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Hexaaquamagnesium(II) bis[*N*-(6-amino-3,4-dihydro-3-methyl-5-nitroso-4-oxopyrimidin-2-yl)glycinate] dihydrate

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P. Arranz Mascarós,[a]* Justo Cobo Domingo,[a] M. Godino Salido,[a] M. D. Gutiérrez Valero,[a] R. López Garzón[a] and John Nicolson Low[b]

[a]Departamento de Química Inorgánica y Orgánica, Universidad de Jaén, 23071 Jaén, Spain, and [b]Department of Applied Physics and Electronic and Mechanical Engineering, University of Dundee, Nethergate, Dundee DD1 4HN, Scotland
Correspondence e-mail: j.n.low@dundee.ac.uk

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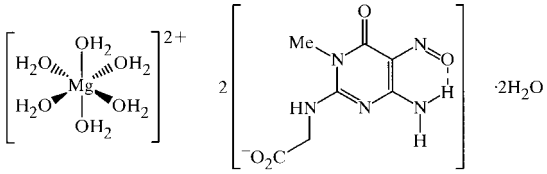
The analysis of the title compound, $[Mg(H_2O)_6](C_7H_8N_5O_4)_2\cdot 2H_2O$, continues our study of the reactivity of metal ions with N-protected amino acids. The Mg ion lies on an inversion centre with Mg—O 2.0437 (10)-2.0952 (10) Å. The $[Mg(H_2O)_6]^{2+}$cations, anions and water molecules are linked by an extensive hydrogen-bond network.

Comment

The title compound, hexaaquamagnesium(II) bis[*N*-(6-amino-3,4-dihydro-3-methyl-5-nitroso-4-oxopyrimidin-2-yl)-glycinate] dihydrate, (I), continues our study of the reactivity of metal ions with N-protected amino acids. These reactions occur in several biological processes (Bonamartini Corradi, 1992). This type of compound shows great versatility in the formation of hydrogen-bonded complexes as a result of the presence of numerous hydrogen-bond donor and acceptor groups. Divalent magnesium ions shows a rich coordination ability to low-molecular weight metabolites, nucleic acid derivatives, and carrier ligands and in all cases, water molecules of coordination are involved in the binding interactions (Cowan, 1995). In this case, the Mg ion sits on a crystallographic centre of symmetry and is coordinated to six water molecules (three unique and three symmetry related); the anion is not coordinated to the Mg cation. Examination of the structure with *PLATON* (Spek, 1999) showed that there were no solvent-accessible voids in the crystal lattice.



(I)

Experimental

The ligand N-(6-amino-3,4-dihydro-3-methyl-5-nitroso-4-oxopyrimidin-2-yl)glycine was prepared according to the method previously reported (Low *et al.*, 1997). Complex (I) was obtained from aqueous solution at pH *ca* 6.2, $MgCl_2$(3 mmol) was dissolved in KCl 0.5 M (25 ml) and added to a solution of the potassium salt of the ligand (1 mmol) in the minimum amount of water (20 ml). A violet crystalline precipitate appeared and was filtered off and washed with water, ethanol and diethyl ether and stored under an anhydrous environment. Analysis, calculated for $C_{14}H_{32}MgN_{10}O_{16}$: C 27.08, H 5.01, N 22.08%; found C 26.66, H 5.15, N 21.99%.

Crystal data

$[Mg(H_2O)_6](C_7H_8N_5O_4)_2\cdot 2H_2O$	$Z = 1$
$M_r = 620.81$	$D_x = 1.593$ Mg m^{-3}
Triclinic, $P\overline{1}$	Mo $K\alpha$ radiation
$a = 7.3152$ (3) Å	Cell parameters from 2947 reflections
$b = 7.5917$ (4) Å	$\theta = 1.73$–$27.50°$
$c = 12.3024$ (6) Å	$\mu = 0.164$ mm^{-1}
$\alpha = 86.661$ (3)°	$T = 150.0$ (1) K
$\beta = 73.172$ (3)°	Block, pink
$\gamma = 81.79$ (3)°	0.25 × 0.25 × 0.25 mm
$V = 647.15$ (5) Å^3	

Data collection

Kappa–CCD diffractometer	2428 reflections with $I > 2\sigma(I)$
φ s and ω scans with κ offset scans	$R_{int} = 0.034$
Absorption correction: multi-scan (*SORTAV*; Blessing, 1995, 1997)	$\theta_{max} = 27.50°$
$T_{min} = 0.960$, $T_{max} = 0.960$	$h = -9 \rightarrow 8$
8396 measured reflections	$k = -9 \rightarrow 7$
2947 independent reflections	$l = -15 \rightarrow 15$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0622P)^2 + 0.0773P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.0384$	$(\Delta/\sigma)_{max} = 0.001$
$wR(F^2) = 0.1099$	$\Delta\rho_{max} = 0.349$ e Å^{-3}
$S = 1.061$	$\Delta\rho_{min} = -0.280$ e Å^{-3}
2947 reflections	
212 parameters	
H-atom parameters constrained	

Molecule (I) crystallized in the triclinic system; space group $P\overline{1}$ assumed and confirmed by the analysis. H atoms were treated as riding atoms with C—H 0.98 to 0.99 Å, N—H 0.88 Å, The water of crystallization O—H distance was set by *DFIX* to 0.82 Å after location of the H atoms on a difference Fourier map.

Data collection: *KappaCCD server software* (Nonius, 1997); cell refinement: *DENZO* (Otwinowski & Minor, 1997); data reduction: *DENZO* (Otwinowski & Minor, 1997); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997*a*);

program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXL*97 and *WordPerfect* macro *PRPKAPPA* (Ferguson, 1999).

X-ray data were collected at the EPSRC, X-ray Crystallographic Service, University of Southampton using a Enraf–Nonius KappaCCD diffractometer. The authors thank the staff for all their help and advice.

References

Blessing, R. H. (1995). *Acta Cryst.* A**51**, 33–38.
Blessing, R. H. (1997). *J. Appl. Cryst.* **30**, 421–426.
Bonamartini Corradi, A. (1992). *Coord. Chem. Rev.* **117**, 45–98.
Cowan, J. A. (1995). In *Chemistry of Magnesium*. New York: VCH publishers Inc.
Ferguson, G. (1999). *PRPKAPPA*. University of Guelph, Canada.
Low, J. N., Ferguson, G., López, R., Arranz, P., Cobo, J., Melguizo, M., Nogueras, M. & Sánchez, R. (1997). *Acta Cryst.* C**53**, 890–892.
Nonius (1997). *KappaCCD Server Software*. Windows 3.11 Version, Nonius BV, Delft, The Netherlands.
Otwinowski, Z. & Minor, W. (1997). *Methods Enzymol.* **276**, 307- 326.
Sheldrick, G. M. (1997*a*). *SHELXS*97. University of Göttingen, Germany.
Sheldrick, G. M. (1997*b*). *SHELXL*97. University of Göttingen, Germany.
Spek, A. L. (1999). *PLATON*. January 1999 version. University of Utrecht, The Netherlands.