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Poly[bis(μ_2-quinoline-3-carboxylato-κ^2N:O)zinc(II)]

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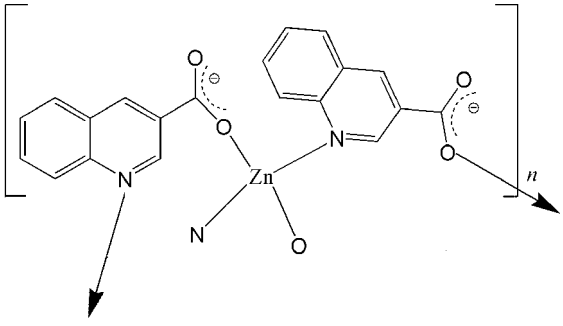
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.003 Å; R factor = 0.036; wR factor = 0.097; data-to-parameter ratio = 14.4.

In the title compound, $[Zn(L)_2]_n$ (HL is quinoline-3-carboxylic acid, $C_{10}H_7NO_2$), the Zn^{II} atom is coordinated by two N atoms from two bis-monodentate L^- ligands and two O atoms from two bis-monodentate L^- ligands, forming a slightly distorted tetrahedral geometry. Each bis-monodentate ligand links two Zn atoms, constructing a two-dimensional layer parallel to the (100) plane. The layers pack together into an *abab* pattern. These layers are linked by π–π interactions [face-to-face separation 3.59 (1) Å] into a supramolecular structure.

Related literature

For related literature, see: Odoko *et al.* (2001); Okabe & Muranishi (2003); Lin *et al.* (1998); Tong *et al.* (2003).



Experimental

Crystal data

$[Zn(C_{10}H_6NO_2)_2]$
M_r = 409.69
Monoclinic, $C2/c$
a = 28.7995 (17) Å
b = 8.0475 (5) Å
c = 15.2845 (9) Å
β = 114.262 (1)°
V = 3229.5 (3) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 1.55 mm^{-1}
T = 293 (2) K
0.15 × 0.10 × 0.04 mm

Data collection

Bruker APEX CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.801, T_{max} = 0.941
12965 measured reflections
3505 independent reflections
3139 reflections with $I > 2\sigma(I)$
R_{int} = 0.030

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.036
$wR(F^2)$ = 0.097
S = 1.07
3505 reflections
244 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 1.47 e Å^{-3}
$\Delta\rho_{min}$ = −0.30 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Zn1—O1	1.927 (2)	Zn1—N1^{ii}	2.097 (2)
Zn1—O4^{i}	1.963 (2)	Zn1—N2	2.102 (2)
O1—Zn1—O4^{i}	138.54 (7)	O1—Zn1—N2	100.00 (7)
O1—Zn1—N1^{ii}	110.34 (7)	O4^{i}—Zn1—N2	100.73 (7)
O4^{i}—Zn1—N1^{ii}	100.64 (7)	N1^{ii}—Zn1—N2	100.45 (7)

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

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1997); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: KP2135).

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supplementary materials

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Poly[bis(μ_2-quinoline-3-carboxylato-κ^2N:O)zinc(II)]

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Comment

Organic nitriles ligands and their hydroxlyate derivatives (carboxylates) have been widely used for hydrothermal synthesis of coordination polymers (Lin, *et al.*, 1998; Tong, *et al.*, 2003). Notably, these kinds of ligand reactions, relatively straight forward in the context of reaction chemistry, have become an important approach in the crystal engineering of metal-organic frameworks exhibiting novel physical properties. In the title compound, (I), the quin-3 − c group evidently results from the hydrolysis of quinoline-3-carbonitrile. The quin-3 − c ligands used in this work exhibit bridging mode different from other quinoline derivatives (Odoko, *et al*., 2001; Okabe & Muranishi, 2003). To the best of our knowledge, this is the first isolated quin-3 − c coordination polymer.

There are one Zn^{II} atom and two quin-3 − c ligands in the asymmetric unit. The Zn^{II} atom has a tetrahedral environment formed by two N atoms [Co – N 2.097 (2) − 2.102 (2) Å] and two O atoms [Co – O 1.927 (2) − 1.963 (2) Å] belonging to for different quin-3 − c ligands. The quin-3 − c ion binds to zinc in a bridge mode, through the carboxylate O atom and the quinoline N atom. The carboxylato group is monodentate. Each Zn^{II} atom is connected by four ditopic quin-3 − c ligands, which construct a two-dimensional layer parallel to the (100) plane (Fig. 2) and generate two-dimensional square grids based on the (4, 4) topology. The quinoline rings of quin-3 − c penetrating into the adjacent layers are parallel to each other, and face-to-face separations are about 3.59 (1) Å (the second quinoline rings symmetry code: x, y, 1 − z) indicating π···π interaction.

Experimental

Quinoline-3-carbonitrile (1 mmol, 0.154 g), $Zn(NO_3)_2{\cdot}6H_2O$ (0.5 mmol, 0.10 g) in water (10 ml). The mixture solution was stirred for 30 min at room temperature. The mixed solution were added to 15 ml sealed teflon-lined stainless steel vessels and the teflon-lined stainless steel vessels was left at 433 K vacuum case for 3 d under autogenous pressure. After cooled to room temperature, colourless crystals were obtained (yield: 80%, based on Zn).

Refinement

All other H atoms were positioned geometrically and refined as riding, with C–H distances of 0.93 Å and U_{iso}(H) = 1.2 U_{eq}(C).

Figures

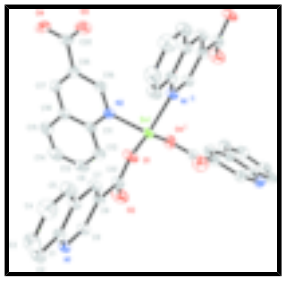

Fig. 1. The molecular stucture of (I) showing the coordination geometry around zinc with the 50% probability ellipsoids for non-H atoms. Hydrogen atoms have been omitted. [Symmetry codes: (i) x, $2 - y$, $z - 1/2$; (ii) x, $y + 1$, z.]

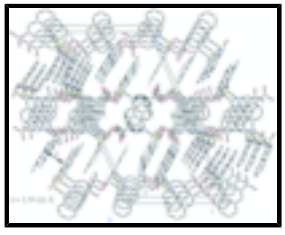

Fig. 2. Packing diagram of (I); hydrogen atoms have been omited.

Poly[bis(μ$_2$-quinoline-3-carboxylato-κ^2*N*:*O*)zinc(II)]

Crystal data

$[Zn(C_{10}H_6NO_2)_2]$	F_{000} = 1664
M_r = 409.69	D_x = 1.685 Mg m^{-3}
Monoclinic, *C*2/*c*	Mo *K*α radiation λ = 0.71073 Å
a = 28.7995 (17) Å	Cell parameters from 3505 reflections
b = 8.0475 (5) Å	θ = 1.6–27.0º
c = 15.2845 (9) Å	μ = 1.55 mm^{-1}
β = 114.2620 (10)º	*T* = 293 (2) K
V = 3229.5 (3) Å^3	Block, yellow
Z = 8	0.15 × 0.10 × 0.04 mm

Data collection

Bruker SMART CCD area-detector diffractometer	3505 independent reflections
Radiation source: fine-focus sealed tube	3139 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.030
T = 293(2) K	θ_{max} = 27.0º
phi and ω scans	θ_{min} = 1.6º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	*h* = −35→36
T_{min} = 0.801, T_{max} = 0.941	*k* = −10→10
12965 measured reflections	*l* = −19→19

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.036$	H-atom parameters constrained
$wR(F^2) = 0.097$	$w = 1/[\sigma^2(F_o^2) + (0.0609P)^2 + 2.5142P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.07$	$(\Delta/\sigma)_{max} = 0.001$
3505 reflections	$\Delta\rho_{max} = 1.47$ e Å^{-3}
244 parameters	$\Delta\rho_{min} = -0.30$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

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	0.126630 (9)	0.87864 (3)	0.431899 (16)	0.02379 (11)
N2	0.08079 (7)	0.8761 (2)	0.50917 (13)	0.0245 (4)
O4	0.07901 (6)	1.0274 (2)	0.80930 (11)	0.0339 (4)
O3	0.14500 (7)	1.0907 (2)	0.77747 (13)	0.0414 (4)
C19	0.10001 (8)	0.9447 (3)	0.59501 (15)	0.0271 (4)
H19A	0.1312	0.9988	0.6141	0.033*
C17	0.03160 (9)	0.8594 (3)	0.63348 (16)	0.0297 (5)
H17A	0.0155	0.8544	0.6752	0.036*
C16	0.00951 (8)	0.7822 (3)	0.54283 (15)	0.0276 (4)
C18	0.07678 (8)	0.9417 (3)	0.65969 (15)	0.0265 (4)
C20	0.10280 (9)	1.0280 (3)	0.75489 (15)	0.0300 (5)
C12	0.01183 (9)	0.7247 (3)	0.38800 (15)	0.0305 (5)
H12A	0.0278	0.7340	0.3462	0.037*
C14	−0.05816 (10)	0.6271 (3)	0.4220 (2)	0.0411 (6)
H14A	−0.0889	0.5703	0.4019	0.049*
C11	0.03451 (8)	0.7944 (2)	0.48051 (14)	0.0242 (4)
C13	−0.03377 (10)	0.6432 (3)	0.35961 (18)	0.0374 (5)
H13A	−0.0488	0.5979	0.2983	0.045*

C15	−0.03718 (9)	0.6940 (3)	0.51180 (18)	0.0362 (5)
H15A	−0.0535	0.6819	0.5528	0.043*
N1	0.17247 (7)	0.0863 (2)	0.49329 (13)	0.0232 (3)
O1	0.16472 (6)	0.67676 (19)	0.47914 (12)	0.0349 (4)
O2	0.10349 (7)	0.5261 (2)	0.36969 (13)	0.0435 (4)
C8	0.17215 (8)	0.3862 (2)	0.49059 (16)	0.0242 (4)
C9	0.15142 (8)	0.2295 (2)	0.45446 (15)	0.0244 (4)
H9A	0.1210	0.2263	0.3998	0.029*
C10	0.14361 (9)	0.5398 (3)	0.44045 (16)	0.0274 (4)
C6	0.24106 (8)	0.2430 (3)	0.61467 (15)	0.0256 (4)
C7	0.21666 (8)	0.3917 (2)	0.57096 (16)	0.0270 (5)
H7A	0.2309	0.4937	0.5969	0.032*
C2	0.24291 (9)	−0.0598 (3)	0.61506 (17)	0.0326 (5)
H2A	0.2283	−0.1611	0.5886	0.039*
C1	0.21828 (8)	0.0899 (2)	0.57371 (15)	0.0233 (4)
C3	0.28822 (9)	−0.0562 (3)	0.69407 (18)	0.0394 (6)
H3A	0.3045	−0.1554	0.7204	0.047*
C4	0.31046 (10)	0.0950 (3)	0.7359 (2)	0.0415 (6)
H4A	0.3410	0.0951	0.7903	0.050*
C5	0.28758 (8)	0.2421 (3)	0.69749 (17)	0.0345 (5)
H5A	0.3026	0.3420	0.7257	0.041*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn1	0.02945 (17)	0.01509 (15)	0.02426 (16)	0.00046 (8)	0.00844 (11)	0.00107 (8)
N2	0.0269 (9)	0.0225 (9)	0.0220 (9)	−0.0012 (6)	0.0080 (7)	0.0001 (6)
O4	0.0402 (9)	0.0345 (9)	0.0235 (7)	0.0045 (7)	0.0095 (7)	−0.0047 (6)
O3	0.0431 (10)	0.0376 (9)	0.0365 (9)	−0.0101 (8)	0.0094 (8)	−0.0105 (7)
C19	0.0285 (11)	0.0237 (11)	0.0262 (10)	−0.0040 (8)	0.0084 (9)	−0.0016 (8)
C17	0.0337 (12)	0.0296 (11)	0.0277 (11)	0.0002 (9)	0.0147 (9)	−0.0003 (8)
C16	0.0282 (11)	0.0231 (10)	0.0285 (10)	−0.0003 (8)	0.0087 (9)	−0.0007 (8)
C18	0.0318 (11)	0.0222 (10)	0.0223 (10)	0.0010 (8)	0.0079 (8)	−0.0006 (8)
C20	0.0392 (12)	0.0195 (10)	0.0237 (10)	0.0059 (9)	0.0052 (9)	−0.0010 (8)
C12	0.0350 (12)	0.0253 (11)	0.0264 (11)	0.0001 (9)	0.0078 (9)	−0.0014 (8)
C14	0.0285 (12)	0.0366 (14)	0.0487 (15)	−0.0099 (10)	0.0061 (11)	−0.0057 (10)
C11	0.0268 (10)	0.0165 (9)	0.0252 (10)	0.0012 (7)	0.0066 (8)	0.0004 (7)
C13	0.0383 (13)	0.0297 (12)	0.0308 (12)	−0.0034 (10)	0.0008 (10)	−0.0054 (9)
C15	0.0296 (12)	0.0355 (13)	0.0436 (13)	−0.0054 (9)	0.0150 (10)	−0.0026 (10)
N1	0.0254 (9)	0.0157 (8)	0.0264 (9)	−0.0003 (6)	0.0085 (7)	0.0011 (6)
O1	0.0412 (9)	0.0132 (7)	0.0431 (9)	0.0018 (6)	0.0102 (8)	0.0008 (6)
O2	0.0402 (10)	0.0279 (9)	0.0456 (10)	0.0076 (7)	0.0006 (8)	0.0077 (7)
C8	0.0283 (11)	0.0140 (9)	0.0306 (11)	0.0028 (7)	0.0124 (9)	0.0025 (7)
C9	0.0242 (10)	0.0187 (10)	0.0273 (10)	−0.0007 (8)	0.0074 (8)	0.0003 (8)
C10	0.0321 (11)	0.0174 (10)	0.0327 (11)	0.0050 (8)	0.0134 (9)	0.0039 (8)
C6	0.0255 (10)	0.0204 (10)	0.0291 (11)	−0.0001 (8)	0.0094 (9)	0.0004 (8)
C7	0.0304 (11)	0.0170 (10)	0.0313 (11)	−0.0025 (8)	0.0102 (9)	−0.0021 (7)
C2	0.0342 (12)	0.0216 (11)	0.0381 (12)	0.0029 (9)	0.0109 (10)	0.0038 (9)

C1	0.0234 (10)	0.0201 (9)	0.0256 (10)	0.0020 (7)	0.0093 (8)	0.0027 (7)
C3	0.0368 (13)	0.0324 (13)	0.0423 (13)	0.0124 (10)	0.0093 (11)	0.0135 (10)
C4	0.0288 (12)	0.0443 (14)	0.0386 (14)	0.0045 (10)	0.0010 (11)	0.0052 (11)
C5	0.0299 (11)	0.0299 (12)	0.0355 (12)	−0.0029 (9)	0.0052 (10)	−0.0024 (9)

Geometric parameters (Å, °)

Zn1—O1	1.927 (2)	C13—H13A	0.9300
Zn1—O4^{i}	1.963 (2)	C15—H15A	0.9300
Zn1—N1^{ii}	2.097 (2)	N1—C9	1.323 (3)
Zn1—N2	2.102 (2)	N1—C1	1.385 (3)
N2—C19	1.317 (3)	N1—Zn1^{iv}	2.0974 (17)
N2—C11	1.386 (3)	O1—C10	1.280 (3)
O4—C20	1.277 (3)	O2—C10	1.221 (3)
O4—Zn1^{iii}	1.9626 (15)	C8—C7	1.364 (3)
O3—C20	1.227 (3)	C8—C9	1.407 (3)
C19—C18	1.403 (3)	C8—C10	1.508 (3)
C19—H19A	0.9300	C9—H9A	0.9300
C17—C18	1.365 (3)	C6—C7	1.410 (3)
C17—C16	1.410 (3)	C6—C1	1.415 (3)
C17—H17A	0.9300	C6—C5	1.415 (3)
C16—C11	1.414 (3)	C7—H7A	0.9300
C16—C15	1.419 (3)	C2—C3	1.366 (3)
C18—C20	1.505 (3)	C2—C1	1.409 (3)
C12—C13	1.370 (3)	C2—H2A	0.9300
C12—C11	1.408 (3)	C3—C4	1.401 (4)
C12—H12A	0.9300	C3—H3A	0.9300
C14—C15	1.362 (4)	C4—C5	1.365 (3)
C14—C13	1.404 (4)	C4—H4A	0.9300
C14—H14A	0.9300	C5—H5A	0.9300
O1—Zn1—O4^{i}	138.54 (7)	C14—C15—C16	120.1 (2)
O1—Zn1—N1^{ii}	110.34 (7)	C14—C15—H15A	119.9
O4^{i}—Zn1—N1^{ii}	100.64 (7)	C16—C15—H15A	119.9
O1—Zn1—N2	100.00 (7)	C9—N1—C1	118.26 (18)
O4^{i}—Zn1—N2	100.73 (7)	C9—N1—Zn1^{iv}	113.89 (14)
N1^{ii}—Zn1—N2	100.45 (7)	C1—N1—Zn1^{iv}	127.47 (14)
C19—N2—C11	118.00 (18)	C10—O1—Zn1	117.62 (14)
C19—N2—Zn1	116.85 (14)	C7—C8—C9	118.22 (18)
C11—N2—Zn1	124.84 (14)	C7—C8—C10	123.04 (18)
C20—O4—Zn1^{iii}	105.61 (14)	C9—C8—C10	118.7 (2)
N2—C19—C18	124.6 (2)	N1—C9—C8	124.18 (19)
N2—C19—H19A	117.7	N1—C9—H9A	117.9
C18—C19—H19A	117.7	C8—C9—H9A	117.9
C18—C17—C16	119.6 (2)	O2—C10—O1	125.8 (2)
C18—C17—H17A	120.2	O2—C10—C8	119.73 (19)
C16—C17—H17A	120.2	O1—C10—C8	114.51 (19)
C17—C16—C11	118.84 (19)	C7—C6—C1	118.64 (18)

C17—C16—C15	122.2 (2)	C7—C6—C5	122.1 (2)
C11—C16—C15	119.0 (2)	C1—C6—C5	119.22 (19)
C17—C18—C19	118.3 (2)	C8—C7—C6	120.00 (18)
C17—C18—C20	122.9 (2)	C8—C7—H7A	120.0
C19—C18—C20	118.8 (2)	C6—C7—H7A	120.0
O3—C20—O4	123.6 (2)	C3—C2—C1	120.0 (2)
O3—C20—C18	120.3 (2)	C3—C2—H2A	120.0
O4—C20—C18	116.2 (2)	C1—C2—H2A	120.0
C13—C12—C11	119.9 (2)	N1—C1—C2	120.02 (19)
C13—C12—H12A	120.1	N1—C1—C6	120.68 (18)
C11—C12—H12A	120.1	C2—C1—C6	119.30 (19)
C15—C14—C13	120.6 (2)	C2—C3—C4	120.9 (2)
C15—C14—H14A	119.7	C2—C3—H3A	119.5
C13—C14—H14A	119.7	C4—C3—H3A	119.5
N2—C11—C12	119.71 (19)	C5—C4—C3	120.5 (2)
N2—C11—C16	120.66 (18)	C5—C4—H4A	119.8
C12—C11—C16	119.63 (19)	C3—C4—H4A	119.8
C12—C13—C14	120.7 (2)	C4—C5—C6	120.1 (2)
C12—C13—H13A	119.6	C4—C5—H5A	120.0
C14—C13—H13A	119.6	C6—C5—H5A	120.0

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

Fig. 1

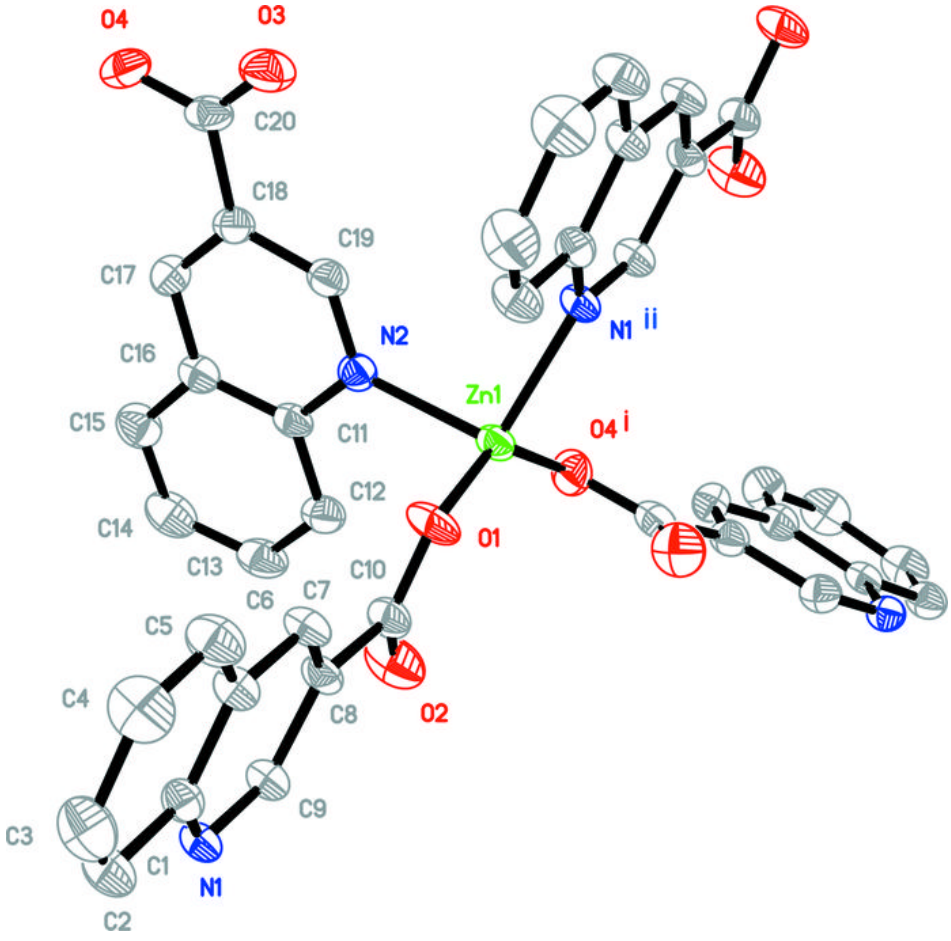
O4
O3
C20
C18
C19
C17
N2
C16
C15
C11
C12
C14
C13
C10
C7
C6
C5
C4
C8
O2
C9
C3
C1
N1
C2
Zn1
O1
O4 i
N1 ii

Fig. 2