## metal-organic compounds

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### [1-(4-Hydroxy-2-oxidobenzylidene)-4phenylthiosemicarbazonato- $\kappa^3 N, O, S$ ]-(1,10-phenanthroline- $\kappa^2 N, N'$ )zinc(II)– 4,4'-bipyridine (2/1)

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Key indicators: single-crystal X-ray study; T = 140 K; mean  $\sigma$ (C–C) = 0.007 Å; R factor = 0.047; wR factor = 0.117; data-to-parameter ratio = 12.4.

The  $Zn^{II}$  atom in the title compound,  $[Zn(C_{14}H_{11}N_3O_2S)-(C_{12}H_8N_2)]\cdot 0.5C_{10}H_8N_2$ , is *N*,*N*'-chelated by the *N*-heterocycle and *N*,*O*,*S*-chelated by the deprotonated Schiff base in a square-pyramidal environment. The hydroxy group of the Schiff base is a hydrogen-bond donor to 4,4'-bipyridine, which is located about a center of inversion, resulting in the formation of a supramolecular trimeric unit.

#### **Related literature**

For [1-(4-hydroxy-2-oxidobenzylidene)-4-phenylthiosemicarbazonato](1,10-phenanthroline)zinc dimethyl sulfoxide disolvate hydrate, see: Tan *et al.* (2009). For other *N*-heterocyclic adducts of zinc 1-(2-oxidobenzylidene)-4-phenylthiosemicarbonates, see: Deng *et al.* (2007); Seena & Kurup (2008).

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#### **Experimental**

#### Crystal data

$$\begin{split} & [\text{Zn}(\text{C}_{14}\text{H}_{11}\text{N}_3\text{O}_2\text{S})(\text{C}_{12}\text{H}_8\text{N}_2)] \cdots \qquad \beta = 92.417 ~ (3)^\circ \\ & 0.5\text{C}_{10}\text{H}_8\text{N}_2 \qquad \qquad V = 2663.7 ~ (2) ~ \text{\AA}^3 \\ & M_r = 608.98 \qquad \qquad Z = 4 \\ & \text{Monoclinic, $P2_1/c$} \qquad & \text{Mo $K$$\alpha$ radiation} \\ & a = 11.6372 ~ (6) ~ \text{\AA} \qquad \qquad \mu = 1.04 ~ \text{mm}^{-1} \\ & b = 9.8376 ~ (5) ~ \text{\AA} \qquad \qquad T = 140 ~ \text{K} \\ & c = 23.288 ~ (1) ~ \text{\AA} \qquad \qquad 0.10 \times 0.04 \times 0.02 ~ \text{mm} \end{split}$$

#### Data collection

Bruker SMART APEX diffractometer Absorption correction: multi-scan (SADABS; Sheldrick, 1996)  $T_{min} = 0.903, T_{max} = 0.979$ 

#### Refinement

| $R[F^2 > 2\sigma(F^2)] = 0.047$ | H atoms treated by a mixture of                            |
|---------------------------------|------------------------------------------------------------|
| $wR(F^2) = 0.117$               | independent and constrained                                |
| S = 0.98                        | refinement                                                 |
| 4681 reflections                | $\Delta \rho_{\rm max} = 0.38 \ {\rm e} \ {\rm \AA}^{-3}$  |
| 378 parameters                  | $\Delta \rho_{\rm min} = -0.40 \text{ e } \text{\AA}^{-3}$ |
| 2 restraints                    |                                                            |

14867 measured reflections

 $R_{\rm int} = 0.089$ 

4681 independent reflections

2918 reflections with  $I > 2\sigma(I)$ 

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

| $D - H \cdots A$ | D-H      | $H \cdot \cdot \cdot A$ | $D \cdots A$ | $D - \mathbf{H} \cdot \cdot \cdot A$ |
|------------------|----------|-------------------------|--------------|--------------------------------------|
| O2−H2···N6       | 0.84 (5) | 2.01 (5)                | 2.839 (6)    | 168 (6)                              |

Data collection: *APEX2* (Bruker, 2008); cell refinement: *SAINT* (Bruker, 2008); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2009).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: TK2484).

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supplementary materials

Acta Cryst. (2009). E65, m920 [doi:10.1107/S1600536809026245]

[1-(4-Hydroxy-2-oxidobenzylidene)-4-phenylthiosemicarbazonato- $\kappa^3 N, O, S$ ](1,10-phenanthroline- $\kappa^2 N, N'$ )zinc(II)-4,4'-bipyridine (2/1)

K. W. Tan, C. H. Ng, M. J. Maah and S. W. Ng

#### Experimental

Zinc acetate monohydrate (0.22 g, 1 mmol), 2,4-dihydroxybenzaldehyde 4-phenylthiosemicarbazone (0.29 g, 1 mmol) and 1,10-phenanthroline (0.18 g, 1 mmol) were heated in ethanol (50 ml). The product was isolated and reacted with 4,4'-bipyridine (0.15 g, 1 mmol) in DMF to give a yellow solution. A small amount of tiny crystals were isolated when the mixture was set aside for a week.

#### Refinement

Carbon-bound H-atoms were placed in calculated positions (C—H 0.95 Å) and were included in the refinement in the riding model approximation with U(H) set to  $1.2U_{eq}(C)$ . The amino- and hydroxy H-atoms were refined with distance restraints of O–H 0.84±0.01 Å and N–H 0.88±0.01 Å, respectively; their temperature factors were refined.

Figures



Fig. 1. Thermal ellipsoid (Barbour, 2001) plot of  $Zn(C_{12}H_8N_2)(C_{14}H_{11}N_3O_2S)$ . 0.5 $C_{10}H_8N_2$  at the 70% probability level. Only atoms comprising the asymmetric unit are labelled; the 4,4'-bipyridine molecule is located about a center of inversion. Hydrogen atoms are drawn as spheres of arbitrary radii.

# [1-(4-Hydroxy-2-oxidobenzylidene)-4-phenylthiosemicarbazonato- $\kappa^3 N$ , *O*, *S*](1,10-phenanthroline- $\kappa^2 N$ , *N*')zinc(II)-4,4'-bipyridine (2/1)

Crystal data

 $[Zn(C_{14}H_{11}N_{3}O_{2}S)(C_{12}H_{8}N_{2})] \cdot 0.5C_{10}H_{8}N_{2}$  $F_{000} = 12$  $M_r = 608.98$  $D_x = 1.51$ Monoclinic,  $P2_1/c$ Mo Ka rateHall symbol: -P 2ybcCell paraa = 11.6372 (6) Å $\theta = 2.4-2$ b = 9.8376 (5) Å $\mu = 1.04$ c = 23.288 (1) ÅT = 140 H $\beta = 92.417$  (3)°Prism, yetV = 2663.7 (2) Å<sup>3</sup> $0.10 \times 0.4$ 

| $F_{000} = 1252$                               |
|------------------------------------------------|
| $D_{\rm x} = 1.519 {\rm ~Mg~m}^{-3}$           |
| Mo K $\alpha$ radiation, $\lambda = 0.71073$ Å |
| Cell parameters from 1335 reflections          |
| $\theta = 2.4 - 20.2^{\circ}$                  |
| $\mu = 1.04 \text{ mm}^{-1}$                   |
| T = 140  K                                     |
| Prism, yellow                                  |
| $0.10\times0.04\times0.02~mm$                  |

#### Data collection

| Bruker SMART APEX<br>diffractometer                            | 4681 independent reflections           |
|----------------------------------------------------------------|----------------------------------------|
| Radiation source: fine-focus sealed tube                       | 2918 reflections with $I > 2\sigma(I)$ |
| Monochromator: graphite                                        | $R_{\rm int} = 0.089$                  |
| T = 140  K                                                     | $\theta_{\text{max}} = 25.0^{\circ}$   |
| ω scans                                                        | $\theta_{\min} = 1.8^{\circ}$          |
| Absorption correction: Multi-scan<br>(SADABS; Sheldrick, 1996) | $h = -13 \rightarrow 13$               |
| $T_{\min} = 0.903, T_{\max} = 0.979$                           | $k = -11 \rightarrow 11$               |
| 14867 measured reflections                                     | $l = -27 \rightarrow 27$               |

#### Refinement

| Refinement on $F^2$                                            | Secondary atom site location: difference Fourier map                      |
|----------------------------------------------------------------|---------------------------------------------------------------------------|
| Least-squares matrix: full                                     | Hydrogen site location: inferred from neighbouring sites                  |
| $R[F^2 > 2\sigma(F^2)] = 0.047$                                | H atoms treated by a mixture of independent and constrained refinement    |
| $wR(F^2) = 0.117$                                              | $w = 1/[\sigma^2(F_o^2) + (0.0515P)^2]$<br>where $P = (F_o^2 + 2F_c^2)/3$ |
| <i>S</i> = 0.98                                                | $(\Delta/\sigma)_{\text{max}} = 0.001$                                    |
| 4681 reflections                                               | $\Delta \rho_{max} = 0.38 \text{ e} \text{ Å}^{-3}$                       |
| 378 parameters                                                 | $\Delta \rho_{min} = -0.40 \text{ e } \text{\AA}^{-3}$                    |
| 2 restraints                                                   | Extinction correction: none                                               |
| Primary atom site location: structure-invariant direct methods |                                                                           |

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters  $(Å^2)$ 

|     | x            | у            | Ζ            | $U_{\rm iso}*/U_{\rm eq}$ |
|-----|--------------|--------------|--------------|---------------------------|
| Zn1 | 0.67107 (4)  | 0.62440 (5)  | 0.56348 (2)  | 0.02152 (16)              |
| S1  | 0.82614 (10) | 0.50702 (12) | 0.52318 (5)  | 0.0236 (3)                |
| 01  | 0.5106 (2)   | 0.6211 (3)   | 0.58865 (12) | 0.0257 (7)                |
| 02  | 0.2250 (3)   | 0.7085 (4)   | 0.72356 (16) | 0.0416 (9)                |
| H2  | 0.188 (5)    | 0.738 (6)    | 0.6945 (16)  | 0.07 (2)*                 |
| N1  | 0.7189 (3)   | 0.5107 (4)   | 0.63475 (15) | 0.0216 (9)                |
| N2  | 0.8294 (3)   | 0.4544 (4)   | 0.63924 (15) | 0.0256 (9)                |
| N3  | 0.9923 (3)   | 0.4067 (4)   | 0.59142 (16) | 0.0263 (10)               |
| Н3  | 1.029 (3)    | 0.427 (5)    | 0.5604 (12)  | 0.036 (15)*               |
| N4  | 0.6154 (3)   | 0.7367 (4)   | 0.48877 (15) | 0.0218 (9)                |
| N5  | 0.7320 (3)   | 0.8198 (4)   | 0.58516 (15) | 0.0222 (9)                |
| N6  | 0.1202 (3)   | 0.8459 (4)   | 0.62781 (18) | 0.0371 (11)               |
| C1  | 0.4781 (4)   | 0.6105 (5)   | 0.64195 (18) | 0.0242 (10)               |
| C2  | 0.3686 (4)   | 0.6607 (5)   | 0.6553 (2)   | 0.0272 (12)               |
| H2A | 0.3205       | 0.6984       | 0.6254       | 0.033*                    |

| C3         0.3294 (4)         0.6565 (5)         0.7103 (2)         0.0327 (13)           C4         0.3969 (4)         0.5966 (5)         0.7542 (2)         0.0380 (14)           B4         0.303         0.5929         0.7922         0.046*           C5         0.5007 (4)         0.5436 (6)         0.7423 (2)         0.0364 (13)           B5A         0.5445 (4)         0.5492 (5)         0.68749 (19)         0.0259 (11)           C7         0.6604 (4)         0.4965 (5)         0.6806 (19)         0.0259 (11)           C7         0.6604 (1)         0.4594 (3)         0.5907 (19)         0.0217 (11)           C9         1.0617 (4)         0.3594 (5)         0.6887 (19)         0.0217 (11)           C9         1.0617 (4)         0.3299 (5)         0.7278 (2)         0.0353 (13)           H10         0.9378         0.2239 (5)         0.7278 (2)         0.0353 (13)           H11         1.0642         0.1921         0.7573         0.044*           C12         1.2121 (4)         0.2249 (5)         0.6781 (2)         0.0376 (14)           H13         1.3346         0.3377         0.757         0.045*           C14         1.812 (4)         0.3749 (5)         0.63541 (19)                                                                             |     |            |            |              |             |
|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-----|------------|------------|--------------|-------------|
| C4         0.3969 (4)         0.5966 (5)         0.7542 (2)         0.0380 (14)           H4         0.3703         0.5929         0.7922         0.046*           C5         0.5007 (4)         0.5345 (6)         0.7423 (2)         0.0364 (13)           H5A         0.5445         0.5004         0.7724         0.044*           C6         0.5469 (4)         0.5492 (5)         0.68749 (19)         0.0251 (11)           C7         0.6604 (4)         0.4965 (5)         0.6889 (19)         0.0217 (11)           C9         1.0617 (4)         0.3594 (5)         0.6888 (19)         0.0237 (11)           C10         1.0185 (4)         0.2294 (5)         0.728 (19)         0.0321 (12)           H10         0.9378         0.2231         0.6887 (19)         0.0321 (12)           H11         1.0642         0.1291         0.7594         0.042*           C12         1.2121 (4)         0.3249 (5)         0.7242 (2)         0.0356 (13)           H12         1.2633         0.2211         0.7573         0.445*           C14         1.812 (4)         0.3749         0.63541 (19)         0.032*           C14         1.812 (4)         0.3749         0.63541 (19)         0.032*     <                                                                                     | C3  | 0.3294 (4) | 0.6565 (5) | 0.7103 (2)   | 0.0327 (13) |
| H40.37030.59290.79220.046*C50.5007 (4)0.5436 (6)0.7423 (2)0.0364 (13)H5A0.5469 (4)0.5492 (5)0.68749 (19)0.0251 (11)C60.6604 (4)0.4965 (5)0.68069 (19)0.0259 (11)H70.6064 (4)0.44770.71200.031*C80.8810 (4)0.4554 (4)0.59072 (19)0.0217 (11)C91.0617 (4)0.3594 (5)0.68859 (19)0.0237 (11)C101.0185 (4)0.2924 (5)0.68857 (19)0.0231 (12)H100.93780.28230.6887 (10)0.034*C111.0937 (4)0.2399 (5)0.7278 (2)0.0353 (13)H111.06420.19210.75940.042*C121.2121 (4)0.2566 (5)0.7242 (2)0.0376 (14)H131.33460.33770.67570.045*C141.1812 (4)0.3749 (5)0.6341 (19)0.0235 (11)H141.2160.42020.60340.033*C150.5563 (4)0.6950 (5)0.44181 (19)0.235 (11)H150.5157 (4)0.7832 (6)0.3990 (2)0.036 (14)H160.47270.74990.36640.044*C170.5390 (4)0.914 (6)0.4048 (2)0.0331 (13)H170.51250.98130.37590.404*C160.5157 (4)0.9459 (5)0.4336 (19)0.0281 (12)C190.6260 (4)1.1078 (5)0.4628 (2)0.0367 (13)<                                                                                                                                                                                                                                                                                                                                                                                                                               | C4  | 0.3969 (4) | 0.5966 (5) | 0.7542 (2)   | 0.0380 (14) |
| CS         0.5007 (4)         0.5436 (6)         0.742 (2)         0.0364 (13)           HSA         0.5445         0.5004         0.7724         0.044*           C6         0.5669 (4)         0.5492 (5)         0.6879 (19)         0.0259 (11)           C7         0.6604 (4)         0.4955 (3)         0.68069 (19)         0.0217 (11)           C8         0.8810 (4)         0.4554 (4)         0.59072 (19)         0.0217 (11)           C9         1.0617 (4)         0.3594 (5)         0.68859 (19)         0.0237 (11)           C10         1.0185 (4)         0.2392 (5)         0.7272 (2)         0.0353 (13)           H11         1.0642         0.1921         0.7594         0.042*           C12         1.2121 (4)         0.2260 (5)         0.7242 (2)         0.0356 (13)           H11         1.0642         0.1921         0.7594         0.042*           C13         1.2540 (4)         0.3249 (5)         0.6781 (2)         0.0354 (13)           H13         1.3346         0.3377         0.6757         0.045*           C14         1.1812 (4)         0.3749 (5)         0.63541 (19)         0.0276 (11)           H14         1.216         0.4202         0.6364         0.039*<                                                                                | H4  | 0.3703     | 0.5929     | 0.7922       | 0.046*      |
| HSA0.54450.50040.77240.044*C60.5469 (4)0.5492 (5)0.68749 (19)0.0259 (11)C70.6604 (4)0.4965 (5)0.68069 (19)0.0259 (11)H70.69540.44770.71200.031*C80.8810 (4)0.4554 (4)0.59072 (19)0.0217 (11)C91.0617 (4)0.2924 (5)0.6855 (19)0.0281 (12)H100.93780.28230.68870.034*C111.0937 (4)0.2999 (5)0.7278 (2)0.0353 (13)H111.06420.19210.75340.042*C121.2121 (4)0.2560 (5)0.724 (2)0.0356 (13)H121.26330.22110.75330.044*C131.2540 (4)0.3249 (5)0.6781 (2)0.0376 (14)H131.33460.33770.65541 (19)0.0276 (11)H141.21160.42020.60340.03*C150.5563 (4)0.6950 (5)0.44181 (19)0.276 (11)H150.54120.60060.43740.036* (14)H160.47270.74990.36640.044*C170.5390 (4)0.9144 (6)0.448 (2)0.031 (13)H170.51250.98130.37590.464*C180.6018 (4)0.9676 (5)0.45326 (19)0.0281 (12)C190.6260 (4)1.1078 (5)0.4562 (2)0.0367 (13)H190.59701.17310.45920.3361 (19)0.241C200.6895 (4) <td>C5</td> <td>0.5007 (4)</td> <td>0.5436 (6)</td> <td>0.7423 (2)</td> <td>0.0364 (13)</td>                                                                                                                                                                                                                                                                                                                                                           | C5  | 0.5007 (4) | 0.5436 (6) | 0.7423 (2)   | 0.0364 (13) |
| C6         0.5469 (4)         0.5492 (5)         0.68749 (19)         0.0251 (11)           C7         0.6604 (4)         0.4965 (5)         0.68069 (19)         0.0257 (11)           H7         0.6554         0.4477         0.7120         0.014"           C8         0.8810 (4)         0.4554 (4)         0.59072 (19)         0.0217 (11)           C9         1.0617 (4)         0.2394 (5)         0.68556 (19)         0.0237 (11)           C10         1.0185 (4)         0.2399 (5)         0.7278 (2)         0.0353 (13)           H11         1.0642         0.1921         0.7594         0.042*           C12         1.2121 (4)         0.3249 (5)         0.6781 (2)         0.0356 (13)           H12         1.2633         0.2211         0.7533         0.444*           C13         1.2540 (4)         0.3249 (5)         0.6781 (2)         0.0356 (14)           H13         1.3346         0.3377         0.6574         0.034*           C14         1.812 (4)         0.3749 (5)         0.6341 (19)         0.0253 (11)           H14         1.2116         0.4505 (5)         0.44181 (19)         0.253 (11)           H15         0.5513 (4)         0.6950 (5)         0.4418 (2)         <                                                                            | H5A | 0.5445     | 0.5004     | 0.7724       | 0.044*      |
| C7 $0.6604$ (4) $0.4965$ (5) $0.68069$ (19) $0.0259$ (11)H7 $0.0594$ $0.4477$ $0.7120$ $0.031*$ C8 $0.8810$ (4) $0.4554$ (4) $0.59072$ (19) $0.0217$ (11)C9 $1.0617$ (4) $0.3594$ (5) $0.63889$ (19) $0.02237$ (11)C10 $1.0185$ (4) $0.2294$ (5) $0.68556$ (19) $0.0281$ (12)H10 $0.9378$ $0.2239$ (5) $0.7278$ (2) $0.0334^*$ C11 $1.0937$ (4) $0.2399$ (5) $0.7278$ (2) $0.0353$ (13)H11 $1.0642$ $0.1921$ $0.7594$ $0.042^*$ C12 $1.2121$ (4) $0.2566$ (5) $0.7242$ (2) $0.0356$ (13)H12 $1.2633$ $0.2211$ $0.7533$ $0.044^*$ C13 $1.2540$ (4) $0.3249$ (5) $0.63541$ (19) $0.0276$ (11)H13 $1.3346$ $0.3377$ $0.6757$ $0.045^*$ C14 $1.1812$ (4) $0.3749$ (5) $0.63541$ (19) $0.0276$ (11)H14 $1.2116$ $0.4202$ $0.6034$ $0.033^*$ C15 $0.5563$ (4) $0.6950$ (5) $0.44181$ (19) $0.0253$ (11)H15 $0.5412$ $0.6006$ $0.3374$ $0.3374$ C16 $0.5157$ (4) $0.7822$ (6) $0.3990$ (2) $0.0365$ (14)H16 $0.4727$ $0.7499$ $0.364$ $0.0311$ (13)H17 $0.5125$ $0.9813$ $0.3759$ $0.444^*$ C19 $0.6260$ (4) $1.1078$ (5) $0.6325$ (19) $0.0281$ (12)C16 $0.7797$ (1) <t< td=""><td>C6</td><td>0.5469 (4)</td><td>0.5492 (5)</td><td>0.68749 (19)</td><td>0.0261 (11)</td></t<>                                                                                                                                     | C6  | 0.5469 (4) | 0.5492 (5) | 0.68749 (19) | 0.0261 (11) |
| H70.69540.44770.71200.031*C80.8810 (4)0.4554 (4)0.59072 (19)0.0217 (11)C91.0617 (4)0.3594 (5)0.63889 (19)0.0221 (12)C101.0185 (4)0.2924 (5)0.68855 (19)0.0281 (12)H100.93780.28230.68870.034*C111.0937 (4)0.2399 (5)0.7278 (2)0.0353 (13)H111.06420.19210.75940.042*C121.212 (4)0.2566 (5)0.7242 (2)0.0357 (14)H131.2540 (4)0.2249 (5)0.6781 (2)0.0376 (14)H131.33460.33770.67570.045*C141.1812 (4)0.3749 (5)0.63541 (19)0.0276 (11)H141.21160.42020.60340.033*C150.5563 (4)0.6950 (5)0.44181 (19)0.0253 (11)H150.5120.69060.43740.030*C160.5157 (4)0.7832 (6)0.3990 (2)0.0365 (14)H160.47270.74990.36640.044*C170.5390 (4)0.9194 (6)0.4048 (2)0.0331 (13)H170.51250.98130.37590.044*C180.6018 (4)0.9676 (5)0.45336 (19)0.0281 (12)C190.6260 (4)1.1078 (5)0.5625 (2)0.0367 (13)H190.59701.17310.43590.044*C200.6885 (4)1.493 (5)0.5162 (0)0.0318 (13)H220.7194 <td>C7</td> <td>0.6604 (4)</td> <td>0.4965 (5)</td> <td>0.68069 (19)</td> <td>0.0259 (11)</td>                                                                                                                                                                                                                                                                                                                                                | C7  | 0.6604 (4) | 0.4965 (5) | 0.68069 (19) | 0.0259 (11) |
| C8         0.8810 (4)         0.4554 (4)         0.59072 (19)         0.0217 (11)           C9         1.0617 (4)         0.3594 (5)         0.63889 (19)         0.0237 (11)           C10         1.0185 (4)         0.2924 (5)         0.68857 (19)         0.034*           C11         1.0937 (4)         0.2399 (5)         0.7278 (2)         0.0353 (13)           H11         1.0642         0.1921         0.7594         0.042*           C12         1.2121 (4)         0.2566 (5)         0.7242 (2)         0.0356 (13)           H12         1.2633         0.2211         0.7533         0.044*           C13         1.2540 (4)         0.3249 (5)         0.6781 (2)         0.0376 (14)           H13         1.3346         0.3377         0.6757         0.045*           C14         1.1812 (4)         0.3749 (5)         0.6034         0.033*           C15         0.5563 (4)         0.6950 (5)         0.44181 (19)         0.0255 (11)           H14         1.2116         0.4202         0.6034         0.036*           C15         0.5563 (4)         0.7932 (6)         0.3990 (2)         0.036* (14)           H14         1.2116         0.4202         0.3939 (2)         0.6364 (14) </td <td>H7</td> <td>0.6954</td> <td>0.4477</td> <td>0.7120</td> <td>0.031*</td> | H7  | 0.6954     | 0.4477     | 0.7120       | 0.031*      |
| C9         1.0617 (4)         0.3594 (5)         0.63889 (19)         0.0237 (11)           C10         1.0185 (4)         0.2924 (5)         0.68556 (19)         0.0281 (12)           H10         0.9378         0.2823         0.6887         0.0334 (12)           H11         1.0937 (4)         0.2399 (5)         0.7278 (2)         0.0353 (13)           H11         1.0642         0.1921         0.7594         0.042*           C12         1.2121 (4)         0.2266 (5)         0.7242 (2)         0.0356 (13)           H12         1.2633         0.2211         0.7533         0.044*           C13         1.2540 (4)         0.3349 (5)         0.6757         0.045*           C14         1.1812 (4)         0.3749 (5)         0.63541 (19)         0.0226 (11)           H14         1.2116         0.4202         0.6034         0.033*           C15         0.5563 (4)         0.6950 (5)         0.44181 (19)         0.0253 (11)           H15         0.5412         0.6006         0.4374         0.030*           C16         0.5157 (4)         0.7832 (6)         0.3990 (2)         0.0365 (14)           H17         0.5125         0.813         0.3759         0.444*                                                                                                  | C8  | 0.8810 (4) | 0.4554 (4) | 0.59072 (19) | 0.0217 (11) |
| C10         1.0185 (4)         0.2924 (5)         0.68556 (19)         0.0281 (12)           H10         0.9378         0.2823         0.6887         0.034*           C11         1.0937 (4)         0.2399 (5)         0.7278 (2)         0.0353 (13)           H11         1.0642         0.1921         0.7594         0.042*           C12         1.2121 (4)         0.2566 (5)         0.7242 (2)         0.0356 (13)           H12         1.2633         0.2211         0.7533         0.044*           C13         1.2540 (4)         0.3249 (5)         0.6781 (2)         0.0376 (14)           H13         1.3346         0.3377         0.6757         0.045*           C14         1.812 (4)         0.3749 (5)         0.6341 (19)         0.0276 (11)           H14         1.2116         0.4005         0.44181 (19)         0.0253 (11)           H15         0.5563 (4)         0.6096         0.4374         0.030*           C16         0.5157 (4)         0.7832 (6)         0.3990 (2)         0.0356 (14)           H16         0.4727         0.7499         0.3664         0.044*           C17         0.5390 (4)         0.9194 (6)         0.4048 (2)         0.0351 (12)                                                                                                    | C9  | 1.0617 (4) | 0.3594 (5) | 0.63889 (19) | 0.0237 (11) |
| H100.93780.28230.68870.034*C111.0937 (4)0.2399 (5)0.7278 (2)0.0353 (13)H111.06420.19210.75940.042*C121.2121 (4)0.2566 (5)0.7242 (2)0.0356 (13)H121.26330.22110.75330.044*C131.2540 (4)0.3249 (5)0.6781 (2)0.0376 (14)H131.33460.33770.67570.045*C141.1812 (4)0.3749 (5)0.63541 (19)0.0276 (11)H141.21160.40200.60340.033*C150.5563 (4)0.6950 (5)0.44181 (19)0.0253 (11)H150.54120.60060.43740.030*C160.5157 (4)0.7892 (6)0.3990 (2)0.0361 (4)H160.47270.74990.36640.044*C170.5390 (4)0.9194 (6)0.4048 (2)0.0331 (13)H170.51250.98130.37590.040*C180.6018 (4)0.9676 (5)0.45336 (19)0.0281 (12)C190.6260 (4)1.17310.43590.044*C200.6895 (4)1.1493 (5)0.5093 (2)0.0380 (14)H200.70801.24290.51360.046*C210.7297 (4)1.0533 (5)0.525 (2)0.0307 (12)C220.81211.18300.61040.041*C230.8244 (4)0.9928 (5)0.6427 (2)0.339 (13)H230.86811.01610.6767<                                                                                                                                                                                                                                                                                                                                                                                                                                                                   | C10 | 1.0185 (4) | 0.2924 (5) | 0.68556 (19) | 0.0281 (12) |
| C11         1.0937 (4)         0.2399 (5)         0.7278 (2)         0.0353 (13)           H11         1.0642         0.1921         0.7594         0.042*           C12         1.2121 (4)         0.2566 (5)         0.7242 (2)         0.0365 (13)           H12         1.2633         0.2211         0.7533         0.044*           C13         1.2540 (4)         0.3249 (5)         0.6781 (2)         0.0376 (14)           H13         1.3346         0.3377         0.6757         0.045*           C14         1.812 (4)         0.3749 (5)         0.63541 (19)         0.0276 (11)           H14         1.2116         0.4202         0.6034         0.033*           C15         0.5563 (4)         0.6950 (5)         0.44181 (19)         0.0225 (11)           H15         0.5412         0.6006         0.4374         0.030*           C16         0.5157 (4)         0.7892 (6)         0.3990 (2)         0.0365 (13)           H16         0.4727         0.7499         0.3664         0.044*           C17         0.530 (4)         0.9676 (5)         0.4533 (6)         0.021 (12)           C18         0.6018 (4)         0.9676 (5)         0.4528 (2)         0.0380 (14)                                                                                                   | H10 | 0.9378     | 0.2823     | 0.6887       | 0.034*      |
| H111.06420.19210.75940.042*C121.2121 (4)0.2566 (5)0.7242 (2)0.0365 (13)H121.26330.22110.75330.044*C131.2540 (4)0.3249 (5)0.6781 (2)0.0376 (14)H131.33460.33770.67570.045*C141.1812 (4)0.3749 (5)0.63541 (19)0.0276 (11)H141.21160.42020.60340.033*C150.5563 (4)0.6950 (5)0.44181 (19)0.0253 (11)H150.54120.60060.43740.030*C160.5157 (4)0.7832 (6)0.3990 (2)0.0365 (14)H160.47270.74990.36640.044*C170.5390 (4)0.9194 (6)0.4048 (2)0.0331 (13)H170.51250.98130.37590.040*C180.6018 (4)0.9676 (5)0.45336 (19)0.0281 (12)C190.6260 (4)1.1078 (5)0.4628 (2)0.0367 (13)H190.59701.17310.43590.044*C200.6895 (4)1.1493 (5)0.5093 (2)0.0345 (13)H220.81211.8300.61040.041*C230.8224 (4)0.9928 (5)0.6427 (2)0.0339 (13)H240.81370.79120.65990.035*C250.7022 (4)0.9150 (4)0.54532 (19)0.0221 (10)C240.81370.79120.6990.035*C250.7022 (4)0.9150 (4)0.543                                                                                                                                                                                                                                                                                                                                                                                                                                                              | C11 | 1.0937 (4) | 0.2399 (5) | 0.7278 (2)   | 0.0353 (13) |
| C12         1.2121 (4)         0.2566 (5)         0.7242 (2)         0.0365 (13)           H12         1.2633         0.2211         0.7533         0.044*           C13         1.2540 (4)         0.3249 (5)         0.6781 (2)         0.0376 (14)           H13         1.3346         0.3377         0.6757         0.045*           C14         1.1812 (4)         0.3749 (5)         0.63541 (19)         0.0276 (11)           H14         1.2116         0.4202         0.6034         0.033*           C15         0.5563 (4)         0.6950 (5)         0.44181 (19)         0.0253 (11)           H15         0.5412         0.6006         0.4374         0.030*           C16         0.5157 (4)         0.7832 (6)         0.3990 (2)         0.0365 (14)           H16         0.4727         0.7499         0.3664         0.044*           C17         0.5390 (4)         0.9194 (6)         0.4048 (2)         0.0331 (13)           H17         0.5125         0.9813         0.3759         0.404*           C18         0.6018 (4)         0.9676 (5)         0.45336 (19)         0.2281 (12)           C19         0.5260 (4)         1.1493 (5)         0.5093 (2)         0.0380 (14) <td>H11</td> <td>1.0642</td> <td>0.1921</td> <td>0.7594</td> <td>0.042*</td>                 | H11 | 1.0642     | 0.1921     | 0.7594       | 0.042*      |
| H121.26330.22110.75330.044*C131.2540 (4)0.3249 (5)0.6781 (2)0.0376 (14)H131.33460.33770.67570.045*C141.1812 (4)0.3749 (5)0.63541 (19)0.0276 (11)H141.21160.42020.60340.033*C150.5563 (4)0.6950 (5)0.44181 (19)0.0223 (11)H150.54120.60060.43740.030*C160.5157 (4)0.7832 (6)0.3990 (2)0.0365 (14)H160.47270.74990.36640.044*C170.5390 (4)0.9194 (6)0.0408 (2)0.0331 (13)H170.51250.98130.37590.040*C180.6018 (4)0.9676 (5)0.45336 (19)0.0281 (12)C190.6260 (4)1.1078 (5)0.4628 (2)0.0367 (13)H190.59701.17310.43590.044*C200.6895 (4)1.1493 (5)0.5093 (2)0.0380 (14)H200.70801.24290.51360.046*C210.7297 (4)1.0533 (5)0.5525 (2)0.0337 (13)H220.81211.18300.61040.041*C230.8244 (4)0.9928 (5)0.6427 (2)0.0339 (13)H230.86811.01610.67670.041*C240.7919 (4)0.8584 (5)0.65216 (19)0.0221 (10)C250.7022 (4)0.9150 (4)0.54532 (19)0.0212 (10)C260.6384 (4)0.8                                                                                                                                                                                                                                                                                                                                                                                                                                                     | C12 | 1.2121 (4) | 0.2566 (5) | 0.7242 (2)   | 0.0365 (13) |
| C13         1.2540 (4)         0.3249 (5)         0.6781 (2)         0.0376 (14)           H13         1.3346         0.3377         0.6757         0.045*           C14         1.1812 (4)         0.3749 (5)         0.63341 (19)         0.0276 (11)           H14         1.2116         0.4202         0.6034         0.033*           C15         0.5563 (4)         0.6950 (5)         0.44181 (19)         0.0253 (11)           H15         0.5412         0.6006         0.4374         0.030*           C16         0.5157 (4)         0.7892 (6)         0.3990 (2)         0.0365 (14)           H16         0.4727         0.7499         0.3664         0.044*           C17         0.5390 (4)         0.9194 (6)         0.4048 (2)         0.0331 (13)           H17         0.5125         0.9813         0.3759         0.040*           C19         0.6260 (4)         1.1078 (5)         0.4628 (2)         0.0357 (13)           H19         0.5970         1.1731         0.4359         0.044*           C20         0.6895 (4)         1.1493 (5)         0.5093 (2)         0.0380 (14)           H20         0.7080         1.2429         0.5136         0.4642                                                                                                                 | H12 | 1.2633     | 0.2211     | 0.7533       | 0.044*      |
| H131.33460.33770.67570.045*C141.1812 (4)0.3749 (5)0.63541 (19)0.0276 (11)H141.21160.42020.60340.033*C150.5563 (4)0.6950 (5)0.44181 (19)0.0253 (11)H150.54120.60060.43740.030*C160.5157 (4)0.7832 (6)0.3990 (2)0.0365 (14)H160.47270.74990.36640.044*C170.5390 (4)0.9194 (6)0.4048 (2)0.0331 (13)H170.51250.98130.37590.040*C180.6018 (4)0.9676 (5)0.45336 (19)0.0281 (12)C190.6260 (4)1.1078 (5)0.4628 (2)0.0367 (13)H190.59701.17310.43590.044*C200.6895 (4)1.1493 (5)0.5093 (2)0.0380 (14)H200.70801.24290.51360.046*C210.7297 (4)1.0533 (5)0.5525 (2)0.0307 (12)C220.7924 (4)1.0906 (5)0.6035 (2)0.0339 (13)H230.86811.01610.67670.041*C240.7919 (4)0.8584 (5)0.65126 (19)0.0221 (10)C250.7022 (4)0.9150 (4)0.54532 (19)0.0221 (10)C260.6384 (4)0.8709 (5)0.44330.048*C250.7022 (4)0.9150 (4)0.54532 (19)0.0221 (10)C260.6384 (4)0.8709 (5)0.5679 (2)0.0343 (13)H23 <td>C13</td> <td>1.2540 (4)</td> <td>0.3249 (5)</td> <td>0.6781 (2)</td> <td>0.0376 (14)</td>                                                                                                                                                                                                                                                                                                                                         | C13 | 1.2540 (4) | 0.3249 (5) | 0.6781 (2)   | 0.0376 (14) |
| C141.1812 (4)0.3749 (5)0.63541 (19)0.0276 (11)H141.21160.42020.60340.033*C150.5563 (4)0.6950 (5)0.44181 (19)0.0253 (11)H150.54120.60060.43740.030*C160.5157 (4)0.7832 (6)0.3990 (2)0.0365 (14)H160.47270.74990.36640.044*C170.5390 (4)0.9194 (6)0.4048 (2)0.0331 (13)H170.51250.98130.37590.040*C180.6018 (4)0.9676 (5)0.45336 (19)0.0281 (12)C190.6260 (4)1.1078 (5)0.4628 (2)0.0367 (13)H190.59701.17310.43590.044*C200.6895 (4)1.1493 (5)0.5093 (2)0.0307 (12)C220.7924 (4)1.0906 (5)0.6035 (2)0.0347 (13)H220.81211.18300.61040.041*C230.8244 (4)0.9928 (5)0.6427 (2)0.0339 (13)H230.86811.01610.67670.041*C240.7919 (4)0.8584 (5)0.6427 (12)0.0339 (13)H230.86811.01610.67670.041*C240.7919 (4)0.8584 (5)0.64232 (19)0.0221 (10)C250.7022 (4)0.9150 (4)0.54532 (19)0.0212 (10)C260.6384 (4)0.8709 (5)0.44430.048*C250.7022 (4)0.9150 (4)0.54532 (19)0.0212 (10)C26 <td>H13</td> <td>1.3346</td> <td>0.3377</td> <td>0.6757</td> <td>0.045*</td>                                                                                                                                                                                                                                                                                                                                                         | H13 | 1.3346     | 0.3377     | 0.6757       | 0.045*      |
| H141.21160.42020.60340.033*C150.5563 (4)0.6950 (5)0.44181 (19)0.0253 (11)H150.54120.60060.43740.030*C160.5157 (4)0.7832 (6)0.3990 (2)0.0365 (14)H160.47270.74990.36640.044*C170.5390 (4)0.9194 (6)0.4048 (2)0.0331 (13)H170.51250.98130.37590.040*C180.6018 (4)0.9676 (5)0.45336 (19)0.0281 (12)C190.6260 (4)1.1078 (5)0.4628 (2)0.0367 (13)H190.59701.17310.43590.044*C200.6895 (4)1.1493 (5)0.5093 (2)0.0380 (14)H200.70801.24290.51360.046*C210.7297 (4)1.0533 (5)0.525 (2)0.0307 (12)C220.7924 (4)1.0906 (5)0.6035 (2)0.0345 (13)H220.81211.18300.61040.041*C230.8244 (4)0.9928 (5)0.63216 (19)0.0224 (12)H240.81370.79120.65990.035*C250.7022 (4)0.9150 (4)0.54532 (19)0.0212 (10)C260.6384 (4)0.8709 (5)0.44430.044*C280.0887 (4)1.03190.64430.044*C280.087 (4)1.03190.64430.044*C290.0256 (4)0.9736 (5)0.5379 (2)0.0345 (13)H280.10171.1361<                                                                                                                                                                                                                                                                                                                                                                                                                                                          | C14 | 1.1812 (4) | 0.3749 (5) | 0.63541 (19) | 0.0276 (11) |
| C150.5563 (4)0.6950 (5)0.44181 (19)0.0253 (11)H150.54120.60060.43740.030*C160.5157 (4)0.7832 (6)0.3990 (2)0.0365 (14)H160.47270.74990.36640.044*C170.5390 (4)0.9194 (6)0.4048 (2)0.0331 (13)H170.51250.98130.37590.040*C180.6018 (4)0.9676 (5)0.45336 (19)0.0281 (12)C190.6260 (4)1.1078 (5)0.4628 (2)0.0367 (13)H190.59701.17310.43590.044*C200.6895 (4)1.1493 (5)0.5093 (2)0.0380 (14)H200.70801.24290.51360.046*C210.7297 (4)1.0533 (5)0.5525 (2)0.0307 (12)C220.924 (4)1.0906 (5)0.6035 (2)0.0345 (13)H220.81211.18300.61040.041*C230.8244 (4)0.9928 (5)0.63216 (19)0.0224 (12)H240.81370.79120.65990.035*C250.7022 (4)0.9150 (4)0.54532 (19)0.0212 (10)C260.6384 (4)0.8709 (5)0.44430.048*C280.087 (4)1.03190.64430.041*C290.0256 (4)0.9783 (5)0.5379 (2)0.0345 (13)H280.10171.13610.56240.041*C290.0256 (4)0.8298 (5)0.5377 (19)0.0281 (12)C300.0133 (5) <td>H14</td> <td>1.2116</td> <td>0.4202</td> <td>0.6034</td> <td>0.033*</td>                                                                                                                                                                                                                                                                                                                                                                  | H14 | 1.2116     | 0.4202     | 0.6034       | 0.033*      |
| H150.54120.60060.43740.030*C160.5157 (4)0.7832 (6)0.3990 (2)0.0365 (14)H160.47270.74990.36640.044*C170.5390 (4)0.9194 (6)0.4048 (2)0.0331 (13)H170.51250.98130.37590.040*C180.6018 (4)0.9676 (5)0.45336 (19)0.0281 (12)C190.6260 (4)1.1078 (5)0.4628 (2)0.0367 (13)H190.59701.17310.43590.044*C200.6895 (4)1.1493 (5)0.5093 (2)0.0380 (14)H200.70801.24290.51360.046*C210.7297 (4)1.0533 (5)0.5525 (2)0.0307 (12)C220.81211.18300.61040.041*C230.8244 (4)0.9928 (5)0.6427 (2)0.0339 (13)H230.86811.01610.67670.041*C240.7919 (4)0.8584 (5)0.63216 (19)0.0224 (10)C250.7022 (4)0.9150 (4)0.54532 (19)0.0202 (10)C260.6384 (4)0.8709 (5)0.49423 (18)0.0212 (10)C270.1329 (4)0.9783 (5)0.6168 (2)0.0398 (14)H270.17491.03190.64430.048*C280.0887 (4)1.0418 (5)0.5679 (2)0.0343 (13)H280.10171.13610.56240.041*C290.0256 (4)0.9682 (5)0.5379 (2)0.0343 (13)H280.1017<                                                                                                                                                                                                                                                                                                                                                                                                                                            | C15 | 0.5563 (4) | 0.6950 (5) | 0.44181 (19) | 0.0253 (11) |
| C160.5157 (4)0.7832 (6)0.3990 (2)0.0365 (14)H160.47270.74990.36640.044*C170.5390 (4)0.9194 (6)0.4048 (2)0.0331 (13)H170.51250.98130.37590.040*C180.6018 (4)0.9676 (5)0.45336 (19)0.0281 (12)C190.6260 (4)1.1078 (5)0.4628 (2)0.0367 (13)H190.59701.17310.43590.044*C200.6895 (4)1.1493 (5)0.5093 (2)0.0380 (14)H200.70801.24290.51360.046*C210.7297 (4)1.0533 (5)0.5525 (2)0.0307 (12)C220.7924 (4)1.0906 (5)0.6035 (2)0.0345 (13)H220.81211.18300.61040.041*C230.8244 (4)0.9928 (5)0.6427 (2)0.0339 (13)H230.86811.01610.67670.041*C240.7919 (4)0.8584 (5)0.63216 (19)0.0224 (12)H240.81370.79120.65990.035*C250.7022 (4)0.9150 (4)0.54532 (19)0.0202 (10)C260.6384 (4)0.8709 (5)0.49423 (18)0.0212 (10)C260.6384 (4)0.8709 (5)0.6168 (2)0.0398 (14)H270.1329 (4)0.9783 (5)0.6168 (2)0.0343 (13)H280.10171.13610.56240.041*C290.0256 (4)0.9682 (5)0.5379 (2)0.0347 (13)H3                                                                                                                                                                                                                                                                                                                                                                                                                                   | H15 | 0.5412     | 0.6006     | 0.4374       | 0.030*      |
| H160.47270.74990.36640.044*C170.5390 (4)0.9194 (6)0.4048 (2)0.0331 (13)H170.51250.98130.37590.040*C180.6018 (4)0.9676 (5)0.45336 (19)0.0281 (12)C190.6260 (4)1.1078 (5)0.4628 (2)0.0367 (13)H190.59701.17310.43590.044*C200.6895 (4)1.1493 (5)0.5093 (2)0.0380 (14)H200.70801.24290.51360.046*C210.7297 (4)1.0533 (5)0.5525 (2)0.0307 (12)C220.7924 (4)1.0906 (5)0.6035 (2)0.0345 (13)H220.81211.18300.61040.041*C230.8244 (4)0.9928 (5)0.6427 (2)0.0339 (13)H230.86811.01610.67670.041*C240.7919 (4)0.8584 (5)0.63216 (19)0.0224 (12)H240.81370.79120.65990.035*C250.7022 (4)0.9150 (4)0.54532 (19)0.0202 (10)C260.6384 (4)0.8709 (5)0.49423 (18)0.0212 (10)C270.1329 (4)0.9783 (5)0.6168 (2)0.0398 (14)L270.17491.03190.64430.048*C280.0887 (4)1.0418 (5)0.5679 (2)0.0343 (13)H280.10171.13610.56240.041*C290.0256 (4)0.9682 (5)0.5379 (2)0.0347 (13)H30-0.0280                                                                                                                                                                                                                                                                                                                                                                                                                                            | C16 | 0.5157 (4) | 0.7832 (6) | 0.3990 (2)   | 0.0365 (14) |
| C170.5390 (4)0.9194 (6)0.4048 (2)0.0331 (13)H170.51250.98130.37590.040*C180.6018 (4)0.9676 (5)0.45336 (19)0.0281 (12)C190.6260 (4)1.1078 (5)0.4628 (2)0.0367 (13)H190.59701.17310.43590.044*C200.6895 (4)1.1493 (5)0.5093 (2)0.0380 (14)H200.70801.24290.51360.046*C210.7297 (4)1.0533 (5)0.5525 (2)0.0307 (12)C220.7924 (4)1.0906 (5)0.6035 (2)0.0345 (13)H220.81211.18300.61040.041*C230.8244 (4)0.9928 (5)0.6427 (2)0.0339 (13)H230.86811.01610.67670.041*C240.7919 (4)0.8584 (5)0.63216 (19)0.0224 (12)H240.81370.79120.65990.035*C250.7022 (4)0.9150 (4)0.54532 (19)0.0202 (10)C260.6384 (4)0.8709 (5)0.49423 (18)0.0212 (10)C270.1329 (4)0.9783 (5)0.6168 (2)0.0398 (14)H270.17491.03190.64430.048*C280.0887 (4)1.0418 (5)0.5679 (2)0.0343 (13)H280.10171.13610.56240.041*C290.0256 (4)0.9682 (5)0.52677 (19)0.0281 (12)C300.0133 (5)0.8298 (5)0.5379 (2)0.0347 (13)                                                                                                                                                                                                                                                                                                                                                                                                                                   | H16 | 0.4727     | 0.7499     | 0.3664       | 0.044*      |
| H170.51250.98130.37590.040*C180.6018 (4)0.9676 (5)0.45336 (19)0.0281 (12)C190.6260 (4)1.1078 (5)0.4628 (2)0.0367 (13)H190.59701.17310.43590.044*C200.6895 (4)1.1493 (5)0.5093 (2)0.0380 (14)H200.70801.24290.51360.046*C210.7297 (4)1.0533 (5)0.5525 (2)0.0307 (12)C220.7924 (4)1.0906 (5)0.6035 (2)0.0345 (13)H220.81211.18300.61040.041*C230.8244 (4)0.9928 (5)0.6427 (2)0.0339 (13)H230.86811.01610.67670.041*C240.7919 (4)0.8584 (5)0.63216 (19)0.0224 (12)H240.81370.79120.65990.035*C250.7022 (4)0.9150 (4)0.54532 (19)0.0202 (10)C260.6384 (4)0.8709 (5)0.49423 (18)0.0212 (10)C270.1329 (4)0.9783 (5)0.6168 (2)0.0398 (14)H270.17491.03190.64430.048*C280.0887 (4)1.0418 (5)0.5679 (2)0.0343 (13)H280.10171.13610.56240.041*C290.0256 (4)0.9682 (5)0.5379 (2)0.0347 (13)H30-0.02800.77360.51100.042*C310.0606 (4)0.7748 (5)0.5876 (2)0.0378 (13)H310.504<                                                                                                                                                                                                                                                                                                                                                                                                                                            | C17 | 0.5390 (4) | 0.9194 (6) | 0.4048 (2)   | 0.0331 (13) |
| C180.6018 (4)0.9676 (5)0.45336 (19)0.0281 (12)C190.6260 (4)1.1078 (5)0.4628 (2)0.0367 (13)H190.59701.17310.43590.044*C200.6895 (4)1.1493 (5)0.5093 (2)0.0380 (14)H200.70801.24290.51360.046*C210.7297 (4)1.0533 (5)0.5525 (2)0.0307 (12)C220.7924 (4)1.0906 (5)0.6035 (2)0.0345 (13)H220.81211.18300.61040.041*C230.8244 (4)0.9928 (5)0.6427 (2)0.0339 (13)H230.86811.01610.67670.041*C240.7919 (4)0.8584 (5)0.63216 (19)0.0204 (12)H240.81370.79120.65990.035*C250.7022 (4)0.9150 (4)0.54532 (19)0.0202 (10)C260.6384 (4)0.8709 (5)0.49423 (18)0.0212 (10)C270.1329 (4)0.9783 (5)0.6168 (2)0.0398 (14)H270.17491.03190.64430.048*C280.0887 (4)1.0418 (5)0.5679 (2)0.0343 (13)H280.10171.13610.56240.041*C290.0256 (4)0.9682 (5)0.5379 (2)0.0347 (13)H30-0.02800.77360.51100.042*C310.0606 (4)0.7748 (5)0.5876 (2)0.0378 (13)H310.05040.68020.59380.045*                                                                                                                                                                                                                                                                                                                                                                                                                                                     | H17 | 0.5125     | 0.9813     | 0.3759       | 0.040*      |
| C190.6260 (4)1.1078 (5)0.4628 (2)0.0367 (13)H190.59701.17310.43590.044*C200.6895 (4)1.1493 (5)0.5093 (2)0.0380 (14)H200.70801.24290.51360.046*C210.7297 (4)1.0533 (5)0.5525 (2)0.0307 (12)C220.7924 (4)1.0906 (5)0.6035 (2)0.0345 (13)H220.81211.18300.61040.041*C230.8244 (4)0.9928 (5)0.6427 (2)0.0339 (13)H230.86811.01610.67670.041*C240.7919 (4)0.8584 (5)0.63216 (19)0.0224 (12)H240.81370.79120.65990.035*C250.7022 (4)0.9150 (4)0.54532 (19)0.0202 (10)C260.6384 (4)0.8709 (5)0.49423 (18)0.0212 (10)C270.1329 (4)0.9783 (5)0.6168 (2)0.398 (14)H270.17491.03190.64430.048*C280.0887 (4)1.0418 (5)0.5679 (2)0.0343 (13)H280.10171.13610.56240.041*C290.0256 (4)0.9682 (5)0.5379 (2)0.0347 (13)H30-0.02800.77360.51100.042*C310.0606 (4)0.7748 (5)0.5876 (2)0.0378 (13)H310.05040.68020.59380.045*                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                    | C18 | 0.6018 (4) | 0.9676 (5) | 0.45336 (19) | 0.0281 (12) |
| H190.59701.17310.43590.044*C200.6895 (4)1.1493 (5)0.5093 (2)0.0380 (14)H200.70801.24290.51360.046*C210.7297 (4)1.0533 (5)0.5525 (2)0.0307 (12)C220.7924 (4)1.0906 (5)0.6035 (2)0.0345 (13)H220.81211.18300.61040.041*C230.8244 (4)0.9928 (5)0.6427 (2)0.0339 (13)H230.86811.01610.67670.041*C240.7919 (4)0.8584 (5)0.63216 (19)0.0224 (12)H240.81370.79120.65990.035*C250.7022 (4)0.9150 (4)0.54532 (19)0.0202 (10)C260.6384 (4)0.8709 (5)0.49423 (18)0.0212 (10)C270.1329 (4)0.9783 (5)0.6168 (2)0.0398 (14)H270.17491.03190.64430.048*C280.0887 (4)1.0418 (5)0.5679 (2)0.0343 (13)H280.10171.13610.56240.041*C290.0256 (4)0.9682 (5)0.5379 (2)0.0347 (13)H30-0.02800.77360.51100.422*C310.0606 (4)0.7748 (5)0.5876 (2)0.0378 (13)H310.05040.68020.59380.045*                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                               | C19 | 0.6260 (4) | 1.1078 (5) | 0.4628 (2)   | 0.0367 (13) |
| C200.6895 (4)1.1493 (5)0.5093 (2)0.0380 (14)H200.70801.24290.51360.046*C210.7297 (4)1.0533 (5)0.5525 (2)0.0307 (12)C220.7924 (4)1.0906 (5)0.6035 (2)0.0345 (13)H220.81211.18300.61040.041*C230.8244 (4)0.9928 (5)0.6427 (2)0.0339 (13)H230.86811.01610.67670.041*C240.7919 (4)0.8584 (5)0.63216 (19)0.0294 (12)H240.81370.79120.65990.035*C250.7022 (4)0.9150 (4)0.54532 (19)0.0202 (10)C260.6384 (4)0.8709 (5)0.49423 (18)0.0212 (10)C270.1329 (4)0.9783 (5)0.6168 (2)0.0398 (14)H270.17491.03190.64430.041*C280.0887 (4)1.0418 (5)0.5679 (2)0.0343 (13)H280.10171.13610.56240.041*C290.0256 (4)0.9682 (5)0.5379 (2)0.0347 (13)H30-0.02800.77360.51100.042*C310.0606 (4)0.7748 (5)0.5876 (2)0.0378 (13)H310.05040.68020.59380.045*                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                          | H19 | 0.5970     | 1.1731     | 0.4359       | 0.044*      |
| H200.70801.24290.51360.046*C210.7297 (4)1.0533 (5)0.5525 (2)0.0307 (12)C220.7924 (4)1.0906 (5)0.6035 (2)0.0345 (13)H220.81211.18300.61040.041*C230.8244 (4)0.9928 (5)0.6427 (2)0.0339 (13)H230.86811.01610.67670.041*C240.7919 (4)0.8584 (5)0.63216 (19)0.0294 (12)H240.81370.79120.65990.035*C250.7022 (4)0.9150 (4)0.54532 (19)0.0202 (10)C260.6384 (4)0.8709 (5)0.49423 (18)0.0212 (10)C270.1329 (4)0.9783 (5)0.6168 (2)0.0398 (14)H270.17491.03190.64430.048*C280.0887 (4)1.0418 (5)0.5679 (2)0.0343 (13)H280.10171.13610.56240.041*C290.0256 (4)0.9682 (5)0.5379 (2)0.0347 (13)H30-0.02800.77360.51100.042*C310.0606 (4)0.7748 (5)0.5876 (2)0.0378 (13)H310.05040.68020.59380.045*                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                      | C20 | 0.6895 (4) | 1.1493 (5) | 0.5093 (2)   | 0.0380 (14) |
| C210.7297 (4)1.0533 (5)0.5525 (2)0.0307 (12)C220.7924 (4)1.0906 (5)0.6035 (2)0.0345 (13)H220.81211.18300.61040.041*C230.8244 (4)0.9928 (5)0.6427 (2)0.0339 (13)H230.86811.01610.67670.041*C240.7919 (4)0.8584 (5)0.63216 (19)0.0294 (12)H240.81370.79120.65990.035*C250.7022 (4)0.9150 (4)0.54532 (19)0.0202 (10)C260.6384 (4)0.8709 (5)0.49423 (18)0.0212 (10)C270.1329 (4)0.9783 (5)0.6168 (2)0.0348 (14)H270.17491.03190.64430.048*C280.0887 (4)1.0418 (5)0.5679 (2)0.0343 (13)H280.10171.13610.56240.041*C290.0256 (4)0.9682 (5)0.5379 (2)0.0347 (13)H30-0.02800.77360.51100.042*C310.0606 (4)0.7748 (5)0.5876 (2)0.0378 (13)H310.05040.68020.59380.045*                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                 | H20 | 0.7080     | 1.2429     | 0.5136       | 0.046*      |
| C220.7924 (4)1.0906 (5)0.6035 (2)0.0345 (13)H220.81211.18300.61040.041*C230.8244 (4)0.9928 (5)0.6427 (2)0.0339 (13)H230.86811.01610.67670.041*C240.7919 (4)0.8584 (5)0.63216 (19)0.0294 (12)H240.81370.79120.65990.035*C250.7022 (4)0.9150 (4)0.54532 (19)0.0202 (10)C260.6384 (4)0.8709 (5)0.49423 (18)0.0212 (10)C270.1329 (4)0.9783 (5)0.6168 (2)0.0398 (14)H270.17491.03190.64430.048*C280.0887 (4)1.0418 (5)0.5679 (2)0.0343 (13)H280.10171.13610.56240.041*C290.0256 (4)0.9682 (5)0.5379 (2)0.0347 (13)H30-0.02800.77360.51100.042*C310.0606 (4)0.7748 (5)0.5876 (2)0.0378 (13)H310.05040.68020.59380.045*                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                             | C21 | 0.7297 (4) | 1.0533 (5) | 0.5525 (2)   | 0.0307 (12) |
| H220.81211.18300.61040.041*C230.8244 (4)0.9928 (5)0.6427 (2)0.0339 (13)H230.86811.01610.67670.041*C240.7919 (4)0.8584 (5)0.63216 (19)0.0294 (12)H240.81370.79120.65990.035*C250.7022 (4)0.9150 (4)0.54532 (19)0.0202 (10)C260.6384 (4)0.8709 (5)0.49423 (18)0.0212 (10)C270.1329 (4)0.9783 (5)0.6168 (2)0.0398 (14)H270.17491.03190.64430.048*C280.0887 (4)1.0418 (5)0.5679 (2)0.0343 (13)H280.10171.13610.56240.041*C290.0256 (4)0.9682 (5)0.52677 (19)0.0281 (12)C300.0133 (5)0.8298 (5)0.5379 (2)0.0347 (13)H30-0.02800.77360.51100.042*C310.0606 (4)0.7748 (5)0.5876 (2)0.0378 (13)H310.05040.68020.59380.045*                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                           | C22 | 0.7924 (4) | 1.0906 (5) | 0.6035 (2)   | 0.0345 (13) |
| C230.8244 (4)0.9928 (5)0.6427 (2)0.0339 (13)H230.86811.01610.67670.041*C240.7919 (4)0.8584 (5)0.63216 (19)0.0294 (12)H240.81370.79120.65990.035*C250.7022 (4)0.9150 (4)0.54532 (19)0.0202 (10)C260.6384 (4)0.8709 (5)0.49423 (18)0.0212 (10)C270.1329 (4)0.9783 (5)0.6168 (2)0.0398 (14)H270.17491.03190.64430.048*C280.0887 (4)1.0418 (5)0.5679 (2)0.0343 (13)H280.10171.13610.56240.041*C290.0256 (4)0.9682 (5)0.5379 (2)0.0347 (13)H30-0.02800.77360.51100.042*C310.0606 (4)0.7748 (5)0.5876 (2)0.0378 (13)H310.05040.68020.59380.045*                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                    | H22 | 0.8121     | 1.1830     | 0.6104       | 0.041*      |
| H230.86811.01610.67670.041*C240.7919 (4)0.8584 (5)0.63216 (19)0.0294 (12)H240.81370.79120.65990.035*C250.7022 (4)0.9150 (4)0.54532 (19)0.0202 (10)C260.6384 (4)0.8709 (5)0.49423 (18)0.0212 (10)C270.1329 (4)0.9783 (5)0.6168 (2)0.0398 (14)H270.17491.03190.64430.048*C280.0887 (4)1.0418 (5)0.5679 (2)0.0343 (13)H280.10171.13610.56240.041*C290.0256 (4)0.9682 (5)0.52677 (19)0.0281 (12)C300.0133 (5)0.8298 (5)0.5379 (2)0.0347 (13)H30-0.02800.77360.51100.042*C310.0606 (4)0.7748 (5)0.5876 (2)0.0378 (13)H310.05040.68020.59380.045*                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                  | C23 | 0.8244 (4) | 0.9928 (5) | 0.6427 (2)   | 0.0339 (13) |
| C240.7919 (4)0.8584 (5)0.63216 (19)0.0294 (12)H240.81370.79120.65990.035*C250.7022 (4)0.9150 (4)0.54532 (19)0.0202 (10)C260.6384 (4)0.8709 (5)0.49423 (18)0.0212 (10)C270.1329 (4)0.9783 (5)0.6168 (2)0.0398 (14)H270.17491.03190.64430.048*C280.0887 (4)1.0418 (5)0.5679 (2)0.0343 (13)H280.10171.13610.56240.041*C290.0256 (4)0.9682 (5)0.5379 (2)0.0347 (13)H30-0.02800.77360.51100.042*C310.0606 (4)0.7748 (5)0.5876 (2)0.0378 (13)H310.05040.68020.59380.045*                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                           | H23 | 0.8681     | 1.0161     | 0.6767       | 0.041*      |
| H240.81370.79120.65990.035*C250.7022 (4)0.9150 (4)0.54532 (19)0.0202 (10)C260.6384 (4)0.8709 (5)0.49423 (18)0.0212 (10)C270.1329 (4)0.9783 (5)0.6168 (2)0.0398 (14)H270.17491.03190.64430.048*C280.0887 (4)1.0418 (5)0.5679 (2)0.0343 (13)H280.10171.13610.56240.041*C290.0256 (4)0.9682 (5)0.52677 (19)0.0281 (12)C300.0133 (5)0.8298 (5)0.5379 (2)0.0347 (13)H30-0.02800.77360.51100.042*C310.0606 (4)0.7748 (5)0.5876 (2)0.0378 (13)H310.05040.68020.59380.045*                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                           | C24 | 0.7919 (4) | 0.8584 (5) | 0.63216 (19) | 0.0294 (12) |
| C250.7022 (4)0.9150 (4)0.54532 (19)0.0202 (10)C260.6384 (4)0.8709 (5)0.49423 (18)0.0212 (10)C270.1329 (4)0.9783 (5)0.6168 (2)0.0398 (14)H270.17491.03190.64430.048*C280.0887 (4)1.0418 (5)0.5679 (2)0.0343 (13)H280.10171.13610.56240.041*C290.0256 (4)0.9682 (5)0.52677 (19)0.0281 (12)C300.0133 (5)0.8298 (5)0.5379 (2)0.0347 (13)H30-0.02800.77360.51100.042*C310.0606 (4)0.7748 (5)0.5876 (2)0.0378 (13)H310.05040.68020.59380.045*                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                      | H24 | 0.8137     | 0.7912     | 0.6599       | 0.035*      |
| C260.6384 (4)0.8709 (5)0.49423 (18)0.0212 (10)C270.1329 (4)0.9783 (5)0.6168 (2)0.0398 (14)H270.17491.03190.64430.048*C280.0887 (4)1.0418 (5)0.5679 (2)0.0343 (13)H280.10171.13610.56240.041*C290.0256 (4)0.9682 (5)0.52677 (19)0.0281 (12)C300.0133 (5)0.8298 (5)0.5379 (2)0.0347 (13)H30-0.02800.77360.51100.042*C310.0606 (4)0.7748 (5)0.5876 (2)0.0378 (13)H310.05040.68020.59380.045*                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                    | C25 | 0.7022 (4) | 0.9150 (4) | 0.54532 (19) | 0.0202 (10) |
| C270.1329 (4)0.9783 (5)0.6168 (2)0.0398 (14)H270.17491.03190.64430.048*C280.0887 (4)1.0418 (5)0.5679 (2)0.0343 (13)H280.10171.13610.56240.041*C290.0256 (4)0.9682 (5)0.52677 (19)0.0281 (12)C300.0133 (5)0.8298 (5)0.5379 (2)0.0347 (13)H30-0.02800.77360.51100.042*C310.0606 (4)0.7748 (5)0.5876 (2)0.0378 (13)H310.05040.68020.59380.045*                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                  | C26 | 0.6384 (4) | 0.8709 (5) | 0.49423 (18) | 0.0212 (10) |
| H270.17491.03190.64430.048*C280.0887 (4)1.0418 (5)0.5679 (2)0.0343 (13)H280.10171.13610.56240.041*C290.0256 (4)0.9682 (5)0.52677 (19)0.0281 (12)C300.0133 (5)0.8298 (5)0.5379 (2)0.0347 (13)H30-0.02800.77360.51100.042*C310.0606 (4)0.7748 (5)0.5876 (2)0.0378 (13)H310.05040.68020.59380.045*                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                              | C27 | 0.1329 (4) | 0.9783 (5) | 0.6168 (2)   | 0.0398 (14) |
| C280.0887 (4)1.0418 (5)0.5679 (2)0.0343 (13)H280.10171.13610.56240.041*C290.0256 (4)0.9682 (5)0.52677 (19)0.0281 (12)C300.0133 (5)0.8298 (5)0.5379 (2)0.0347 (13)H30-0.02800.77360.51100.042*C310.0606 (4)0.7748 (5)0.5876 (2)0.0378 (13)H310.05040.68020.59380.045*                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                         | H27 | 0.1749     | 1.0319     | 0.6443       | 0.048*      |
| H280.10171.13610.56240.041*C290.0256 (4)0.9682 (5)0.52677 (19)0.0281 (12)C300.0133 (5)0.8298 (5)0.5379 (2)0.0347 (13)H30-0.02800.77360.51100.042*C310.0606 (4)0.7748 (5)0.5876 (2)0.0378 (13)H310.05040.68020.59380.045*                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                     | C28 | 0.0887 (4) | 1.0418 (5) | 0.5679 (2)   | 0.0343 (13) |
| C290.0256 (4)0.9682 (5)0.52677 (19)0.0281 (12)C300.0133 (5)0.8298 (5)0.5379 (2)0.0347 (13)H30-0.02800.77360.51100.042*C310.0606 (4)0.7748 (5)0.5876 (2)0.0378 (13)H310.05040.68020.59380.045*                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                | H28 | 0.1017     | 1.1361     | 0.5624       | 0.041*      |
| C300.0133 (5)0.8298 (5)0.5379 (2)0.0347 (13)H30-0.02800.77360.51100.042*C310.0606 (4)0.7748 (5)0.5876 (2)0.0378 (13)H310.05040.68020.59380.045*                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                              | C29 | 0.0256 (4) | 0.9682 (5) | 0.52677 (19) | 0.0281 (12) |
| H30-0.02800.77360.51100.042*C310.0606 (4)0.7748 (5)0.5876 (2)0.0378 (13)H310.05040.68020.59380.045*                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                          | C30 | 0.0133 (5) | 0.8298 (5) | 0.5379 (2)   | 0.0347 (13) |
| C310.0606 (4)0.7748 (5)0.5876 (2)0.0378 (13)H310.05040.68020.59380.045*                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                      | H30 | -0.0280    | 0.7736     | 0.5110       | 0.042*      |
| H31 0.0504 0.6802 0.5938 0.045*                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                              | C31 | 0.0606 (4) | 0.7748 (5) | 0.5876 (2)   | 0.0378 (13) |
|                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                              | H31 | 0.0504     | 0.6802     | 0.5938       | 0.045*      |

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

|                | $U^{11}$      | $U^{22}$    | $U^{33}$    | $U^{12}$     | $U^{13}$    | $U^{23}$     |
|----------------|---------------|-------------|-------------|--------------|-------------|--------------|
| Zn1            | 0.0209 (3)    | 0.0191 (3)  | 0.0250 (3)  | 0.0013 (3)   | 0.0065 (2)  | 0.0033 (3)   |
| S1             | 0.0228 (7)    | 0.0254 (7)  | 0.0230 (6)  | 0.0049 (5)   | 0.0050 (5)  | 0.0021 (5)   |
| 01             | 0.0252 (18)   | 0.0252 (17) | 0.0272 (17) | 0.0055 (16)  | 0.0083 (14) | 0.0099 (16)  |
| 02             | 0.028 (2)     | 0.058 (3)   | 0.041 (2)   | 0.0082 (19)  | 0.0113 (19) | -0.001 (2)   |
| N1             | 0.019 (2)     | 0.020 (2)   | 0.026 (2)   | 0.0015 (17)  | 0.0051 (17) | -0.0013 (17) |
| N2             | 0.022 (2)     | 0.029 (2)   | 0.026 (2)   | 0.0051 (18)  | 0.0033 (18) | 0.0001 (18)  |
| N3             | 0.025 (2)     | 0.033 (3)   | 0.022 (2)   | 0.0056 (19)  | 0.0056 (19) | 0.0049 (19)  |
| N4             | 0.024 (2)     | 0.020 (2)   | 0.022 (2)   | 0.0007 (17)  | 0.0064 (17) | -0.0015 (17) |
| N5             | 0.022 (2)     | 0.025 (2)   | 0.020 (2)   | 0.0028 (17)  | 0.0074 (18) | 0.0015 (17)  |
| N6             | 0.024 (2)     | 0.044 (3)   | 0.044 (3)   | 0.005 (2)    | 0.010 (2)   | -0.012 (2)   |
| C1             | 0.022 (3)     | 0.023 (3)   | 0.028 (3)   | -0.006 (2)   | 0.011 (2)   | -0.005 (2)   |
| C2             | 0.021 (3)     | 0.033 (3)   | 0.028 (3)   | -0.001 (2)   | 0.006 (2)   | 0.004 (2)    |
| C3             | 0.018 (3)     | 0.044 (3)   | 0.037 (3)   | -0.002 (2)   | 0.009 (2)   | -0.005 (2)   |
| C4             | 0.032 (3)     | 0.062 (4)   | 0.020 (3)   | 0.000 (3)    | 0.009 (2)   | -0.003 (3)   |
| C5             | 0.025 (3)     | 0.058 (4)   | 0.027 (3)   | 0.000 (3)    | 0.001 (2)   | -0.001 (3)   |
| C6             | 0.022 (3)     | 0.035 (3)   | 0.022 (2)   | -0.003 (2)   | 0.002 (2)   | -0.004 (2)   |
| C7             | 0.029 (3)     | 0.029 (3)   | 0.020 (2)   | 0.001 (2)    | 0.004 (2)   | 0.004 (2)    |
| C8             | 0.020 (3)     | 0.017 (3)   | 0.028 (3)   | 0.000 (2)    | 0.003 (2)   | 0.000 (2)    |
| С9             | 0.024 (3)     | 0.023 (3)   | 0.025 (2)   | 0.008 (2)    | 0.001 (2)   | -0.002 (2)   |
| C10            | 0.027 (3)     | 0.026 (3)   | 0.031 (3)   | 0.007 (2)    | -0.003 (2)  | 0.002 (2)    |
| C11            | 0.036 (3)     | 0.043 (3)   | 0.027 (3)   | 0.010 (3)    | 0.001 (2)   | 0.002 (3)    |
| C12            | 0.032 (3)     | 0.051 (4)   | 0.026 (3)   | 0.013 (3)    | -0.002 (2)  | -0.002 (3)   |
| C13            | 0.026 (3)     | 0.050 (4)   | 0.036 (3)   | 0.007 (3)    | -0.001 (3)  | -0.009 (3)   |
| C14            | 0.027 (3)     | 0.028 (3)   | 0.028 (2)   | 0.001 (2)    | 0.005 (2)   | -0.003 (2)   |
| C15            | 0.024 (3)     | 0.026 (3)   | 0.026 (3)   | 0.002 (2)    | 0.007 (2)   | -0.007 (2)   |
| C16            | 0.027 (3)     | 0.064 (4)   | 0.019 (3)   | 0.008 (3)    | 0.001 (2)   | -0.006 (3)   |
| C17            | 0.028 (3)     | 0.050 (4)   | 0.022 (3)   | 0.013 (3)    | 0.010 (2)   | 0.012 (2)    |
| C18            | 0.027 (3)     | 0.032 (3)   | 0.027 (3)   | 0.009 (2)    | 0.012 (2)   | 0.008 (2)    |
| C19            | 0.025 (3)     | 0.033 (3)   | 0.052 (3)   | 0.010 (3)    | 0.015 (3)   | 0.021 (3)    |
| C20            | 0.028 (3)     | 0.021 (3)   | 0.067 (4)   | 0.005 (2)    | 0.022 (3)   | 0.009 (3)    |
| C21            | 0.024 (3)     | 0.029 (3)   | 0.040 (3)   | 0.002 (2)    | 0.016 (2)   | -0.005 (3)   |
| C22            | 0.024 (3)     | 0.029 (3)   | 0.052 (3)   | -0.007 (2)   | 0.015 (3)   | -0.016 (3)   |
| C23            | 0.028 (3)     | 0.037 (3)   | 0.037 (3)   | -0.009 (3)   | 0.005 (2)   | -0.015 (3)   |
| C24            | 0.027 (3)     | 0.037 (3)   | 0.025 (3)   | 0.000 (2)    | 0.006 (2)   | -0.001 (2)   |
| C25            | 0.017 (2)     | 0.014 (2)   | 0.030 (3)   | -0.0016 (19) | 0.012 (2)   | -0.001 (2)   |
| C26            | 0.018 (2)     | 0.020 (2)   | 0.026 (2)   | 0.007 (2)    | 0.0075 (19) | -0.001 (2)   |
| C27            | 0.028 (3)     | 0.038 (3)   | 0.053 (4)   | 0.002 (3)    | -0.002 (3)  | -0.022 (3)   |
| C28            | 0.032 (3)     | 0.024 (3)   | 0.047 (3)   | 0.002 (2)    | 0.002 (3)   | -0.012 (3)   |
| C29            | 0.018 (3)     | 0.029 (3)   | 0.038 (3)   | -0.003 (2)   | 0.011 (2)   | -0.012 (2)   |
| C30            | 0.039 (3)     | 0.026 (3)   | 0.041 (3)   | -0.006 (2)   | 0.009 (3)   | -0.007 (2)   |
| C31            | 0.035 (3)     | 0.028 (3)   | 0.051 (3)   | -0.007 (3)   | 0.011 (3)   | -0.003 (3)   |
| Geometric para | meters (Å. °) |             |             |              |             |              |

Zn1—O1 1.981 (3) C11—C12 1.394 (7)

| Zn1—N1                    | 2.058 (4)   | C11—H11                     | 0.9500    |
|---------------------------|-------------|-----------------------------|-----------|
| Zn1—N5                    | 2.103 (4)   | C12—C13                     | 1.373 (7) |
| Zn1—N4                    | 2.138 (3)   | C12—H12                     | 0.9500    |
| Zn1—S1                    | 2.3692 (12) | C13—C14                     | 1.370 (6) |
| S1—C8                     | 1.748 (4)   | С13—Н13                     | 0.9500    |
| 01—C1                     | 1.317 (5)   | C14—H14                     | 0.9500    |
| O2—C3                     | 1.365 (6)   | C15—C16                     | 1.389 (6) |
| O2—H2                     | 0.84 (5)    | C15—H15                     | 0.9500    |
| N1—C7                     | 1.299 (5)   | C16—C17                     | 1.373 (7) |
| N1—N2                     | 1.401 (5)   | C16—H16                     | 0.9500    |
| N2—C8                     | 1.302 (5)   | C17—C18                     | 1.402 (7) |
| N3—C8                     | 1.380 (6)   | C17—H17                     | 0.9500    |
| N3—C9                     | 1.419 (6)   | C18—C26                     | 1.399 (6) |
| N3—H3                     | 0.88 (3)    | C18—C19                     | 1.423 (7) |
| N4—C15                    | 1.332 (5)   | C19—C20                     | 1.347 (7) |
| N4—C26                    | 1.352 (6)   | С19—Н19                     | 0.9500    |
| N5—C24                    | 1.328 (5)   | C20—C21                     | 1.445 (7) |
| N5—C25                    | 1.353 (5)   | С20—Н20                     | 0.9500    |
| N6—C27                    | 1.336 (7)   | C21—C25                     | 1.406 (6) |
| N6—C31                    | 1.340 (6)   | C21—C22                     | 1.414 (7) |
| C1—C2                     | 1.413 (6)   | C22—C23                     | 1.368 (7) |
| C1—C6                     | 1.434 (6)   | C22—H22                     | 0.9500    |
| C2—C3                     | 1.379 (6)   | C23—C24                     | 1.394 (7) |
| C2—H2A                    | 0.9500      | С23—Н23                     | 0.9500    |
| C3—C4                     | 1.392 (7)   | C24—H24                     | 0.9500    |
| C4—C5                     | 1.356 (7)   | C25—C26                     | 1.442 (6) |
| C4—H4                     | 0.9500      | C27—C28                     | 1.379 (7) |
| C5—C6                     | 1.406 (6)   | С27—Н27                     | 0.9500    |
| C5—H5A                    | 0.9500      | C28—C29                     | 1.386 (6) |
| C6—C7                     | 1.435 (6)   | C28—H28                     | 0.9500    |
| С7—Н7                     | 0.9500      | C29—C30                     | 1.394 (7) |
| C9—C10                    | 1.384 (6)   | C29_C29 <sup>i</sup>        | 1.495 (9) |
| C9—C14                    | 1 405 (6)   | $C_{2}^{(2)} = C_{2}^{(2)}$ | 1 371 (7) |
| C10-C11                   | 1 388 (6)   | C30—H30                     | 0.9500    |
| C10—H10                   | 0.9500      | C31—H31                     | 0.9500    |
| $\Omega_1 = Z_{n1} = N_1$ | 88 77 (13)  | $C_{13}$ $C_{12}$ $C_{11}$  | 1193(5)   |
| 01 - 7n1 - N5             | 104 84 (13) | C13 - C12 - H12             | 120.3     |
| N1—Zn1—N5                 | 103.07 (14) | C11—C12—H12                 | 120.3     |
| $\Omega_1 = Zn_1 = N4$    | 89 56 (13)  | $C_{14}$ $C_{13}$ $C_{12}$  | 120.9(5)  |
| N1 - Zn1 - N4             | 177 58 (14) | C14-C13-H13                 | 119.6     |
| N5—Zn1—N4                 | 79 07 (14)  | C12—C13—H13                 | 119.6     |
| $\Omega_1 = Zn_1 = S_1$   | 148 49 (10) | C13—C14—C9                  | 120 2 (5) |
| N1 - Zn1 - S1             | 82.54 (10)  | C13—C14—H14                 | 1199      |
| N5-Zn1-S1                 | 106.62 (10) | C9—C14—H14                  | 119.9     |
| N4-Zn1-S1                 | 98.00 (10)  | N4—C15—C16                  | 123.0 (5) |
| C8 - S1 - Zn1             | 92.34 (15)  | N4—C15—H15                  | 118.5     |
| C1 - O1 - Zn1             | 1263(3)     | C16—C15—H15                 | 118.5     |
| $C_3 = O_2 = H_2$         | 113 (4)     | C17—C16—C15                 | 118.6 (5) |
|                           | ( · )       |                             |           |

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| C7—N1—N2              | 114.0 (4) | С17—С16—Н16                | 120.7     |
|-----------------------|-----------|----------------------------|-----------|
| C7—N1—Zn1             | 126.1 (3) | C15-C16-H16                | 120.7     |
| N2—N1—Zn1             | 119.4 (3) | C16—C17—C18                | 120.2 (5) |
| C8—N2—N1              | 112.8 (4) | С16—С17—Н17                | 119.9     |
| C8—N3—C9              | 128.7 (4) | С18—С17—Н17                | 119.9     |
| C8—N3—H3              | 114 (3)   | C26—C18—C17                | 116.9 (4) |
| С9—N3—H3              | 116 (3)   | C26—C18—C19                | 120.0 (5) |
| C15—N4—C26            | 118.1 (4) | C17—C18—C19                | 123.0 (5) |
| C15—N4—Zn1            | 129.6 (3) | C20-C19-C18                | 121.1 (5) |
| C26—N4—Zn1            | 112.1 (3) | С20—С19—Н19                | 119.4     |
| C24—N5—C25            | 118.6 (4) | С18—С19—Н19                | 119.4     |
| C24—N5—Zn1            | 128.2 (3) | C19—C20—C21                | 120.8 (5) |
| C25—N5—Zn1            | 113.2 (3) | С19—С20—Н20                | 119.6     |
| C27—N6—C31            | 115.6 (5) | C21—C20—H20                | 119.6     |
| O1—C1—C2              | 118.5 (4) | C25—C21—C22                | 117.3 (5) |
| O1—C1—C6              | 123.8 (4) | C25—C21—C20                | 118.9 (5) |
| C2—C1—C6              | 117.7 (4) | C22—C21—C20                | 123.8 (5) |
| C3—C2—C1              | 122.0 (4) | C23—C22—C21                | 119.6 (5) |
| C3—C2—H2A             | 119.0     | C23—C22—H22                | 120.2     |
| C1—C2—H2A             | 119.0     | C21—C22—H22                | 120.2     |
| O2—C3—C2              | 122.1 (4) | C22—C23—C24                | 119.0 (5) |
| O2—C3—C4              | 118.2 (4) | С22—С23—Н23                | 120.5     |
| C2—C3—C4              | 119.7 (4) | С24—С23—Н23                | 120.5     |
| C5—C4—C3              | 119.5 (4) | N5—C24—C23                 | 123.0 (5) |
| С5—С4—Н4              | 120.2     | N5-C24-H24                 | 118.5     |
| C3—C4—H4              | 120.2     | C23—C24—H24                | 118.5     |
| C4—C5—C6              | 123.3 (5) | N5-C25-C21                 | 122.5 (4) |
| С4—С5—Н5А             | 118.4     | N5-C25-C26                 | 117.8 (4) |
| С6—С5—Н5А             | 118.4     | C21—C25—C26                | 119.8 (4) |
| C5—C6—C1              | 117.7 (4) | N4—C26—C18                 | 123.1 (4) |
| C5—C6—C7              | 118.3 (4) | N4—C26—C25                 | 117.6 (4) |
| C1—C6—C7              | 123.9 (4) | C18—C26—C25                | 119.2 (4) |
| N1—C7—C6              | 124.6 (4) | N6—C27—C28                 | 124.0 (5) |
| N1—C7—H7              | 117.7     | N6—C27—H27                 | 118.0     |
| С6—С7—Н7              | 117.7     | C28—C27—H27                | 118.0     |
| N2—C8—N3              | 117.0 (4) | C27—C28—C29                | 120.2 (5) |
| N2—C8—S1              | 128.2 (4) | С27—С28—Н28                | 119.9     |
| N3—C8—S1              | 114.7 (3) | C29—C28—H28                | 119.9     |
| C10—C9—C14            | 119.4 (4) | C28—C29—C30                | 115.9 (5) |
| C10—C9—N3             | 123.7 (4) | C28—C29—C29 <sup>i</sup>   | 122.6 (5) |
| C14—C9—N3             | 116.8 (4) | C30—C29—C29 <sup>i</sup>   | 121.5 (5) |
| C9—C10—C11            | 1196(5)   | $C_{31} - C_{30} - C_{29}$ | 120 1 (5) |
| C9—C10—H10            | 120.2     | $C_{31} - C_{30} - H_{30}$ | 119.9     |
| C11—C10—H10           | 120.2     | C29—C30—H30                | 119.9     |
| C10-C11-C12           | 120.6 (5) | N6—C31—C30                 | 124.1 (5) |
| C10—C11—H11           | 119.7     | N6—C31—H31                 | 117.9     |
| C12—C11—H11           | 119.7     | С30—С31—Н31                | 117.9     |
| $01 7n1 81 C^{\circ}$ | -00.8 (2) | $C_8 N_3 C_9 C_{10}$       | 22.2 (7)  |
| 01 -LIII-51-C0        | JU.0 (2)  | 0 -10 -01                  | JJ.4 (1)  |

| N1—Zn1—S1—C8  | -15.58 (18) | C8—N3—C9—C14    | -151.2 (5) |
|---------------|-------------|-----------------|------------|
| N5—Zn1—S1—C8  | 85.89 (18)  | C14—C9—C10—C11  | -0.9 (7)   |
| N4—Zn1—S1—C8  | 166.81 (18) | N3-C9-C10-C11   | 174.7 (4)  |
| N1—Zn1—O1—C1  | 27.9 (4)    | C9-C10-C11-C12  | 1.4 (7)    |
| N5—Zn1—O1—C1  | -75.3 (4)   | C10-C11-C12-C13 | -0.5 (8)   |
| N4—Zn1—O1—C1  | -153.8 (4)  | C11-C12-C13-C14 | -0.9 (8)   |
| S1—Zn1—O1—C1  | 101.5 (4)   | C12—C13—C14—C9  | 1.4 (7)    |
| O1—Zn1—N1—C7  | -18.6 (4)   | C10-C9-C14-C13  | -0.5 (7)   |
| N5—Zn1—N1—C7  | 86.4 (4)    | N3-C9-C14-C13   | -176.3 (4) |
| S1—Zn1—N1—C7  | -168.2 (4)  | C26—N4—C15—C16  | -1.2 (7)   |
| O1—Zn1—N1—N2  | 169.6 (3)   | Zn1—N4—C15—C16  | 173.0 (3)  |
| N5—Zn1—N1—N2  | -85.5 (3)   | N4-C15-C16-C17  | 1.1 (7)    |
| S1—Zn1—N1—N2  | 19.9 (3)    | C15-C16-C17-C18 | -0.5 (7)   |
| C7—N1—N2—C8   | 172.2 (4)   | C16-C17-C18-C26 | 0.2 (7)    |
| Zn1—N1—N2—C8  | -14.9 (5)   | C16-C17-C18-C19 | -178.2 (5) |
| O1—Zn1—N4—C15 | -73.6 (4)   | C26-C18-C19-C20 | 3.6 (7)    |
| N5—Zn1—N4—C15 | -178.8 (4)  | C17—C18—C19—C20 | -178.1 (5) |
| S1—Zn1—N4—C15 | 75.7 (4)    | C18—C19—C20—C21 | -3.3 (7)   |
| O1—Zn1—N4—C26 | 101.0 (3)   | C19—C20—C21—C25 | 0.3 (7)    |
| N5—Zn1—N4—C26 | -4.3 (3)    | C19—C20—C21—C22 | -177.2 (5) |
| S1—Zn1—N4—C26 | -109.7 (3)  | C25—C21—C22—C23 | 0.8 (7)    |
| O1—Zn1—N5—C24 | 95.4 (4)    | C20—C21—C22—C23 | 178.3 (4)  |
| N1—Zn1—N5—C24 | 3.2 (4)     | C21—C22—C23—C24 | -1.5 (7)   |
| N4—Zn1—N5—C24 | -178.0 (4)  | C25—N5—C24—C23  | 0.9 (7)    |
| S1—Zn1—N5—C24 | -82.8 (4)   | Zn1—N5—C24—C23  | -177.7 (3) |
| O1—Zn1—N5—C25 | -83.3 (3)   | C22—C23—C24—N5  | 0.7 (7)    |
| N1—Zn1—N5—C25 | -175.5 (3)  | C24—N5—C25—C21  | -1.7 (6)   |
| N4—Zn1—N5—C25 | 3.3 (3)     | Zn1—N5—C25—C21  | 177.1 (3)  |
| S1—Zn1—N5—C25 | 98.5 (3)    | C24—N5—C25—C26  | 179.2 (4)  |
| Zn1—O1—C1—C2  | 156.0 (3)   | Zn1—N5—C25—C26  | -2.0 (5)   |
| Zn1—O1—C1—C6  | -24.9 (6)   | C22-C21-C25-N5  | 0.9 (7)    |
| O1—C1—C2—C3   | -178.3 (4)  | C20-C21-C25-N5  | -176.8 (4) |
| C6—C1—C2—C3   | 2.5 (7)     | C22-C21-C25-C26 | 180.0 (4)  |
| C1—C2—C3—O2   | 178.1 (4)   | C20-C21-C25-C26 | 2.3 (7)    |
| C1—C2—C3—C4   | -2.6 (8)    | C15—N4—C26—C18  | 0.9 (6)    |
| O2—C3—C4—C5   | 179.7 (5)   | Zn1-N4-C26-C18  | -174.4 (3) |
| C2—C3—C4—C5   | 0.3 (8)     | C15—N4—C26—C25  | 179.8 (4)  |
| C3—C4—C5—C6   | 2.0 (8)     | Zn1—N4—C26—C25  | 4.6 (5)    |
| C4—C5—C6—C1   | -2.1 (8)    | C17-C18-C26-N4  | -0.3 (6)   |
| C4—C5—C6—C7   | 176.5 (5)   | C19-C18-C26-N4  | 178.0 (4)  |
| O1—C1—C6—C5   | -179.3 (4)  | C17—C18—C26—C25 | -179.3 (4) |
| C2—C1—C6—C5   | -0.2 (7)    | C19—C18—C26—C25 | -0.9 (6)   |
| O1—C1—C6—C7   | 2.2 (7)     | N5-C25-C26-N4   | -1.8 (6)   |
| C2—C1—C6—C7   | -178.7 (4)  | C21-C25-C26-N4  | 179.0 (4)  |
| N2—N1—C7—C6   | 177.8 (4)   | N5-C25-C26-C18  | 177.2 (4)  |
| Zn1—N1—C7—C6  | 5.5 (7)     | C21—C25—C26—C18 | -2.0 (6)   |
| C5—C6—C7—N1   | -170.8 (5)  | C31—N6—C27—C28  | 0.2 (7)    |
| C1—C6—C7—N1   | 7.7 (8)     | N6—C27—C28—C29  | 0.8 (8)    |
| N1—N2—C8—N3   | 177.6 (4)   | C27—C28—C29—C30 | -1.4 (7)   |

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| N1—N2—C8—S1                                  | -4.2 (6)   | C27–               | -C28-C29-C29 <sup>i</sup> |              | 179.3 (5)  |
|----------------------------------------------|------------|--------------------|---------------------------|--------------|------------|
| C9—N3—C8—N2                                  | -2.7 (7)   | C28–               | -C29-C30-C31              |              | 1.1 (7)    |
| C9—N3—C8—S1                                  | 178.8 (4)  | C29 <sup>i</sup> - |                           |              | -179.6 (5) |
| Zn1—S1—C8—N2                                 | 16.5 (4)   | C27–               | -N6-C31-C30               |              | -0.5 (7)   |
| Zn1—S1—C8—N3                                 | -165.2 (3) | C29–               | -C30-C31-N6               |              | -0.1 (8)   |
| Symmetry codes: (i) $-x$ , $-y+2$ , $-z+1$ . |            |                    |                           |              |            |
|                                              |            |                    |                           |              |            |
| <i>Hydrogen-bond geometry</i> $(A, \circ)$   |            |                    |                           |              |            |
| D—H···A                                      | D          | Р—Н                | H…A                       | $D \cdots A$ | D—H···A    |
| O2—H2…N6                                     | 0.         | .84 (5)            | 2.01 (5)                  | 2.839 (6)    | 168 (6)    |



Fig. 1