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# Tetra-$\mu$-benzoato-bis{[4-(pyrrolidin-1-yl)-pyridine]zinc(II)}

**Seung Man Yu,[a] Kyosang Koo,[b] Pan-Gi Kim,[c] Cheal Kim[a]* and Youngmee Kim[d]***

[a]Department of Fine Chemistry, and Eco-Product and Materials Education Center, Seoul National University of Technology, Seoul 139-743, Republic of Korea, [b]Korea Division of Forest Disaster Management, Korea Forest Research Institute, Seoul 130-712, Republic of Korea, [c]Department of Forest & Environment Resources, Kyungpook National University, Sangju 742-711, Republic of Korea, and [d]Department of Chemistry and Nano Science, Ewha Womans University, Seoul 120-750, Republic of Korea
Correspondence e-mail: chealkim@sunt.ac.kr, ymeekim@ewha.ac.kr

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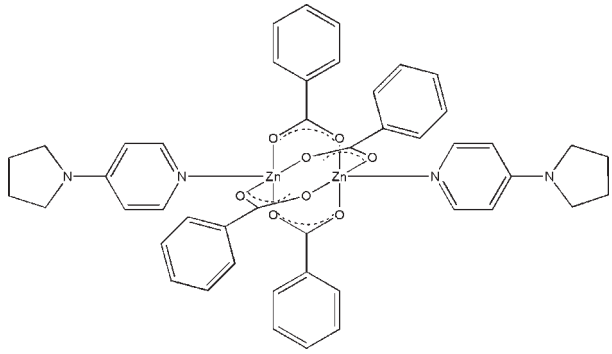
Key indicators: single-crystal X-ray study; $T$ = 293 K; mean $\sigma$(C–C) = 0.009 Å; disorder in main residue; $R$ factor = 0.053; $wR$ factor = 0.179; data-to-parameter ratio = 15.4.

The central part of the title centrosymmetric dinuclear complex, $[Zn_2(C_7H_5O_2)_4(C_9H_{12}N_2)_2]$, has a paddle-wheel conformation with four benzoate ligands bridging two symmetry-related $Zn^{II}$ ions. The distorted square-pyramidal coordination environment around the $Zn^{II}$ ion is completed by an N atom from a 4-(pyrrolidin-1-yl)pyridine ligand. The Zn···Zn separation of 2.9826 (12) Å does not represent a formal direct metal–metal bond. The $Zn^{II}$ ion is displaced by 0.381 (1) Å from the mean plane of the four basal O atoms. Two of the C atoms of the pyrrolidine ring are disordered over two sites with refined occupancies of 0.53 (2) and 0.47 (2).

## Related literature

For crystal structures containing the $[Zn_2(O_2CPh)_4]$ unit, see: Necefoglu *et al.* (2002); Zeleňák *et al.* (2004); Karmakar *et al.* (2006); Ohmura *et al.* (2005). For the crystal structures of copper(II) and zinc(II) benzoates with quinoxaline, 6-methylquinoline, 3-methylquinoline, di-2-pyridyl ketone and *trans*-1-(2-pyridyl)-2-(4-pyridyl)ethylene, see: Lee *et al.* (2008); Yu *et al.* (2008, 2009); Park *et al.* (2008); Shin *et al.* (2009); Song *et al.* (2009). For transition metal ions as the major cation contributors to the inorganic composition of natural water and biological fluids, see: Daniele *et al.* (2008); Parkin (2004); Tshuva & Lippard (2004).



## Experimental

### Crystal data

$[Zn_2(C_7H_5O_2)_4(C_9H_{12}N_2)_2]$
$M_r$ = 911.59
Monoclinic, $P2_1/n$
$a$ = 11.0021 (11) Å
$b$ = 11.4303 (11) Å
$c$ = 16.9508 (16) Å
$\beta$ = 93.869 (2)°
$V$ = 2126.8 (4) Å$^3$
$Z$ = 2
Mo $K\alpha$ radiation
$\mu$ = 1.19 mm$^{-1}$
$T$ = 293 K
0.08 × 0.08 × 0.01 mm

### Data collection

Bruker SMART CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 1997)
$T_{min}$ = 0.909, $T_{max}$ = 0.988
11271 measured reflections
4159 independent reflections
2284 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.068

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.053
$wR(F^2)$ = 0.179
$S$ = 0.90
4159 reflections
270 parameters
7 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.94 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.71 e Å$^{-3}$

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); 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*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LH2962).

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# supplementary materials

*Acta Cryst.* (2010). E**66**, m61-m62 [ **doi:10.1107/S1600536809052714** ]

# Tetra-$\mu$-benzoato-bis{[4-(pyrrolidin-1-yl)pyridine]zinc(II)}

**S. M. Yu, K. Koo, P.-G. Kim, C. Kim and Y. Kim**

## Comment

Recently, great attention has been paid to transition metal ions as the major cation contributors to the inorganic composition of natural water and biological fluids (Daniele, *et al.*, 2008; Parkin, 2004; Tshuva & Lippard, 2004). Some biologically active molecules that have potential interactions with transition metal ions are amino acids, proteins, sugars, nucleotides, fulvic acids and humic acids. In particular, the study on the interaction of transition metal ions with fulvic acids and humic acids, mainly found in soil, is being extensively investigated. As models to examine these interactions we have previously used copper(II) and zinc(II) benzoates as building blocks and reported the structures of copper(II) and zinc(II) benzoates with quinoxaline, 6-methylquinoline, 3-methylquinoline, di-2-pyridylketone, and*trans*-1-(2-pyridyl)-2-(4-pyridyl)ethylene (Lee, *et al.*, 2008; Yu, *et al.*, 2008; Park, *et al.*, 2008; Shin, *et al.*, 2009; Yu, *et al.*, 2009; Song, *et al.*, 2009). The related paddle-wheel type structures for Zn complexes have been previouly reported (Necefoglu, *et al.*, 2002; Zeleňák, *et al.*,2004; Kamakar, *et al.*, 2006; Ohmura, *et al.*, 2005). In this work, we have employed zinc(II) benzoate as a building block and 4-(pyrrolidin-1-yl)pyridine as a ligand. We report herein the structure of the title complex.

The molecular structure of the title complex is shown in Fig. 1. The asymmetric unit contains half of the complex with the formula unit being generated by an inversion center. The central part of the complex had a paddle-wheel type conformation four benzoate ligands bridging two symmetry related $Zn^{II}$ ions. The distorted square-pyramidal coordination environment around the unique $Zn^{II}$ ion is completed by an N atom from a 4-(pyrrolidin-1-yl)pyridine ligand. The $Zn^{II}$ ion is displaced by 0.381 (1) Å from the mean plane of the four basal oxygen atoms.

## Experimental

30.4 mg (0.1 mmol) of $Zn(NO_3)_2{\cdot}6H_2O$ and 28.0 mg (0.2 mmol) of $C_6H_5COONH_4$ were dissolved in 4 ml $H_2O$ and carefully layered by 4 ml me thanol solution of 4-(pyrrolidin-1-yl)pyridine (30.3 mg, 0.2 mmol). Suitable crystals of the title compound for X-ray analysis were obtained in a few weeks.

## Refinement

H atoms were placed in calculated positions with C—H distances of 0.93 Å (pyridine) and 0.97 Å (pyrrolidine). They were included in the refinement in a riding-motion approximation with Uĩso~(H) = 1.2U~eq~(C). The atoms C37/C37A and C38/C38A are disorder components both with refined occupancies of 0.53 (2) and 0.47 (2).

## Figures

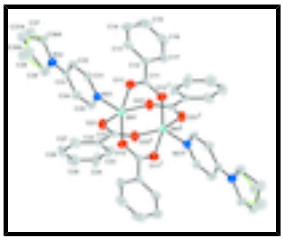

Fig. 1. The molecular structure of the title complex showing the atom-labeling scheme. Displacement ellipsoids are shown at the 30% probability level. H atoms have been omitted for clarity. The disordered part of pyrrol group is shown by green bonds [Symmetry code: (i) -*x*, -*y* + 1, -*z*].

## Tetra-μ-benzoato-bis{[4-(pyrrolidin-1-yl)pyridine]zinc(II)}

### *Crystal data*

| | |
|---|---|
| $[Zn_2(C_7H_5O_2)_4(C_9H_{12}N_2)_2]$ | $F(000) = 944$ |
| $M_r = 911.59$ | $D_x = 1.423$ Mg m$^{-3}$ |
| Monoclinic, $P2_1/n$ | Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å |
| Hall symbol: -P 2yn | Cell parameters from 1481 reflections |
| $a = 11.0021$ (11) Å | $\theta = 2.3$–$19.2°$ |
| $b = 11.4303$ (11) Å | $\mu = 1.19$ mm$^{-1}$ |
| $c = 16.9508$ (16) Å | $T = 293$ K |
| $\beta = 93.869$ (2)° | Plate, colorless |
| $V = 2126.8$ (4) Å$^3$ | 0.08 × 0.08 × 0.01 mm |
| $Z = 2$ | |

### *Data collection*

| | |
|---|---|
| Bruker SMART CCD diffractometer | 4159 independent reflections |
| Radiation source: fine-focus sealed tube | 2284 reflections with $I > 2\sigma(I)$ |
| graphite | $R_{int} = 0.068$ |
| φ and ω scans | $\theta_{max} = 26.0°$, $\theta_{min} = 2.1°$ |
| Absorption correction: multi-scan (*SADABS*; Bruker, 1997) | $h = -13 \rightarrow 13$ |
| $T_{min} = 0.909$, $T_{max} = 0.988$ | $k = -13 \rightarrow 14$ |
| 11271 measured reflections | $l = -17 \rightarrow 20$ |

### *Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Primary atom site location: structure-invariant direct methods |
| Least-squares matrix: full | Secondary atom site location: difference Fourier map |
| $R[F^2 > 2\sigma(F^2)] = 0.053$ | Hydrogen site location: inferred from neighbouring sites |
| $wR(F^2) = 0.179$ | H-atom parameters constrained |
| $S = 0.90$ | $w = 1/[\sigma^2(F_o^2) + (0.1079P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$ |

| | |
|---|---|
| 4159 reflections | $(\Delta/\sigma)_{max} < 0.001$ |
| 270 parameters | $\Delta\rho_{max} = 0.94$ e Å$^{-3}$ |
| 7 restraints | $\Delta\rho_{min} = -0.71$ 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 | 0.11885 (5) | 0.44449 (5) | 0.02560 (4) | 0.0380 (2) | |
| O11 | 0.1576 (4) | 0.5331 (3) | −0.0760 (2) | 0.0524 (11) | |
| O12 | 0.0192 (4) | 0.3879 (4) | 0.1160 (2) | 0.0574 (11) | |
| O21 | 0.1591 (3) | 0.5941 (3) | 0.0872 (2) | 0.0528 (10) | |
| O22 | 0.0201 (4) | 0.3274 (3) | −0.0446 (2) | 0.0562 (11) | |
| N31 | 0.2720 (4) | 0.3488 (4) | 0.0436 (2) | 0.0389 (10) | |
| N32 | 0.5772 (4) | 0.1339 (4) | 0.0637 (3) | 0.0494 (12) | |
| C11 | 0.0949 (5) | 0.5977 (5) | −0.1189 (3) | 0.0409 (13) | |
| C12 | 0.1545 (5) | 0.6638 (4) | −0.1822 (3) | 0.0428 (14) | |
| C13 | 0.2792 (6) | 0.6570 (5) | −0.1882 (3) | 0.0556 (16) | |
| H13 | 0.3250 | 0.6061 | −0.1554 | 0.067* | |
| C14 | 0.3364 (7) | 0.7242 (6) | −0.2419 (4) | 0.072 (2) | |
| H14 | 0.4207 | 0.7224 | −0.2436 | 0.086* | |
| C15 | 0.2653 (9) | 0.7955 (7) | −0.2942 (5) | 0.089 (3) | |
| H15 | 0.3025 | 0.8385 | −0.3325 | 0.107* | |
| C16 | 0.1429 (8) | 0.8024 (6) | −0.2898 (4) | 0.074 (2) | |
| H16 | 0.0974 | 0.8523 | −0.3236 | 0.089* | |
| C17 | 0.0854 (6) | 0.7365 (5) | −0.2356 (3) | 0.0542 (15) | |
| H17 | 0.0011 | 0.7397 | −0.2342 | 0.065* | |
| C21 | 0.0822 (6) | 0.6758 (5) | 0.0839 (3) | 0.0444 (14) | |
| C22 | 0.1148 (5) | 0.7854 (4) | 0.1296 (3) | 0.0384 (13) | |
| C23 | 0.0408 (6) | 0.8808 (5) | 0.1229 (4) | 0.0638 (18) | |
| H23 | −0.0297 | 0.8774 | 0.0894 | 0.077* | |
| C24 | 0.0676 (7) | 0.9824 (6) | 0.1645 (5) | 0.084 (3) | |
| H24 | 0.0174 | 1.0476 | 0.1580 | 0.101* | |
| C25 | 0.1670 (8) | 0.9853 (6) | 0.2142 (5) | 0.082 (2) | |
| H25 | 0.1835 | 1.0527 | 0.2438 | 0.098* | |
| C26 | 0.2463 (7) | 0.8915 (6) | 0.2234 (4) | 0.0710 (19) | |
| H26 | 0.3159 | 0.8950 | 0.2576 | 0.085* | |

| | | | | | |
|---|---|---|---|---|---|
| C27 | 0.2173 (6) | 0.7926 (5) | 0.1794 (4) | 0.0579 (17) | |
| H27 | 0.2695 | 0.7286 | 0.1838 | 0.069* | |
| C31 | 0.3724 (5) | 0.3727 (5) | 0.0069 (3) | 0.0455 (14) | |
| H31 | 0.3719 | 0.4391 | −0.0249 | 0.055* | |
| C32 | 0.4768 (5) | 0.3064 (5) | 0.0126 (4) | 0.0531 (16) | |
| H32 | 0.5441 | 0.3287 | −0.0142 | 0.064* | |
| C33 | 0.4810 (5) | 0.2046 (5) | 0.0591 (3) | 0.0422 (13) | |
| C34 | 0.3747 (5) | 0.1802 (5) | 0.0984 (4) | 0.0517 (16) | |
| H34 | 0.3719 | 0.1152 | 0.1312 | 0.062* | |
| C35 | 0.2759 (5) | 0.2528 (5) | 0.0879 (3) | 0.0478 (15) | |
| H35 | 0.2066 | 0.2335 | 0.1136 | 0.057* | |
| C36 | 0.6859 (5) | 0.1549 (5) | 0.0198 (4) | 0.0573 (17) | |
| H36A | 0.7297 | 0.2235 | 0.0398 | 0.069* | 0.47 (2) |
| H36B | 0.6639 | 0.1656 | −0.0361 | 0.069* | 0.47 (2) |
| C37 | 0.7631 (14) | 0.0439 (11) | 0.0341 (9) | 0.054 (4)* | 0.47 (2) |
| H37A | 0.7416 | −0.0159 | −0.0050 | 0.065* | 0.47 (2) |
| H37B | 0.8495 | 0.0607 | 0.0340 | 0.065* | 0.47 (2) |
| C38 | 0.7273 (7) | 0.008 (2) | 0.1161 (9) | 0.067 (6)* | 0.47 (2) |
| H38A | 0.7685 | 0.0566 | 0.1567 | 0.080* | 0.47 (2) |
| H38B | 0.7467 | −0.0731 | 0.1268 | 0.080* | 0.47 (2) |
| C39 | 0.5882 (5) | 0.0289 (5) | 0.1122 (4) | 0.0607 (18) | |
| H39A | 0.5441 | −0.0362 | 0.0872 | 0.073* | 0.47 (2) |
| H39B | 0.5595 | 0.0420 | 0.1643 | 0.073* | 0.47 (2) |
| H36C | 0.7113 | 0.2360 | 0.0238 | 0.069* | 0.53 (2) |
| H36D | 0.6710 | 0.1345 | −0.0355 | 0.069* | 0.53 (2) |
| C37A | 0.7824 (9) | 0.0733 (12) | 0.0611 (11) | 0.073 (5)* | 0.53 (2) |
| H37C | 0.8362 | 0.0425 | 0.0231 | 0.088* | 0.53 (2) |
| H37D | 0.8310 | 0.1156 | 0.1016 | 0.088* | 0.53 (2) |
| C38A | 0.7126 (9) | −0.0257 (12) | 0.0979 (11) | 0.063 (5)* | 0.53 (2) |
| H38C | 0.7539 | −0.0514 | 0.1473 | 0.076* | 0.53 (2) |
| H38D | 0.7034 | −0.0919 | 0.0622 | 0.076* | 0.53 (2) |
| H39C | 0.5231 | −0.0254 | 0.0971 | 0.073* | 0.53 (2) |
| H39D | 0.5839 | 0.0486 | 0.1676 | 0.073* | 0.53 (2) |

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

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Zn1 | 0.0382 (4) | 0.0339 (3) | 0.0421 (4) | 0.0065 (3) | 0.0043 (3) | 0.0011 (3) |
| O11 | 0.061 (3) | 0.051 (2) | 0.047 (2) | 0.011 (2) | 0.011 (2) | 0.017 (2) |
| O12 | 0.055 (3) | 0.064 (3) | 0.056 (3) | 0.007 (2) | 0.016 (2) | 0.016 (2) |
| O21 | 0.052 (3) | 0.040 (2) | 0.064 (3) | 0.007 (2) | −0.011 (2) | −0.010 (2) |
| O22 | 0.054 (3) | 0.050 (2) | 0.063 (3) | −0.002 (2) | −0.010 (2) | −0.014 (2) |
| N31 | 0.038 (3) | 0.038 (2) | 0.041 (3) | 0.005 (2) | 0.002 (2) | 0.005 (2) |
| N32 | 0.043 (3) | 0.052 (3) | 0.053 (3) | 0.016 (2) | 0.006 (2) | 0.010 (2) |
| C11 | 0.055 (4) | 0.034 (3) | 0.035 (3) | −0.005 (3) | 0.012 (3) | −0.003 (2) |
| C12 | 0.053 (4) | 0.037 (3) | 0.039 (3) | −0.004 (3) | 0.012 (3) | −0.004 (3) |
| C13 | 0.063 (4) | 0.061 (4) | 0.044 (3) | −0.008 (3) | 0.013 (3) | −0.005 (3) |
| C14 | 0.073 (5) | 0.076 (5) | 0.068 (5) | −0.023 (4) | 0.027 (4) | −0.015 (4) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C15 | 0.135 (8) | 0.071 (5) | 0.066 (5) | −0.035 (5) | 0.046 (6) | 0.000 (4) |
| C16 | 0.109 (7) | 0.066 (5) | 0.046 (4) | −0.005 (4) | 0.004 (4) | 0.018 (3) |
| C17 | 0.063 (4) | 0.051 (4) | 0.048 (4) | −0.004 (3) | −0.001 (3) | 0.008 (3) |
| C21 | 0.062 (4) | 0.035 (3) | 0.037 (3) | −0.002 (3) | 0.017 (3) | 0.004 (2) |
| C22 | 0.037 (3) | 0.041 (3) | 0.037 (3) | −0.007 (2) | 0.005 (3) | −0.005 (2) |
| C23 | 0.047 (4) | 0.049 (4) | 0.096 (5) | 0.006 (3) | 0.003 (4) | −0.018 (4) |
| C24 | 0.062 (5) | 0.060 (5) | 0.128 (7) | 0.012 (4) | −0.026 (5) | −0.038 (5) |
| C25 | 0.103 (7) | 0.052 (4) | 0.093 (6) | −0.013 (4) | 0.022 (5) | −0.028 (4) |
| C26 | 0.083 (5) | 0.068 (5) | 0.059 (4) | −0.015 (4) | −0.016 (4) | −0.013 (4) |
| C27 | 0.080 (5) | 0.038 (3) | 0.054 (4) | 0.000 (3) | 0.000 (4) | 0.002 (3) |
| C31 | 0.040 (3) | 0.046 (3) | 0.050 (3) | 0.003 (3) | 0.001 (3) | 0.015 (3) |
| C32 | 0.048 (4) | 0.055 (4) | 0.058 (4) | 0.004 (3) | 0.016 (3) | 0.012 (3) |
| C33 | 0.042 (3) | 0.041 (3) | 0.044 (3) | 0.009 (3) | 0.001 (3) | −0.001 (3) |
| C34 | 0.053 (4) | 0.043 (3) | 0.061 (4) | 0.011 (3) | 0.012 (3) | 0.017 (3) |
| C35 | 0.043 (3) | 0.043 (3) | 0.059 (4) | 0.005 (3) | 0.016 (3) | 0.011 (3) |
| C36 | 0.047 (4) | 0.064 (4) | 0.062 (4) | 0.015 (3) | 0.013 (3) | 0.006 (3) |
| C39 | 0.061 (4) | 0.050 (4) | 0.072 (4) | 0.017 (3) | 0.006 (4) | 0.009 (3) |
| C36A | 0.047 (4) | 0.064 (4) | 0.062 (4) | 0.015 (3) | 0.013 (3) | 0.006 (3) |
| C39A | 0.061 (4) | 0.050 (4) | 0.072 (4) | 0.017 (3) | 0.006 (4) | 0.009 (3) |

*Geometric parameters (Å, °)*

| | | | |
|---|---|---|---|
| Zn1—N31 | 2.014 (4) | C23—H23 | 0.9300 |
| Zn1—O21 | 2.036 (4) | C24—C25 | 1.335 (11) |
| Zn1—O12 | 2.048 (4) | C24—H24 | 0.9300 |
| Zn1—O22 | 2.053 (4) | C25—C26 | 1.384 (11) |
| Zn1—O11 | 2.068 (4) | C25—H25 | 0.9300 |
| Zn1—Zn1$^{i}$ | 2.9826 (12) | C26—C27 | 1.380 (8) |
| O11—C11 | 1.216 (6) | C26—H26 | 0.9300 |
| O12—C11$^{i}$ | 1.270 (6) | C27—H27 | 0.9300 |
| O21—C21 | 1.260 (6) | C31—C32 | 1.374 (7) |
| O22—C21$^{i}$ | 1.268 (7) | C31—H31 | 0.9300 |
| N31—C35 | 1.329 (6) | C32—C33 | 1.404 (7) |
| N31—C31 | 1.333 (6) | C32—H32 | 0.9300 |
| N32—C33 | 1.330 (6) | C33—C34 | 1.412 (7) |
| N32—C39 | 1.454 (7) | C34—C35 | 1.370 (7) |
| N32—C36 | 1.470 (7) | C34—H34 | 0.9300 |
| C11—O12$^{i}$ | 1.270 (6) | C35—H35 | 0.9300 |
| C11—C12 | 1.500 (7) | C36—C37 | 1.536 (7) |
| C12—C13 | 1.384 (8) | C36—H36A | 0.9700 |
| C12—C17 | 1.413 (8) | C36—H36B | 0.9700 |
| C13—C14 | 1.375 (8) | C37—C38 | 1.525 (10) |
| C13—H13 | 0.9300 | C37—H37A | 0.9700 |
| C14—C15 | 1.403 (11) | C37—H37B | 0.9700 |
| C14—H14 | 0.9300 | C38—C39 | 1.545 (7) |
| C15—C16 | 1.356 (10) | C38—H38A | 0.9700 |
| C15—H15 | 0.9300 | C38—H38B | 0.9700 |
| C16—C17 | 1.374 (8) | C39—H39A | 0.9700 |

| | | | |
|---|---|---|---|
| C16—H16 | 0.9300 | C39—H39B | 0.9700 |
| C17—H17 | 0.9300 | C37A—C38A | 1.524 (10) |
| C21—O22$^{i}$ | 1.268 (7) | C37A—H37C | 0.9700 |
| C21—C22 | 1.504 (7) | C37A—H37D | 0.9700 |
| C22—C23 | 1.361 (8) | C38A—H38C | 0.9700 |
| C22—C27 | 1.364 (8) | C38A—H38D | 0.9700 |
| C23—C24 | 1.380 (9) | | |
| N31—Zn1—O21 | 103.14 (17) | C25—C24—H24 | 120.6 |
| N31—Zn1—O12 | 101.53 (16) | C23—C24—H24 | 120.6 |
| O21—Zn1—O12 | 89.46 (17) | C24—C25—C26 | 122.3 (7) |
| N31—Zn1—O22 | 97.95 (17) | C24—C25—H25 | 118.9 |
| O21—Zn1—O22 | 158.90 (16) | C26—C25—H25 | 118.9 |
| O12—Zn1—O22 | 86.50 (17) | C27—C26—C25 | 117.0 (7) |
| N31—Zn1—O11 | 100.06 (16) | C27—C26—H26 | 121.5 |
| O21—Zn1—O11 | 88.04 (16) | C25—C26—H26 | 121.5 |
| O12—Zn1—O11 | 158.27 (16) | C22—C27—C26 | 122.3 (6) |
| O22—Zn1—O11 | 88.11 (16) | C22—C27—H27 | 118.8 |
| N31—Zn1—Zn1$^{i}$ | 169.40 (13) | C26—C27—H27 | 118.8 |
| O21—Zn1—Zn1$^{i}$ | 87.02 (11) | N31—C31—C32 | 124.7 (5) |
| O12—Zn1—Zn1$^{i}$ | 81.31 (12) | N31—C31—H31 | 117.7 |
| O22—Zn1—Zn1$^{i}$ | 71.90 (12) | C32—C31—H31 | 117.7 |
| O11—Zn1—Zn1$^{i}$ | 77.01 (12) | C31—C32—C33 | 119.5 (5) |
| C11—O11—Zn1 | 130.8 (4) | C31—C32—H32 | 120.2 |
| C11$^{i}$—O12—Zn1 | 124.6 (4) | C33—C32—H32 | 120.2 |
| C21—O21—Zn1 | 118.5 (4) | N32—C33—C32 | 122.2 (5) |
| C21$^{i}$—O22—Zn1 | 137.7 (4) | N32—C33—C34 | 122.2 (5) |
| C35—N31—C31 | 115.9 (4) | C32—C33—C34 | 115.6 (5) |
| C35—N31—Zn1 | 122.0 (3) | C35—C34—C33 | 119.6 (5) |
| C31—N31—Zn1 | 122.0 (4) | C35—C34—H34 | 120.2 |
| C33—N32—C39 | 124.8 (4) | C33—C34—H34 | 120.2 |
| C33—N32—C36 | 122.8 (5) | N31—C35—C34 | 124.7 (5) |
| C39—N32—C36 | 112.4 (4) | N31—C35—H35 | 117.6 |
| O11—C11—O12$^{i}$ | 125.3 (5) | C34—C35—H35 | 117.6 |
| O11—C11—C12 | 118.4 (5) | N32—C36—C37 | 104.2 (6) |
| O12$^{i}$—C11—C12 | 116.3 (5) | N32—C36—H36A | 110.9 |
| C13—C12—C17 | 118.6 (5) | C37—C36—H36A | 110.9 |
| C13—C12—C11 | 120.5 (6) | N32—C36—H36B | 110.9 |
| C17—C12—C11 | 120.8 (5) | C37—C36—H36B | 110.9 |
| C14—C13—C12 | 121.2 (7) | H36A—C36—H36B | 108.9 |
| C14—C13—H13 | 119.4 | C38—C37—C36 | 100.9 (9) |
| C12—C13—H13 | 119.4 | C38—C37—H37A | 111.6 |
| C13—C14—C15 | 118.8 (7) | C36—C37—H37A | 111.6 |
| C13—C14—H14 | 120.6 | C38—C37—H37B | 111.6 |
| C15—C14—H14 | 120.6 | C36—C37—H37B | 111.6 |
| C16—C15—C14 | 120.8 (6) | H37A—C37—H37B | 109.4 |
| C16—C15—H15 | 119.6 | C37—C38—C39 | 103.7 (8) |
| C14—C15—H15 | 119.6 | C37—C38—H38A | 111.0 |

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|---|---|---|---|
| C15—C16—C17 | 120.6 (7) | C39—C38—H38A | 111.0 |
| C15—C16—H16 | 119.7 | C37—C38—H38B | 111.0 |
| C17—C16—H16 | 119.7 | C39—C38—H38B | 111.0 |
| C16—C17—C12 | 119.9 (6) | H38A—C38—H38B | 109.0 |
| C16—C17—H17 | 120.0 | N32—C39—C38 | 101.2 (8) |
| C12—C17—H17 | 120.0 | N32—C39—H39A | 111.5 |
| O21—C21—O22$^{i}$ | 124.9 (5) | C38—C39—H39A | 111.5 |
| O21—C21—C22 | 117.3 (6) | N32—C39—H39B | 111.5 |
| O22$^{i}$—C21—C22 | 117.9 (5) | C38—C39—H39B | 111.5 |
| C23—C22—C27 | 118.0 (5) | H39A—C39—H39B | 109.3 |
| C23—C22—C21 | 120.2 (5) | C38A—C37A—H37C | 110.4 |
| C27—C22—C21 | 121.8 (5) | C38A—C37A—H37D | 110.4 |
| C22—C23—C24 | 121.6 (7) | H37C—C37A—H37D | 108.6 |
| C22—C23—H23 | 119.2 | C37A—C38A—H38C | 111.0 |
| C24—C23—H23 | 119.2 | C37A—C38A—H38D | 111.0 |
| C25—C24—C23 | 118.8 (7) | H38C—C38A—H38D | 109.0 |
| N31—Zn1—O11—C11 | 173.5 (5) | C14—C15—C16—C17 | −2.3 (11) |
| O21—Zn1—O11—C11 | −83.5 (5) | C15—C16—C17—C12 | 2.2 (10) |
| O12—Zn1—O11—C11 | 0.1 (8) | C13—C12—C17—C16 | −2.8 (9) |
| O22—Zn1—O11—C11 | 75.8 (5) | C11—C12—C17—C16 | 175.6 (5) |
| Zn1$^{i}$—Zn1—O11—C11 | 3.9 (5) | Zn1—O21—C21—O22$^{i}$ | 0.0 (7) |
| N31—Zn1—O12—C11$^{i}$ | −162.7 (4) | Zn1—O21—C21—C22 | −179.7 (3) |
| O21—Zn1—O12—C11$^{i}$ | 94.0 (5) | O21—C21—C22—C23 | 174.1 (5) |
| O22—Zn1—O12—C11$^{i}$ | −65.2 (5) | O22$^{i}$—C21—C22—C23 | −5.6 (7) |
| O11—Zn1—O12—C11$^{i}$ | 10.7 (8) | O21—C21—C22—C27 | −6.7 (7) |
| Zn1$^{i}$—Zn1—O12—C11$^{i}$ | 7.0 (4) | O22$^{i}$—C21—C22—C27 | 173.6 (5) |
| N31—Zn1—O21—C21 | 176.1 (4) | C27—C22—C23—C24 | 0.3 (9) |
| O12—Zn1—O21—C21 | −82.2 (4) | C21—C22—C23—C24 | 179.5 (6) |
| O22—Zn1—O21—C21 | −3.3 (7) | C22—C23—C24—C25 | −2.0 (12) |
| O11—Zn1—O21—C21 | 76.2 (4) | C23—C24—C25—C26 | 2.4 (13) |
| Zn1$^{i}$—Zn1—O21—C21 | −0.8 (4) | C24—C25—C26—C27 | −1.0 (12) |
| N31—Zn1—O22—C21$^{i}$ | −175.1 (5) | C23—C22—C27—C26 | 1.1 (9) |
| O21—Zn1—O22—C21$^{i}$ | 4.4 (8) | C21—C22—C27—C26 | −178.1 (5) |
| O12—Zn1—O22—C21$^{i}$ | 83.8 (5) | C25—C26—C27—C22 | −0.8 (10) |
| O11—Zn1—O22—C21$^{i}$ | −75.2 (5) | C35—N31—C31—C32 | −0.5 (9) |
| Zn1$^{i}$—Zn1—O22—C21$^{i}$ | 1.8 (5) | Zn1—N31—C31—C32 | −175.5 (5) |
| O21—Zn1—N31—C35 | 110.2 (4) | N31—C31—C32—C33 | 0.8 (10) |
| O12—Zn1—N31—C35 | 18.1 (5) | C39—N32—C33—C32 | 178.5 (6) |
| O22—Zn1—N31—C35 | −70.0 (4) | C36—N32—C33—C32 | −1.1 (9) |
| O11—Zn1—N31—C35 | −159.4 (4) | C39—N32—C33—C34 | −3.7 (9) |
| Zn1$^{i}$—Zn1—N31—C35 | −86.5 (8) | C36—N32—C33—C34 | 176.7 (6) |
| O21—Zn1—N31—C31 | −75.2 (5) | C31—C32—C33—N32 | 176.6 (6) |
| O12—Zn1—N31—C31 | −167.3 (4) | C31—C32—C33—C34 | −1.3 (9) |
| O22—Zn1—N31—C31 | 104.7 (4) | N32—C33—C34—C35 | −176.4 (6) |
| O11—Zn1—N31—C31 | 15.2 (5) | C32—C33—C34—C35 | 1.6 (9) |

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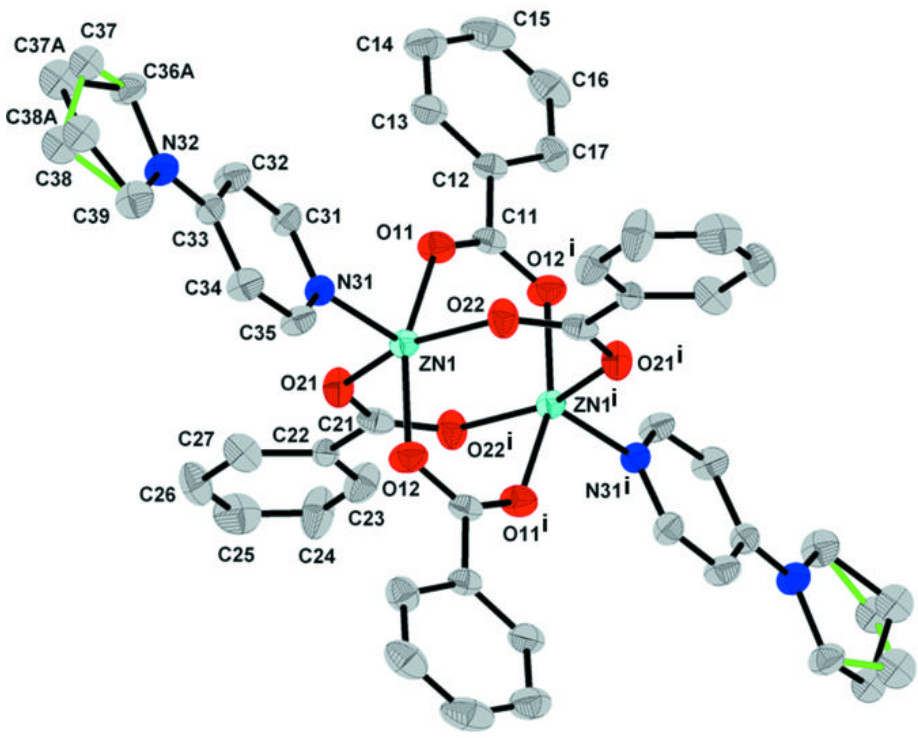
|---|---|---|---|
| $Zn1^{i}$—Zn1—N31—C31 | 88.1 (8) | C31—N31—C35—C34 | 0.8 (9) |
| Zn1—O11—C11—$O12^{i}$ | −10.9 (9) | Zn1—N31—C35—C34 | 175.8 (5) |
| Zn1—O11—C11—C12 | 171.0 (3) | C33—C34—C35—N31 | −1.4 (10) |
| O11—C11—C12—C13 | −4.1 (8) | C33—N32—C36—C37 | −172.3 (9) |
| $O12^{i}$—C11—C12—C13 | 177.6 (5) | C39—N32—C36—C37 | 8.1 (10) |
| O11—C11—C12—C17 | 177.5 (5) | N32—C36—C37—C38 | −30.5 (16) |
| $O12^{i}$—C11—C12—C17 | −0.7 (7) | C36—C37—C38—C39 | 42 (2) |
| C17—C12—C13—C14 | 3.6 (9) | C33—N32—C39—C38 | −162.0 (9) |
| C11—C12—C13—C14 | −174.8 (5) | C36—N32—C39—C38 | 17.6 (10) |
| C12—C13—C14—C15 | −3.6 (9) | C37—C38—C39—N32 | −36.8 (17) |
| C13—C14—C15—C16 | 3.0 (11) | | |

Symmetry codes: (i) −*x*, −*y*+1, −*z*.

**Fig. 1**


C37
C37A
C36A
C38A
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ZN1
O21
O21i
ZN1i
C21
C22
C27
O22i
C26
O12
N31i
C23
O11i
C25
C24