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Synthesis and structure of *catena*-poly[[[aqua-zinc(II)]- μ -2-([amino(sulfanidyl)methylidene]-amino}imino)-2-phenylacetato- κ^4 O,N,S:O'] monohydrate]

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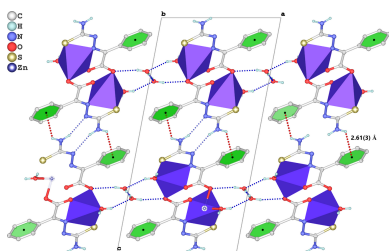
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In the polymeric title compound, $[[\text{Zn}(\text{C}_9\text{H}_7\text{N}_3\text{O}_2\text{S})(\text{H}_2\text{O})]\cdot\text{H}_2\text{O}]_n$, the dianion of phenylglyoxylic acid thiosemicarbazone (benzketozone) chelates one Zn^{II} cation through carboxylate O, azomethine N and thiolate S atoms and bridges to the next Zn^{II} ion through its second carboxylate O atom. Each Zn^{II} ion is five-coordinate, with the aqua ligand completing the coordination sphere, which has a shape intermediate between square-pyramidal and trigonal-bipyramidal. The coordination motif generates a chain extending parallel to [010], with an adjacent $\text{Zn}\cdots\text{Zn}$ separation of 4.8378 (4) Å. $\text{O}-\text{H}\cdots\text{O}$, $\text{O}-\text{H}\cdots\text{S}$ and $\text{N}-\text{H}\cdots\text{N}$ hydrogen bonds connect the polymeric chains and non-coordinating water molecules into a three-periodic network; a weak $\text{N}-\text{H}\cdots\pi$ contact is also present. Hirshfeld surface analysis identifies $\text{H}\cdots\text{H}$ (34.8%), $\text{C}\cdots\text{H}/\text{H}\cdots\text{C}$ (16.1%), $\text{H}\cdots\text{S}/\text{S}\cdots\text{H}$ (13.2%), $\text{O}\cdots\text{H}/\text{H}\cdots\text{O}$ (11.0%) and $\text{N}\cdots\text{H}/\text{H}\cdots\text{N}$ (8.4%) as the principal contact contributions.

1. Chemical context

Thiosemicarbazones are versatile Schiff-base ligands whose coordination behaviour is strongly influenced by the parent carbonyl compound, the central metal cation and the degree of ligand deprotonation. They commonly bind through the azomethine N and thione/thiolate S atoms, while additional donor groups can lead to tridentate or higher-denticity coordination modes (Casas *et al.*, 2000; Lobana *et al.*, 2009; Dilworth & Hueting, 2012). Their structural diversity, together with the broad biological activity of thiosemicarbazone derivatives and their metal complexes, continues to attract considerable interest (Zahra *et al.*, 2025). Anticancer, antimicrobial, antiviral, antimalarial and antioxidant activities have been reported, together with interactions involving albumin, DNA and biologically relevant enzymes (Devi *et al.*, 2024; Nascimento *et al.*, 2024; Chen *et al.*, 2025; Ucar *et al.*, 2025). Selected radiometal bis(thiosemicarbazone) complexes have also been investigated for diagnostic PET/SPECT imaging and therapeutic applications (Dilworth & Hueting, 2012).

Thiosemicarbazones derived from α -keto carboxylic acids are particularly attractive because the carboxylate group provides an additional O-donor site. Deprotonation of both the carboxyl group and the hydrazinic N atom thus can generate a dianionic O,N,S donor set, while the second carboxylate O atom may participate in bridging, thereby

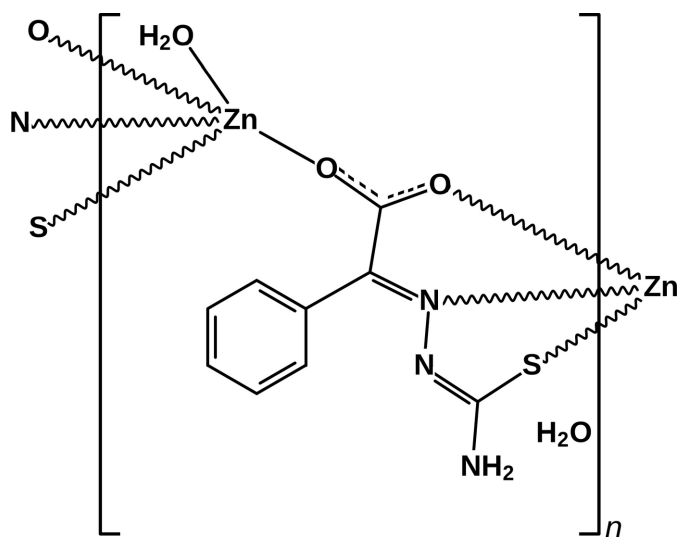


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allowing both discrete chelating modes and the formation of coordination polymers. Glyoxylic acid thiosemicarbazone (H_2GAT) illustrates this structural diversity: Co^{II} and Ni^{II} form mononuclear octahedral bis-chelate complexes (Huseynova *et al.*, 2018a), Zn^{II} gives discrete complexes under some conditions (Huseynova *et al.*, 2020, 2022), whereas Cu^{II} and Zn^{II} can form one-periodic polymers through hydrazinic-N and carboxylate-O bridging, respectively (Burshtein *et al.*, 1987; Huseynova *et al.*, 2019a,b). Related Zn^{II} coordination polymers have also been investigated using crystallographic, Hirshfeld surface and theoretical approaches (Rasulovich *et al.*, 2024; Nuralieva *et al.*, 2025).

The aryl-substituted analogue phenylglyoxylic acid thiosemicarbazone (H_2PGTS ; benzketozone) has previously been structurally characterized as its free monohydrate (Tillaeva *et al.*, 2022), but its metal coordination chemistry remains much less explored.



In this context, the title compound, (I), was synthesized and its crystal structure determined by single-crystal X-ray diffraction, with intermolecular interactions quantified by Hirshfeld surface analysis.

2. Structural commentary

The asymmetric unit of (I) contains one Zn^{II} cation, one doubly deprotonated phenylglyoxylic acid thiosemicarbazone ligand, one aqua ligand and one non-coordinating water molecule (Fig. 1). Zn1 is five-coordinate, bonded to the carboxylate atom O1 and the water O atom O1W in the asymmetric unit and to atoms O2^i , N1^i and S1^i of a symmetry-related ligand [symmetry code: (i) $-x + 1, y - \frac{1}{2}, -z + \frac{1}{2}$]. The coordination environment, with $\tau_5 = 0.42$ (Addison *et al.*, 1984), is between the ideal square-pyramidal ($\tau_5 = 0$) and trigonal-bipyramidal ($\tau_5 = 1$) limits, and therefore slightly closer to square-pyramidal. In this description, S1^i and O2^i define the axial direction [$\text{S1}^i-\text{Zn1}-\text{O2}^i = 155.77(4)^\circ$], whereas O1 , O1W and N1^i form the equatorial set of atoms. The three equatorial angles sum up to $358.69(12)^\circ$, and Zn1 is

displaced by $0.132(1) \text{ \AA}$ from the O1/O1W/N1^i least-squares plane. The $\text{Zn}-\text{O}$ distances are $2.0052(13)$, $2.0350(15)$ and $2.0976(13) \text{ \AA}$, while $\text{Zn}-\text{N1}^i$ and $\text{Zn}-\text{S1}^i$ are $2.1042(15)$ and $2.3907(5) \text{ \AA}$, respectively. The two fused five-membered chelate rings, $\text{Zn1/N1}^i/\text{N2}^i/\text{C9}^i/\text{S1}^i$ and $\text{Zn1/N1}^i/\text{C7}^i/\text{C8}^i/\text{O2}^i$, are nearly planar, with maximum deviations of $0.053(2) \text{ \AA}$ (C9^i) and $0.074(1) \text{ \AA}$ (O2^i), respectively, and bite angles of $79.98(4)$ and $77.11(5)^\circ$.

The ligand is doubly deprotonated, specifically at the carboxyl group and at the hydrazinic atom N2 , and coordinates in the thiolate form. The $\text{C9}-\text{S1}$ distance of $1.7402(18) \text{ \AA}$ lies between values expected for localized $\text{C}=\text{S}$ and $\text{C}-\text{S}$ bonds. The $\text{N2}-\text{C9}$ and $\text{N3}-\text{C9}$ distances [$1.328(2)$ and $1.339(3) \text{ \AA}$] are very similar, indicating substantial delocalization over the thioamide fragment. The azomethine bond $\text{N1}=\text{C7}$ [$1.284(2) \text{ \AA}$] and the $\text{N1}-\text{N2}$ bond [$1.365(2) \text{ \AA}$] are unexceptional. The two carboxylate $\text{C}-\text{O}$ distances [$\text{C8}-\text{O1} = 1.270(2)$ and $\text{C8}-\text{O2} = 1.245(2) \text{ \AA}$] are consistent with a deprotonated carboxylate group. The least-squares planes through $\text{S1/N1/N2/N3/C1/C7/C9}$ and O1/O2/C1/C7/C8 are roughly coplanar, forming a dihedral angle of $7.89(7)^\circ$. This is consistent with the torsion angles $\text{Zn1}-\text{N1}^i-\text{N2}^i-\text{C9}^i = -3.3(2)^\circ$ and $\text{N1}-\text{C7}-\text{C8}-\text{O2} = 7.1(2)^\circ$.

The phenyl ring is almost perpendicular to the chelating part of the ligand: it forms dihedral angles of $70.99(8)$ and $78.56(9)^\circ$ with the thiosemicarbazide ($\text{S1/N1/N2/N3/C1/C7/C9}$) and carboxylate (O1/O2/C1/C7/C8) planes, respectively, and the $\text{C2}-\text{C1}-\text{C7}-\text{N1}$ torsion angle is $71.5(2)^\circ$.

Because the two carboxylate O atoms coordinate to adjacent Zn^{II} cations, each ligand bridges two metal ions and the structure forms a one-periodic coordination polymer. The chain is generated by the 2_1 screw axis and propagates parallel to $[010]$, with an adjacent $\text{Zn1} \cdots \text{Zn1}^i$ separation of $4.8378(4) \text{ \AA}$ (Fig. 2). The bridging carboxylate group adopts a *syn-anti* mode, as shown by the torsion angles $\text{Zn1}-\text{O1}-\text{C8}-\text{O2} = -9.7(2)^\circ$ and $\text{Zn1}-\text{O2}^i-\text{C8}^i-\text{O1}^i =$

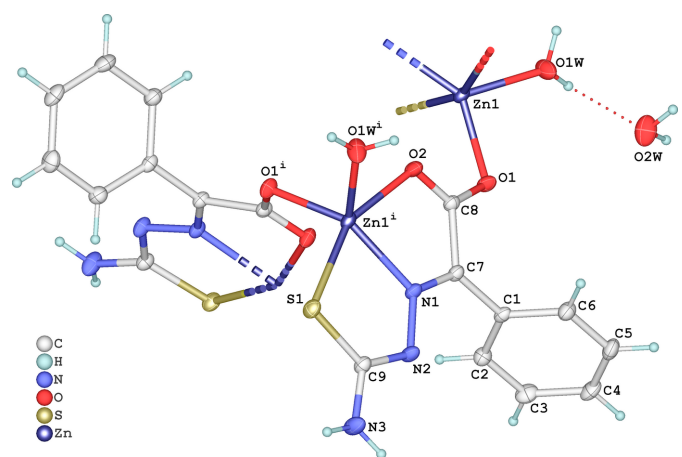


Figure 1
The coordination environment of Zn1 in compound (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level, and H atoms are shown as spheres of arbitrary radius. The red dotted line indicates the $\text{O}-\text{H} \cdots \text{O}$ hydrogen bond to the non-coordinating water molecule. [Symmetry code: (i) $-x + 1, y - \frac{1}{2}, -z + \frac{1}{2}$.]

Table 1

Hydrogen-bond geometry (Å, °).

 C_g is the centroid of the C1–C6 ring.

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O1W—H1WA $\cdots$ O2W	0.84 (1)	2.02 (2)	2.809 (3)	155 (3)
O1W—H1WB $\cdots$ S1 ⁱ	0.84 (1)	2.33 (1)	3.1718 (17)	175 (3)
O2W—H2WA $\cdots$ O1 ⁱⁱⁱ	0.84 (1)	2.19 (1)	3.011 (2)	168 (4)
O2W—H2WB $\cdots$ O2W ⁱⁱⁱ	0.84 (1)	2.18 (1)	3.0162 (14)	178 (4)
N3—H3B $\cdots$ N2 ⁱⁱⁱ	0.86 (1)	2.28 (1)	3.106 (2)	162 (2)
N3—H3A $\cdots$ Cg ⁱⁱⁱ	0.85 (1)	2.61 (3)	3.173 (2)	125 (2)

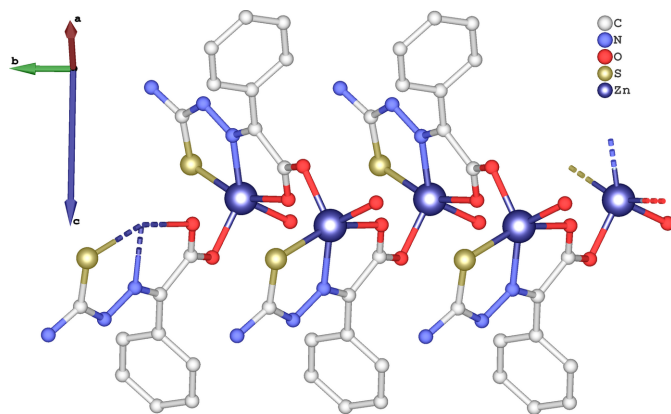
Symmetry codes: (i) $-x+1, y-\frac{3}{2}, -z+\frac{1}{2}$; (ii) $-x, y-\frac{1}{2}, -z+\frac{1}{2}$; (iii) $-x+1, -y+2, -z+1$.

165.62 (15)°. Consecutive phenyl rings protrude alternately towards opposite sides of the chain.

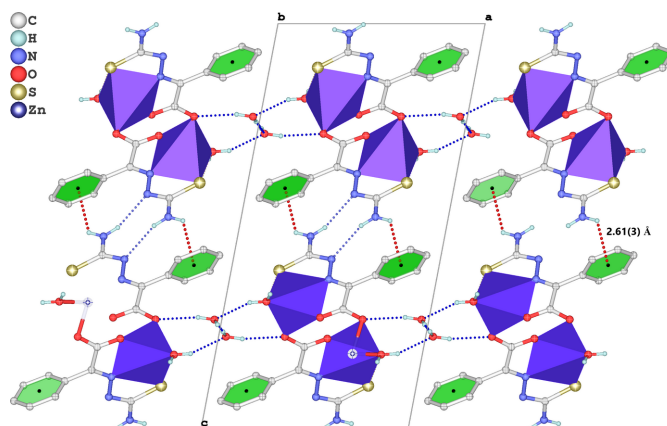
2.1. Supramolecular features

Hydrogen-bonding involves both water molecules and the terminal amino group N3 (Table 1). Within each coordination chain, the aqua ligand O1W donates H1WB to the thiolate atom S1 of a screw axis-related repeat unit; this nearly linear O—H $\cdots$ S contact is the only conventional hydrogen bond within an individual polymeric chain. The second H atom of the aqua ligand, H1WA, is donated to the non-coordinating water molecule O2W, which in turn acts as a double donor: H2WA is directed to the carboxylate atom O1 of a neighbouring coordination chain, while H2WB is donated to a symmetry-related non-coordinating water molecule. Consequently, the non-coordinating water molecules form a hydrogen-bonded chain extending parallel to [010] and simultaneously cross-link neighbouring Zn^{II} coordination chains.

The terminal amino group N3 provides an additional interchain linkage: N3—H3B $\cdots$ N2 hydrogen bonds between inversion-related chains generate a centrosymmetric $R_2^2(8)$ motif (Etter *et al.*, 1990). The second amino H atom, H3A, does not participate in a conventional hydrogen bond but is directed towards the centroid C_g of the C1–C6 phenyl ring of the same inversion-related chain, consistent with a weak

**Figure 2**

Part of the polymeric chain in (I), propagating parallel to [010] through carboxylate bridges and the tridentate O,N,S-chelation of the ligand. H atoms have been omitted for clarity.

**Figure 3**

Part of the crystal structure of (I), viewed along the b axis, showing the hydrogen bonds (dashed lines) that link neighbouring chains and the non-coordinating water molecules. H atoms not involved in hydrogen bonding have been omitted for clarity.

N—H $\cdots$ π contact (Table 1). No significant π – π stacking is observed between the phenyl rings. The shortest centroid-to-centroid separation, 5.6580 (9) Å, occurs between rings related by translation along the b axis; although these rings are parallel, their centroids are laterally offset by 5.019 (2) Å, so that there is no face-to-face overlap. Thus, the supramolecular assembly is governed primarily by O—H $\cdots$ O, O—H $\cdots$ S and N—H $\cdots$ N hydrogen bonds, assisted by the weak N—H $\cdots$ π contact. The intrachain O—H $\cdots$ S interactions, together with the water- and amine-mediated interchain contacts, link the mono-periodic coordination polymers into a tri-periodic hydrogen-bonded network (Fig. 3).

3. Hirshfeld surface analysis

To quantify the intermolecular contacts contributing to the crystal packing, a Hirshfeld surface analysis (McKinnon *et al.*, 2007; Spackman & Jayatilaka, 2009) was performed using *CrystalExplorer* (Spackman *et al.*, 2021). The surface was generated for the complex part of the asymmetric unit, *i.e.* one $[\text{Zn}(\text{C}_9\text{H}_7\text{N}_3\text{O}_2\text{S})(\text{H}_2\text{O})]$ repeat unit of the coordination chain. The non-coordinating water molecule was excluded from this fragment in order to examine its interactions with the polymeric chain; however, it was retained as a neighbouring molecule, so that its contacts with the repeat unit, both as a hydrogen-bond donor and as an acceptor, are mapped onto the surface and included in the fingerprint plots. Because the polymer is truncated at the bridging carboxylate group, the Zn $\cdots$ O, Zn $\cdots$ H and Zn $\cdots$ C contacts (6.1% in total) arise mainly from this truncation rather than from genuine intermolecular packing contacts.

The Hirshfeld surface mapped over d_{norm} is shown in Fig. 4. The most intense red regions, located near the Zn^{II} cation and the carboxylate O atoms, correspond to the Zn—O coordination bonds to the adjacent units of the chain, which are cut by the truncation of the polymer. The other red spots correspond to the O—H $\cdots$ O, O—H $\cdots$ S and N—H $\cdots$ N hydrogen bonds listed in Table 1. The contacts with the non-coordi-

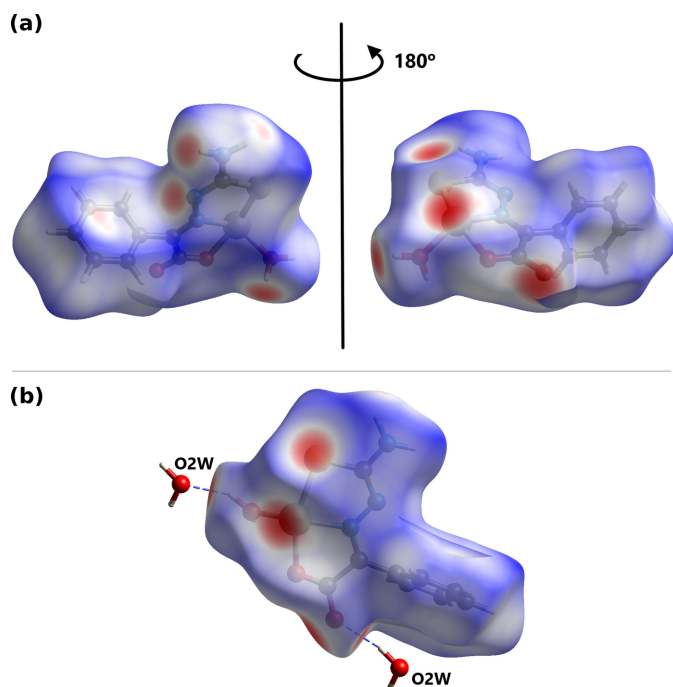


Figure 4
The Hirshfeld surface of (I) mapped over d_{norm} : (a) two views related by a 180° rotation and (b) a view showing the O—H...O hydrogen bonds (dashed lines) to the neighbouring non-coordinating water molecules (O2W).

nating water molecule are shown explicitly in Fig. 4b: O2W accepts a hydrogen bond from the aqua ligand and donates a hydrogen bond to the carboxylate atom O1 of a neighbouring

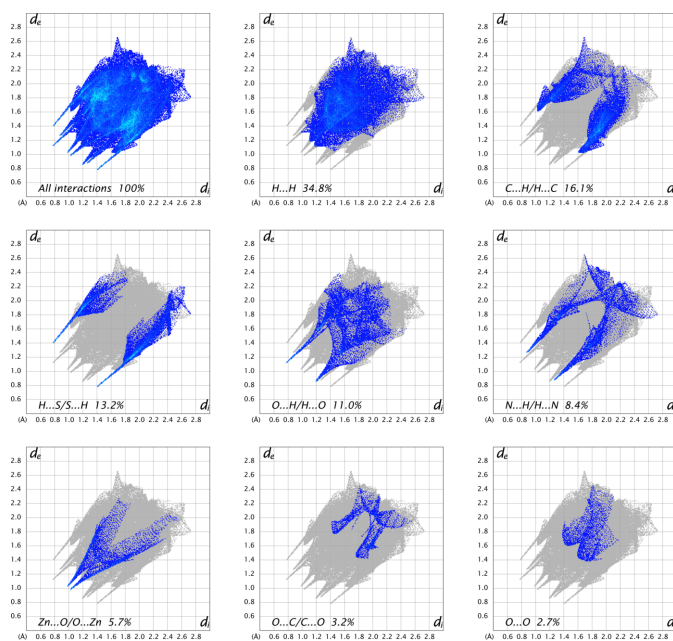


Figure 5
Two-dimensional fingerprint plots for (I), showing the full fingerprint plot and those delineated into H...H, C...H/H...C, H...S/S...H, O...H/H...O, N...H/H...N, Zn...O/O...Zn, O...C/C...O and O...O contacts, and their relative percentage contributions.

chain, and both interactions appear as distinct red spots on the surface. The remaining surface is predominantly white to blue, indicating contacts close to or longer than the sum of the van der Waals radii.

The two-dimensional fingerprint plots (Spackman & McKinnon, 2002) for the full surface and those delineated into the principal contact types, together with their percentage contributions, are shown in Fig. 5. H...H contacts make the largest contribution, followed by C...H/H...C, H...S/S...H, O...H/H...O and N...H/H...N contacts; each of the remaining contact types not shown in Fig. 5 contributes less than 2%. The relatively large H...S/S...H contribution reflects the exposed thiolate S atom, which both coordinates to Zn^{II} and acts as an acceptor in the O—H...S hydrogen bond. Overall, the crystal packing is dominated by contacts involving H atoms, consistent with the hydrogen-bonding network described above, while the very small C...C contribution (0.6%) confirms the absence of significant π – π stacking.

4. Database survey

A search of the Cambridge Structural Database (CSD, Version 6.01, November 2025, including the February 2026 updates; Groom *et al.*, 2016) was carried out using *ConQuest*, restricted to metal-containing structures and using the α -oxo-carboxylate thiosemicarbazone fragment O—C(O)—C—N—N—C(S)—N with all bond types unspecified. The search returned 97 hits. In most of them, the substituent at the azomethine C atom is H, methyl, ethyl or 2-carboxyethyl, corresponding to derivatives of glyoxylic, pyruvic, 2-oxobutyric or 2-oxoglutaric acid. The closest aryl-substituted analogue is PIZTOH (Sonawane *et al.*, 1994), which carries a benzyl substituent. No metal complex with a phenyl group directly bonded to the azomethine C atom was found, so that compound (I) is the first structurally characterized metal complex of this ligand type.

Comparison with the free ligand, $\text{H}_2\text{PGTS}\cdot\text{H}_2\text{O}$ (GEJFAG; Tillaeva *et al.*, 2022), shows the changes caused by deprotonation and coordination. In GEJFAG, the ligand is neutral, with protonated carboxyl and hydrazinic N2 groups, and the C9—S1 bond [1.690 (2) Å] corresponds to a thione form. In the crystal structure of (I), C9—S1 is lengthened to 1.7402 (18) Å, consistent with the thiolate form. At the same time, N2—C9 is shortened from 1.351 (3) to 1.328 (2) Å and N3—C9 is lengthened from 1.306 (3) to 1.339 (3) Å, so that the two C—N bonds of the thioamide fragment become nearly equal, indicating charge delocalization after deprotonation of N2. Coordination also changes the ligand conformation considerably. In GEJFAG, the phenyl ring forms dihedral angles of $22.6 (1)^\circ$ and $47.9 (1)^\circ$ with the thiosemicarbazide (S1/N1/N2/N3/C1/C7/C9) and carboxyl (O1/O2/C1/C7/C8) planes, respectively, and the C2—C1—C7—N1 torsion angle is $-27.2 (3)^\circ$. In (I), the corresponding values are $70.99 (8)^\circ$, $78.56 (9)^\circ$ and $71.5 (2)^\circ$. This rotation is presumably required to relieve steric repulsion between the phenyl ring and the planar, fused O,N,S-chelate system.

Among complexes of the parent glyoxylic acid thiosemicarbazone (H_2GAT), both discrete and polymeric structures are known. Co^{II} and Ni^{II} form mononuclear octahedrally coordinated bis-chelates (ODOWUC and ODOXAJ; Huseynova *et al.*, 2018). Ni^{II} also forms discrete bis-chelates, $[\text{Zn}(\text{HGAT})_2] \cdot x\text{H}_2\text{O}$ (FOTPAI, $x = 5/3$; Huseynova *et al.*, 2020; VADFEP, $x = 3/2$; Huseynova *et al.*, 2022), in which two monoanionic ligands coordinate to the overall six-coordinate Zn^{II} cation. In FOTPAI, the $\text{Zn}-\text{O}$ [2.105 (3)–2.197 (3) Å], $\text{Zn}-\text{N}$ [2.138 (3)–2.175 (3) Å] and $\text{Zn}-\text{S}$ [2.4974 (12)–2.5874 (13) Å] bonds are all longer than the corresponding bonds in the structure of (I) [2.0052 (13)–2.0976 (13), 2.1042 (15) and 2.3907 (5) Å, respectively], as expected for the lower coordination number and the dianionic ligand in (I).

Only nine of the 97 hits are one-periodic coordination polymers: six Cu, two Pb and one Zn complexes. The Zn^{II} polymer of H_2GAT (LOXNAQ; Huseynova *et al.*, 2019*b*) is the closest analogue of (I). In both structures, the dianionic ligand chelates one five-coordinate Zn^{II} cation through the O, N,S donor set, a water molecule completes the coordination sphere, and the second carboxylate O atom bridges to the next Zn^{II} ion. Unlike in (I), however, LOXNAQ contains no non-coordinating water molecule, so that the water-mediated cross-linking of the chains observed in (I) is absent. A different mode of chain propagation is found in the Cu^{II} polymer of the same ligand (GERPAU, Burshtein *et al.*, 1987; redetermined as GERPAU01, Huseynova *et al.*, 2019*a*). Here, the square-pyramidally coordinated Cu^{II} cations are linked through the hydrazinic N atom, and the carboxylate group acts only as a chelating donor. Replacing the H atom of H_2GAT by a phenyl group in (I) therefore does not change the carboxylate-bridged chain motif. However, the phenyl rings, which protrude alternately to opposite sides of the chain, prevent close packing of the chains and preclude $\pi-\pi$ stacking, so that the chains are linked only through hydrogen bonds involving the water molecules and the amino group.

5. Synthesis and crystallization

The ligand $\text{H}_2\text{PGTS} \cdot \text{H}_2\text{O}$ was prepared according to the published procedure (Tillaeva *et al.*, 2022). A solution of $\text{Zn}(\text{CH}_3\text{COO})_2 \cdot 2\text{H}_2\text{O}$ (0.220 g, 1.00 mmol) in water (5 ml) was added to a solution of $\text{H}_2\text{PGTS} \cdot \text{H}_2\text{O}$ (0.242 g, 1.00 mmol) in ethanol (5 ml). The reaction mixture was stirred at 333 K at 500 rpm for 10 min and then allowed to evaporate slowly at room temperature. After 5 d, colourless block-shaped crystals suitable for single-crystal X-ray diffraction were obtained (yield 55%). Analysis calculated for $\text{C}_9\text{H}_{11}\text{N}_3\text{O}_4\text{SZn}$ ($M_r = 322.64$): C, 33.50; H, 3.44; N, 13.02; S, 9.94%. Found: C, 33.45; H, 3.39; N, 12.98; S, 9.97%.

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. H atoms attached to C atoms were placed in calculated positions ($\text{C}-\text{H} = 0.93$ Å) and refined using a riding model, with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$. The H atoms

Table 2

Experimental details.

Crystal data	
Chemical formula	$[\text{Zn}(\text{C}_9\text{H}_7\text{N}_3\text{O}_2\text{S})(\text{H}_2\text{O})] \cdot \text{H}_2\text{O}$
M_r	322.64
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	291
a, b, c (Å)	10.5337 (1), 5.6580 (1), 21.0089 (3)
β (°)	100.760 (1)
V (Å ³)	1230.11 (3)
Z	4
Radiation type	Cu $K\alpha$
μ (mm ^{−1})	4.49
Crystal size (mm)	0.3 × 0.2 × 0.12
Data collection	
Diffractometer	Xcalibur, Ruby
Absorption correction	Multi-scan (<i>CrysAlis PRO</i> ; Rigaku OD, 2023)
$T_{\text{min}}, T_{\text{max}}$	0.572, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	7561, 2514, 2354
R_{int}	0.029
$(\sin \theta/\lambda)_{\text{max}}$ (Å ^{−1})	0.630
Refinement	
$R[F^2 > 2\sigma(F^2)], wR(F^2), S$	0.028, 0.078, 1.06
No. of reflections	2514
No. of parameters	188
No. of restraints	6
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{\text{max}}, \Delta\rho_{\text{min}}$ (e Å ^{−3})	0.29, −0.31

Computer programs: *CrysAlis PRO* (Rigaku OD, 2023), *SHELXT* (Sheldrick, 2015*a*), *SHELXL* (Sheldrick, 2015*b*), *OLEX2* (Dolomanov *et al.*, 2009) and *publCIF* (Westrip, 2010).

of the aqua ligand, the non-coordinating water molecule and of the amino group were located in difference-Fourier maps and refined with restrained O—H and N—H distances of 0.85 (1) and 0.86 (1) Å, respectively. Their positional and isotropic displacement parameters were refined independently. A total of six distance restraints were applied.

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supporting information

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Synthesis and structure of *catena*-poly[[[aquazinc(II)]- μ -2-([amino(sulfanidyl)methylidene]amino)imino)-2-phenylacetato- $\kappa^4 O, N, S: O'$] monohydrate]

Javokhirkhon Akhatov, Gulnora Tillaeva, Khayit Turaev, Odyl Choriyev, Maftuna Primkulova, Bakhtiyar Ibragimov and Jamshid Mengnorovich Ashurov

Computing details

catena-Poly[[[aquazinc(II)]- μ -2-([amino(sulfanidyl)methylidene]amino)imino)-2-phenylacetato- $\kappa^4 O, N, S: O'$] monohydrate]

Crystal data

[Zn(C₉H₇N₃O₂S)(H₂O)]·H₂O

$M_r = 322.64$

Monoclinic, $P2_1/c$

$a = 10.5337$ (1) Å

$b = 5.6580$ (1) Å

$c = 21.0089$ (3) Å

$\beta = 100.760$ (1)°

$V = 1230.11$ (3) Å³

$Z = 4$

$F(000) = 656$

$D_x = 1.742$ Mg m⁻³

Cu $K\alpha$ radiation, $\lambda = 1.54184$ Å

Cell parameters from 5766 reflections

$\theta = 4.2$ – 76.1°

$\mu = 4.49$ mm⁻¹

$T = 291$ K

Block, colourless

$0.3 \times 0.2 \times 0.12$ mm

Data collection

Xcalibur, Ruby

diffractometer

Radiation source: Enhance (Cu) X-ray Source

Graphite monochromator

Detector resolution: 10.2576 pixels mm⁻¹

ω scans

Absorption correction: multi-scan

(CrysAlisPro; Rigaku OD, 2023)

$T_{\min} = 0.572$, $T_{\max} = 1.000$

7561 measured reflections

2514 independent reflections

2354 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.029$

$\theta_{\max} = 76.4^\circ$, $\theta_{\min} = 4.3^\circ$

$h = -13 \rightarrow 13$

$k = -7 \rightarrow 5$

$l = -22 \rightarrow 26$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.028$

$wR(F^2) = 0.078$

$S = 1.06$

2514 reflections

188 parameters

6 restraints

Hydrogen site location: mixed

H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0492P)^2 + 0.2444P]$

where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} < 0.001$

$\Delta\rho_{\max} = 0.29$ e Å⁻³

$\Delta\rho_{\min} = -0.31$ e Å⁻³

Extinction correction: SHELXL2025/1
 (Sheldrick 2015b),
 $F_c^* = k F_c [1 + 0.001 x F_c^2 \lambda^3 / \sin(2\theta)]^{-1/4}$
 Extinction coefficient: 0.0015 (2)

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 ($\text{\AA}^2$)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Zn1	0.33743 (2)	0.15367 (4)	0.18671 (2)	0.02765 (12)
S1	0.76756 (4)	0.93004 (9)	0.39192 (2)	0.03347 (14)
O1	0.32015 (13)	0.3021 (2)	0.27135 (6)	0.0330 (3)
O1W	0.19866 (16)	−0.0979 (3)	0.18463 (10)	0.0505 (4)
H1WA	0.1198 (13)	−0.091 (6)	0.1870 (17)	0.074 (10)*
H1WB	0.210 (3)	−0.227 (3)	0.1666 (15)	0.073 (10)*
O2	0.52699 (13)	0.3937 (2)	0.27595 (7)	0.0339 (3)
N1	0.51936 (14)	0.6934 (3)	0.37017 (7)	0.0271 (3)
N2	0.52557 (16)	0.8524 (3)	0.41950 (8)	0.0324 (4)
N3	0.64759 (19)	1.1381 (4)	0.47600 (10)	0.0444 (5)
C1	0.29820 (16)	0.5810 (3)	0.38054 (8)	0.0271 (4)
C2	0.21642 (19)	0.7747 (4)	0.36741 (9)	0.0340 (4)
H2	0.238097	0.898891	0.342474	0.041*
C3	0.1029 (2)	0.7831 (4)	0.39137 (11)	0.0410 (5)
H3	0.047601	0.911604	0.381886	0.049*
C4	0.0713 (2)	0.6005 (4)	0.42947 (10)	0.0413 (5)
H4	−0.004767	0.607332	0.445818	0.050*
C5	0.1526 (2)	0.4085 (4)	0.44320 (10)	0.0417 (5)
H5	0.131217	0.286301	0.468878	0.050*
C6	0.2663 (2)	0.3973 (4)	0.41872 (10)	0.0349 (4)
H6	0.320883	0.267589	0.427841	0.042*
C7	0.41709 (17)	0.5678 (3)	0.35307 (8)	0.0267 (4)
C8	0.42359 (17)	0.4086 (3)	0.29632 (8)	0.0274 (4)
C9	0.63595 (17)	0.9720 (3)	0.42991 (8)	0.0300 (4)
O2W	−0.03563 (18)	−0.1447 (4)	0.22900 (11)	0.0613 (5)
H2WA	−0.1165 (10)	−0.148 (6)	0.2234 (19)	0.081 (11)*
H2WB	−0.016 (4)	−0.283 (3)	0.2415 (19)	0.088 (12)*
H3A	0.7214 (14)	1.202 (4)	0.4853 (13)	0.044 (7)*
H3B	0.5869 (19)	1.153 (4)	0.4977 (11)	0.046 (7)*

Atomic displacement parameters ($\text{\AA}^2$)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn1	0.02673 (16)	0.03423 (18)	0.02422 (16)	−0.00090 (9)	0.01046 (10)	−0.00270 (9)
S1	0.0263 (2)	0.0425 (3)	0.0332 (2)	−0.00429 (17)	0.00958 (17)	−0.00229 (18)

O1	0.0305 (7)	0.0431 (7)	0.0263 (6)	−0.0046 (5)	0.0078 (5)	−0.0097 (5)
O1W	0.0379 (8)	0.0392 (8)	0.0795 (12)	−0.0112 (7)	0.0243 (8)	−0.0157 (8)
O2	0.0345 (7)	0.0385 (7)	0.0324 (7)	−0.0053 (6)	0.0155 (5)	−0.0094 (6)
N1	0.0258 (7)	0.0354 (8)	0.0211 (7)	−0.0024 (6)	0.0070 (5)	−0.0035 (6)
N2	0.0296 (8)	0.0430 (9)	0.0260 (7)	−0.0071 (6)	0.0091 (6)	−0.0111 (6)
N3	0.0385 (10)	0.0562 (12)	0.0412 (10)	−0.0172 (8)	0.0145 (8)	−0.0212 (9)
C1	0.0244 (8)	0.0367 (9)	0.0208 (7)	−0.0034 (7)	0.0058 (6)	−0.0052 (7)
C2	0.0327 (9)	0.0378 (10)	0.0319 (9)	0.0002 (8)	0.0071 (7)	0.0019 (8)
C3	0.0300 (10)	0.0527 (12)	0.0403 (11)	0.0087 (9)	0.0066 (8)	−0.0028 (9)
C4	0.0290 (9)	0.0630 (13)	0.0349 (10)	−0.0016 (9)	0.0137 (8)	−0.0040 (9)
C5	0.0421 (11)	0.0508 (12)	0.0364 (10)	−0.0075 (9)	0.0181 (9)	0.0036 (9)
C6	0.0357 (10)	0.0388 (10)	0.0324 (9)	0.0021 (8)	0.0115 (8)	0.0030 (8)
C7	0.0261 (8)	0.0335 (9)	0.0212 (8)	−0.0021 (7)	0.0064 (6)	−0.0014 (7)
C8	0.0307 (9)	0.0309 (9)	0.0215 (8)	−0.0005 (7)	0.0069 (6)	−0.0004 (7)
C9	0.0289 (8)	0.0377 (10)	0.0237 (8)	−0.0021 (7)	0.0060 (6)	−0.0012 (7)
O2W	0.0398 (10)	0.0780 (14)	0.0641 (12)	−0.0045 (9)	0.0040 (8)	0.0210 (10)

Geometric parameters (Å, °)

Zn1—S1 ⁱ	2.3907 (5)	C1—C2	1.389 (3)
Zn1—O1	2.0052 (13)	C1—C6	1.392 (3)
Zn1—O1W	2.0350 (15)	C1—C7	1.475 (2)
Zn1—O2 ⁱ	2.0976 (13)	C2—H2	0.9300
Zn1—N1 ⁱ	2.1042 (15)	C2—C3	1.382 (3)
S1—C9	1.7402 (18)	C3—H3	0.9300
O1—C8	1.270 (2)	C3—C4	1.385 (3)
O1W—H1WA	0.843 (10)	C4—H4	0.9300
O1W—H1WB	0.844 (10)	C4—C5	1.380 (3)
O2—C8	1.245 (2)	C5—H5	0.9300
N1—N2	1.365 (2)	C5—C6	1.391 (3)
N1—C7	1.284 (2)	C6—H6	0.9300
N2—C9	1.328 (2)	C7—C8	1.506 (2)
N3—C9	1.339 (3)	O2W—H2WA	0.838 (10)
N3—H3A	0.847 (10)	O2W—H2WB	0.840 (10)
N3—H3B	0.856 (10)		
O1—Zn1—S1 ⁱ	103.41 (4)	C1—C2—H2	120.0
O1—Zn1—O1W	97.37 (7)	C3—C2—C1	120.07 (19)
O1—Zn1—O2 ⁱ	97.49 (6)	C3—C2—H2	120.0
O1—Zn1—N1 ⁱ	130.72 (6)	C2—C3—H3	119.9
O1W—Zn1—S1 ⁱ	101.83 (6)	C2—C3—C4	120.2 (2)
O1W—Zn1—O2 ⁱ	87.34 (7)	C4—C3—H3	119.9
O1W—Zn1—N1 ⁱ	130.60 (7)	C3—C4—H4	119.9
O2 ⁱ —Zn1—S1 ⁱ	155.77 (4)	C5—C4—C3	120.11 (19)
O2 ⁱ —Zn1—N1 ⁱ	77.11 (5)	C5—C4—H4	119.9
N1 ⁱ —Zn1—S1 ⁱ	79.98 (4)	C4—C5—H5	119.9
C9—S1—Zn1 ⁱⁱ	95.78 (6)	C4—C5—C6	120.1 (2)
C8—O1—Zn1	110.63 (11)	C6—C5—H5	119.9

Zn1—O1W—H1WA	133 (2)	C1—C6—H6	120.1
Zn1—O1W—H1WB	117 (2)	C5—C6—C1	119.77 (19)
H1WA—O1W—H1WB	107 (3)	C5—C6—H6	120.1
C8—O2—Zn1 ⁱⁱ	113.71 (11)	N1—C7—C1	126.26 (16)
N2—N1—Zn1 ⁱⁱ	124.33 (11)	N1—C7—C8	113.11 (15)
C7—N1—Zn1 ⁱⁱ	115.78 (12)	C1—C7—C8	120.49 (15)
C7—N1—N2	119.72 (15)	O1—C8—C7	116.67 (15)
C9—N2—N1	112.18 (15)	O2—C8—O1	124.32 (16)
C9—N3—H3A	115.1 (18)	O2—C8—C7	118.99 (16)
C9—N3—H3B	118.7 (18)	N2—C9—S1	127.08 (14)
H3A—N3—H3B	125 (3)	N2—C9—N3	115.87 (17)
C2—C1—C6	119.74 (17)	N3—C9—S1	117.02 (14)
C2—C1—C7	120.16 (17)	H2WA—O2W—H2WB	102 (3)
C6—C1—C7	120.10 (17)		
Zn1 ⁱⁱ —S1—C9—N2	8.01 (18)	C1—C2—C3—C4	1.1 (3)
Zn1 ⁱⁱ —S1—C9—N3	−174.01 (16)	C1—C7—C8—O1	4.7 (3)
Zn1—O1—C8—O2	−9.7 (2)	C1—C7—C8—O2	−176.99 (17)
Zn1—O1—C8—C7	168.47 (12)	C2—C1—C6—C5	0.3 (3)
Zn1 ⁱⁱ —O2—C8—O1	165.62 (15)	C2—C1—C7—N1	71.5 (2)
Zn1 ⁱⁱ —O2—C8—C7	−12.5 (2)	C2—C1—C7—C8	−103.8 (2)
Zn1 ⁱⁱ —N1—N2—C9	−3.3 (2)	C2—C3—C4—C5	−0.6 (3)
Zn1 ⁱⁱ —N1—C7—C1	−173.36 (14)	C3—C4—C5—C6	−0.1 (3)
Zn1 ⁱⁱ —N1—C7—C8	2.2 (2)	C4—C5—C6—C1	0.3 (3)
N1—N2—C9—S1	−4.4 (2)	C6—C1—C2—C3	−1.0 (3)
N1—N2—C9—N3	177.57 (17)	C6—C1—C7—N1	−109.7 (2)
N1—C7—C8—O1	−171.16 (16)	C6—C1—C7—C8	75.0 (2)
N1—C7—C8—O2	7.1 (2)	C7—N1—N2—C9	−178.26 (17)
N2—N1—C7—C1	2.1 (3)	C7—C1—C2—C3	177.80 (18)
N2—N1—C7—C8	177.66 (15)	C7—C1—C6—C5	−178.50 (17)

Symmetry codes: (i) $-x+1, y-1/2, -z+1/2$; (ii) $-x+1, y+1/2, -z+1/2$.

Hydrogen-bond geometry ($\text{\AA}$, $^\circ$)

Cg is the centroid of the C1—C6 ring.

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O1W—H1WA $\cdots$ O2W	0.84 (1)	2.02 (2)	2.809 (3)	155 (3)
O1W—H1WB $\cdots$ S1 ⁱⁱⁱ	0.84 (1)	2.33 (1)	3.1718 (17)	175 (3)
O2W—H2WA $\cdots$ O1 ^{iv}	0.84 (1)	2.19 (1)	3.011 (2)	168 (4)
O2W—H2WB $\cdots$ O2W ^{iv}	0.84 (1)	2.18 (1)	3.0162 (14)	178 (4)
N3—H3B $\cdots$ N2 ^v	0.86 (1)	2.28 (1)	3.106 (2)	162 (2)
N3—H3A $\cdots$ Cg ^v	0.85 (1)	2.61 (3)	3.173 (2)	125 (2)

Symmetry codes: (iii) $-x+1, y-3/2, -z+1/2$; (iv) $-x, y-1/2, -z+1/2$; (v) $-x+1, -y+2, -z+1$.