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catena-Poly[[diaquamagnesium(II)]-bis-(μ-5-ammonioisophthalato-κ^2O^1:O^3)]

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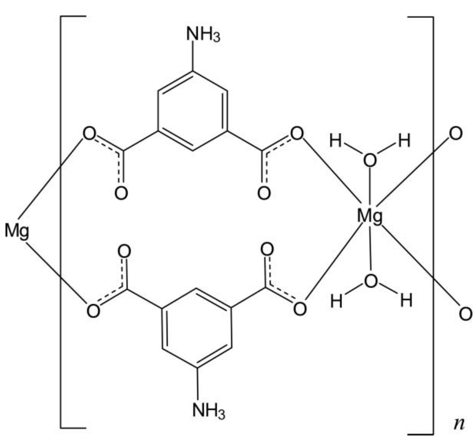
Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.003 Å; R factor = 0.049; wR factor = 0.136; data-to-parameter ratio = 14.9.

In the title compound, $[Mg(C_8H_6NO_4)_2(H_2O)_2]_n$, the Mg^{II} ion lies on a twofold roatation axis and is coordinated in a slightly distorted octahedral environment. Pairs of bridging ammoniumisophthalate ligands connect symmetry-related Mg^{II} ions, forming chains along [010]. In the crystal, intermolecular O—H···O and N—H···O hydrogen bonds link these chains into a three-dimensional network. The centroids of pairs of symmetry-related benzene rings within a chain are separated by 3.5707 (12) Å.

Related literature

For general background to metal coordination polymers, see: Kitagawa *et al.* (2004). For related structures, see: Zeng *et al.* (2007); Kongshaug & Fjellvåg (2006).



Experimental

Crystal data

$[Mg(C_8H_6NO_4)_2(H_2O)_2]$
M_r = 420.62
Monoclinic, $P2/n$
a = 6.9987 (2) Å
b = 9.9434 (3) Å
c = 11.3809 (3) Å
β = 94.730 (2)°
V = 789.31 (4) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.18 mm^{-1}
T = 295 K
0.10 × 0.08 × 0.08 mm

Data collection

Bruker APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2008)
T_{min} = 0.982, T_{max} = 0.986
6693 measured reflections
1963 independent reflections
1228 reflections with $I > 2\sigma(I)$
R_{int} = 0.047

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.049
$wR(F^2)$ = 0.136
S = 1.00
1963 reflections
132 parameters
2 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.36 e Å^{-3}
$\Delta\rho_{min}$ = −0.29 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O1W—H1WA···O3^{i}	0.85	2.04	2.883 (2)	175
N1—H1A···O1^{ii}	0.89	1.85	2.726 (2)	166
N1—H1B···O2^{iii}	0.89	2.19	2.919 (3)	138
N1—H1B···O4^{iv}	0.89	2.26	3.009 (3)	142
N1—H1C···O3^{v}	0.89	2.00	2.869 (2)	165

Symmetry codes: (i) $-x, -y+2, -z+1$; (ii) $x+\frac{1}{2}, -y+2, z+\frac{1}{2}$; (iii) $-x, -y+2, -z+2$; (iv) $-x, -y+3, -z+2$; (v) $x+\frac{1}{2}, -y+3, z+\frac{1}{2}$.

Data collection: *APEX2* (Bruker, 2010); cell refinement: *SAINT* (Bruker, 2009); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *DIAMOND* (Brandenburg, 2010); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LH5144).

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supporting information

Acta Cryst. (2010). E**66**, m1437 [https://doi.org/10.1107/S1600536810040250]

catena-Poly[[diaquamagnesium(II)]-bis(μ-5-ammonioisophthalato-κ^2O^1:O^3)]

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S1. Comment

The synthesis of metal coordination polymers has been an intense research area due to their interesting topologies and potential applications (Kitagawa, *et al.*, 2004). The crystal structures of 5-aminoisophthalic acid complexes with sodium (Zeng, *et al.*, 2007) and zinc (Kongshaug, *et al.*, 2006) have already been reported. In our continuous investigation in this area we report herein the structure of a new Mg coordination polymer based on the 5-amineisophthalato ligand.

The asymmetric unit of the title compound consists of half a an Mg^{II} ion, one 5-ammoniumisophthalato ligand and one coordinated water molecule. The Mg^{II} ion lies on a twofold roatation axis and is coordinated in a slightly distorted octahedral coordination environment (see Fig. 1). Pairs of bridging ammoniumisophthalato ligands connect symmetry related Mg^{II} ions to form one-dimensional chains along [010]. In the crystal structure, intermolecular O-H···O and N-H···O hydrogen bonds link these chains into a three-dimensional network (Fig. 2). The centroids of pairs of symmetry related benzene rings within a chain are separated by 3.5707 (12)Å.

S2. Experimental

Solvothermal reactions were carried out at 423 K for 2 d in a Teflon-lined acid digestion bomb with an internal volume of 23 ml followed by slow cooling at 6 K/h to room temperature. A single-phase product consisting of transparent brown crystals of was obtained from a mixture of 5-aminoisophthalic acid ($C_8H_7NO_4$, 0.0724 g, 0.4 mmol), $Mg(NO_3)_2.6H_2O$ (0.1026 g, 0.4 mmol), and DMF (5.0 ml) and H_2O (1.0 ml).

S3. Refinement

H atoms were constrained to ideal geometries, with C—H = 0.93 Å and U_{iso}(H) = 1.2U_{eq}(C); O—H = 0.85 Å and U_{iso}(H) = 1.5U_{eq}(N); N—H = 0.89 Å and U_{iso}(H) = 1.5U_{eq}(N). The aqua H atoms are clearly visible in difference Fourier maps and this clarifies that one of the H atoms does not have an acceptor.

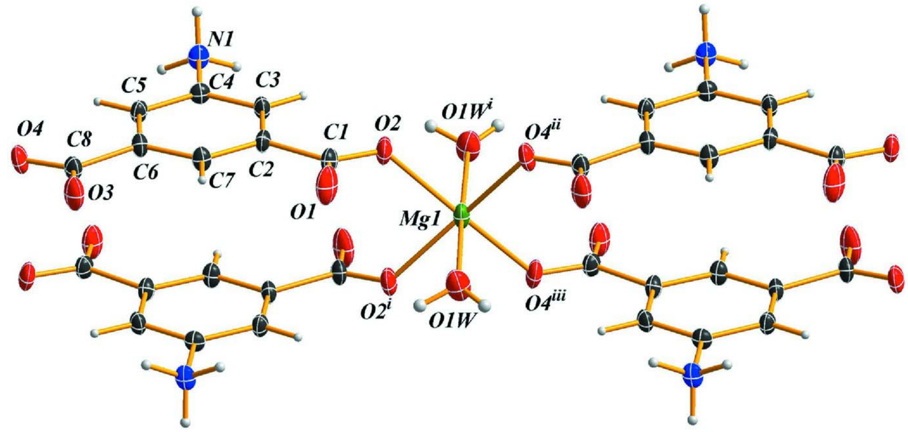

Figure 1

Part of the one-dimensional chain title compound with labelling and displacement ellipsoids drawn at the 50% probability level. Symmetry codes: (i) -*x* + 1/2, *y*, -*z* + 3/2; (ii) *x*, *y* - 1, *z*; (iii) -*x* + 1/2, *y* - 1, -*z* + 3/2.

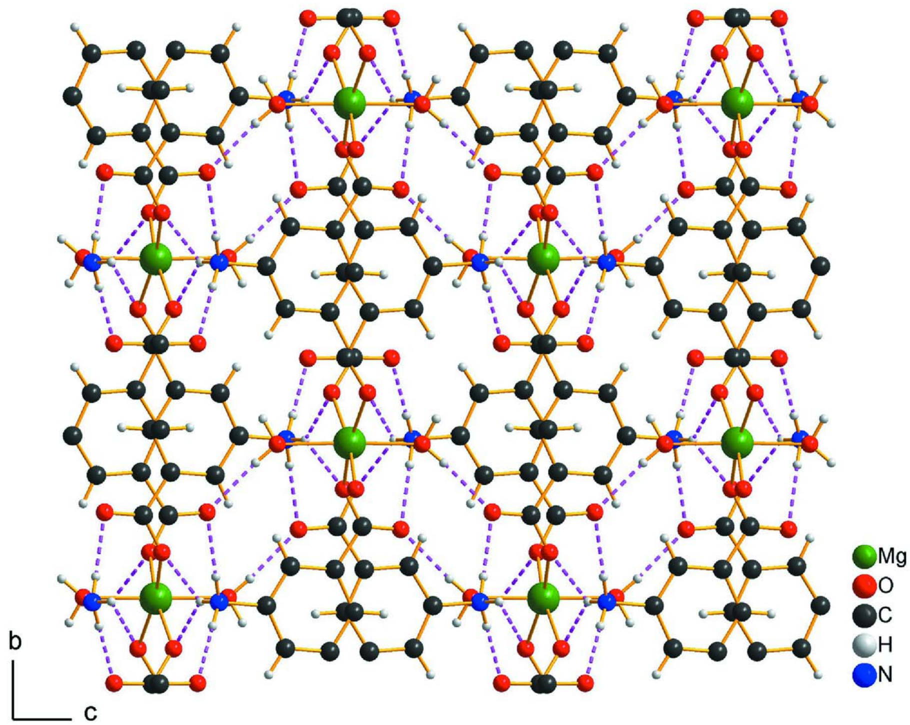

Figure 2

Part of the crystal structure of the title compound with view along the crystallographic *a* axis with hydrogen bonds shown as dashed lines.

catena-Poly[[diaquamagnesium(II)]-bis(μ-5-ammonioisophthalato- κ^2O^1:O^3)]

Crystal data

$[Mg(C_8H_6NO_4)_2(H_2O)_2]$	a = 6.9987 (2) Å
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Monoclinic, $P2/n$	c = 11.3809 (3) Å
Hall symbol: -P 2yac	β = 94.730 (2)°

V = 789.31 (4) Å^3
Z = 2
F(000) = 436
D_x = 1.770 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 1773 reflections
θ = 2.7–28.1°
μ = 0.18 mm^{-1}
T = 295 K
Columnar, colourless
0.10 × 0.08 × 0.08 mm

Data collection

Bruker APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 8.3333 pixels mm^{-1}
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2008)
T_{min} = 0.982, T_{max} = 0.986
6693 measured reflections
1963 independent reflections
1228 reflections with $I > 2\sigma(I)$
R_{int} = 0.047
θ_{max} = 28.3°, θ_{min} = 2.1°
$h = -9 \rightarrow 9$
$k = -13 \rightarrow 12$
$l = -15 \rightarrow 15$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.049
$wR(F^2)$ = 0.136
S = 1.00
1963 reflections
132 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
$w = 1/[\sigma^2(F_o^2) + (0.0686P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.36 e Å^{-3}
$\Delta\rho_{min}$ = −0.29 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 (Å^2)

	x	y	z	U_{iso}*/U_{eq}
Mg1	0.2500	0.72884 (11)	0.7500	0.0186 (3)
O1	−0.0895 (3)	0.97847 (17)	0.64235 (14)	0.0356 (5)
O2	0.0658 (2)	0.87721 (15)	0.79595 (13)	0.0242 (4)
O3	−0.1076 (3)	1.47494 (16)	0.61801 (14)	0.0294 (5)
O4	0.0357 (2)	1.59288 (15)	0.76552 (13)	0.0240 (4)
C1	−0.0008 (4)	0.9804 (2)	0.74109 (19)	0.0192 (5)
C2	0.0340 (3)	1.1145 (2)	0.80116 (18)	0.0165 (5)
C3	0.1175 (3)	1.1241 (2)	0.91552 (18)	0.0175 (5)
H3A	0.1514	1.0469	0.9585	0.021*
C4	0.1497 (3)	1.2498 (2)	0.96473 (18)	0.0164 (5)

C5	0.1056 (3)	1.3660 (2)	0.90294 (18)	0.0173 (5)
H5A	0.1308	1.4495	0.9376	0.021*
C6	0.0226 (3)	1.3570 (2)	0.78786 (18)	0.0169 (5)
C7	−0.0154 (3)	1.2315 (2)	0.73840 (19)	0.0177 (5)
H7A	−0.0746	1.2253	0.6624	0.021*
C8	−0.0199 (3)	1.4837 (2)	0.71758 (18)	0.0186 (5)
O1W	0.1775 (3)	0.72574 (17)	0.56326 (14)	0.0317 (5)
H1WA	0.1547	0.6707	0.5072	0.048*
H1WB	0.1906	0.8003	0.5266	0.048*
N1	0.2340 (3)	1.26019 (18)	1.08656 (15)	0.0203 (5)
H1A	0.3092	1.1894	1.1034	0.030*
H1B	0.1409	1.2622	1.1353	0.030*
H1C	0.3031	1.3352	1.0949	0.030*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Mg1	0.0252 (7)	0.0106 (5)	0.0192 (5)	0.000	−0.0031 (5)	0.000
O1	0.0543 (14)	0.0189 (10)	0.0303 (10)	−0.0015 (9)	−0.0166 (9)	−0.0080 (7)
O2	0.0343 (11)	0.0106 (8)	0.0274 (9)	0.0030 (7)	0.0011 (8)	−0.0002 (6)
O3	0.0446 (13)	0.0171 (9)	0.0245 (8)	0.0021 (8)	−0.0098 (8)	0.0042 (7)
O4	0.0346 (11)	0.0114 (8)	0.0253 (8)	−0.0057 (7)	−0.0013 (8)	0.0006 (6)
C1	0.0233 (14)	0.0113 (11)	0.0227 (11)	−0.0023 (10)	−0.0008 (10)	−0.0037 (9)
C2	0.0190 (13)	0.0094 (11)	0.0209 (11)	0.0001 (9)	0.0009 (10)	−0.0015 (8)
C3	0.0241 (14)	0.0109 (11)	0.0173 (10)	0.0005 (9)	0.0009 (10)	0.0018 (8)
C4	0.0171 (12)	0.0174 (12)	0.0142 (10)	−0.0007 (9)	−0.0014 (9)	−0.0010 (8)
C5	0.0228 (14)	0.0115 (11)	0.0175 (10)	−0.0007 (9)	0.0004 (10)	−0.0031 (8)
C6	0.0183 (13)	0.0114 (11)	0.0206 (11)	0.0009 (9)	−0.0010 (10)	0.0021 (8)
C7	0.0209 (13)	0.0146 (11)	0.0167 (10)	−0.0012 (10)	−0.0044 (9)	0.0002 (8)
C8	0.0236 (14)	0.0137 (12)	0.0183 (11)	0.0018 (10)	0.0001 (10)	0.0032 (8)
O1W	0.0477 (13)	0.0250 (10)	0.0211 (8)	−0.0054 (9)	−0.0047 (8)	−0.0004 (7)
N1	0.0260 (12)	0.0177 (10)	0.0162 (9)	0.0003 (8)	−0.0043 (8)	−0.0009 (7)

Geometric parameters (Å, º)

Mg1—O4^{i}	2.0375 (17)	C3—C4	1.380 (3)
Mg1—O4^{ii}	2.0375 (17)	C3—H3A	0.9300
Mg1—O2	2.0550 (17)	C4—C5	1.375 (3)
Mg1—O2^{iii}	2.0550 (17)	C4—N1	1.465 (3)
Mg1—O1W	2.1441 (16)	C5—C6	1.391 (3)
Mg1—O1W^{iii}	2.1441 (16)	C5—H5A	0.9300
O1—C1	1.238 (3)	C6—C7	1.386 (3)
O2—C1	1.270 (3)	C6—C8	1.509 (3)
O3—C8	1.246 (3)	C7—H7A	0.9300
O4—C8	1.262 (3)	O1W—H1WA	0.8459
O4—Mg1^{iv}	2.0374 (17)	O1W—H1WB	0.8589
C1—C2	1.508 (3)	N1—H1A	0.8900
C2—C3	1.385 (3)	N1—H1B	0.8900

C2—C7	1.394 (3)	N1—H1C	0.8900
O4^{i}—Mg1—O4^{ii}	96.86 (11)	C2—C3—H3A	120.5
O4^{i}—Mg1—O2	88.43 (7)	C5—C4—C3	122.1 (2)
O4^{ii}—Mg1—O2	168.54 (7)	C5—C4—N1	118.73 (19)
O4^{i}—Mg1—O2^{iii}	168.54 (7)	C3—C4—N1	119.18 (19)
O4^{ii}—Mg1—O2^{iii}	88.43 (7)	C4—C5—C6	119.1 (2)
O2—Mg1—O2^{iii}	88.24 (10)	C4—C5—H5A	120.4
O4^{i}—Mg1—O1W	87.75 (7)	C6—C5—H5A	120.4
O4^{ii}—Mg1—O1W	91.16 (7)	C7—C6—C5	119.4 (2)
O2—Mg1—O1W	99.23 (7)	C7—C6—C8	120.9 (2)
O2^{iii}—Mg1—O1W	81.96 (7)	C5—C6—C8	119.6 (2)
O4^{i}—Mg1—O1W^{iii}	91.16 (7)	C6—C7—C2	120.8 (2)
O4^{ii}—Mg1—O1W^{iii}	87.75 (7)	C6—C7—H7A	119.6
O2—Mg1—O1W^{iii}	81.96 (7)	C2—C7—H7A	119.6
O2^{iii}—Mg1—O1W^{iii}	99.23 (7)	O3—C8—O4	124.4 (2)
O1W—Mg1—O1W^{iii}	178.35 (11)	O3—C8—C6	119.0 (2)
C1—O2—Mg1	131.89 (15)	O4—C8—C6	116.66 (19)
C8—O4—Mg1^{iv}	137.42 (15)	Mg1—O1W—H1WA	140.5
O1—C1—O2	124.7 (2)	Mg1—O1W—H1WB	116.3
O1—C1—C2	118.4 (2)	H1WA—O1W—H1WB	102.3
O2—C1—C2	116.89 (19)	C4—N1—H1A	109.5
C3—C2—C7	119.4 (2)	C4—N1—H1B	109.5
C3—C2—C1	121.77 (19)	H1A—N1—H1B	109.5
C7—C2—C1	118.78 (19)	C4—N1—H1C	109.5
C4—C3—C2	119.06 (19)	H1A—N1—H1C	109.5
C4—C3—H3A	120.5	H1B—N1—H1C	109.5

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1*W*—H1*WA*···O3^{v}	0.85	2.04	2.883 (2)	175
N1—H1*A*···O1^{vi}	0.89	1.85	2.726 (2)	166
N1—H1*B*···O2^{vii}	0.89	2.19	2.919 (3)	138
N1—H1*B*···O4^{viii}	0.89	2.26	3.009 (3)	142
N1—H1*C*···O3^{ix}	0.89	2.00	2.869 (2)	165

Symmetry codes: (v) $-x, -y+2, -z+1$; (vi) $x+1/2, -y+2, z+1/2$; (vii) $-x, -y+2, -z+2$; (viii) $-x, -y+3, -z+2$; (ix) $x+1/2, -y+3, z+1/2$.