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# *catena*-Poly[[diaqua(2,2′-bipyridine-$\kappa^2N,N'$)zinc]-$\mu$-2,2′-[1,4-phenylenebis(sulfanediyl)]diacetato-$\kappa^2O:O'$]

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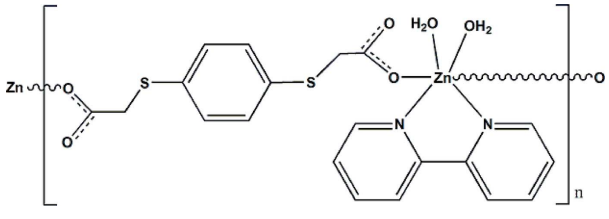
Key indicators: single-crystal X-ray study; $T$ = 296 K; mean $\sigma$(C–C) = 0.002 Å; $R$ factor = 0.025; $wR$ factor = 0.070; data-to-parameter ratio = 16.7.

In the polymeric title complex, $[Zn(C_{10}H_8O_4S_2)(C_{10}H_8N_2)(H_2O)_2]_n$, the $Zn^{2+}$ ion lies on a twofold rotation axis and exhibits an octahedral environment, in which it is coordinated by two *trans* O atoms from two symmetry-related 2,2′-[1,4-phenylenebis(sulfanediyl)]diacetate anions, two N atoms from one 2,2′-bipyridine ligand, and two *cis* O atoms from water molecules. The dihedral angle between the two pyridine rings is 11.5 (1)°. Adjacent $Zn^{2+}$ ions are bridged in a monodentate manner by the diacetate anions, forming a chain structure extending parallel to [101], and are further linked into the final three-dimensional structure by O—H···O hydrogen bonds between the coordinating water molecules as donor and the non-coordinating carboxylate O atoms as acceptor atoms.

## Related literature

For background to 1,4-benzenebis(thioacetic acid), including its synthesis and coordination behaviour, see: Yin & Feng (2009); Yin *et al.* (2009); Chen *et al.* (2010); Wang *et al.* (2011*a*,*b*); Jiang *et al.* (2012).




## Experimental

### Crystal data

$[Zn(C_{10}H_8O_4S_2)(C_{10}H_8N_2)(H_2O)_2]$
$M_r$ = 513.87
Monoclinic, $C2/c$
$a$ = 20.4396 (8) Å
$b$ = 12.8695 (8) Å
$c$ = 7.9798 (4) Å
$\beta$ = 90.765 (3)°
$V$ = 2098.88 (19) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 1.41 mm$^{-1}$
$T$ = 296 K
0.22 × 0.16 × 0.11 mm

### Data collection

Bruker APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min}$ = 0.761, $T_{max}$ = 0.853
16253 measured reflections
2448 independent reflections
2237 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.026

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.025
$wR(F^2)$ = 0.070
$S$ = 1.04
2448 reflections
147 parameters
3 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.31 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.31 e Å$^{-3}$

**Table 1**
Selected bond lengths (Å).

| | | | |
|---|---|---|---|
| Zn1—O1$W$ | 2.0896 (11) | Zn1—O1 | 2.1529 (10) |
| Zn1—N1 | 2.1477 (13) | | |

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| O1$W$—H1$WA$···O2$^{i}$ | 0.83 (1) | 1.90 (2) | 2.7107 (15) | 170 (2) |
| O1$W$—H1$WB$···O2 | 0.82 (1) | 1.86 (2) | 2.6582 (16) | 164 (2) |

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

Data collection: *APEX2* (Bruker, 2006); cell refinement: *SAINT* (Bruker, 2006); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008) and *DIAMOND* (Crystal Impact, 2008); software used to prepare material for publication: *publCIF* (Westrip, 2010).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: WM2568).

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# supplementary materials

*Acta Cryst.* (2012). E**68**, m105 [ **doi:10.1107/S1600536811055310** ]

# *catena*-Poly[[diaqua(2,2'-bipyridine-$\kappa^2N,N'$)zinc]-$\mu$-2,2'-[1,4-phenylenebis(sulfanediyl)]diacetato-$\kappa^2O:O'$]

**H. Lin and X.-J. Wang**

## Comment

1,4-Benzenebis(thioacetic acid), ($C_{10}H_{10}O_4S_2$), is a flexible aromatic multi-carboxylate ligand, which can be prepared from 1,4-benzenebisthiol (Yin & Feng, 2009). Compared with rigid ligands, these flexible aromatic carboxylate ligands contain more coordination sites (*viz.* S and O atoms) to construct various extended structures with different metal ions. Recently, some complexes derived from 1,4-benzenebis(thioacetic acid) with bipyridine ligands have been reported (Yin *et al.*, 2009; Chen *et al.*, 2010; Wang *et al.*, 2011*a,b*; Jiang *et al.*, 2012). Here we report the synthesis and structure of a new complex, $[Zn(C_{10}H_8O_4S_2)(C_{10}H_8N_2)(H_2O)_2]_n$, (I).

Complex (I) is isotypic with its Co(II) analogue (Jiang *et al.*, 2012). A view on the molecular structure of (I), showing the coordination environment of the $Zn^{2+}$ ion, is presented in Fig. 1. The asymmetric unit consists of one $Zn^{2+}$ ion (situated on a twofold rotation axis), half of a $[C_{10}H_8O_4S_2]^{2-}$ anion, half of a 2,2'-bipy molecule, and one coordinating water molecule. The $Zn^{2+}$ ion is six-coordinated by two O atoms from two symmetry-related $[C_{10}H_8O_4S_2]^{2-}$ anions (Zn—O 2.1529 (10) Å), two N atoms from one chelating 2,2'-bipy molecule (Zn—N 2.1477 (13) Å), and two water molecules (Zn—O 2.0896 (11) Å) to form a slightly distorted octahedral geometry. The two pyridine rings in the bipy ligand are almost parallel with a dihedral angle of 11.5 (1)°. As shown in Fig. 2, adjacent $Zn^{2+}$ ions are monodentately linked by the $[C_{10}H_8O_4S_2]^{2-}$ anions to form a chain structure running parallel to [101]. The chains are further linked by O—H···O hydrogen bonds to form the final three-dimensional supramolecular architecture (Fig. 3).

## Experimental

A mixture of 1,4-benzenebis(thioacetic acid) (0.103 g, 0.4 mmol), $ZnCl_2.6H_2O$ (0.054 g, 0.4 mmol), 2,2'-bipy (0.031 g, 0.2 mmol), and $Na_2CO_3$ (0.042 g, 0.4 mmol) in $H_2O$ (16 ml)/$C_2H_5OH$ (2 ml) was placed in a 25 ml Teflon-lined stainless steel vessel and heated at 433 K for 72 h, then cooled to room temperature over 3 d. Colourless crystals suitable for X-ray analysis were obtained.

## Refinement

The carbon-bound H-atoms were positioned geometrically and included in the refinement using a riding model [aromatic C—H 0.93Å and aliphatic C—H 0.97 Å, $U_{iso}$(H) = 1.2$U_{eq}$(C)]. The oxygen-bound H-atoms were located in difference Fourier maps and refined with an O—H distance restrained to 0.85 Å and $U_{iso}$(H) = 1.2$U_{eq}$(O).

## Figures

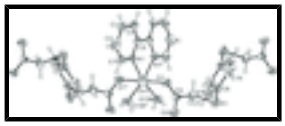

Fig. 1. The molecular structure of (I). Displacement ellipsoids are drawn at the 30% probability level. [Symmetry codes: (i) -*x* + 1,*y*,-*z* + 1/2.]

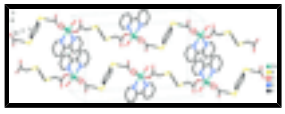

Fig. 2. The chain structure of the title complex. All H atoms have been omitted for clarity.

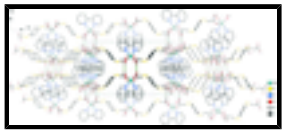

Fig. 3. The three-dimensional supramolecular structure built through O—H···O hydrogen bonds (dashed lines).

## *catena*-Poly[[diaqua(2,2'-bipyridine-κ$^2$*N*,*N*')zinc]- μ-2,2'-[1,4-phenylenebis(sulfanediyl)]diacetato-κ$^2$*O*:*O*']

*Crystal data*

| | |
|---|---|
| $[Zn(C_{10}H_8O_4S_2)(C_{10}H_8N_2)(H_2O)_2]$ | $F(000) = 1056$ |
| $M_r = 513.87$ | $D_x = 1.626$ Mg m$^{-3}$ |
| Monoclinic, *C*2/*c* | Mo *K*α radiation, λ = 0.71073 Å |
| Hall symbol: -C 2yc | Cell parameters from 7952 reflections |
| *a* = 20.4396 (8) Å | θ = 1.9–27.7° |
| *b* = 12.8695 (8) Å | μ = 1.41 mm$^{-1}$ |
| *c* = 7.9798 (4) Å | *T* = 296 K |
| β = 90.765 (3)° | Block, colourless |
| *V* = 2098.88 (19) Å$^3$ | 0.22 × 0.16 × 0.11 mm |
| *Z* = 4 | |

*Data collection*

| | |
|---|---|
| Bruker APEXII CCD diffractometer | 2448 independent reflections |
| Radiation source: fine-focus sealed tube | 2237 reflections with $I > 2\sigma(I)$ |
| graphite | $R_{int} = 0.026$ |
| ω scans | $\theta_{max} = 27.7°$, $\theta_{min} = 1.9°$ |
| Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996) | *h* = −26→26 |
| $T_{min} = 0.761$, $T_{max} = 0.853$ | *k* = −15→16 |
| 16253 measured reflections | *l* = −10→10 |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Primary atom site location: structure-invariant direct methods |
| Least-squares matrix: full | Secondary atom site location: difference Fourier map |
| $R[F^2 > 2\sigma(F^2)] = 0.025$ | Hydrogen site location: inferred from neighbouring sites |

| | |
|---|---|
| $wR(F^2) = 0.070$ | H atoms treated by a mixture of independent and constrained refinement |
| $S = 1.04$ | $w = 1/[\sigma^2(F_o^2) + (0.043P)^2 + 0.7442P]$ where $P = (F_o^2 + 2F_c^2)/3$ |
| 2448 reflections | $(\Delta/\sigma)_{max} = 0.001$ |
| 147 parameters | $\Delta\rho_{max} = 0.31$ e Å$^{-3}$ |
| 3 restraints | $\Delta\rho_{min} = -0.31$ e Å$^{-3}$ |

*Special details*

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

**Refinement**. Refinement of $F^2$ against ALL reflections. The weighted *R*-factor *wR* and goodness of fit *S* are based on $F^2$, conventional *R*-factors *R* are based on *F*, with *F* set to zero for negative $F^2$. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on $F^2$ are statistically about twice as large as those based on *F*, and *R*- factors based on ALL data will be even larger.

*Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å$^2$)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| Zn1 | 0.5000 | 0.725191 (16) | 0.2500 | 0.03569 (9) |
| S1 | 0.676748 (19) | 0.62114 (4) | 0.78141 (5) | 0.04863 (12) |
| N1 | 0.44065 (7) | 0.85617 (9) | 0.31662 (16) | 0.0391 (3) |
| O1W | 0.57320 (6) | 0.61941 (8) | 0.18683 (14) | 0.0435 (3) |
| H1WA | 0.5703 (10) | 0.5693 (13) | 0.123 (2) | 0.052* |
| H1WB | 0.5785 (10) | 0.5933 (15) | 0.2793 (18) | 0.052* |
| O1 | 0.54190 (6) | 0.72445 (7) | 0.49896 (13) | 0.0398 (2) |
| O2 | 0.57240 (6) | 0.55857 (8) | 0.50514 (13) | 0.0446 (3) |
| C1 | 0.38250 (9) | 0.85086 (14) | 0.3913 (2) | 0.0484 (4) |
| H1A | 0.3633 | 0.7861 | 0.4061 | 0.058* |
| C2 | 0.34980 (10) | 0.93842 (17) | 0.4477 (2) | 0.0597 (5) |
| H2A | 0.3089 | 0.9329 | 0.4966 | 0.072* |
| C3 | 0.37950 (11) | 1.03389 (15) | 0.4292 (3) | 0.0618 (5) |
| H3A | 0.3594 | 1.0937 | 0.4688 | 0.074* |
| C4 | 0.43876 (10) | 1.03996 (13) | 0.3523 (2) | 0.0532 (4) |
| H4A | 0.4592 | 1.1040 | 0.3391 | 0.064* |
| C5 | 0.46836 (8) | 0.94978 (11) | 0.29374 (19) | 0.0403 (3) |
| C6 | 0.56711 (6) | 0.64669 (10) | 0.56961 (17) | 0.0319 (3) |
| C7 | 0.59312 (7) | 0.66315 (13) | 0.74760 (18) | 0.0395 (3) |
| H7A | 0.5652 | 0.6258 | 0.8245 | 0.047* |
| H7B | 0.5901 | 0.7365 | 0.7746 | 0.047* |
| C8 | 0.71752 (7) | 0.69346 (13) | 0.6228 (2) | 0.0408 (3) |
| C9 | 0.71738 (8) | 0.65950 (13) | 0.4586 (2) | 0.0479 (4) |
| H9A | 0.6958 | 0.5983 | 0.4300 | 0.057* |
| C10 | 0.75080 (8) | 0.78402 (14) | 0.6640 (2) | 0.0475 (4) |

| | | | | |
|---|---|---|---|---|
| H10A | 0.7518 | 0.8070 | 0.7745 | 0.057* |

*Atomic displacement parameters (Å$^2$)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Zn1 | 0.04999 (16) | 0.02228 (13) | 0.03467 (14) | 0.000 | −0.00485 (10) | 0.000 |
| S1 | 0.0406 (2) | 0.0562 (3) | 0.0490 (2) | 0.00141 (17) | −0.00659 (17) | 0.01881 (18) |
| N1 | 0.0518 (7) | 0.0284 (6) | 0.0367 (6) | 0.0019 (5) | −0.0129 (5) | −0.0020 (5) |
| O1W | 0.0664 (7) | 0.0291 (5) | 0.0349 (5) | 0.0064 (5) | −0.0039 (5) | −0.0045 (4) |
| O1 | 0.0540 (6) | 0.0316 (5) | 0.0336 (5) | 0.0051 (4) | −0.0085 (5) | −0.0008 (4) |
| O2 | 0.0661 (7) | 0.0290 (5) | 0.0385 (5) | 0.0007 (5) | −0.0048 (5) | 0.0043 (4) |
| C1 | 0.0531 (9) | 0.0449 (9) | 0.0468 (9) | 0.0033 (7) | −0.0084 (7) | −0.0017 (7) |
| C2 | 0.0590 (11) | 0.0643 (12) | 0.0555 (11) | 0.0169 (9) | −0.0085 (8) | −0.0076 (9) |
| C3 | 0.0744 (13) | 0.0478 (10) | 0.0626 (11) | 0.0254 (9) | −0.0234 (9) | −0.0171 (8) |
| C4 | 0.0680 (11) | 0.0309 (8) | 0.0600 (10) | 0.0107 (7) | −0.0274 (9) | −0.0082 (7) |
| C5 | 0.0546 (8) | 0.0258 (6) | 0.0398 (7) | 0.0028 (6) | −0.0231 (6) | −0.0023 (5) |
| C6 | 0.0324 (6) | 0.0328 (7) | 0.0304 (6) | −0.0034 (5) | 0.0012 (5) | 0.0042 (5) |
| C7 | 0.0400 (7) | 0.0479 (8) | 0.0307 (7) | 0.0045 (6) | −0.0003 (6) | 0.0028 (6) |
| C8 | 0.0310 (7) | 0.0437 (8) | 0.0475 (8) | 0.0024 (6) | −0.0010 (6) | 0.0051 (7) |
| C9 | 0.0418 (8) | 0.0454 (9) | 0.0564 (10) | −0.0066 (7) | 0.0025 (7) | −0.0064 (7) |
| C10 | 0.0420 (8) | 0.0553 (10) | 0.0452 (9) | −0.0039 (7) | 0.0003 (7) | −0.0075 (7) |

*Geometric parameters (Å, °)*

| | | | |
|---|---|---|---|
| Zn1—O1W$^{i}$ | 2.0896 (11) | C2—C3 | 1.379 (3) |
| Zn1—O1W | 2.0896 (11) | C2—H2A | 0.9300 |
| Zn1—N1$^{i}$ | 2.1477 (13) | C3—C4 | 1.367 (3) |
| Zn1—N1 | 2.1477 (13) | C3—H3A | 0.9300 |
| Zn1—O1$^{i}$ | 2.1529 (10) | C4—C5 | 1.392 (2) |
| Zn1—O1 | 2.1529 (10) | C4—H4A | 0.9300 |
| S1—C8 | 1.7861 (16) | C5—C5$^{i}$ | 1.478 (4) |
| S1—C7 | 1.8095 (15) | C6—C7 | 1.5247 (19) |
| N1—C1 | 1.339 (2) | C7—H7A | 0.9700 |
| N1—C5 | 1.3447 (19) | C7—H7B | 0.9700 |
| O1W—H1WA | 0.825 (14) | C8—C9 | 1.382 (2) |
| O1W—H1WB | 0.817 (14) | C8—C10 | 1.387 (2) |
| O1—C6 | 1.2557 (16) | C9—C10$^{ii}$ | 1.388 (2) |
| O2—C6 | 1.2506 (17) | C9—H9A | 0.9300 |
| C1—C2 | 1.388 (3) | C10—C9$^{ii}$ | 1.388 (2) |
| C1—H1A | 0.9300 | C10—H10A | 0.9300 |
| O1W$^{i}$—Zn1—O1W | 98.69 (7) | C1—C2—H2A | 120.8 |
| O1W$^{i}$—Zn1—N1$^{i}$ | 168.43 (5) | C4—C3—C2 | 119.51 (17) |
| O1W—Zn1—N1$^{i}$ | 92.47 (5) | C4—C3—H3A | 120.2 |
| O1W$^{i}$—Zn1—N1 | 92.47 (5) | C2—C3—H3A | 120.2 |
| O1W—Zn1—N1 | 168.43 (5) | C3—C4—C5 | 119.63 (17) |
| N1$^{i}$—Zn1—N1 | 76.59 (7) | C3—C4—H4A | 120.2 |

| | | | |
|---|---|---|---|
| O1W$^{i}$—Zn1—O1$^{i}$ | 86.70 (4) | C5—C4—H4A | 120.2 |
| O1W—Zn1—O1$^{i}$ | 92.97 (4) | N1—C5—C4 | 121.03 (16) |
| N1$^{i}$—Zn1—O1$^{i}$ | 89.66 (4) | N1—C5—C5$^{i}$ | 115.91 (9) |
| N1—Zn1—O1$^{i}$ | 90.74 (4) | C4—C5—C5$^{i}$ | 123.05 (11) |
| O1W$^{i}$—Zn1—O1 | 92.97 (4) | O2—C6—O1 | 125.11 (13) |
| O1W—Zn1—O1 | 86.70 (4) | O2—C6—C7 | 118.57 (12) |
| N1$^{i}$—Zn1—O1 | 90.74 (4) | O1—C6—C7 | 116.32 (12) |
| N1—Zn1—O1 | 89.66 (4) | C6—C7—S1 | 114.48 (10) |
| O1$^{i}$—Zn1—O1 | 179.49 (5) | C6—C7—H7A | 108.6 |
| C8—S1—C7 | 100.80 (7) | S1—C7—H7A | 108.6 |
| C1—N1—C5 | 118.97 (14) | C6—C7—H7B | 108.6 |
| C1—N1—Zn1 | 125.31 (11) | S1—C7—H7B | 108.6 |
| C5—N1—Zn1 | 115.42 (11) | H7A—C7—H7B | 107.6 |
| Zn1—O1W—H1WA | 127.8 (14) | C9—C8—C10 | 119.04 (15) |
| Zn1—O1W—H1WB | 97.9 (14) | C9—C8—S1 | 120.80 (13) |
| H1WA—O1W—H1WB | 104.3 (17) | C10—C8—S1 | 120.15 (13) |
| C6—O1—Zn1 | 125.00 (9) | C8—C9—C10$^{ii}$ | 120.52 (16) |
| N1—C1—C2 | 122.49 (17) | C8—C9—H9A | 119.7 |
| N1—C1—H1A | 118.8 | C10$^{ii}$—C9—H9A | 119.7 |
| C2—C1—H1A | 118.8 | C8—C10—C9$^{ii}$ | 120.43 (16) |
| C3—C2—C1 | 118.3 (2) | C8—C10—H10A | 119.8 |
| C3—C2—H2A | 120.8 | C9$^{ii}$—C10—H10A | 119.8 |
| O1W$^{i}$—Zn1—N1—C1 | 7.41 (13) | C2—C3—C4—C5 | 0.0 (3) |
| O1W—Zn1—N1—C1 | −157.1 (2) | C1—N1—C5—C4 | 2.5 (2) |
| N1$^{i}$—Zn1—N1—C1 | −176.39 (15) | Zn1—N1—C5—C4 | −171.45 (11) |
| O1$^{i}$—Zn1—N1—C1 | 94.13 (13) | C1—N1—C5—C5$^{i}$ | −178.37 (15) |
| O1—Zn1—N1—C1 | −85.55 (13) | Zn1—N1—C5—C5$^{i}$ | 7.63 (19) |
| O1W$^{i}$—Zn1—N1—C5 | −179.03 (10) | C3—C4—C5—N1 | −2.3 (2) |
| O1W—Zn1—N1—C5 | 16.4 (3) | C3—C4—C5—C5$^{i}$ | 178.72 (18) |
| N1$^{i}$—Zn1—N1—C5 | −2.82 (7) | Zn1—O1—C6—O2 | 1.0 (2) |
| O1$^{i}$—Zn1—N1—C5 | −92.30 (10) | Zn1—O1—C6—C7 | −179.21 (9) |
| O1—Zn1—N1—C5 | 88.01 (10) | O2—C6—C7—S1 | 51.79 (17) |
| O1W$^{i}$—Zn1—O1—C6 | 63.39 (12) | O1—C6—C7—S1 | −128.01 (12) |
| O1W—Zn1—O1—C6 | −35.15 (12) | C8—S1—C7—C6 | 55.61 (13) |
| N1$^{i}$—Zn1—O1—C6 | −127.58 (12) | C7—S1—C8—C9 | −80.93 (14) |
| N1—Zn1—O1—C6 | 155.84 (12) | C7—S1—C8—C10 | 100.14 (14) |
| O1$^{i}$—Zn1—O1—C6 | 14.13 (13) | C10—C8—C9—C10$^{ii}$ | −1.0 (3) |
| C5—N1—C1—C2 | −0.6 (2) | S1—C8—C9—C10$^{ii}$ | −179.94 (13) |
| Zn1—N1—C1—C2 | 172.80 (13) | C9—C8—C10—C9$^{ii}$ | 1.0 (3) |
| N1—C1—C2—C3 | −1.7 (3) | S1—C8—C10—C9$^{ii}$ | 179.95 (13) |
| C1—C2—C3—C4 | 1.9 (3) | | |

Symmetry codes: (i) −*x*+1, *y*, −*z*+1/2; (ii) −*x*+3/2, −*y*+3/2, −*z*+1.

*Hydrogen-bond geometry (Å, °)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| O1W—H1WA···O2$^{iii}$ | 0.83 (1) | 1.90 (2) | 2.7107 (15) | 170.(2) |
| O1W—H1WB···O2 | 0.82 (1) | 1.86 (2) | 2.6582 (16) | 164 (2) |

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

**Fig. 1**

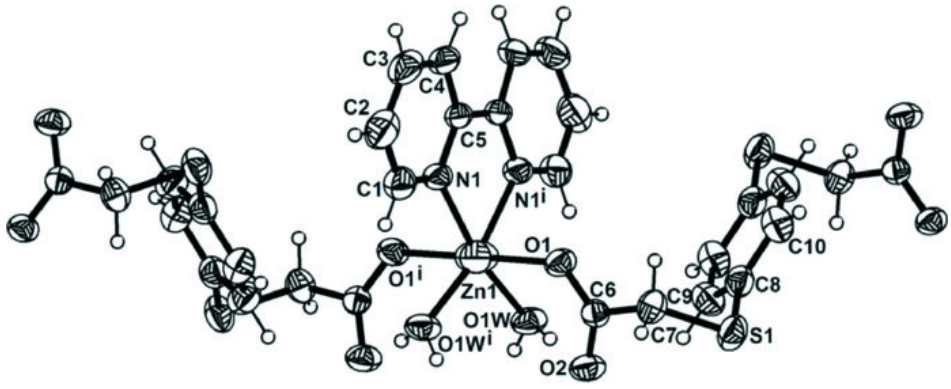

**Fig. 2**

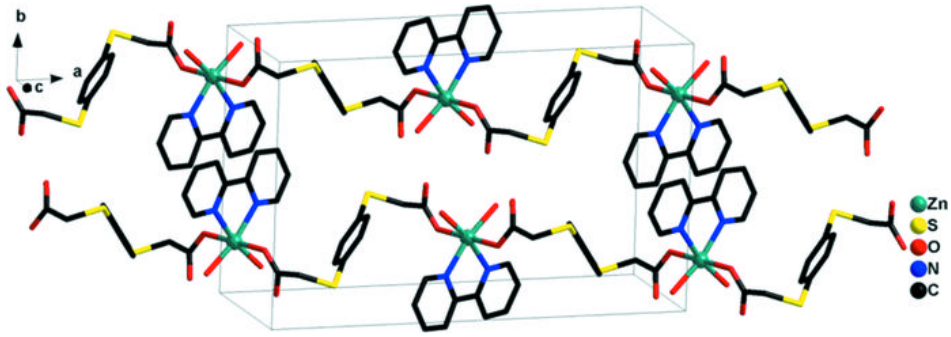

**Fig. 3**