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Triaqua(pyridine-2,6-dicarboxylato)magnesium(II) dihydrate

Hossein Aghabozorg,[a]* Pouya Ghasemikhah,[a] Mohammad Ghadermazi,[b] Janet Soleimannejad[c] and Harry Adams[d]

[a]Department of Chemistry, Teacher Training University, 49 Mofateh Avenue, 15614 Tehran, Iran, [b]Department of Chemistry, Faculty of Science, Kurdistan University, Sanandaj, Iran, [c]Department of Chemistry, Faculty of Science, Ilam University, Ilam, Iran, and [d]Department of Chemistry, University of Sheffield, Sheffield S3 7HF, England

Correspondence e-mail: haghabozorg@yahoo.com

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Key indicators

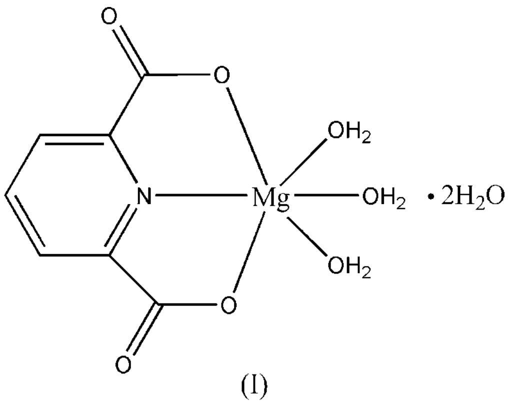
Single-crystal X-ray study
T = 150 K
Mean σ(C–C) = 0.001 Å
R factor = 0.027
wR factor = 0.079
Data-to-parameter ratio = 17.1

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

The reaction of magnesium(II) nitrate hexahydrate with the proton-transfer compound (pipzH_2)(pydc) [pipz is piperazine and pydcH_2 is pyridine-2,6-dicarboxylic acid] in aqueous solution leads to the formation of the title compound, $[Mg(C_7H_3O_4)(H_2O)_3]\cdot 2H_2O$. The piperazinium cation is not incorporated in this crystal structure. The Mg^{II} atom has a distorted octahedral coordination environment. There are many intermolecular O—H$\cdots$O hydrogen bonds involving the $(pydc)^{2-}$ species and water molecules in the crystal structure.

Comment

Hydrogen bonding plays a key role in chemical, catalytic and biochemical processes, as well as in supramolecular chemistry and crystal engineering (Epstein & Shubina, 2002). In order to study the hydrogen-bonding patterns in proton-transfer compounds, our research group has selected pyridine-2,6-dicarboxylic acid (pydcH_2) and 1,10-phenanthroline-2,9-dicarboxylic acid (phendcH_2) as proton donors, and 2,6-pyridinediamine (pyda), creatinine (creat) and 1,10-phenanthroline (phen) as proton acceptors. This has resulted in the formation of new proton-transfer systems, such as (pydaH)(pydcH) (Aghabozorg *et al.*, 2005), (creatH)(pydcH) (Moghimi *et al.*, 2005) and (creatH)(phendcH) (Soleimannejad *et al.*, 2005). The dicarboxylate fragments of the resulting proton-transfer compounds can function as suitable ligands in the synthesis of organo–metal complexes (Moghimi *et al.*, 2002*a*,*b*, 2005; Ranjbar *et al.*, 2003; Ranjbar, Aghabozorg & Moghimi, 2002; Ranjbar, Taghavipur *et al.*, 2002; Ranjbar *et al.*, 2001). Here, we report the crystal structure of the title mononuclear complex, $[Mg(pydc)(H_2O)_3]\cdot 2H_2O$, (I), in which the $(pydc)^{2-}$ species acts as a tridentate ligand through two O atoms and one N atom.



(I)

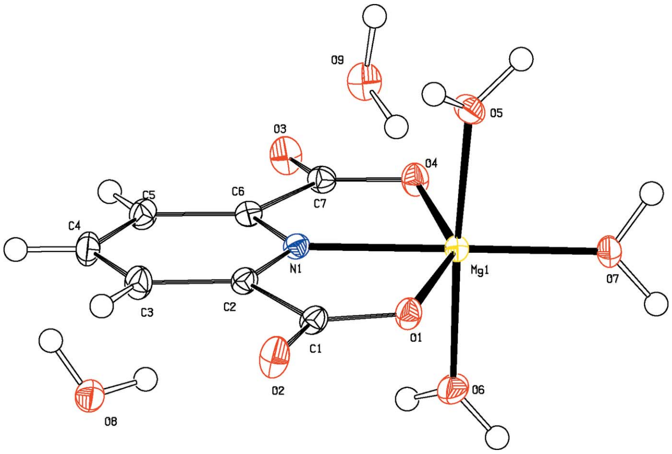


Figure 1
The molecular structure of the title complex, with displacement ellipsoids drawn at the 50% probability level and H atoms shown as small spheres.

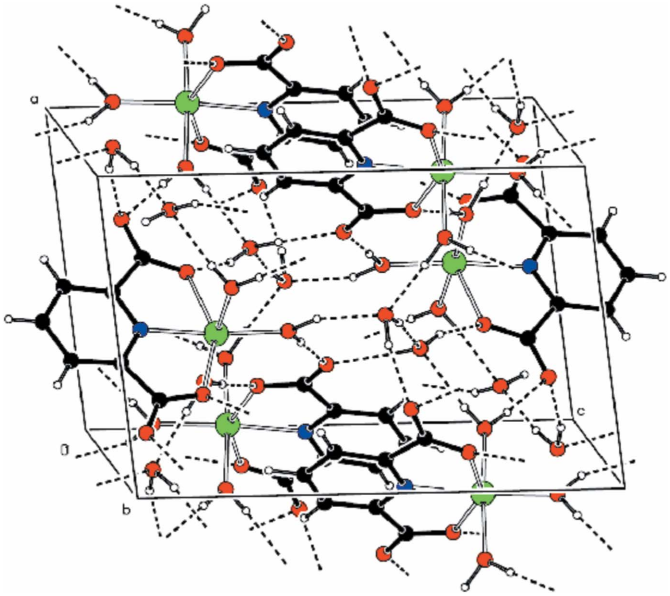


Figure 2
The crystal packing of (I). Hydrogen bonds are shown as dashed lines.

The structure of (I) is shown in Fig. 1 and geometric parameters are given in Table 1. The coordination geometry around the Mg^{II} atom is distorted octahedral. The bond angles show small deviations from 90 and 180°.

Details of the strongest hydrogen bonds are given in Table 2. In the crystal structure of (I), three coordinated water molecules and two uncoordinated water molecules are involved in the hydrogen bonds in the crystal structure. Four O atoms of the carboxylate groups create hydrogen bonds to adjacent molecules (Fig. 2 and Table 2).

Experimental

The reaction of $(pipzH_2)(pydc)$ (200 mg, 0.797 mmol) with $Mg(NO_3)_2\cdot6H_2O$ (122.2 mg, 0.477 mmol) in water (20 ml) gave colourless crystals of $[Mg(pydc)(H_2O)_3]\cdot2H_2O$, (I). X-ray diffraction quality crystals were obtained by slow evaporation of the solvent at room temperature.

Crystal data

$[Mg(C_7H_3O_4)(H_2O)_3]\cdot2H_2O$
$M_r = 279.49$
Monoclinic, $P2_1/n$
$a = 8.9229$ (7) Å
$b = 9.9459$ (8) Å
$c = 13.2508$ (10) Å
$\beta = 97.383$ (4)°
$V = 1166.21$ (16) $Å^3$
$Z = 4$
Mo $K\alpha$ radiation
$\mu = 0.19$ mm^{-1}
$T = 150$ (2) K
0.22 × 0.19 × 0.17 mm

Data collection

Bruker APEXII diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1997*a*)
$T_{min} = 0.879$, $T_{max} = 0.968$
27484 measured reflections
2780 independent reflections
2596 reflections with $I > 2\sigma(I)$
$R_{int} = 0.022$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.028$
$wR(F^2) = 0.079$
$S = 1.06$
2780 reflections
163 parameters
H-atom parameters constrained
$\Delta\rho_{max} = 0.36$ e $Å^{-3}$
$\Delta\rho_{min} = -0.33$ e $Å^{-3}$

Table 1
Selected geometric parameters (Å, °).

Mg1—O7	2.0086 (8)	Mg1—O1	2.1700 (8)
Mg1—O6	2.0356 (8)	O1—C1	1.2692 (13)
Mg1—O5	2.0523 (8)	O2—C1	1.2475 (13)
Mg1—N1	2.1065 (9)	O3—C7	1.2491 (13)
Mg1—O4	2.1542 (8)	O4—C7	1.2695 (13)
O7—Mg1—O6	88.68 (3)	O5—Mg1—O4	92.19 (3)
O7—Mg1—O5	88.17 (3)	N1—Mg1—O4	74.26 (3)
O6—Mg1—O5	176.49 (4)	O7—Mg1—O1	110.27 (4)
O7—Mg1—N1	175.10 (4)	O6—Mg1—O1	90.68 (3)
O6—Mg1—N1	88.96 (3)	O5—Mg1—O1	88.96 (3)
O5—Mg1—N1	94.30 (3)	N1—Mg1—O1	74.05 (3)
O7—Mg1—O4	101.45 (4)	O4—Mg1—O1	148.28 (3)
O6—Mg1—O4	89.95 (3)		
O2—C1—C2—C3	−0.56 (16)	C5—C6—C7—O3	−4.86 (15)
O1—C1—C2—C3	178.03 (10)	C5—C6—C7—O4	175.73 (10)

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O5—H5*A*···O9	0.95	1.85	2.7919 (11)	173
O5—H5*B*···O1^{i}	0.95	1.79	2.7395 (10)	177
O6—H6*A*···O8^{ii}	0.95	1.87	2.8084 (11)	167
O6—H6*B*···O3^{iii}	0.95	1.73	2.6678 (11)	171
O7—H7*A*···O9^{iv}	0.95	1.96	2.8674 (11)	160
O7—H7*B*···O2^{i}	0.95	1.72	2.6683 (11)	176
O8—H8*A*···O2	0.95	1.77	2.7145 (11)	171
O8—H8*B*···O4^{v}	0.95	1.87	2.7905 (11)	161
O9—H9*B*···O8^{vi}	0.95	1.84	2.7815 (11)	170
O9—H9*A*···O3^{vii}	0.95	1.92	2.8424 (12)	162

Symmetry codes: (i) $-x+\frac{3}{2}, y+\frac{1}{2}, -z+\frac{3}{2}$; (ii) $-x+2, -y+1, -z+1$; (iii) $-x+\frac{5}{2}, y-\frac{1}{2}, -z+\frac{3}{2}$; (iv) $x+\frac{1}{2}, -y+\frac{3}{2}, z+\frac{1}{2}$; (v) $x-\frac{1}{2}, -y+\frac{3}{2}, z-\frac{1}{2}$; (vi) $-x+1, -y+1, -z+1$; (vii) $x-1, y, z$.

H atoms were positioned geometrically and refined with a riding model (including torsional freedom for methyl groups), with O—H and C—H distances equal to 0.95 Å, and with $U_{iso}(H) = 1.2$ (1.5 for methyl groups) times $U_{eq}(C,O)$.

m1488 Aghabozorg *et al.* • $[Mg(C_7H_3O_4)(H_2O)_3]\cdot2H_2O$ *Acta Cryst.* (2007). E**63**, m1487–m1489

Data collection: *SMART* (Bruker, 1998); cell refinement: *SMART*; data reduction: *SAINT-Plus* (Bruker, 1998); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*b*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*b*); molecular graphics: *SHELXTL* (Sheldrick, 1998); software used to prepare material for publication: *SHELXTL*.

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References

Aghabozorg, H., Akbari Saei, A. & Ramezanipour, F. (2005). *Acta Cryst.* E**61**, o3242–o3244.

Bruker (1998). *SAINT-Plus* (Version 6.01) and *SMART* (Version 5.059). Bruker AXS Inc., Madison, Wisconsin, USA.

Epstein, L. M. & Shubina, E. S. (2002). *Coord. Chem. Rev.* **231**, 165–181.

Moghimi, A., Ranjbar, M., Aghabozorg, H., Jalili, F., Shamsipur, M. & Chadha, R. K. (2002*a*). *Can. J. Chem.* **80**, 1687–1696.

Moghimi, A., Ranjbar, M., Aghabozorg, H., Jalili, F., Shamsipur, M. & Chadha, R. K. (2002*b*). *J. Chem. Res. (S)*, pp. 477–479.

Moghimi, A., Sharif, M. A., Shokrollahi, A., Shamsipur, M. & Aghabozorg, H. (2005). *Z. Anorg. Allg. Chem.* **631**, 902–908.

Ranjbar, M., Aghabozorg, H., Moghimi, A. & Yanovsky, A. (2001). *Z. Kristallogr. New Cryst. Struct.* **216**, 626–628.

Ranjbar, M., Aghabozorg, H. & Moghimi, A. (2002). *Acta Cryst.* E**58**, m304–m306.

Ranjbar, M., Moghimi, A. & Aghabozorg, H. (2003). *Anal. Sci.* **19**, 803–804.

Ranjbar, M., Taghavipur, M., Aghabozorg, H., Moghimi, A., Jalili, F. & Shamsipur, M. (2002). *Pol. J. Chem.* **76**, 785–794.

Sheldrick, G. M. (1997*a*). *SADABS*. Version 2.01. Bruker AXS Inc., Madison, Wisconsin, USA.

Sheldrick, G. M. (1997*b*). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.

Sheldrick, G. M. (1998). *SHELXTL*. Version 5.10. Bruker AXS Inc., Madison, Wisconsin, USA.

Soleimannejad, J., Sharif, M. A., Sheshmani, S., Alizadeh, R., Moghimi, A. & Aghabozorg, H. (2005). *Anal. Sci.* **21**, x49–x50.

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