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## Structure Reports

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**Poly[ $\mu_2$ -benzene-1,3-dicarboxylato- $\kappa^2$ O:O'- $\mu_2$ -1,3-di-4-pyridylpropane- $\kappa^2$ N:N'-zinc(II)]**

Jin-Feng Huang,<sup>a</sup> Yu-Mei Dai,<sup>a\*</sup> Jian-Rong Lin,<sup>a</sup> Hui Lin<sup>a</sup> and En Tang<sup>b,c</sup>

<sup>a</sup>College of Chemistry and Materials, Fujian Normal University, Fuzhou 350007, People's Republic of China, <sup>b</sup>State Key Laboratory of Structural Chemistry, Fujian Institute of Research on the Structure of Matter, Chinese Academy of Sciences, Fuzhou, Fujian 350002, People's Republic of China, and <sup>c</sup>Conjugate and Medicinal Chemistry Laboratory, Department of Radiology, Brigham and Women's Hospital and Harvard Medical School, Boston, MA 02115, USA  
Correspondence e-mail: dym@fjnu.edu.cn

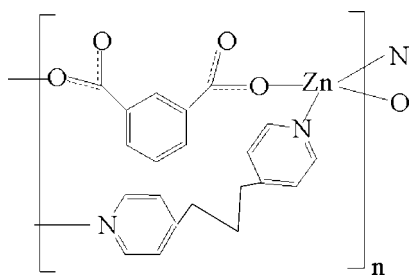
Received 13 December 2007; accepted 16 January 2008

Key indicators: single-crystal X-ray study;  $T = 293$  K; mean  $\sigma(\text{C}-\text{C}) = 0.004$  Å;  $R$  factor = 0.041;  $wR$  factor = 0.116; data-to-parameter ratio = 17.0.

The title compound,  $[\text{Zn}(\text{C}_8\text{H}_4\text{O}_4)(\text{C}_{13}\text{H}_{14}\text{N}_2)]_n$ , was obtained by the hydrothermal reaction of  $\text{Zn}(\text{OAc})_2 \cdot \text{H}_2\text{O}$  with 1,3-di-4-pyridylpropane (bpp) and isophthalic acid ( $\text{H}_2\text{ip}$ ). The  $\text{Zn}^{\text{II}}$  ion is coordinated by two bpp and two ip ligands in a distorted tetrahedral environment. Each ligand coordinates in a bridging mode to connect  $\text{Zn}^{\text{II}}$  ions into a three-dimensional diamondoid-type structure.

## Related literature

For related literature, see: Dai *et al.* (2005); Evans *et al.* (1999); Tang *et al.* (2004); Fujita *et al.* (1994).



## Experimental

## Crystal data

$[\text{Zn}(\text{C}_8\text{H}_4\text{O}_4)(\text{C}_{13}\text{H}_{14}\text{N}_2)]$

$M_r = 427.76$

Monoclinic,  $P2_1/c$

$a = 11.0418$  (13) Å

$b = 11.1924$  (14) Å

$c = 16.8687$  (17) Å

$\beta = 115.249$  (7)°

$V = 1885.5$  (4) Å<sup>3</sup>

$Z = 4$

Mo  $K\alpha$  radiation

$\mu = 1.33$  mm<sup>-1</sup>

$T = 293$  (2) K

$0.30 \times 0.20 \times 0.10$  mm

## Data collection

Bruker SMART CCD

diffractometer

Absorption correction: multi-scan

(*SADABS*; Sheldrick, 1996)

$T_{\text{min}} = 0.733$ ,  $T_{\text{max}} = 0.875$

14111 measured reflections

4328 independent reflections

3887 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.020$

## Refinement

$R[F^2 > 2\sigma(F^2)] = 0.040$

$wR(F^2) = 0.115$

$S = 1.04$

4328 reflections

254 parameters

H-atom parameters constrained

$\Delta\rho_{\text{max}} = 0.73$  e Å<sup>-3</sup>

$\Delta\rho_{\text{min}} = -0.76$  e Å<sup>-3</sup>

Table 1

Selected geometric parameters (Å, °).

|                         |             |                         |            |
|-------------------------|-------------|-------------------------|------------|
| Zn1—O2                  | 1.9511 (17) | Zn1—N2                  | 2.041 (2)  |
| Zn1—O4 <sup>i</sup>     | 1.9621 (17) | Zn1—N1                  | 2.051 (2)  |
| O2—Zn1—O4 <sup>i</sup>  | 101.92 (7)  | O2—Zn1—N1               | 109.01 (8) |
| O2—Zn1—N2               | 114.19 (8)  | O4 <sup>i</sup> —Zn1—N1 | 100.98 (8) |
| O4 <sup>i</sup> —Zn1—N2 | 122.01 (8)  | N2—Zn1—N1               | 107.55 (8) |

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

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINTE* (Siemens, 1997); data reduction: *SAINTE*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; 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: LH2583).

## References

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**supplementary materials**

*Acta Cryst.* (2008). E64, m386 [ doi:10.1107/S1600536808001621 ]

## Poly[ $\mu_2$ -benzene-1,3-dicarboxylato- $\kappa^2 O:O'$ - $\mu_2$ -1,3-di-4-pyridylpropane- $\kappa^2 N:N'$ -zinc(II)]

J.-F. Huang, Y.-M. Dai, J.-R. Lin, H. Lin and E. Tang

### Comment

A large family of coordination polymers has been developed recently owing to their potential applications as functional solid materials and their intriguing architectures or topologies (Evans *et al.*, 1999; Fujita *et al.*, 1994). It is now well understood that the hydrothermal crystallization of metal centers with multidentate N- or O-donor ligands, which possess more rich coordination sites and a wide variety of shapes to facilitate the formation of various networks, is one of the useful approaches to assembly desired new materials. An impressive literature of one-, two- and three-dimensional frameworks based on these ligands (Dai *et al.*, 2005; Tang *et al.*, 2004) with various structural motifs, such as helical, brick wall, ladder, honeycomb, square grid, parquet, and diamondoid, have been reported to date. Here we report the synthesis and crystal structure of the title compound (I).

In (I) [Fig. 1] each  $Zn^{II}$  ion coordinates to two pyridine N atoms of two bpp ligands and two carboxylate groups of two ip ligands, in monodentate modes, giving a distorted tetrahedral coordination environment. Both bpp and ip ligands coordinate in bridging modes to form a three-dimensional diamondoid structure with  $Zn \cdots Zn$  separations of 9.425 and 12.745 Å and forming cavities within the structure (Fig. 2).

### Experimental

A mixture of  $Zn(Ac)_2 \cdot H_2O$  (1.00 mmol, 0.22 g), bpp (1.00 mmol, 0.19 g),  $H_2ip$  (1.00 mmol, 0.16 g) and  $H_2O$  (15 ml) was vigorously stirred until the pH was adjusted to 6 by adding 10% NaOH. This mixture was heated at 433 K for 3 days in a sealed 25 ml Teflon-lined stainless steel vessel under autogenous pressure. After cooling to room temperature at 50 K  $h^{-1}$ , orange prism-shaped crystals were isolated, which were washed with ethanol and dried in air.

### Refinement

H atoms were positioned geometrically and refined using a riding model [ $C-H$  0.93–0.97 Å and  $U_{iso}(H) = 1.2U_{eq}(C)$ ].

### Figures

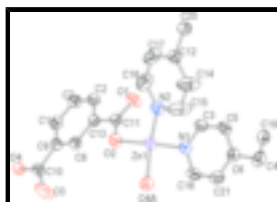


Fig. 1. The asymmetric unit showing 30% probability displacement ellipsoids. A symmetry related O atom is shown to complete the tetrahedral coordination [symmetry code: (A)  $x, 5/2 - y, 1/2 + z$ ]. H atoms are not shown.

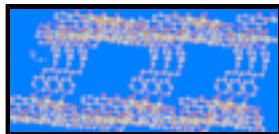


Fig. 2. Part of the crystal structure of the title compound.

## Poly[ $\mu_2$ -benzene-1,3-dicarboxylato- $\kappa^2$ O:O'- $\mu_2$ -1,3-di-4-\ pyridylpropane- $\kappa^2$ N:N'-zinc(II)]

### Crystal data

[Zn(C<sub>8</sub>H<sub>4</sub>O<sub>4</sub>)(C<sub>13</sub>H<sub>14</sub>N<sub>2</sub>)]

$M_r = 427.76$

Monoclinic,  $P2_1/c$

Hall symbol: -P 2ybc

$a = 11.0418$  (13) Å

$b = 11.1924$  (14) Å

$c = 16.8687$  (17) Å

$\beta = 115.249$  (7)°

$V = 1885.5$  (4) Å<sup>3</sup>

$Z = 4$

$F_{000} = 880$

$D_x = 1.507$  Mg m<sup>-3</sup>

Mo  $K\alpha$  radiation

$\lambda = 0.71073$  Å

Cell parameters from 4994 reflections

$\theta = 3.2$ – $27.5$ °

$\mu = 1.33$  mm<sup>-1</sup>

$T = 293$  (2) K

Prism, orange

$0.30 \times 0.20 \times 0.10$  mm

### Data collection

Bruker SMART CCD  
diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

$T = 293$ (2) K

$\omega$  scans

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

$T_{\min} = 0.733$ ,  $T_{\max} = 0.875$

14111 measured reflections

4328 independent reflections

3887 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.020$

$\theta_{\text{max}} = 27.5$ °

$\theta_{\text{min}} = 3.2$ °

$h = -14 \rightarrow 14$

$k = -11 \rightarrow 14$

$l = -21 \rightarrow 21$

### Refinement

Refinement on  $F^2$

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.040$

$wR(F^2) = 0.115$

$S = 1.04$

4328 reflections

254 parameters

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

$w = 1/[\sigma^2(F_o^2) + (0.0695P)^2 + 1.1112P]$

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

$(\Delta/\sigma)_{\text{max}} = 0.002$

$\Delta\rho_{\text{max}} = 0.73$  e Å<sup>-3</sup>

$\Delta\rho_{\text{min}} = -0.76$  e Å<sup>-3</sup>

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

|      | <i>x</i>     | <i>y</i>     | <i>z</i>      | $U_{\text{iso}}^*/U_{\text{eq}}$ |
|------|--------------|--------------|---------------|----------------------------------|
| Zn1  | 0.21026 (3)  | 1.06213 (2)  | 0.850451 (16) | 0.03187 (11)                     |
| O1   | 0.1788 (2)   | 0.88899 (17) | 0.71665 (12)  | 0.0485 (5)                       |
| O2   | 0.2385 (2)   | 1.07900 (15) | 0.74443 (11)  | 0.0405 (4)                       |
| O3   | 0.2086 (3)   | 1.3428 (2)   | 0.50730 (17)  | 0.0828 (9)                       |
| O4   | 0.22045 (18) | 1.27148 (16) | 0.38941 (11)  | 0.0412 (4)                       |
| N1   | 0.0122 (2)   | 1.02485 (18) | 0.81573 (13)  | 0.0346 (4)                       |
| N2   | 0.3207 (2)   | 0.92958 (18) | 0.93261 (13)  | 0.0379 (5)                       |
| C1   | 0.1641 (2)   | 1.0385 (2)   | 0.43263 (15)  | 0.0375 (5)                       |
| H1A  | 0.1559       | 1.0490       | 0.3759        | 0.045*                           |
| C2   | 0.1551 (2)   | 0.9102 (2)   | 0.54416 (16)  | 0.0354 (5)                       |
| H2A  | 0.1387       | 0.8354       | 0.5616        | 0.042*                           |
| C3   | -0.0341 (3)  | 0.9129 (2)   | 0.81017 (17)  | 0.0388 (5)                       |
| H3A  | 0.0255       | 0.8498       | 0.8201        | 0.047*                           |
| C4   | -0.4016 (3)  | 0.9562 (3)   | 0.7578 (2)    | 0.0491 (7)                       |
| H4A  | -0.4054      | 0.9442       | 0.8137        | 0.059*                           |
| H4B  | -0.4533      | 1.0272       | 0.7313        | 0.059*                           |
| C5   | -0.1657 (3)  | 0.8869 (2)   | 0.79050 (16)  | 0.0410 (5)                       |
| H5A  | -0.1931      | 0.8078       | 0.7875        | 0.049*                           |
| C6   | -0.2578 (2)  | 0.9791 (2)   | 0.77504 (15)  | 0.0370 (5)                       |
| C7   | 0.1420 (3)   | 0.9271 (2)   | 0.45968 (17)  | 0.0407 (6)                       |
| H7A  | 0.1182       | 0.8632       | 0.4207        | 0.049*                           |
| C8   | 0.2136 (2)   | 1.1160 (2)   | 0.57552 (14)  | 0.0333 (5)                       |
| H8A  | 0.2380       | 1.1798       | 0.6146        | 0.040*                           |
| C9   | 0.1985 (2)   | 1.1341 (2)   | 0.49008 (14)  | 0.0332 (5)                       |
| C10  | 0.2109 (3)   | 1.2590 (2)   | 0.46194 (16)  | 0.0403 (5)                       |
| C11  | 0.2035 (2)   | 0.9872 (2)   | 0.69431 (14)  | 0.0322 (5)                       |
| C12  | 0.4479 (2)   | 0.7383 (2)   | 1.04535 (15)  | 0.0353 (5)                       |
| C13  | 0.1929 (2)   | 1.0050 (2)   | 0.60318 (14)  | 0.0302 (4)                       |
| C14  | 0.3843 (5)   | 0.8270 (3)   | 1.0680 (2)    | 0.0765 (12)                      |
| H14A | 0.3829       | 0.8252       | 1.1227        | 0.092*                           |
| C15  | 0.3220 (5)   | 0.9198 (3)   | 1.0112 (2)    | 0.0780 (13)                      |
| H15A | 0.2790       | 0.9782       | 1.0290        | 0.094*                           |
| C16  | 0.3822 (3)   | 0.8432 (3)   | 0.91049 (19)  | 0.0596 (9)                       |

## supplementary materials

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|      |             |            |              |            |
|------|-------------|------------|--------------|------------|
| H16A | 0.3829      | 0.8469     | 0.8556       | 0.072*     |
| C17  | 0.4451 (3)  | 0.7481 (3) | 0.96411 (18) | 0.0575 (8) |
| H17A | 0.4862      | 0.6900     | 0.9446       | 0.069*     |
| C18  | -0.0769 (3) | 1.1138 (2) | 0.79964 (17) | 0.0413 (5) |
| H18A | -0.0472     | 1.1921     | 0.8027       | 0.050*     |
| C19  | -0.4686 (3) | 0.8497 (2) | 0.69901 (16) | 0.0424 (6) |
| H19A | -0.4147     | 0.7790     | 0.7231       | 0.051*     |
| H19B | -0.5554     | 0.8365     | 0.6990       | 0.051*     |
| C20  | 0.5127 (2)  | 0.6335 (2) | 1.10512 (16) | 0.0393 (5) |
| H20A | 0.5996      | 0.6190     | 1.1055       | 0.047*     |
| H20B | 0.4582      | 0.5630     | 1.0811       | 0.047*     |
| C21  | -0.2100 (3) | 1.0941 (2) | 0.77886 (18) | 0.0429 (6) |
| H21A | -0.2682     | 1.1586     | 0.7673       | 0.051*     |

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

|     | $U^{11}$     | $U^{22}$     | $U^{33}$     | $U^{12}$      | $U^{13}$     | $U^{23}$     |
|-----|--------------|--------------|--------------|---------------|--------------|--------------|
| Zn1 | 0.03897 (18) | 0.03055 (17) | 0.02643 (16) | -0.00058 (10) | 0.01427 (12) | 0.00286 (9)  |
| O1  | 0.0735 (13)  | 0.0335 (9)   | 0.0400 (9)   | -0.0039 (9)   | 0.0257 (9)   | 0.0072 (8)   |
| O2  | 0.0602 (11)  | 0.0360 (9)   | 0.0325 (8)   | -0.0046 (8)   | 0.0266 (8)   | -0.0023 (7)  |
| O3  | 0.166 (3)    | 0.0358 (11)  | 0.0722 (15)  | -0.0180 (14)  | 0.0749 (18)  | -0.0039 (11) |
| O4  | 0.0501 (10)  | 0.0401 (9)   | 0.0381 (9)   | 0.0086 (8)    | 0.0233 (8)   | 0.0138 (7)   |
| N1  | 0.0386 (10)  | 0.0289 (9)   | 0.0346 (9)   | -0.0028 (8)   | 0.0139 (8)   | -0.0002 (8)  |
| N2  | 0.0436 (11)  | 0.0367 (11)  | 0.0306 (10)  | 0.0021 (8)    | 0.0131 (9)   | 0.0055 (8)   |
| C1  | 0.0402 (12)  | 0.0450 (13)  | 0.0271 (10)  | 0.0023 (10)   | 0.0143 (9)   | 0.0005 (10)  |
| C2  | 0.0417 (12)  | 0.0290 (11)  | 0.0362 (11)  | -0.0001 (9)   | 0.0173 (10)  | 0.0000 (9)   |
| C3  | 0.0459 (13)  | 0.0282 (11)  | 0.0433 (13)  | 0.0008 (10)   | 0.0198 (11)  | 0.0017 (10)  |
| C4  | 0.0458 (14)  | 0.0557 (17)  | 0.0506 (15)  | -0.0129 (12)  | 0.0250 (13)  | -0.0232 (13) |
| C5  | 0.0525 (14)  | 0.0300 (12)  | 0.0417 (13)  | -0.0090 (10)  | 0.0213 (11)  | -0.0047 (10) |
| C6  | 0.0410 (12)  | 0.0406 (13)  | 0.0301 (10)  | -0.0072 (10)  | 0.0160 (9)   | -0.0095 (10) |
| C7  | 0.0514 (15)  | 0.0356 (13)  | 0.0346 (12)  | -0.0032 (10)  | 0.0180 (11)  | -0.0090 (10) |
| C8  | 0.0411 (12)  | 0.0304 (11)  | 0.0301 (10)  | -0.0019 (9)   | 0.0167 (9)   | -0.0020 (9)  |
| C9  | 0.0369 (11)  | 0.0338 (12)  | 0.0306 (10)  | 0.0009 (9)    | 0.0160 (9)   | 0.0043 (9)   |
| C10 | 0.0510 (14)  | 0.0363 (13)  | 0.0370 (12)  | -0.0009 (10)  | 0.0221 (11)  | 0.0055 (10)  |
| C11 | 0.0365 (11)  | 0.0316 (11)  | 0.0301 (10)  | 0.0039 (9)    | 0.0157 (9)   | 0.0031 (9)   |
| C12 | 0.0342 (11)  | 0.0348 (12)  | 0.0343 (11)  | 0.0005 (9)    | 0.0121 (9)   | 0.0042 (9)   |
| C13 | 0.0324 (10)  | 0.0300 (11)  | 0.0296 (10)  | 0.0029 (8)    | 0.0146 (8)   | 0.0019 (8)   |
| C14 | 0.145 (4)    | 0.0503 (18)  | 0.0402 (15)  | 0.042 (2)     | 0.046 (2)    | 0.0145 (13)  |
| C15 | 0.148 (4)    | 0.0481 (17)  | 0.0414 (16)  | 0.046 (2)     | 0.044 (2)    | 0.0115 (13)  |
| C16 | 0.0671 (19)  | 0.078 (2)    | 0.0407 (14)  | 0.0318 (17)   | 0.0300 (14)  | 0.0196 (14)  |
| C17 | 0.0651 (18)  | 0.069 (2)    | 0.0436 (14)  | 0.0355 (16)   | 0.0278 (14)  | 0.0143 (14)  |
| C18 | 0.0454 (13)  | 0.0274 (12)  | 0.0484 (14)  | -0.0035 (10)  | 0.0175 (11)  | -0.0010 (10) |
| C19 | 0.0398 (13)  | 0.0458 (14)  | 0.0429 (13)  | -0.0119 (11)  | 0.0190 (11)  | -0.0146 (11) |
| C20 | 0.0399 (13)  | 0.0367 (13)  | 0.0417 (12)  | 0.0067 (10)   | 0.0179 (10)  | 0.0076 (10)  |
| C21 | 0.0429 (14)  | 0.0339 (12)  | 0.0493 (14)  | 0.0026 (11)   | 0.0172 (12)  | -0.0044 (11) |

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

|        |             |        |        |
|--------|-------------|--------|--------|
| Zn1—O2 | 1.9511 (17) | C5—H5A | 0.9300 |
|--------|-------------|--------|--------|

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|                          |             |                        |             |
|--------------------------|-------------|------------------------|-------------|
| Zn1—O4 <sup>i</sup>      | 1.9621 (17) | C6—C21                 | 1.383 (4)   |
| Zn1—N2                   | 2.041 (2)   | C7—H7A                 | 0.9300      |
| Zn1—N1                   | 2.051 (2)   | C8—C9                  | 1.393 (3)   |
| O1—C11                   | 1.230 (3)   | C8—C13                 | 1.381 (3)   |
| O2—C11                   | 1.281 (3)   | C8—H8A                 | 0.9300      |
| O3—C10                   | 1.218 (3)   | C9—C10                 | 1.501 (3)   |
| O4—C10                   | 1.279 (3)   | C11—C13                | 1.504 (3)   |
| O4—Zn1 <sup>ii</sup>     | 1.9621 (17) | C12—C14                | 1.361 (4)   |
| N1—C18                   | 1.343 (3)   | C12—C17                | 1.362 (3)   |
| N1—C3                    | 1.342 (3)   | C12—C20                | 1.513 (3)   |
| N2—C16                   | 1.323 (4)   | C14—C15                | 1.381 (4)   |
| N2—C15                   | 1.324 (4)   | C14—H14A               | 0.9300      |
| C1—C9                    | 1.384 (3)   | C15—H15A               | 0.9300      |
| C1—C7                    | 1.384 (4)   | C16—C17                | 1.377 (4)   |
| C1—H1A                   | 0.9300      | C16—H16A               | 0.9300      |
| C2—C7                    | 1.383 (3)   | C17—H17A               | 0.9300      |
| C2—C13                   | 1.392 (3)   | C18—C21                | 1.376 (4)   |
| C2—H2A                   | 0.9300      | C18—H18A               | 0.9300      |
| C3—C5                    | 1.376 (4)   | C19—C20 <sup>iii</sup> | 1.519 (3)   |
| C3—H3A                   | 0.9300      | C19—H19A               | 0.9700      |
| C4—C19                   | 1.524 (3)   | C19—H19B               | 0.9700      |
| C4—C6                    | 1.509 (4)   | C20—C19 <sup>iv</sup>  | 1.519 (3)   |
| C4—H4A                   | 0.9700      | C20—H20A               | 0.9700      |
| C4—H4B                   | 0.9700      | C20—H20B               | 0.9700      |
| C5—C6                    | 1.393 (4)   | C21—H21A               | 0.9300      |
| O2—Zn1—O4 <sup>i</sup>   | 101.92 (7)  | C1—C9—C10              | 122.2 (2)   |
| O2—Zn1—N2                | 114.19 (8)  | O3—C10—O4              | 123.3 (2)   |
| O4 <sup>i</sup> —Zn1—N2  | 122.01 (8)  | O3—C10—C9              | 119.3 (2)   |
| O2—Zn1—N1                | 109.01 (8)  | O4—C10—C9              | 117.4 (2)   |
| O4 <sup>i</sup> —Zn1—N1  | 100.98 (8)  | O1—C11—O2              | 123.9 (2)   |
| N2—Zn1—N1                | 107.55 (8)  | O1—C11—C13             | 120.0 (2)   |
| C11—O2—Zn1               | 113.99 (14) | O2—C11—C13             | 116.04 (19) |
| C10—O4—Zn1 <sup>ii</sup> | 114.07 (17) | C14—C12—C17            | 115.5 (2)   |
| C18—N1—C3                | 117.0 (2)   | C14—C12—C20            | 122.2 (2)   |
| C18—N1—Zn1               | 120.43 (17) | C17—C12—C20            | 122.3 (2)   |
| C3—N1—Zn1                | 122.55 (17) | C8—C13—C2              | 119.1 (2)   |
| C16—N2—C15               | 115.7 (2)   | C8—C13—C11             | 120.8 (2)   |
| C16—N2—Zn1               | 124.72 (18) | C2—C13—C11             | 120.0 (2)   |
| C15—N2—Zn1               | 119.2 (2)   | C12—C14—C15            | 121.2 (3)   |
| C9—C1—C7                 | 120.0 (2)   | C12—C14—H14A           | 119.4       |
| C9—C1—H1A                | 120.0       | C15—C14—H14A           | 119.4       |
| C7—C1—H1A                | 120.0       | N2—C15—C14             | 123.1 (3)   |
| C7—C2—C13                | 120.1 (2)   | N2—C15—H15A            | 118.4       |
| C7—C2—H2A                | 120.0       | C14—C15—H15A           | 118.4       |
| C13—C2—H2A               | 120.0       | N2—C16—C17             | 123.7 (2)   |
| N1—C3—C5                 | 123.1 (2)   | N2—C16—H16A            | 118.1       |
| N1—C3—H3A                | 118.5       | C17—C16—H16A           | 118.1       |

## supplementary materials

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|            |           |                              |           |
|------------|-----------|------------------------------|-----------|
| C5—C3—H3A  | 118.5     | C16—C17—C12                  | 120.8 (3) |
| C19—C4—C6  | 115.9 (2) | C16—C17—H17A                 | 119.6     |
| C19—C4—H4A | 108.3     | C12—C17—H17A                 | 119.6     |
| C6—C4—H4A  | 108.3     | N1—C18—C21                   | 122.9 (2) |
| C19—C4—H4B | 108.3     | N1—C18—H18A                  | 118.5     |
| C6—C4—H4B  | 108.3     | C21—C18—H18A                 | 118.5     |
| H4A—C4—H4B | 107.4     | C20 <sup>iii</sup> —C19—C4   | 113.2 (2) |
| C3—C5—C6   | 120.0 (2) | C20 <sup>iii</sup> —C19—H19A | 108.9     |
| C3—C5—H5A  | 120.0     | C4—C19—H19A                  | 108.9     |
| C6—C5—H5A  | 120.0     | C20 <sup>iii</sup> —C19—H19B | 108.9     |
| C5—C6—C21  | 116.6 (2) | C4—C19—H19B                  | 108.9     |
| C5—C6—C4   | 122.3 (2) | H19A—C19—H19B                | 107.7     |
| C21—C6—C4  | 121.1 (2) | C12—C20—C19 <sup>iv</sup>    | 114.5 (2) |
| C2—C7—C1   | 120.5 (2) | C12—C20—H20A                 | 108.6     |
| C2—C7—H7A  | 119.8     | C19 <sup>iv</sup> —C20—H20A  | 108.6     |
| C1—C7—H7A  | 119.8     | C12—C20—H20B                 | 108.6     |
| C9—C8—C13  | 121.1 (2) | C19 <sup>iv</sup> —C20—H20B  | 108.6     |
| C9—C8—H8A  | 119.5     | H20A—C20—H20B                | 107.6     |
| C13—C8—H8A | 119.5     | C18—C21—C6                   | 120.4 (2) |
| C8—C9—C1   | 119.2 (2) | C18—C21—H21A                 | 119.8     |
| C8—C9—C10  | 118.4 (2) | C6—C21—H21A                  | 119.8     |

Symmetry codes: (i)  $x, -y+5/2, z+1/2$ ; (ii)  $x, -y+5/2, z-1/2$ ; (iii)  $x-1, -y+3/2, z-1/2$ ; (iv)  $x+1, -y+3/2, z+1/2$ .



Fig. 2

