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## Key indicators

Single-crystal X-ray study  
 $T = 293$  K  
Mean  $\sigma(\text{C}-\text{C}) = 0.004$  Å  
 $R$  factor = 0.040  
 $wR$  factor = 0.088  
Data-to-parameter ratio = 16.9For details of how these key indicators were  
automatically derived from the article, see  
<http://journals.iucr.org/e>.Bis(1,10-phenanthroline- $\kappa^2\text{N},\text{N}$ )bis(thiosalicylato-  
 $1\kappa^2\text{O},\text{O}':2\kappa^2\text{O}',\text{S}$ )dizinc(II)

In the title compound,  $[\text{Zn}_2(\text{C}_7\text{H}_4\text{O}_2\text{S})_2(\text{C}_{12}\text{H}_8\text{N}_2)_2]$ , the Zn complex forms a centrosymmetric dimer with a Zn...Zn separation of 3.580 (1) Å. Each Zn atom is coordinated by two N atoms from the 1,10-phenanthroline (phen) ligand and by three O atoms and one S atom from the thiosalicylate ligands in a highly distorted octahedral geometry, with Zn–N distances of 2.119 (2) and 2.166 (2) Å, Zn–O distances in the range 2.161 (2)–2.329 (2) Å, and a Zn–S distance of 2.3034 (12) Å. There are  $\pi$ – $\pi$  stacking interactions between the phen rings, forming a stacking arrangement along the  $c$  axis in the crystal structure.

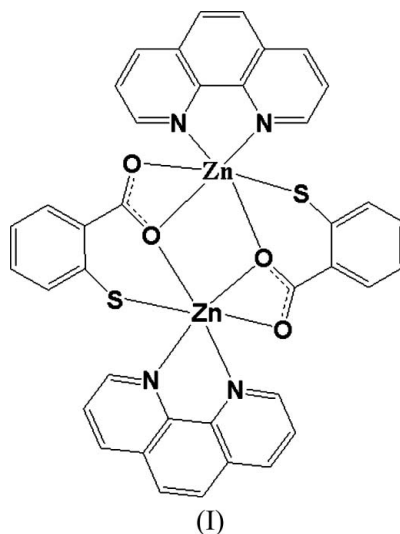
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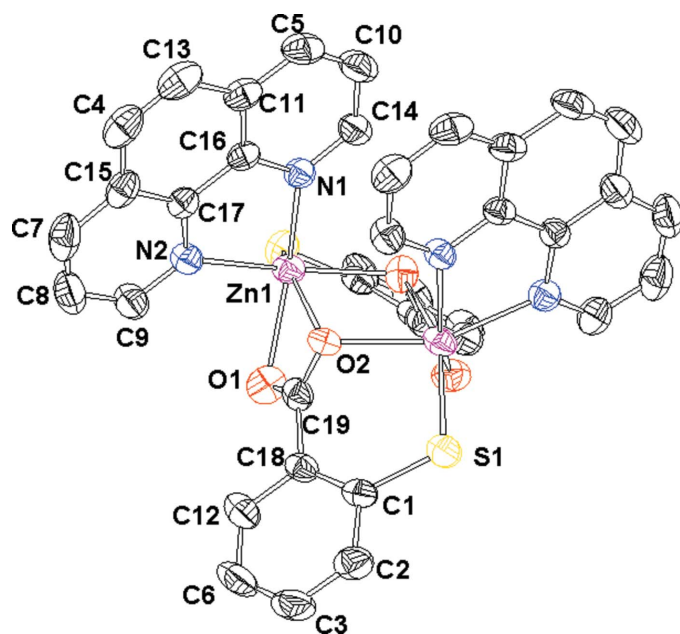
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## Comment

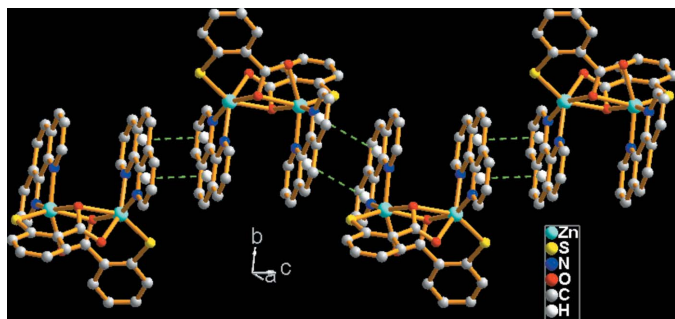
The design and synthesis of supramolecular coordination polymer networks organized and held together by means of coordination covalent bonds, hydrogen bonds and  $\pi$ – $\pi$  stacking interactions, has been a field of rapid growth because of their special physical properties and potential application in functional materials (Atwood *et al.*, 1996; Barton *et al.*, 1999). A number of promising supramolecular complexes have been designed and constructed from long flexible ligands (Luo *et al.*, 2003). While attempting to prepare a complex containing 2,2-dithiodibenzoic acid ligands *via* a hydrothermal reaction, we did not obtain the expected complex but instead obtained the title compound, (I).



As shown in Fig. 1, each Zn atom in (I) is six-coordinated *via* two N atoms from the phen ligand and three O atoms and one S atom from the thiosalicylate ligands in a highly distorted octahedral geometry, with Zn–N distances of 2.119 (2) and


**Figure 1**

A view of the title molecule, showing the atom-labelling scheme and with displacement ellipsoids at the 40% probability level. Unlabelled atoms are related to labelled atoms by the symmetry operator  $1 - x, y/2 - z$ . H atoms have been omitted.


**Figure 2**

The extended structure of (I), formed through  $\pi$ - $\pi$  interactions between the phen rings (dashed lines). H atoms have been omitted.

2.166 (2) Å, Zn—O distances in the range 2.161 (2)–2.329 (2) Å, and a Zn—S distance of 2.3034 (12) Å.

The Zn complex forms a centrosymmetric dimer with a Zn···Zn separation of 3.580 (1) Å, indicating no direct metal-metal interaction. There are  $\pi$ - $\pi$  stacking interactions between phen ligands, as shown in Fig. 2. Adjacent rings of phen are approximately parallel; the perpendicular spacing of the rings is 3.479 (4) Å, and the ring centroid-to-centroid distance is 3.700 (6) Å, close to the sum of the van der Waals radii of two C atoms (Bondi, 1964). Neighbouring dimers are connected by  $\pi$ - $\pi$  interactions, forming a stacking arrangement.

## Experimental

Zn(CH<sub>3</sub>CO<sub>2</sub>)<sub>2</sub>·2H<sub>2</sub>O (1 mmol), 2,2-dithiodibenzoic acid (0.5 mmol) and 1,10-phenanthroline (1 mmol) were mixed in H<sub>2</sub>O (15 ml) and heated at 433 K for 3 d in a sealed 25 ml Teflon-lined stainless steel vessel under autogenous pressure. After cooling to room temperature

at 5 K h<sup>-1</sup>, yellow prismatic crystals of (I) were isolated, which were washed with water and dried in air.

## Crystal data

[Zn<sub>2</sub>(C<sub>7</sub>H<sub>4</sub>O<sub>2</sub>S)<sub>2</sub>(C<sub>12</sub>H<sub>8</sub>N<sub>2</sub>)<sub>2</sub>]  
*M<sub>r</sub>* = 795.53  
 Monoclinic, *C*2/*c*  
*a* = 18.785 (11) Å  
*b* = 9.581 (5) Å  
*c* = 18.523 (10) Å  
 $\beta$  = 90.924 (17)°  
*V* = 3333 (3) Å<sup>3</sup>  
*Z* = 4

*D<sub>x</sub>* = 1.585 Mg m<sup>-3</sup>  
 Mo *K*α radiation  
 Cell parameters from 826 reflections  
 $\theta$  = 3.1–27.5°  
 $\mu$  = 1.61 mm<sup>-1</sup>  
*T* = 293 (2) K  
 Prism, yellow  
 0.40 × 0.25 × 0.10 mm

## Data collection

Bruker SMART CCD diffractometer  
 $\omega$  scans  
 Absorption correction: multi-scan (SADABS; Sheldrick, 1996)  
*T<sub>min</sub>* = 0.623, *T<sub>max</sub>* = 0.851  
 6321 measured reflections

3829 independent reflections  
 3302 reflections with *I* > 2σ(*I*)  
*R<sub>int</sub>* = 0.021  
 $\theta_{\max}$  = 27.5°  
*h* = -24 → 24  
*k* = -12 → 12  
*l* = -23 → 24

## Refinement

Refinement on *F*<sup>2</sup>  
*R* [*F*<sup>2</sup> > 2σ(*F*<sup>2</sup>)] = 0.040  
*wR* (*F*<sup>2</sup>) = 0.088  
*S* = 1.10  
 3829 reflections  
 226 parameters  
 H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0345P)^2 + 3.4919P]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\max} = 0.001$   
 $\Delta\rho_{\max} = 0.38 \text{ e \AA}^{-3}$   
 $\Delta\rho_{\min} = -0.38 \text{ e \AA}^{-3}$

**Table 1**

Selected bond lengths (Å).

|                     |           |                     |             |
|---------------------|-----------|---------------------|-------------|
| Zn1—N1              | 2.119 (2) | Zn1—S1 <sup>i</sup> | 2.3034 (12) |
| Zn1—O2 <sup>i</sup> | 2.161 (2) | Zn1—O2              | 2.329 (2)   |
| Zn1—N2              | 2.166 (2) | S1—Zn1 <sup>i</sup> | 2.3034 (12) |
| Zn1—O1              | 2.254 (2) | O2—Zn1 <sup>i</sup> | 2.161 (2)   |

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

C-bound H atoms were positioned geometrically and refined as riding on their parent atoms, with C—H = 0.93 Å and *U*<sub>iso</sub>(H) = 1.2*U*<sub>eq</sub>(C).

Data collection: SMART (Siemens, 1996); cell refinement: SMART and SAINT (Siemens, 1994); data reduction: SAINT; program(s) used to solve structure: SHELXTL (Siemens, 1994); program(s) used to refine structure: SHELXTL; molecular graphics: SHELXTL; software used to prepare material for publication: SHELXTL.

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