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# Tetrakis[$\mu$-4-(dimethylamino)benzoato-$\kappa^2O$:$O'$]bis[(*N*,*N*-diethylnicotinamide-$\kappa N^1$)zinc(II)]

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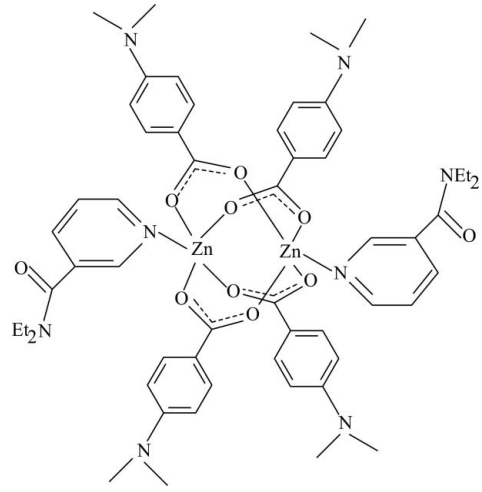
Key indicators: single-crystal X-ray study; $T$ = 294 K; mean $\sigma$(C–C) = 0.003 Å; $R$ factor = 0.033; $wR$ factor = 0.090; data-to-parameter ratio = 19.7.

The title molecule, $[Zn_2(C_9H_{10}NO_2)_4(C_{10}H_{14}N_2O)_2]$, is a centrosymmetric binuclear complex, with Zn atoms [Zn$\cdots$Zn′ = 2.8927 (4) Å] bridged by four carboxylate groups from the dimethylaminobenzoate (DMAB) ligands. The four carboxyl O atoms around the Zn atom form a distorted square-planar arrangement; the distorted square-pyramidal coordination geometry is completed by the pyridine N atom of the *N*,*N*-diethylnicotinamide (DENA) ligand. The Zn atom is displaced by 0.3326 (2) Å from the plane of the four O atoms, with an average Zn—O distance of 2.0416 (12) Å. The dihedral angles between the carboxylate groups and the adjacent benzene rings are 5.31 (8) and 11.00 (9)°, while the pyridine ring is oriented at dihedral angles of 66.26 (6) and 37.88 (7)° with respect to the benzene rings. Weak intramolecular C—H$\cdots$O and intermolecular C—H$\cdots\pi$ interactions are present.

## Related literature

For general background to niacin and the nicotinic acid derivative *N*,*N*-diethylnicotinamide (DENA), see: Bigoli *et al.* (1972); Krishnamachari (1974). For related structures, see: Hökelek *et al.* (1995, 2009*a*,*b*); Speier & Fulop (1989); Usubaliev *et al.* (1980).



## Experimental

### Crystal data

$[Zn_2(C_9H_{10}NO_2)_4(C_{10}H_{14}N_2O)_2]$
$M_r$ = 1143.96
Triclinic, $P\overline{1}$
$a$ = 9.2731 (6) Å
$b$ = 13.2340 (8) Å
$c$ = 13.4756 (8) Å
$\alpha$ = 112.348 (3)°
$\beta$ = 109.236 (2)°
$\gamma$ = 95.728 (2)°
$V$ = 1395.33 (16) Å$^3$
$Z$ = 1
Mo $K\alpha$ radiation
$\mu$ = 0.92 mm$^{-1}$
$T$ = 294 K
0.52 × 0.35 × 0.25 mm

### Data collection

Bruker Kappa APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
$T_{min}$ = 0.681, $T_{max}$ = 0.791
24970 measured reflections
6877 independent reflections
5749 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.029

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.033
$wR(F^2)$ = 0.090
$S$ = 1.06
6877 reflections
349 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.24 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.43 e Å$^{-3}$

**Table 1**
Selected bond lengths (Å).

| | | | |
|---|---|---|---|
| Zn1—O1 | 2.0265 (12) | Zn1—O5 | 2.0459 (12) |
| Zn1—O2 | 2.0269 (12) | Zn1—N3 | 2.0446 (13) |
| Zn1—O4 | 2.0669 (12) | | |

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

| $D$—H$\cdots A$ | $D$—H | H$\cdots A$ | $D\cdots A$ | $D$—H$\cdots A$ |
|---|---|---|---|---|
| C23—H23$\cdots$O5 | 0.93 | 2.54 | 3.122 (2) | 121 |
| C8—H8$A\cdots Cg3^{i}$ | 0.96 | 2.77 | 3.629 (3) | 150 |

Symmetry code: (i) $-x+1, -y, -z+1$. $Cg3$ is the centroid of the N3/C19–C23 ring.

Data collection: *APEX2* (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: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999) and *PLATON* (Spek, 2009).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU2669).

## References

Bigoli, F., Braibanti, A., Pellinghelli, M. A. & Tiripicchio, A. (1972). *Acta Cryst.* B**28**, 962–966.
Bruker (2005). *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
Bruker (2007). *APEX2* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Farrugia, L. J. (1999). *J. Appl. Cryst.* **32**, 837–838.
Hökelek, T., Necefoğlu, H. & Balcı, M. (1995). *Acta Cryst.* C**51**, 2020–2023.
Hökelek, T., Yılmaz, F., Tercan, B., Aybirdi, Ö. & Necefoğlu, H. (2009*a*). *Acta Cryst.* E**65**, m955–m956.
Hökelek, T., Yılmaz, F., Tercan, B., Aybirdi, Ö. & Necefoğlu, H. (2009*b*). *Acta Cryst.* E**65**, m1328–m1329.
Krishnamachari, K. A. V. R. (1974). *Am. J. Clin. Nutr.* **27**, 108–111.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Speier, G. & Fulop, V. (1989). *J. Chem. Soc. Dalton Trans.* pp. 2331–2333.
Spek, A. L. (2009). *Acta Cryst.* D**65**, 148–155.
Usubaliev, B. T., Movsumov, E. M., Musaev, F. N., Nadzhafov, G. N., Amiraslanov, I. R. & Mamedov, Kh. S. (1980). *Koord. Khim.* **6**, 1091–1096.

# supporting information

*Acta Cryst.* (2009). E**65**, m1582–m1583 [doi:10.1107/S1600536809047473]

## Tetrakis[$\mu$-4-(dimethylamino)benzoato-$\kappa^2O$:$O'$]bis[(*N*,*N*-diethylnicotinamide-$\kappa N^1$)zinc(II)]

**Tuncer Hökelek, Hakan Dal, Barış Tercan, Özgür Aybirdi and Hacali Necefoğlu**

### S1. Comment

As a part of our ongoing investigation on transition metal complexes of nicotinamide (NA), one form of niacin (Krishnamachari, 1974), and/or the nicotinic acid derivative *N*,*N*-diethylnicotinamide (DENA), an important respiratory stimulant (Bigoli *et al.*, 1972), the title compound was synthesized and its crystal structure is reported herein.

The title compound is a binuclear compound, consisting of two DENA and four dimethylaminobenzoate (DMAB) ligands. The crystal structures of similar complexes of $Cu^{2+}$ and $Zn^{2+}$ ions, $[Cu(C_6H_5COO)_2(C_5H_5N)]_2$ (Usubaliev *et al.*, 1980); $[Cu(C_6H_5CO_2)_2(py)]_2$ (Speier & Fulop, 1989), $[Cu_2(C_6H_5COO)_4(C_{10}H_{14}N_2O)_2]$ (Hökelek *et al.*, 1995), $[Zn_2(C_{11}H_{14}NO_2)_4(C_{10}H_{14}N_2O)_2]$ (Hökelek *et al.*, 2009*a*) and $[Zn_2(C_8H_8NO_2)_4(C_{10}H_{14}N_2O)_2].2H_2O$ (Hökelek *et al.*, 2009*b*) have also been determined. In these structures, the benzoate ion acts as a bidentate ligand.

The title dimeric complex, $[Zn_2(DMAB)_4(DENA)_2]$, has a centre of symmetry and two $Zn^{II}$ atoms surrounded by four DMAB groups and two DENA ligands (Fig. 1). The DENA ligands are coordinated to Zn atoms through pyridine N atoms only. The DMAB groups act as bridging ligands. The Zn···Zn′ distance is 2.8927 (4) Å. The average Zn—O distance is 2.0416 (12) Å (Table 1), and four O atoms of the bridging DMAB ligands around each Zn atom form a distorted square plane. The Zn atom lies 0.3326 (2) Å below the least-squares plane. The average O—Zn—O bond angle is 88.48 (6)°. A distorted square-pyramidal arrangement around each Zn atom is completed by the pyridine N atom of DENA ligand at 2.0446 (13) Å from the Zn atom. The N3—Zn1···Zn1′ angle is 163.64 (6)° and the dihedral angle between plane through Zn1, O1, O4, C1, Zn1′, O1′, O4′, C1′ and the plane through Zn1, O2, O5, C10, Zn1′, O2′, O5′, C10′ is 89.47 (7)°. The dihedral angles between the planar carboxylate groups and the adjacent benzene rings A (C2—C7) and B (C11—C16) are 5.31 (8)° and 11.00 (9)°, respectively, while that between rings A and B is A/B = 83.70 (6)°. Ring C (N3/C19—C23) is oriented with respect to rings A and B at dihedral angles A/C = 66.26 (6) and B/C = 37.88 (7) °.

Weak intramolecular C—H···O and C—H···$\pi$ interactions (Table 2) are present, in which they may be effective in the stabilization of the structure.

### S2. Experimental

The title compound was prepared by the reaction of $ZnSO_4.H_2O$ (0.9 g, 5 mmol) in $H_2O$ (50 ml) and DENA (1.78 g, 10 mmol) in $H_2O$ (50 ml) with sodium *p*-dimethylaminobenzoate (1.88 g, 10 mmol) in $H_2O$ (100 ml). The mixture was filtered and set aside to crystallize at ambient temperature for one week, giving colorless single crystals.

### S3. Refinement

H atoms were positioned geometrically with C—H = 0.93, 0.97 and 0.96 Å, for aromatic, methylene and methyl H atoms, respectively, and constrained to ride on their parent atoms, with $U_{iso}(H) = xU_{eq}(C)$, where $x = 1.5$ for methyl H and $x = 1.2$ for all other H atoms.

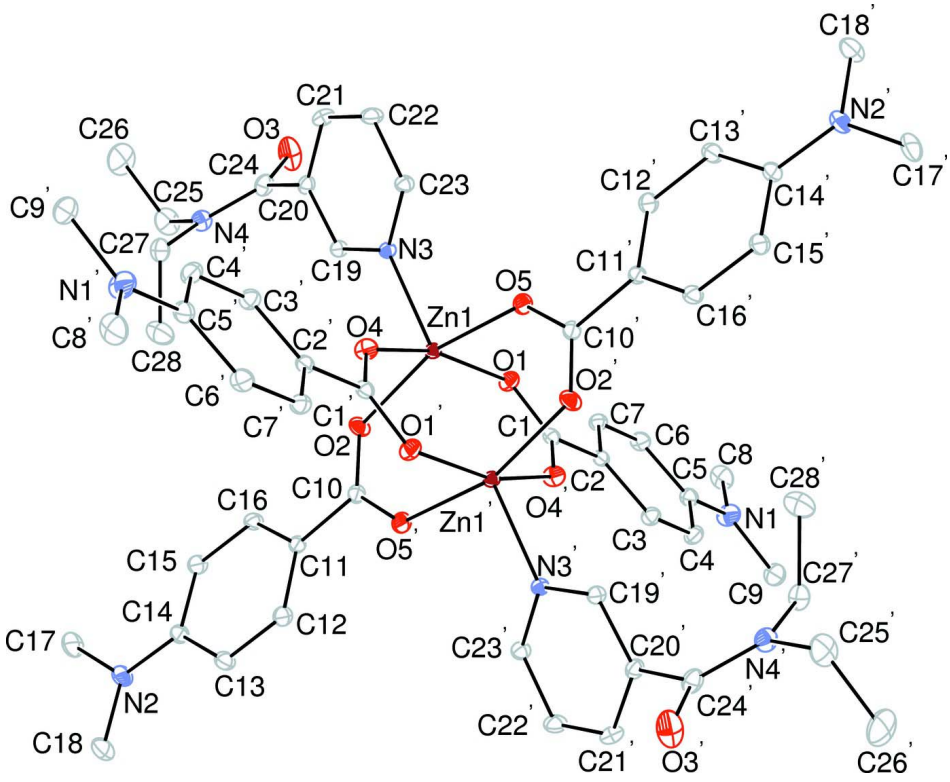


**Figure 1**

The molecular structure of the title molecule with the atom-numbering scheme. Displacement ellipsoids are drawn at the 15% probability level. Primed atoms are generated by the symmetry operator:(′) 1-*x*, 1-*y*, 1-*z*.

**Tetrakis[$\mu$-4-(dimethylamino)benzoato-$\kappa^2O$:$O'$]bis[(*N*,*N*-diethylnicotinamide-$\kappa N^1$)zinc(II)]**

*Crystal data*

$[Zn_2(C_9H_{10}NO_2)_4(C_{10}H_{14}N_2O)_2]$
$M_r$ = 1143.96
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a$ = 9.2731 (6) Å
$b$ = 13.2340 (8) Å
$c$ = 13.4756 (8) Å
$\alpha$ = 112.348 (3)°
$\beta$ = 109.236 (2)°
$\gamma$ = 95.728 (2)°
$V$ = 1395.33 (16) Å$^3$
$Z$ = 1
$F$(000) = 600
$D_x$ = 1.361 Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda$ = 0.71073 Å
Cell parameters from 9870 reflections
$\theta$ = 2.4–28.3°
$\mu$ = 0.92 mm$^{-1}$
$T$ = 294 K
Block, colorless
0.52 × 0.35 × 0.25 mm

*Data collection*

Bruker Kappa APEXII CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\varphi$ and $\omega$ scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
$T_{min}$ = 0.681, $T_{max}$ = 0.791
24970 measured reflections
6877 independent reflections
5749 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.029
$\theta_{max}$ = 28.3°, $\theta_{min}$ = 1.7°
$h$ = −12→12
$k$ = −16→17
$l$ = −17→17

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.033$
$wR(F^2) = 0.090$
$S = 1.06$
6877 reflections
349 parameters
0 restraints
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
$w = 1/[\sigma^2(F_o^2) + (0.0476P)^2 + 0.2013P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.24$ e Å$^{-3}$
$\Delta\rho_{min} = -0.43$ 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 (Å²)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| Zn1 | 0.647429 (19) | 0.587023 (15) | 0.565621 (14) | 0.03318 (7) |
| N1 | 0.0447 (2) | 0.97057 (18) | 0.3697 (2) | 0.0740 (6) |
| N2 | 0.3784 (2) | 0.63356 (17) | 1.11287 (14) | 0.0626 (5) |
| N3 | 0.88138 (15) | 0.67128 (11) | 0.64273 (11) | 0.0336 (3) |
| N4 | 1.16916 (19) | 0.90139 (14) | 1.01779 (14) | 0.0529 (4) |
| O1 | 0.52598 (14) | 0.69380 (11) | 0.52284 (11) | 0.0495 (3) |
| O2 | 0.58984 (16) | 0.62604 (11) | 0.70601 (11) | 0.0514 (3) |
| O3 | 1.2203 (3) | 1.00113 (14) | 0.92564 (15) | 0.0984 (7) |
| O4 | 0.69851 (15) | 0.44310 (11) | 0.57910 (12) | 0.0515 (3) |
| O5 | 0.63255 (15) | 0.51278 (12) | 0.39761 (10) | 0.0542 (3) |
| C1 | 0.3792 (2) | 0.65704 (15) | 0.46130 (14) | 0.0387 (4) |
| C2 | 0.29154 (19) | 0.73827 (14) | 0.43619 (14) | 0.0375 (4) |
| C3 | 0.1306 (2) | 0.70435 (16) | 0.36591 (16) | 0.0466 (4) |
| H3 | 0.0769 | 0.6287 | 0.3333 | 0.056* |
| C4 | 0.0491 (2) | 0.77940 (18) | 0.34350 (18) | 0.0533 (5) |
| H4 | −0.0584 | 0.7536 | 0.2961 | 0.064* |
| C5 | 0.1243 (2) | 0.89438 (17) | 0.39039 (18) | 0.0499 (4) |
| C6 | 0.2864 (2) | 0.92796 (17) | 0.46138 (18) | 0.0512 (5) |
| H6 | 0.3409 | 1.0035 | 0.4947 | 0.061* |
| C7 | 0.3659 (2) | 0.85148 (16) | 0.48263 (16) | 0.0453 (4) |
| H7 | 0.4734 | 0.8767 | 0.5299 | 0.054* |
| C8 | 0.1256 (3) | 1.0887 (2) | 0.4196 (2) | 0.0767 (7) |
| H8A | 0.0508 | 1.1301 | 0.3992 | 0.115* |
| H8B | 0.2045 | 1.0961 | 0.3895 | 0.115* |
| H8C | 0.1752 | 1.1183 | 0.5032 | 0.115* |

| | | | | |
|---|---|---|---|---|
| C9 | −0.1234 (3) | 0.9381 (2) | 0.3032 (2) | 0.0778 (7) |
| H9A | −0.1586 | 1.0036 | 0.3019 | 0.117* |
| H9B | −0.1759 | 0.9056 | 0.3388 | 0.117* |
| H9C | −0.1478 | 0.8836 | 0.2247 | 0.117* |
| C10 | 0.4677 (2) | 0.56674 (16) | 0.69715 (14) | 0.0418 (4) |
| C11 | 0.43798 (19) | 0.58899 (15) | 0.80439 (14) | 0.0398 (4) |
| C12 | 0.3197 (2) | 0.51570 (17) | 0.80381 (15) | 0.0486 (4) |
| H12 | 0.2529 | 0.4548 | 0.7334 | 0.058* |
| C13 | 0.2979 (2) | 0.53000 (18) | 0.90376 (17) | 0.0531 (5) |
| H13 | 0.2169 | 0.4791 | 0.8997 | 0.064* |
| C14 | 0.3962 (2) | 0.62048 (17) | 1.01199 (15) | 0.0478 (4) |
| C15 | 0.5102 (2) | 0.69743 (18) | 1.01119 (15) | 0.0530 (5) |
| H15 | 0.5735 | 0.7608 | 1.0805 | 0.064* |
| C16 | 0.5308 (2) | 0.68143 (17) | 0.91032 (15) | 0.0474 (4) |
| H16 | 0.6087 | 0.7337 | 0.9131 | 0.057* |
| C17 | 0.4929 (3) | 0.7180 (2) | 1.22593 (18) | 0.0795 (7) |
| H17A | 0.4760 | 0.7042 | 1.2867 | 0.119* |
| H17B | 0.4808 | 0.7918 | 1.2350 | 0.119* |
| H17C | 0.5977 | 0.7140 | 1.2310 | 0.119* |
| C18 | 0.2607 (3) | 0.5536 (2) | 1.1128 (2) | 0.0754 (7) |
| H18A | 0.2701 | 0.5743 | 1.1916 | 0.113* |
| H18B | 0.2763 | 0.4793 | 1.0808 | 0.113* |
| H18C | 0.1572 | 0.5539 | 1.0661 | 0.113* |
| C19 | 0.94694 (19) | 0.75356 (14) | 0.75189 (14) | 0.0369 (4) |
| H19 | 0.8823 | 0.7750 | 0.7921 | 0.044* |
| C20 | 1.1054 (2) | 0.80823 (15) | 0.80792 (15) | 0.0427 (4) |
| C21 | 1.2004 (2) | 0.77375 (18) | 0.74711 (18) | 0.0539 (5) |
| H21 | 1.3080 | 0.8089 | 0.7816 | 0.065* |
| C22 | 1.1348 (2) | 0.68765 (18) | 0.63601 (18) | 0.0537 (5) |
| H22 | 1.1976 | 0.6621 | 0.5951 | 0.064* |
| C23 | 0.9753 (2) | 0.63968 (15) | 0.58606 (15) | 0.0416 (4) |
| H23 | 0.9305 | 0.5829 | 0.5097 | 0.050* |
| C24 | 1.1705 (2) | 0.91161 (17) | 0.92357 (17) | 0.0536 (5) |
| C25 | 1.2270 (3) | 1.0051 (2) | 1.1274 (2) | 0.0837 (8) |
| H25A | 1.1758 | 0.9954 | 1.1766 | 0.100* |
| H25B | 1.1973 | 1.0667 | 1.1101 | 0.100* |
| C26 | 1.4002 (4) | 1.0362 (3) | 1.1927 (3) | 0.1230 (13) |
| H26A | 1.4314 | 1.1060 | 1.2619 | 0.184* |
| H26B | 1.4518 | 1.0449 | 1.1442 | 0.184* |
| H26C | 1.4299 | 0.9777 | 1.2144 | 0.184* |
| C27 | 1.1366 (3) | 0.79420 (19) | 1.02381 (18) | 0.0609 (5) |
| H27A | 1.2212 | 0.7969 | 1.0912 | 0.073* |
| H27B | 1.1368 | 0.7341 | 0.9545 | 0.073* |
| C28 | 0.9820 (4) | 0.7661 (3) | 1.0327 (3) | 0.0990 (9) |
| H28A | 0.9775 | 0.7036 | 1.0522 | 0.149* |
| H28B | 0.8967 | 0.7463 | 0.9591 | 0.149* |
| H28C | 0.9729 | 0.8306 | 1.0926 | 0.149* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Zn1 | 0.02904 (10) | 0.03429 (12) | 0.03032 (10) | 0.00543 (7) | 0.01153 (7) | 0.00929 (8) |
| N1 | 0.0647 (12) | 0.0723 (13) | 0.1079 (16) | 0.0331 (10) | 0.0319 (11) | 0.0608 (12) |
| N2 | 0.0671 (11) | 0.0820 (13) | 0.0420 (9) | 0.0147 (10) | 0.0313 (8) | 0.0238 (9) |
| N3 | 0.0325 (6) | 0.0324 (7) | 0.0342 (7) | 0.0087 (5) | 0.0142 (5) | 0.0120 (6) |
| N4 | 0.0554 (10) | 0.0441 (9) | 0.0426 (8) | 0.0082 (7) | 0.0161 (7) | 0.0065 (7) |
| O1 | 0.0403 (7) | 0.0488 (8) | 0.0577 (8) | 0.0151 (6) | 0.0144 (6) | 0.0253 (6) |
| O2 | 0.0586 (8) | 0.0561 (8) | 0.0402 (7) | 0.0107 (6) | 0.0297 (6) | 0.0145 (6) |
| O3 | 0.1420 (17) | 0.0466 (10) | 0.0616 (10) | −0.0197 (10) | 0.0089 (10) | 0.0166 (8) |
| O4 | 0.0514 (7) | 0.0395 (7) | 0.0664 (8) | 0.0141 (6) | 0.0237 (6) | 0.0253 (6) |
| O5 | 0.0479 (7) | 0.0726 (9) | 0.0298 (6) | 0.0141 (7) | 0.0151 (5) | 0.0108 (6) |
| C1 | 0.0444 (9) | 0.0414 (10) | 0.0387 (9) | 0.0150 (7) | 0.0233 (7) | 0.0191 (8) |
| C2 | 0.0395 (8) | 0.0417 (9) | 0.0381 (8) | 0.0118 (7) | 0.0197 (7) | 0.0202 (7) |
| C3 | 0.0426 (9) | 0.0424 (10) | 0.0513 (10) | 0.0073 (8) | 0.0159 (8) | 0.0204 (8) |
| C4 | 0.0403 (9) | 0.0593 (13) | 0.0585 (12) | 0.0129 (9) | 0.0130 (8) | 0.0296 (10) |
| C5 | 0.0522 (11) | 0.0547 (12) | 0.0596 (12) | 0.0221 (9) | 0.0271 (9) | 0.0358 (10) |
| C6 | 0.0538 (11) | 0.0411 (10) | 0.0640 (12) | 0.0108 (8) | 0.0240 (9) | 0.0284 (9) |
| C7 | 0.0398 (9) | 0.0465 (10) | 0.0510 (10) | 0.0085 (8) | 0.0173 (8) | 0.0241 (9) |
| C8 | 0.0995 (19) | 0.0644 (16) | 0.0989 (19) | 0.0435 (14) | 0.0491 (16) | 0.0549 (15) |
| C9 | 0.0682 (15) | 0.104 (2) | 0.0950 (19) | 0.0481 (15) | 0.0366 (14) | 0.0672 (17) |
| C10 | 0.0423 (9) | 0.0517 (11) | 0.0345 (8) | 0.0217 (8) | 0.0190 (7) | 0.0166 (8) |
| C11 | 0.0367 (8) | 0.0509 (10) | 0.0323 (8) | 0.0161 (7) | 0.0164 (7) | 0.0153 (7) |
| C12 | 0.0471 (10) | 0.0517 (11) | 0.0359 (9) | 0.0081 (8) | 0.0150 (8) | 0.0107 (8) |
| C13 | 0.0522 (11) | 0.0602 (12) | 0.0469 (10) | 0.0069 (9) | 0.0250 (9) | 0.0210 (9) |
| C14 | 0.0488 (10) | 0.0608 (12) | 0.0391 (9) | 0.0194 (9) | 0.0243 (8) | 0.0203 (9) |
| C15 | 0.0483 (10) | 0.0634 (13) | 0.0322 (9) | 0.0059 (9) | 0.0166 (8) | 0.0075 (9) |
| C16 | 0.0410 (9) | 0.0574 (12) | 0.0374 (9) | 0.0070 (8) | 0.0191 (7) | 0.0128 (8) |
| C17 | 0.0939 (18) | 0.100 (2) | 0.0390 (11) | 0.0174 (15) | 0.0317 (12) | 0.0223 (12) |
| C18 | 0.0869 (17) | 0.0942 (19) | 0.0689 (15) | 0.0242 (14) | 0.0474 (14) | 0.0456 (15) |
| C19 | 0.0358 (8) | 0.0342 (9) | 0.0345 (8) | 0.0068 (7) | 0.0140 (6) | 0.0097 (7) |
| C20 | 0.0384 (9) | 0.0404 (10) | 0.0390 (9) | 0.0039 (7) | 0.0071 (7) | 0.0160 (8) |
| C21 | 0.0300 (8) | 0.0586 (12) | 0.0637 (12) | 0.0058 (8) | 0.0136 (8) | 0.0234 (10) |
| C22 | 0.0401 (9) | 0.0651 (13) | 0.0621 (12) | 0.0180 (9) | 0.0298 (9) | 0.0249 (10) |
| C23 | 0.0402 (9) | 0.0431 (10) | 0.0391 (9) | 0.0123 (7) | 0.0197 (7) | 0.0122 (8) |
| C24 | 0.0504 (11) | 0.0419 (11) | 0.0454 (10) | 0.0019 (8) | 0.0044 (8) | 0.0113 (8) |
| C25 | 0.108 (2) | 0.0578 (15) | 0.0513 (13) | 0.0038 (14) | 0.0278 (13) | −0.0016 (11) |
| C26 | 0.110 (3) | 0.107 (3) | 0.0625 (17) | −0.029 (2) | −0.0102 (16) | 0.0001 (16) |
| C27 | 0.0666 (13) | 0.0592 (13) | 0.0478 (11) | 0.0142 (10) | 0.0150 (10) | 0.0215 (10) |
| C28 | 0.100 (2) | 0.110 (2) | 0.110 (2) | 0.0161 (18) | 0.0574 (19) | 0.061 (2) |

*Geometric parameters (Å, º)*

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|---|---|---|---|
| Zn1—Zn1$^{i}$ | 2.8927 (4) | C11—C16 | 1.388 (2) |
| Zn1—O1 | 2.0265 (12) | C12—C13 | 1.373 (3) |
| Zn1—O2 | 2.0269 (12) | C12—H12 | 0.9300 |
| Zn1—O4 | 2.0669 (12) | C13—H13 | 0.9300 |

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| Zn1—O5 | 2.0459 (12) | C14—N2 | 1.371 (2) |
| Zn1—N3 | 2.0446 (13) | C14—C13 | 1.404 (3) |
| O1—C1 | 1.263 (2) | C14—C15 | 1.399 (3) |
| O2—C10 | 1.255 (2) | C15—C16 | 1.374 (2) |
| O4—C1$^{i}$ | 1.255 (2) | C15—H15 | 0.9300 |
| O5—C10$^{i}$ | 1.266 (2) | C16—H16 | 0.9300 |
| N1—C9 | 1.438 (3) | C17—H17A | 0.9600 |
| N1—C8 | 1.447 (3) | C17—H17B | 0.9600 |
| N2—C18 | 1.443 (3) | C17—H17C | 0.9600 |
| N2—C17 | 1.449 (3) | C18—H18A | 0.9600 |
| N3—C19 | 1.334 (2) | C18—H18B | 0.9600 |
| N3—C23 | 1.336 (2) | C18—H18C | 0.9600 |
| N4—C25 | 1.463 (3) | C19—C20 | 1.377 (2) |
| N4—C27 | 1.459 (3) | C19—H19 | 0.9300 |
| C1—O4$^{i}$ | 1.255 (2) | C20—C21 | 1.388 (3) |
| C2—C1 | 1.484 (2) | C20—C24 | 1.503 (2) |
| C2—C3 | 1.392 (2) | C21—H21 | 0.9300 |
| C2—C7 | 1.381 (2) | C22—C21 | 1.369 (3) |
| C3—C4 | 1.369 (3) | C22—H22 | 0.9300 |
| C3—H3 | 0.9300 | C23—C22 | 1.370 (2) |
| C4—C5 | 1.403 (3) | C23—H23 | 0.9300 |
| C4—H4 | 0.9300 | C24—O3 | 1.214 (3) |
| C5—N1 | 1.366 (2) | C24—N4 | 1.331 (3) |
| C6—C5 | 1.402 (3) | C25—C26 | 1.478 (4) |
| C6—H6 | 0.9300 | C25—H25A | 0.9700 |
| C7—C6 | 1.371 (3) | C25—H25B | 0.9700 |
| C7—H7 | 0.9300 | C26—H26A | 0.9600 |
| C8—H8A | 0.9600 | C26—H26B | 0.9600 |
| C8—H8B | 0.9600 | C26—H26C | 0.9600 |
| C8—H8C | 0.9600 | C27—C28 | 1.500 (3) |
| C9—H9A | 0.9600 | C27—H27A | 0.9700 |
| C9—H9B | 0.9600 | C27—H27B | 0.9700 |
| C9—H9C | 0.9600 | C28—H28A | 0.9600 |
| C10—O5$^{i}$ | 1.266 (2) | C28—H28B | 0.9600 |
| C11—C10 | 1.485 (2) | C28—H28C | 0.9600 |
| C11—C12 | 1.386 (3) | | |

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| O1—Zn1—O2 | 89.01 (6) | C13—C12—H12 | 118.9 |
| O1—Zn1—O4 | 161.34 (5) | C12—C13—C14 | 120.84 (18) |
| O1—Zn1—O5 | 88.39 (6) | C12—C13—H13 | 119.6 |
| O1—Zn1—N3 | 106.31 (5) | C14—C13—H13 | 119.6 |
| O2—Zn1—O4 | 89.28 (6) | N2—C14—C13 | 121.29 (18) |
| O2—Zn1—O5 | 161.09 (6) | N2—C14—C15 | 121.92 (18) |
| O2—Zn1—N3 | 101.76 (5) | C15—C14—C13 | 116.77 (16) |
| O5—Zn1—O4 | 87.23 (6) | C16—C15—C14 | 121.46 (18) |
| N3—Zn1—O4 | 92.23 (5) | C16—C15—H15 | 119.3 |
| N3—Zn1—O5 | 96.95 (5) | C14—C15—H15 | 119.3 |
| C1—O1—Zn1 | 118.82 (11) | C11—C16—H16 | 119.2 |

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| C10—O2—Zn1 | 119.77 (11) | C15—C16—C11 | 121.52 (18) |
| C1$^{i}$—O4—Zn1 | 135.03 (12) | C15—C16—H16 | 119.2 |
| C10$^{i}$—O5—Zn1 | 134.43 (12) | N2—C17—H17A | 109.5 |
| C5—N1—C8 | 120.9 (2) | N2—C17—H17B | 109.5 |
| C5—N1—C9 | 121.6 (2) | N2—C17—H17C | 109.5 |
| C9—N1—C8 | 117.41 (19) | H17A—C17—H17B | 109.5 |
| C14—N2—C17 | 120.85 (19) | H17A—C17—H17C | 109.5 |
| C14—N2—C18 | 121.51 (19) | H17B—C17—H17C | 109.5 |
| C18—N2—C17 | 116.96 (18) | N2—C18—H18A | 109.5 |
| C19—N3—Zn1 | 121.99 (11) | N2—C18—H18B | 109.5 |
| C19—N3—C23 | 118.04 (14) | N2—C18—H18C | 109.5 |
| C23—N3—Zn1 | 119.85 (11) | H18A—C18—H18B | 109.5 |
| C24—N4—C25 | 117.08 (19) | H18A—C18—H18C | 109.5 |
| C24—N4—C27 | 124.81 (17) | H18B—C18—H18C | 109.5 |
| C27—N4—C25 | 117.48 (18) | N3—C19—C20 | 123.28 (15) |
| O1—C1—C2 | 117.78 (15) | N3—C19—H19 | 118.4 |
| O4$^{i}$—C1—O1 | 124.74 (16) | C20—C19—H19 | 118.4 |
| O4$^{i}$—C1—C2 | 117.47 (15) | C19—C20—C21 | 117.52 (16) |
| C3—C2—C1 | 121.68 (16) | C19—C20—C24 | 121.55 (16) |
| C7—C2—C1 | 121.40 (15) | C21—C20—C24 | 120.41 (16) |
| C7—C2—C3 | 116.92 (16) | C20—C21—H21 | 120.2 |
| C2—C3—H3 | 119.1 | C22—C21—C20 | 119.63 (16) |
| C4—C3—C2 | 121.76 (17) | C22—C21—H21 | 120.2 |
| C4—C3—H3 | 119.1 | C21—C22—C23 | 118.90 (17) |
| C3—C4—C5 | 121.46 (18) | C21—C22—H22 | 120.6 |
| C3—C4—H4 | 119.3 | C23—C22—H22 | 120.6 |
| C5—C4—H4 | 119.3 | N3—C23—C22 | 122.60 (16) |
| N1—C5—C4 | 122.23 (19) | N3—C23—H23 | 118.7 |
| N1—C5—C6 | 121.32 (19) | C22—C23—H23 | 118.7 |
| C6—C5—C4 | 116.45 (17) | O3—C24—N4 | 123.26 (19) |
| C5—C6—H6 | 119.4 | O3—C24—C20 | 117.73 (19) |
| C7—C6—C5 | 121.22 (18) | N4—C24—C20 | 119.00 (18) |
| C7—C6—H6 | 119.4 | N4—C25—C26 | 113.3 (2) |
| C2—C7—H7 | 118.9 | N4—C25—H25A | 108.9 |
| C6—C7—C2 | 122.19 (17) | N4—C25—H25B | 108.9 |
| C6—C7—H7 | 118.9 | C26—C25—H25A | 108.9 |
| N1—C8—H8A | 109.5 | C26—C25—H25B | 108.9 |
| N1—C8—H8B | 109.5 | H25A—C25—H25B | 107.7 |
| N1—C8—H8C | 109.5 | C25—C26—H26A | 109.5 |
| H8A—C8—H8B | 109.5 | C25—C26—H26B | 109.5 |
| H8A—C8—H8C | 109.5 | C25—C26—H26C | 109.5 |
| H8B—C8—H8C | 109.5 | H26A—C26—H26B | 109.5 |
| N1—C9—H9A | 109.5 | H26A—C26—H26C | 109.5 |
| N1—C9—H9B | 109.5 | H26B—C26—H26C | 109.5 |
| N1—C9—H9C | 109.5 | N4—C27—C28 | 113.8 (2) |
| H9A—C9—H9B | 109.5 | N4—C27—H27A | 108.8 |
| H9A—C9—H9C | 109.5 | N4—C27—H27B | 108.8 |
| H9B—C9—H9C | 109.5 | C28—C27—H27A | 108.8 |

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| O2—C10—O5$^{i}$ | 124.39 (16) | C28—C27—H27B | 108.8 |
| O2—C10—C11 | 118.63 (15) | H27A—C27—H27B | 107.7 |
| O5$^{i}$—C10—C11 | 116.98 (16) | C27—C28—H28A | 109.5 |
| C12—C11—C10 | 121.20 (16) | C27—C28—H28B | 109.5 |
| C12—C11—C16 | 117.10 (16) | C27—C28—H28C | 109.5 |
| C16—C11—C10 | 121.66 (16) | H28A—C28—H28B | 109.5 |
| C11—C12—H12 | 118.9 | H28A—C28—H28C | 109.5 |
| C13—C12—C11 | 122.17 (17) | H28B—C28—H28C | 109.5 |
| | | | |
| O2—Zn1—O1—C1 | −86.30 (13) | C3—C2—C7—C6 | 0.1 (3) |
| O4—Zn1—O1—C1 | −1.5 (2) | C2—C3—C4—C5 | 0.0 (3) |
| O5—Zn1—O1—C1 | 74.97 (13) | C3—C4—C5—N1 | −179.4 (2) |
| N3—Zn1—O1—C1 | 171.73 (12) | C3—C4—C5—C6 | −0.2 (3) |
| O1—Zn1—O2—C10 | 92.13 (14) | C4—C5—N1—C8 | 179.9 (2) |
| O4—Zn1—O2—C10 | −69.29 (14) | C4—C5—N1—C9 | 3.2 (3) |
| O5—Zn1—O2—C10 | 10.0 (3) | C6—C5—N1—C8 | 0.7 (3) |
| N3—Zn1—O2—C10 | −161.42 (14) | C6—C5—N1—C9 | −176.0 (2) |
| O1—Zn1—O4—C1$^{i}$ | 4.3 (3) | C7—C6—C5—N1 | 179.6 (2) |
| O2—Zn1—O4—C1$^{i}$ | 89.10 (17) | C7—C6—C5—C4 | 0.3 (3) |
| O5—Zn1—O4—C1$^{i}$ | −72.31 (17) | C2—C7—C6—C5 | −0.2 (3) |
| N3—Zn1—O4—C1$^{i}$ | −169.16 (17) | C12—C11—C10—O2 | −169.73 (18) |
| O1—Zn1—O5—C10$^{i}$ | −88.02 (18) | C12—C11—C10—O5$^{i}$ | 9.4 (3) |
| O2—Zn1—O5—C10$^{i}$ | −5.8 (3) | C16—C11—C10—O2 | 7.8 (3) |
| O4—Zn1—O5—C10$^{i}$ | 73.84 (18) | C16—C11—C10—O5$^{i}$ | −173.06 (17) |
| N3—Zn1—O5—C10$^{i}$ | 165.75 (17) | C10—C11—C12—C13 | 175.00 (17) |
| O1—Zn1—N3—C19 | 75.41 (13) | C16—C11—C12—C13 | −2.7 (3) |
| O1—Zn1—N3—C23 | −108.69 (13) | C10—C11—C16—C15 | −175.32 (17) |
| O2—Zn1—N3—C19 | −17.02 (14) | C12—C11—C16—C15 | 2.3 (3) |
| O2—Zn1—N3—C23 | 158.88 (13) | C11—C12—C13—C14 | −0.2 (3) |
| O4—Zn1—N3—C19 | −106.75 (13) | C13—C14—N2—C17 | 171.8 (2) |
| O4—Zn1—N3—C23 | 69.15 (13) | C13—C14—N2—C18 | 1.6 (3) |
| O5—Zn1—N3—C19 | 165.77 (13) | C15—C14—N2—C17 | −9.6 (3) |
| O5—Zn1—N3—C23 | −18.33 (14) | C15—C14—N2—C18 | −179.8 (2) |
| Zn1—O1—C1—O4$^{i}$ | −2.1 (2) | N2—C14—C13—C12 | −178.00 (19) |
| Zn1—O1—C1—C2 | 176.98 (10) | C15—C14—C13—C12 | 3.3 (3) |
| Zn1—O2—C10—O5$^{i}$ | −5.9 (3) | N2—C14—C15—C16 | 177.68 (19) |
| Zn1—O2—C10—C11 | 173.11 (11) | C13—C14—C15—C16 | −3.7 (3) |
| Zn1—N3—C19—C20 | 176.95 (13) | C14—C15—C16—C11 | 0.9 (3) |
| Zn1—N3—C23—C22 | −175.48 (15) | N3—C19—C20—C21 | −1.0 (3) |
| C19—N3—C23—C22 | 0.6 (3) | N3—C19—C20—C24 | 170.73 (17) |
| C23—N3—C19—C20 | 1.0 (2) | C19—C20—C21—C22 | −0.5 (3) |
| C24—N4—C25—C26 | −86.0 (3) | C24—C20—C21—C22 | −172.34 (19) |
| C27—N4—C25—C26 | 85.3 (3) | C19—C20—C24—O3 | −111.7 (2) |
| C24—N4—C27—C28 | −110.6 (2) | C19—C20—C24—N4 | 67.5 (2) |
| C25—N4—C27—C28 | 78.8 (3) | C21—C20—C24—O3 | 59.8 (3) |
| C3—C2—C1—O1 | 177.84 (16) | C21—C20—C24—N4 | −121.0 (2) |
| C3—C2—C1—O4$^{i}$ | −3.0 (2) | C23—C22—C21—C20 | 2.0 (3) |
| C7—C2—C1—O1 | −2.8 (2) | N3—C23—C22—C21 | −2.0 (3) |

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| C7—C2—C1—O4$^{i}$ | 176.30 (16) | O3—C24—N4—C25 | 1.9 (3) |
| C1—C2—C3—C4 | 179.40 (17) | O3—C24—N4—C27 | −168.7 (2) |
| C7—C2—C3—C4 | 0.1 (3) | C20—C24—N4—C25 | −177.29 (19) |
| C1—C2—C7—C6 | −179.29 (17) | C20—C24—N4—C27 | 12.1 (3) |

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

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| C23—H23···O5 | 0.93 | 2.54 | 3.122 (2) | 121 |
| C8—H8*A*···*Cg*3$^{ii}$ | 0.96 | 2.77 | 3.629 (3) | 150 |

Symmetry code: (ii) −*x*+1, −*y*, −*z*+1.