Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

catena-Poly[[bis(1-vinylimidazole-κN^3)-zinc(II)]-μ-phthalato-$\kappa^2O^1:O^2$]

Rong-Xun Li,[a,b] Shao-Xiang Li,[b] Qi-Ye Wu,[c] Guang-Ye Liu[b] and Fa-Qian Liu[b]*

[a]School of Materials Science and Engineering, University of Science and Technology Beijing, Beijing 100083, People's Republic of China, [b]Key Laboratory of Advanced Materials, Qingdao University of Science and Technology, Qingdao 266042, People's Republic of China, and [c]School of Polymer Science and Engineering, Qingdao University of Science and Technology, Qingdao 266042, People's Republic of China
Correspondence e-mail: qdplastics@163.com

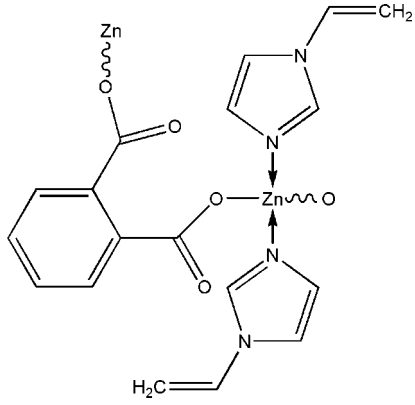
Received 25 October 2007; accepted 26 October 2007

Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.012 Å; R factor = 0.045; wR factor = 0.139; data-to-parameter ratio = 19.4.

The title compound, $[Zn(C_8H_4O_4)(C_5H_6N_2)_2]_n$, in the solid state comprises polymeric zigzag chains extending along the c axis. Each Zn^{II} ion is coordinated by two N [Zn—N = 1.991 (6) and 2.031 (5) Å] and two O [Zn—O = 1.912 (5) and 1.965 (5) Å] atoms in a distorted tetrahedral geometry. Weak C—H···O interactions contribute to the crystal packing stability.

Related literature

In the corresponding compound [Zn(phthalato)(1-*H*-imidazole)$_2$] the Zn^{II} ions also have a distorted tetrahedral environment (Liu *et al.*, 2002).



Experimental

Crystal data

$[Zn(C_8H_4O_4)(C_5H_6N_2)_2]$
M_r = 417.72
Monoclinic, $P2_1/c$
a = 8.4110 (17) Å
b = 16.329 (3) Å
c = 14.083 (3) Å
β = 100.87 (3)°
V = 1899.5 (7) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.32 mm^{-1}
T = 293 (2) K
0.40 × 0.10 × 0.10 mm

Data collection

Bruker SMART 1K CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2004)
T_{min} = 0.620, T_{max} = 0.879
3729 measured reflections
3678 independent reflections
2090 reflections with $I > 2\sigma(I)$
R_{int} = 0.015

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.139
S = 1.08
3678 reflections
190 parameters
133 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 1.02 e Å^{-3}
$\Delta\rho_{min}$ = −1.09 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C9—H9A···O1	0.93	2.51	3.435 (10)	170
C14—H14A···O4^{i}	0.93	2.25	3.166 (8)	167
C18—H18A···O4^{i}	0.93	2.49	3.405 (11)	169

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

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2001); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL* and local programs.

This work was supported by the Natural Science Foundation of Shandong Province (grant No. Y2006B12).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CV2329).

References

Bruker (2001). *SMART* (Version 5.628) and *SAINT* (Version 6.45). Bruker AXS Inc., Madison, Wisconsin, USA.
Liu, Q. Y., Liu, P., Wang, J. & Chen, Y. (2002). *Chin. J. Struct. Chem.* **21**, 509–512.
Sheldrick, G. M. (2001). *SHELXTL*. Version 5.0. Bruker AXS Inc., Madison, Wisconsin, USA.
Sheldrick, G. M. (2004). *SADABS*. University of Göttingen, Germany.

  doi:10.1107/S160053680705355X

supplementary materials

Acta Cryst. (2007). E**63**, m2874 [**doi:10.1107/S160053680705355X**]

catena-Poly[[bis(1-vinylimidazole-κN^3)zinc(II)]-μ-phthalato-$\kappa^2O^1:O^2$\]

R.-X. Li, S.-X. Li, Q.-Y. Wu, G.-Y. Liu and F.-Q. Liu

Comment

In the title compound, (I) (Fig. 1), the zinc(II) centers are bridged by the carboxylate group of *o*-phthalate and saturated by 1-vinylimidazole. Each Zn^{II} ion is coordinated by two N [Zn—N1 = 1.993 (3) Å, Zn—N3 = 2.031 (5) Å] and two O [Zn—O2 = 1.912 (5) Å, Zn—O3 = 1.965 (5) Å] atoms in a distorted tetrahedral geometry. All these values agree well with those observed in [Zn(phthalato)(1-*H*-imidazole)$_2$] (Liu *et al.*, 2002), where Zn^{II} ions also have a distorted tetrahedral environment. Each *o*-phthalate in (I) dianion acts as a bidentate ligand to bridge two Zn^{II} ions through the two monodentate carboxylate groups, building a zigzag infinate chain structure along the *c* axis. The metal-metal distances across each polymer backbone are 7.1397 (18) Å.

In the crystal, weak C—H···O interactions (Table 1) contribute to the crystal packing stability.

Experimental

The reaction of $ZnCl_2$ (0.68 g, 5 mmol) with *o*-phthalic acid (0.83 g, 5 mmol) in an aqueous-alcohol (3:1) solution (40 ml) at 363 K for 30 minutes produced a blue solution, to which 1-vinylimidazole (0.94 g, 10 mmol) was added. The reaction solution was kept at room temperature after stirring for an hour at 333 K. Colourless crystals were obtained after a few days.

Refinement

All H atoms were positioned geometrically (C—H 0.93 Å) and allowed to ride on their parent atoms with U_{iso}(H) = 1.2 U_{eq}(C).

Figures

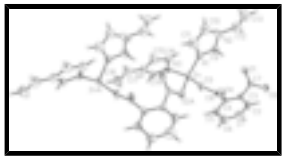


Fig. 1. A portion of the polymeric chain in the title compound showing the atomic numbering and 30% probability displacement ellipsoids [symmetry code: (A) *x*,-*y* + 1/2,*z* + 1/2].

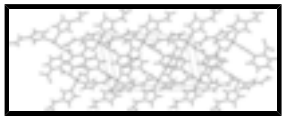


Fig. 2. The packing of (I), viewed down the *b* axis.

catena-Poly[[bis(1-vinylimidazole-κN^3)zinc(II)]-μ-phthalato-κ$^2O^1$:O^2]

Crystal data

$[Zn(C_8H_4O_4)(C_5H_6N_2)_2]$	F_{000} = 856
M_r = 417.72	D_x = 1.461 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 3025 reflections
a = 8.4110 (17) Å	θ = 2.5–25.1º
b = 16.329 (3) Å	μ = 1.32 mm^{-1}
c = 14.083 (3) Å	T = 293 (2) K
β = 100.87 (3)º	Block, colourless
V = 1899.5 (7) Å^3	0.40 × 0.10 × 0.10 mm
Z = 4	

Data collection

Bruker SMART 1K CCD area-detector diffractometer	3678 independent reflections
Radiation source: fine-focus sealed tube	2090 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.015
T = 293(2) K	θ_{max} = 26.0º
thin–slice ω scans	θ_{min} = 1.9º
Absorption correction: multi-scan (SADABS; Sheldrick, 2004)	h = −10→10
T_{min} = 0.620, T_{max} = 0.879	k = 0→20
3729 measured reflections	l = 0→17

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.045	H-atom parameters constrained
$wR(F^2)$ = 0.139	$w = 1/[\sigma^2(F_o^2) + (0.1041P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.08	$(\Delta/\sigma)_{max} < 0.001$
3678 reflections	$\Delta\rho_{max}$ = 1.03 e Å^{-3}
190 parameters	$\Delta\rho_{min}$ = −1.09 e Å^{-3}
133 restraints	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

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}
Zn	0.11543 (10)	0.21386 (5)	0.54220 (5)	0.0456 (3)
O1	0.0879 (6)	0.1714 (3)	0.2024 (3)	0.0524 (12)
O2	0.2671 (6)	0.2117 (3)	0.1147 (3)	0.0608 (14)
O3	0.2286 (6)	0.1414 (3)	0.4655 (3)	0.0570 (14)
O4	0.2799 (7)	0.2508 (3)	0.3833 (3)	0.0567 (14)
N1	−0.0828 (8)	0.2607 (4)	0.4605 (4)	0.0562 (16)
N2	−0.2745 (10)	0.2885 (5)	0.3388 (6)	0.087 (2)
N3	0.0464 (7)	0.1306 (3)	0.6335 (4)	0.0459 (13)
N4	0.0425 (8)	0.0561 (4)	0.7615 (5)	0.059
C1	0.5666 (14)	0.0239 (7)	0.2496 (8)	0.105
H1A	0.6262	−0.0093	0.2156	0.125*
C2	0.4515 (10)	0.0729 (5)	0.1993 (6)	0.068 (2)
H2A	0.4353	0.0730	0.1322	0.082*
C3	0.3591 (8)	0.1219 (4)	0.2441 (4)	0.0469 (16)
C4	0.3852 (8)	0.1234 (4)	0.3456 (5)	0.0452 (16)
C5	0.5051 (10)	0.0725 (5)	0.3981 (6)	0.064 (2)
H5A	0.5227	0.0727	0.4653	0.077*
C6	0.5999 (12)	0.0208 (6)	0.3497 (7)	0.087 (3)
H6A	0.6798	−0.0132	0.3834	0.104*
C7	0.2259 (8)	0.1715 (4)	0.1859 (4)	0.0422 (16)
C8	0.2909 (8)	0.1767 (5)	0.3999 (5)	0.0439 (16)
C9	−0.1283 (10)	0.2505 (5)	0.3651 (6)	0.067 (2)
H9A	−0.0713	0.2229	0.3245	0.080*
C10	−0.3184 (13)	0.3235 (7)	0.4126 (7)	0.089
H10A	−0.4129	0.3530	0.4128	0.107*
C11	−0.1980 (14)	0.3083 (7)	0.4892 (8)	0.099
H11A	−0.1946	0.3275	0.5517	0.119*
C12	−0.3286 (13)	0.2862 (6)	0.2280 (8)	0.101
H12A	−0.2862	0.2467	0.1922	0.121*
C13	−0.4307 (12)	0.3378 (7)	0.1850 (8)	0.101
H13A	−0.4734	0.3774	0.2205	0.121*
H13B	−0.4625	0.3359	0.1181	0.121*
C14	0.0926 (8)	0.1266 (4)	0.7271 (5)	0.0464 (16)

H14A	0.1520	0.1669	0.7649	0.056*
C15	−0.0419 (11)	0.0139 (6)	0.6833 (6)	0.080
H15A	−0.0898	−0.0373	0.6848	0.097*
C16	−0.0421 (10)	0.0598 (5)	0.6052 (6)	0.064
H16A	−0.0927	0.0468	0.5425	0.077*
C17	0.0665 (12)	0.0246 (7)	0.8540 (7)	0.087
H17A	0.0191	−0.0257	0.8626	0.105*
C18	0.1471 (12)	0.0584 (6)	0.9271 (7)	0.090 (3)
H18A	0.1964	0.1087	0.9214	0.108*
H18B	0.1579	0.0333	0.9873	0.108*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn	0.0559 (5)	0.0507 (5)	0.0273 (4)	0.0043 (4)	0.0006 (3)	−0.0008 (4)
O1	0.057 (3)	0.051 (3)	0.048 (3)	0.003 (3)	0.007 (2)	0.011 (2)
O2	0.068 (3)	0.073 (4)	0.041 (3)	0.007 (3)	0.008 (2)	0.016 (3)
O3	0.086 (4)	0.054 (3)	0.035 (3)	0.009 (3)	0.020 (3)	0.005 (2)
O4	0.085 (4)	0.044 (3)	0.040 (3)	0.016 (3)	0.010 (3)	−0.003 (2)
N1	0.061 (4)	0.063 (4)	0.041 (3)	−0.003 (3)	0.001 (3)	0.004 (3)
N2	0.079 (5)	0.084 (5)	0.080 (4)	0.001 (4)	−0.031 (4)	0.010 (4)
N3	0.055 (3)	0.047 (3)	0.037 (3)	0.006 (3)	0.009 (3)	−0.002 (2)
N4	0.059	0.059	0.059	0.000	0.011	0.000
C1	0.105	0.105	0.105	0.000	0.020	0.000
C2	0.092 (6)	0.069 (5)	0.048 (4)	0.016 (4)	0.022 (4)	0.004 (4)
C3	0.056 (4)	0.052 (4)	0.032 (3)	−0.002 (3)	0.005 (3)	0.001 (3)
C4	0.056 (4)	0.045 (4)	0.034 (3)	0.000 (3)	0.006 (3)	0.007 (3)
C5	0.074 (5)	0.062 (5)	0.052 (4)	0.018 (4)	0.001 (4)	0.014 (3)
C6	0.077 (6)	0.098 (6)	0.084 (5)	0.031 (5)	0.013 (4)	0.008 (5)
C7	0.051 (4)	0.040 (4)	0.031 (3)	−0.001 (3)	−0.002 (3)	−0.001 (3)
C8	0.043 (4)	0.050 (4)	0.031 (3)	0.001 (3)	−0.010 (3)	−0.004 (3)
C9	0.063 (4)	0.074 (5)	0.059 (4)	−0.014 (4)	−0.001 (4)	0.009 (4)
C10	0.089	0.089	0.089	0.000	0.017	0.000
C11	0.099	0.099	0.099	0.000	0.019	0.000
C12	0.101	0.101	0.101	0.000	0.019	0.000
C13	0.101	0.101	0.101	0.000	0.019	0.000
C14	0.061 (4)	0.042 (3)	0.037 (3)	0.006 (3)	0.012 (3)	0.002 (3)
C15	0.080	0.080	0.080	0.000	0.015	0.000
C16	0.064	0.064	0.064	0.000	0.012	0.000
C17	0.087	0.087	0.087	0.000	0.016	0.000
C18	0.103 (8)	0.082 (7)	0.082 (7)	0.005 (6)	0.009 (6)	0.010 (6)

Geometric parameters (Å, °)

Zn—O2^{i}	1.912 (5)	C3—C4	1.406 (8)
Zn—O3	1.965 (5)	C3—C7	1.495 (7)
Zn—N1	1.991 (6)	C4—C5	1.404 (9)
Zn—N3	2.031 (5)	C4—C8	1.483 (9)

O1—C7	1.226 (8)	C5—C6	1.420 (11)
O2—C7	1.299 (8)	C5—H5A	0.9300
O2—Zn^{ii}	1.912 (5)	C6—H6A	0.9300
O3—C8	1.282 (8)	C9—H9A	0.9300
O4—C8	1.232 (8)	C10—C11	1.356 (14)
N1—C9	1.335 (9)	C10—H10A	0.9300
N1—C11	1.363 (12)	C11—H11A	0.9300
N2—C10	1.299 (12)	C12—C13	1.272 (8)
N2—C9	1.365 (11)	C12—H12A	0.9300
N2—C12	1.541 (12)	C13—H13A	0.9300
N3—C14	1.303 (8)	C13—H13B	0.9300
N3—C16	1.392 (9)	C14—H14A	0.9300
N4—C14	1.348 (9)	C15—C16	1.330 (11)
N4—C15	1.377 (10)	C15—H15A	0.9300
N4—C17	1.379 (10)	C16—H16A	0.9300
C1—C2	1.350 (13)	C17—C18	1.250 (12)
C1—C6	1.385 (12)	C17—H17A	0.9300
C1—H1A	0.9300	C18—H18A	0.9300
C2—C3	1.351 (10)	C18—H18B	0.9300
C2—H2A	0.9300		
O2^{i}—Zn—O3	109.4 (2)	C5—C6—H6A	121.8
O2^{i}—Zn—N1	117.8 (3)	O1—C7—O2	123.2 (6)
O3—Zn—N1	110.7 (2)	O1—C7—C3	122.2 (6)
O2^{i}—Zn—N3	109.3 (2)	O2—C7—C3	114.6 (6)
O3—Zn—N3	99.9 (2)	O4—C8—O3	123.5 (7)
N1—Zn—N3	108.4 (2)	O4—C8—C4	120.5 (6)
C7—O2—Zn^{ii}	119.0 (4)	O3—C8—C4	116.0 (6)
C8—O3—Zn	115.6 (4)	N1—C9—N2	106.8 (8)
C9—N1—C11	106.5 (8)	N1—C9—H9A	126.6
C9—N1—Zn	125.7 (6)	N2—C9—H9A	126.6
C11—N1—Zn	127.8 (6)	N2—C10—C11	105.9 (10)
C10—N2—C9	111.1 (8)	N2—C10—H10A	127.0
C10—N2—C12	138.3 (9)	C11—C10—H10A	127.0
C9—N2—C12	110.1 (9)	C10—C11—N1	109.5 (10)
C14—N3—C16	106.9 (6)	C10—C11—H11A	125.3
C14—N3—Zn	127.4 (5)	N1—C11—H11A	125.3
C16—N3—Zn	125.2 (5)	C13—C12—N2	120.6 (11)
C14—N4—C15	106.8 (7)	C13—C12—H12A	119.7
C14—N4—C17	131.2 (8)	N2—C12—H12A	119.7
C15—N4—C17	122.0 (8)	C12—C13—H13A	120.0
C2—C1—C6	122.9 (11)	C12—C13—H13B	120.0
C2—C1—H1A	118.6	H13A—C13—H13B	120.0
C6—C1—H1A	118.6	N3—C14—N4	110.6 (6)
C3—C2—C1	121.7 (8)	N3—C14—H14A	124.7
C3—C2—H2A	119.2	N4—C14—H14A	124.7
C1—C2—H2A	119.2	C16—C15—N4	107.5 (9)
C2—C3—C4	119.4 (6)	C16—C15—H15A	126.3
C2—C3—C7	120.1 (6)	N4—C15—H15A	126.3

C4—C3—C7	120.4 (6)	C15—C16—N3	108.3 (8)
C3—C4—C5	118.9 (7)	C15—C16—H16A	125.9
C3—C4—C8	122.5 (6)	N3—C16—H16A	125.9
C5—C4—C8	118.5 (6)	C18—C17—N4	124.9 (10)
C4—C5—C6	120.8 (7)	C18—C17—H17A	117.5
C4—C5—H5A	119.6	N4—C17—H17A	117.5
C6—C5—H5A	119.6	C17—C18—H18A	120.0
C1—C6—C5	116.3 (9)	C17—C18—H18B	120.0
C1—C6—H6A	121.8	H18A—C18—H18B	120.0
O2^{i}—Zn—O3—C8	−64.4 (5)	C2—C3—C7—O2	−47.7 (9)
N1—Zn—O3—C8	67.0 (5)	C4—C3—C7—O2	134.8 (7)
N3—Zn—O3—C8	−179.0 (5)	Zn—O3—C8—O4	−1.2 (9)
O2^{i}—Zn—N1—C9	121.9 (6)	Zn—O3—C8—C4	176.4 (4)
O3—Zn—N1—C9	−5.0 (7)	C3—C4—C8—O4	−52.7 (10)
N3—Zn—N1—C9	−113.5 (7)	C5—C4—C8—O4	127.3 (7)
O2^{i}—Zn—N1—C11	−58.4 (8)	C3—C4—C8—O3	129.7 (7)
O3—Zn—N1—C11	174.7 (7)	C5—C4—C8—O3	−50.4 (9)
N3—Zn—N1—C11	66.2 (8)	C11—N1—C9—N2	−3.2 (10)
O2^{i}—Zn—N3—C14	0.9 (6)	Zn—N1—C9—N2	176.6 (5)
O3—Zn—N3—C14	115.7 (6)	C10—N2—C9—N1	2.0 (11)
N1—Zn—N3—C14	−128.6 (6)	C12—N2—C9—N1	175.0 (7)
O2^{i}—Zn—N3—C16	−169.2 (5)	C9—N2—C10—C11	0.1 (12)
O3—Zn—N3—C16	−54.5 (6)	C12—N2—C10—C11	−169.9 (11)
N1—Zn—N3—C16	61.3 (6)	N2—C10—C11—N1	−2.1 (12)
C6—C1—C2—C3	−0.8 (13)	C9—N1—C11—C10	3.4 (11)
C1—C2—C3—C4	1.3 (10)	Zn—N1—C11—C10	−176.4 (6)
C1—C2—C3—C7	−176.2 (8)	C10—N2—C12—C13	12.3 (19)
C2—C3—C4—C5	−1.1 (10)	C9—N2—C12—C13	−157.8 (10)
C7—C3—C4—C5	176.3 (7)	C16—N3—C14—N4	1.4 (8)
C2—C3—C4—C8	178.8 (7)	Zn—N3—C14—N4	−170.2 (4)
C7—C3—C4—C8	−3.7 (10)	C15—N4—C14—N3	−0.5 (9)
C3—C4—C5—C6	0.5 (12)	C17—N4—C14—N3	177.9 (8)
C8—C4—C5—C6	−179.4 (8)	C14—N4—C15—C16	−0.8 (10)
C2—C1—C6—C5	0.2 (15)	C17—N4—C15—C16	−179.3 (8)
C4—C5—C6—C1	−0.1 (14)	N4—C15—C16—N3	1.6 (10)
Zn^{ii}—O2—C7—O1	8.7 (9)	C14—N3—C16—C15	−1.9 (9)
Zn^{ii}—O2—C7—C3	−173.8 (4)	Zn—N3—C16—C15	169.9 (6)
C2—C3—C7—O1	129.9 (8)	C14—N4—C17—C18	−1.1 (17)
C4—C3—C7—O1	−47.6 (10)	C15—N4—C17—C18	177.0 (11)

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

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C9—H9A···O1	0.93	2.51	3.435 (10)	170
C14—H14A···O4^{i}	0.93	2.25	3.166 (8)	167
C18—H18A···O4^{i}	0.93	2.49	3.405 (11)	169

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

Fig. 1

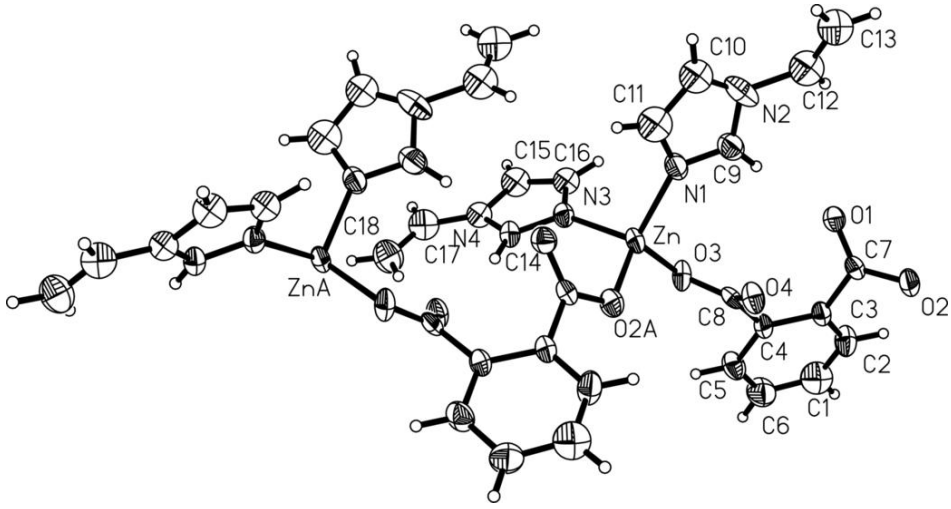


Fig. 2