Synthesis, crystal structure and Hirshfeld surface analysis of a zinc(II) coordination polymer of 5-phenyl-1,3,4-oxadiazole-2-thiolate

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A new zinc coordination polymer with 5-phenyl-1,3,4-oxadiazole-2-thiolate, namely, \(\text{catena-poly[Zn(II)-bis(\mu_2-5-phenyl-1,3,4-oxadiazole-2-thiolato)-\kappa^2N^3:S\kappa^2S:N]}\). \([\text{Zn(C_8H_5N_2OS)_(2)}]_n\), was synthesized. The single-crystal X-ray diffraction analysis shows that the polymeric structure crystallizes in the centrosymmetric monoclinic \(C2/c\) space group. The \(\text{Zn}^{II}\) atom is coordinated to two S and two N atoms from four crystallographically independent (L) ligands, forming zigzag chains along the [001] direction. This polymer complex forms an eight-membered \([\text{Zn–S–C–N–Zn–S–C–N}]\) chair-like ring with two \(\text{Zn}^{II}\) atoms and two ligand molecules. On the Hirshfeld surface, the largest contributions come from the short contacts such as van der Waals forces, including H\(\cdots\)C, H\(\cdots\)H and S\(\cdots\)H. Interactions including N\(\cdots\)H, O\(\cdots\)H and C\(\cdots\)C contacts were also observed; however, their contribution to the overall stability of the crystal lattice is minor.

1. Chemical context

Among heterocyclic organic compounds, 1,3,4-oxadiazoles have become an important class of heterocycles because of their broad spectrum of biological activity (De Oliveira et al., 2012; Vaidya et al., 2020). Scientists have identified many properties of 1,3,4-oxadiazole derivatives, such as antimicrobial (Bala et al., 2014; Zachariah et al., 2015; Ahmed et al., 2017; Razzaqova et al., 2019), antituberculosis (Makane et al., 2019; Wang et al., 2022), anticancer (Alam, 2022; Vaidya et al., 2020; Zhang et al., 2005), anti-inflammatory (Abd-Ellah et al., 2017), analgesic (Husain & Ajmal, 2009), herbicidal (Sun et al., 2014; Duan et al., 2011) and antifungal (Zhang et al., 2013; Capoci et al., 2019) activities. Heterocyclic thiones are an important type of compound in coordination chemistry because of their potential multifunctional donor sites, namely either exocyclic sulfur or endocyclic nitrogen (Reddy et al., 2011; Wang et al., 2010). The presence of the 1,3,4-oxadiazole ring affects the physicochemical and pharmacokinetic properties of the entire compound. An exciting feature of these metal complexes is that they can be mononuclear (Singh et al., 2008; Oulila et al., 2012), binuclear (Xiao et al., 2011; Wang et al., 2007) and/or polymeric (Beghidja et al., 2007).

Oxadiazole ligands are ideal objects for creating new coordination compounds with great potential in various fields. Scientists have written extensive literature on the biological properties of oxadiazole-based complex compounds,
especially on their anticancer effects. In addition to these, in the field of electrical engineering, metal complexes bearing oxadiazole ligands have been used as emitting particles in light-emitting diodes. The introduction of various functionalized oxadiazole ligands makes it easy to control the emission color, thermal stability, and film-forming properties of such complexes (Salassa & Terenzi, 2019).

Herein, we report on the synthesis and crystal structure of a new polymeric complex, $[\text{Zn}_n \text{L}_2]^n$, with $L = 5$-phenyl-1,3,4-oxadiazole-2-thiol.

2. Structural commentary

The single crystal X-ray structure of 5-phenyl-1,3,4-oxadiazole-2-thiolate Zn$^{\text{II}}$ shows a polymeric structure that crystallizes in the centrosymmetric monoclinic space group $C2/c$ (Table 2). As seen in Fig. 1, its asymmetric unit contains half a zinc atom and one ligand anion. The central Zn$^{\text{II}}$ atom has a distorted tetrahedral environment comprising two sulfur and two nitrogen atoms. It is coordinated by four crystallographically independent ($\text{L}^n$) ligands, forming zigzag chains along the [001] direction, which are linked by two sulfur atoms and two nitrogen atoms of four ligands. The Zn$^1$–S$^1$ and Zn$^1$–N$^1$ bond lengths are 2.3370 (5) Å, 2.0184 (14) Å, respectively. In this case, the bond angles of the atom forming the tetrahedral polyhedron are slightly different from the angles of the ideal tetrahedron [N$^1$–Zn$^1$–N$^1$ = 111.37 (9)$^\circ$],

![Figure 1](image1)

**Figure 1**
The molecular structure of $[\text{Zn}_n \text{L}_2]$ with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level and H atoms are displayed as small spheres of arbitrary radii.

| D—H—A         | D—H    | H—A    | D···A       | D—H···A    |
|---------------|--------|--------|-------------|-----------|
| C6—H6···S$^1$ | 1.00 (3)| 2.86 (3)| 3.608 (2)   | 132 (2)   |

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

It is known from the literature (Razzoqova et al., 2019) that the sulfur atom in the 1,3,4-oxadiazole-2-thione molecule is attached to the ring by a double bond. In this polymer complex synthesized based on Zn$^{\text{II}}$ ion, the oxadiazole derivative transforms into the thiol tautomeric form and binds to the Zn ion. The N1 atom in the ligand molecule, on the other hand, forms a bond with another Zn$^{\text{II}}$ ion due to its high electron-donating property, resulting in an eight-membered [Zn–S–C–N–Zn–S–C–N] chair-like ring with two Zn$^{\text{II}}$ atoms and two ligand molecules (Fig. 2). The dihedral angle between the mean planes of the phenyl (C3–C8) and oxadiazole (C1/O1/C2/N2/N1) rings of the ligand molecule is 13.42 (8)$^\circ$. The conformation of the oxadiazole-thiol fragment of the ligand is approximately planar (r.m.s. deviation 0.006 Å), with a maximum deviation from the least-squares plane of 0.009 (1) Å for atom O1. The dihedral angle between the planes of the two neighboring independent oxadiazole-thiol (C1/O1/C2/N2/N1/S1) fragments is 64.10 (9)$^\circ$.

3. Supramolecular features

The $[(\text{Zn}_n \text{L}_2)_n]$ unit is given as a monomer of the polymeric chain that extends parallel to the c-axis. Along the polymeric chain, the hydrophilic groups are concentrated within the core of the chain while the phenyl rings project approximately normal to the chain. Neighboring chains across the ab plane are loosely connected via a rather weak C6—H6···S$^1$ hydrogen bond (Table 1, Fig. 3).

![Figure 2](image2)

**Figure 2**
The view of the molecular packing showing the polymeric chain extended along the c-axis.
4. Hirshfeld surface analysis

To further investigate the intermolecular interactions present in the title compound, a Hirshfeld surface analysis was performed, and the two-dimensional fingerprint plots were generated with CrystalExplorer17 (Turner et al., 2017). The Hirshfeld surface mapped over \( d_{\text{norm}} \) and corresponding colors representing various interactions are shown in Fig. 4. We chose the \( \text{Zn}_2 \text{L}_2 \) molecular fragment as the monomer unit for calculating the Hirshfeld surface of this polymer complex. The large red areas on the Hirshfeld surface correspond to the \( \text{Zn} \cdots \text{C} / \text{C} / \text{C} / \text{N} \) interactions. The two-dimensional (2D) fingerprint plots (McKinnon et al., 2007) are shown in Fig. 5. On the Hirshfeld surface, the largest contributions (19.2%, 19.5% and 19%) come from short contacts such as van der Waals forces, \( \text{H} \cdots \text{H}, \text{C} \cdots \text{H} \) and \( \text{S} \cdots \text{H} \) contacts. \( \text{N} \cdots \text{H} \) (8.1%), \( \text{O} \cdots \text{H} \) (8%) and \( \text{C} \cdots \text{C} \) (4.7%) contacts are also observed. These interactions play a crucial role in the overall stabilization of the crystal packing.

5. Database survey

A survey of the Cambridge Structural Database (CSD, version 5.43, update of November 2021; Groom et al., 2016) revealed that crystal structures had been reported for complexes of 1,3,4-oxadiazole derivatives and a number of metal ions, including zinc, copper, nickel, manganese, cadmium, cobalt and silver. No polymer complexes containing \([\text{M} \cdots \text{S} \cdots \text{C} \cdots \text{N} \cdots \text{M} \cdots \text{S} \cdots \text{C} \cdots \text{N}]\) eight-membered cyclization have been reported. The structures of complexes of Pt, Sn and Au based on 5-phenyl-1,3,4-oxadiazole-2-thiole with additional ligands have been deposited in the CSD (FATNIZ, Al-Jibori et al., 2012; HAXTAC, Ma et al., 2005; and YIVVEG, Chaves et al., 2014). However, no complexes containing only the zinc ion and 5-phenyl-1,3,4-oxadiazole-2-thiolate have been documented in the CSD.

6. Synthesis and crystallization

\( \text{ZnCl}_2 \) (0.136 g, 0.001 mol) and 5-phenyl-1,3,4-oxadiazole-2-thiol (ligand) (0.354 g, 0.002 mol) were dissolved separately in ethanol (10 mL). To a solution of the ligand, an aqueous...
solution of KOH (0.112 g, 0.002 mol) was added. The obtained solutions were mixed together and stirred at 323 K for 20 min. A white precipitate was obtained. The precipitate was filtered and allowed to dry. The solid residue was dissolved in DMF to crystallize for the single crystal X-ray diffraction studies. X-ray quality single crystals were produced after 10 days by slow evaporation of the solution.

7. Refinement
Crystal data, data collection and structure refinement details are summarized in Table 2. All the hydrogen atoms were located in difference-Fourier maps and refined isotropically.

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Synthesis, crystal structure and Hirshfeld surface analysis of a zinc(II) coordination polymer of 5-phenyl-1,3,4-oxadiazole-2-thiolate

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Computing details

Data collection: CrysAlis PRO (Rigaku OD, 2020); cell refinement: CrysAlis PRO (Rigaku OD, 2020); data reduction: CrysAlis PRO (Rigaku OD, 2020); program(s) used to solve structure: SHELXT2014/5 (Sheldrick, 2015a); program(s) used to refine structure: SHELXL2016/6 (Sheldrick, 2015b); molecular graphics: OLEX2 (Dolomanov et al., 2009); software used to prepare material for publication: OLEX2 (Dolomanov et al., 2009).

catena-Poly[ zinc(II)-bis(μ₂-5-phenyl-1,3,4-oxadiazole-2-thiolato)-κ²N³: S²: N³]

Crystal data

\[\text{[Zn(C}_8\text{H}_5\text{N}_2\text{O}_3\text{S}]_{\text{2}}}\]  
\(M_r = 419.79\)

Monoclinic, \(C_2/c\)

\(a = 20.4223\ (3) \AA\)

\(b = 11.3260\ (2) \AA\)

\(c = 7.4019\ (1) \AA\)

\(\beta = 98.310\ (1)\)°

\(V = 1694.11\ (5) \AA^3\)

\(Z = 4\)

Data collection

XtaLAB Synergy, single source at home/near, HyPix3000 diffractometer

Radiation source: micro-focus sealed X-ray tube, PhotonJet (Cu) X-ray Source

Mirror monochromator

Detector resolution: 10.0000 pixels mm⁻¹

\(\omega\) scans

Absorption correction: multi-scan

(CrysAlisPro; Rigaku OD, 2020)

Refinement

Refinement on \(F^2\)

Least-squares matrix: full

\(R(F^2 > 2\sigma(F^2)) = 0.026\)

\(wR(F^2) = 0.073\)

\(S = 1.09\)

1634 reflections

\(T_{\text{min}} = 0.099, T_{\text{max}} = 1.000\)

7033 measured reflections

1536 reflections with \(I > 2\sigma(I)\)

\(R_{\text{int}} = 0.028\)

\(\theta_{\text{max}} = 71.5°, \theta_{\text{min}} = 4.4°\)

\(h = -25\rightarrow 23\)

\(k = -13\rightarrow 13\)

\(l = -9\rightarrow 8\)

134 parameters

0 restraints

Primary atom site location: structure-invariant direct methods

Hydrogen site location: difference Fourier map

All H-atom parameters refined
\[ w = 1/[\sigma^2(F_o^2) + (0.0425P)^2 + 0.6399P] \]
\[ \Delta p_{\text{max}} = 0.26 \text{ e Å}^{-3} \]
\[ \Delta p_{\text{min}} = -0.33 \text{ e Å}^{-3} \]
\[ \Delta\sigma_{\text{max}} = 0.001 \]

**Special details**

**Geometry.** All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

**Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)**

| Atom | x      | y      | z      | Uiso*/Ueq |
|------|--------|--------|--------|-----------|
| Zn1  | 0.500000 | 0.42861 (3) | 0.750000 | 0.03700 (13) |
| S1   | 0.52858 (2) | 0.70338 (4) | 0.49120 (6) | 0.04489 (15) |
| O1   | 0.64980 (6) | 0.66497 (11) | 0.66937 (16) | 0.0378 (3) |
| N1   | 0.57974 (7) | 0.52907 (14) | 0.7241 (2) | 0.0381 (3) |
| N2   | 0.64167 (7) | 0.49941 (14) | 0.8226 (2) | 0.0402 (3) |
| C2   | 0.68103 (8) | 0.58151 (15) | 0.7854 (2) | 0.0360 (4) |
| C3   | 0.75171 (8) | 0.59280 (16) | 0.8505 (2) | 0.0370 (4) |
| C1   | 0.58617 (8) | 0.62555 (15) | 0.6334 (2) | 0.0362 (4) |
| C8   | 0.78515 (9) | 0.49670 (18) | 0.9351 (3) | 0.0442 (4) |
| C4   | 0.78562 (10) | 0.69688 (18) | 0.8287 (3) | 0.0472 (4) |
| C7   | 0.85194 (10) | 0.5044 (2) | 0.9992 (3) | 0.0572 (5) |
| C5   | 0.85239 (11) | 0.7043 (2) | 0.8940 (3) | 0.0578 (5) |
| C6   | 0.88524 (10) | 0.6091 (2) | 0.9798 (3) | 0.0613 (6) |
| H8   | 0.7634 (11) | 0.4299 (18) | 0.946 (3) | 0.042 (6)* |
| H5   | 0.8723 (13) | 0.772 (3) | 0.874 (3) | 0.068 (7)* |
| H4   | 0.7642 (12) | 0.761 (2) | 0.771 (3) | 0.059 (7)* |
| H7   | 0.8758 (14) | 0.443 (2) | 1.056 (4) | 0.074 (8)* |
| H6   | 0.9339 (15) | 0.614 (3) | 1.020 (4) | 0.088 (9)* |

**Atomic displacement parameters (Å²)**

|          | U^11    | U^22    | U^33    | U^12    | U^13    | U^23    |
|----------|---------|---------|---------|---------|---------|---------|
| Zn1      | 0.02217 (18) | 0.0460 (2) | 0.0416 (2) | 0.0000  | 0.00048 (13) | 0.0000  |
| S1       | 0.0363 (3) | 0.0440 (3) | 0.0508 (3) | 0.00848 (17) | -0.00577 (19) | -0.00479 (18) |
| O1       | 0.0309 (6) | 0.0384 (6) | 0.0423 (6) | -0.0034 (5) | -0.0009 (5) | 0.0004 (5) |
| N1       | 0.0228 (7) | 0.0461 (8) | 0.0440 (8) | -0.0019 (6) | 0.0001 (6) | 0.0003 (6) |
| N2       | 0.0243 (7) | 0.0483 (8) | 0.0462 (8) | -0.0030 (6) | -0.0012 (6) | 0.0056 (6) |
| C2       | 0.0291 (8) | 0.0410 (9) | 0.0368 (8) | -0.0004 (6) | 0.0010 (7) | -0.0010 (6) |
| C3       | 0.0276 (8) | 0.0468 (9) | 0.0359 (8) | -0.0050 (7) | 0.0019 (6) | -0.0033 (7) |
| C1       | 0.0273 (8) | 0.0418 (9) | 0.0386 (8) | 0.0008 (7) | 0.0013 (6) | -0.0070 (7) |
| C8       | 0.0357 (9) | 0.0498 (11) | 0.0459 (9) | -0.0059 (8) | 0.0012 (7) | 0.0053 (8) |
| C4       | 0.0380 (10) | 0.0446 (10) | 0.0578 (11) | -0.0048 (8) | 0.0027 (8) | 0.0008 (9) |
| C7       | 0.0363 (10) | 0.0697 (14) | 0.0620 (12) | 0.0004 (10) | -0.0044 (9) | 0.0124 (11) |
| C5       | 0.0393 (11) | 0.0591 (13) | 0.0741 (14) | -0.0179 (9) | 0.0052 (10) | -0.0027 (11) |
| C6       | 0.0288 (10) | 0.0797 (15) | 0.0722 (14) | -0.0108 (10) | -0.0035 (9) | 0.0046 (12) |
### Geometric parameters (Å, °)

| Bond/Angle | Value     | Value     | Value     |
|------------|-----------|-----------|-----------|
| Zn1—S1i    | 2.3370 (5) | C3—C8     | 1.385 (3) |
| Zn1—S1ii   | 2.3370 (5) | C3—C4     | 1.388 (3) |
| Zn1—N1     | 2.0184 (14)| C8—C7     | 1.381 (3) |
| Zn1—N1iii  | 2.0184 (14)| C8—H8     | 0.89 (2)  |
| S1—C1      | 1.7059 (17)| C4—C5     | 1.382 (3) |
| O1—C2      | 1.371 (2)  | C4—H4     | 0.92 (3)  |
| O1—C1      | 1.3635 (19)| C7—C6     | 1.384 (3) |
| N1—N2      | 1.4062 (18)| C7—H7     | 0.92 (3)  |
| N1—C1      | 1.299 (2)  | C5—C6     | 1.376 (4) |
| N2—C2      | 1.285 (2)  | C5—H5     | 0.89 (3)  |
| C2—C3      | 1.460 (2)  | C6—H6     | 1.00 (3)  |
| S1i—Zn1—S1ii| 100.46 (3)| O1—C1—S1  | 120.26 (13)|
| N1—Zn1—S1i| 108.51 (4) | N1—C1—S1  | 129.90 (13)|
| N1—Zn1—S1i| 113.82 (4) | N1—C1—O1  | 109.83 (14)|
| N1—Zn1—S1i| 108.50 (4) | C3—C8—H8  | 119.3 (14)|
| N1—Zn1—S1i| 113.82 (5) | C7—C8—C3  | 120.24 (19)|
| Zn1i—S1—Zn1i| 111.37 (9)| C7—C8—H8  | 120.5 (14)|
| C1—S1—Zn1i| 102.39 (6) | C3—C4—H4  | 120.8 (16)|
| C1—O1—C2  | 103.92 (13)| C5—C4—C3  | 119.6 (2) |
| N2—N1—Zn1 | 119.57 (11)| C5—C4—H4  | 119.6 (16)|
| C1—N1—Zn1 | 131.80 (12)| C8—C7—C6  | 119.6 (2) |
| C1—N1—N2  | 108.57 (13)| C8—C7—H7  | 122.8 (17)|
| C2—N2—N1  | 105.05 (14)| C6—C7—H7  | 117.6 (17)|
| O1—C2—C3  | 119.65 (15)| C4—C5—H5  | 116.4 (17)|
| N2—C2—O1  | 112.61 (14)| C6—C5—C4  | 120.3 (2) |
| N2—C2—C3  | 127.75 (16)| C6—C5—H5  | 123.3 (17)|
| C8—C3—C2  | 118.67 (16)| C7—C6—H6  | 119.8 (18)|
| C8—C3—C4  | 119.85 (17)| C5—C6—C7  | 120.33 (19)|
| C4—C3—C2  | 121.48 (17)| C5—C6—H6  | 119.8 (18)|
| Zn1i—S1—C1—O1| 116.48 (12)| C2—O1—C1—S1| −179.75 (12)|
| Zn1i—S1—C1—N1| −65.24 (17)| C2—O1—C1—N1| 1.66 (18)|
| Zn1—N1—N2—C2| −176.89 (12)| C2—C3—C8—C7| −179.66 (19)|
| Zn1—N1—C1—S1| −2.7 (3)   | C2—C3—C4—C5| 179.34 (19)|
| Zn1—N1—C1—O1| 175.68 (11)| C3—C8—C7—C6| 0.5 (3) |
| O1—C2—C3—C8| −166.60 (16)| C3—C4—C5—C6| 0.2 (3) |
| O1—C2—C3—C4| 13.2 (3)   | C1—O1—C2—N2| −1.25 (19)|
| N1—N2—C2—O1| 0.4 (2)    | C1—O1—C2—C3| 178.37 (15)|
| N1—N2—C2—C3| −179.19 (17)| C1—N1—N2—C2| 0.68 (19)|
| N2—N1—C1—S1| −179.91 (13)| C8—C3—C4—C5| −0.9 (3) |
| N2—N1—C1—O1| −1.49 (19) | C8—C7—C6—C5| −1.2 (4) |
| N2—C2—C3—C8| 13.0 (3)   | C4—C3—C8—C7| 0.6 (3) |
| N2—C2—C3—C4| −167.27 (19)| C4—C5—C6—C7| 0.9 (4) |

Symmetry codes: (i) −x+1, −y+1, −z+1; (ii) x, −y+1, z+1/2; (iii) −x+1, y, −z+3/2.
Hydrogen-bond geometry (Å, °)

| D—H···A | D—H | H···A | D···A | D—H···A |
|---|---|---|---|---|
| C6—H6···S1^iv | 1.00 (3) | 2.86 (3) | 3.608 (2) | 132 (2) |

Symmetry code: (iv) x+1/2, -y+3/2, z+1/2.