

catena-Poly[[bis(1-ethylimidazole- κ N³)-zinc(II)]- μ -phthalato- κ^2 O¹:O²]

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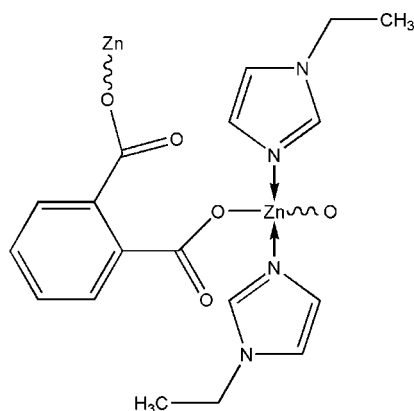
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Key indicators: single-crystal X-ray study; $T = 293$ K; mean $\sigma(\text{C}-\text{C}) = 0.015$ Å; R factor = 0.060; wR factor = 0.183; data-to-parameter ratio = 11.4.

In the solid state, the title compound, $[\text{Zn}(\text{C}_8\text{H}_4\text{O}_4)(\text{C}_5\text{H}_8\text{N}_2)_2]_n$, exhibits polymeric zigzag chains extended along the c axis. Each Zn^{II} ion is coordinated by two N and two O atoms in a distorted tetrahedral geometry. Weak C—H...O interactions contribute to the crystal packing stability.

Related literature

For related literature, see: Liu *et al.* (2002).



Experimental

Crystal data

$[\text{Zn}(\text{C}_8\text{H}_4\text{O}_4)(\text{C}_5\text{H}_8\text{N}_2)_2]$

$M_r = 419.75$

Orthorhombic, $Pca2_1$

$a = 10.209$ (2) Å

$b = 13.870$ (3) Å

$c = 13.583$ (3) Å

$V = 1923.3$ (7) Å³

$Z = 4$

Mo $K\alpha$ radiation

$\mu = 1.31$ mm⁻¹

$T = 293$ (2) K

$0.40 \times 0.10 \times 0.10$ mm

Data collection

Bruker SMART 1K CCD area-detector diffractometer
Absorption correction: multi-scan (SADABS; Sheldrick, 2004)
 $T_{\text{min}} = 0.623$, $T_{\text{max}} = 0.880$

2616 measured reflections
2125 independent reflections
1404 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.012$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.060$

$wR(F^2) = 0.183$

$S = 1.02$

2125 reflections

186 parameters

62 restraints

H-atom parameters constrained

$\Delta\rho_{\text{max}} = 0.73$ e Å⁻³

$\Delta\rho_{\text{min}} = -0.91$ e Å⁻³

Absolute structure: Flack (1983),

145 Friedel pairs

Flack parameter: 0.02 (5)

Table 1

Selected bond lengths (Å).

Zn—O2	1.974 (6)	Zn—N1	1.993 (8)
Zn—O3	1.976 (7)	Zn—N3	2.028 (8)

Table 2

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C5—H5A...O1 ⁱ	0.93	2.42	3.309 (13)	159
C7—H7A...O2 ⁱⁱ	0.97	2.52	3.317 (13)	140
C9—H9A...O1	0.93	2.41	3.113 (12)	133
C10—H10A...O4	0.93	2.42	3.090 (15)	129
C16—H16A...O2 ⁱⁱⁱ	0.93	2.59	3.478 (14)	159

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

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.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HG2326).

References

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supplementary materials

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

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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-ethylimidazole. Each Zn^{II} ion is coordinated by two N [Zn—N1 = 1.993 (8), Zn—N3 = 2.028 (8) Å] and two O [Zn—O2 = 1.974 (6), Zn—O3 = 1.976 (7) 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). Each *o*-phthalate dianion acts as a bidentate ligand to bridge two Zn^{II} atoms through two monodentate carboxylate groups, building a zigzag infinite chain structure along the *c* axis. The metal-metal distances across each polymer backbone are 6.889 (3) Å. In the crystal, Weak C—H...O interactions contribute to the crystal packing stability.

Experimental

The reaction of ZnCl₂ (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-ethylimidazole (0.95 g, 10 mmol) was added. The reaction solution was kept at room temperature after stirring for an hour at 333 K. colorless crystals were obtained after a few days.

Refinement

H atoms were positioned geometrically (C—H = 0.93–0.97 Å) and allowed to ride on their parent atoms with $U_{\text{iso}}(\text{H}) = 1.2$ times $U_{\text{eq}}(\text{C})$.

Figures

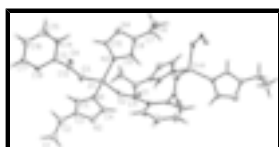


Fig. 1. A portion of the polymeric chain in the title compound showing atomic numbering and 30% probability displacement ellipsoids [symmetry codes: (A) $-x + 1/2, y, z - 1/2$. Fig. 2. The packing of (I), viewed down the *a* axis.



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Crystal data

[Zn(C₈H₄O₄)(C₅H₈N₂)₂]

$M_r = 419.75$

$F_{000} = 864$

$D_x = 1.450 \text{ Mg m}^{-3}$

supplementary materials

Orthorhombic, $Pca2_1$

Hall symbol: P 2c -2ac

$a = 10.209$ (2) Å

$b = 13.870$ (3) Å

$c = 13.583$ (3) Å

$V = 1923.3$ (7) Å³

$Z = 4$

Mo $K\alpha$ radiation

$\lambda = 0.71073$ Å

Cell parameters from 3025 reflections

$\theta = 2.5$ – 25.1°

$\mu = 1.31$ mm⁻¹

$T = 293$ (2) K

Block, colorless

$0.40 \times 0.10 \times 0.10$ mm

Data collection

Bruker SMART 1K CCD area-detector diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

$T = 293$ (2) K

thin-slice ω scans

Absorption correction: multi-scan (SADABS; Sheldrick, 2004)

$T_{\min} = 0.623$, $T_{\max} = 0.880$

2616 measured reflections

2125 independent reflections

1404 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.012$

$\theta_{\text{max}} = 26.0^\circ$

$\theta_{\text{min}} = 1.5^\circ$

$h = 0 \rightarrow 12$

$k = 0 \rightarrow 17$

$l = 0 \rightarrow 16$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.060$

$wR(F^2) = 0.183$

$S = 1.02$

2125 reflections

186 parameters

62 restraints

Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$$w = 1/[\sigma^2(F_o^2) + (0.0962P)^2 + 2.22P]$$

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

$(\Delta/\sigma)_{\text{max}} = 0.006$

$\Delta\rho_{\text{max}} = 0.73$ e Å⁻³

$\Delta\rho_{\text{min}} = -0.91$ e Å⁻³

Extinction correction: none

Absolute structure: Flack (1983), 145 Friedel pairs

Flack parameter: 0.02 (5)

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 (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Zn	0.19333 (9)	0.74668 (7)	0.75914 (15)	0.0293 (3)
O1	0.3715 (7)	0.7223 (5)	0.5888 (5)	0.0359 (16)
O2	0.3432 (6)	0.8244 (5)	0.7131 (5)	0.0346 (15)
O3	0.1449 (7)	0.8235 (5)	0.8761 (5)	0.0406 (17)
O4	-0.0256 (8)	0.7258 (5)	0.8876 (6)	0.0401 (17)
N1	0.2555 (9)	0.6214 (5)	0.8137 (7)	0.0377 (17)
N2	0.3722 (10)	0.4877 (7)	0.8343 (9)	0.060
N3	0.0552 (7)	0.7507 (5)	0.6519 (7)	0.0294 (17)
N4	-0.1320 (9)	0.7819 (7)	0.5765 (9)	0.055
C1	0.4036 (12)	0.4780 (9)	1.0816 (11)	0.060
H1A	0.3777	0.4604	1.1471	0.090*
H1B	0.4203	0.5461	1.0790	0.090*
H1C	0.4817	0.4435	1.0640	0.090*
C2	0.2942 (11)	0.4526 (9)	1.0096 (10)	0.055
H2B	0.3016	0.3847	0.9935	0.066*
H2C	0.2110	0.4616	1.0429	0.066*
C3	0.2910 (10)	0.5061 (7)	0.9196 (9)	0.041
C4	0.3455 (9)	0.5592 (7)	0.7707 (9)	0.045
H4B	0.3814	0.5660	0.7082	0.054*
C5	0.2333 (10)	0.5884 (7)	0.9032 (8)	0.042 (2)
H5A	0.1822	0.6204	0.9495	0.051*
C6	-0.1131 (13)	0.7339 (10)	0.3451 (11)	0.062 (3)
H6A	-0.0954	0.7436	0.2764	0.093*
H6B	-0.2057	0.7378	0.3564	0.093*
H6C	-0.0819	0.6715	0.3647	0.093*
C7	-0.0448 (12)	0.8101 (8)	0.4040 (8)	0.049 (3)
H7A	0.0423	0.8196	0.3771	0.059*
H7B	-0.0922	0.8703	0.3968	0.059*
C8	-0.0330 (10)	0.7880 (7)	0.5088 (8)	0.036
C9	0.0760 (10)	0.7683 (6)	0.5575 (8)	0.035 (2)
H9A	0.1585	0.7670	0.5285	0.042*
C10	-0.0729 (10)	0.7633 (8)	0.6662 (9)	0.045 (3)
H10A	-0.1156	0.7600	0.7266	0.054*
C11	0.3983 (9)	0.7972 (6)	0.6299 (7)	0.031 (2)
C12	0.0351 (9)	0.7984 (7)	0.9131 (7)	0.031
C13	-0.0231 (8)	0.8647 (5)	0.9879 (6)	0.021
C14	-0.1150 (10)	0.9321 (7)	0.9505 (8)	0.042 (2)
H14A	-0.1335	0.9334	0.8835	0.050*
C15	-0.1767 (11)	0.9953 (8)	1.0126 (10)	0.054 (3)
H15A	-0.2393	1.0377	0.9881	0.065*
C16	-0.1455 (12)	0.9963 (9)	1.1132 (10)	0.056
H16A	-0.1861	1.0399	1.1553	0.067*

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C17	-0.0560 (10)	0.9333 (7)	1.1485 (7)	0.039 (2)
H17A	-0.0359	0.9345	1.2153	0.046*
C18	0.0063 (8)	0.8675 (6)	1.0892 (7)	0.0271 (18)

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn	0.0352 (5)	0.0290 (5)	0.0237 (5)	0.0015 (4)	-0.0025 (6)	0.0013 (5)
O1	0.046 (4)	0.032 (3)	0.030 (4)	-0.010 (3)	0.009 (3)	-0.004 (3)
O2	0.047 (4)	0.042 (4)	0.015 (3)	-0.002 (3)	0.003 (3)	0.004 (3)
O3	0.053 (4)	0.037 (4)	0.032 (4)	0.001 (3)	0.009 (3)	-0.004 (3)
O4	0.051 (5)	0.041 (4)	0.029 (4)	-0.010 (3)	-0.006 (4)	-0.009 (3)
N1	0.038 (4)	0.040 (4)	0.035 (4)	0.003 (3)	0.001 (4)	-0.001 (3)
N2	0.060	0.060	0.060	0.000	0.000	0.000
N3	0.022 (4)	0.037 (4)	0.029 (5)	0.001 (3)	-0.003 (3)	-0.002 (3)
N4	0.055	0.055	0.055	0.000	0.000	0.000
C1	0.060	0.060	0.060	0.000	0.000	0.000
C2	0.055	0.055	0.055	0.000	0.000	0.000
C3	0.041	0.041	0.041	0.000	0.000	0.000
C4	0.045	0.045	0.045	0.000	0.000	0.000
C5	0.042 (5)	0.044 (4)	0.041 (5)	0.004 (4)	-0.002 (4)	0.004 (4)
C6	0.064 (7)	0.087 (7)	0.035 (6)	-0.005 (5)	0.000 (5)	-0.011 (5)
C7	0.047 (5)	0.059 (6)	0.041 (5)	0.000 (5)	0.001 (5)	0.004 (5)
C8	0.036	0.036	0.036	0.000	0.000	0.000
C9	0.030 (5)	0.044 (5)	0.030 (6)	0.000 (4)	-0.004 (4)	0.011 (4)
C10	0.029 (5)	0.079 (8)	0.027 (6)	0.004 (5)	0.003 (4)	0.004 (5)
C11	0.043 (5)	0.024 (4)	0.026 (5)	-0.004 (4)	-0.004 (4)	0.012 (4)
C12	0.031	0.031	0.031	0.000	0.000	0.000
C13	0.021	0.021	0.021	0.000	0.000	0.000
C14	0.055 (6)	0.034 (5)	0.036 (6)	0.006 (5)	-0.001 (5)	0.012 (4)
C15	0.062 (7)	0.031 (5)	0.070 (9)	0.011 (5)	-0.014 (6)	0.005 (6)
C16	0.056	0.056	0.056	0.000	0.000	0.000
C17	0.054 (6)	0.039 (5)	0.023 (5)	0.002 (4)	0.004 (5)	0.000 (4)
C18	0.029 (4)	0.034 (4)	0.019 (4)	-0.003 (3)	-0.007 (4)	0.000 (4)

Geometric parameters (\AA , $^\circ$)

Zn—O2	1.974 (6)	C5—H5A	0.9300
Zn—O3	1.976 (7)	C6—C7	1.498 (18)
Zn—N1	1.993 (8)	C6—H6A	0.9600
Zn—N3	2.028 (8)	C6—H6B	0.9600
O1—C11	1.211 (12)	C6—H6C	0.9600
O2—C11	1.318 (12)	C7—C8	1.461 (16)
O3—C12	1.277 (12)	C7—H7A	0.9700
O4—C12	1.232 (12)	C7—H7B	0.9700
N1—C5	1.318 (14)	C8—C9	1.322 (14)
N1—C4	1.389 (13)	C9—H9A	0.9300
N2—C4	1.343 (15)	C10—H10A	0.9300

N2—C3	1.448 (16)	C11—C18 ⁱ	1.485 (12)
N3—C9	1.323 (14)	C12—C13	1.493 (12)
N3—C10	1.333 (14)	C13—C18	1.409 (12)
N4—C8	1.369 (14)	C13—C14	1.419 (13)
N4—C10	1.384 (15)	C14—C15	1.370 (17)
C1—C2	1.526 (17)	C14—H14A	0.9300
C1—H1A	0.9600	C15—C16	1.403 (18)
C1—H1B	0.9600	C15—H15A	0.9300
C1—H1C	0.9600	C16—C17	1.352 (15)
C2—C3	1.430 (17)	C16—H16A	0.9300
C2—H2B	0.9700	C17—C18	1.374 (13)
C2—H2C	0.9700	C17—H17A	0.9300
C3—C5	1.305 (14)	C18—C11 ⁱⁱ	1.485 (12)
C4—H4B	0.9300		
O2—Zn—O3	98.9 (3)	H6A—C6—H6C	109.5
O2—Zn—N1	110.3 (3)	H6B—C6—H6C	109.5
O3—Zn—N1	104.5 (3)	C8—C7—C6	114.3 (10)
O2—Zn—N3	107.2 (3)	C8—C7—H7A	108.7
O3—Zn—N3	112.9 (3)	C6—C7—H7A	108.7
N1—Zn—N3	120.8 (3)	C8—C7—H7B	108.7
C11—O2—Zn	116.5 (6)	C6—C7—H7B	108.7
C12—O3—Zn	112.9 (6)	H7A—C7—H7B	107.6
C5—N1—C4	106.6 (9)	C9—C8—N4	105.8 (10)
C5—N1—Zn	126.2 (7)	C9—C8—C7	126.9 (10)
C4—N1—Zn	126.6 (7)	N4—C8—C7	127.3 (10)
C4—N2—C3	105.6 (9)	C8—C9—N3	112.8 (10)
C9—N3—C10	105.9 (9)	C8—C9—H9A	123.6
C9—N3—Zn	126.1 (7)	N3—C9—H9A	123.6
C10—N3—Zn	125.5 (8)	N3—C10—N4	108.9 (10)
C8—N4—C10	106.3 (9)	N3—C10—H10A	125.5
C2—C1—H1A	109.5	N4—C10—H10A	125.5
C2—C1—H1B	109.5	O1—C11—O2	123.0 (8)
H1A—C1—H1B	109.5	O1—C11—C18 ⁱ	122.7 (9)
C2—C1—H1C	109.5	O2—C11—C18 ⁱ	114.3 (8)
H1A—C1—H1C	109.5	O4—C12—O3	123.6 (9)
H1B—C1—H1C	109.5	O4—C12—C13	119.6 (8)
C3—C2—C1	116.4 (10)	O3—C12—C13	116.7 (8)
C3—C2—H2B	108.2	C18—C13—C14	118.2 (8)
C1—C2—H2B	108.2	C18—C13—C12	126.6 (8)
C3—C2—H2C	108.2	C14—C13—C12	115.2 (8)
C1—C2—H2C	108.2	C15—C14—C13	120.4 (10)
H2B—C2—H2C	107.3	C15—C14—H14A	119.8
C5—C3—C2	127.6 (11)	C13—C14—H14A	119.8
C5—C3—N2	106.0 (10)	C14—C15—C16	120.1 (11)
C2—C3—N2	125.5 (10)	C14—C15—H15A	120.0
N2—C4—N1	108.8 (10)	C16—C15—H15A	120.0
N2—C4—H4B	125.6	C17—C16—C15	119.5 (12)
N1—C4—H4B	125.6	C17—C16—H16A	120.2

supplementary materials

C3—C5—N1	112.6 (10)	C15—C16—H16A	120.2
C3—C5—H5A	123.7	C16—C17—C18	122.3 (10)
N1—C5—H5A	123.7	C16—C17—H17A	118.9
C7—C6—H6A	109.5	C18—C17—H17A	118.9
C7—C6—H6B	109.5	C17—C18—C13	119.5 (8)
H6A—C6—H6B	109.5	C17—C18—C11 ⁱⁱ	121.4 (8)
C7—C6—H6C	109.5	C13—C18—C11 ⁱⁱ	119.0 (8)
O3—Zn—O2—C11	-176.2 (6)	C10—N4—C8—C7	-177.7 (11)
N1—Zn—O2—C11	74.6 (7)	C6—C7—C8—C9	111.4 (13)
N3—Zn—O2—C11	-58.8 (6)	C6—C7—C8—N4	-67.4 (15)
O2—Zn—O3—C12	169.3 (6)	N4—C8—C9—N3	-0.6 (12)
N1—Zn—O3—C12	-76.9 (7)	C7—C8—C9—N3	-179.6 (10)
N3—Zn—O3—C12	56.3 (7)	C10—N3—C9—C8	-2.5 (12)
O2—Zn—N1—C5	122.8 (9)	Zn—N3—C9—C8	-165.5 (7)
O3—Zn—N1—C5	17.4 (9)	C9—N3—C10—N4	4.5 (12)
N3—Zn—N1—C5	-111.1 (9)	Zn—N3—C10—N4	167.7 (7)
O2—Zn—N1—C4	-47.0 (9)	C8—N4—C10—N3	-4.9 (13)
O3—Zn—N1—C4	-152.4 (8)	Zn—O2—C11—O1	-9.0 (12)
N3—Zn—N1—C4	79.1 (9)	Zn—O2—C11—C18 ⁱ	169.3 (6)
O2—Zn—N3—C9	23.5 (8)	Zn—O3—C12—O4	9.5 (12)
O3—Zn—N3—C9	131.3 (7)	Zn—O3—C12—C13	-167.5 (6)
N1—Zn—N3—C9	-104.1 (8)	O4—C12—C13—C18	99.1 (12)
O2—Zn—N3—C10	-136.4 (8)	O3—C12—C13—C18	-83.8 (11)
O3—Zn—N3—C10	-28.6 (9)	O4—C12—C13—C14	-82.3 (11)
N1—Zn—N3—C10	96.1 (9)	O3—C12—C13—C14	94.9 (10)
C1—C2—C3—C5	-87.3 (16)	C18—C13—C14—C15	-2.5 (14)
C1—C2—C3—N2	80.3 (15)	C12—C13—C14—C15	178.7 (9)
C4—N2—C3—C5	-5.0 (13)	C13—C14—C15—C16	2.4 (17)
C4—N2—C3—C2	-174.8 (10)	C14—C15—C16—C17	-1.1 (18)
C3—N2—C4—N1	1.7 (12)	C15—C16—C17—C18	-0.1 (17)
C5—N1—C4—N2	2.2 (12)	C16—C17—C18—C13	0.0 (15)
Zn—N1—C4—N2	173.6 (7)	C16—C17—C18—C11 ⁱⁱ	-178.3 (9)
C2—C3—C5—N1	176.2 (10)	C14—C13—C18—C17	1.3 (13)
N2—C3—C5—N1	6.8 (13)	C12—C13—C18—C17	179.9 (8)
C4—N1—C5—C3	-5.8 (12)	C14—C13—C18—C11 ⁱⁱ	179.6 (8)
Zn—N1—C5—C3	-177.2 (7)	C12—C13—C18—C11 ⁱⁱ	-1.7 (13)
C10—N4—C8—C9	3.3 (12)		

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

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

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C5—H5A \cdots O1 ⁱⁱ	0.93	2.42	3.309 (13)	159
C7—H7A \cdots O2 ⁱ	0.97	2.52	3.317 (13)	140
C9—H9A \cdots O1	0.93	2.41	3.113 (12)	133
C10—H10A \cdots O4	0.93	2.42	3.090 (15)	129
C16—H16A \cdots O2 ⁱⁱⁱ	0.93	2.59	3.478 (14)	159

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

Fig. 1

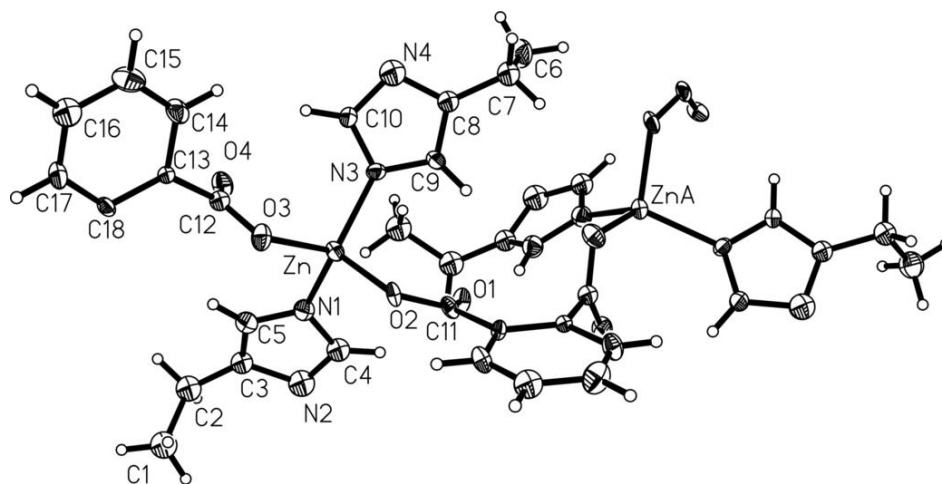


Fig. 2

