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Key indicators

Single-crystal X-ray study
 $T = 293\text{ K}$
Mean $\sigma(\text{C}-\text{C}) = 0.004\text{ \AA}$
 R factor = 0.038
 wR factor = 0.100
Data-to-parameter ratio = 17.7For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.

Bis(1,10-phenanthroline)dithiocyanatozinc(II)

The title compound, $[\text{Zn}(\text{NCS})_2(\text{C}_{12}\text{H}_8\text{N}_2)_2]$, is a mononuclear zinc complex, in which the Zn atom is located on a twofold rotation axis. The zinc^{II} cation has a slightly distorted octahedral geometry containing four N atoms from two 1,10-phenanthroline molecules and two N atoms from two thiocyanate anions.

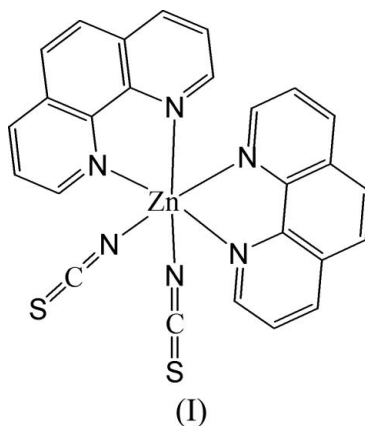
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Comment

For many decades the thiocyanate anion has been one of the most widely used ligands, due to its versatile coordination modes with different metals (Tarafder *et al.*, 1989; Goher *et al.*, 2000). Several methods for the synthesis of the title complex, (I), have been reported (Schilt & Fritsch, 1966; Chakravorti & Subrahmanyam, 1992), and some properties of the complex have also been studied (Lorant, 1970; Syamal & Kale, 1977). However, to the best of our knowledge, the crystal structure has not been reported. In this paper, the crystal structure of (I) is reported, and its coordination mode is discussed.



The title compound crystallizes in the centrosymmetric orthorhombic space group $Pbcn$ with four formula units in the unit cell. The structure determination indicates that the coordination environment of the zinc(II) cation is defined by two N atoms from two thiocyanate anions and four N atoms from two phenanthroline (phen) molecules (Fig. 1), each of which are related by a twofold rotation. The metal ion shows a slightly distorted octahedral geometry, with the two bidentate chelating phen, as well as the two monodentate *N*-donor thiocyanate anions, in a *cis* arrangement. The two phen ligands are almost perpendicular to each other, with a dihedral angle of $89.6(1)^\circ$.

The Zn–N(phen) distances (Table 1) of 2.222(2) and 2.193(2) Å are near to the values found in other zinc complex with 1,10-phenanthroline (Zhu *et al.*, 2005). The Zn–

N(thiocyanate) distance of 2.063 (3) Å is similar to the values in related compounds (Wu, 2004).

Experimental

A mixture of Zn(NO₃)₂·6H₂O (0.149 g, 0.5 mmol) and 1,10-phenanthroline (0.198 g, 1 mmol) in methanol (20 ml) was heated at reflux for 0.5 h, then sodium thiocyanate (0.081 g, 1 mmol) was added to the solution and the mixture was heated at reflux for a further 2 h. Pale-yellow crystals were obtained by evaporating the solution for several days at room temperature (yield: 48%, based on Zn). Analysis calculated for C₂₆H₁₆N₆S₂Zn: C 57.62, H 2.98, N 15.51%; found: C 57.79, H 2.86, N 15.62%.

Crystal data

[Zn(NCS) ₂ (C ₁₂ H ₈ N ₂) ₂]	Mo Kα radiation
<i>M_r</i> = 541.98	Cell parameters from 2969 reflections
Orthorhombic, <i>Pbcn</i>	<i>θ</i> = 2.3–28.3°
<i>a</i> = 13.147 (5) Å	<i>μ</i> = 1.26 mm ⁻¹
<i>b</i> = 10.088 (5) Å	<i>T</i> = 293 (2) K
<i>c</i> = 17.549 (5) Å	Plate, yellow
<i>V</i> = 2327.5 (16) Å ³	0.53 × 0.19 × 0.07 mm
<i>Z</i> = 4	
<i>D_x</i> = 1.547 Mg m ⁻³	

Data collection

Bruker APEX CCD area-detector diffractometer	2901 independent reflections
<i>ω</i> scans	1505 reflections with <i>I</i> > 2σ(<i>I</i>)
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	<i>R_{int}</i> = 0.067
<i>T_{min}</i> = 0.595, <i>T_{max}</i> = 0.915	<i>θ_{max}</i> = 28.3°
13350 measured reflections	<i>h</i> = -9 → 17
	<i>k</i> = -13 → 13
	<i>l</i> = -23 → 22

Refinement

Refinement on <i>F</i> ²	H-atom parameters constrained
<i>R</i> [<i>F</i> ² > 2σ(<i>F</i> ²)] = 0.038	<i>w</i> = 1/[σ ² (<i>F_o</i> ²) + (0.0467 <i>P</i>) ²]
<i>wR</i> (<i>F</i> ²) = 0.100	where <i>P</i> = (<i>F_o</i> ² + 2 <i>F_c</i> ²)/3
<i>S</i> = 0.92	(Δ/σ) _{max} < 0.001
2810 reflections	Δρ _{max} = 0.34 e Å ⁻³
159 parameters	Δρ _{min} = -0.31 e Å ⁻³

Table 1
Selected geometric parameters (Å, °).

Zn–N3	2.063 (3)	Zn–N1	2.222 (2)
Zn–N2	2.193 (2)		
N3 ⁱ –Zn–N3	95.11 (14)	N2–Zn–N1 ⁱ	90.44 (8)
N3 ⁱ –Zn–N2	91.41 (10)	N3–Zn–N1	89.13 (10)
N2–Zn–N2 ⁱ	159.93 (12)	N2–Zn–N1	75.24 (8)
N3–Zn–N1 ⁱ	166.58 (10)	N1 ⁱ –Zn–N1	89.63 (12)

Symmetry code: (i) -x + 1, y, -z + ½.

All H atoms on C atoms were positioned geometrically and refined as riding atoms, with C–H = 0.93 Å and *U*_{iso}(H) = 1.2*U*_{eq}(C).

Data collection: SMART (Bruker, 1997); cell refinement: SAINT (Bruker, 1999); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics:

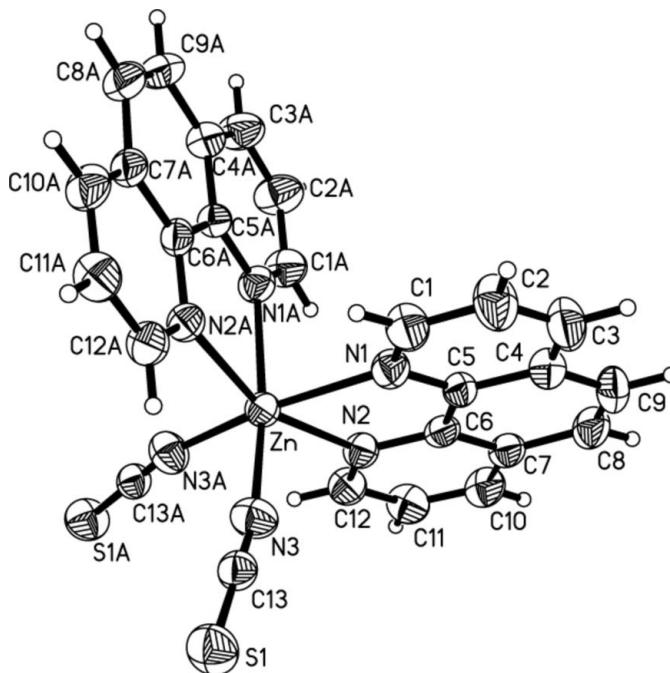


Figure 1
View of (I), with displacement ellipsoids drawn at the 30% probability level. The suffix A denotes the symmetry position -x + 1, y, -z + ½.

SHELXTL-Plus (Sheldrick, 1990); software used to prepare material for publication: SHELXL97.

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