Acta Crystallographica Section E
Structure Reports
Online

ISSN 1600-5368

trans-Diaquabis(5-methylpyrazine-2-carboxylato-κ^2*O*,*N*)zinc(II)

Michał Gryz,[a] Wojciech Starosta[b] and Janusz Leciejewicz[b]*

[a]Office for Medicinal Products, Medical Devices and Biocides, ul. Ząbkowska 41, 03-736 Warszawa, Poland, and [b]Institute of Nuclear Chemistry and Technology, ul. Dorodna 16, 03-195 Warszawa, Poland

Correspondence e-mail: jlec@ichtj.waw.pl

Received 26 March 2007
Accepted 4 April 2007

Key indicators

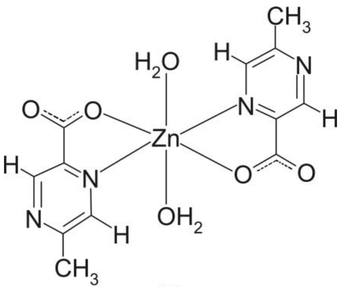
Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.002 Å
R factor = 0.031
wR factor = 0.085
Data-to-parameter ratio = 16.1

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

The crystal structure of the title compound, [Zn($C_6H_5N_2O_2$)$_2$(H_2O)$_2$], consists of discrete mononuclear complex molecules. The Zn^{II} ion is located on an inversion centre and is coordinated in a *trans* mode by the *N*,*O*-bonding groups donated by two 3-methylpyrazine-2-carboxylate ligands [Zn—N = 2.109 (1) Å and Zn—O = 2.090 (1) Å] and by two aqua O atoms [Zn—O = 2.129 (2) Å]. The coordination geometry around the Zn^{II} ion is slightly distorted octahedral. The crystal structure is stabilized by a network of O—H···O hydrogen bonds operating between the coordinated water molecules and carboxylate O atoms.

Comment

The crystal structure of the title compound, (I), contains discrete mononuclear complex molecules in which Zn^{II} ions, situated on inversion centres, are chelated by two 5-methylpyrazine-2-carboxylate ligands in a *trans* mode and bonded by two water molecules. The coordination geometry around the Zn^{II} ion is slightly distorted octahedral. The ligand chelation proceeds *via* its *N*,*O*-bonding group. The pyrazine ring is essentially planar [r.m.s. deviation 0.0176 (2) Å] and the carboxylate group deviates from this ring plane by 3.5 (1)°. The molecular structure is shown in Fig. 1 and relevant bond distances and angles for the Zn^{II} coordination octahedron are listed in Table 1. The bond distances and angles within the ligand molecule are in fair agreement with those reported for the parent acid (Vishweshwar *et al.* 2002).



(I)

Coordinated water molecules and carboxylate O atoms participate in a network of O—H···O hydrogen bonds (Table 2) which are responsible for the stability of the crystal structure (Fig. 2).

Experimental

Zinc carbonate in a small excess was added with constant stirring to a hot aqueous solution (50 ml) containing 5-methylpyrazine-2-

carboxylic acid (Aldrich) (0.01 mol), then filtered off. After a few days, colourless well shaped single crystals in the form of rectangular blocks deposited in the mother liquid. They were separated off, washed with cold ethanol and dried in air at room temperature.

Crystal data

$[Zn(C_6H_5N_2O_2)_2(H_2O)_2]$
M_r = 375.64
Triclinic, $P\overline{1}$
a = 5.1405 (10) Å
b = 6.4312 (13) Å
c = 12.234 (2) Å
α = 104.67 (3)°
β = 90.61 (3)°
γ = 109.44 (3)°
V = 366.97 (13) Å^3
Z = 1
Mo $K\alpha$ radiation
μ = 1.71 mm^{-1}
T = 293 (2) K
0.48 × 0.12 × 0.10 mm

Data collection

Kuma KM-4 four-circle diffractometer
Absorption correction: analytical (*CrysAlis RED*; Oxford Diffraction, 2002)
T_{min} = 0.758, T_{max} = 0.813
2381 measured reflections
2157 independent reflections
2070 reflections with $I > 2\sigma(I)$
R_{int} = 0.010
3 standard reflections every 200 reflections intensity decay: 0.2%

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.031
$wR(F^2)$ = 0.085
S = 1.10
2157 reflections
134 parameters
All H-atom parameters refined
$\Delta\rho_{max}$ = 0.95 e Å^{-3}
$\Delta\rho_{min}$ = −0.80 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Zn1—O1	2.0901 (12)	Zn1—O3	2.1287 (16)
Zn1—N1	2.1085 (13)		
O1^{i}—Zn1—O1	180	N1—Zn1—O3	92.44 (6)
O1—Zn1—N1	79.23 (5)	O1—Zn1—O3^{i}	89.36 (5)
O1—Zn1—N1^{i}	100.77 (5)	N1—Zn1—O3^{i}	87.56 (6)
N1—Zn1—N1^{i}	180	O3—Zn1—O3^{i}	180
O1—Zn1—O3	90.64 (5)		

Symmetry code: (i) $-x+2, -y+1, -z+1$.

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

D—H···A	D—H	H···A	D···A	D—H···A
O3—H31···O2^{ii}	0.75 (4)	1.96 (4)	2.679 (2)	162 (3)
O3—H32···O1^{iii}	0.77 (3)	1.99 (3)	2.7374 (18)	161 (3)

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

All H atoms were located in a difference Fourier map and refined with isotropic displacement parameters, giving C—H distances in the range 0.88 (5)–0.94 (3) Å.

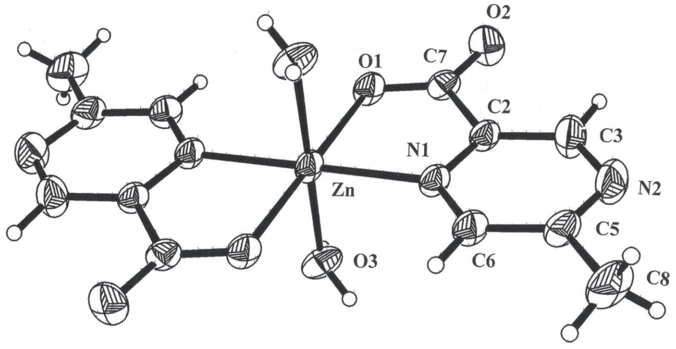


Figure 1
The molecular structure of (I), with the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level. Unlablled atoms are related by the symmetry operator ($2-x$, $1-y$, $1-z$).

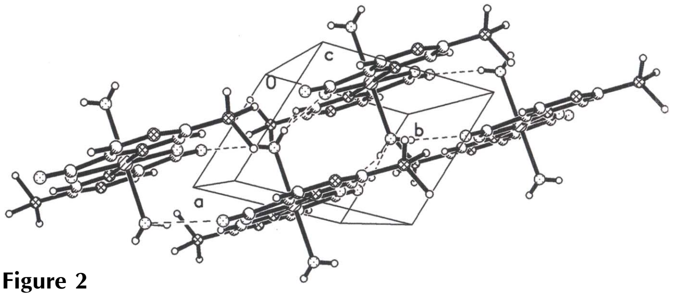


Figure 2
Part of the crystal structure of (I), with hydrogen bonds indicated by dashed lines.

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

This work was supported by the Ministry of Scientific Research and Information Technology (grant No. 3 T09 078 28).

References

Kuma (2001). *DATAPROC*. Version 10.0.7. Kuma Diffraction, Wrocław, Poland.
Kuma Diffraction (1996). *KM-4 Software*. Kuma Diffraction, Wrocław, Poland.
Oxford Diffraction (2002). *CrysAlis RED*. Version 1.69. Oxford Diffraction Ltd., Abingdon, Oxfordshire, England.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Siemens (1992). *XP*. Version 4.3. Siemens Analytical X-ray Instruments Inc., Karlsruhe, Germany.
Vishweshwar, P., Nangla, A. & Lynch, V. M. (2002). *J. Org. Chem.* **67**, 555–565.

Acta Cryst. (2007). E**63**, m1402–m1403 Gryz *et al.* • $[Zn(C_6H_5N_2O_2)_2(H_2O)_2]$ **m1403**