142 (9)
O4	0.0439 (10)	0.0482 (12)	0.0465 (10)	−0.0193 (9)	−0.0060 (8)	−0.0195 (8)
O5	0.0475 (10)	0.0436 (11)	0.0446 (10)	−0.0091 (9)	−0.0108 (8)	−0.0158 (8)

Geometric parameters (Å, °)

C1—N1	1.361 (4)	C10—O1	1.244 (3)
C1—C6	1.384 (4)	C10—O2	1.283 (3)
C1—C2	1.406 (4)	C10—Mg1	2.831 (3)
C2—C3	1.370 (4)	C11—O5	1.389 (3)
C2—H2	0.9300	C11—H11A	0.9600
C3—C4	1.422 (4)	C11—H11B	0.9600
C3—H3	0.9300	C11—H11C	0.9600
C4—C5	1.373 (4)	Mg1—O1	1.9913 (17)
C4—H4	0.9300	Mg1—O1^{i}	1.9913 (17)
C5—C6	1.401 (4)	Mg1—O3^{i}	2.081 (2)
C5—H5	0.9300	Mg1—O3	2.081 (2)
C6—C7	1.406 (4)	Mg1—N1	2.267 (3)
C7—C8	1.357 (4)	Mg1—N1^{i}	2.267 (3)
C7—H7	0.9300	O3—H3A	0.9600
C8—C9	1.366 (4)	O3—H3B	0.9600
C8—H8	0.9300	O4—H4A	0.8500
C9—N1	1.360 (4)	O4—H4B	0.8500
C9—C10	1.513 (4)	O5—H5C	0.9599
N1—C1—C6	121.5 (3)	C9—C10—Mg1	82.07 (17)
N1—C1—C2	117.4 (3)	O5—C11—H11A	109.5
C6—C1—C2	121.1 (3)	O5—C11—H11B	109.5
C3—C2—C1	118.7 (3)	H11A—C11—H11B	109.5
C3—C2—H2	120.6	O5—C11—H11C	109.5
C1—C2—H2	120.6	H11A—C11—H11C	109.5
C2—C3—C4	121.2 (3)	H11B—C11—H11C	109.5
C2—C3—H3	119.4	O1—Mg1—O1^{i}	180.0
C4—C3—H3	119.4	O1—Mg1—O3^{i}	87.67 (8)
C5—C4—C3	118.9 (3)	O1^{i}—Mg1—O3^{i}	92.33 (8)
C5—C4—H4	120.6	O1—Mg1—O3	92.33 (8)
C3—C4—H4	120.6	O1^{i}—Mg1—O3	87.67 (8)
C4—C5—C6	120.9 (3)	O3^{i}—Mg1—O3	180.0
C4—C5—H5	119.5	O1—Mg1—N1	76.97 (8)
C6—C5—H5	119.5	O1^{i}—Mg1—N1	103.03 (8)
C1—C6—C5	119.2 (3)	O3^{i}—Mg1—N1	90.70 (8)
C1—C6—C7	119.6 (3)	O3—Mg1—N1	89.30 (8)
C5—C6—C7	121.2 (3)	O1—Mg1—N1^{i}	103.03 (8)
C8—C7—C6	118.5 (3)	O1^{i}—Mg1—N1^{i}	76.97 (8)
C8—C7—H7	120.7	O3^{i}—Mg1—N1^{i}	89.30 (8)

C6—C7—H7	120.7	O3—Mg1—N1^{i}	90.70 (8)
C7—C8—C9	119.6 (3)	N1—Mg1—N1^{i}	180.0
C7—C8—H8	120.2	C9—N1—C1	117.0 (3)
C9—C8—H8	120.2	C9—N1—Mg1	110.26 (18)
N1—C9—C8	123.7 (3)	C1—N1—Mg1	132.7 (2)
N1—C9—C10	112.9 (3)	C10—O1—Mg1	120.38 (19)
C8—C9—C10	123.3 (3)	Mg1—O3—H3A	109.4
O1—C10—O2	124.2 (3)	Mg1—O3—H3B	109.2
O1—C10—C9	119.4 (3)	H3A—O3—H3B	109.5
O2—C10—C9	116.4 (3)	H4A—O4—H4B	109.5
O2—C10—Mg1	161.3 (2)	C11—O5—H5C	109.1

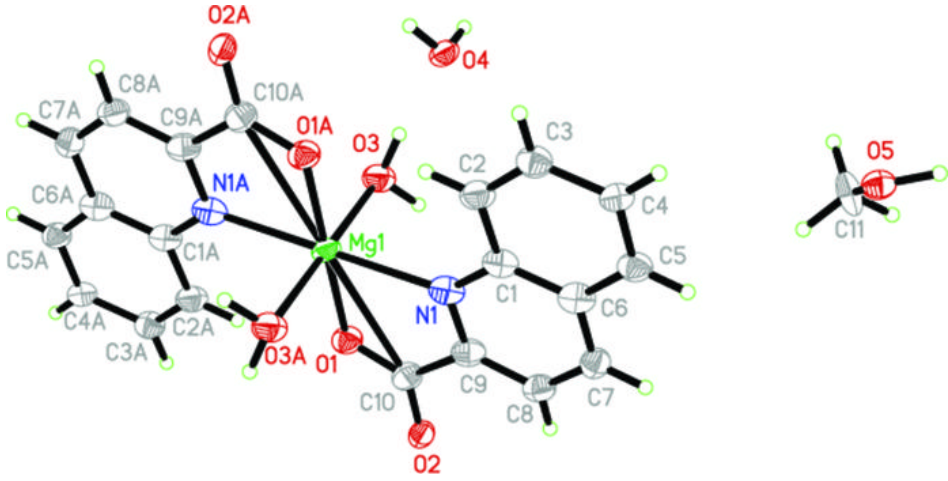
Symmetry codes: (i) −*x*+1, −*y*, −*z*+2.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O3—H3A···O2^{ii}	0.96	1.74	2.696 (3)	171
O3—H3B···O4	0.96	1.76	2.713 (3)	175
O4—H4A···O5^{iii}	0.85	1.99	2.759 (3)	149
O4—H4B···O5^{iv}	0.85	2.21	2.968 (3)	149
O5—H5C···O2^{v}	0.96	1.77	2.665 (3)	153

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

Fig. 1


O2A
O4
C8A
C10A
C7A
C9A
O1A
O3
C3
C2
O5
N1A
C4
C6A
Mg1
C5
C5A
C1A
C1
N1
C6
C4A
C2A
C3A
O3A
O1
C9
C10
C8
C7
C11
O2