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Key indicators

Single-crystal X-ray study
 $T = 293\text{ K}$
Mean $\sigma(\text{C}-\text{C}) = 0.002\text{ \AA}$
 R factor = 0.042
 wR factor = 0.137
Data-to-parameter ratio = 16.4For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.Bis[hexaquamagnesium(II)] pyrazine-2,3,5,6-tetra-
carboxylate tetrahydrate

The unit cell of the title compound, $[\text{Mg}(\text{H}_2\text{O})_6]_2(\text{C}_8\text{N}_2\text{O}_8) \cdot 4\text{H}_2\text{O}$, contains two hexaquamagnesium(II) cations, one fully deprotonated pyrazine-2,3,5,6-tetracarboxylate $[(2,3,5,6\text{-PZTC})^{4-}]$ anion with its geometrical centre situated at the inversion centre and four solvent water molecules. The magnesium(II) ion is surrounded by six water molecules with their O atoms located at the apices of a fairly regular octahedron. Mg—O bond distances range from 2.036 (1) to 2.113 (1) Å (mean value 2.065 Å). The carboxylate groups are inclined to the pyrazine ring by 22.8 (1) and 99.1 (1)°. A three-dimensional network of hydrogen bonds is built up between the coordinated water molecules and the carboxylate O atoms.

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Comment

The unit cell of the title compound, (I), contains two $[\text{Mg}(\text{H}_2\text{O})_6]^{2+}$ cations, one fully deprotonated pyrazine-2,3,5,6-tetracarboxylate $[(2,3,5,6\text{-PZTC})^{4-}]$ anion and four solvent water molecules. Fig. 1 shows the molecules with the atom-numbering scheme; Fig. 2 shows the packing of the molecules. The geometrical centre of the $(2,3,5,6\text{-PZTC})^{4-}$ anion is situated at a centre of symmetry. The deprotonated carboxylic groups are inclined to the plane of the pyrazine ring by 22.8 (1) and 99.1 (1)°. The bond distances and bond angles within the $(2,3,5,6\text{-PZTC})^{4-}$ anion do not differ from those reported in structures of 3d transition metal ion complexes with this ligand (Marioni *et al.*, 1986, 1994; Graf *et al.*, 1993). The magnesium ion and the surrounding six coordinated water molecules are located in general positions. The coordination polyhedron around the Mg^{II} ion is a fairly regular octahedron with typical bond distances and angles (Table 1). Four solvent water molecules complete the contents of the unit cell. The

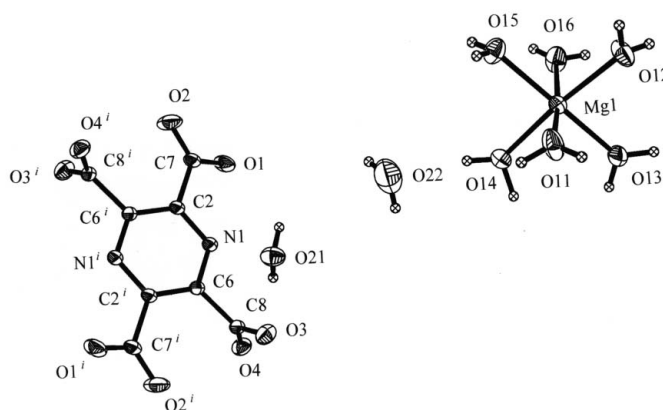


Figure 1

Atom-labelling scheme for the title compound. Non-H atoms are shown as 50% probability displacement ellipsoids. [Symmetry code: (i) $-x + 2, -y, -z$.]

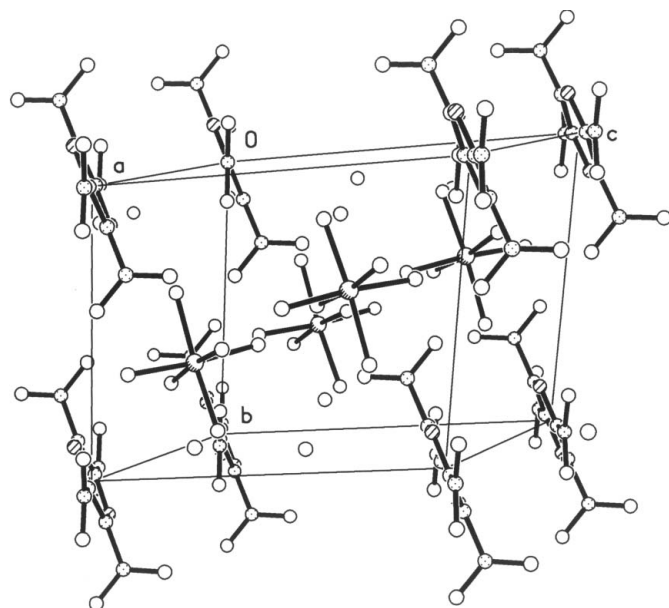
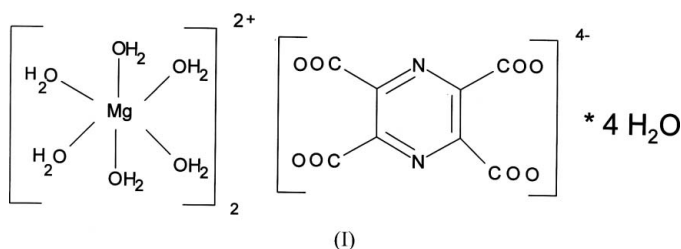


Figure 2
Packing of molecules in the unit cell of compound (I). H atoms have been omitted.

coordinated water molecules act as donors in a three-dimensional network of rather weak hydrogen bonds with $O-H \cdots O > 2.7 \text{ \AA}$. The acceptors are the carboxylate O atoms of the anion molecules. Both solvent water molecules are donors for hydrogen bonds. The geometrical parameters of the hydrogen bond system are given in Table 2. Among metal complexes with pyrazine 2,3,5,6-tetracarboxylate, an ionic pattern has been reported in the Mn^{II} compound (Marioni *et al.*, 1994). Its monoclinic structure contains $[Mn(H_2O)_6]^{2+}$ cations and doubly deprotonated $[H_2(2,3,5,6-PZTC)]^{2-}$ anions. Separate $[Mg(H_2O)_6]^{2+}$ cations have also been observed in the structure of the copper complex $[Mg(H_2O)_6]^{2+} \cdot [Cu(2,3,5,6-PZTC)(H_2O)_2]^{2-} \cdot 2H_2O$, in which the ligand molecules are fully deprotonated and bridge the Cu^{II} ions to form catenated polyanions (Graf *et al.*, 1993).



Experimental

A hot aqueous solution (50 ml) containing magnesium acetate tetrahydrate (2 mmol) was added with constant stirring to a hot aqueous solution (50 ml) containing pyrazine-2,3,5,6-tetracarboxylic acid (1 mmol). After boiling for 1 h, the solution was left to crystallize at room temperature. After several days, colourless crystals were found in the mother liquid.

Crystal data

$[Mg(H_2O)_6]_2(C_8N_2O_8) \cdot 4H_2O$
 $M_r = 588.98$
 Triclinic, $P\bar{1}$
 $a = 6.7467 (13) \text{ \AA}$
 $b = 9.1779 (18) \text{ \AA}$
 $c = 10.731 (2) \text{ \AA}$
 $\alpha = 102.95 (3)^\circ$
 $\beta = 103.29 (3)^\circ$
 $\gamma = 100.02 (3)^\circ$
 $V = 612.2 (2) \text{ \AA}^3$

$Z = 1$
 $D_x = 1.598 \text{ Mg m}^{-3}$
 Mo $K\alpha$ radiation
 Cell parameters from 25 reflections
 $\theta = 6-15^\circ$
 $\mu = 0.21 \text{ mm}^{-1}$
 $T = 293 (2) \text{ K}$
 Rectangular block, colourless
 $0.30 \times 0.25 \times 0.20 \text{ mm}$

Data collection

Kuma KM-4 four-circle diffractometer
 $\omega/2\theta$ scans
 Absorption correction: analytical (CrysAlis RED; Oxford Diffraction, 2000)
 $T_{\min} = 0.955$, $T_{\max} = 0.977$
 3839 measured reflections
 3565 independent reflections

2752 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.018$
 $\theta_{\max} = 30.1^\circ$
 $h = 0 \rightarrow 9$
 $k = -12 \rightarrow 12$
 $l = -14 \rightarrow 14$
 3 standard reflections every 200 reflections
 intensity decay: 3.1%

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.042$
 $wR(F^2) = 0.137$
 $S = 1.14$
 3565 reflections
 217 parameters
 H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0859P)^2 + 0.0954P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} = 0.001$
 $\Delta\rho_{\max} = 0.60 \text{ e \AA}^{-3}$
 $\Delta\rho_{\min} = -0.56 \text{ e \AA}^{-3}$

Table 1

Selected geometric parameters (\AA , $^\circ$).

Mg1—O11	2.0359 (14)	Mg1—O14	2.0654 (13)
Mg1—O12	2.0437 (13)	Mg1—O13	2.0748 (15)
Mg1—O15	2.0523 (15)	Mg1—O16	2.1130 (14)
O11—Mg1—O12	89.20 (6)	O15—Mg1—O13	174.97 (6)
O15—Mg1—O14	91.09 (6)	O14—Mg1—O13	86.74 (6)
O12—Mg1—O13	87.90 (6)	O15—Mg1—O16	84.34 (6)

Table 2

Hydrogen-bonding geometry (\AA , $^\circ$).

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
O11—H112 \cdots O4 ⁱⁱ	0.86 (3)	1.94 (3)	2.7935 (18)	174 (2)
O11—H111 \cdots O1 ⁱⁱⁱ	0.85 (4)	1.86 (4)	2.7037 (18)	171 (3)
O12—H121 \cdots O4 ^{iv}	0.85 (3)	1.97 (3)	2.8074 (17)	172 (3)
O12—H122 \cdots O1 ⁱⁱ	0.86 (4)	1.86 (4)	2.7103 (19)	168 (3)
O13—H132 \cdots N1 ^{iv}	0.86 (3)	2.10 (3)	2.9084 (18)	156 (3)
O14—H142 \cdots O22	0.90 (3)	1.96 (3)	2.846 (2)	167 (3)
O14—H141 \cdots O4 ^v	0.95 (3)	1.85 (3)	2.782 (2)	165 (3)
O15—H151 \cdots O21 ^{vi}	0.83 (3)	1.91 (3)	2.7323 (19)	174 (2)
O15—H152 \cdots O21 ^{vii}	0.85 (3)	1.89 (3)	2.7185 (18)	165 (3)
O16—H162 \cdots O3 ^{iv}	0.848 (16)	1.928 (16)	2.7739 (18)	175 (3)
O21—H212 \cdots O2 ^{viii}	0.88 (3)	1.83 (3)	2.7135 (18)	175 (3)

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

H atoms were found in Fourier maps and refined with isotropic displacement parameters. The U values of the H atoms bonded to O16 and O22 were set to $1.2U_{\text{eq}}$ of the parent atom. The positional parameters of the H atoms bonded to O22 were not refined. The O—H distances for the H atoms bonded to O16 were restrained to $0.82 (2) \text{ \AA}$.

Data collection: *KM-4 Software* (Kuma, 1996); cell refinement: *KM-4 Software*; data reduction: *DATAPROC* (Kuma, 2001); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); structure refinement and publication software: *SHELXL97* (Sheldrick, 1997); molecular graphics: *XP* (Siemens, 1992).

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