# metal-organic compounds

# Poly[[μ2-2,2′-diethyl-1,1′-(butane-1,4-diyl)diimidazole-κ²N³:N³′](μ2-5-hydroxy-isophthalato-κ²O¹:O³)zinc]

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In the title coordination polymer, $[Zn(C_8H_4O_5)(C_{14}H_{22}N_4)]_n$, the $Zn^{II}$ cation is coordinated by an $O_2N_2$ donor set in a distorted tetrahedral geometry. The $Zn^{II}$ ions are linked by $\mu_2$-OH-bdc (OH-$H_2$bdc = 5-hydroxyisophthalic acid) and bbie ligands [bbie = 2,2′-diethyl-1,1′-(butane-1,4-diyl)diimidazole], forming a two-dimensional layer parallel to the *ab* plane. The layers are further connected through intermolecular C—H···O and O—H···O hydrogen bonds, forming a three-dimensional supramolecular structure. In the bbie ligand, the two C atoms in the ethyl group are each disordered over two positions with a site-occupancy ratio of 0.69:0.31.

## Related literature

For background information on bis(imidazole) ligands, see: Kan *et al.* (2011); Liu *et al.* (2007).
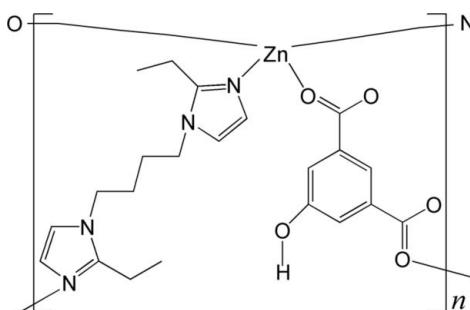


## Experimental

### Crystal data

| | |
|---|---|
| $[Zn(C_8H_4O_5)(C_{14}H_{22}N_4)]$ | $a$ = 13.5120 (12) Å |
| $M_r$ = 491.84 | $b$ = 12.765 (1) Å |
| Monoclinic, $P2_1/n$ | $c$ = 13.5910 (12) Å |

| | |
|---|---|
| $\beta$ = 103.933 (2)° | $\mu$ = 1.12 mm$^{-1}$ |
| $V$ = 2275.2 (3) Å$^3$ | $T$ = 293 K |
| $Z$ = 4 | 0.28 × 0.24 × 0.21 mm |
| Mo $K\alpha$ radiation | |

### Data collection

| | |
|---|---|
| Bruker SMART APEX CCD area-detector diffractometer | 13890 measured reflections |
| Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996) | 5467 independent reflections |
| $T_{min}$ = 0.73, $T_{max}$ = 0.79 | 3988 reflections with $I > 2\sigma(I)$ |
| | $R_{int}$ = 0.034 |

### Refinement

| | |
|---|---|
| $R[F^2 > 2\sigma(F^2)]$ = 0.036 | 309 parameters |
| $wR(F^2)$ = 0.087 | H-atom parameters constrained |
| $S$ = 1.03 | $\Delta\rho_{max}$ = 0.32 e Å$^{-3}$ |
| 5467 reflections | $\Delta\rho_{min}$ = −0.29 e Å$^{-3}$ |

**Table 1**
Selected geometric parameters (Å, °).

| Zn1—O1 | 1.9662 (15) | Zn1—N4$^{ii}$ | 2.0020 (18) |
|---|---|---|---|
| Zn1—O4$^{i}$ | 1.9682 (14) | Zn1—N1 | 2.0286 (17) |

| O1—Zn1—O4$^{i}$ | 102.54 (6) | O1—Zn1—N1 | 115.96 (7) |
|---|---|---|---|
| O1—Zn1—N4$^{ii}$ | 117.20 (7) | O4$^{i}$—Zn1—N1 | 98.33 (6) |
| O4$^{i}$—Zn1—N4$^{ii}$ | 118.18 (7) | N4$^{ii}$—Zn1—N1 | 103.59 (7) |

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

**Table 2**
Hydrogen-bond geometry (Å, °).

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| C10—H10···O1$^{iii}$ | 0.93 | 2.62 | 3.417 (3) | 144 |
| C14—H14···O5$^{iii}$ | 0.93 | 2.49 | 3.398 (3) | 166 |
| O5—H5···O2$^{iv}$ | 0.82 | 1.88 | 2.697 (2) | 171 |

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

Data collection: *SMART* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT*; 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*.

## References

Bruker (2007). *SMART* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.

Kan, W.-Q., Liu, Y.-Y., Yang, J., Liu, Y.-Y. & Ma, J.-F. (2011). *CrystEngComm*, **13**, 4256–4269.

Liu, Y.-Y., Ma, J.-F. & Zhang, L.-P. (2007). *Acta Cryst.* E**63**, m2317.

Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.

Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.

# supporting information

# Poly[[*μ*₂-2,2′-diethyl-1,1′-(butane-1,4-diyl)diimidazole-*κ*²*N*³:*N*³′](*μ*₂-5-hydroxy-isophthalato-*κ*²*O*¹:*O*³)zinc]

## Ying-Ying Liu, Xing Wang and Yong-Sheng Yan

## S1. Comment

As part of an investigation of the transition metal application there is a need to prepare further examples of these compounds. In this paper, the structure of the title compound, (I), is described.

As shown in Fig. 1, the $Zn^{II}$ ions is four-coordinated by two oxygen atoms from two oxygen atoms of two OH-bdc anions and two nitrogen atoms of two bbie ligands. Each carboxylate group of OH-bdc acts in a monodentate mode, and the hydroxyl group is not involved in coordination. The bbie molecule coordinates to two $Zn^{II}$ cations through its two aromatic N atoms, thus acing as a bridging bidentate ligand. As illustrated in Fig. 2, The $Zn^{II}$ cations are connected by OH-bdc and bbie ligands to form a layer parallel to the *ab* plane. There exist hydrogen-binding interactions among adjacent layers. The layers are further connected by these hydrogen bonds to a 3D supramolecular architecture.

## S2. Experimental

The ligand bbie was synthesized according to the literature Liu *et al.*, (2007), but 2-phenylimidazole was replaced by 2-ethylimidazole. A mixture of $ZnCO_3$ (0.050 g, 0.40 mmol), OH—$H^2$bdc (0.043 g, 0.40 mmol), bbie (0.099 g, 0.40 mmol), and water (8 ml) was sealed in a Teflon reactor (18 ml) and heated at 140 °C for 3 days. After the mixture had been cooled to room temperature at 10 °C.h⁻¹, colorless crystals of (I) were obtained. Yield: 43%.

## S3. Refinement

Disorderd bbie ligand was refined using C17 and C18 atoms split over two sites, with a total occupancy of 1. A 11 H-atoms bound to carbon were refined using a riding model with d(C—H) = 0.93 Å, $U_{iso}$ = 1.2$U_{eq}$(C) for aromatic and 0.97 Å, $U_{iso}$ = 1.5$U_{eq}$(C) for $CH_2$ atoms. Hydroxyl H atoms were refined using a riding model with d(O—H) = 0.82 Å, $U_{iso}$ =1.5$U_{eq}$(O).
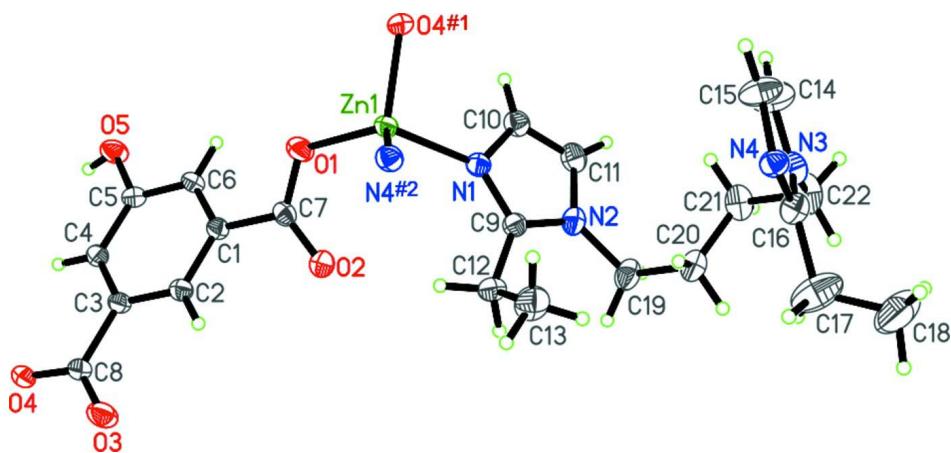
**Figure 1**

A view of the local coordination of the $Zn^{II}$ cation of (I). Displacement ellipsoids are drawn at the 30% probability level.
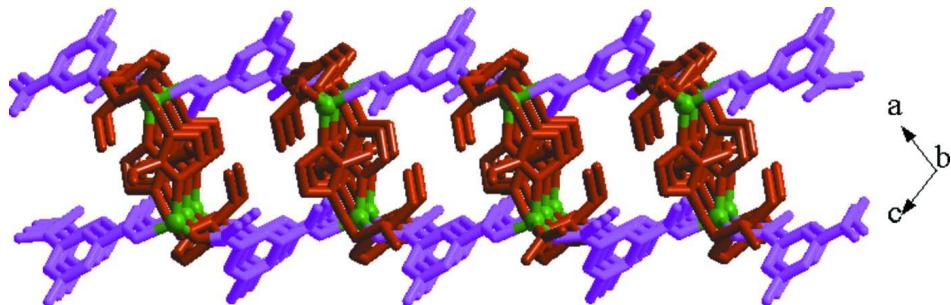


**Figure 2**

View of the two-dimensional layer of (I).

**Poly[[μ₂-2,2′-diethyl-1,1′-(butane-1,4-diyl)diimidazole- $\kappa^2N^3$:$N^{3′}$]($μ_2$-5-hydroxyisophthalato- $\kappa^2O^1$:$O^3$)zinc]**

*Crystal data*
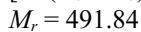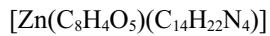
| | |
|---|---|
| [Zn($C_8H_4O_5$)($C_{14}H_{22}N_4$)] | $F(000) = 1024$ |
| $M_r = 491.84$ | $D_x = 1.436$ Mg m$^{-3}$ |
| Monoclinic, $P2_1/n$ | Mo $K\alpha$ radiation, $\lambda = 0.71069$ Å |
| Hall symbol: -P 2yn | Cell parameters from 3988 reflections |
| $a = 13.5120$ (12) Å | $\theta = 1.9$–28.3° |
| $b = 12.765$ (1) Å | $\mu = 1.12$ mm$^{-1}$ |
| $c = 13.5910$ (12) Å | $T = 293$ K |
| $\beta = 103.933$ (2)° | Block, colorless |
| $V = 2275.2$ (3) Å$^3$ | 0.28 × 0.24 × 0.21 mm |
| $Z = 4$ | |

*Data collection*

| | |
|---|---|
| Bruker SMART APEX CCD area-detector diffractometer | 13890 measured reflections |
| | 5467 independent reflections |
| Radiation source: fine-focus sealed tube | 3988 reflections with $I > 2\sigma(I)$ |
| Graphite monochromator | $R_{int} = 0.034$ |
| $\omega$ scans | $\theta_{max} = 28.3°$, $\theta_{min} = 1.9°$ |
| Absorption correction: multi-scan | $h = -13 \rightarrow 17$ |
| (*SADABS*; Sheldrick, 1996) | $k = -14 \rightarrow 17$ |
| $T_{min} = 0.73$, $T_{max} = 0.79$ | $l = -18 \rightarrow 18$ |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Secondary atom site location: difference Fourier map |
| Least-squares matrix: full | |
| $R[F^2 > 2\sigma(F^2)] = 0.036$ | Hydrogen site location: inferred from neighbouring sites |
| $wR(F^2) = 0.087$ | |
| $S = 1.03$ | H-atom parameters constrained |
| 5467 reflections | $w = 1/[\sigma^2(F_o^2) + (0.0374P)^2 + 0.1596P]$ |
| 309 parameters | where $P = (F_o^2 + 2F_c^2)/3$ |
| 0 restraints | $(\Delta/\sigma)_{max} = 0.001$ |
| Primary atom site location: structure-invariant direct methods | $\Delta\rho_{max} = 0.32$ e Å$^{-3}$ |
| | $\Delta\rho_{min} = -0.29$ 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* | $U_{iso}$*/$U_{eq}$ | Occ. (<1) |
|---|---|---|---|---|---|
| Zn1 | 0.582734 (18) | 0.485563 (18) | 0.336590 (17) | 0.03285 (9) | |
| C1 | 0.35185 (15) | 0.26820 (15) | 0.21865 (15) | 0.0328 (4) | |
| C2 | 0.30834 (15) | 0.23700 (16) | 0.11970 (15) | 0.0354 (5) | |
| H2 | 0.3183 | 0.2771 | 0.0658 | 0.042* | |
| C3 | 0.24997 (15) | 0.14625 (16) | 0.10089 (15) | 0.0339 (5) | |
| C4 | 0.23245 (15) | 0.08795 (16) | 0.18177 (15) | 0.0338 (5) | |
| H4 | 0.1928 | 0.0276 | 0.1695 | 0.041* | |
| C5 | 0.27431 (15) | 0.12020 (16) | 0.28070 (15) | 0.0349 (5) | |
| C6 | 0.33484 (16) | 0.20925 (16) | 0.29951 (15) | 0.0358 (5) | |
| H6 | 0.3640 | 0.2296 | 0.3659 | 0.043* | |
| C7 | 0.41726 (16) | 0.36460 (16) | 0.23657 (16) | 0.0349 (5) | |
| C8 | 0.20549 (16) | 0.11336 (17) | −0.00696 (16) | 0.0368 (5) | |
| C9 | 0.48306 (15) | 0.70092 (16) | 0.27233 (15) | 0.0355 (5) | |
| C10 | 0.51820 (17) | 0.67354 (18) | 0.43504 (16) | 0.0414 (5) | |
| H10 | 0.5403 | 0.6413 | 0.4978 | 0.050* | |
| C11 | 0.47890 (18) | 0.77010 (18) | 0.41969 (18) | 0.0466 (6) | |
| H11 | 0.4683 | 0.8162 | 0.4691 | 0.056* | |
| C12 | 0.46889 (18) | 0.68667 (19) | 0.16100 (16) | 0.0464 (6) | |
| H12A | 0.4015 | 0.7119 | 0.1275 | 0.056* | |
| H12B | 0.4707 | 0.6122 | 0.1472 | 0.056* | |
| C13 | 0.5467 (2) | 0.7414 (2) | 0.1135 (2) | 0.0665 (8) | |
| H13A | 0.5387 | 0.7173 | 0.0451 | 0.100* | |
| H13B | 0.6144 | 0.7255 | 0.1521 | 0.100* | |
| H13C | 0.5360 | 0.8158 | 0.1134 | 0.100* | |
| C14 | 0.7862 (2) | 1.0000 (2) | 0.4101 (2) | 0.0739 (9) | |

| H14 | 0.7847 | 0.9867 | 0.4770 | 0.089* | |
|---|---|---|---|---|---|
| C15 | 0.8584 (2) | 0.9700 (2) | 0.36442 (19) | 0.0632 (7) | |
| H15 | 0.9166 | 0.9323 | 0.3950 | 0.076* | |
| C16 | 0.74705 (18) | 1.05462 (18) | 0.25407 (18) | 0.0443 (5) | |
| C17 | 0.6885 (7) | 1.1012 (7) | 0.1514 (6) | 0.062 (2) | 0.688 (10) |
| H17A | 0.7064 | 1.0627 | 0.0966 | 0.074* | 0.688 (10) |
| H17B | 0.6158 | 1.0932 | 0.1447 | 0.074* | 0.688 (10) |
| C18 | 0.7127 (4) | 1.2139 (4) | 0.1428 (5) | 0.097 (2) | 0.688 (10) |
| H18A | 0.6750 | 1.2404 | 0.0786 | 0.146* | 0.688 (10) |
| H18B | 0.7844 | 1.2218 | 0.1479 | 0.146* | 0.688 (10) |
| H18C | 0.6943 | 1.2523 | 0.1965 | 0.146* | 0.688 (10) |
| C18′ | 0.6330 (13) | 1.0952 (16) | 0.0904 (14) | 0.156 (10) | 0.312 (10) |
| H18D | 0.6135 | 1.1524 | 0.0439 | 0.234* | 0.312 (10) |
| H18E | 0.5741 | 1.0694 | 0.1105 | 0.234* | 0.312 (10) |
| H18F | 0.6617 | 1.0400 | 0.0580 | 0.234* | 0.312 (10) |
| C17′ | 0.7098 (17) | 1.132 (2) | 0.1811 (16) | 0.099 (10) | 0.312 (10) |
| H17C | 0.7669 | 1.1615 | 0.1592 | 0.119* | 0.312 (10) |
| H17D | 0.6797 | 1.1873 | 0.2129 | 0.119* | 0.312 (10) |
| C19 | 0.41398 (18) | 0.88519 (17) | 0.2671 (2) | 0.0536 (6) | |
| H19A | 0.3650 | 0.9129 | 0.3021 | 0.064* | |
| H19B | 0.3777 | 0.8693 | 0.1981 | 0.064* | |
| C20 | 0.49432 (19) | 0.96907 (18) | 0.26511 (19) | 0.0514 (6) | |
| H20A | 0.5474 | 0.9382 | 0.2374 | 0.062* | |
| H20B | 0.4627 | 1.0245 | 0.2195 | 0.062* | |
| C21 | 0.5432 (2) | 1.01699 (19) | 0.3666 (2) | 0.0540 (7) | |
| H21A | 0.5752 | 0.9619 | 0.4125 | 0.065* | |
| H21B | 0.4905 | 1.0484 | 0.3945 | 0.065* | |
| C22 | 0.6228 (2) | 1.1000 (2) | 0.3613 (2) | 0.0618 (7) | |
| H22A | 0.5939 | 1.1500 | 0.3084 | 0.074* | |
| H22B | 0.6408 | 1.1377 | 0.4252 | 0.074* | |
| N1 | 0.52069 (13) | 0.62938 (13) | 0.34288 (12) | 0.0348 (4) | |
| N2 | 0.45730 (14) | 0.78804 (13) | 0.31714 (14) | 0.0407 (4) | |
| N3 | 0.71500 (15) | 1.05383 (16) | 0.34053 (15) | 0.0490 (5) | |
| N4 | 0.83402 (14) | 1.00315 (13) | 0.26584 (13) | 0.0379 (4) | |
| O1 | 0.48724 (12) | 0.36689 (12) | 0.31780 (11) | 0.0484 (4) | |
| O2 | 0.40181 (12) | 0.43621 (12) | 0.17278 (11) | 0.0460 (4) | |
| O3 | 0.21788 (14) | 0.16868 (13) | −0.07723 (11) | 0.0565 (5) | |
| O4 | 0.15489 (12) | 0.02734 (11) | −0.01974 (10) | 0.0400 (4) | |
| O5 | 0.26148 (12) | 0.06464 (12) | 0.36316 (10) | 0.0482 (4) | |
| H5 | 0.2121 | 0.0257 | 0.3459 | 0.072* | |

*Atomic displacement parameters (Å$^2$)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Zn1 | 0.03576 (15) | 0.03453 (14) | 0.02655 (13) | −0.00202 (10) | 0.00417 (10) | 0.00010 (10) |
| C1 | 0.0291 (11) | 0.0328 (11) | 0.0340 (11) | −0.0004 (8) | 0.0028 (9) | −0.0028 (9) |
| C2 | 0.0374 (12) | 0.0369 (11) | 0.0307 (10) | −0.0007 (9) | 0.0057 (9) | 0.0014 (9) |
| C3 | 0.0328 (11) | 0.0366 (11) | 0.0297 (10) | 0.0016 (9) | 0.0023 (9) | −0.0023 (9) |

| | | | | | |
|----|----|----|----|----|----|
| C4 | 0.0302 (11) | 0.0338 (11) | 0.0350 (11) | −0.0027 (9) | 0.0032 (9) | −0.0004 (9) |
| C5 | 0.0334 (11) | 0.0396 (12) | 0.0310 (11) | 0.0013 (9) | 0.0062 (9) | 0.0041 (9) |
| C6 | 0.0372 (12) | 0.0393 (12) | 0.0274 (10) | −0.0012 (9) | 0.0006 (9) | −0.0048 (9) |
| C7 | 0.0341 (12) | 0.0373 (11) | 0.0342 (11) | −0.0003 (9) | 0.0095 (9) | −0.0065 (9) |
| C8 | 0.0360 (12) | 0.0382 (12) | 0.0326 (11) | 0.0019 (9) | 0.0014 (9) | −0.0008 (9) |
| C9 | 0.0331 (11) | 0.0359 (11) | 0.0365 (11) | −0.0023 (9) | 0.0065 (9) | 0.0013 (9) |
| C10 | 0.0458 (13) | 0.0450 (13) | 0.0352 (12) | −0.0027 (10) | 0.0130 (10) | −0.0027 (10) |
| C11 | 0.0515 (15) | 0.0464 (14) | 0.0465 (14) | −0.0030 (11) | 0.0211 (12) | −0.0109 (11) |
| C12 | 0.0518 (14) | 0.0470 (14) | 0.0370 (12) | 0.0041 (11) | 0.0042 (11) | 0.0047 (10) |
| C13 | 0.089 (2) | 0.0669 (18) | 0.0512 (15) | −0.0035 (16) | 0.0321 (15) | 0.0076 (13) |
| C14 | 0.076 (2) | 0.112 (3) | 0.0406 (15) | 0.0171 (18) | 0.0274 (15) | 0.0192 (15) |
| C15 | 0.0628 (18) | 0.088 (2) | 0.0404 (14) | 0.0194 (15) | 0.0163 (13) | 0.0225 (14) |
| C16 | 0.0472 (14) | 0.0423 (13) | 0.0471 (13) | 0.0010 (11) | 0.0186 (11) | 0.0030 (11) |
| C17 | 0.060 (4) | 0.074 (4) | 0.044 (4) | 0.027 (3) | −0.001 (3) | 0.006 (3) |
| C18 | 0.090 (4) | 0.082 (4) | 0.112 (5) | 0.013 (3) | 0.011 (3) | 0.059 (3) |
| C18′ | 0.092 (12) | 0.26 (2) | 0.110 (13) | 0.064 (14) | 0.018 (10) | 0.090 (14) |
| C17′ | 0.066 (12) | 0.19 (3) | 0.055 (12) | 0.051 (13) | 0.036 (10) | 0.035 (12) |
| C19 | 0.0472 (15) | 0.0385 (13) | 0.0748 (18) | 0.0058 (11) | 0.0140 (13) | 0.0050 (12) |
| C20 | 0.0549 (16) | 0.0382 (13) | 0.0642 (17) | 0.0024 (11) | 0.0202 (13) | 0.0052 (12) |
| C21 | 0.0518 (15) | 0.0517 (15) | 0.0673 (17) | −0.0062 (12) | 0.0312 (14) | −0.0104 (13) |
| C22 | 0.0590 (17) | 0.0528 (16) | 0.086 (2) | −0.0054 (13) | 0.0416 (15) | −0.0192 (14) |
| N1 | 0.0374 (10) | 0.0359 (10) | 0.0310 (9) | −0.0003 (8) | 0.0081 (8) | −0.0001 (8) |
| N2 | 0.0395 (11) | 0.0332 (10) | 0.0507 (11) | 0.0010 (8) | 0.0133 (9) | −0.0009 (8) |
| N3 | 0.0498 (12) | 0.0519 (12) | 0.0509 (12) | −0.0039 (10) | 0.0231 (10) | −0.0098 (10) |
| N4 | 0.0409 (11) | 0.0412 (10) | 0.0325 (9) | 0.0015 (8) | 0.0104 (8) | 0.0013 (8) |
| O1 | 0.0477 (10) | 0.0477 (9) | 0.0418 (9) | −0.0153 (8) | −0.0048 (7) | 0.0006 (7) |
| O2 | 0.0533 (10) | 0.0365 (9) | 0.0454 (9) | −0.0049 (7) | 0.0066 (8) | 0.0031 (7) |
| O3 | 0.0758 (12) | 0.0585 (11) | 0.0317 (8) | −0.0190 (9) | 0.0063 (8) | 0.0016 (8) |
| O4 | 0.0453 (9) | 0.0381 (8) | 0.0312 (8) | −0.0052 (7) | −0.0013 (7) | −0.0039 (6) |
| O5 | 0.0563 (10) | 0.0549 (10) | 0.0313 (8) | −0.0147 (8) | 0.0066 (7) | 0.0049 (7) |

*Geometric parameters (Å, º)*

| | | | |
|----|----|----|----|
| Zn1—O1 | 1.9662 (15) | C14—H14 | 0.9300 |
| Zn1—O4[i] | 1.9682 (14) | C15—N4 | 1.367 (3) |
| Zn1—N4[ii] | 2.0020 (18) | C15—H15 | 0.9300 |
| Zn1—N1 | 2.0286 (17) | C16—N4 | 1.322 (3) |
| C1—C2 | 1.390 (3) | C16—N3 | 1.347 (3) |
| C1—C6 | 1.396 (3) | C16—C17′ | 1.40 (3) |
| C1—C7 | 1.500 (3) | C16—C17 | 1.547 (9) |
| C2—C3 | 1.390 (3) | C17—C18 | 1.486 (12) |
| C2—H2 | 0.9300 | C17—H17A | 0.9700 |
| C3—C4 | 1.394 (3) | C17—H17B | 0.9700 |
| C3—C8 | 1.504 (3) | C18—H18A | 0.9600 |
| C4—C5 | 1.390 (3) | C18—H18B | 0.9600 |
| C4—H4 | 0.9300 | C18—H18C | 0.9600 |
| C5—O5 | 1.372 (2) | C18′—C17′ | 1.48 (3) |
| C5—C6 | 1.388 (3) | C18′—H18D | 0.9600 |

| | | | |
|---|---|---|---|
| C6—H6 | 0.9300 | C18′—H18E | 0.9600 |
| C7—O2 | 1.243 (2) | C18′—H18F | 0.9600 |
| C7—O1 | 1.269 (2) | C17′—H17C | 0.9700 |
| C8—O3 | 1.231 (3) | C17′—H17D | 0.9700 |
| C8—O4 | 1.283 (2) | C19—N2 | 1.467 (3) |
| C9—N1 | 1.333 (2) | C19—C20 | 1.530 (3) |
| C9—N2 | 1.353 (3) | C19—H19A | 0.9700 |
| C9—C12 | 1.490 (3) | C19—H19B | 0.9700 |
| C10—C11 | 1.338 (3) | C20—C21 | 1.508 (3) |
| C10—N1 | 1.381 (3) | C20—H20A | 0.9700 |
| C10—H10 | 0.9300 | C20—H20B | 0.9700 |
| C11—N2 | 1.373 (3) | C21—C22 | 1.524 (3) |
| C11—H11 | 0.9300 | C21—H21A | 0.9700 |
| C12—C13 | 1.530 (3) | C21—H21B | 0.9700 |
| C12—H12A | 0.9700 | C22—N3 | 1.466 (3) |
| C12—H12B | 0.9700 | C22—H22A | 0.9700 |
| C13—H13A | 0.9600 | C22—H22B | 0.9700 |
| C13—H13B | 0.9600 | N4—Zn1ⁱⁱⁱ | 2.0020 (18) |
| C13—H13C | 0.9600 | O4—Zn1ⁱᵛ | 1.9682 (14) |
| C14—C15 | 1.333 (4) | O5—H5 | 0.8200 |
| C14—N3 | 1.362 (3) | | |
| | | | |
| O1—Zn1—O4ⁱ | 102.54 (6) | C18—C17—H17A | 109.3 |
| O1—Zn1—N4ⁱⁱ | 117.20 (7) | C16—C17—H17A | 109.3 |
| O4ⁱ—Zn1—N4ⁱⁱ | 118.18 (7) | C18—C17—H17B | 109.3 |
| O1—Zn1—N1 | 115.96 (7) | C16—C17—H17B | 109.3 |
| O4ⁱ—Zn1—N1 | 98.33 (6) | H17A—C17—H17B | 108.0 |
| N4ⁱⁱ—Zn1—N1 | 103.59 (7) | C17—C18—H18A | 109.5 |
| C2—C1—C6 | 119.72 (18) | C17—C18—H18B | 109.5 |
| C2—C1—C7 | 119.17 (18) | H18A—C18—H18B | 109.5 |
| C6—C1—C7 | 121.11 (17) | C17—C18—H18C | 109.5 |
| C3—C2—C1 | 120.38 (19) | H18A—C18—H18C | 109.5 |
| C3—C2—H2 | 119.8 | H18B—C18—H18C | 109.5 |
| C1—C2—H2 | 119.8 | C17′—C18′—H18D | 109.5 |
| C2—C3—C4 | 119.76 (18) | C17′—C18′—H18E | 109.5 |
| C2—C3—C8 | 119.19 (19) | H18D—C18′—H18E | 109.5 |
| C4—C3—C8 | 121.04 (18) | C17′—C18′—H18F | 109.5 |
| C5—C4—C3 | 119.87 (19) | H18D—C18′—H18F | 109.5 |
| C5—C4—H4 | 120.1 | H18E—C18′—H18F | 109.5 |
| C3—C4—H4 | 120.1 | C16—C17′—C18′ | 115 (2) |
| O5—C5—C6 | 117.24 (17) | C16—C17′—H17C | 108.4 |
| O5—C5—C4 | 122.36 (19) | C18′—C17′—H17C | 108.4 |
| C6—C5—C4 | 120.36 (19) | C16—C17′—H17D | 108.4 |
| C5—C6—C1 | 119.87 (18) | C18′—C17′—H17D | 108.4 |
| C5—C6—H6 | 120.1 | H17C—C17′—H17D | 107.5 |
| C1—C6—H6 | 120.1 | N2—C19—C20 | 113.23 (19) |
| O2—C7—O1 | 123.70 (19) | N2—C19—H19A | 108.9 |
| O2—C7—C1 | 119.78 (18) | C20—C19—H19A | 108.9 |

| O1—C7—C1 | 116.52 (18) | N2—C19—H19B | 108.9 |
|---|---|---|---|
| O3—C8—O4 | 123.61 (19) | C20—C19—H19B | 108.9 |
| O3—C8—C3 | 119.93 (19) | H19A—C19—H19B | 107.7 |
| O4—C8—C3 | 116.46 (18) | C21—C20—C19 | 115.1 (2) |
| N1—C9—N2 | 109.52 (18) | C21—C20—H20A | 108.5 |
| N1—C9—C12 | 125.47 (19) | C19—C20—H20A | 108.5 |
| N2—C9—C12 | 124.99 (19) | C21—C20—H20B | 108.5 |
| C11—C10—N1 | 109.3 (2) | C19—C20—H20B | 108.5 |
| C11—C10—H10 | 125.4 | H20A—C20—H20B | 107.5 |
| N1—C10—H10 | 125.4 | C20—C21—C22 | 113.4 (2) |
| C10—C11—N2 | 106.9 (2) | C20—C21—H21A | 108.9 |
| C10—C11—H11 | 126.5 | C22—C21—H21A | 108.9 |
| N2—C11—H11 | 126.5 | C20—C21—H21B | 108.9 |
| C9—C12—C13 | 116.1 (2) | C22—C21—H21B | 108.9 |
| C9—C12—H12A | 108.3 | H21A—C21—H21B | 107.7 |
| C13—C12—H12A | 108.3 | N3—C22—C21 | 111.8 (2) |
| C9—C12—H12B | 108.3 | N3—C22—H22A | 109.3 |
| C13—C12—H12B | 108.3 | C21—C22—H22A | 109.3 |
| H12A—C12—H12B | 107.4 | N3—C22—H22B | 109.3 |
| C12—C13—H13A | 109.5 | C21—C22—H22B | 109.3 |
| C12—C13—H13B | 109.5 | H22A—C22—H22B | 107.9 |
| H13A—C13—H13B | 109.5 | C9—N1—C10 | 106.52 (17) |
| C12—C13—H13C | 109.5 | C9—N1—Zn1 | 132.81 (14) |
| H13A—C13—H13C | 109.5 | C10—N1—Zn1 | 120.54 (14) |
| H13B—C13—H13C | 109.5 | C9—N2—C11 | 107.76 (18) |
| C15—C14—N3 | 107.1 (2) | C9—N2—C19 | 127.13 (19) |
| C15—C14—H14 | 126.4 | C11—N2—C19 | 125.11 (19) |
| N3—C14—H14 | 126.4 | C16—N3—C14 | 106.8 (2) |
| C14—C15—N4 | 109.7 (2) | C16—N3—C22 | 129.2 (2) |
| C14—C15—H15 | 125.1 | C14—N3—C22 | 124.1 (2) |
| N4—C15—H15 | 125.1 | C16—N4—C15 | 105.6 (2) |
| N4—C16—N3 | 110.7 (2) | C16—N4—Zn1ᶦᶦᶦ | 127.12 (15) |
| N4—C16—C17′ | 126.3 (9) | C15—N4—Zn1ᶦᶦᶦ | 127.13 (17) |
| N3—C16—C17′ | 119.1 (9) | C7—O1—Zn1 | 117.32 (14) |
| N4—C16—C17 | 123.1 (4) | C8—O4—Zn1ᶦᵛ | 109.05 (13) |
| N3—C16—C17 | 126.0 (4) | C5—O5—H5 | 109.5 |
| C18—C17—C16 | 111.6 (6) | | |
| | | | |
| C6—C1—C2—C3 | −1.4 (3) | O1—Zn1—N1—C9 | −91.05 (19) |
| C7—C1—C2—C3 | 178.03 (18) | O4ᶦ—Zn1—N1—C9 | 160.56 (18) |
| C1—C2—C3—C4 | 1.9 (3) | N4ᶦᶦ—Zn1—N1—C9 | 38.8 (2) |
| C1—C2—C3—C8 | −178.86 (19) | O1—Zn1—N1—C10 | 93.79 (16) |
| C2—C3—C4—C5 | −0.7 (3) | O4ᶦ—Zn1—N1—C10 | −14.60 (17) |
| C8—C3—C4—C5 | −179.88 (18) | N4ᶦᶦ—Zn1—N1—C10 | −136.36 (16) |
| C3—C4—C5—O5 | −178.50 (19) | N1—C9—N2—C11 | −0.5 (2) |
| C3—C4—C5—C6 | −1.0 (3) | C12—C9—N2—C11 | 178.1 (2) |
| O5—C5—C6—C1 | 179.13 (18) | N1—C9—N2—C19 | 179.53 (19) |
| C4—C5—C6—C1 | 1.5 (3) | C12—C9—N2—C19 | −1.9 (3) |

| | | | |
|---|---|---|---|
| C2—C1—C6—C5 | −0.3 (3) | C10—C11—N2—C9 | 0.7 (2) |
| C7—C1—C6—C5 | −179.75 (19) | C10—C11—N2—C19 | −179.3 (2) |
| C2—C1—C7—O2 | 28.3 (3) | C20—C19—N2—C9 | −95.4 (3) |
| C6—C1—C7—O2 | −152.2 (2) | C20—C19—N2—C11 | 84.6 (3) |
| C2—C1—C7—O1 | −151.0 (2) | N4—C16—N3—C14 | 0.6 (3) |
| C6—C1—C7—O1 | 28.4 (3) | C17′—C16—N3—C14 | −158.6 (11) |
| C2—C3—C8—O3 | −2.7 (3) | C17—C16—N3—C14 | 176.4 (5) |
| C4—C3—C8—O3 | 176.5 (2) | N4—C16—N3—C22 | −179.4 (2) |
| C2—C3—C8—O4 | 177.98 (19) | C17′—C16—N3—C22 | 21.4 (12) |
| C4—C3—C8—O4 | −2.8 (3) | C17—C16—N3—C22 | −3.7 (6) |
| N1—C10—C11—N2 | −0.7 (3) | C15—C14—N3—C16 | 0.0 (3) |
| N1—C9—C12—C13 | −104.2 (3) | C15—C14—N3—C22 | 180.0 (2) |
| N2—C9—C12—C13 | 77.4 (3) | C21—C22—N3—C16 | 105.4 (3) |
| N3—C14—C15—N4 | −0.6 (4) | C21—C22—N3—C14 | −74.7 (3) |
| N4—C16—C17—C18 | −96.2 (6) | N3—C16—N4—C15 | −1.0 (3) |
| N3—C16—C17—C18 | 88.6 (7) | C17′—C16—N4—C15 | 156.4 (12) |
| C17′—C16—C17—C18 | 10 (3) | C17—C16—N4—C15 | −176.8 (5) |
| N4—C16—C17′—C18′ | 99.1 (17) | N3—C16—N4—Zn1ⁱⁱⁱ | −177.31 (14) |
| N3—C16—C17′—C18′ | −105.3 (15) | C17′—C16—N4—Zn1ⁱⁱⁱ | −19.9 (12) |
| C17—C16—C17′—C18′ | 9.4 (19) | C17—C16—N4—Zn1ⁱⁱⁱ | 6.8 (5) |
| N2—C19—C20—C21 | −69.9 (3) | C14—C15—N4—C16 | 0.9 (3) |
| C19—C20—C21—C22 | 179.9 (2) | C14—C15—N4—Zn1ⁱⁱⁱ | 177.28 (19) |
| C20—C21—C22—N3 | −70.7 (3) | O2—C7—O1—Zn1 | −5.3 (3) |
| N2—C9—N1—C10 | 0.1 (2) | C1—C7—O1—Zn1 | 173.94 (13) |
| C12—C9—N1—C10 | −178.5 (2) | O4ⁱ—Zn1—O1—C7 | 168.10 (15) |
| N2—C9—N1—Zn1 | −175.60 (14) | N4ⁱⁱ—Zn1—O1—C7 | −60.73 (17) |
| C12—C9—N1—Zn1 | 5.8 (3) | N1—Zn1—O1—C7 | 62.23 (17) |
| C11—C10—N1—C9 | 0.4 (2) | O3—C8—O4—Zn1ⁱᵛ | −10.2 (3) |
| C11—C10—N1—Zn1 | 176.70 (15) | C3—C8—O4—Zn1ⁱᵛ | 169.17 (14) |

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

*Hydrogen-bond geometry (Å, º)*

| D—H···A | D—H | H···A | D···A | D—H···A |
|---|---|---|---|---|
| C10—H10···O1ᵛ | 0.93 | 2.62 | 3.417 (3) | 144 |
| C14—H14···O5ᵛ | 0.93 | 2.49 | 3.398 (3) | 166 |
| O5—H5···O2ᵛⁱ | 0.82 | 1.88 | 2.697 (2) | 171 |

Symmetry codes: (v) −*x*+1, −*y*+1, −*z*+1; (vi) −*x*+1/2, *y*−1/2, −*z*+1/2.