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catena-Poly[[diaquabis[(4-nitrophenylsulfinyl)acetato-κO]zinc(II)]-μ-4,4′-bipyridine-$\kappa^2 N{:}N'$]

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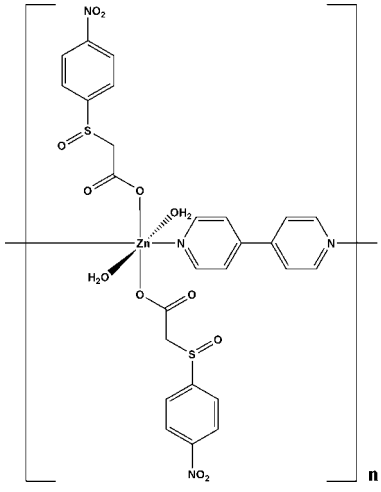
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.006 Å; R factor = 0.029; wR factor = 0.077; data-to-parameter ratio = 16.2.

In the title coordination polymer, $[Zn(C_8H_6NO_5S)_2(C_{10}H_8N_2)(H_2O)_2]_n$, each Zn^{II} ion is in a slightly distorted octahedral coordination environment, formed by two carboxylate O atoms from two (4-nitrophenylsulfinyl)acetate ligands, two N atoms from bipyridine ligands and two water molecules. The Zn^{II} ions and the bipryidine ligands lie on crystallographic twofold axes with the Zn^{II} ions linked by bipyridine ligands into a one-dimensional chain structure. In the crystal structure, intermolecular O—H···O hydrogen bonds link one-dimensional chains into a three-dimensional network.

Related literature

For synthetic background, see: Ghosh *et al.* (2005), and for previously published structures related to the topic, see: Glidewell *et al.* (2002, 2003). For preparation details, see: Nobles & Thompson (1965).



Experimental

Crystal data

$[Zn(C_8H_6NO_5S)_2(C_{10}H_8N_2)(H_2O)_2]$
M_r = 713.98
Orthorhombic, *Fdd*2
a = 20.079 (4) Å
b = 25.646 (5) Å
c = 11.485 (2) Å
V = 5914 (2) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 1.04 mm^{-1}
T = 293 (2) K
0.28 × 0.23 × 0.20 mm

Data collection

Rigaku RAXIS-RAPID diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.761, T_{max} = 0.822
14073 measured reflections
3335 independent reflections
3138 reflections with $I > 2\sigma(I)$
R_{int} = 0.027

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.029
$wR(F^2)$ = 0.077
S = 1.07
3335 reflections
206 parameters
13 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.55 e Å^{-3}
$\Delta\rho_{min}$ = −0.32 e Å^{-3}
Absolute structure: Flack (1983)
Flack parameter: 0.022 (14)

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O6—H12···O1^{i}	0.85	1.88	2.731 (4)	176
O6—H11···O2^{ii}	0.85	1.83	2.655 (4)	162

Symmetry codes: (i) $x+\frac{1}{4}, -y+\frac{7}{4}, z-\frac{1}{4}$; (ii) $-x, -y+2, z$.

Data collection: *RAPID-AUTO* (Rigaku, 1998); cell refinement: *RAPID-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LH2371).

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supplementary materials

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catena-Poly[[diaquabis[(4-nitrophenylsulfinyl)acetato-κO]zinc(II)]-μ-4,4'-bipyridine-$\kappa^2 N$:N']

Y.-J. Hou, Y.-H. Yu, Z.-Z. Sun, B.-Y. Li and G.-F. Hou

Comment

4,4'-Bipyridine and organic aromatic carboxylic acid ligands are often used in syntheses to bridge metal atoms and these compound can demonstrate fascinating network topologies and potential application in the field of host–guest chemistry, ion exchange and catalysis (Ghosh *et al.*, 2005). Simple carboxylic acids containing the 4-nitrophenyl group exhibit a variety of supramolecular aggregation patterns (Glidewell *et al.*, 2002). Recently, our attention has been focused on 4-nitrophenyl-sulfinyl acetic acid, whose crystal structure has been reported previously (Glidewell *et al.*, 2003).

Complex(I) consists of linear chains formed through 4,4'-bipy ligands linking six-coordinate Zn^{II} ions (Fig. 1). The ZnII ion has slightly distorted octahedral geometry. Two N donors of two 4,4'-bipy ligands and two coordinated water molecules lie in the equatorial plane, while two O-atom donors of two (4-nitrophenylsulfinyl)acetate ligands are in the axial positions.

These one-dimensional chains are connected into a three dimensional network *via* intermolecular O—H···O hydrogen bonds(Table 1),(Fig. 2).

Experimental

(4-Nitrophenylsulfanyl)acetic acid was prepared by a nucleophilic reaction of chloroacetic acid and 4-nitrothiophenol under basic conditions. (4-nitrophenylsulfanyl)acetic acid was then oxidized using 30% aqueous hydrogen peroxide in acetic anhydride solution, producing 4-nitrophenylsulfinyl acetic acid (Nobles & Thompson, 1965). Zinc nitrate hexahydrate (0.586 g, 2 mmol) and (4-nitrophenylsulfinyl)acetic acid (0.458 g, 2 mmol) and 4,4'-bipyridine (0.312 g, 2 mmol) were dissolved in water and the pH was adjusted to 6 with 0.01*M* sodium hydroxide, colorless crystals separated from the filtered solution after several days.

Refinement

H atoms bound to C atoms were placed in calculated positions and treated as riding on their parent atoms, withwith C—H = 0.93 Å (aromatic C) or C—H = 0.97 Å (methylene C), and with U_{iso}(H) = 1.2Ueq(C). Water H atoms were initially located in a difference Fourier map but they were treated as riding on their parent atoms with O—H = 0.85 Å and with U_{iso}(H) = 1.5Ueq(O).

Figures

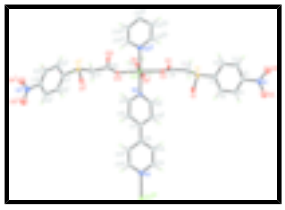

Fig. 1. Part of the polymeric structure of the title complex, with the atomlabelling scheme. Displacement ellipsoids are drawn at the 30% probability level and H atoms are represented as spheres of arbitrary radii. [Symmetry codes: (I) −*x*, −*y* + 2, *z*; (II) *x*, *y*,*z* − 1; (III)-*x*, −*y* + 2, *z* − 1, (IV) *x*, *y*, *z* + 1].

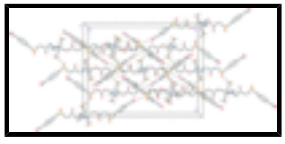

Fig. 2. A partial packing plot of (I). Dashed lines indicate the donor to acceptor non-bonded contacts invloved in hydrogen bonding. H atoms have been omitted.

catena-Poly[[diaquabis[(4-nitrophenylsulfinyl)acetato-κ*O*]zinc(II)]- μ-4,4'-bipyridine-κ^2*N*:*N*']

Crystal data

$[Zn(C_8H_6NO_5S)_2(C_{10}H_8N_2)(H_2O)_2]$	F_{000} = 2928
M_r = 713.98	D_x = 1.604 Mg m^{-3}
Orthorhombic, *Fdd*2	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: F 2 -2d	Cell parameters from 12942 reflections
a = 20.079 (4) Å	θ = 6.3–54.9º
b = 25.646 (5) Å	μ = 1.04 mm^{-1}
c = 11.485 (2) Å	*T* = 293 (2) K
V = 5914 (2) Å^3	Block, colourless
Z = 8	0.28 × 0.23 × 0.20 mm

Data collection

Rigaku RAXIS-RAPID diffractometer	3335 independent reflections
Radiation source: fine-focus sealed tube	3138 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.027
T = 293(2) K	θ_{max} = 27.4º
ω scans	θ_{min} = 3.1º
Absorption correction: multi-scan (ABSCOR; Higashi, 1995)	*h* = −26→26
T_{min} = 0.761, T_{max} = 0.822	*k* = −33→33
14073 measured reflections	*l* = −14→14

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)]$ = 0.029	$w = 1/[\sigma^2(F_o^2) + (0.047P)^2 + 4.1913P]$

	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.077$	$(\Delta/\sigma)_{max} = 0.005$
$S = 1.07$	$\Delta\rho_{max} = 0.55$ e Å^{-3}
3335 reflections	$\Delta\rho_{min} = -0.31$ e Å^{-3}
206 parameters	Extinction correction: none
13 restraints	Absolute structure: Flack (1983)
Primary atom site location: structure-invariant direct methods	Flack parameter: 0.022 (14)
Secondary atom site location: difference Fourier map	

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}
C1	0.02856 (17)	0.72739 (13)	0.5181 (3)	0.0284 (7)
C2	0.0666 (2)	0.70549 (15)	0.4295 (3)	0.0362 (8)
H1	0.0647	0.7189	0.3544	0.043*
C3	0.10728 (19)	0.66355 (14)	0.4545 (3)	0.0374 (9)
H2	0.1334	0.6484	0.3969	0.045*
C4	0.1084 (2)	0.64463 (14)	0.5672 (3)	0.0338 (8)
C5	0.0714 (2)	0.66611 (15)	0.6570 (3)	0.0398 (9)
H3	0.0733	0.6524	0.7319	0.048*
C6	0.0315 (2)	0.70887 (15)	0.6312 (3)	0.0364 (8)
H4	0.0069	0.7250	0.6897	0.044*
C7	0.03217 (17)	0.83002 (12)	0.4745 (4)	0.0310 (7)
H5	0.0590	0.8310	0.5448	0.037*
H6	0.0614	0.8232	0.4091	0.037*
C8	−0.00307 (18)	0.88235 (12)	0.4576 (3)	0.0280 (7)
C9	0.0212 (2)	1.04111 (14)	0.7267 (4)	0.0370 (8)
H7	0.0369	1.0699	0.6860	0.044*
C10	0.0210 (2)	1.04293 (17)	0.8483 (4)	0.0414 (9)
H8	0.0349	1.0729	0.8869	0.050*
C11	0.0000	1.0000	0.9105 (5)	0.0300 (13)
C12	0.0000	1.0000	1.0404 (5)	0.0359 (14)
C13	0.0321 (2)	0.96088 (16)	1.1036 (4)	0.0383 (9)
H9	0.0536	0.9338	1.0650	0.046*
C14	0.03179 (19)	0.96264 (14)	1.2234 (4)	0.0355 (8)

H10	0.0545	0.9369	1.2643	0.043*
N1	0.1489 (2)	0.59871 (17)	0.5925 (4)	0.0506 (9)
N2	0.0000	1.0000	0.6666 (4)	0.0264 (10)
N3	0.0000	1.0000	1.2837 (4)	0.0308 (11)
O1	−0.06561 (15)	0.78963 (11)	0.5975 (3)	0.0472 (7)
O2	−0.06099 (15)	0.88136 (10)	0.4182 (3)	0.0446 (7)
O3	0.03031 (12)	0.92181 (8)	0.4850 (2)	0.0302 (5)
O4	0.1760 (2)	0.57580 (17)	0.5154 (4)	0.0837 (12)
O5	0.1539 (2)	0.58524 (18)	0.6938 (4)	0.0845 (12)
O6	0.10205 (11)	1.02344 (9)	0.4739 (2)	0.0324 (5)
H12	0.1267	1.0044	0.4314	0.049*
H11	0.0976	1.0551	0.4537	0.049*
S2	−0.02931 (4)	0.77903 (3)	0.48577 (9)	0.0311 (2)
Zn1	0.0000	1.0000	0.47672 (3)	0.02310 (14)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0334 (17)	0.0190 (14)	0.0327 (19)	−0.0014 (12)	0.0014 (15)	0.0027 (13)
C2	0.046 (2)	0.0311 (17)	0.0318 (18)	0.0040 (16)	0.0073 (17)	0.0063 (15)
C3	0.0390 (19)	0.0333 (18)	0.040 (2)	0.0061 (15)	0.0095 (16)	−0.0009 (15)
C4	0.0373 (18)	0.0277 (17)	0.0365 (19)	0.0073 (15)	−0.0023 (16)	0.0044 (15)
C5	0.048 (2)	0.039 (2)	0.0323 (19)	0.0122 (18)	0.0004 (17)	0.0072 (16)
C6	0.043 (2)	0.0346 (19)	0.032 (2)	0.0091 (16)	0.0062 (16)	0.0000 (15)
C7	0.0333 (16)	0.0209 (14)	0.0387 (17)	−0.0012 (12)	0.0007 (16)	−0.0004 (15)
C8	0.0412 (17)	0.0217 (14)	0.021 (2)	0.0032 (14)	0.0011 (14)	−0.0002 (12)
C9	0.056 (2)	0.0340 (18)	0.0209 (16)	−0.0072 (17)	−0.0033 (18)	0.0036 (15)
C10	0.065 (3)	0.037 (2)	0.0219 (19)	−0.010 (2)	−0.0070 (18)	−0.0022 (16)
C11	0.034 (3)	0.039 (3)	0.017 (3)	0.000 (2)	0.000	0.000
C12	0.046 (4)	0.041 (4)	0.020 (3)	−0.004 (2)	0.000	0.000
C13	0.052 (2)	0.039 (2)	0.0238 (18)	0.0089 (17)	0.0028 (17)	−0.0022 (16)
C14	0.0454 (19)	0.0375 (18)	0.0236 (17)	0.0085 (15)	0.0011 (18)	0.0042 (15)
N1	0.058 (2)	0.048 (2)	0.046 (2)	0.0266 (18)	0.0021 (18)	0.0042 (17)
N2	0.035 (3)	0.027 (2)	0.017 (2)	0.0019 (16)	0.000	0.000
N3	0.038 (3)	0.035 (3)	0.019 (2)	−0.0026 (17)	0.000	0.000
O1	0.0427 (15)	0.0356 (15)	0.063 (2)	0.0060 (12)	0.0208 (15)	0.0064 (14)
O2	0.0513 (15)	0.0249 (12)	0.0578 (17)	0.0043 (11)	−0.0216 (14)	−0.0069 (12)
O3	0.0410 (12)	0.0197 (9)	0.0299 (12)	0.0006 (9)	−0.0014 (12)	−0.0005 (10)
O4	0.0909 (16)	0.0800 (16)	0.0802 (17)	0.0424 (12)	0.0035 (13)	−0.0019 (12)
O5	0.0888 (16)	0.0848 (16)	0.0797 (17)	0.0400 (12)	0.0001 (13)	0.0060 (13)
O6	0.0356 (12)	0.0293 (11)	0.0323 (12)	0.0041 (9)	0.0041 (12)	0.0017 (11)
S2	0.0310 (4)	0.0203 (3)	0.0418 (5)	−0.0003 (3)	−0.0009 (4)	0.0015 (4)
Zn1	0.0327 (3)	0.0192 (2)	0.0174 (2)	−0.0002 (2)	0.000	0.000

Geometric parameters (Å, °)

C1—C6	1.384 (5)	C11—C10^{i}	1.379 (5)
C1—C2	1.391 (5)	C11—C12	1.492 (6)

C1—S2	1.801 (3)	C12—C13^{i}	1.396 (5)
C2—C3	1.381 (5)	C12—C13	1.396 (5)
C2—H1	0.9300	C13—C14	1.377 (6)
C3—C4	1.383 (5)	C13—H9	0.9300
C3—H2	0.9300	C14—N3	1.343 (5)
C4—C5	1.384 (6)	C14—H10	0.9300
C4—N1	1.460 (5)	N1—O4	1.194 (6)
C5—C6	1.390 (5)	N1—O5	1.217 (6)
C5—H3	0.9300	N2—C9^{i}	1.330 (4)
C6—H4	0.9300	N2—Zn1	2.181 (4)
C7—C8	1.530 (4)	N3—C14^{i}	1.343 (5)
C7—S2	1.803 (3)	N3—Zn1^{ii}	2.217 (5)
C7—H5	0.9700	O1—S2	1.500 (3)
C7—H6	0.9700	O3—Zn1	2.098 (2)
C8—O2	1.248 (5)	O6—Zn1	2.136 (2)
C8—O3	1.254 (4)	O6—H12	0.8500
C9—N2	1.330 (4)	O6—H11	0.8501
C9—C10	1.397 (6)	Zn1—O3^{i}	2.098 (2)
C9—H7	0.9300	Zn1—O6^{i}	2.136 (2)
C10—C11	1.379 (5)	Zn1—N3^{iii}	2.217 (5)
C10—H8	0.9300		
C6—C1—C2	121.6 (3)	C13—C12—C11	121.3 (3)
C6—C1—S2	118.3 (3)	C14—C13—C12	119.6 (4)
C2—C1—S2	120.0 (3)	C14—C13—H9	120.2
C3—C2—C1	119.2 (4)	C12—C13—H9	120.2
C3—C2—H1	120.4	N3—C14—C13	122.7 (4)
C1—C2—H1	120.4	N3—C14—H10	118.6
C2—C3—C4	118.5 (3)	C13—C14—H10	118.6
C2—C3—H2	120.7	O4—N1—O5	122.0 (4)
C4—C3—H2	120.7	O4—N1—C4	120.3 (4)
C3—C4—C5	123.3 (3)	O5—N1—C4	117.7 (4)
C3—C4—N1	118.5 (4)	C9—N2—C9^{i}	117.5 (5)
C5—C4—N1	118.1 (3)	C9—N2—Zn1	121.3 (2)
C4—C5—C6	117.7 (3)	C9^{i}—N2—Zn1	121.3 (2)
C4—C5—H3	121.1	C14—N3—C14^{i}	117.9 (5)
C6—C5—H3	121.1	C14—N3—Zn1^{ii}	121.0 (3)
C1—C6—C5	119.6 (4)	C14^{i}—N3—Zn1^{ii}	121.0 (3)
C1—C6—H4	120.2	C8—O3—Zn1	127.2 (2)
C5—C6—H4	120.2	Zn1—O6—H12	113.9
C8—C7—S2	109.2 (2)	Zn1—O6—H11	100.0
C8—C7—H5	109.8	H12—O6—H11	117.0
S2—C7—H5	109.8	O1—S2—C1	105.68 (17)
C8—C7—H6	109.8	O1—S2—C7	105.22 (18)
S2—C7—H6	109.8	C1—S2—C7	96.11 (15)
H5—C7—H6	108.3	O3—Zn1—O3^{i}	174.79 (15)
O2—C8—O3	127.3 (3)	O3—Zn1—O6^{i}	90.57 (9)

O2—C8—C7	117.3 (3)	$O3^{i}$—Zn1—$O6^{i}$	89.50 (9)
O3—C8—C7	115.4 (3)	O3—Zn1—O6	89.50 (9)
N2—C9—C10	122.9 (4)	$O3^{i}$—Zn1—O6	90.57 (9)
N2—C9—H7	118.5	$O6^{i}$—Zn1—O6	178.29 (15)
C10—C9—H7	118.5	O3—Zn1—N2	87.39 (7)
C11—C10—C9	119.5 (4)	$O3^{i}$—Zn1—N2	87.39 (7)
C11—C10—H8	120.3	$O6^{i}$—Zn1—N2	90.86 (7)
C9—C10—H8	120.3	O6—Zn1—N2	90.86 (7)
$C10^{i}$—C11—C10	117.6 (5)	O3—Zn1—$N3^{iii}$	92.61 (7)
$C10^{i}$—C11—C12	121.2 (3)	$O3^{i}$—Zn1—$N3^{iii}$	92.61 (7)
C10—C11—C12	121.2 (3)	$O6^{i}$—Zn1—$N3^{iii}$	89.14 (7)
$C13^{i}$—C12—C13	117.4 (5)	O6—Zn1—$N3^{iii}$	89.14 (7)
$C13^{i}$—C12—C11	121.3 (3)	N2—Zn1—$N3^{iii}$	180.000 (3)

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

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O6—H12···$O1^{iv}$	0.85	1.88	2.731 (4)	176
O6—H11···$O2^{i}$	0.85	1.83	2.655 (4)	162

Symmetry codes: (iv) *x*+1/4, −*y*+7/4, *z*−1/4; (i) −*x*, −*y*+2, *z*.

Fig. 1

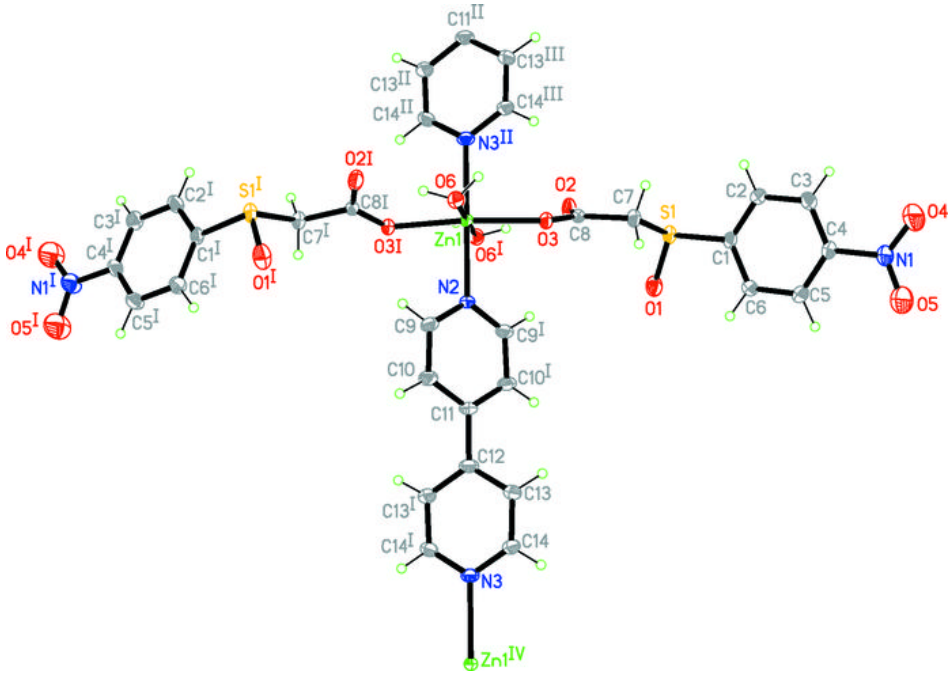
C11II
C13III
C13II
C14III
C14II
N3II
O2I
O6
O2
C7
S1
C2
C3
O4
S1I
C2I
C8I
C3I
C4
N1
C4I
C1I
C7I
O3I
Zn1
O6I
O3
C8
C1
O4I
N1I
O1I
O1
C6I
C5
O5
O5I
C5I
N2
C9
C9I
C10
C10I
C11
C12
C13
C13I
C14
C14I
N3
Zn1IV

Fig. 2