Acta Cryst E CRYSTALLOGRAPHIC COMMUNICATIONS

ISSN 2056-9890

Received 19 March 2015
Accepted 25 March 2015

Edited by W. Imhof, University Koblenz-Landau, Germany

**Keywords**: crystal structure; thiosemicarbazone–$Zn^{II}$ complex; hydrogen-bonded polymer

**CCDC reference**: 1056177
**Supporting information**: this article has supporting information at journals.iucr.org/e

# Crystal structure of bis[*N*-phenyl-2-(1,2,3,4-tetrahydronaphthalen-1-ylidene)hydrazinecarbothioamidato-$\kappa^2N^2,S$]zinc dimethyl sulfoxide monosolvate

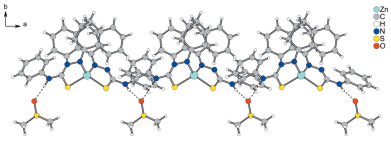
**Genelane Cruz Santana,[a] Iara de Fátima Gimenez,[a]* Christian Näther,[b] Inke Jess[b] and Adriano Bof de Oliveira[c]**

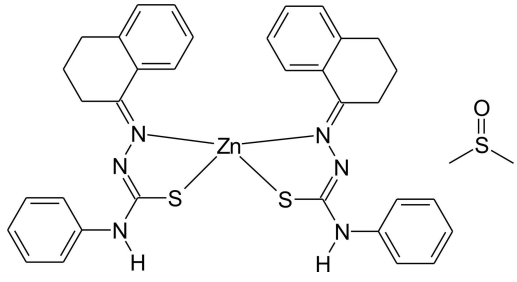
[a]Programa de Pós-Graduação em Ciência e Engenharia de Materiais, Universidade Federal de Sergipe, Av. Marechal Rondon s/n, 49100-000 São Cristóvão-SE, Brazil, [b]Institut für Anorganische Chemie, Christian-Albrechts-Universität zu Kiel, Max-Eyth Strasse 2, D-24118 Kiel, Germany, and [c]Departamento de Química, Universidade Federal de Sergipe, Av. Marechal Rondon s/n, 49100-000 São Cristóvão-SE, Brazil. *Correspondence e-mail: iara.gimenez@gmail.com

The reaction of the *N*-phenyl-2-(1,2,3,4-tetrahydronaphthalen-1-ylidene)hydrazinecarbothioamide ligand with zinc acetate dihydrate in a 2:1 molar ratio yielded a yellow solid, which was crystallized from DMSO to obtain the title compound, $[Zn(C_{17}H_{16}N_3S)_2]\cdot C_2H_6OS$. The $Zn^{II}$ ion is four-coordinated in a distorted tetrahedral environment by two deprotonated ligands. Each ligand acts as an *N*,*S*-donor, forming a five-membered metallacycle. The maximum deviation from the mean plane of the N–N–C–S chelate group is 0.0029 (14) Å for the *N*-donor atom of one ligand and 0.0044 (14) Å for the non-coordinating N atom of the second. The dihedral angle between the planes of the two chelate groups is 72.80 (07)°. Bond lengths in the ligands are compared with those in the crystal structure of the free ligand. In the crystal, complex molecules are connected by dimethyl sulfoxide solvate molecules *via* N—H···O hydrogen-bonding interactions, building a one-dimensional hydrogen-bonded polymer along the *a*-axis direction. The S atom and one C atom of the dimethyl sulfoxide solvate molecules are disordered over two sets of sites with an occupancy ratio of 0.6:0.4.

## 1. Chemical context

In a continuation of our on-going research on the supramolecular chemistry of thiosemicarbazone derivatives and their complexes, we report herein the synthesis and crystal structure of a $Zn^{II}$ complex with the *N*-phenyl-2-(1,2,3,4-tetrahydronaphthalen-1-ylidene)hydrazinecarbothioamidate ligand. Thiosemicarbazone derivatives are *N*,*S*-donors with a wide range of coordination modes and a variety of applications in biological inorganic chemistry (Lobana *et al.* 2009; Ferraz *et al.* 2012).





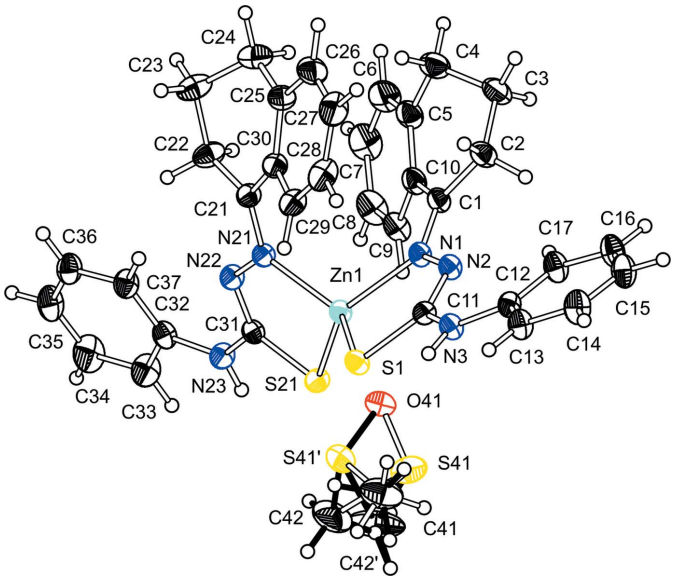



**Figure 1**
The molecular structure of the title compound with atom labeling and displacement ellipsoids drawn at the 30% probability level. Disorder is shown with open and full bonds.

## 2. Structural commentary

The molecular structure of the title compound consists of one $Zn^{II}$ ion, four-coordinated in a distorted tetrahedral environment by two deprotonated thiosemicarbazone ligands in a bidentate chelating mode, and one disordered DMSO solvate molecule (Fig. 1). The *N*,*S*-donor atoms together with the central zinc atom form five-membered metallacycles (Fig. 1). The maximum deviation from the mean plane of the N1—N2—C11—S1 chelate group is 0.0029 (14) Å for the N1 donor atom. For the N21—N22—C31—S21 chelate group, the maximum deviation is 0.0044 (14) Å for atom N22. The dihedral angle between the planes of the two chelate groups is 72.80 (7)°, clearly showing the distorted tetrahedral geometry.

The acidic hydrogen of the hydrazine fragment is lost by the reaction with the acetate anion. The negative charge of the deprotonated ligand is delocalized over the N—N—C—S entity, as indicated by their intermediate bond lengths. The bond lengths in the ligand are also affected by the coordination with the metal atom, especially the C—S bond length, which is consistent with increased single-bond character. In the crystal structure of the free ligand (de Oliveira *et al.*, 2014), selected bond lengths are N—N = 1.3846 (14), N—C = 1.3642 (16) and C—S = 1.6773 (13) Å. For the ligands in the title $Zn^{II}$ complex, the bond lengths are N1—N2 = 1.400 (3)/N21—N22 = 1.393 (3) Å, N2—C11 = 1.303 (3)/N22—C31 = 1.304 (3) Å and C11—S1 = 1.755 (2)/C31—S21 = 1.749 (2) Å.

Neither of the coordinating ligands is planar. For one ligand, the dihedral angles between the aromatic rings (C5–C10 and C12–C17) is 58.25 (11)°. In the second ligand, the corresponding angle is 49.99 (11)° between the C25–C30 and C32–C37 rings. In addition, the aliphatic rings are also not planar. The maximum deviation from the mean plane for the C1–C5/C10 ring is 0.355 (3) Å for C3 and for the C21–C25/C30 ring the maximum deviation is 0.359 (3) Å for C23, with both of the aliphatic rings having an envelope conformation

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

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N3—H3*N*···O41 | 0.88 | 2.08 | 2.945 (3) | 168 |
| N23—H23*N*···O41$^{i}$ | 0.88 | 2.03 | 2.903 (3) | 173 |

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

## 3. Supramolecular features

In the crystal, the $Zn^{II}$ complex molecules and the DMSO solvent molecules build a monomeric entity. The DMSO molecule bridges two complex molecules *via* intermolecular N—H···O hydrogen-bonding interactions, building a one-dimensional hydrogen-bonded polymer along the *a*-axis direction (Fig. 2, Table 1).

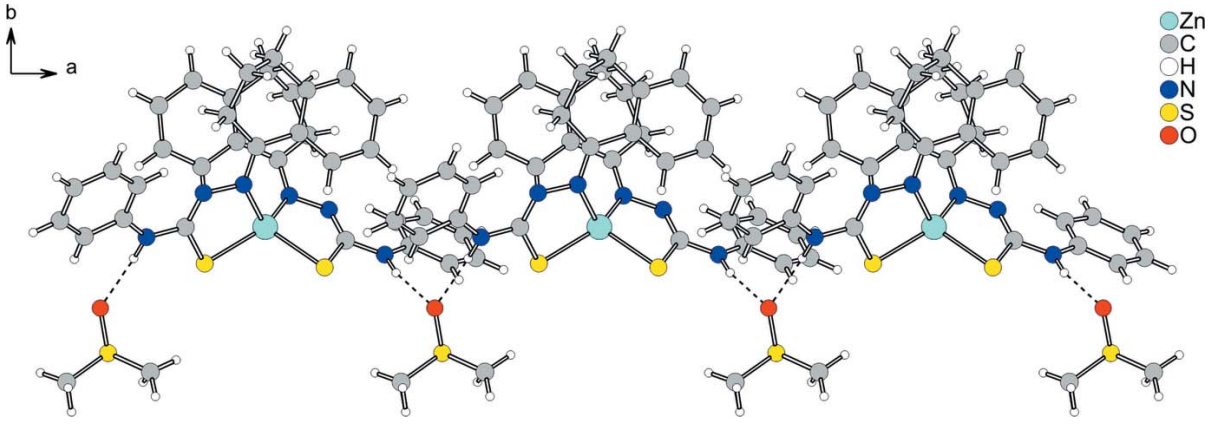



**Figure 2**
View of the one-dimensional hydrogen-bonded polymer that elongates along the *a*-axis direction. Intermolecular hydrogen bonding (for details, see Table 1) is shown as dashed lines. The minor occupancy components of the disordered atoms are not shown for clarity.

## 4. Synthesis and crystallization

Starting materials were commercially available and used without further purification. The ligand synthesis was adapted from a procedure reported previously (Freund & Schander, 1902). A mixture of *N*-phenyl-2-(1,2,3,4-tetrahydronaphthalen-1-ylidene)hydrazinecarbothioamide dissolved in THF (2 mmol/40 mL) with zinc acetate dihydrate dissolved in ethanol (1 mmol/30 mL) was refluxed for 4 h under continuous stirring. An orange solid was obtained, filtered and washed with ethanol. Suitable crystals for X-ray diffraction were obtained in DMSO by slow evaporation of the solvent.

## 5. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. The C—H and N—H hydrogen atoms were positioned with idealized geometry and refined isotropically with $U_{iso}$(H) = 1.2 $U_{eq}$(C) (1.5 for methyl H atoms) using a riding model with C—H = 0.95 Å for aromatic, C—H = 0.99 Å for methylene, C—H = 0.98 Å for methyl and N—H = 0.88 Å. In the DMSO solvate molecule, the S atom and methylene C atom C42 and attached H atoms are disordered and were refined using a split model with an occupancy ratio of 0.4:0.6.

**Table 2**
Experimental details.

| | |
|---|---|
| Crystal data | |
| Chemical formula | $[Zn(C_{17}H_{16}N_3S)_2]\cdot C_2H_6OS$ |
| $M_r$ | 732.27 |
| Crystal system, space group | Monoclinic, $P2_1/n$ |
| Temperature (K) | 200 |
| $a$, $b$, $c$ (Å) | 10.6320 (4), 17.2695 (5), 19.4067 (7) |
| $\beta$ (°) | 94.223 (3) |
| $V$ (Å$^3$) | 3553.6 (2) |
| $Z$ | 4 |
| Radiation type | Mo $K\alpha$ |
| $\mu$ (mm$^{-1}$) | 0.91 |
| Crystal size (mm) | 0.14 × 0.10 × 0.06 |
| | |
| Data collection | |
| Diffractometer | STOE IPDS1 |
| Absorption correction | Numerical (*X-SHAPE* and *X-RED32*; Stoe & Cie, 2008) |
| $T_{min}$, $T_{max}$ | 0.793, 0.916 |
| No. of measured, independent and observed [$I > 2\sigma(I)$] reflections | 45253, 6947, 6171 |
| $R_{int}$ | 0.041 |
| (sin $\theta/\lambda)_{max}$ (Å$^{-1}$) | 0.617 |
| | |
| Refinement | |
| $R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, $S$ | 0.042, 0.097, 1.06 |
| No. of reflections | 6947 |
| No. of parameters | 442 |
| H-atom treatment | H-atom parameters constrained |
| $\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å$^{-3}$) | 0.80, −0.68 |

Computer programs: *X-AREA* and *X-RED32* (Stoe & Cie, 2008), *SHELXS97* (Sheldrick, 2008), *SHELXL2013-2* (Sheldrick, 2015), *DIAMOND* (Brandenburg, 2006) and *publCIF* (Westrip, 2010).

## Acknowledgements

We gratefully acknowledge the financial support by the State of Schleswig–Holstein, Germany. We thank Professor Dr Wolfgang Bensch for access to his experimental facilities. IFG and GCS thank CNPq for the award of a researcher scholarship and CAPES for the award of a PhD scholarship, respectively. ABO thanks Renan Lira de Farias, Universidade Federal de Sergipe, Brazil, for his support in the laboratory.

## References

Brandenburg, K. (2006). *DIAMOND*. Crystal Impact GbR, Bonn, Germany.
Ferraz, K. S. O., Silva, N. F., Da Silva, J. G., Speziali, N. L., Mendes, I. C. & Beraldo, H. (2012). *J. Mol. Struct.* **1008**, 102–107.
Freund, M. & Schander, A. (1902). *Ber. Dtsch. Chem. Ges.* **35**, 2602–2606.
Lobana, T. S., Sharma, R., Bawa, G. & Khanna, S. (2009). *Coord. Chem. Rev.* **253**, 977–1055.
Oliveira, A. B. de, Feitosa, B. R. S., Näther, C. & Jess, I. (2014). *Acta Cryst.* E**70**, o205.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Sheldrick, G. M. (2015). *Acta Cryst.* C**71**, 3–8.
Stoe & Cie (2008). *X-SHAPE*, *X-AREA* and *X-RED32*. Stoe & Cie, Darmstadt, Germany.
Westrip, S. P. (2010). *J. Appl. Cryst.* **43**, 920–925.

# supporting information

*Acta Cryst.* (2015). E**71**, 440-442 [https://doi.org/10.1107/S205698901500612X]

## Crystal structure of bis[*N*-phenyl-2-(1,2,3,4-tetrahydronaphthalen-1-yl-idene)hydrazinecarbothioamidato-$\kappa^2N^2$,*S*]zinc dimethyl sulfoxide monosolvate

**Genelane Cruz Santana, Iara de Fátima Gimenez, Christian Näther, Inke Jess and Adriano Bof de Oliveira**

### Computing details

Data collection: *X-AREA* (Stoe & Cie, 2008); cell refinement: *X-AREA* (Stoe & Cie, 2008); data reduction: *X-RED32* (Stoe & Cie, 2008); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL2013-2*(Sheldrick, 2015); molecular graphics: *DIAMOND* (Brandenburg, 2006); software used to prepare material for publication: *publCIF* (Westrip, 2010).

### Bis[*N*-phenyl-2-(1,2,3,4-tetrahydronaphthalen-1-ylidene)hydrazinecarbothioamidato-$\kappa^2N^2$,*S*]zinc dimethyl sulfoxide monosolvate

*Crystal data*

$[Zn(C_{17}H_{16}N_3S)_2]\cdot C_2H_6OS$
$M_r$ = 732.27
Monoclinic, $P2_1/n$
$a$ = 10.6320 (4) Å
$b$ = 17.2695 (5) Å
$c$ = 19.4067 (7) Å
$\beta$ = 94.223 (3)°
$V$ = 3553.6 (2) Å$^3$
$Z$ = 4
$F(000)$ = 1528
$D_x$ = 1.369 Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda$ = 0.71073 Å
$\theta$ = 1.6–26.0°
$\mu$ = 0.91 mm$^{-1}$
$T$ = 200 K
Prism, orange
0.14 × 0.10 × 0.06 mm

*Data collection*

STOE IPDS-1 diffractometer
Radiation source: fine-focus sealed tube, STOE IPDS-1
Graphite monochromator
$\varphi$ scans
Absorption correction: numerical (X-SHAPE and X-RED32; Stoe & Cie, 2008)
$T_{min}$ = 0.793, $T_{max}$ = 0.916
45253 measured reflections
6947 independent reflections
6171 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.041
$\theta_{max}$ = 26.0°, $\theta_{min}$ = 1.6°
$h$ = −13→13
$k$ = −21→21
$l$ = −23→23

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.097
$S$ = 1.06
6947 reflections
442 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

$w = 1/[\sigma^2(F_o^2) + (0.0382P)^2 + 2.9458P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.80$ e Å$^{-3}$
$\Delta\rho_{min} = -0.68$ 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* | $U_{iso}$*/$U_{eq}$ | Occ. (<1) |
|---|---|---|---|---|---|
| Zn1 | 0.75764 (2) | 0.193873 (16) | 0.627860 (14) | 0.03590 (9) | |
| C1 | 0.7188 (2) | 0.31745 (15) | 0.73748 (13) | 0.0415 (5) | |
| C2 | 0.6288 (3) | 0.36245 (17) | 0.77834 (15) | 0.0518 (7) | |
| H2A | 0.6079 | 0.3311 | 0.8186 | 0.062* | |
| H2B | 0.5497 | 0.3711 | 0.7491 | 0.062* | |
| C3 | 0.6803 (3) | 0.44078 (18) | 0.80402 (17) | 0.0635 (8) | |
| H3A | 0.6101 | 0.4736 | 0.8177 | 0.076* | |
| H3B | 0.7399 | 0.4331 | 0.8451 | 0.076* | |
| C4 | 0.7473 (3) | 0.48091 (18) | 0.74761 (18) | 0.0633 (8) | |
| H4A | 0.6883 | 0.4883 | 0.7062 | 0.076* | |
| H4B | 0.7777 | 0.5324 | 0.7638 | 0.076* | |
| C5 | 0.8570 (3) | 0.43171 (18) | 0.72969 (15) | 0.0555 (7) | |
| C6 | 0.9733 (3) | 0.4637 (2) | 0.71835 (19) | 0.0716 (10) | |
| H6 | 0.9831 | 0.5184 | 0.7190 | 0.086* | |
| C7 | 1.0752 (3) | 0.4175 (2) | 0.7061 (2) | 0.0784 (11) | |
| H7 | 1.1535 | 0.4406 | 0.6973 | 0.094* | |
| C8 | 1.0638 (3) | 0.3377 (2) | 0.70660 (18) | 0.0684 (9) | |
| H8 | 1.1345 | 0.3059 | 0.6994 | 0.082* | |
| C9 | 0.9483 (3) | 0.30455 (18) | 0.71767 (15) | 0.0524 (7) | |
| H9 | 0.9404 | 0.2498 | 0.7186 | 0.063* | |
| C10 | 0.8434 (2) | 0.35090 (16) | 0.72747 (14) | 0.0467 (6) | |
| N1 | 0.68571 (18) | 0.25148 (12) | 0.70903 (10) | 0.0374 (4) | |
| N2 | 0.56703 (18) | 0.22579 (12) | 0.72604 (10) | 0.0390 (4) | |
| C11 | 0.5176 (2) | 0.16915 (14) | 0.68884 (12) | 0.0365 (5) | |
| S1 | 0.58047 (6) | 0.11959 (4) | 0.62029 (3) | 0.04070 (15) | |
| N3 | 0.40074 (18) | 0.14264 (13) | 0.70263 (11) | 0.0407 (5) | |
| H3N | 0.3667 | 0.1097 | 0.6721 | 0.049* | |
| C12 | 0.3262 (2) | 0.15955 (15) | 0.75765 (13) | 0.0399 (5) | |
| C13 | 0.2066 (2) | 0.12656 (17) | 0.75371 (14) | 0.0493 (6) | |
| H13 | 0.1790 | 0.0964 | 0.7146 | 0.059* | |

| | | | | | |
|---|---|---|---|---|---|
| C14 | 0.1274 (3) | 0.1373 (2) | 0.80637 (16) | 0.0582 (8) | |
| H14 | 0.0455 | 0.1150 | 0.8027 | 0.070* | |
| C15 | 0.1657 (3) | 0.1799 (2) | 0.86376 (15) | 0.0580 (8) | |
| H15 | 0.1117 | 0.1865 | 0.9002 | 0.070* | |
| C16 | 0.2836 (3) | 0.2128 (2) | 0.86770 (15) | 0.0577 (8) | |
| H16 | 0.3107 | 0.2425 | 0.9073 | 0.069* | |
| C17 | 0.3644 (2) | 0.20369 (18) | 0.81488 (14) | 0.0508 (7) | |
| H17 | 0.4450 | 0.2276 | 0.8182 | 0.061* | |
| C21 | 0.7844 (2) | 0.34196 (15) | 0.54269 (13) | 0.0408 (5) | |
| C22 | 0.8717 (3) | 0.39974 (16) | 0.51388 (18) | 0.0555 (7) | |
| H22A | 0.9047 | 0.3781 | 0.4716 | 0.067* | |
| H22B | 0.9442 | 0.4084 | 0.5480 | 0.067* | |
| C23 | 0.8086 (3) | 0.47694 (18) | 0.4965 (2) | 0.0655 (9) | |
| H23A | 0.8736 | 0.5160 | 0.4876 | 0.079* | |
| H23B | 0.7518 | 0.4715 | 0.4540 | 0.079* | |
| C24 | 0.7336 (3) | 0.50397 (18) | 0.55528 (19) | 0.0675 (9) | |
| H24A | 0.7906 | 0.5108 | 0.5975 | 0.081* | |
| H24B | 0.6939 | 0.5546 | 0.5434 | 0.081* | |
| C25 | 0.6338 (3) | 0.44571 (17) | 0.56840 (15) | 0.0532 (7) | |
| C26 | 0.5159 (3) | 0.4675 (2) | 0.58907 (18) | 0.0674 (9) | |
| H26 | 0.4992 | 0.5206 | 0.5971 | 0.081* | |
| C27 | 0.4235 (3) | 0.4135 (2) | 0.59806 (18) | 0.0718 (10) | |
| H27 | 0.3456 | 0.4293 | 0.6146 | 0.086* | |
| C28 | 0.4430 (3) | 0.3370 (2) | 0.58337 (17) | 0.0627 (8) | |
| H28 | 0.3776 | 0.3002 | 0.5875 | 0.075* | |
| C29 | 0.5585 (2) | 0.31397 (17) | 0.56250 (15) | 0.0495 (6) | |
| H29 | 0.5712 | 0.2612 | 0.5509 | 0.059* | |
| C30 | 0.6571 (2) | 0.36679 (16) | 0.55815 (14) | 0.0440 (6) | |
| N21 | 0.82246 (17) | 0.27193 (12) | 0.55813 (10) | 0.0365 (4) | |
| N22 | 0.94220 (18) | 0.25641 (12) | 0.53682 (11) | 0.0402 (5) | |
| C31 | 0.9966 (2) | 0.19343 (14) | 0.56117 (12) | 0.0370 (5) | |
| S21 | 0.93916 (6) | 0.12624 (4) | 0.61853 (3) | 0.04147 (15) | |
| N23 | 1.11279 (19) | 0.17498 (13) | 0.53992 (11) | 0.0438 (5) | |
| H23N | 1.1506 | 0.1358 | 0.5618 | 0.053* | |
| C32 | 1.1814 (2) | 0.20924 (16) | 0.48819 (13) | 0.0434 (6) | |
| C33 | 1.2983 (3) | 0.1765 (2) | 0.47906 (17) | 0.0627 (8) | |
| H33 | 1.3285 | 0.1346 | 0.5073 | 0.075* | |
| C34 | 1.3711 (3) | 0.2057 (2) | 0.4282 (2) | 0.0763 (11) | |
| H34 | 1.4511 | 0.1833 | 0.4222 | 0.092* | |
| C35 | 1.3300 (3) | 0.2660 (2) | 0.38675 (17) | 0.0636 (8) | |
| H35 | 1.3804 | 0.2853 | 0.3521 | 0.076* | |
| C36 | 1.2150 (3) | 0.29789 (19) | 0.39610 (15) | 0.0551 (7) | |
| H36 | 1.1853 | 0.3396 | 0.3674 | 0.066* | |
| C37 | 1.1408 (3) | 0.27054 (18) | 0.44670 (14) | 0.0499 (6) | |
| H37 | 1.0616 | 0.2941 | 0.4528 | 0.060* | |
| S41 | 0.22794 (16) | −0.03767 (8) | 0.62486 (9) | 0.0732 (4) | 0.60 |
| S41′ | 0.2187 (2) | −0.01998 (12) | 0.55185 (11) | 0.0653 (5) | 0.40 |
| O41 | 0.25110 (17) | 0.04499 (11) | 0.60282 (11) | 0.0521 (5) | |

| | | | | | |
|---|---|---|---|---|---|
| C41 | 0.1008 (4) | −0.0730 (2) | 0.5786 (3) | 0.0915 (13) | |
| H41A | 0.0241 | −0.0510 | 0.5958 | 0.137* | 0.60 |
| H41B | 0.0990 | −0.1295 | 0.5831 | 0.137* | 0.60 |
| H41C | 0.1051 | −0.0591 | 0.5298 | 0.137* | 0.60 |
| H41D | 0.0243 | −0.0413 | 0.5780 | 0.137* | 0.40 |
| H41E | 0.1230 | −0.0914 | 0.6257 | 0.137* | 0.40 |
| H41F | 0.0857 | −0.1175 | 0.5477 | 0.137* | 0.40 |
| C42 | 0.3516 (9) | −0.0914 (6) | 0.5996 (7) | 0.124 (5) | 0.60 |
| H42A | 0.4297 | −0.0742 | 0.6249 | 0.186* | 0.60 |
| H42B | 0.3586 | −0.0846 | 0.5499 | 0.186* | 0.60 |
| H42C | 0.3372 | −0.1462 | 0.6095 | 0.186* | 0.60 |
| C42′ | 0.3297 (14) | −0.0806 (9) | 0.5512 (7) | 0.099 (5) | 0.40 |
| H42D | 0.4055 | −0.0550 | 0.5366 | 0.148* | 0.40 |
| H42E | 0.3053 | −0.1226 | 0.5190 | 0.148* | 0.40 |
| H42F | 0.3471 | −0.1019 | 0.5978 | 0.148* | 0.40 |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Zn1 | 0.03107 (14) | 0.03978 (16) | 0.03778 (15) | 0.00053 (11) | 0.00889 (10) | −0.00104 (11) |
| C1 | 0.0421 (13) | 0.0436 (14) | 0.0397 (13) | −0.0017 (11) | 0.0089 (10) | −0.0057 (11) |
| C2 | 0.0520 (15) | 0.0492 (15) | 0.0560 (17) | −0.0006 (13) | 0.0169 (13) | −0.0114 (13) |
| C3 | 0.075 (2) | 0.0528 (17) | 0.0647 (19) | −0.0011 (15) | 0.0165 (16) | −0.0208 (15) |
| C4 | 0.074 (2) | 0.0467 (16) | 0.070 (2) | −0.0102 (15) | 0.0093 (16) | −0.0144 (14) |
| C5 | 0.0604 (17) | 0.0546 (17) | 0.0519 (16) | −0.0159 (14) | 0.0073 (13) | −0.0132 (13) |
| C6 | 0.074 (2) | 0.065 (2) | 0.077 (2) | −0.0324 (18) | 0.0117 (18) | −0.0151 (17) |
| C7 | 0.059 (2) | 0.093 (3) | 0.084 (3) | −0.037 (2) | 0.0168 (18) | −0.018 (2) |
| C8 | 0.0451 (16) | 0.088 (2) | 0.073 (2) | −0.0164 (16) | 0.0134 (15) | −0.0212 (19) |
| C9 | 0.0423 (14) | 0.0620 (18) | 0.0538 (16) | −0.0092 (13) | 0.0091 (12) | −0.0149 (14) |
| C10 | 0.0465 (14) | 0.0509 (15) | 0.0436 (14) | −0.0117 (12) | 0.0088 (11) | −0.0099 (12) |
| N1 | 0.0317 (10) | 0.0431 (11) | 0.0382 (11) | −0.0032 (8) | 0.0080 (8) | −0.0028 (9) |
| N2 | 0.0320 (10) | 0.0451 (11) | 0.0409 (11) | −0.0039 (9) | 0.0105 (8) | −0.0023 (9) |
| C11 | 0.0306 (11) | 0.0390 (12) | 0.0403 (13) | 0.0008 (9) | 0.0056 (9) | 0.0017 (10) |
| S1 | 0.0355 (3) | 0.0431 (3) | 0.0445 (3) | −0.0037 (2) | 0.0101 (2) | −0.0067 (3) |
| N3 | 0.0321 (10) | 0.0481 (12) | 0.0426 (11) | −0.0056 (9) | 0.0077 (8) | −0.0052 (9) |
| C12 | 0.0324 (12) | 0.0481 (14) | 0.0401 (13) | 0.0029 (10) | 0.0077 (10) | 0.0038 (11) |
| C13 | 0.0359 (13) | 0.0656 (18) | 0.0471 (15) | −0.0077 (12) | 0.0076 (11) | −0.0030 (13) |
| C14 | 0.0334 (13) | 0.086 (2) | 0.0565 (17) | −0.0080 (14) | 0.0122 (12) | 0.0018 (16) |
| C15 | 0.0414 (14) | 0.085 (2) | 0.0495 (16) | 0.0000 (14) | 0.0177 (12) | −0.0010 (15) |
| C16 | 0.0495 (15) | 0.080 (2) | 0.0454 (15) | −0.0046 (15) | 0.0145 (12) | −0.0091 (14) |
| C17 | 0.0369 (13) | 0.0702 (19) | 0.0466 (15) | −0.0075 (12) | 0.0116 (11) | −0.0066 (13) |
| C21 | 0.0384 (13) | 0.0400 (13) | 0.0445 (14) | 0.0022 (10) | 0.0065 (10) | 0.0026 (11) |
| C22 | 0.0417 (14) | 0.0459 (15) | 0.080 (2) | −0.0006 (12) | 0.0100 (14) | 0.0135 (14) |
| C23 | 0.0528 (17) | 0.0469 (16) | 0.097 (3) | −0.0012 (13) | 0.0082 (17) | 0.0203 (17) |
| C24 | 0.072 (2) | 0.0432 (16) | 0.087 (2) | 0.0092 (15) | −0.0019 (18) | 0.0014 (16) |
| C25 | 0.0564 (16) | 0.0471 (15) | 0.0562 (17) | 0.0139 (13) | 0.0043 (13) | 0.0021 (13) |
| C26 | 0.072 (2) | 0.064 (2) | 0.066 (2) | 0.0321 (17) | 0.0086 (16) | −0.0015 (16) |
| C27 | 0.0560 (19) | 0.093 (3) | 0.069 (2) | 0.0343 (19) | 0.0194 (16) | 0.0174 (19) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C28 | 0.0392 (14) | 0.080 (2) | 0.071 (2) | 0.0158 (14) | 0.0134 (14) | 0.0230 (17) |
| C29 | 0.0378 (13) | 0.0543 (16) | 0.0568 (16) | 0.0100 (12) | 0.0077 (12) | 0.0111 (13) |
| C30 | 0.0400 (13) | 0.0463 (14) | 0.0461 (14) | 0.0088 (11) | 0.0067 (11) | 0.0040 (11) |
| N21 | 0.0307 (9) | 0.0397 (11) | 0.0400 (11) | 0.0036 (8) | 0.0087 (8) | 0.0016 (9) |
| N22 | 0.0303 (10) | 0.0461 (12) | 0.0456 (12) | 0.0034 (9) | 0.0115 (8) | 0.0040 (9) |
| C31 | 0.0307 (11) | 0.0425 (13) | 0.0384 (12) | 0.0028 (10) | 0.0063 (9) | −0.0032 (10) |
| S21 | 0.0358 (3) | 0.0414 (3) | 0.0485 (4) | 0.0060 (2) | 0.0114 (3) | 0.0056 (3) |
| N23 | 0.0335 (10) | 0.0502 (12) | 0.0487 (12) | 0.0082 (9) | 0.0098 (9) | 0.0067 (10) |
| C32 | 0.0302 (12) | 0.0564 (16) | 0.0447 (14) | −0.0015 (11) | 0.0100 (10) | −0.0048 (12) |
| C33 | 0.0385 (14) | 0.083 (2) | 0.068 (2) | 0.0139 (15) | 0.0157 (13) | 0.0114 (17) |
| C34 | 0.0399 (16) | 0.109 (3) | 0.084 (2) | 0.0103 (17) | 0.0283 (16) | 0.006 (2) |
| C35 | 0.0452 (16) | 0.092 (2) | 0.0559 (18) | −0.0123 (16) | 0.0208 (13) | −0.0027 (17) |
| C36 | 0.0493 (15) | 0.0673 (19) | 0.0500 (16) | −0.0089 (14) | 0.0131 (12) | 0.0024 (14) |
| C37 | 0.0398 (14) | 0.0617 (17) | 0.0499 (15) | 0.0004 (12) | 0.0142 (11) | 0.0033 (13) |
| S41 | 0.0817 (10) | 0.0498 (7) | 0.0839 (10) | −0.0036 (7) | −0.0225 (8) | 0.0050 (7) |
| S41′ | 0.0815 (14) | 0.0555 (11) | 0.0591 (12) | −0.0035 (10) | 0.0072 (10) | −0.0126 (9) |
| O41 | 0.0462 (10) | 0.0444 (10) | 0.0654 (12) | 0.0011 (8) | 0.0033 (9) | −0.0082 (9) |
| C41 | 0.071 (2) | 0.068 (2) | 0.135 (4) | −0.0099 (19) | 0.010 (2) | −0.023 (2) |
| C42 | 0.067 (4) | 0.062 (5) | 0.238 (14) | 0.028 (4) | −0.021 (8) | −0.031 (8) |
| C42′ | 0.093 (10) | 0.084 (8) | 0.125 (11) | 0.029 (7) | 0.042 (9) | −0.024 (9) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| Zn1—N1 | 2.057 (2) | C23—H23A | 0.9900 |
| Zn1—N21 | 2.064 (2) | C23—H23B | 0.9900 |
| Zn1—S21 | 2.2745 (6) | C24—C25 | 1.498 (4) |
| Zn1—S1 | 2.2747 (7) | C24—H24A | 0.9900 |
| C1—N1 | 1.303 (3) | C24—H24B | 0.9900 |
| C1—C10 | 1.471 (3) | C25—C26 | 1.396 (4) |
| C1—C2 | 1.503 (3) | C25—C30 | 1.402 (4) |
| C2—C3 | 1.529 (4) | C26—C27 | 1.375 (5) |
| C2—H2A | 0.9900 | C26—H26 | 0.9500 |
| C2—H2B | 0.9900 | C27—C28 | 1.370 (5) |
| C3—C4 | 1.517 (4) | C27—H27 | 0.9500 |
| C3—H3A | 0.9900 | C28—C29 | 1.380 (4) |
| C3—H3B | 0.9900 | C28—H28 | 0.9500 |
| C4—C5 | 1.504 (4) | C29—C30 | 1.397 (4) |
| C4—H4A | 0.9900 | C29—H29 | 0.9500 |
| C4—H4B | 0.9900 | N21—N22 | 1.393 (3) |
| C5—C6 | 1.387 (4) | N22—C31 | 1.304 (3) |
| C5—C10 | 1.403 (4) | C31—N23 | 1.368 (3) |
| C6—C7 | 1.380 (5) | C31—S21 | 1.749 (2) |
| C6—H6 | 0.9500 | N23—C32 | 1.414 (3) |
| C7—C8 | 1.384 (5) | N23—H23N | 0.8800 |
| C7—H7 | 0.9500 | C32—C37 | 1.380 (4) |
| C8—C9 | 1.386 (4) | C32—C33 | 1.388 (4) |
| C8—H8 | 0.9500 | C33—C34 | 1.392 (4) |
| C9—C10 | 1.397 (4) | C33—H33 | 0.9500 |

| | | | |
|---|---|---|---|
| C9—H9 | 0.9500 | C34—C35 | 1.367 (5) |
| N1—N2 | 1.400 (3) | C34—H34 | 0.9500 |
| N2—C11 | 1.303 (3) | C35—C36 | 1.365 (4) |
| C11—N3 | 1.369 (3) | C35—H35 | 0.9500 |
| C11—S1 | 1.755 (2) | C36—C37 | 1.387 (4) |
| N3—C12 | 1.407 (3) | C36—H36 | 0.9500 |
| N3—H3N | 0.8800 | C37—H37 | 0.9500 |
| C12—C17 | 1.383 (4) | S41—O41 | 1.516 (2) |
| C12—C13 | 1.390 (3) | S41—C41 | 1.682 (4) |
| C13—C14 | 1.383 (4) | S41—C42 | 1.709 (9) |
| C13—H13 | 0.9500 | S41′—O41 | 1.518 (3) |
| C14—C15 | 1.371 (4) | S41′—C42′ | 1.578 (13) |
| C14—H14 | 0.9500 | S41′—C41 | 1.666 (4) |
| C15—C16 | 1.373 (4) | C41—H41A | 0.9800 |
| C15—H15 | 0.9500 | C41—H41B | 0.9800 |
| C16—C17 | 1.394 (4) | C41—H41C | 0.9800 |
| C16—H16 | 0.9500 | C41—H41D | 0.9800 |
| C17—H17 | 0.9500 | C41—H41E | 0.9800 |
| C21—N21 | 1.303 (3) | C41—H41F | 0.9800 |
| C21—C30 | 1.471 (3) | C42—H42A | 0.9800 |
| C21—C22 | 1.499 (4) | C42—H42B | 0.9800 |
| C22—C23 | 1.519 (4) | C42—H42C | 0.9800 |
| C22—H22A | 0.9900 | C42′—H42D | 0.9800 |
| C22—H22B | 0.9900 | C42′—H42E | 0.9800 |
| C23—C24 | 1.513 (5) | C42′—H42F | 0.9800 |

| | | | |
|---|---|---|---|
| N1—Zn1—N21 | 110.30 (8) | H24A—C24—H24B | 108.2 |
| N1—Zn1—S21 | 132.43 (6) | C26—C25—C30 | 118.3 (3) |
| N21—Zn1—S21 | 87.53 (5) | C26—C25—C24 | 122.0 (3) |
| N1—Zn1—S1 | 88.25 (6) | C30—C25—C24 | 119.6 (3) |
| N21—Zn1—S1 | 129.85 (6) | C27—C26—C25 | 121.3 (3) |
| S21—Zn1—S1 | 114.13 (3) | C27—C26—H26 | 119.4 |
| N1—C1—C10 | 120.3 (2) | C25—C26—H26 | 119.4 |
| N1—C1—C2 | 120.9 (2) | C28—C27—C26 | 120.4 (3) |
| C10—C1—C2 | 118.7 (2) | C28—C27—H27 | 119.8 |
| C1—C2—C3 | 113.8 (2) | C26—C27—H27 | 119.8 |
| C1—C2—H2A | 108.8 | C27—C28—C29 | 119.4 (3) |
| C3—C2—H2A | 108.8 | C27—C28—H28 | 120.3 |
| C1—C2—H2B | 108.8 | C29—C28—H28 | 120.3 |
| C3—C2—H2B | 108.8 | C28—C29—C30 | 121.2 (3) |
| H2A—C2—H2B | 107.7 | C28—C29—H29 | 119.4 |
| C4—C3—C2 | 110.2 (2) | C30—C29—H29 | 119.4 |
| C4—C3—H3A | 109.6 | C29—C30—C25 | 119.0 (2) |
| C2—C3—H3A | 109.6 | C29—C30—C21 | 121.9 (2) |
| C4—C3—H3B | 109.6 | C25—C30—C21 | 119.1 (2) |
| C2—C3—H3B | 109.6 | C21—N21—N22 | 112.67 (19) |
| H3A—C3—H3B | 108.1 | C21—N21—Zn1 | 130.06 (16) |
| C5—C4—C3 | 108.8 (3) | N22—N21—Zn1 | 115.18 (14) |

| | | | |
|---|---|---|---|
| C5—C4—H4A | 109.9 | C31—N22—N21 | 116.34 (19) |
| C3—C4—H4A | 109.9 | N22—C31—N23 | 118.1 (2) |
| C5—C4—H4B | 109.9 | N22—C31—S21 | 128.12 (18) |
| C3—C4—H4B | 109.9 | N23—C31—S21 | 113.76 (18) |
| H4A—C4—H4B | 108.3 | C31—S21—Zn1 | 92.77 (8) |
| C6—C5—C10 | 118.9 (3) | C31—N23—C32 | 129.9 (2) |
| C6—C5—C4 | 121.8 (3) | C31—N23—H23N | 115.1 |
| C10—C5—C4 | 119.2 (3) | C32—N23—H23N | 115.1 |
| C7—C6—C5 | 121.1 (3) | C37—C32—C33 | 118.8 (2) |
| C7—C6—H6 | 119.4 | C37—C32—N23 | 125.4 (2) |
| C5—C6—H6 | 119.4 | C33—C32—N23 | 115.7 (3) |
| C6—C7—C8 | 120.3 (3) | C32—C33—C34 | 119.5 (3) |
| C6—C7—H7 | 119.9 | C32—C33—H33 | 120.3 |
| C8—C7—H7 | 119.9 | C34—C33—H33 | 120.3 |
| C7—C8—C9 | 119.5 (3) | C35—C34—C33 | 121.5 (3) |
| C7—C8—H8 | 120.3 | C35—C34—H34 | 119.2 |
| C9—C8—H8 | 120.3 | C33—C34—H34 | 119.2 |
| C8—C9—C10 | 120.6 (3) | C36—C35—C34 | 118.6 (3) |
| C8—C9—H9 | 119.7 | C36—C35—H35 | 120.7 |
| C10—C9—H9 | 119.7 | C34—C35—H35 | 120.7 |
| C9—C10—C5 | 119.5 (3) | C35—C36—C37 | 121.2 (3) |
| C9—C10—C1 | 121.9 (3) | C35—C36—H36 | 119.4 |
| C5—C10—C1 | 118.6 (3) | C37—C36—H36 | 119.4 |
| C1—N1—N2 | 113.40 (19) | C32—C37—C36 | 120.3 (3) |
| C1—N1—Zn1 | 130.03 (16) | C32—C37—H37 | 119.9 |
| N2—N1—Zn1 | 114.81 (14) | C36—C37—H37 | 119.9 |
| C11—N2—N1 | 116.18 (19) | O41—S41—C41 | 109.37 (19) |
| N2—C11—N3 | 118.5 (2) | O41—S41—C42 | 106.6 (4) |
| N2—C11—S1 | 128.70 (18) | C41—S41—C42 | 104.8 (4) |
| N3—C11—S1 | 112.77 (18) | O41—S41′—C42′ | 111.2 (6) |
| C11—S1—Zn1 | 92.06 (8) | O41—S41′—C41 | 110.1 (2) |
| C11—N3—C12 | 130.5 (2) | C42′—S41′—C41 | 102.6 (7) |
| C11—N3—H3N | 114.8 | S41—O41—S41′ | 56.91 (12) |
| C12—N3—H3N | 114.8 | S41′—C41—S41 | 51.17 (14) |
| C17—C12—C13 | 118.9 (2) | S41′—C41—H41A | 123.9 |
| C17—C12—N3 | 125.1 (2) | S41—C41—H41A | 109.5 |
| C13—C12—N3 | 115.9 (2) | S41′—C41—H41B | 126.5 |
| C14—C13—C12 | 120.5 (3) | S41—C41—H41B | 109.5 |
| C14—C13—H13 | 119.7 | H41A—C41—H41B | 109.5 |
| C12—C13—H13 | 119.7 | S41′—C41—H41C | 58.3 |
| C15—C14—C13 | 120.8 (3) | S41—C41—H41C | 109.5 |
| C15—C14—H14 | 119.6 | H41A—C41—H41C | 109.5 |
| C13—C14—H14 | 119.6 | H41B—C41—H41C | 109.5 |
| C14—C15—C16 | 118.9 (3) | S41′—C41—H41D | 109.5 |
| C14—C15—H15 | 120.6 | S41—C41—H41D | 115.9 |
| C16—C15—H15 | 120.6 | H41B—C41—H41D | 122.4 |
| C15—C16—C17 | 121.4 (3) | H41C—C41—H41D | 87.2 |
| C15—C16—H16 | 119.3 | S41′—C41—H41E | 109.5 |

| | | | |
|---|---|---|---|
| C17—C16—H16 | 119.3 | S41—C41—H41E | 59.4 |
| C12—C17—C16 | 119.5 (3) | H41A—C41—H41E | 87.5 |
| C12—C17—H17 | 120.2 | H41B—C41—H41E | 66.3 |
| C16—C17—H17 | 120.2 | H41C—C41—H41E | 162.6 |
| N21—C21—C30 | 119.9 (2) | H41D—C41—H41E | 109.5 |
| N21—C21—C22 | 120.9 (2) | S41′—C41—H41F | 109.5 |
| C30—C21—C22 | 119.1 (2) | S41—C41—H41F | 134.4 |
| C21—C22—C23 | 113.1 (2) | H41A—C41—H41F | 114.2 |
| C21—C22—H22A | 109.0 | H41C—C41—H41F | 67.7 |
| C23—C22—H22A | 109.0 | H41D—C41—H41F | 109.5 |
| C21—C22—H22B | 109.0 | H41E—C41—H41F | 109.5 |
| C23—C22—H22B | 109.0 | S41—C42—H42A | 109.5 |
| H22A—C22—H22B | 107.8 | S41—C42—H42B | 109.5 |
| C24—C23—C22 | 110.6 (3) | H42A—C42—H42B | 109.5 |
| C24—C23—H23A | 109.5 | S41—C42—H42C | 109.5 |
| C22—C23—H23A | 109.5 | H42A—C42—H42C | 109.5 |
| C24—C23—H23B | 109.5 | H42B—C42—H42C | 109.5 |
| C22—C23—H23B | 109.5 | S41′—C42′—H42D | 109.5 |
| H23A—C23—H23B | 108.1 | S41′—C42′—H42E | 109.5 |
| C25—C24—C23 | 109.9 (3) | H42D—C42′—H42E | 109.5 |
| C25—C24—H24A | 109.7 | S41′—C42′—H42F | 109.5 |
| C23—C24—H24A | 109.7 | H42D—C42′—H42F | 109.5 |
| C25—C24—H24B | 109.7 | H42E—C42′—H42F | 109.5 |
| C23—C24—H24B | 109.7 | | |

| | | | |
|---|---|---|---|
| N1—C1—C2—C3 | −176.3 (3) | C23—C24—C25—C30 | 33.3 (4) |
| C10—C1—C2—C3 | 1.0 (4) | C30—C25—C26—C27 | −1.2 (5) |
| C1—C2—C3—C4 | 42.4 (4) | C24—C25—C26—C27 | 177.2 (3) |
| C2—C3—C4—C5 | −61.7 (4) | C25—C26—C27—C28 | −3.4 (5) |
| C3—C4—C5—C6 | −138.1 (3) | C26—C27—C28—C29 | 3.0 (5) |
| C3—C4—C5—C10 | 38.9 (4) | C27—C28—C29—C30 | 2.0 (5) |
| C10—C5—C6—C7 | −1.0 (5) | C28—C29—C30—C25 | −6.6 (4) |
| C4—C5—C6—C7 | 176.0 (3) | C28—C29—C30—C21 | 173.8 (3) |
| C5—C6—C7—C8 | −1.6 (6) | C26—C25—C30—C29 | 6.0 (4) |
| C6—C7—C8—C9 | 1.7 (6) | C24—C25—C30—C29 | −172.4 (3) |
| C7—C8—C9—C10 | 0.8 (5) | C26—C25—C30—C21 | −174.3 (3) |
| C8—C9—C10—C5 | −3.4 (4) | C24—C25—C30—C21 | 7.2 (4) |
| C8—C9—C10—C1 | 178.3 (3) | N21—C21—C30—C29 | −26.2 (4) |
| C6—C5—C10—C9 | 3.4 (4) | C22—C21—C30—C29 | 158.1 (3) |
| C4—C5—C10—C9 | −173.7 (3) | N21—C21—C30—C25 | 154.2 (3) |
| C6—C5—C10—C1 | −178.2 (3) | C22—C21—C30—C25 | −21.5 (4) |
| C4—C5—C10—C1 | 4.7 (4) | C30—C21—N21—N22 | 176.8 (2) |
| N1—C1—C10—C9 | −30.4 (4) | C22—C21—N21—N22 | −7.6 (3) |
| C2—C1—C10—C9 | 152.3 (3) | C30—C21—N21—Zn1 | −20.7 (4) |
| N1—C1—C10—C5 | 151.3 (3) | C22—C21—N21—Zn1 | 154.9 (2) |
| C2—C1—C10—C5 | −26.0 (4) | N1—Zn1—N21—C21 | −29.8 (2) |
| C10—C1—N1—N2 | 177.2 (2) | S21—Zn1—N21—C21 | −164.6 (2) |
| C2—C1—N1—N2 | −5.6 (3) | S1—Zn1—N21—C21 | 75.6 (2) |

| | | | |
|---|---|---|---|
| C10—C1—N1—Zn1 | −18.9 (4) | N1—Zn1—N21—N22 | 132.36 (16) |
| C2—C1—N1—Zn1 | 158.3 (2) | S21—Zn1—N21—N22 | −2.39 (15) |
| N21—Zn1—N1—C1 | −32.0 (2) | S1—Zn1—N21—N22 | −122.19 (14) |
| S21—Zn1—N1—C1 | 74.0 (2) | C21—N21—N22—C31 | 167.8 (2) |
| S1—Zn1—N1—C1 | −164.2 (2) | Zn1—N21—N22—C31 | 2.5 (3) |
| N21—Zn1—N1—N2 | 131.70 (16) | N21—N22—C31—N23 | 178.2 (2) |
| S21—Zn1—N1—N2 | −122.29 (14) | N21—N22—C31—S21 | −1.0 (3) |
| S1—Zn1—N1—N2 | −0.55 (15) | N22—C31—S21—Zn1 | −0.7 (2) |
| C1—N1—N2—C11 | 166.6 (2) | N23—C31—S21—Zn1 | −179.98 (18) |
| Zn1—N1—N2—C11 | 0.1 (3) | N1—Zn1—S21—C31 | −114.08 (11) |
| N1—N2—C11—N3 | −179.0 (2) | N21—Zn1—S21—C31 | 1.45 (10) |
| N1—N2—C11—S1 | 0.7 (3) | S1—Zn1—S21—C31 | 134.57 (8) |
| N2—C11—S1—Zn1 | −0.9 (2) | N22—C31—N23—C32 | −8.0 (4) |
| N3—C11—S1—Zn1 | 178.75 (17) | S21—C31—N23—C32 | 171.3 (2) |
| N1—Zn1—S1—C11 | 0.64 (10) | C31—N23—C32—C37 | −0.9 (5) |
| N21—Zn1—S1—C11 | −114.62 (11) | C31—N23—C32—C33 | 180.0 (3) |
| S21—Zn1—S1—C11 | 137.18 (8) | C37—C32—C33—C34 | −0.5 (5) |
| N2—C11—N3—C12 | −9.2 (4) | N23—C32—C33—C34 | 178.7 (3) |
| S1—C11—N3—C12 | 171.1 (2) | C32—C33—C34—C35 | −0.1 (6) |
| C11—N3—C12—C17 | −6.5 (4) | C33—C34—C35—C36 | 0.2 (6) |
| C11—N3—C12—C13 | 175.6 (3) | C34—C35—C36—C37 | 0.3 (5) |
| C17—C12—C13—C14 | −0.4 (4) | C33—C32—C37—C36 | 1.0 (4) |
| N3—C12—C13—C14 | 177.7 (3) | N23—C32—C37—C36 | −178.1 (3) |
| C12—C13—C14—C15 | −0.8 (5) | C35—C36—C37—C32 | −1.0 (5) |
| C13—C14—C15—C16 | 1.0 (5) | O41—S41—O41—S41′ | 0 (47) |
| C14—C15—C16—C17 | −0.1 (5) | C41—S41—O41—S41′ | −43.9 (2) |
| C13—C12—C17—C16 | 1.3 (4) | C42—S41—O41—S41′ | 68.9 (4) |
| N3—C12—C17—C16 | −176.6 (3) | O41—S41′—O41—S41 | 0 (58) |
| C15—C16—C17—C12 | −1.0 (5) | C42′—S41′—O41—S41 | −68.3 (6) |
| N21—C21—C22—C23 | 177.7 (3) | C41—S41′—O41—S41 | 44.7 (2) |
| C30—C21—C22—C23 | −6.7 (4) | O41—S41′—C41—S41 | −42.94 (17) |
| C21—C22—C23—C24 | 46.8 (4) | C42′—S41′—C41—S41 | 75.5 (6) |
| C22—C23—C24—C25 | −60.0 (4) | O41—S41—C41—S41′ | 42.81 (18) |
| C23—C24—C25—C26 | −145.1 (3) | C42—S41—C41—S41′ | −71.1 (5) |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N3—H3*N*···O41 | 0.88 | 2.08 | 2.945 (3) | 168 |
| N23—H23*N*···O41$^{i}$ | 0.88 | 2.03 | 2.903 (3) | 173 |

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