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catena-Poly[[bis(1-methylimidazole-κN^3)-zinc(II)]-μ-isophthalato-κ^2O^1:O^3]

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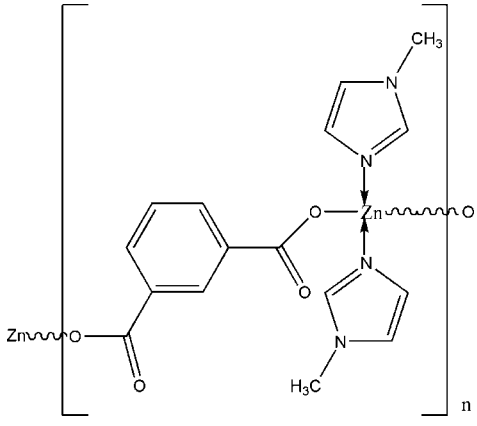
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.009 Å; R factor = 0.068; wR factor = 0.207; data-to-parameter ratio = 13.5.

In the solid state, the title compound, $[Zn(C_8H_4O_4)(C_4H_6N_2)_2]_n$, exhibits the existence of polymeric zigzag chains extending along the *a* axis. Each Zn^{II} ion is coordinated by two N atoms [Zn—N = 1.996 (6) and 2.032 (5) Å] and two O atoms [Zn—O = 1.930 (4) and 1.976 (4) Å] in a distorted tetrahedral geometry. Weak C—H···O interactions contribute to the crystal packing stability.

Related literature

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



Experimental

Crystal data

$[Zn(C_8H_4O_4)(C_4H_6N_2)_2]$
M_r = 393.72
Orthorhombic, *Pbca*
a = 9.6820 (19) Å
b = 13.224 (3) Å
c = 26.983 (5) Å
V = 3454.8 (12) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 1.45 mm^{-1}
T = 293 (2) K
0.20 × 0.10 × 0.10 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
Absorption correction: none
3091 measured reflections
2967 independent reflections
2041 reflections with $I > 2\sigma(I)$
R_{int} = 0.035
3 standard reflections
every 100 reflections
intensity decay: none

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.068
$wR(F^2)$ = 0.207
S = 1.05
2967 reflections
220 parameters
40 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.50 e Å^{-3}
$\Delta\rho_{min}$ = −0.61 e Å^{-3}

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C1—H1*A*···O3^{i}	0.96	2.55	3.423 (10)	150
C4—H4*B*···O3^{i}	0.93	2.31	3.150 (9)	150
C11—H11*A*···O2^{ii}	0.93	2.54	3.457 (8)	171

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

Data collection: *CAD-4 Software* (Enraf–Nonius, 1989); cell refinement: *CAD-4 Software*; data reduction: *NRCVAX* (Gabe *et al.*, 1989); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL/PC* (Sheldrick, 2008); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CV2451).

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supplementary materials

Acta Cryst. (2008). E**64**, m1335 [**doi:10.1107/S160053680803078X**]

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

J. Zhao

Comment

In the title compound, (I) (Fig. 1), the zinc(II) centers are bridged by carboxylate groups of isophthalate ligands. Each Zn^{II} ion is coordinated by two N [Zn—N2 = 1.996 (6) Å, Zn—N4 = 2.032 (5) Å] and two O [Zn—O1 = 1.930 (4) Å, Zn—O4 = 1.976 (4) Å] atoms in a distorted tetrahedral geometry. All these values agree well with those observed in [Zn(isophthalato)(1-*H*-imidazole)$_2$] (Yang *et al.*, 2002). Each isophthalate dianion in (I) acts as a bidentate ligand to bridge two Zn^{II} atoms through two monodentate carboxylate groups, building a zigzag polymeric chain along the *a* axis. The metal–metal distance across each polymer backbone is 9.682 (7) Å.

In the crystal, weak C—H···O interactions contribute to the crystal packing stability. In the corresponding zinc compound [Zn(isophthalato)(1-*H*-imidazole)$_2$] (Yang *et al.*, 2002), the Zn^{II} ions have a distorted tetrahedral environment.

Experimental

The reaction of $ZnCl_2$(0.68 g, 5 mmol) with isophthalic 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-methylimidazole (0.82 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

H atoms were positioned geometrically (C—H = 0.93 or 0.96 Å) and allowed to ride on their parent atoms with U_{iso}(H) = 1.2 or 1.5 times U_{eq}(C).

Figures

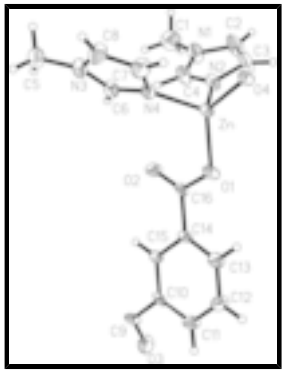


Fig. 1. A portion of the polymeric chain in (I) showing the atomic numbering and 30% probability displacement ellipsoids.

catena-Poly[[bis(1-methylimidazole-κN^3)zinc(II)]-μ-isophthalato- κ^2*O*^{1}:*O*^{3}]

Crystal data

$[Zn(C_8H_4O_4)(C_4H_6N_2)_2]$	$F(000) = 1616$
$M_r = 393.72$	$D_x = 1.514$ Mg m^{-3}
Orthorhombic, *Pbca*	Mo *K*α radiation, λ = 0.71073 Å
Hall symbol: -P 2ac 2ab	Cell parameters from 25 reflections
a = 9.6820 (19) Å	θ = 10–14°
b = 13.224 (3) Å	μ = 1.45 mm^{-1}
c = 26.983 (5) Å	*T* = 293 K
V = 3454.8 (12) Å^3	Block, colourless
Z = 8	0.20 × 0.10 × 0.10 mm

Data collection

Enraf–Nonius CAD-4 diffractometer	$R_{int} = 0.036$
Radiation source: fine-focus sealed tube	$\theta_{max} = 25.2°$, $\theta_{min} = 1.5°$
graphite	*h* = 0→11
ω scans	*k* = 0→15
3091 measured reflections	*l* = 0→32
2967 independent reflections	3 standard reflections every 100 reflections
2041 reflections with $I > 2\sigma(I)$	intensity decay: none

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.068$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.207$	H-atom parameters constrained
S = 1.05	$w = 1/[\sigma^2(F_o^2) + (0.1255P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
2967 reflections	$(\Delta/\sigma)_{max} < 0.001$
220 parameters	$\Delta\rho_{max} = 0.50$ e Å^{-3}
40 restraints	$\Delta\rho_{min} = -0.61$ 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}
Zn	0.18405 (6)	0.12667 (5)	0.12048 (3)	0.0338 (3)
N1	0.1883 (6)	0.3348 (5)	0.2326 (2)	0.0594 (17)
N2	0.1689 (5)	0.2071 (4)	0.1829 (2)	0.0434 (13)
N3	0.2381 (6)	0.3608 (4)	0.0199 (2)	0.0461 (14)
N4	0.1948 (5)	0.2244 (4)	0.06251 (18)	0.0358 (12)
O1	0.3326 (4)	0.0294 (4)	0.11870 (16)	0.0460 (12)
O2	0.4748 (4)	0.1603 (3)	0.12273 (18)	0.0510 (13)
O3	1.0442 (4)	−0.0567 (4)	0.1520 (2)	0.0680 (16)
O4	−0.0041 (4)	0.0763 (3)	0.10656 (16)	0.0440 (11)
C1	0.2355 (10)	0.4326 (6)	0.2511 (3)	0.081
H1A	0.3017	0.4605	0.2284	0.122*
H1B	0.2777	0.4239	0.2830	0.122*
H1C	0.1581	0.4776	0.2539	0.122*
C2	0.0944 (8)	0.2711 (7)	0.2534 (3)	0.079 (3)
H2A	0.0483	0.2798	0.2833	0.094*
C3	0.0821 (8)	0.1945 (7)	0.2223 (3)	0.071 (2)
H3A	0.0229	0.1399	0.2267	0.086*
C4	0.2306 (8)	0.2910 (6)	0.1911 (2)	0.0523 (18)
H4B	0.2976	0.3181	0.1703	0.063*
C5	0.2982 (8)	0.4589 (5)	0.0065 (3)	0.060 (2)
H5A	0.3727	0.4745	0.0288	0.089*
H5B	0.2287	0.5104	0.0089	0.089*
H5C	0.3326	0.4560	−0.0268	0.089*
C6	0.2723 (6)	0.3054 (5)	0.0588 (2)	0.0408 (15)
H6A	0.3427	0.3218	0.0809	0.049*
C7	0.1029 (8)	0.2310 (5)	0.0239 (3)	0.0568 (19)
H7A	0.0326	0.1849	0.0175	0.068*
C8	0.1294 (8)	0.3137 (5)	−0.0030 (3)	0.059 (2)
H8A	0.0835	0.3349	−0.0315	0.070*
C9	0.9641 (6)	−0.0064 (5)	0.1281 (2)	0.0361 (14)
C10	0.8172 (5)	−0.0403 (5)	0.1219 (2)	0.0328 (14)
C11	0.7891 (7)	−0.1438 (5)	0.1187 (2)	0.0436 (16)
H11A	0.8608	−0.1907	0.1190	0.052*
C12	0.6544 (7)	−0.1755 (5)	0.1151 (3)	0.060 (2)
H12A	0.6356	−0.2443	0.1126	0.072*
C13	0.5473 (7)	−0.1080 (5)	0.1151 (3)	0.0510 (18)
H13A	0.4572	−0.1318	0.1121	0.061*
C14	0.5702 (5)	−0.0054 (4)	0.1195 (2)	0.0301 (12)
C15	0.7082 (5)	0.0286 (4)	0.1222 (2)	0.0321 (13)
H15A	0.7265	0.0975	0.1242	0.039*

C16	0.4545 (6)	0.0702 (5)	0.1210 (2)	0.0340 (14)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn	0.0166 (4)	0.0401 (4)	0.0446 (5)	0.0005 (3)	−0.0007 (3)	0.0023 (3)
N1	0.067 (4)	0.058 (3)	0.053 (3)	−0.018 (3)	0.016 (3)	−0.013 (3)
N2	0.032 (3)	0.056 (3)	0.043 (3)	−0.008 (2)	0.006 (2)	0.001 (2)
N3	0.051 (3)	0.052 (3)	0.035 (3)	−0.008 (3)	0.003 (3)	0.003 (3)
N4	0.024 (2)	0.043 (3)	0.041 (3)	−0.009 (2)	−0.009 (2)	0.006 (2)
O1	0.019 (2)	0.057 (3)	0.062 (3)	0.004 (2)	0.0020 (19)	0.003 (2)
O2	0.021 (2)	0.036 (2)	0.096 (4)	−0.0011 (19)	−0.001 (2)	0.004 (2)
O3	0.023 (2)	0.075 (3)	0.106 (4)	−0.001 (2)	−0.013 (3)	0.041 (3)
O4	0.020 (2)	0.049 (3)	0.063 (3)	−0.0021 (19)	−0.004 (2)	0.008 (2)
C1	0.081	0.081	0.081	0.000	0.000	0.000
C2	0.068 (5)	0.100 (6)	0.068 (5)	−0.024 (4)	0.038 (4)	−0.019 (4)
C3	0.064 (5)	0.081 (5)	0.069 (5)	−0.030 (4)	0.031 (4)	−0.006 (4)
C4	0.052 (4)	0.071 (4)	0.033 (3)	−0.010 (3)	0.015 (3)	−0.005 (3)
C5	0.069 (5)	0.054 (4)	0.056 (5)	−0.010 (4)	0.008 (4)	0.004 (4)
C6	0.034 (3)	0.051 (4)	0.037 (4)	−0.006 (3)	0.001 (3)	0.003 (3)
C7	0.053 (4)	0.054 (4)	0.063 (5)	−0.009 (4)	−0.017 (4)	0.005 (4)
C8	0.061 (5)	0.060 (5)	0.054 (5)	−0.004 (4)	−0.017 (4)	0.017 (4)
C9	0.017 (3)	0.046 (3)	0.045 (4)	0.006 (3)	0.000 (3)	−0.007 (3)
C10	0.011 (3)	0.054 (4)	0.033 (3)	−0.002 (2)	0.002 (2)	0.005 (3)
C11	0.026 (3)	0.041 (4)	0.064 (4)	0.005 (3)	−0.006 (3)	−0.007 (3)
C12	0.029 (4)	0.031 (3)	0.119 (7)	−0.006 (3)	−0.005 (4)	−0.006 (4)
C13	0.024 (3)	0.042 (4)	0.087 (5)	−0.005 (3)	−0.002 (3)	−0.007 (3)
C14	0.015 (3)	0.037 (3)	0.038 (3)	0.002 (2)	−0.004 (2)	0.001 (3)
C15	0.017 (3)	0.034 (3)	0.046 (4)	−0.001 (2)	−0.002 (2)	0.005 (3)
C16	0.012 (3)	0.049 (4)	0.041 (3)	0.001 (3)	0.001 (2)	0.008 (3)

Geometric parameters (Å, °)

Zn—O1	1.930 (4)	C3—H3A	0.9300
Zn—O4	1.976 (4)	C4—H4B	0.9300
Zn—N2	1.996 (6)	C5—H5A	0.9600
Zn—N4	2.032 (5)	C5—H5B	0.9600
N1—C4	1.327 (8)	C5—H5C	0.9600
N1—C2	1.360 (9)	C6—H6A	0.9300
N1—C1	1.459 (10)	C7—C8	1.339 (9)
N2—C4	1.279 (8)	C7—H7A	0.9300
N2—C3	1.367 (8)	C8—H8A	0.9300
N3—C6	1.322 (8)	C9—O4^{ii}	1.277 (8)
N3—C8	1.371 (9)	C9—C10	1.501 (7)
N3—C5	1.468 (8)	C10—C15	1.395 (8)
N4—C6	1.311 (7)	C10—C11	1.399 (9)
N4—C7	1.372 (8)	C11—C12	1.373 (8)
O1—C16	1.299 (7)	C11—H11A	0.9300

O2—C16	1.209 (8)	C12—C13	1.368 (9)
O3—C9	1.207 (7)	C12—H12A	0.9300
O4—C9^{i}	1.277 (8)	C13—C14	1.381 (8)
C1—H1A	0.9600	C13—H13A	0.9300
C1—H1B	0.9600	C14—C15	1.411 (7)
C1—H1C	0.9600	C14—C16	1.502 (8)
C2—C3	1.319 (11)	C15—H15A	0.9300
C2—H2A	0.9300		
O1—Zn—O4	117.23 (19)	H5A—C5—H5B	109.5
O1—Zn—N2	115.5 (2)	N3—C5—H5C	109.5
O4—Zn—N2	105.80 (19)	H5A—C5—H5C	109.5
O1—Zn—N4	111.51 (19)	H5B—C5—H5C	109.5
O4—Zn—N4	96.63 (18)	N4—C6—N3	111.7 (6)
N2—Zn—N4	108.3 (2)	N4—C6—H6A	124.2
C4—N1—C2	106.5 (6)	N3—C6—H6A	124.2
C4—N1—C1	125.3 (7)	C8—C7—N4	109.9 (6)
C2—N1—C1	128.2 (7)	C8—C7—H7A	125.1
C4—N2—C3	104.9 (6)	N4—C7—H7A	125.1
C4—N2—Zn	125.0 (5)	C7—C8—N3	105.8 (6)
C3—N2—Zn	129.6 (5)	C7—C8—H8A	127.1
C6—N3—C8	107.4 (5)	N3—C8—H8A	127.1
C6—N3—C5	125.9 (6)	O3—C9—O4^{ii}	124.1 (6)
C8—N3—C5	126.5 (6)	O3—C9—C10	120.2 (6)
C6—N4—C7	105.2 (5)	O4^{ii}—C9—C10	115.7 (5)
C6—N4—Zn	127.4 (4)	C15—C10—C11	119.5 (5)
C7—N4—Zn	126.2 (4)	C15—C10—C9	121.5 (6)
C16—O1—Zn	113.5 (4)	C11—C10—C9	118.9 (5)
C9^{i}—O4—Zn	115.1 (4)	C12—C11—C10	119.2 (6)
N1—C1—H1A	109.5	C12—C11—H11A	120.4
N1—C1—H1B	109.5	C10—C11—H11A	120.4
H1A—C1—H1B	109.5	C13—C12—C11	121.4 (6)
N1—C1—H1C	109.5	C13—C12—H12A	119.3
H1A—C1—H1C	109.5	C11—C12—H12A	119.3
H1B—C1—H1C	109.5	C12—C13—C14	121.2 (6)
C3—C2—N1	105.9 (7)	C12—C13—H13A	119.4
C3—C2—H2A	127.0	C14—C13—H13A	119.4
N1—C2—H2A	127.0	C13—C14—C15	118.0 (5)
C2—C3—N2	110.2 (7)	C13—C14—C16	122.4 (5)
C2—C3—H3A	124.9	C15—C14—C16	119.5 (5)
N2—C3—H3A	124.9	C10—C15—C14	120.5 (5)
N2—C4—N1	112.4 (6)	C10—C15—H15A	119.7
N2—C4—H4B	123.8	C14—C15—H15A	119.7
N1—C4—H4B	123.8	O2—C16—O1	124.0 (6)
N3—C5—H5A	109.5	O2—C16—C14	122.4 (5)
N3—C5—H5B	109.5	O1—C16—C14	113.6 (5)
O1—Zn—N2—C4	89.0 (6)	Zn—N4—C6—N3	−169.7 (4)
O4—Zn—N2—C4	−139.6 (6)	C8—N3—C6—N4	0.9 (8)
N4—Zn—N2—C4	−36.9 (6)	C5—N3—C6—N4	176.2 (6)

O1—Zn—N2—C3	−100.1 (7)	C6—N4—C7—C8	1.9 (8)
O4—Zn—N2—C3	31.4 (7)	Zn—N4—C7—C8	170.1 (5)
N4—Zn—N2—C3	134.1 (7)	N4—C7—C8—N3	−1.4 (9)
O1—Zn—N4—C6	−81.7 (5)	C6—N3—C8—C7	0.3 (9)
O4—Zn—N4—C6	155.6 (5)	C5—N3—C8—C7	−175.0 (6)
N2—Zn—N4—C6	46.5 (6)	O3—C9—C10—C15	141.9 (7)
O1—Zn—N4—C7	112.7 (6)	O4^{ii}—C9—C10—C15	−38.6 (9)
O4—Zn—N4—C7	−10.0 (6)	O3—C9—C10—C11	−34.3 (9)
N2—Zn—N4—C7	−119.1 (6)	O4^{ii}—C9—C10—C11	145.2 (6)
O4—Zn—O1—C16	170.5 (4)	C15—C10—C11—C12	1.0 (10)
N2—Zn—O1—C16	−63.7 (4)	C9—C10—C11—C12	177.3 (6)
N4—Zn—O1—C16	60.4 (4)	C10—C11—C12—C13	−0.7 (12)
O1—Zn—O4—C9^{i}	44.5 (5)	C11—C12—C13—C14	−1.0 (12)
N2—Zn—O4—C9^{i}	−86.0 (4)	C12—C13—C14—C15	2.4 (11)
N4—Zn—O4—C9^{i}	162.9 (4)	C12—C13—C14—C16	−178.4 (6)
C4—N1—C2—C3	−2.1 (10)	C11—C10—C15—C14	0.3 (9)
C1—N1—C2—C3	177.6 (8)	C9—C10—C15—C14	−175.9 (5)
N1—C2—C3—N2	1.5 (11)	C13—C14—C15—C10	−2.0 (10)
C4—N2—C3—C2	−0.2 (10)	C16—C14—C15—C10	178.7 (5)
Zn—N2—C3—C2	−172.6 (6)	Zn—O1—C16—O2	−1.8 (8)
C3—N2—C4—N1	−1.2 (9)	Zn—O1—C16—C14	−180.0 (4)
Zn—N2—C4—N1	171.6 (5)	C13—C14—C16—O2	−176.8 (7)
C2—N1—C4—N2	2.1 (9)	C15—C14—C16—O2	2.4 (9)
C1—N1—C4—N2	−177.6 (7)	C13—C14—C16—O1	1.4 (8)
C7—N4—C6—N3	−1.7 (7)	C15—C14—C16—O1	−179.4 (5)

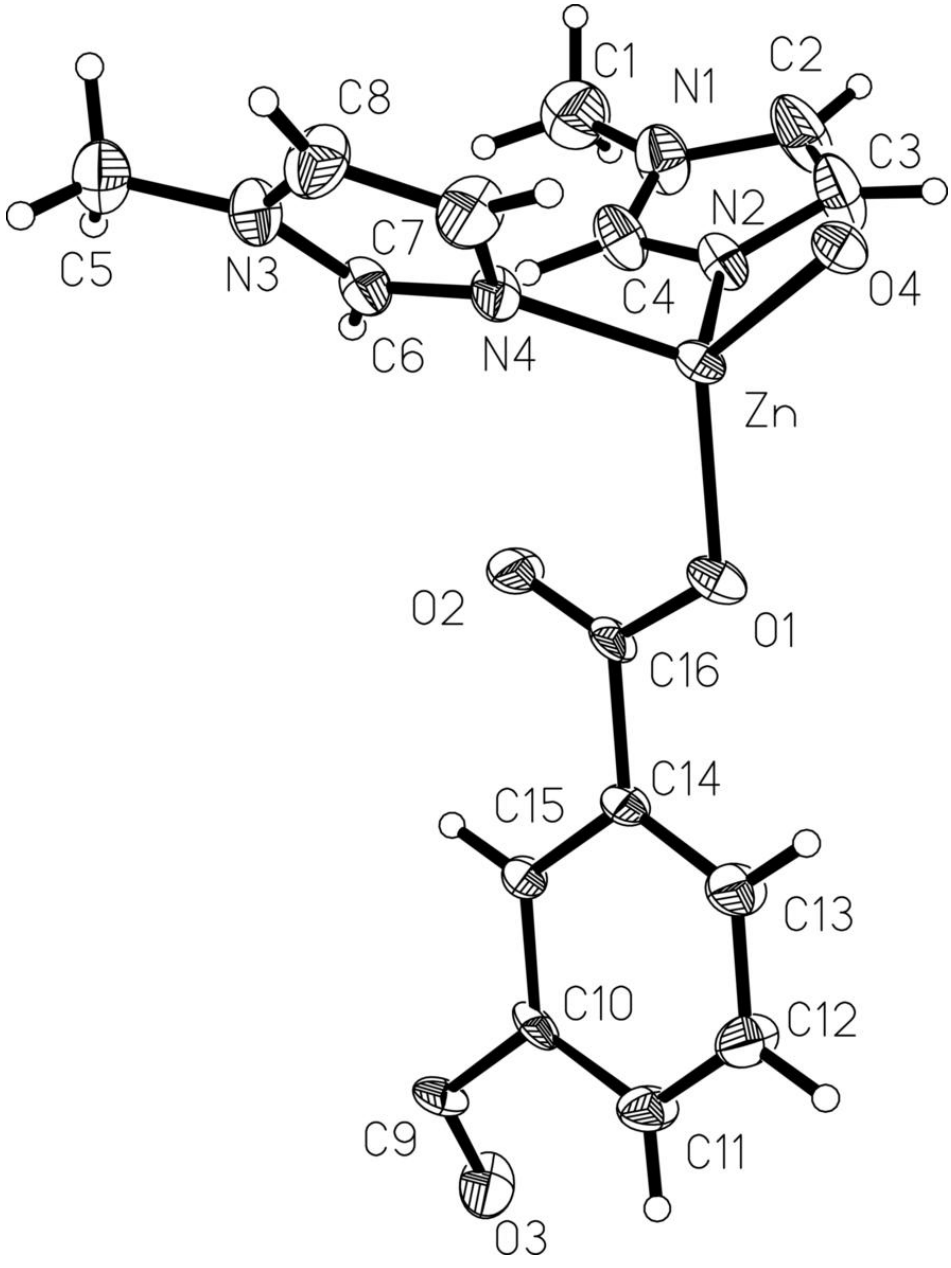
Symmetry codes: (i) *x*−1, *y*, *z*; (ii) *x*+1, *y*, *z*.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C1—H1A···O3^{iii}	0.96	2.55	3.423 (10)	150
C4—H4B···O3^{iii}	0.93	2.31	3.150 (9)	150
C11—H11A···O2^{iv}	0.93	2.54	3.457 (8)	171

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

Fig. 1


C1
N1
C2
C8
C3
N2
C7
C5
N3
C4
O4
C6
N4
Zn
O2
O1
C16
C14
C15
C13
C10
C12
C9
C11
O3