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Poly[(μ_2-1,3-di-4-pyridylpropane-κ^2N:N')(μ_2-terephthalato-κ^2O:O')-zinc(II)]

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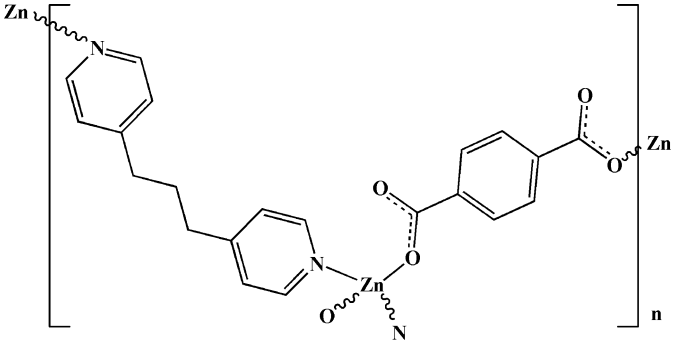
Key indicators: single-crystal X-ray study; T = 273 K; mean σ(C–C) = 0.005 Å; R factor = 0.036; wR factor = 0.095; data-to-parameter ratio = 13.2.

In the title compound, $[Zn(C_8H_4O_4)(C_{13}H_{14}N_2)]_n$, each Zn atom is coordinated by two terephthalate and two 1,3-di-4-pyridylpropane ligands in a distorted tetrahedral fashion. As a result, undulating layers are formed perpendicular to the b axis.

Related literature

For related literature, see: Dai *et al.* (2004).



Experimental

Crystal data

$[Zn(C_8H_4O_4)(C_{13}H_{14}N_2)]$
M_r = 427.74
Orthorhombic, *Pbca*
a = 11.7563 (4) Å
b = 16.3925 (5) Å
c = 19.7019 (7) Å
V = 3796.9 (2) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 1.32 mm^{-1}
T = 273 (2) K
0.20 × 0.14 × 0.10 mm

Data collection

Siemens SMART 1K CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.800, T_{max} = 0.850
28979 measured reflections
3350 independent reflections
2358 reflections with $I > 2\sigma(I)$
R_{int} = 0.084

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.036
$wR(F^2)$ = 0.096
S = 0.94
3350 reflections
253 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.79 e Å^{-3}
$\Delta\rho_{min}$ = −0.48 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Zn1—O3^{i}	1.952 (2)	Zn1—N1	2.058 (2)
Zn1—O2	2.005 (2)	Zn1—N2^{ii}	2.068 (3)
O3^{i}—Zn1—O2	119.62 (9)	O2—Zn1—N2^{ii}	97.03 (10)
O3^{i}—Zn1—N1	122.05 (10)	N1—Zn1—N2^{ii}	103.10 (9)
O2—Zn1—N1	105.80 (9)	C7—O2—Zn1	102.9 (2)

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

Data collection: *SMART* (Siemens, 1996*a*); cell refinement: *SAINT* (Siemens, 1996*a*); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Siemens, 1996*b*); 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: BT2419).

References

Dai, J.-C., Wu, X.-T., Hu, S.-M., Fu, Z.-Y., Zhang, J.-J., Du, W.-X., Zhang, H.-H. & Sun, R.-Q. (2004). *Eur. J. Inorg. Chem.* pp. 2096–2106.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Siemens (1996*a*). *SMART* and *SAINT*. Versions 4.0. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.
Siemens (1996*b*). *SHELXTL*. Version 5.06. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.

supplementary materials

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Poly[(μ_2-1,3-di-4-pyridylpropane-κ^2N:N')(μ_2-terephthalato-κ^2O:O')zinc(II)]

E Yang, X.-C. Song, Y.-D. Lin and S.-Z. Shen

Comment

Ligands containing O– or N-donors can bind metal centers. Thus, they serve as building blocks to construct supramolecular architectures. Herein we report the structure of $[Zn(tp)(bpp)]_n$ (tp = terephthalate, bpp = 1,3-di-4-pyridylpropane).

As shown in Figure 1, the asymmetric unit of the title compound is composed of a four-coordinate Zn(II)center, a tp ligand and a bpp ligand, in which each Zinc center is coordinated in a distorted tetrahedral geometry to two tp ligands and two bpp ligands through two carboxylate groups and two nitrogen donors. An isostructural compound Cd(tp)(bpp) has been reported (Dai *et al.*, 2004).

Experimental

A mixture of $Zn(NO_3)_2$ (0.145 g, 0.5 mmol), Na_2CO_3 (0.05 g, 0.5 mmol), terephthalate (0.08 g, 0.5 mmol), 1,3-di-4-pyridylpropane (0.09 g, 0.5 mmol) and H_2O (10 ml) was sealed in a 25 ml stainless-steel reactor with a Teflon-lined stainless steel reactor and was heated at 393 K for 3 d. On completion of the reaction, the reactor was cooled slowly to room temperature and the mixture was filtered, giving colorless single crystals suitable for X-ray analysis.

Refinement

All H atoms were placed at calculated positions, and refined with isotropic displacement parameters, using a riding model [C—H 0.93Å and U_{iso}(H) = 1.2U_{eq}(C)].

Figures

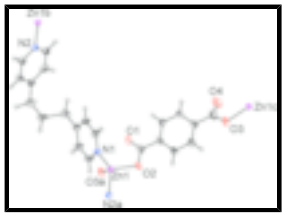

Fig. 1. A view of the title compound, showing 50% probability displacement ellipsoids [symmetry code: (*a*) −1 + *x*,*y*,*z*; (*b*) 1 + *x*,*y*,*z*; (*c*) *x*,1/2 − *y*,-1/2 + *z*.].

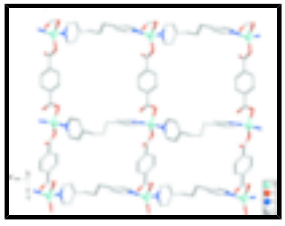

Fig. 2. Packing diagram of the title compound.

Poly[(μ$_2$-1,3-di-4-pyridylpropane-κ^2*N*:*N*')(μ$_2$-terephthalato- κ^2*O*:*O*')zinc(II)]

Crystal data

$[Zn(C_8H_4O_4)(C_{13}H_{14}N_2)]$	F_{000} = 1760
M_r = 427.74	D_x = 1.497 Mg m^{-3}
Orthorhombic, *Pbca*	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: -P 2ac 2ab	θ = 2.1–25.0º
a = 11.7563 (4) Å	μ = 1.32 mm^{-1}
b = 16.3925 (5) Å	*T* = 273 (2) K
c = 19.7019 (7) Å	Prism, colorless
V = 3796.9 (2) Å^3	0.20 × 0.14 × 0.10 mm
Z = 8	

Data collection

Siemens SMART 1K CCD area-detector diffractometer	3350 independent reflections
Radiation source: fine-focus sealed tube	2358 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.084
T = 273(2) K	θ_{max} = 25.0º
φ and ω scans	θ_{min} = 2.1º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	*h* = −13→13
T_{min} = 0.800, T_{max} = 0.850	*k* = −19→19
28979 measured reflections	*l* = −22→23

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
$wR(F^2)$ = 0.096	$w = 1/[\sigma^2(F_o^2) + (0.0511P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 0.94	$(\Delta/\sigma)_{max}$ = 0.001
3350 reflections	$\Delta\rho_{max}$ = 0.79 e Å^{-3}
253 parameters	$\Delta\rho_{min}$ = −0.48 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	0.03302 (3)	0.11133 (2)	0.628053 (18)	0.02148 (13)
O1	0.13272 (19)	0.23097 (12)	0.56729 (11)	0.0316 (6)
O2	−0.01621 (18)	0.15596 (12)	0.53795 (11)	0.0292 (5)
O3	0.0110 (2)	0.32360 (13)	0.20996 (12)	0.0348 (6)
O4	0.1115 (3)	0.42520 (19)	0.25268 (15)	0.0705 (10)
N1	0.1814 (2)	0.04851 (14)	0.60977 (13)	0.0215 (6)
N2	0.9127 (2)	0.01958 (15)	0.63451 (13)	0.0232 (6)
C1	0.0592 (3)	0.24763 (17)	0.45592 (17)	0.0220 (7)
C2	−0.0246 (3)	0.22873 (18)	0.40925 (17)	0.0255 (7)
H2A	−0.0842	0.1945	0.4217	0.031*
C3	−0.0204 (3)	0.26049 (18)	0.34390 (18)	0.0288 (8)
H3A	−0.0761	0.2464	0.3125	0.035*
C4	0.0664 (3)	0.31303 (19)	0.32547 (17)	0.0285 (8)
C5	0.1504 (3)	0.3327 (2)	0.37208 (18)	0.0309 (8)
H5A	0.2086	0.3682	0.3600	0.037*
C6	0.1473 (3)	0.29935 (18)	0.43646 (17)	0.0264 (8)
H6A	0.2048	0.3116	0.4672	0.032*
C7	0.0599 (3)	0.21031 (18)	0.52526 (17)	0.0259 (8)
C8	0.0673 (3)	0.3545 (2)	0.2571 (2)	0.0440 (10)
C9	0.1854 (3)	−0.03344 (18)	0.60805 (18)	0.0295 (8)
H9A	0.1177	−0.0623	0.6123	0.035*
C10	0.2853 (3)	−0.07658 (19)	0.60027 (19)	0.0317 (9)
H10A	0.2839	−0.1333	0.5988	0.038*
C11	0.3881 (3)	−0.03531 (18)	0.59467 (17)	0.0238 (7)
C12	0.3835 (3)	0.04878 (18)	0.59680 (18)	0.0288 (8)
H12A	0.4501	0.0790	0.5928	0.035*
C13	0.2810 (3)	0.08814 (19)	0.60476 (18)	0.0297 (8)
H13A	0.2807	0.1448	0.6068	0.036*
C14	0.5000 (2)	−0.07953 (19)	0.58788 (18)	0.0281 (8)
H14A	0.5587	−0.0406	0.5757	0.034*
H14B	0.4943	−0.1190	0.5514	0.034*
C15	0.5349 (3)	−0.12322 (18)	0.65255 (19)	0.0298 (8)
H15A	0.4779	−0.1639	0.6636	0.036*
H15B	0.5372	−0.0841	0.6895	0.036*
C16	0.6511 (3)	−0.16502 (19)	0.6468 (2)	0.0342 (9)
H16A	0.6632	−0.1994	0.6863	0.041*
H16B	0.6521	−0.1996	0.6069	0.041*
C17	0.7464 (3)	−0.10311 (19)	0.64198 (17)	0.0267 (8)

C18	0.7910 (3)	−0.0679 (2)	0.69933 (18)	0.0340 (9)
H18A	0.7660	−0.0847	0.7418	0.041*
C19	0.8727 (3)	−0.0077 (2)	0.69445 (18)	0.0327 (8)
H19A	0.9012	0.0151	0.7342	0.039*
C20	0.7884 (3)	−0.07596 (18)	0.58023 (18)	0.0287 (8)
H20A	0.7619	−0.0988	0.5400	0.034*
C21	0.8697 (3)	−0.01512 (18)	0.57826 (17)	0.0255 (8)
H21A	0.8957	0.0026	0.5362	0.031*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn1	0.0232 (2)	0.0222 (2)	0.0190 (2)	0.00177 (16)	−0.00028 (17)	−0.00100 (16)
O1	0.0448 (15)	0.0261 (12)	0.0240 (14)	0.0051 (11)	−0.0072 (12)	0.0018 (11)
O2	0.0345 (13)	0.0268 (11)	0.0262 (14)	0.0001 (11)	0.0032 (11)	0.0076 (11)
O3	0.0539 (16)	0.0316 (12)	0.0189 (13)	−0.0003 (11)	−0.0016 (12)	0.0017 (11)
O4	0.085 (2)	0.0718 (19)	0.055 (2)	−0.0278 (18)	−0.0141 (18)	0.0243 (17)
N1	0.0203 (14)	0.0214 (13)	0.0228 (16)	−0.0028 (11)	0.0007 (12)	−0.0019 (12)
N2	0.0205 (14)	0.0287 (14)	0.0205 (16)	0.0023 (12)	0.0001 (12)	0.0017 (13)
C1	0.0280 (19)	0.0168 (15)	0.0214 (18)	0.0058 (13)	0.0034 (15)	−0.0008 (13)
C2	0.0313 (19)	0.0207 (15)	0.0245 (19)	−0.0027 (14)	0.0012 (16)	0.0009 (15)
C3	0.038 (2)	0.0252 (17)	0.0232 (19)	0.0006 (16)	−0.0050 (17)	−0.0031 (15)
C4	0.033 (2)	0.0289 (18)	0.023 (2)	0.0028 (15)	0.0037 (16)	0.0044 (15)
C5	0.0260 (18)	0.0377 (19)	0.029 (2)	−0.0033 (15)	0.0033 (16)	0.0079 (17)
C6	0.0237 (18)	0.0296 (17)	0.026 (2)	0.0025 (14)	−0.0024 (15)	0.0000 (16)
C7	0.033 (2)	0.0210 (16)	0.0234 (19)	0.0119 (15)	0.0032 (16)	−0.0009 (15)
C8	0.052 (3)	0.045 (2)	0.035 (3)	−0.006 (2)	−0.002 (2)	0.011 (2)
C9	0.0195 (17)	0.0247 (17)	0.044 (2)	−0.0044 (14)	0.0008 (16)	−0.0018 (16)
C10	0.0233 (19)	0.0201 (16)	0.052 (2)	−0.0008 (14)	0.0017 (17)	−0.0055 (17)
C11	0.0230 (18)	0.0279 (17)	0.0203 (18)	−0.0016 (14)	0.0000 (15)	−0.0023 (15)
C12	0.0206 (18)	0.0265 (17)	0.039 (2)	−0.0057 (14)	0.0010 (16)	0.0011 (17)
C13	0.029 (2)	0.0210 (16)	0.039 (2)	−0.0021 (15)	−0.0015 (16)	−0.0024 (15)
C14	0.0195 (18)	0.0287 (17)	0.036 (2)	−0.0005 (14)	0.0030 (15)	−0.0086 (16)
C15	0.0194 (17)	0.0265 (17)	0.044 (2)	0.0004 (14)	0.0048 (16)	−0.0012 (16)
C16	0.0244 (19)	0.0278 (18)	0.050 (3)	−0.0006 (15)	0.0047 (17)	0.0024 (17)
C17	0.0197 (17)	0.0250 (16)	0.035 (2)	0.0071 (14)	0.0026 (15)	0.0022 (16)
C18	0.030 (2)	0.045 (2)	0.026 (2)	−0.0064 (17)	0.0025 (17)	0.0096 (17)
C19	0.032 (2)	0.045 (2)	0.021 (2)	−0.0058 (17)	−0.0010 (16)	0.0012 (17)
C20	0.0231 (18)	0.0309 (18)	0.032 (2)	0.0004 (15)	−0.0003 (16)	−0.0087 (16)
C21	0.0244 (18)	0.0331 (18)	0.0191 (19)	0.0000 (15)	0.0031 (15)	−0.0018 (15)

Geometric parameters (Å, °)

Zn1—O3^{i}	1.952 (2)	C9—C10	1.380 (4)
Zn1—O2	2.005 (2)	C9—H9A	0.9300
Zn1—N1	2.058 (2)	C10—C11	1.389 (4)
Zn1—N2^{ii}	2.068 (3)	C10—H10A	0.9300
O1—C7	1.239 (4)	C11—C12	1.380 (4)

O2—C7	1.287 (4)	C11—C14	1.508 (4)
O3—C8	1.248 (4)	C12—C13	1.375 (4)
O3—Zn1^{iii}	1.952 (2)	C12—H12A	0.9300
O4—C8	1.273 (4)	C13—H13A	0.9300
N1—C13	1.342 (4)	C14—C15	1.518 (5)
N1—C9	1.345 (4)	C14—H14A	0.9700
N2—C21	1.345 (4)	C14—H14B	0.9700
N2—C19	1.348 (4)	C15—C16	1.533 (4)
N2—Zn1^{iv}	2.068 (3)	C15—H15A	0.9700
C1—C2	1.382 (4)	C15—H15B	0.9700
C1—C6	1.392 (4)	C16—C17	1.515 (4)
C1—C7	1.497 (4)	C16—H16A	0.9700
C2—C3	1.390 (5)	C16—H16B	0.9700
C2—H2A	0.9300	C17—C18	1.373 (5)
C3—C4	1.384 (4)	C17—C20	1.386 (5)
C3—H3A	0.9300	C18—C19	1.380 (4)
C4—C5	1.386 (5)	C18—H18A	0.9300
C4—C8	1.509 (5)	C19—H19A	0.9300
C5—C6	1.382 (4)	C20—C21	1.381 (4)
C5—H5A	0.9300	C20—H20A	0.9300
C6—H6A	0.9300	C21—H21A	0.9300
O3^{i}—Zn1—O2	119.62 (9)	C11—C10—H10A	120.0
O3^{i}—Zn1—N1	122.05 (10)	C12—C11—C10	116.7 (3)
O2—Zn1—N1	105.80 (9)	C12—C11—C14	121.1 (3)
O3^{i}—Zn1—N2^{ii}	104.82 (10)	C10—C11—C14	122.1 (3)
O2—Zn1—N2^{ii}	97.03 (10)	C13—C12—C11	120.4 (3)
N1—Zn1—N2^{ii}	103.10 (9)	C13—C12—H12A	119.8
C7—O2—Zn1	102.9 (2)	C11—C12—H12A	119.8
C8—O3—Zn1^{iii}	108.9 (2)	N1—C13—C12	123.0 (3)
C13—N1—C9	116.8 (3)	N1—C13—H13A	118.5
C13—N1—Zn1	120.7 (2)	C12—C13—H13A	118.5
C9—N1—Zn1	122.2 (2)	C11—C14—C15	112.8 (3)
C21—N2—C19	116.8 (3)	C11—C14—H14A	109.0
C21—N2—Zn1^{iv}	120.9 (2)	C15—C14—H14A	109.0
C19—N2—Zn1^{iv}	122.3 (2)	C11—C14—H14B	109.0
C2—C1—C6	118.9 (3)	C15—C14—H14B	109.0
C2—C1—C7	121.3 (3)	H14A—C14—H14B	107.8
C6—C1—C7	119.7 (3)	C14—C15—C16	113.0 (3)
C1—C2—C3	120.5 (3)	C14—C15—H15A	109.0
C1—C2—H2A	119.8	C16—C15—H15A	109.0
C3—C2—H2A	119.8	C14—C15—H15B	109.0
C4—C3—C2	120.1 (3)	C16—C15—H15B	109.0
C4—C3—H3A	119.9	H15A—C15—H15B	107.8
C2—C3—H3A	119.9	C17—C16—C15	111.4 (3)
C3—C4—C5	119.7 (3)	C17—C16—H16A	109.4
C3—C4—C8	121.3 (3)	C15—C16—H16A	109.4
C5—C4—C8	118.8 (3)	C17—C16—H16B	109.4

C6—C5—C4	119.8 (3)	C15—C16—H16B	109.4
C6—C5—H5A	120.1	H16A—C16—H16B	108.0
C4—C5—H5A	120.1	C18—C17—C20	116.8 (3)
C5—C6—C1	120.9 (3)	C18—C17—C16	120.8 (3)
C5—C6—H6A	119.6	C20—C17—C16	122.3 (3)
C1—C6—H6A	119.6	C17—C18—C19	120.6 (3)
O1—C7—O2	122.7 (3)	C17—C18—H18A	119.7
O1—C7—C1	120.1 (3)	C19—C18—H18A	119.7
O2—C7—C1	117.2 (3)	N2—C19—C18	122.8 (3)
O3—C8—O4	122.4 (4)	N2—C19—H19A	118.6
O3—C8—C4	118.5 (3)	C18—C19—H19A	118.6
O4—C8—C4	118.3 (4)	C21—C20—C17	120.2 (3)
N1—C9—C10	123.0 (3)	C21—C20—H20A	119.9
N1—C9—H9A	118.5	C17—C20—H20A	119.9
C10—C9—H9A	118.5	N2—C21—C20	122.8 (3)
C9—C10—C11	120.0 (3)	N2—C21—H21A	118.6
C9—C10—H10A	120.0	C20—C21—H21A	118.6

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

Fig. 1

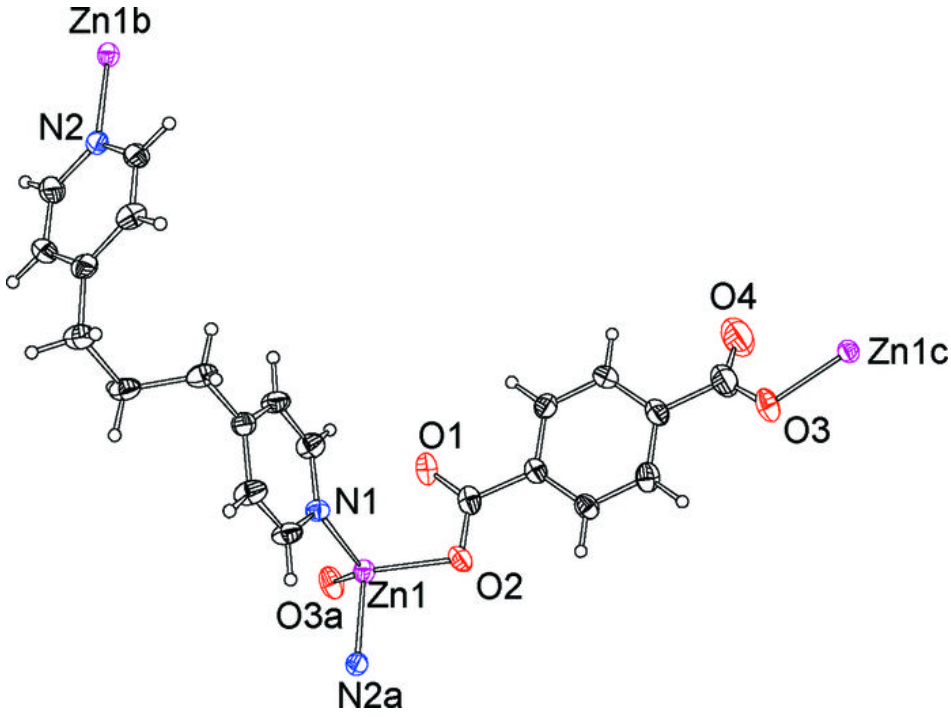

Fig. 2