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# Bis(5,5-diphenylhydantoinato-$\kappa N^3$)-(ethylenediamine)zinc(II)

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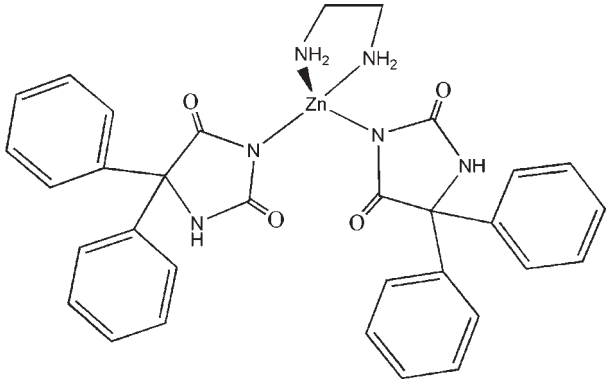
Key indicators: single-crystal X-ray study; $T$ = 298 K; mean $\sigma$(C–C) = 0.005 Å; $R$ factor = 0.034; $wR$ factor = 0.089; data-to-parameter ratio = 13.2.

In the title compound, $[Zn(C_{15}H_{11}N_2O_2)_2(C_2H_8N_2)]$, the $Zn^{II}$ atom is coordinated in a distorted tetrahedral geometry. Intramolecular N—H···O, C—H···O and C—H···N hydrogen bonds occur. In the crystal, molecules are linked by intermolecular N—H···O hydrogen bonds, forming a three-dimensional network.

## Related literature

5,5-Diphenylimidazoline-2,4-dione (phenytoin) is widely used in the treatment of epilepsy and should be an excellent ligand for transition metal complexes, see: Milne *et al.* (1999); Akitsu & Einaga (2005); Akitsu *et al.* (1997). For complexes with 5,5-diphenylhydantoinate, see: Hu, Xu, Wang & Xu (2006); Hu, Xu, Xu & Wang (2006).




## Experimental

### Crystal data

$[Zn(C_{15}H_{11}N_2O_2)_2(C_2H_8N_2)]$
$M_r$ = 627.99
Triclinic, $P\overline{1}$
$a$ = 9.702 (1) Å
$b$ = 13.052 (2) Å
$c$ = 13.293 (2) Å
$\alpha$ = 109.114 (2)°
$\beta$ = 109.462 (2)°
$\gamma$ = 93.020(10)°
$V$ = 1473.1 (3) Å$^3$
$Z$ = 2
Mo $K\alpha$ radiation
$\mu$ = 0.88 mm$^{-1}$
$T$ = 298 K
0.50 × 0.46 × 0.32 mm

### Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min}$ = 0.667, $T_{max}$ = 0.766
7725 measured reflections
5124 independent reflections
4452 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.017

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.034
$wR(F^2)$ = 0.089
$S$ = 1.03
5124 reflections
388 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.61 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.45 e Å$^{-3}$

**Table 1**
Hydrogen-bond geometry (Å, °).

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| N6—H6$B$···O2 | 0.90 | 2.18 | 2.858 (3) | 132 |
| C9—H9···O2 | 0.93 | 2.36 | 2.992 (3) | 125 |
| C11—H11···N1 | 0.93 | 2.52 | 2.860 (4) | 102 |
| C24—H24···O4 | 0.93 | 2.39 | 3.042 (4) | 127 |
| C26—H26···N3 | 0.93 | 2.51 | 2.854 (4) | 102 |
| N1—H1···O1$^{i}$ | 0.86 | 2.16 | 3.008 (3) | 167 |
| N3—H3···O3$^{ii}$ | 0.86 | 2.04 | 2.843 (3) | 156 |
| N5—H5$A$···O4$^{iii}$ | 0.90 | 1.97 | 2.855 (3) | 170 |
| N5—H5$B$···O1$^{iii}$ | 0.90 | 2.18 | 3.003 (3) | 152 |

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

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); 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: BX2240).

## References

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# supporting information

*Acta Cryst.* (2009). E**65**, m1426 [https://doi.org/10.1107/S160053680904313X]

## Bis(5,5-diphenylhydantoinato-$\kappa N^3$)(ethylenediamine)zinc(II)

**Xilan Hu, Xingyou Xu, Daqi Wang and Yu Zhang**

### S1. Comment

5,5-diphenylimidazoline-2,4-dione (phenytoin) compound is a widely used drug in the treatment of epilepsy and should be an excellent ligand for transition metal complex (Milne *et al.*, 1999; Akitsu, Komorita, Kushi *et al.*,1997; Akitsu, Einaga, 2005). We have designed and synthesized a series of complexes with 5,5-diphenylhydantoinate (Hu, Xu, Wang *et al.*, 2006). We report here the crystal structure of the title compound (I). The compound (Fig. 1) consists of $[Zn(pht)_2(en)]$ (pht=5,5-diphenylhydantoinato; en=ethylendiamine) complex neutral molecule. The Zn atom is coordinated by two nitrogen atoms from two pht ligands and two nitrogen atoms from two en ligands and is in a distorted tetrahedron $ZnN_4$ coordination environment.The Zn—N bond distances lie in the range of 1.9506 (18)Å to 2.057 (2) Å. There are intra- and intermolecular N—H···O=C hydrogen bonds, forming a three-dimensional network in the crystal structure, Table 1.

### S2. Experimental

To a solution of pht (1.00 mmol) in methanol (10 ml) was added zinc(II) acetate tetrahydrate (0.5 mmol) and the solution of Ethylenediamine(0.5 mmol) in methanol (10 ml). Then the mixture was sealed in a 25 ml stainless steel vessel with Teflon linear and heated to 393 K for 50 h the fill rate being 80%. After cooling to room temperature, the colorless single crystals were obtained by slow evaporation from the filtrate.

### S3. Refinement

The space group was uniquely assigned from the systematic absences. All H atoms were placed at calculated positions, with N—H = 0.86–0.90 Å, and with $U_{iso}$(H) values were set at 1.2$U_{eq}$, and C—H = 0.93Å (phenyl), 0.97Å (methylene), respectively, and with $U_{iso}$(H) values were set at 1.2 $U_{eq}$(C) (phenyl,methylene).

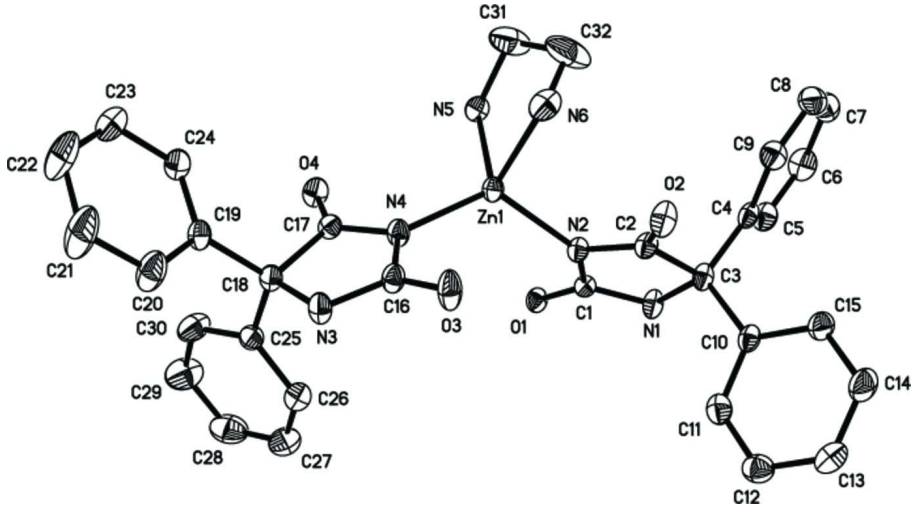


**Figure 1**

The molecular structure of the title complex. Displacement ellipsoids are drawn at the 30% probability level. The H-atom have been omitted for clarity.

**Bis(5,5-diphenylhydantoinato-$\kappa N^3$)(ethylenediamine)zinc(II)**

*Crystal data*

$[Zn(C_{15}H_{11}N_2O_2)_2(C_2H_8N_2)]$
$M_r = 627.99$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 9.702$ (1) Å
$b = 13.0520$ (15) Å
$c = 13.2930$ (16) Å
$\alpha = 109.114$ (2)°
$\beta = 109.462$ (2)°
$\gamma = 93.302$ (1)°
$V = 1473.1$ (3) Å$^3$
$Z = 2$
$F(000) = 652$
$D_x = 1.416$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 4727 reflections
$\theta = 2.6$–27.7°
$\mu = 0.88$ mm$^{-1}$
$T = 298$ K
Block, colorless
0.50 × 0.46 × 0.32 mm

*Data collection*

Bruker SMART CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\varphi$ and $\omega$ scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.667$, $T_{max} = 0.766$
7725 measured reflections
5124 independent reflections
4452 reflections with $I > 2\sigma(I)$
$R_{int} = 0.017$
$\theta_{max} = 25.0°$, $\theta_{min} = 1.7°$
$h = -11 \rightarrow 11$
$k = -15 \rightarrow 15$
$l = -14 \rightarrow 15$

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.034$
$wR(F^2) = 0.089$
$S = 1.03$
5124 reflections
388 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

$w = 1/[\sigma^2(F_o^2) + (0.0432P)^2 + 0.9132P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$

$\Delta\rho_{max} = 0.61$ e Å$^{-3}$
$\Delta\rho_{min} = -0.45$ 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* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| Zn1 | −0.00468 (3) | 0.61290 (2) | 0.37871 (2) | 0.02823 (10) |
| N1 | 0.4053 (2) | 0.53299 (18) | 0.37370 (16) | 0.0358 (5) |
| H1 | 0.4894 | 0.5154 | 0.4032 | 0.043* |
| N2 | 0.1898 (2) | 0.59269 (15) | 0.36211 (16) | 0.0290 (4) |
| N3 | −0.0141 (3) | 0.92085 (15) | 0.58602 (18) | 0.0380 (5) |
| H3 | 0.0040 | 0.9910 | 0.6028 | 0.046* |
| N4 | −0.0279 (2) | 0.74051 (15) | 0.49503 (17) | 0.0328 (4) |
| N5 | −0.1098 (2) | 0.46617 (15) | 0.36800 (17) | 0.0335 (4) |
| H5A | −0.0432 | 0.4228 | 0.3835 | 0.040* |
| H5B | −0.1548 | 0.4787 | 0.4190 | 0.040* |
| N6 | −0.1472 (2) | 0.5694 (2) | 0.21093 (19) | 0.0480 (6) |
| H6A | −0.2288 | 0.5998 | 0.2067 | 0.058* |
| H6B | −0.1020 | 0.5906 | 0.1699 | 0.058* |
| O1 | 0.33097 (18) | 0.56196 (14) | 0.52547 (13) | 0.0337 (4) |
| O2 | 0.1300 (2) | 0.61465 (16) | 0.18764 (15) | 0.0455 (5) |
| O3 | 0.0303 (2) | 0.86389 (14) | 0.41865 (17) | 0.0510 (5) |
| O4 | −0.1104 (2) | 0.66928 (13) | 0.60608 (16) | 0.0401 (4) |
| C1 | 0.3111 (2) | 0.56151 (18) | 0.42891 (19) | 0.0278 (5) |
| C2 | 0.2089 (3) | 0.5866 (2) | 0.2636 (2) | 0.0318 (5) |
| C3 | 0.3484 (3) | 0.5354 (2) | 0.25864 (19) | 0.0319 (5) |
| C4 | 0.2992 (3) | 0.4187 (2) | 0.1657 (2) | 0.0333 (5) |
| C5 | 0.3729 (3) | 0.3350 (2) | 0.1842 (2) | 0.0433 (6) |
| H5 | 0.4527 | 0.3499 | 0.2528 | 0.052* |
| C6 | 0.3292 (4) | 0.2292 (2) | 0.1016 (3) | 0.0537 (7) |
| H6 | 0.3807 | 0.1741 | 0.1151 | 0.064* |
| C7 | 0.2103 (4) | 0.2046 (2) | −0.0001 (3) | 0.0523 (7) |
| H7 | 0.1812 | 0.1334 | −0.0550 | 0.063* |
| C8 | 0.1354 (3) | 0.2864 (2) | −0.0196 (2) | 0.0498 (7) |
| H8 | 0.0545 | 0.2705 | −0.0878 | 0.060* |
| C9 | 0.1796 (3) | 0.3926 (2) | 0.0618 (2) | 0.0420 (6) |
| H9 | 0.1288 | 0.4476 | 0.0470 | 0.050* |
| C10 | 0.4530 (3) | 0.6143 (2) | 0.2406 (2) | 0.0325 (5) |

| | | | | |
|---|---|---|---|---|
| C11 | 0.5446 (3) | 0.7065 (2) | 0.3331 (2) | 0.0440 (6) |
| H11 | 0.5478 | 0.7163 | 0.4064 | 0.053* |
| C12 | 0.6311 (3) | 0.7837 (2) | 0.3181 (3) | 0.0490 (7) |
| H12 | 0.6919 | 0.8447 | 0.3811 | 0.059* |
| C13 | 0.6278 (3) | 0.7708 (2) | 0.2107 (3) | 0.0500 (7) |
| H13 | 0.6852 | 0.8233 | 0.2006 | 0.060* |
| C14 | 0.5390 (3) | 0.6797 (3) | 0.1181 (3) | 0.0553 (8) |
| H14 | 0.5364 | 0.6706 | 0.0451 | 0.066* |
| C15 | 0.4527 (3) | 0.6011 (2) | 0.1331 (2) | 0.0469 (7) |
| H15 | 0.3943 | 0.5391 | 0.0701 | 0.056* |
| C16 | −0.0009 (3) | 0.84551 (19) | 0.4940 (2) | 0.0346 (6) |
| C17 | −0.0734 (3) | 0.74627 (18) | 0.5818 (2) | 0.0303 (5) |
| C18 | −0.0629 (3) | 0.86969 (18) | 0.6538 (2) | 0.0313 (5) |
| C19 | −0.2101 (3) | 0.89940 (19) | 0.6608 (2) | 0.0341 (5) |
| C20 | −0.2238 (4) | 1.0100 (2) | 0.6886 (3) | 0.0608 (9) |
| H20 | −0.1437 | 1.0630 | 0.7039 | 0.073* |
| C21 | −0.3546 (5) | 1.0409 (3) | 0.6938 (4) | 0.0841 (13) |
| H21 | −0.3623 | 1.1150 | 0.7134 | 0.101* |
| C22 | −0.4754 (4) | 0.9628 (3) | 0.6699 (4) | 0.0769 (11) |
| H22 | −0.5651 | 0.9839 | 0.6709 | 0.092* |
| C23 | −0.4618 (3) | 0.8539 (3) | 0.6447 (3) | 0.0568 (8) |
| H23 | −0.5422 | 0.8011 | 0.6295 | 0.068* |
| C24 | −0.3285 (3) | 0.8228 (2) | 0.6420 (2) | 0.0422 (6) |
| H24 | −0.3190 | 0.7494 | 0.6274 | 0.051* |
| C25 | 0.0588 (3) | 0.89167 (19) | 0.7714 (2) | 0.0357 (6) |
| C26 | 0.2070 (3) | 0.9131 (2) | 0.7872 (3) | 0.0530 (7) |
| H26 | 0.2329 | 0.9217 | 0.7286 | 0.064* |
| C27 | 0.3172 (4) | 0.9218 (3) | 0.8887 (3) | 0.0681 (10) |
| H27 | 0.4166 | 0.9367 | 0.8982 | 0.082* |
| C28 | 0.2816 (4) | 0.9088 (3) | 0.9754 (3) | 0.0697 (10) |
| H28 | 0.3562 | 0.9137 | 1.0433 | 0.084* |
| C29 | 0.1353 (4) | 0.8884 (3) | 0.9616 (3) | 0.0718 (10) |
| H29 | 0.1104 | 0.8803 | 1.0208 | 0.086* |
| C30 | 0.0239 (3) | 0.8797 (3) | 0.8599 (3) | 0.0554 (8) |
| H30 | −0.0753 | 0.8657 | 0.8512 | 0.066* |
| C31 | −0.2203 (4) | 0.4122 (3) | 0.2507 (3) | 0.0715 (10) |
| H31A | −0.2261 | 0.3330 | 0.2275 | 0.086* |
| H31B | −0.3172 | 0.4277 | 0.2499 | 0.086* |
| C32 | −0.1855 (5) | 0.4482 (3) | 0.1696 (3) | 0.0890 (14) |
| H32A | −0.2703 | 0.4216 | 0.0975 | 0.107* |
| H32B | −0.1024 | 0.4167 | 0.1557 | 0.107* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Zn1 | 0.03145 (16) | 0.02810 (15) | 0.03137 (16) | 0.01168 (11) | 0.01542 (12) | 0.01390 (11) |
| N1 | 0.0317 (11) | 0.0594 (13) | 0.0302 (11) | 0.0233 (10) | 0.0153 (9) | 0.0273 (10) |
| N2 | 0.0279 (10) | 0.0367 (10) | 0.0280 (10) | 0.0121 (8) | 0.0125 (8) | 0.0160 (8) |

| | | | | | | |
|---|---|---|---|---|---|---|
| N3 | 0.0587 (14) | 0.0218 (9) | 0.0486 (13) | 0.0109 (9) | 0.0358 (11) | 0.0151 (9) |
| N4 | 0.0423 (12) | 0.0242 (9) | 0.0404 (11) | 0.0116 (9) | 0.0239 (10) | 0.0127 (9) |
| N5 | 0.0362 (11) | 0.0334 (10) | 0.0375 (11) | 0.0081 (9) | 0.0163 (9) | 0.0185 (9) |
| N6 | 0.0366 (13) | 0.0734 (16) | 0.0464 (13) | 0.0160 (12) | 0.0117 (11) | 0.0402 (13) |
| O1 | 0.0337 (9) | 0.0471 (10) | 0.0257 (8) | 0.0093 (7) | 0.0127 (7) | 0.0183 (7) |
| O2 | 0.0418 (11) | 0.0743 (13) | 0.0428 (10) | 0.0326 (10) | 0.0212 (9) | 0.0405 (10) |
| O3 | 0.0859 (15) | 0.0372 (10) | 0.0595 (12) | 0.0229 (10) | 0.0542 (12) | 0.0252 (9) |
| O4 | 0.0506 (11) | 0.0293 (9) | 0.0547 (11) | 0.0117 (8) | 0.0299 (9) | 0.0222 (8) |
| C1 | 0.0269 (12) | 0.0297 (11) | 0.0285 (12) | 0.0061 (9) | 0.0102 (10) | 0.0128 (10) |
| C2 | 0.0284 (12) | 0.0412 (13) | 0.0326 (13) | 0.0129 (10) | 0.0130 (10) | 0.0193 (11) |
| C3 | 0.0291 (13) | 0.0496 (14) | 0.0273 (12) | 0.0168 (11) | 0.0129 (10) | 0.0231 (11) |
| C4 | 0.0311 (13) | 0.0462 (14) | 0.0347 (13) | 0.0105 (11) | 0.0181 (11) | 0.0232 (11) |
| C5 | 0.0392 (15) | 0.0525 (16) | 0.0471 (15) | 0.0186 (13) | 0.0187 (13) | 0.0253 (13) |
| C6 | 0.061 (2) | 0.0490 (17) | 0.066 (2) | 0.0235 (15) | 0.0309 (17) | 0.0291 (15) |
| C7 | 0.064 (2) | 0.0444 (16) | 0.0512 (17) | 0.0022 (14) | 0.0278 (16) | 0.0163 (14) |
| C8 | 0.0516 (18) | 0.0568 (17) | 0.0396 (15) | 0.0017 (14) | 0.0126 (13) | 0.0219 (14) |
| C9 | 0.0432 (16) | 0.0499 (16) | 0.0390 (14) | 0.0127 (12) | 0.0145 (12) | 0.0240 (13) |
| C10 | 0.0271 (12) | 0.0461 (14) | 0.0335 (13) | 0.0159 (11) | 0.0146 (10) | 0.0213 (11) |
| C11 | 0.0457 (16) | 0.0524 (16) | 0.0381 (14) | 0.0149 (13) | 0.0185 (13) | 0.0181 (13) |
| C12 | 0.0421 (16) | 0.0460 (16) | 0.0527 (17) | 0.0083 (13) | 0.0136 (13) | 0.0146 (13) |
| C13 | 0.0414 (16) | 0.0540 (17) | 0.067 (2) | 0.0096 (13) | 0.0243 (15) | 0.0329 (16) |
| C14 | 0.0559 (19) | 0.073 (2) | 0.0485 (17) | 0.0045 (16) | 0.0241 (15) | 0.0330 (16) |
| C15 | 0.0444 (16) | 0.0629 (18) | 0.0347 (14) | −0.0003 (13) | 0.0147 (12) | 0.0215 (13) |
| C16 | 0.0427 (15) | 0.0273 (12) | 0.0445 (14) | 0.0128 (10) | 0.0267 (12) | 0.0148 (11) |
| C17 | 0.0305 (13) | 0.0267 (11) | 0.0373 (13) | 0.0088 (10) | 0.0148 (10) | 0.0134 (10) |
| C18 | 0.0386 (14) | 0.0249 (11) | 0.0377 (13) | 0.0078 (10) | 0.0212 (11) | 0.0131 (10) |
| C19 | 0.0419 (14) | 0.0357 (13) | 0.0344 (13) | 0.0146 (11) | 0.0207 (11) | 0.0171 (11) |
| C20 | 0.068 (2) | 0.0454 (16) | 0.101 (3) | 0.0266 (15) | 0.057 (2) | 0.0371 (17) |
| C21 | 0.094 (3) | 0.067 (2) | 0.153 (4) | 0.055 (2) | 0.088 (3) | 0.067 (3) |
| C22 | 0.065 (2) | 0.093 (3) | 0.123 (3) | 0.050 (2) | 0.063 (2) | 0.069 (3) |
| C23 | 0.0432 (17) | 0.071 (2) | 0.068 (2) | 0.0131 (15) | 0.0288 (16) | 0.0306 (17) |
| C24 | 0.0461 (16) | 0.0405 (14) | 0.0478 (16) | 0.0121 (12) | 0.0248 (13) | 0.0179 (12) |
| C25 | 0.0374 (14) | 0.0278 (12) | 0.0418 (14) | 0.0053 (10) | 0.0180 (12) | 0.0096 (11) |
| C26 | 0.0434 (17) | 0.0584 (18) | 0.0517 (17) | 0.0047 (14) | 0.0224 (14) | 0.0095 (14) |
| C27 | 0.0370 (17) | 0.078 (2) | 0.069 (2) | 0.0039 (16) | 0.0139 (16) | 0.0100 (19) |
| C28 | 0.055 (2) | 0.070 (2) | 0.060 (2) | 0.0040 (17) | −0.0032 (17) | 0.0200 (18) |
| C29 | 0.062 (2) | 0.100 (3) | 0.0502 (19) | −0.002 (2) | 0.0093 (17) | 0.0381 (19) |
| C30 | 0.0393 (16) | 0.080 (2) | 0.0496 (17) | 0.0003 (15) | 0.0144 (14) | 0.0311 (16) |
| C31 | 0.078 (2) | 0.059 (2) | 0.053 (2) | −0.0192 (18) | 0.0014 (18) | 0.0198 (16) |
| C32 | 0.110 (3) | 0.081 (3) | 0.0382 (18) | −0.027 (2) | −0.0048 (19) | 0.0157 (18) |

*Geometric parameters (Å, º)*

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| Zn1—N4 | 1.9506 (18) | C11—C12 | 1.381 (4) |
| Zn1—N2 | 1.9941 (19) | C11—H11 | 0.9300 |
| Zn1—N5 | 2.0561 (19) | C12—C13 | 1.370 (4) |
| Zn1—N6 | 2.057 (2) | C12—H12 | 0.9300 |
| N1—C1 | 1.349 (3) | C13—C14 | 1.374 (4) |

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| N1—C3 | 1.455 (3) | C13—H13 | 0.9300 |
| N1—H1 | 0.8600 | C14—C15 | 1.392 (4) |
| N2—C2 | 1.360 (3) | C14—H14 | 0.9300 |
| N2—C1 | 1.390 (3) | C15—H15 | 0.9300 |
| N3—C16 | 1.346 (3) | C17—C18 | 1.558 (3) |
| N3—C18 | 1.457 (3) | C18—C19 | 1.525 (3) |
| N3—H3 | 0.8600 | C18—C25 | 1.535 (4) |
| N4—C17 | 1.348 (3) | C19—C24 | 1.377 (4) |
| N4—C16 | 1.386 (3) | C19—C20 | 1.394 (4) |
| N5—C31 | 1.469 (4) | C20—C21 | 1.370 (4) |
| N5—H5A | 0.9000 | C20—H20 | 0.9300 |
| N5—H5B | 0.9000 | C21—C22 | 1.384 (5) |
| N6—C32 | 1.472 (4) | C21—H21 | 0.9300 |
| N6—H6A | 0.9000 | C22—C23 | 1.374 (5) |
| N6—H6B | 0.9000 | C22—H22 | 0.9300 |
| O1—C1 | 1.231 (3) | C23—C24 | 1.386 (4) |
| O2—C2 | 1.224 (3) | C23—H23 | 0.9300 |
| O3—C16 | 1.226 (3) | C24—H24 | 0.9300 |
| O4—C17 | 1.221 (3) | C25—C30 | 1.379 (4) |
| C2—C3 | 1.555 (3) | C25—C26 | 1.380 (4) |
| C3—C10 | 1.534 (3) | C26—C27 | 1.379 (5) |
| C3—C4 | 1.537 (3) | C26—H26 | 0.9300 |
| C4—C5 | 1.384 (3) | C27—C28 | 1.365 (5) |
| C4—C9 | 1.396 (4) | C27—H27 | 0.9300 |
| C5—C6 | 1.386 (4) | C28—C29 | 1.368 (5) |
| C5—H5 | 0.9300 | C28—H28 | 0.9300 |
| C6—C7 | 1.377 (4) | C29—C30 | 1.386 (4) |
| C6—H6 | 0.9300 | C29—H29 | 0.9300 |
| C7—C8 | 1.371 (4) | C30—H30 | 0.9300 |
| C7—H7 | 0.9300 | C31—C32 | 1.433 (5) |
| C8—C9 | 1.384 (4) | C31—H31A | 0.9700 |
| C8—H8 | 0.9300 | C31—H31B | 0.9700 |
| C9—H9 | 0.9300 | C32—H32A | 0.9700 |
| C10—C15 | 1.382 (3) | C32—H32B | 0.9700 |
| C10—C11 | 1.389 (4) | | |

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| N4—Zn1—N2 | 123.12 (8) | C12—C13—C14 | 119.5 (3) |
| N4—Zn1—N5 | 112.66 (8) | C12—C13—H13 | 120.2 |
| N2—Zn1—N5 | 108.94 (8) | C14—C13—H13 | 120.2 |
| N4—Zn1—N6 | 118.42 (9) | C13—C14—C15 | 120.3 (3) |
| N2—Zn1—N6 | 102.08 (9) | C13—C14—H14 | 119.8 |
| N5—Zn1—N6 | 84.83 (9) | C15—C14—H14 | 119.8 |
| C1—N1—C3 | 112.29 (18) | C10—C15—C14 | 120.7 (3) |
| C1—N1—H1 | 123.9 | C10—C15—H15 | 119.7 |
| C3—N1—H1 | 123.9 | C14—C15—H15 | 119.7 |
| C2—N2—C1 | 108.39 (18) | O3—C16—N3 | 126.6 (2) |
| C2—N2—Zn1 | 120.78 (15) | O3—C16—N4 | 123.3 (2) |
| C1—N2—Zn1 | 129.63 (15) | N3—C16—N4 | 110.1 (2) |

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| C16—N3—C18 | 112.08 (19) | O4—C17—N4 | 126.9 (2) |
| C16—N3—H3 | 124.0 | O4—C17—C18 | 123.8 (2) |
| C18—N3—H3 | 124.0 | N4—C17—C18 | 109.18 (18) |
| C17—N4—C16 | 109.22 (18) | N3—C18—C19 | 111.23 (19) |
| C17—N4—Zn1 | 130.24 (15) | N3—C18—C25 | 112.6 (2) |
| C16—N4—Zn1 | 120.51 (16) | C19—C18—C25 | 113.46 (19) |
| C31—N5—Zn1 | 107.60 (17) | N3—C18—C17 | 99.11 (17) |
| C31—N5—H5A | 110.2 | C19—C18—C17 | 114.35 (19) |
| Zn1—N5—H5A | 110.2 | C25—C18—C17 | 105.10 (18) |
| C31—N5—H5B | 110.2 | C24—C19—C20 | 118.8 (2) |
| Zn1—N5—H5B | 110.2 | C24—C19—C18 | 123.3 (2) |
| H5A—N5—H5B | 108.5 | C20—C19—C18 | 117.9 (2) |
| C32—N6—Zn1 | 103.62 (18) | C21—C20—C19 | 120.3 (3) |
| C32—N6—H6A | 111.0 | C21—C20—H20 | 119.8 |
| Zn1—N6—H6A | 111.0 | C19—C20—H20 | 119.8 |
| C32—N6—H6B | 111.0 | C20—C21—C22 | 120.6 (3) |
| Zn1—N6—H6B | 111.0 | C20—C21—H21 | 119.7 |
| H6A—N6—H6B | 109.0 | C22—C21—H21 | 119.7 |
| O1—C1—N1 | 124.9 (2) | C23—C22—C21 | 119.5 (3) |
| O1—C1—N2 | 124.9 (2) | C23—C22—H22 | 120.3 |
| N1—C1—N2 | 110.25 (19) | C21—C22—H22 | 120.3 |
| O2—C2—N2 | 127.1 (2) | C22—C23—C24 | 120.0 (3) |
| O2—C2—C3 | 123.4 (2) | C22—C23—H23 | 120.0 |
| N2—C2—C3 | 109.58 (18) | C24—C23—H23 | 120.0 |
| N1—C3—C10 | 112.7 (2) | C19—C24—C23 | 120.7 (3) |
| N1—C3—C4 | 111.98 (19) | C19—C24—H24 | 119.7 |
| C10—C3—C4 | 114.11 (18) | C23—C24—H24 | 119.7 |
| N1—C3—C2 | 98.85 (17) | C30—C25—C26 | 118.3 (3) |
| C10—C3—C2 | 108.59 (19) | C30—C25—C18 | 121.1 (2) |
| C4—C3—C2 | 109.47 (19) | C26—C25—C18 | 120.3 (2) |
| C5—C4—C9 | 117.7 (2) | C27—C26—C25 | 120.7 (3) |
| C5—C4—C3 | 120.1 (2) | C27—C26—H26 | 119.6 |
| C9—C4—C3 | 122.2 (2) | C25—C26—H26 | 119.6 |
| C4—C5—C6 | 120.8 (3) | C28—C27—C26 | 120.5 (3) |
| C4—C5—H5 | 119.6 | C28—C27—H27 | 119.7 |
| C6—C5—H5 | 119.6 | C26—C27—H27 | 119.7 |
| C7—C6—C5 | 120.8 (3) | C27—C28—C29 | 119.5 (3) |
| C7—C6—H6 | 119.6 | C27—C28—H28 | 120.2 |
| C5—C6—H6 | 119.6 | C29—C28—H28 | 120.2 |
| C8—C7—C6 | 119.3 (3) | C28—C29—C30 | 120.3 (3) |
| C8—C7—H7 | 120.4 | C28—C29—H29 | 119.9 |
| C6—C7—H7 | 120.4 | C30—C29—H29 | 119.9 |
| C7—C8—C9 | 120.3 (3) | C25—C30—C29 | 120.6 (3) |
| C7—C8—H8 | 119.8 | C25—C30—H30 | 119.7 |
| C9—C8—H8 | 119.8 | C29—C30—H30 | 119.7 |
| C8—C9—C4 | 121.1 (3) | C32—C31—N5 | 112.7 (3) |
| C8—C9—H9 | 119.4 | C32—C31—H31A | 109.1 |
| C4—C9—H9 | 119.4 | N5—C31—H31A | 109.1 |

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|---|---|---|---|
| C15—C10—C11 | 118.0 (2) | C32—C31—H31B | 109.1 |
| C15—C10—C3 | 122.0 (2) | N5—C31—H31B | 109.1 |
| C11—C10—C3 | 119.8 (2) | H31A—C31—H31B | 107.8 |
| C12—C11—C10 | 121.1 (3) | C31—C32—N6 | 111.7 (3) |
| C12—C11—H11 | 119.4 | C31—C32—H32A | 109.3 |
| C10—C11—H11 | 119.4 | N6—C32—H32A | 109.3 |
| C13—C12—C11 | 120.3 (3) | C31—C32—H32B | 109.3 |
| C13—C12—H12 | 119.8 | N6—C32—H32B | 109.3 |
| C11—C12—H12 | 119.8 | H32A—C32—H32B | 107.9 |

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| N4—Zn1—N2—C2 | −118.65 (18) | C3—C10—C11—C12 | −174.7 (2) |
| N5—Zn1—N2—C2 | 106.10 (18) | C10—C11—C12—C13 | 0.2 (4) |
| N6—Zn1—N2—C2 | 17.5 (2) | C11—C12—C13—C14 | −0.8 (4) |
| N4—Zn1—N2—C1 | 75.4 (2) | C12—C13—C14—C15 | 0.1 (5) |
| N5—Zn1—N2—C1 | −59.8 (2) | C11—C10—C15—C14 | −1.7 (4) |
| N6—Zn1—N2—C1 | −148.45 (19) | C3—C10—C15—C14 | 174.0 (3) |
| N2—Zn1—N4—C17 | −118.7 (2) | C13—C14—C15—C10 | 1.1 (5) |
| N5—Zn1—N4—C17 | 15.1 (2) | C18—N3—C16—O3 | 175.9 (3) |
| N6—Zn1—N4—C17 | 111.7 (2) | C18—N3—C16—N4 | −4.2 (3) |
| N2—Zn1—N4—C16 | 63.7 (2) | C17—N4—C16—O3 | −174.0 (3) |
| N5—Zn1—N4—C16 | −162.46 (18) | Zn1—N4—C16—O3 | 4.0 (4) |
| N6—Zn1—N4—C16 | −65.9 (2) | C17—N4—C16—N3 | 6.1 (3) |
| N4—Zn1—N5—C31 | 120.3 (2) | Zn1—N4—C16—N3 | −175.88 (17) |
| N2—Zn1—N5—C31 | −99.4 (2) | C16—N4—C17—O4 | 178.0 (2) |
| N6—Zn1—N5—C31 | 1.6 (2) | Zn1—N4—C17—O4 | 0.2 (4) |
| N4—Zn1—N6—C32 | −137.5 (2) | C16—N4—C17—C18 | −5.5 (3) |
| N2—Zn1—N6—C32 | 83.8 (2) | Zn1—N4—C17—C18 | 176.76 (16) |
| N5—Zn1—N6—C32 | −24.5 (2) | C16—N3—C18—C19 | −119.9 (2) |
| C3—N1—C1—O1 | 177.2 (2) | C16—N3—C18—C25 | 111.5 (2) |
| C3—N1—C1—N2 | −4.1 (3) | C16—N3—C18—C17 | 0.8 (3) |
| C2—N2—C1—O1 | 177.2 (2) | O4—C17—C18—N3 | 179.6 (2) |
| Zn1—N2—C1—O1 | −15.6 (3) | N4—C17—C18—N3 | 2.9 (2) |
| C2—N2—C1—N1 | −1.5 (3) | O4—C17—C18—C19 | −62.1 (3) |
| Zn1—N2—C1—N1 | 165.76 (16) | N4—C17—C18—C19 | 121.2 (2) |
| C1—N2—C2—O2 | −174.8 (2) | O4—C17—C18—C25 | 63.0 (3) |
| Zn1—N2—C2—O2 | 16.6 (4) | N4—C17—C18—C25 | −113.7 (2) |
| C1—N2—C2—C3 | 6.1 (3) | N3—C18—C19—C24 | 132.8 (2) |
| Zn1—N2—C2—C3 | −162.49 (15) | C25—C18—C19—C24 | −99.0 (3) |
| C1—N1—C3—C10 | 121.6 (2) | C17—C18—C19—C24 | 21.6 (3) |
| C1—N1—C3—C4 | −108.2 (2) | N3—C18—C19—C20 | −47.8 (3) |
| C1—N1—C3—C2 | 7.1 (3) | C25—C18—C19—C20 | 80.4 (3) |
| O2—C2—C3—N1 | 173.0 (2) | C17—C18—C19—C20 | −159.1 (2) |
| N2—C2—C3—N1 | −7.9 (2) | C24—C19—C20—C21 | −1.9 (5) |
| O2—C2—C3—C10 | 55.4 (3) | C18—C19—C20—C21 | 178.7 (3) |
| N2—C2—C3—C10 | −125.5 (2) | C19—C20—C21—C22 | −0.9 (6) |
| O2—C2—C3—C4 | −69.8 (3) | C20—C21—C22—C23 | 2.2 (7) |
| N2—C2—C3—C4 | 109.3 (2) | C21—C22—C23—C24 | −0.8 (6) |
| N1—C3—C4—C5 | −32.8 (3) | C20—C19—C24—C23 | 3.4 (4) |

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| C10—C3—C4—C5 | 96.7 (3) | C18—C19—C24—C23 | −177.2 (2) |
| C2—C3—C4—C5 | −141.3 (2) | C22—C23—C24—C19 | −2.1 (5) |
| N1—C3—C4—C9 | 146.4 (2) | N3—C18—C25—C30 | 160.6 (2) |
| C10—C3—C4—C9 | −84.1 (3) | C19—C18—C25—C30 | 33.1 (3) |
| C2—C3—C4—C9 | 37.8 (3) | C17—C18—C25—C30 | −92.6 (3) |
| C9—C4—C5—C6 | 0.3 (4) | N3—C18—C25—C26 | −26.0 (3) |
| C3—C4—C5—C6 | 179.5 (2) | C19—C18—C25—C26 | −153.5 (2) |
| C4—C5—C6—C7 | −0.8 (4) | C17—C18—C25—C26 | 80.9 (3) |
| C5—C6—C7—C8 | 0.4 (4) | C30—C25—C26—C27 | 0.2 (4) |
| C6—C7—C8—C9 | 0.5 (4) | C18—C25—C26—C27 | −173.4 (3) |
| C7—C8—C9—C4 | −1.0 (4) | C25—C26—C27—C28 | 0.4 (5) |
| C5—C4—C9—C8 | 0.6 (4) | C26—C27—C28—C29 | −0.9 (6) |
| C3—C4—C9—C8 | −178.6 (2) | C27—C28—C29—C30 | 0.8 (6) |
| N1—C3—C10—C15 | 155.5 (2) | C26—C25—C30—C29 | −0.4 (5) |
| C4—C3—C10—C15 | 26.3 (3) | C18—C25—C30—C29 | 173.2 (3) |
| C2—C3—C10—C15 | −96.1 (3) | C28—C29—C30—C25 | −0.1 (6) |
| N1—C3—C10—C11 | −28.9 (3) | Zn1—N5—C31—C32 | 23.6 (4) |
| C4—C3—C10—C11 | −158.1 (2) | N5—C31—C32—N6 | −47.9 (5) |
| C2—C3—C10—C11 | 79.5 (3) | Zn1—N6—C32—C31 | 45.3 (4) |
| C15—C10—C11—C12 | 1.0 (4) | | |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N6—H6*B*···O2 | 0.90 | 2.18 | 2.858 (3) | 132 |
| C9—H9···O2 | 0.93 | 2.36 | 2.992 (3) | 125 |
| C11—H11···N1 | 0.93 | 2.52 | 2.860 (4) | 102 |
| C24—H24···O4 | 0.93 | 2.39 | 3.042 (4) | 127 |
| C26—H26···N3 | 0.93 | 2.51 | 2.854 (4) | 102 |
| N1—H1···O1$^{i}$ | 0.86 | 2.16 | 3.008 (3) | 167 |
| N3—H3···O3$^{ii}$ | 0.86 | 2.04 | 2.843 (3) | 156 |
| N5—H5*A*···O4$^{iii}$ | 0.90 | 1.97 | 2.855 (3) | 170 |
| N5—H5*B*···O1$^{iii}$ | 0.90 | 2.18 | 3.003 (3) | 152 |

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