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Tetraaquabis(thiocyanato-κN)zinc(II) bis(2-methylpyrazine 1,4-dioxide)

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Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.005 Å
R factor = 0.037
wR factor = 0.099
Data-to-parameter ratio = 14.7

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

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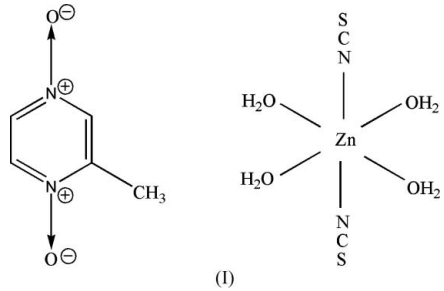
In the title compound, $[Zn(NCS)_2(H_2O)_4]\cdot 2C_5H_6N_2O_2$, the six-coordinated Zn^{II} atom lies on a special position of site symmetry 2/m. The methylpyrazine dioxide molecule lies on a mirror plane and links with the Zn^{II} complex *via* O—H···O hydrogen bonding.

Comment

The isothiocyanate anion and pyrazine 1,4-dioxide can act as either monodentate or bidentate ligands in metal complexes, depending on the reaction conditions and the reacting substances (Sun, Wang & Gao, 2005). In order to understand the relationship between the coordination modes and the metal ions, the title compound, (I), has been synthesized.



(I)

The molecular structure of (I) is shown in Fig. 1. The Zn^{II} atom is located on a twofold axis and a mirror plane, and has an octahedral coordination geometry (Table 1) formed by four water molecules and two isothiocyanate anions. The 2-methylpyrazine 1,4-dioxide molecule is located on a mirror plane, is uncoordinated and links with the Zn^{II} complex *via* O—H···O hydrogen bonding (Table 2). This agrees with the situation found in an Mn^{II} analog (Xu *et al.*, 2005) and a Co^{II} analog (Sun, Shi & Zhang, 2005).

Experimental

2-Methylpyrazine 1,4-dioxide (0.04 g, 0.3 mmol) was added to an aqueous solution (15 ml) containing $Zn(ClO_4)_2\cdot 6H_2O$ (0.11 g, 0.3 mmol) and sodium thiocyanate (0.05 g, 0.6 mmol). The solution was stirred for 5 min. Colorless single crystals of (I) were obtained after three weeks.

Crystal data

$[Zn(NCS)_2(H_2O)_4]\cdot 2C_5H_6N_2O_2$
M_r = 505.83
Monoclinic, $C2/m$
a = 16.985 (6) Å
b = 6.775 (2) Å
c = 10.141 (3) Å
β = 111.879 (4)°
V = 1082.9 (6) Å^3
Z = 2
Mo $K\alpha$ radiation
Cell parameters from 2336 reflections
θ = 2.2–27.0°
μ = 1.38 mm^{-1}
T = 298 (2) K
Prism, colorless
0.22 × 0.12 × 0.08 mm

Data collection

Bruker SMART CCD area-detector diffractometer	1275 independent reflections
φ and ω scans	1198 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	$R_{int} = 0.027$
$T_{min} = 0.752$, $T_{max} = 0.898$	$\theta_{max} = 27.0^\circ$
3156 measured reflections	$h = -21 \rightarrow 15$
	$k = -8 \rightarrow 8$
	$l = -9 \rightarrow 12$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0576P)^2 + 0.4793P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.037$	$(\Delta/\sigma)_{max} = 0.001$
$wR(F^2) = 0.099$	$\Delta\rho_{max} = 0.51$ e Å^{-3}
$S = 1.12$	$\Delta\rho_{min} = -0.84$ e Å^{-3}
1275 reflections	Extinction correction: *SHELXL97*
87 parameters	Extinction coefficient: 0.032 (3)
H-atom parameters constrained	

Table 1
Selected geometric parameters (Å, °).

Zn1—N1	2.088 (3)	Zn1—O1	2.1271 (14)
N1—Zn1—O1	86.74 (7)		

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···O2^{i}	0.84	1.94	2.746 (2)	159
O1—H2···O3^{ii}	0.84	1.89	2.725 (2)	173

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

H atoms of the pyrazine ring were placed in calculated positions, with C—H = 0.93 Å, and refined in riding mode, with U_{iso}(H) = 1.2 U_{eq}(C). H atoms of the methyl group and the water molecules were located in a difference Fourier map and refined as riding in their as-found relative positions, with U_{iso}(H) = 1.5U_{eq}(carrier).

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2001); software used to prepare material for publication: *SHELXTL*.

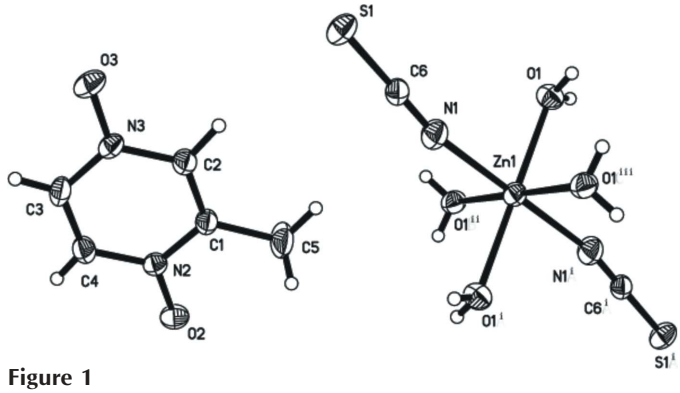


Figure 1
The molecular structure of (I), with 30% probability displacement ellipsoids (arbitrary spheres for H atoms) [symmetry codes: (iii) $-x+1, y, -z+2$; (iv) $-x+1, -y, -z+2$; (v) $x, -y, z$].

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References

Bruker (1997). *SMART* (Version 5.6) and *SAINT* (Version 5. A06). Bruker AXS Inc., Madison, Wisconsin, USA.
Bruker (2001). *SHELXTL*. Version 5.0. Bruker AXS Inc., Madison, Wisconsin, USA.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Sun, H.-L., Wang, Z.-M. & Gao, S. (2005). *Inorg. Chem.* **44**, 2169–2176.
Sun, Y.-M., Shi, J.-M. & Zhang, X. (2005). *Acta Cryst.* E**61**, m1501–m1502.
Wen, X., Shi, J. M. & Zhang, X. (2005). *Acta Cryst.* E**61**, m854–m855.