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Bis[2-amino-1-methyl-1*H*-imidazol-4(5*H*)-one-κN^3]-dithiocyanatozinc(II)

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Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.007 Å
R factor = 0.054
wR factor = 0.143
Data-to-parameter ratio = 16.7

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

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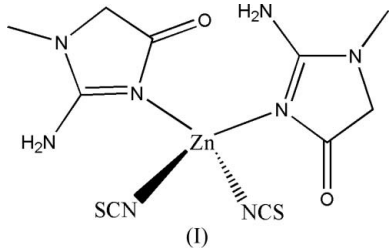
In the title compound, $[Zn(NCS)_2(C_4H_7N_3O)_2]$, the Zn atom is coordinated by two N atoms from two 2-amino-1-methyl-imidazol-4(5*H*)-one (creatinine) ligands and by another two N atoms from two terminal thiocyanate ligands in a slightly distorted tetrahedral geometry. The molecule possesses a crystallographic twofold symmetry axis. In the crystal structure, molecules are linked through intermolecular N—H···O hydrogen bonds to form chains.

Comment

Zinc is the second most abundant transition metal in biology and it functions as the active site of hydrolytic enzymes, such as carboxypeptidase and carbonic anhydrase, where it is in a hard donor coordination environment of nitrogen and oxygen (Lipscomb & Sträter, 1996). Zinc has long been recognized as a structural template in protein folding or as a Lewis acid catalyst that can readily adopt four-, five- or six-coordination (Vallee & Auld, 1993). Recent reports have suggested that zinc is able to play a catalytic role in the activation of thiols as nucleophiles at physiological pH (Matthews & Goulding, 1997; Wilker & Lippard, 1997; Myers *et al.*, 1993). As an extension of the work on the structural investigation of such zinc complexes, the title zinc(II) complex, (I), is reported here.



(I)

Compound (I) is a mononuclear zinc(II) complex (Fig. 1). The molecule possesses a crystallographic twofold symmetry axis. The Zn atom in (I) is four-coordinated by two N atoms from two 2-amino-1-methylimidazolidin-4-one (creatinine) ligands and by another two N atoms from two terminal thiocyanate ligands. This ZnN_4 coordination forms a slightly distorted tetrahedral geometry, with angles subtended at the Zn^{II} atom in the range 105.6 (2)–115.38 (15)° (Table 1). The bond lengths related to the metal centre are typical and comparable to the values in other zinc(II) complexes (McCleverty *et al.*, 1980; Terazono *et al.*, 2002; Neels & Stoeckli-Evans, 1999; Hong, 2007).

In the crystal structure of (I), molecules are linked through intermolecular N—H···O hydrogen bonds (Table 2), forming chains (Fig. 2).

Experimental

2-Amino-1-methylimidazolidin-4-one (1.0 mmol, 114.3 mg), ammonium thiocyanate (1.0 mmol, 76.2 mg) and $Zn(CH_3COO)_2{\cdot}2H_2O$ (0.5 mmol, 109.8 mg) were dissolved in 50 ml of 95% ethanol. The mixture was stirred at room temperature for 30 min to give a clear colourless solution. After keeping the solution in air for two weeks, colourless needle-shaped crystals were formed.

Crystal data

$[Zn(NCS)_2(C_4H_7N_3O)_2]$
M_r = 407.78
Monoclinic, $C2/c$
a = 14.958 (1) Å
b = 11.628 (2) Å
c = 12.794 (2) Å
β = 122.248 (1)°
V = 1882.0 (5) Å^3
Z = 4
D_x = 1.439 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 1.55 mm^{-1}
T = 298 (2) K
Block cut from needle, colourless
0.25 × 0.12 × 0.10 mm

Data collection

Bruker SMART CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.699, T_{max} = 0.861
6880 measured reflections
1872 independent reflections
1668 reflections with $I > 2\sigma(I)$
R_{int} = 0.043
θ_{max} = 26.5°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.054
$wR(F^2)$ = 0.143
S = 1.05
1872 reflections
112 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0951P)^2 + 0.8797P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 1.16 e Å^{-3}
$\Delta\rho_{min}$ = −0.56 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Zn1—N4	1.973 (3)	Zn1—N1	1.995 (2)
N4^{i}—Zn1—N4	105.6 (2)	N4—Zn1—N1	110.79 (12)
N4^{i}—Zn1—N1	106.95 (12)	N1—Zn1—N1^{i}	115.38 (15)

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

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

D—H···A	D—H	H···A	D···A	D—H···A
N3—H3A···N4^{i}	0.90 (5)	2.26 (5)	3.072 (4)	150 (4)
N3—H3B···O1^{ii}	0.90 (5)	1.96 (2)	2.791 (4)	154 (5)

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

Atoms H3*A* and H3*B* were located in a difference Fourier map and refined isotropically, with the N—H and H···H distances restrained to 0.90 (1) and 1.43 (2) Å, respectively, and with U_{iso}(H) values fixed at 0.08 Å^2. The other H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms with C—H distances in the range 0.96–0.97 Å, and with U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(C). The structure contains solvent-accessible voids of 60 Å^3, which might accommodate a disordered water molecule. An unassigned maximum residual electron density was observed 3.25 Å from atom H4*B*.

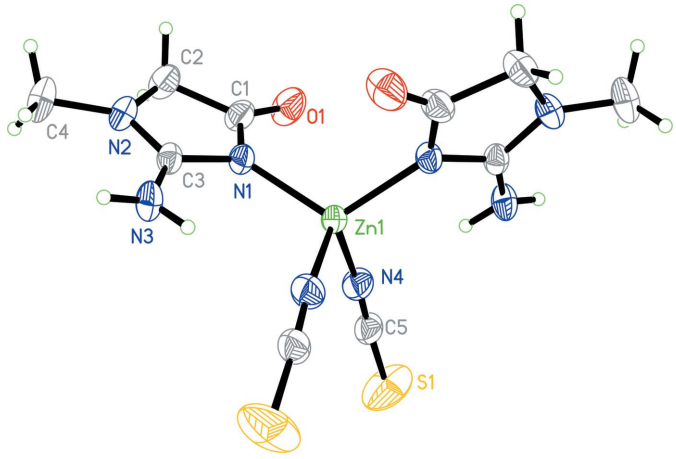


Figure 1
The molecular structure of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level. Unlabelled atoms are at the symmetry position $(-x, y, \frac{1}{2}-z)$.

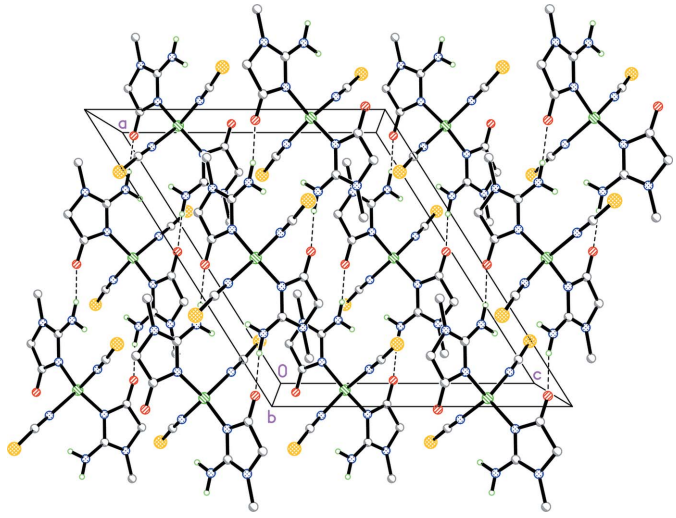


Figure 2
The molecular packing of (I), viewed along the *b* axis. Intermolecular N—H···O hydrogen bonds are shown as dashed lines. C-bound H atoms have been omitted.

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINT* (Bruker, 2002); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXL97*.

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