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(*N*,*N*-Diethylethane-1,2-diamine)dithiocyanatozinc(II)

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In the title compound, $[Zn(NCS)_2(C_6H_{16}N_2)]$, the Zn^{II} atom is coordinated by two N atoms of *N*,*N*-diethylethane-1,2-diamine and by another two N atoms from two terminal thiocyanate ligands in a slightly distorted tetrahedral geometry. In the crystal structure, molecules are linked through intermolecular N—H···S hydrogen bonds, forming chains running along the *b* axis.

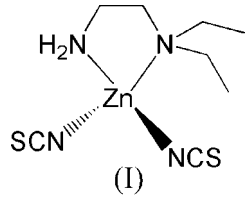
Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.004 Å
R factor = 0.033
wR factor = 0.083
Data-to-parameter ratio = 21.3

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

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 of N and O (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)

Complex (I) is a mononuclear zinc(II) compound (Fig. 1). The Zn^{II} atom is four-coordinated by two N atoms of *N*,*N*-diethylethane-1,2-diamine and 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 88.54 (8)–115.51 (10)° (Table 1). The bond lengths related to the metal centre are typical and are comparable with the values in other zinc(II) complexes (McCleverty *et al.*, 1980; Terazono *et al.*, 2002; Neels & Stoeckli-Evans, 1999).

In the crystal structure of (I), molecules are linked through intermolecular N—H···S hydrogen bonds (Table 2), forming chains running along the *b* axis (Fig.2).

Experimental

All reagents were commercial grade and were used without further purification. *N*,*N*-Diethylethane-1,2-diamine (1.0 mmol, 116.2 mg),

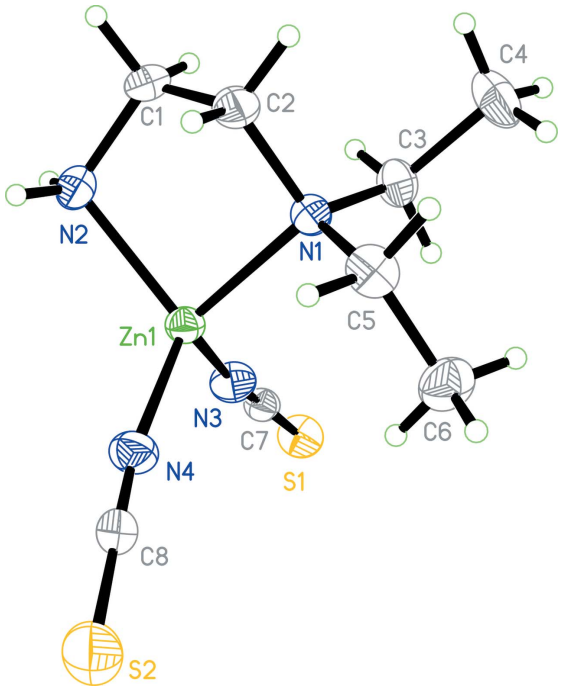


Figure 1
The molecular structure of (I), showing 30% probability displacement ellipsoids and the atom-numbering scheme.

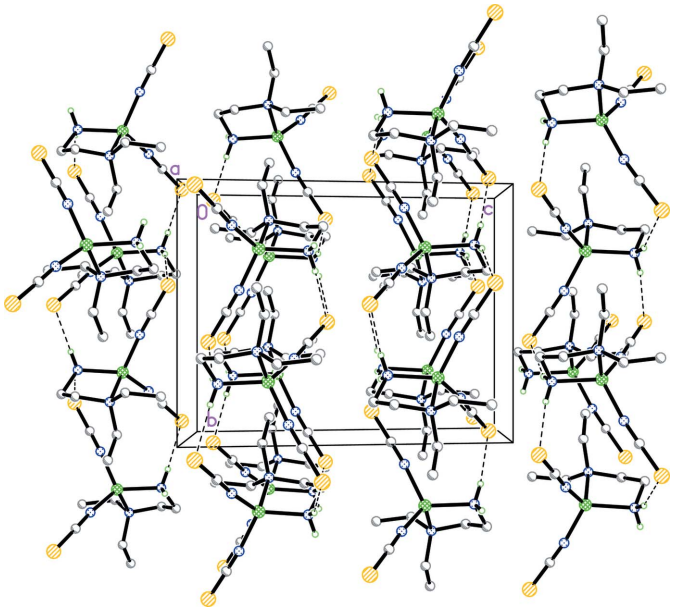


Figure 2
The crystal packing of (I), viewed along the *a* axis. Intermolecular hydrogen bonds are shown as dashed lines.

ammonium thiocyanate (2.0 mmol, 152.3 mg) and $Zn(CH_3COO)_2{\cdot}2H_2O$ (1.0 mmol, 219.5 mg) were dissolved in 95% ethanol (30 ml). The mixture was stirred at room temperature for 30 min to give a clear colourless solution. After keeping the solution in air for a week, colourless block-shaped crystals were formed. Analysis, found: C 32.21, H 5.45, N 18.73%; calculated for $C_8H_{16}N_4S_2Zn$: C 32.27, H 5.42, N 18.82%.

Crystal data

$[Zn(NCS)_2(C_6H_{16}N_2)]$
M_r = 297.74
Monoclinic, $P2_1/c$
a = 9.451 (1) Å
b = 10.574 (1) Å
c = 13.716 (2) Å
β = 100.869 (2)°
V = 1346.1 (3) Å^3
Z = 4
D_x = 1.469 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 2.11 mm^{-1}
T = 298 (2) K
Block, colourless
0.23 × 0.21 × 0.18 mm

Data collection

Bruker SMART CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.642, T_{max} = 0.703
11271 measured reflections
3065 independent reflections
2319 reflections with $I > 2\sigma(I)$
R_{int} = 0.031
θ_{max} = 27.5°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.033
$wR(F^2)$ = 0.083
S = 1.03
3065 reflections
144 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0383P)^2 + 0.1533P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.40 e Å^{-3}
$\Delta\rho_{min}$ = −0.31 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Zn1—N4	1.928 (2)	Zn1—N2	2.023 (2)
Zn1—N3	1.929 (2)	Zn1—N1	2.0727 (18)
N4—Zn1—N3	111.93 (9)	N4—Zn1—N1	110.86 (8)
N4—Zn1—N2	114.65 (9)	N3—Zn1—N1	113.33 (8)
N3—Zn1—N2	115.51 (10)	N2—Zn1—N1	88.54 (8)

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2C···S2^{i}	0.887 (10)	2.652 (12)	3.489 (3)	158 (2)
N2—H2D···S1^{ii}	0.884 (19)	2.739 (13)	3.558 (2)	155 (2)

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

Atoms H2*C* and H2*D* 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 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).

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); 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: *SHELXTL*.

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