

## Poly[tetrakis( $\mu_4$ -4,6-dimethyl-5-nitrobenzene-1,3-dicarboxylato- $\kappa^2O^1:O^1':O^3:O^3'$ )bis(pyridine- $\kappa N$ )dizinc]

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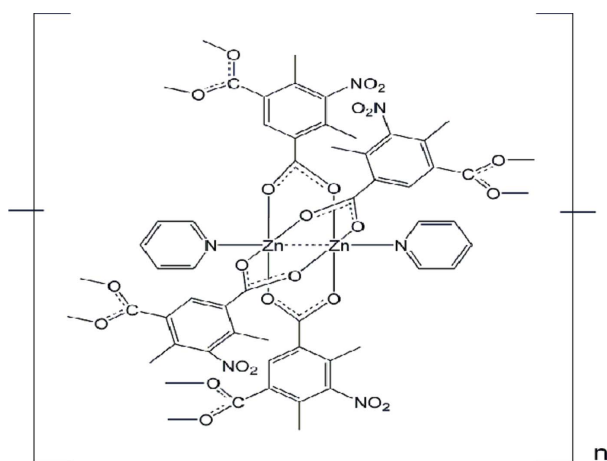
Received 19 January 2011; accepted 7 April 2011

Key indicators: single-crystal X-ray study;  $T = 298$  K; mean  $\sigma(C-C) = 0.004$  Å;  $R$  factor = 0.033;  $wR$  factor = 0.081; data-to-parameter ratio = 16.2.

In the title complex,  $[Zn_2(C_{10}H_7NO_6)_2(C_5H_5N)_2]_n$ , the repeat unit is a centrosymmetric tetra-carboxylato- $O, O'$ -bridged dimer in which each  $Zn^{II}$  atom is five-coordinated by four O atoms from different dianionic 4,6-dimethyl-5-nitroisophthalate ligands [ $Zn-O = 2.0283(18)$ – $2.0540(19)$  Å] and one N atom from a pyridine molecule [ $Zn-N = 2.030(2)$  Å] in the axial site of a slightly distorted square-pyramidal coordination sphere. The  $Zn \cdots Zn$  separation is  $2.9750(6)$  Å. The complex dimers are extended into a two-dimensional polymeric structure parallel to (100) through bridges provided by the second carboxylate group of the ligand.

### Related literature

For the structure of a similar but discrete tetra-carboxylato-bridged  $Zn_2$  dimer, see: Yu *et al.* (2011).



### Experimental

#### Crystal data

$[Zn(C_{10}H_7NO_6)(C_5H_5N)]$   
 $M_r = 381.64$   
 Monoclinic,  $P2_1/c$   
 $a = 10.2947(9)$  Å  
 $b = 11.8526(10)$  Å  
 $c = 12.8501(11)$  Å  
 $\beta = 97.933(2)^\circ$

$V = 1553.0(2)$  Å<sup>3</sup>  
 $Z = 4$   
 Mo  $K\alpha$  radiation  
 $\mu = 1.62$  mm<sup>-1</sup>  
 $T = 298$  K  
 $0.12 \times 0.10 \times 0.08$  mm

#### Data collection

Bruker APEXII CCD area-detector diffractometer  
 Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)  
 $T_{min} = 0.824$ ,  $T_{max} = 0.879$   
 8899 measured reflections  
 3525 independent reflections  
 2750 reflections with  $I > 2\sigma(I)$   
 $R_{int} = 0.029$

#### Refinement

$R[F^2 > 2\sigma(F^2)] = 0.033$   
 $wR(F^2) = 0.081$   
 $S = 1.03$   
 3525 reflections

217 parameters  
 H-atom parameters constrained  
 $\Delta\rho_{max} = 0.43$  e Å<sup>-3</sup>  
 $\Delta\rho_{min} = -0.43$  e Å<sup>-3</sup>

Data collection: *APEX2* (Bruker, 2007); cell refinement: *SAINT-Plus* (Bruker, 2007); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

This work was supported by the Scientific and Technological Project of Shandong Province (2008SGG0809) and Doctoral Foundation of Shandong Province (2009SBS0913).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: ZS2089).

### References

- Bruker (2007). *APEX2* and *SAINT-Plus*. Bruker AXS Inc., Madison, Wisconsin, USA.  
 Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.  
 Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.  
 Yu, Z.-Y., Lin, K.-H., Zhang, F.-F., Shao, M. & Li, M. (2011). *Acta Cryst.* **E67**, m206.

**supplementary materials**

*Acta Cryst.* (2011). E67, m586 [ doi:10.1107/S1600536811013092 ]

**Poly[tetrakis( $\mu$ -4,6-dimethyl-5-nitrobenzene-1,3-dicarboxylato- $\kappa^2 O^1:O^1':O^3:O^3'$ )bis(pyridine- $\kappa N$ )dizinc]**

**Q.-Y. Ma, R.-F. Guan and G.-Z. Li**

**Comment**

The title complex  $[Zn_2(C_{10}H_7NO_6)_2(C_5H_5N)_2]_n$  (I) was obtained by chance when we were attempting to prepare some porous metal-organic framework materials by the reaction of 4,6-dimethyl-5-nitroisophthalic acid with  $Zn(NO_3)_2$ . In (I), the repeating unit is a centrosymmetric tetra-carboxylato  $O, O'$  bridged dimer (Fig. 1) in which each  $Zn^{II}$  is five-coordinated by four O atoms from different dianionic 4,6-dimethyl-5-nitroisophthalate ligands [ $Zn-O$ , 2.0283 (18)–2.0540 (19) Å] and one N atom from a pyridine molecule [ $Zn-N$ , 2.030 (2) Å] in the axial site of a slightly distorted square pyramidal coordination sphere. Each of the Zn atoms has an approximately square-pyramidal environment, with four O atoms in a plane and the pyridine N atom at the apical site. The Zn–Zn separation in the dimer is 2.9750 (6) Å. This dimeric unit is similar to that found in the structure of the tetra-benzoato-bridged but discrete  $Zn_2$  dimer with 4-(dimethylamino)pyridine (Yu *et al.*, 2011). The complex dimers in (I) are extended into a two-dimensional polymer structure through bridges provided by the second carboxylate group of the ligand (Figs. 2, 3).

**Experimental**

4,6-Dimethyl-5-nitroisophthalic acid (2 mg, 0.0046 mmol) and  $Zn(NO_3)_2$  (4 mg, 0.0137 mmol) were dissolved in 1 ml of a mixed DMSO– $H_2O$  solvent (2:1) and 2 drops pyridine were added. This solution was sealed in a Pyrex glass tube and heated to 120° C over a period of 10 h, and then maintained at this temperature for 50 h, after which it was cooled to room temperature over 17 h. Colourless rod crystals were obtained, which were filtered, washed with water and dried in air.

**Refinement**

All H atoms were placed in calculated positions ( $C-H = 0.93-0.96$  Å) and refined in a riding mode with  $U_{iso}(H) = 1.2U_{eq}(C)$ . The methyl H atoms are rotationally disordered over six equal half-occupancy sites.

**Figures**

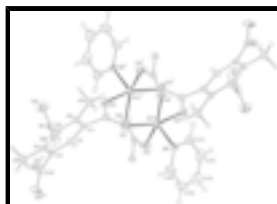


Fig. 1. The atom numbering scheme for the centrosymmetric dimeric unit in the title compound with displacement ellipsoids drawn at the 30% probability level. Symmetry codes are: (i)  $-x+1, -y, -z+1$ ; (ii)  $-x+1, y-1/2, -z-3/2$ ; (iii)  $x, -y+1/2, z+1/2$ . The second set of hydrogen atoms on the 50% rotationally-disordered methyl groups (C8 and C9) are omitted.

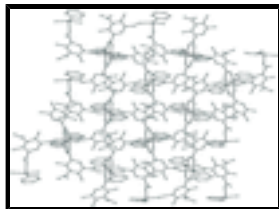


Fig. 2. The two-dimensional polymeric extension of the title compound viewed down the *a* axial direction.

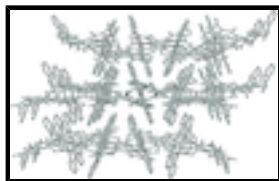


Fig. 3. The packed structure of the title compound viewed down the *c* axial direction.

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### Crystal data

[Zn(C<sub>10</sub>H<sub>7</sub>NO<sub>6</sub>)(C<sub>5</sub>H<sub>5</sub>N)]

$M_r = 381.64$

Monoclinic,  $P2_1/c$

Hall symbol: -P 2ybc

$a = 10.2947$  (9) Å

$b = 11.8526$  (10) Å

$c = 12.8501$  (11) Å

$\beta = 97.933$  (2)°

$V = 1553.0$  (2) Å<sup>3</sup>

$Z = 4$

$F(000) = 776$

$D_x = 1.632$  Mg m<sup>-3</sup>

Mo  $K\alpha$  radiation,  $\lambda = 0.71073$  Å

Cell parameters from 2968 reflections

$\theta = 2.3$ – $26.1$ °

$\mu = 1.62$  mm<sup>-1</sup>

$T = 298$  K

Rod, colourless

$0.12 \times 0.10 \times 0.08$  mm

### Data collection

Bruker APEXII CCD area-detector diffractometer

Radiation source: fine-focus sealed tube graphite

$\phi$  and  $\omega$  scans

Absorption correction: multi-scan (SADABS; Sheldrick, 1996)

$T_{\min} = 0.824$ ,  $T_{\max} = 0.879$

8899 measured reflections

3525 independent reflections

2750 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.029$

$\theta_{\max} = 27.7$ °,  $\theta_{\min} = 2.0$ °

$h = -8 \rightarrow 13$

$k = -15 \rightarrow 15$

$l = -16 \rightarrow 16$

### Refinement

Refinement on  $F^2$

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.033$

$wR(F^2) = 0.081$

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

$S = 1.03$	$w = 1/[\sigma^2(F_o^2) + (0.0353P)^2 + 0.6981P]$
3525 reflections	where $P = (F_o^2 + 2F_c^2)/3$
217 parameters	$(\Delta/\sigma)_{\max} = 0.001$
0 restraints	$\Delta\rho_{\max} = 0.43 \text{ e } \text{\AA}^{-3}$
	$\Delta\rho_{\min} = -0.43 \text{ e } \text{\AA}^{-3}$

*Special details*

**Geometry.** Bond distances, angles etc. have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell esds are taken into account in the estimation of distances, angles and torsion angles

**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 ( $\text{\AA}^2$ )*

	$x$	$y$	$z$	$U_{\text{iso}}^*/U_{\text{eq}}$	Occ. (<1)
Zn1	0.63668 (3)	-0.03544 (2)	0.53898 (2)	0.0233 (1)	
O1	0.65410 (19)	0.13708 (16)	0.54695 (18)	0.0546 (8)	
O2	0.4496 (2)	0.18909 (15)	0.49411 (17)	0.0508 (7)	
O3	0.55390 (18)	-0.03094 (18)	0.67374 (14)	0.0454 (7)	
O4	0.6491 (2)	-0.02213 (19)	0.38329 (14)	0.0499 (7)	
O5	0.7497 (2)	0.62087 (19)	0.42547 (16)	0.0600 (8)	
O6	0.9095 (2)	0.5865 (2)	0.5453 (2)	0.0703 (10)	
N1	0.7959 (2)	0.57613 (18)	0.50579 (17)	0.0352 (7)	
N2	0.8232 (2)	-0.07998 (17)	0.59645 (16)	0.0298 (6)	
C1	0.5998 (2)	0.32743 (18)	0.56737 (17)	0.0245 (7)	
C2	0.6751 (2)	0.39863 (19)	0.51257 (17)	0.0253 (7)	
C3	0.7112 (2)	0.50127 (19)	0.56086 (18)	0.0258 (7)	
C4	0.6795 (2)	0.53868 (18)	0.65714 (17)	0.0253 (7)	
C5	0.5997 (2)	0.46553 (19)	0.70674 (17)	0.0235 (6)	
C6	0.5600 (2)	0.36307 (19)	0.66100 (17)	0.0260 (7)	
C7	0.5647 (3)	0.2080 (2)	0.53197 (18)	0.0283 (7)	
C8	0.7134 (3)	0.3664 (2)	0.4076 (2)	0.0382 (9)	
C9	0.7241 (3)	0.6519 (2)	0.7019 (2)	0.0416 (9)	
C10	0.5618 (2)	0.48883 (19)	0.81384 (17)	0.0259 (7)	
C11	0.9056 (3)	-0.1198 (3)	0.5336 (2)	0.0455 (10)	
C12	1.0338 (3)	-0.1460 (3)	0.5712 (3)	0.0625 (14)	
C13	1.0764 (3)	-0.1350 (3)	0.6760 (3)	0.0739 (15)	
C14	0.9916 (4)	-0.0970 (4)	0.7408 (3)	0.0817 (14)	
C15	0.8655 (3)	-0.0695 (3)	0.6982 (2)	0.0559 (11)	
H6A	0.50520	0.31680	0.69400	0.0310*	
H8A	0.67890	0.29300	0.38790	0.0570*	0.500
H8B	0.80720	0.36510	0.41230	0.0570*	0.500
H8C	0.67830	0.42060	0.35570	0.0570*	0.500

## supplementary materials

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H8D	0.76410	0.42610	0.38270	0.0570*	0.500
H8E	0.63580	0.35410	0.35830	0.0570*	0.500
H8F	0.76460	0.29850	0.41490	0.0570*	0.500
H9A	0.69250	0.66260	0.76810	0.0620*	0.500
H9B	0.69000	0.71040	0.65410	0.0620*	0.500
H9C	0.81820	0.65490	0.71220	0.0620*	0.500
H9D	0.77470	0.68930	0.65480	0.0620*	0.500
H9E	0.77710	0.64150	0.76880	0.0620*	0.500
H9F	0.64890	0.69700	0.71080	0.0620*	0.500
H11A	0.87570	-0.13000	0.46260	0.0550*	
H12A	1.09060	-0.17090	0.52580	0.0750*	
H13A	1.16230	-0.15320	0.70300	0.0890*	
H14A	1.01850	-0.08980	0.81260	0.0980*	
H15A	0.80810	-0.04270	0.74230	0.0670*	

### Atomic displacement parameters ( $\text{\AA}^2$ )

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
Zn1	0.0253 (2)	0.0240 (2)	0.0210 (1)	0.0011 (1)	0.0044 (1)	0.0003 (1)
O1	0.0406 (12)	0.0231 (10)	0.0991 (18)	0.0015 (9)	0.0057 (12)	-0.0082 (10)
O2	0.0471 (12)	0.0278 (10)	0.0708 (14)	-0.0077 (9)	-0.0156 (10)	-0.0060 (9)
O3	0.0346 (10)	0.0791 (15)	0.0245 (9)	0.0051 (10)	0.0108 (8)	0.0017 (9)
O4	0.0510 (12)	0.0788 (15)	0.0218 (9)	0.0216 (11)	0.0114 (9)	0.0125 (9)
O5	0.0789 (16)	0.0588 (14)	0.0439 (12)	-0.0111 (12)	0.0142 (11)	0.0230 (11)
O6	0.0460 (14)	0.0838 (18)	0.0819 (18)	-0.0243 (13)	0.0113 (13)	0.0200 (15)
N1	0.0456 (14)	0.0298 (11)	0.0338 (12)	-0.0076 (10)	0.0185 (10)	-0.0013 (9)
N2	0.0285 (11)	0.0286 (10)	0.0324 (11)	0.0014 (9)	0.0047 (9)	-0.0001 (9)
C1	0.0281 (12)	0.0225 (11)	0.0229 (11)	-0.0012 (9)	0.0036 (9)	-0.0028 (9)
C2	0.0302 (12)	0.0246 (12)	0.0220 (11)	0.0007 (10)	0.0064 (9)	-0.0024 (9)
C3	0.0298 (13)	0.0227 (11)	0.0261 (12)	-0.0020 (9)	0.0077 (10)	0.0036 (9)
C4	0.0317 (13)	0.0204 (11)	0.0239 (11)	-0.0007 (10)	0.0043 (9)	-0.0005 (9)
C5	0.0278 (12)	0.0243 (11)	0.0189 (10)	0.0017 (10)	0.0047 (9)	-0.0002 (9)
C6	0.0303 (13)	0.0243 (12)	0.0244 (12)	-0.0048 (9)	0.0079 (10)	0.0010 (9)
C7	0.0412 (15)	0.0237 (12)	0.0215 (11)	-0.0049 (11)	0.0100 (10)	-0.0010 (9)
C8	0.0552 (18)	0.0334 (14)	0.0293 (13)	0.0001 (12)	0.0171 (12)	-0.0026 (11)
C9	0.0616 (19)	0.0268 (13)	0.0390 (15)	-0.0123 (13)	0.0160 (14)	-0.0078 (11)
C10	0.0355 (14)	0.0236 (12)	0.0195 (11)	0.0024 (10)	0.0075 (10)	0.0011 (9)
C11	0.0412 (17)	0.0514 (18)	0.0456 (16)	0.0133 (14)	0.0122 (13)	0.0050 (14)
C12	0.0423 (19)	0.066 (2)	0.083 (3)	0.0198 (16)	0.0219 (18)	0.004 (2)
C13	0.0309 (18)	0.073 (3)	0.111 (3)	0.0081 (17)	-0.0148 (19)	-0.020 (2)
C14	0.053 (2)	0.110 (3)	0.071 (2)	0.023 (2)	-0.0308 (19)	-0.039 (2)
C15	0.0443 (18)	0.074 (2)	0.0458 (18)	0.0131 (16)	-0.0064 (14)	-0.0239 (16)

### Geometric parameters ( $\text{\AA}$ , $^\circ$ )

Zn1—O1	2.0540 (19)	C5—C10	1.507 (3)
Zn1—O3	2.0336 (18)	C11—C12	1.377 (4)
Zn1—O4	2.0283 (18)	C12—C13	1.364 (5)
Zn1—N2	2.030 (2)	C13—C14	1.363 (5)

Zn1—O2 <sup>i</sup>	2.0450 (19)	C14—C15	1.377 (5)
O1—C7	1.242 (3)	C6—H6A	0.9300
O2—C7	1.238 (4)	C8—H8A	0.9600
O3—C10 <sup>ii</sup>	1.246 (3)	C8—H8B	0.9600
O4—C10 <sup>iii</sup>	1.240 (3)	C8—H8C	0.9600
O5—N1	1.199 (3)	C8—H8D	0.9600
O6—N1	1.215 (3)	C8—H8E	0.9600
N1—C3	1.490 (3)	C8—H8F	0.9600
N2—C11	1.336 (4)	C9—H9A	0.9600
N2—C15	1.326 (3)	C9—H9B	0.9600
C1—C2	1.400 (3)	C9—H9C	0.9600
C1—C6	1.389 (3)	C9—H9D	0.9600
C1—C7	1.515 (3)	C9—H9E	0.9600
C2—C3	1.393 (3)	C9—H9F	0.9600
C2—C8	1.506 (3)	C11—H11A	0.9300
C3—C4	1.395 (3)	C12—H12A	0.9300
C4—C5	1.406 (3)	C13—H13A	0.9300
C4—C9	1.507 (3)	C14—H14A	0.9300
C5—C6	1.386 (3)	C15—H15A	0.9300
O1—Zn1—O3	88.59 (9)	N2—C11—C12	121.7 (3)
O1—Zn1—O4	87.41 (9)	C11—C12—C13	119.1 (3)
O1—Zn1—N2	99.73 (8)	C12—C13—C14	119.3 (3)
O1—Zn1—O2 <sup>i</sup>	158.34 (8)	C13—C14—C15	118.9 (3)
O3—Zn1—O4	158.24 (8)	N2—C15—C14	122.2 (3)
O3—Zn1—N2	100.58 (8)	C1—C6—H6A	119.00
O2 <sup>i</sup> —Zn1—O3	88.82 (8)	C5—C6—H6A	119.00
O4—Zn1—N2	101.18 (8)	C2—C8—H8A	109.00
O2 <sup>i</sup> —Zn1—O4	87.07 (9)	C2—C8—H8B	109.00
O2 <sup>i</sup> —Zn1—N2	101.89 (8)	C2—C8—H8C	109.00
Zn1—O1—C7	127.48 (18)	C2—C8—H8D	109.00
Zn1 <sup>i</sup> —O2—C7	127.43 (17)	C2—C8—H8E	109.00
Zn1—O3—C10 <sup>ii</sup>	129.39 (16)	C2—C8—H8F	109.00
Zn1—O4—C10 <sup>iii</sup>	126.61 (17)	H8A—C8—H8B	110.00
O5—N1—O6	124.0 (2)	H8A—C8—H8C	109.00
O5—N1—C3	118.9 (2)	H8B—C8—H8C	109.00
O6—N1—C3	117.0 (2)	H8D—C8—H8E	109.00
Zn1—N2—C11	121.32 (17)	H8D—C8—H8F	110.00
Zn1—N2—C15	120.00 (19)	H8E—C8—H8F	109.00
C11—N2—C15	118.7 (2)	C4—C9—H9A	109.00
C2—C1—C6	120.2 (2)	C4—C9—H9B	109.00
C2—C1—C7	122.5 (2)	C4—C9—H9C	110.00
C6—C1—C7	117.2 (2)	C4—C9—H9D	110.00
C1—C2—C3	115.8 (2)	C4—C9—H9E	109.00
C1—C2—C8	122.0 (2)	C4—C9—H9F	109.00
C3—C2—C8	122.3 (2)	H9A—C9—H9B	109.00
N1—C3—C2	116.51 (19)	H9A—C9—H9C	109.00
N1—C3—C4	117.13 (19)	H9B—C9—H9C	110.00

## supplementary materials

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C2—C3—C4	126.3 (2)	H9D—C9—H9E	109.00
C3—C4—C5	115.4 (2)	H9D—C9—H9F	110.00
C3—C4—C9	121.7 (2)	H9E—C9—H9F	109.00
C5—C4—C9	122.9 (2)	N2—C11—H11A	119.00
C4—C5—C6	120.3 (2)	C12—C11—H11A	119.00
C4—C5—C10	122.8 (2)	C11—C12—H12A	120.00
C6—C5—C10	116.71 (19)	C13—C12—H12A	120.00
C1—C6—C5	121.9 (2)	C12—C13—H13A	120.00
O1—C7—O2	126.0 (2)	C14—C13—H13A	120.00
O1—C7—C1	116.4 (2)	C13—C14—H14A	121.00
O2—C7—C1	117.6 (2)	C15—C14—H14A	121.00
O3 <sup>iv</sup> —C10—C5	117.08 (19)	N2—C15—H15A	119.00
O4 <sup>v</sup> —C10—C5	117.53 (19)	C14—C15—H15A	119.00
O3 <sup>iv</sup> —C10—O4 <sup>v</sup>	125.3 (2)		
O3—Zn1—O1—C7	-70.9 (2)	C15—N2—C11—C12	-2.4 (5)
O4—Zn1—O1—C7	87.7 (2)	C11—N2—C15—C14	0.8 (5)
N2—Zn1—O1—C7	-171.4 (2)	Zn1—N2—C11—C12	177.4 (3)
O2 <sup>i</sup> —Zn1—O1—C7	12.3 (4)	Zn1—N2—C15—C14	-179.1 (3)
O1—Zn1—O3—C10 <sup>ii</sup>	82.6 (2)	C2—C1—C6—C5	-4.3 (3)
O4—Zn1—O3—C10 <sup>ii</sup>	3.2 (4)	C2—C1—C7—O1	74.4 (3)
N2—Zn1—O3—C10 <sup>ii</sup>	-177.8 (2)	C7—C1—C2—C8	7.3 (3)
O2 <sup>i</sup> —Zn1—O3—C10 <sup>ii</sup>	-75.9 (2)	C7—C1—C6—C5	172.4 (2)
O1—Zn1—O4—C10 <sup>iii</sup>	-75.2 (2)	C6—C1—C2—C3	3.3 (3)
O3—Zn1—O4—C10 <sup>iii</sup>	4.4 (4)	C6—C1—C7—O2	75.5 (3)
N2—Zn1—O4—C10 <sup>iii</sup>	-174.7 (2)	C7—C1—C2—C3	-173.3 (2)
O2 <sup>i</sup> —Zn1—O4—C10 <sup>iii</sup>	83.8 (2)	C6—C1—C2—C8	-176.2 (2)
O1—Zn1—N2—C11	-106.3 (2)	C6—C1—C7—O1	-102.3 (3)
O1—Zn1—N2—C15	73.6 (2)	C2—C1—C7—O2	-107.9 (3)
O3—Zn1—N2—C11	163.4 (2)	C8—C2—C3—C4	179.4 (2)
O3—Zn1—N2—C15	-16.8 (2)	C8—C2—C3—N1	-2.9 (3)
O4—Zn1—N2—C11	-17.0 (2)	C1—C2—C3—C4	0.0 (3)
O4—Zn1—N2—C15	162.8 (2)	C1—C2—C3—N1	177.59 (19)
O2 <sup>i</sup> —Zn1—N2—C11	72.3 (2)	N1—C3—C4—C9	2.4 (3)
O2 <sup>i</sup> —Zn1—N2—C15	-107.8 (2)	C2—C3—C4—C5	-2.2 (3)
O1—Zn1—O2 <sup>i</sup> —C7 <sup>i</sup>	-3.3 (4)	C2—C3—C4—C9	-180.0 (2)
O3—Zn1—O2 <sup>i</sup> —C7 <sup>i</sup>	79.9 (2)	N1—C3—C4—C5	-179.84 (19)
O4—Zn1—O2 <sup>i</sup> —C7 <sup>i</sup>	-78.7 (2)	C3—C4—C5—C6	1.3 (3)
N2—Zn1—O2 <sup>i</sup> —C7 <sup>i</sup>	-179.5 (2)	C9—C4—C5—C6	179.0 (2)
Zn1—O1—C7—O2	-11.5 (4)	C3—C4—C5—C10	176.5 (2)
Zn1—O1—C7—C1	166.09 (17)	C9—C4—C5—C10	-5.8 (3)
Zn1 <sup>i</sup> —O2—C7—O1	8.2 (4)	C10—C5—C6—C1	-173.6 (2)
Zn1 <sup>i</sup> —O2—C7—C1	-169.35 (16)	C4—C5—C10—O3 <sup>iv</sup>	138.0 (2)
Zn1—O3—C10 <sup>ii</sup> —C5 <sup>ii</sup>	169.14 (16)	C4—C5—C10—O4 <sup>v</sup>	-44.5 (3)
Zn1—O3—C10 <sup>ii</sup> —O4 <sup>i</sup>	-8.1 (4)	C6—C5—C10—O3 <sup>iv</sup>	-46.6 (3)



Zn1—O4—C10 <sup>iii</sup> —O3 <sup>i</sup>	-8.2 (4)	C6—C5—C10—O4 <sup>v</sup>	130.9 (2)
Zn1—O4—C10 <sup>iii</sup> —C5 <sup>iii</sup>	169.07 (16)	C4—C5—C6—C1	1.9 (3)
O6—N1—C3—C2	-108.6 (3)	N2—C11—C12—C13	2.5 (5)
O5—N1—C3—C4	-111.8 (3)	C11—C12—C13—C14	-0.8 (6)
O6—N1—C3—C4	69.3 (3)	C12—C13—C14—C15	-0.8 (6)
O5—N1—C3—C2	70.4 (3)	C13—C14—C15—N2	0.8 (6)

Symmetry codes: (i)  $-x+1, -y, -z+1$ ; (ii)  $-x+1, y-1/2, -z+3/2$ ; (iii)  $x, -y+1/2, z-1/2$ ; (iv)  $-x+1, y+1/2, -z+3/2$ ; (v)  $x, -y+1/2, z+1/2$ .

Fig. 1

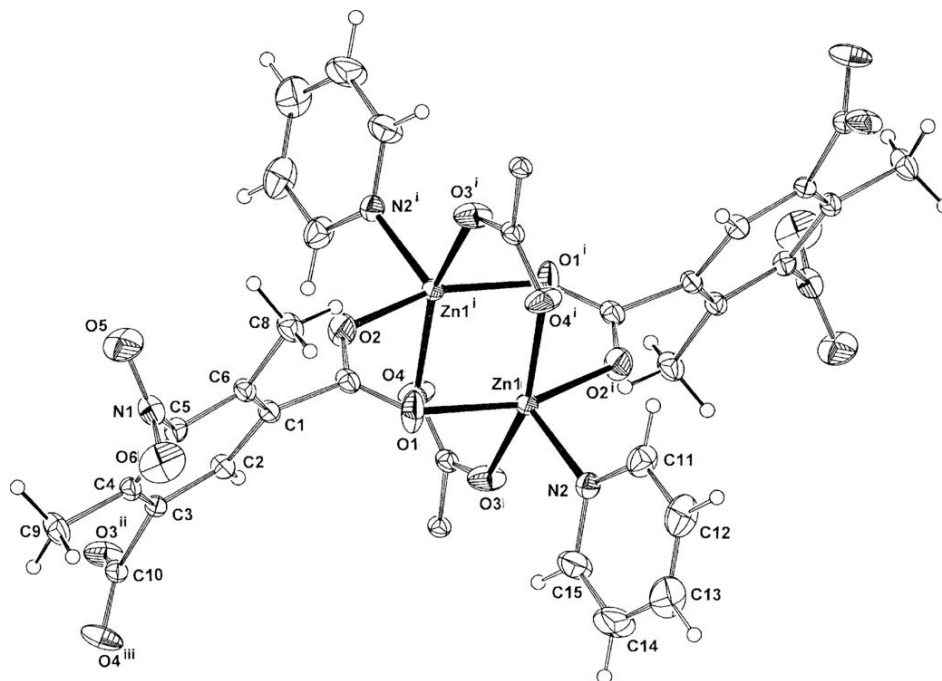


Fig. 2

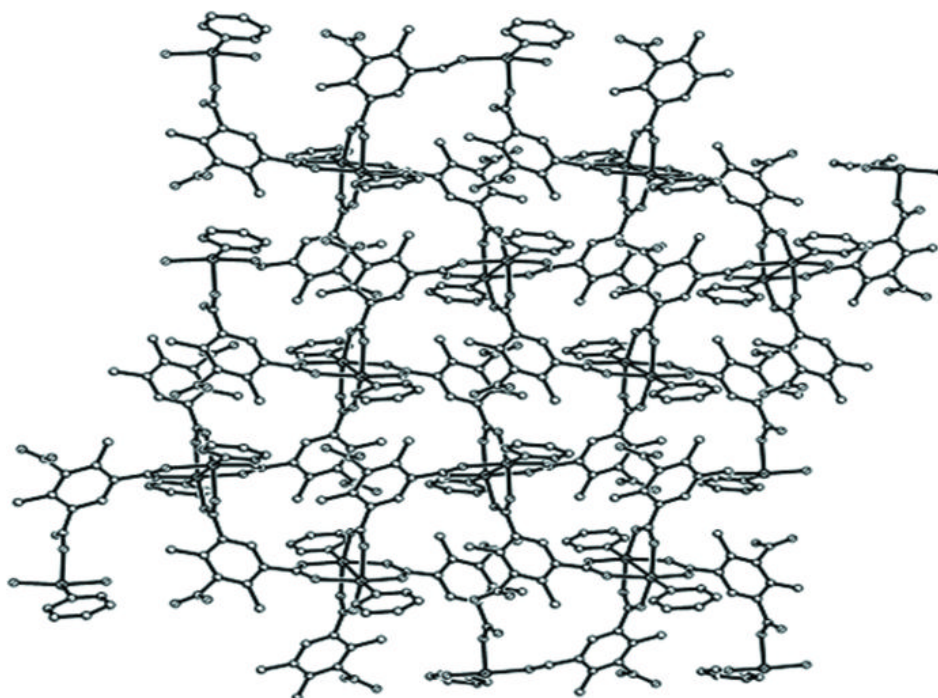


Fig. 3

