data reports





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Crystal structure of bis{2,4-di-tert-butyl-6-[(isopropylimino)methyl]phenolato- $\kappa^2 N,O$ }zinc dichloromethane monosolvate

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Received 17 July 2014; accepted 15 October 2014

Edited by M. Weil, Vienna University of Technology, Austria

In the title compound, $[Zn(C_{18}H_{28}NO)_2] \cdot CH_2Cl_2$, the Zn^{II} atom is *N*,*O*-chelated by two crystallographically independent salicylaldehyde imine ligands, leading to a distorted tetrahedral coordination sphere. The dihedral angle between the planes of the two metallacycles is 88.69 (6)°. Intramolecular non-classical C-H···O hydrogen-bonding interactions are observed. In the crystal, the complex molecules stack into columns along the *a* axis. Dichloromethane solvent molecules are situated in the voids of this arrangement.

Keywords: crystal structure; Schiff base; zinc; tetrahedral coordination.

CCDC reference: 1029220

1. Related literature

For backgroud to poly(lactide) (PLA) and its copolymers, see: Wheaton & Hayes (2011); Chen *et al.* (2006). For the use of bulky ligands coordinating to the active metal site to avoid undesirable transesterification during synthesis of lactides by ring-opening polymerization (ROP), see: Wu *et al.* (2006). For a highly active zinc catalyst for the controlled polymerization of lactides, see: Williams *et al.* (2003); Chamberlain *et al.* (2001). For the preparation of zinc salicylaldehydeimine complexes, see: Chisholm *et al.* (2001).



2. Experimental

2.1. Crystal data

 $[Zn(C_{18}H_{28}NO)_2] \cdot CH_2Cl_2 M_r = 699.12$ Monoclinic, P2₁/n a = 13.6653 (17) Åb = 14.6674 (18) Åc = 19.663 (2) Å $\beta = 104.807 (2)^{\circ}$

2.2. Data collection

Bruker APEAII area-detector
diffractometer
Absorption correction: multi-scan
(SADABS; Bruker, 2007)
$T_{\min} = 0.725, \ T_{\max} = 0.816$

2.3. Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.036$ $wR(F^2) = 0.101$ S = 1.038281 reflections Z = 4Mo K α radiation $\mu = 0.82 \text{ mm}^{-1}$ T = 173 K $0.42 \times 0.41 \times 0.26 \text{ mm}$

V = 3810.4 (8) Å³

22339 measured reflections
8281 independent reflections
6513 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.024$

413 parameters
H-atom parameters constrained
$\Delta \rho_{\rm max} = 0.52 \ {\rm e} \ {\rm \AA}^{-3}$
$\Delta \rho_{\rm min} = -0.37 \text{ e} \text{ Å}^{-3}$

 Table 1

 Hydrogen-bond geometry (Å, °).

$D - H \cdots A$	D-H	$H \cdot \cdot \cdot A$	$D \cdots A$	$D - \mathbf{H} \cdot \cdot \cdot A$
$C4 - H4A \cdots O1$ $C5 - H5C \cdots O1$ $C23 - H23C \cdots O2$ $C24 - H24A \cdots O2$	0.98 0.98 0.98 0.98	2.37 2.32 2.35 2.33	3.018 (3) 2.967 (3) 2.994 (3) 2.986 (3)	123 123 122 124

Data collection: *APEX2* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *publCIF* (Westrip, 2010).

Acknowledgements

This project was supported by the National Torch Program projects of China (grant No. 2011 GH031761).

Supporting information for this paper is available from the IUCr electronic archives (Reference: WM5038).

References

- Bruker (2007). APEX2, SAINT and SADABS. Bruker AXS Inc., Madison, Wisconsin, USA.
- Chamberlain, B. M., Cheng, M., Moore, D. R., Ovitt, T. M., Lobkovsky, E. B. & Coates, G. W. (2001). J. Am. Chem. Soc. 123, 3229–3238.
- Chen, H.-Y., Tang, H.-Y. & Lin, C.-C. (2006). Macromolecules, **39**, 3745–3752.
 Chisholm, M. H., Gallucci, J. C., Zhen, H. & Huffman, J. C. (2001). Inorg. Chem. **40**, 5051–5054.
- Sheldrick, G. M. (2008). Acta Cryst. A64, 112-122.
- Westrip, S. P. (2010). J. Appl. Cryst. 43, 920-925.
- Wheaton, C. A. & Hayes, P. G. (2011). Comments Inorg. Chem. 32, 127-162.
- Williams, C. K., Breyfogle, L. E., Choi, S. K., Nam, W., Young, V. J. Jr, Hillmyer, M. A. & Tolman, W. B. (2003). J. Am. Chem. Soc. 125, 11350– 11359.
- Wu, J.-C., Yu, T.-L., Chen, C.-T. & Lin, C.-C. (2006). Coord. Chem. Rev. 250, 602–626.

supporting information

Acta Cryst. (2014). E70, m390-m391 [doi:10.1107/S1600536814022636]

Crystal structure of bis{2,4-di-*tert*-butyl-6-[(isopropylimino)methyl]phenolato- $\kappa^2 N, O$ }zinc dichloromethane monosolvate

Yuan-Zeng Hao

S1. Experimental

Synthesis of the ligand: Diisopropylamine (2.02 g, 20 mmol) was added dropwise to a solution of the 2,6-di-*tert*-butyl-salicylaldehyde (4.68 g, 20 mmol) in dry ethanol (60 ml) at room temperature over a period of 5 min. The mixture was stirred at 353 K for four hours. Then the solvent was removed by rotary evaporation, and the residue was recrystallizated from methanol. The ligand was isolated as a yellow solid in 20% yield.

Synthesis of the complex: In a Schlenk flask, $ZnEt_2$ (1.22 g, 10 mmol) was added to the solution of the salicylaldehydeimine ligand (10 mmol in tetrahydrofuran) at room temperature. The reaction mixture was stirred in the absence of light for 3 hours at room temperature and was then filtered in the dark and the volume of the solution reduced to 5.0 ml. Pentane was added to afford the product as a light-green solid in *ca*. 50% yield. Single-crystals suitable for X-ray diffraction were grown by slow evaporation of a solution of the title compound in dichlormethane at room temperature.

S2. Refinement

Reflection (011) was affected by the beamstop and was omitted from the refinement. H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms with a C—H distances of 0.95 (aromatic) and 0.99 Å (methylene) and with $U_{iso}(H) = 1.2U_{eq}(C)$, and 0.98 Å for CH₃ [$U_{iso}(H) = 1.5U_{eq}(C)$].



Figure 1

The molecular structure of the title complex with atom labelling and displacement ellipsoids drawn at the 30% probability level.



Figure 2

View of the crystal structure of title compound; H atoms are omitted for clarity.

Bis{2,4-di-tert-butyl-6-[(isopropylimino)methyl]phenolato- $\kappa^2 N, O$ }zinc dichloromethane monosolvate

Crystal data	
$[Zn(C_{18}H_{28}NO)_2]$ ·CH ₂ Cl ₂	F(000) = 1496
$M_r = 699.12$	$D_{\rm x} = 1.219 {\rm Mg} {\rm m}^{-3}$
Monoclinic, $P2_1/n$	Mo <i>K</i> α radiation, $\lambda = 0.71073$ Å
Hall symbol: -P 2yn	Cell parameters from 5049 reflections
a = 13.6653 (17) Å	$\theta = 2.1 - 27.0^{\circ}$
b = 14.6674 (18) Å	$\mu = 0.82 \text{ mm}^{-1}$
c = 19.663 (2) Å	T = 173 K
$\beta = 104.807 \ (2)^{\circ}$	Block, light-green
V = 3810.4 (8) Å ³	$0.42 \times 0.41 \times 0.26 \text{ mm}$
Z = 4	

Data collection

Bruker APEXII area-detector	22339 measured reflections
diffractometer	8281 independent reflections
Radiation source: fine-focus sealed tube	6513 reflections with $I > 2\sigma(I)$
Graphite monochromator	$R_{int} = 0.024$
φ and ω scans	$\theta_{max} = 27.1^{\circ}, \theta_{min} = 1.8^{\circ}$
Absorption correction: multi-scan	$h = -17 \rightarrow 8$
(<i>SADABS</i> ; Bruker, 2007)	$k = -18 \rightarrow 18$
$T_{\min} = 0.725, T_{\max} = 0.816$	$l = -25 \rightarrow 25$
Refinement	
Refinement on F^2	Secondary atom site location: difference Fourier
Least-squares matrix: full	map
$R[F^2 > 2\sigma(F^2)] = 0.036$	Hydrogen site location: inferred from
$wR(F^2) = 0.101$	neighbouring sites
S = 1.02	H-atom parameters constrained
8281 reflections	$w = 1/[\sigma^2(F_o^2) + (0.0501P)^2 + 2.0294P]$
413 parameters	where $P = (F_o^2 + 2F_c^2)/3$
0 restraints	$(\Delta/\sigma)_{max} < 0.001$
Primary atom site location: structure-invariant	$\Delta\rho_{max} = 0.52$ e Å ⁻³
direct methods	$\Delta\rho_{min} = -0.37$ e Å ⁻³

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit *S* are based on F^2 , conventional *R*-factors *R* are based on *F*, with *F* set to zero for negative F^2 . The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating *R*-factors(gt) *etc.* and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on *F*, and *R*- factors based on ALL data will be even larger.

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

	x	v	Z	$U_{\rm iso}*/U_{\rm eq}$	
Znl	0.231421 (16)	0.615892 (14)	0.299369 (11)	0.02227 (7)	
01	0.12145 (10)	0.68715 (9)	0.31431 (7)	0.0271 (3)	
N2	0.36935 (12)	0.66973 (11)	0.33979 (8)	0.0236 (3)	
N1	0.18811 (12)	0.49721 (10)	0.33244 (8)	0.0232 (3)	
02	0.23720 (10)	0.61964 (10)	0.20306 (7)	0.0276 (3)	
C1	0.04377 (14)	0.65800 (13)	0.33501 (9)	0.0220 (4)	
C19	0.31561 (14)	0.63896 (12)	0.17944 (10)	0.0222 (4)	
C2	-0.03878 (15)	0.71885 (13)	0.33494 (9)	0.0236 (4)	
C7	-0.11968 (15)	0.68601 (13)	0.35778 (10)	0.0251 (4)	
H7	-0.1738	0.7269	0.3573	0.030*	
C14	0.03560 (14)	0.56642 (13)	0.35720 (9)	0.0228 (4)	
C13	-0.04928 (15)	0.53872 (13)	0.38081 (10)	0.0244 (4)	
H13	-0.0519	0.4778	0.3967	0.029*	
C15	0.10583 (14)	0.49406 (13)	0.35310 (9)	0.0238 (4)	
H15	0.0889	0.4357	0.3678	0.029*	
C21	0.20705 (15)	0.60533 (13)	0.05374 (10)	0.0264 (4)	

$\begin{array}{cccccccccccccccccccccccccccccccccccc$					
H16 0.2070 0.3606 0.3496 0.033* C18 0.22391 (19) 0.38570 (15) 0.24970 (12) 0.0389 (2) H18A 0.1513 0.3822 0.2268 0.058* H18D 0.2556 0.3267 0.2456 0.058* C24 0.12496 (16) 0.67508 (15) 0.05796 (11) 0.0333 (2) H24A 0.1176 0.6775 0.1062 0.050* H24A 0.1444 0.7354 0.04444 0.050* H24C 0.1444 0.7354 0.04444 0.050* H33 0.4907 0.7113 0.3202 0.029* C34 0.40723 (16) 0.69940 (14) 0.4133 0.035* H23B 0.17481 (18) 0.50939 (14) 0.07091 (11) 0.0355 (12) H23A 0.276 0.4654 0.0681 0.053* H23C 0.1648 0.5089 0.1185 0.053* H23C 0.1648 0.5089 0.1185 0.053* H23B 0.1114<	C16	0.23887 (15)	0.40931 (13)	0.32679 (11)	0.0276 (4)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	H16	0.2070	0.3606	0.3496	0.033*
H18A0.15130.38220.22680.058*H18B0.25560.32670.24560.058*H18C0.25510.43290.22690.058*H18C0.25510.43290.22690.058*H24B0.60040.65690.02600.050*H24B0.60440.65690.02600.050*H24C0.14440.73540.04440.050*C330.42696 (14)0.68492 (13)0.29838 (10)0.0229*C340.40723 (16)0.69940 (14)0.41395 (10)0.0295 (13)H340.47140.73440.41830.035*C330.17481 (18)0.50939 (14)0.07091 (11)0.0353 (14)H23B0.11140.49260.03700.053*H23A0.22760.46540.06810.053*H23B0.11140.49260.03700.053*H23B0.11440.56715 (6)0.15546 (4)0.0742 (10)C110.91415 (5)0.39983 (5)0.22012 (4)0.05636 (22)C110.91415 (5)0.39983 (5)0.22012 (4)0.0563 (22)C110.91415 (5)0.39983 (5)0.22012 (4)0.0564 (20)C6-0.13092 (18)0.87132 (13)0.30842 (11)0.0397 (2)H6A-0.19170.81190.28460.060*H6E-0.13470.87280.36270.060*C200.30799 (14)0.63163 (12)0.10503 (9)0.0216 (2)C310.49349 (15)0.68533 (13)	C18	0.22391 (19)	0.38570 (15)	0.24970 (12)	0.0389 (5)
H18B 0.2556 0.3267 0.2456 0.058^{*} H18C 0.2551 0.4329 0.2269 0.058^{*} C24 $0.12496(16)$ $0.67508(15)$ $0.05796(11)$ 0.0333 H24A 0.1176 0.6775 0.1062 0.050^{*} H24B 0.0604 0.6569 0.0260 0.0250^{*} H24C 0.1444 0.7354 0.0444 0.050^{*} C33 $0.42696(14)$ $0.68492(13)$ $0.29838(10)$ $0.0242(2)$ H33 0.4907 0.7113 0.3202 0.029^{*} C34 $0.40723(16)$ $0.69940(14)$ $0.41395(10)$ $0.0255(2)$ H34 0.4714 0.7344 0.4183 0.035^{*} C23 $0.17481(18)$ $0.50939(14)$ $0.07091(11)$ $0.0355(2)$ H23B 0.1114 0.4926 0.0370 0.053^{*} H23B 0.1114 0.4926 0.0370 0.053^{*} C3 $-0.03675(15)$ $0.81732(13)$ $0.30842(11)$ $0.0278(2)$ C1 $0.91415(5)$ $0.39983(5)$ $0.22012(4)$ 0.0376 C1 $0.91415(5)$ $0.39983(5)$ $0.22012(4)$ 0.0376 C6 $-0.13092(18)$ $0.87132(14)$ $0.31363(14)$ $0.0974(2)$ C6 $-0.1307(18)$ $0.87132(14)$ $0.3163(14)$ $0.0397(2)$ H6A -0.1264 0.9337 0.2264 0.031^{*} C20 $0.30799(14)$ $0.63163(12)$ $0.10503(9)$ $0.0216(2)$ C31 $0.49494(15)$ $0.6298(16)$ <td>H18A</td> <td>0.1513</td> <td>0.3822</td> <td>0.2268</td> <td>0.058*</td>	H18A	0.1513	0.3822	0.2268	0.058*
H18C 0.2551 0.4329 0.2269 0.058^* C24 $0.12496(16)$ $0.67758(15)$ $0.05796(11)$ $0.0333(16)$ H24A 0.1176 0.6775 0.1062 0.050^* H24B 0.0604 0.6569 0.0260 0.050^* H24C 0.1444 0.7354 0.0444 0.050^* C33 $0.42696(14)$ $0.68942(13)$ $0.29838(10)$ $0.0222(6)$ H33 0.4907 0.7113 0.3202 0.029^* C34 $0.40723(16)$ $0.69940(14)$ $0.41395(10)$ $0.0295(6)$ H34 0.4714 0.7344 0.4183 0.035^* C23 $0.17481(18)$ $0.50939(14)$ $0.07091(11)$ $0.0535(2)$ H23A 0.2276 0.4654 0.0681 0.053^* H23C 0.1648 0.5089 0.1185 $0.0254(2)$ C3 $-0.03675(15)$ $0.81732(13)$ $0.30842(11)$ $0.0278(6)$ C11 $0.91415(5)$ $0.3998(5)$ $0.22012(4)$ 0.05363 C12 $0.95759(7)$ $0.56715(6)$ $0.15546(4)$ $0.0742(2)$ C6 $-0.13092(18)$ $0.87132(14)$ $0.31363(14)$ 0.0374 H6A -0.1917 0.8419 0.2846 $0.066*$ H6B -0.1264 0.9337 0.2264 $0.031*$ C20 $0.30799(14)$ $0.63163(12)$ $0.1554(10)$ $0.0255(6)$ H31 0.5554 0.6625 -0.0354 $0.054*$ H22A 0.2268 0.6625 -0.0354 $0.054*$ </td <td>H18B</td> <td>0.2556</td> <td>0.3267</td> <td>0.2456</td> <td>0.058*</td>	H18B	0.2556	0.3267	0.2456	0.058*
$\begin{array}{ccccc} C24 & 0.12496 (16) & 0.67508 (15) & 0.05796 (11) & 0.0333 (1) \\ 124A & 0.1176 & 0.6775 & 0.1062 & 0.050* \\ 124B & 0.0604 & 0.6569 & 0.0260 & 0.050* \\ 124C & 0.1444 & 0.7354 & 0.0444 & 0.050* \\ C33 & 0.42696 (14) & 0.68492 (13) & 0.29838 (10) & 0.0242 (1) \\ 133 & 0.4907 & 0.7113 & 0.3202 & 0.029* \\ C34 & 0.40723 (16) & 0.69940 (14) & 0.41395 (10) & 0.0295 (1) \\ 134 & 0.4714 & 0.7344 & 0.4183 & 0.035* \\ C23 & 0.17481 (18) & 0.50939 (14) & 0.07091 (11) & 0.0355 (1) \\ 123A & 0.2276 & 0.4654 & 0.0681 & 0.053* \\ 123B & 0.1114 & 0.4926 & 0.0370 & 0.053* \\ 123C & 0.1648 & 0.5089 & 0.1185 & 0.055* \\ C3 & -0.03675 (15) & 0.81732 (13) & 0.30842 (11) & 0.0278 (1) \\ C11 & 0.91415 (5) & 0.39983 (5) & 0.22012 (4) & 0.0742 (1) \\ C6 & -0.13092 (18) & 0.87132 (14) & 0.31363 (14) & 0.0397 (1) \\ 166A & -0.1917 & 0.8419 & 0.2846 & 0.066* \\ 16B & -0.1264 & 0.9337 & 0.2969 & 0.066* \\ 16B & -0.1264 & 0.9337 & 0.2969 & 0.066* \\ 16B & -0.1264 & 0.9337 & 0.2969 & 0.066* \\ 16B & -0.1264 & 0.9337 & 0.2969 & 0.066* \\ 16B & -0.1264 & 0.9337 & 0.2969 & 0.066* \\ 16B & -0.1264 & 0.9337 & 0.2969 & 0.066* \\ 16B & -0.1264 & 0.9337 & 0.2969 & 0.066* \\ 16B & -0.1264 & 0.9337 & 0.2969 & 0.066* \\ 16B & -0.1264 & 0.9337 & 0.2969 & 0.066* \\ 16B & -0.1264 & 0.9337 & 0.2569 (11) & 0.0255 (1) \\ 122A & 0.2688 & 0.6625 & -0.0354 & 0.054* \\ 122B & 0.1476 & 0.5888 & -0.0537 & 0.054* \\ 122B & 0.1476 & 0.5888 & -0.0537 & 0.054* \\ 122B & 0.1476 & 0.5888 & -0.0537 & 0.054* \\ 122B & 0.1476 & 0.5888 & -0.0537 & 0.054* \\ 122B & 0.1476 & 0.5888 & -0.0537 & 0.054* \\ 122B & 0.1476 & 0.5888 & -0.0537 & 0.054* \\ 142B & 0.1476 & 0.5888 & -0.0537 & 0.054* \\ 142B & 0.1476 & 0.5888 & -0.0537 & 0.054* \\ 142B & 0.1476 & 0.5888 & -0.0537 & 0.054* \\ 142B & 0.0476 & 0.5888 & -0.0537 & 0.054* \\ 142B & 0.0476 & 0.59850 (13) & 0.38169 (10) & 0.0255 (14) \\ 0.4990 & 0.2216 (15) & 0.6725 (14) & 0.40596 (11) & 0.0268 (16) \\ 0.4622 & 0.3322 & 0.6525 & 0.054* \\ 144 & 0.0233 & 0.7818 & 0.2249 & 0.054* \\ 144 & 0.0233 & 0.7818 & 0.2249 & 0.054* \\ 144 & 0.0316 & 0.8799 & 0.2141 & 0.$	H18C	0.2551	0.4329	0.2269	0.058*
H24A0.11760.67750.10620.050*H24B0.06040.65590.02600.050*H24C0.14440.73540.04440.050*C330.42696 (14)0.68492 (13)0.29838 (10)0.0242 (2H330.49070.71130.32020.029*C340.40723 (16)0.69940 (14)0.41395 (10)0.0255 (2H340.47140.73440.41830.035*C230.17481 (18)0.50939 (14)0.07091 (11)0.0355 (2H23A0.22760.46540.06810.053*H23B0.11140.49260.03700.053*H23C0.16480.50890.11850.053*C3-0.03675 (15)0.81732 (13)0.30842 (11)0.0278 (2C110.91415 (5)0.39983 (5)0.22012 (4)0.05363C20.95759 (7)0.56715 (6)0.15546 (4)0.0397 (2C6-0.13092 (18)0.87132 (14)0.31363 (14)0.0397 (2H6A-0.19170.84190.28460.060*H6B-0.12640.93370.29690.066*H6B-0.13470.87280.36270.060*C200.30799 (14)0.63163 (12)0.10503 (9)0.0216 (2C310.49349 (15)0.68533 (13)0.1956 (10)0.0255 (13)H22B0.14760.5888-0.05370.054*H22B0.14760.59650 (13)0.38169 (10)0.0244 (25C4-0.03558 (18)0.6625	C24	0.12496 (16)	0.67508 (15)	0.05796 (11)	0.0333 (5)
H24B 0.0604 0.6569 0.0260 0.050^{*} H24C 0.1444 0.7354 0.0444 0.050^{*} C33 0.42696 (14) 0.68492 (13) 0.29838 (10) 0.0224 (2)H33 0.4077 0.7113 0.3202 0.029^{*} C34 0.40723 (16) 0.69940 (14) 0.41395 (10) 0.0295 (2)H34 0.4714 0.7344 0.41395 (10) 0.0255 (2)H23A 0.2766 0.4654 0.0681 0.053^{*} H23B 0.1114 0.4926 0.0370 0.053^{*} H23C 0.1648 0.5089 0.1185 0.053^{*} C11 0.91415 (5) 0.39983 (5) 0.2212 (4) 0.05363 C12 0.95759 (7) 0.56715 (6) 0.15546 (4) 0.0742 (2)C6 -0.13092 (18) 0.87132 (14) 0.31363 (14) 0.0397 (2)H6A -0.1917 0.8419 0.2846 0.660^{*} H6E -0.1264 0.9337 0.2969 0.660^{*} H31 0.5554 0.7049 0.2264 0.031^{*} C22 0.21423 (18) 0.6625 -0.0357 0.0564^{*} H22R 0.1476 0.5888 -0.0377 0.054^{*} H22B 0.1476 0.5874 0.0314^{*} C25 0.39349 (15) 0.64874 (13) 0.08192 (10) 0.0255 (H22A 0.2269 0.5661 -0.0279 0.054^{*} H22B 0.1476 0.5888 -0.0337 0.054^{*}	H24A	0.1176	0.6775	0.1062	0.050*
H24C 0.1444 0.7354 0.0444 0.050^* C33 0.42696 (14) 0.68492 (13) 0.29838 (10) 0.0224 (13)H33 0.4907 0.7113 0.3202 0.029^* C34 0.40723 (16) 0.69940 (14) 0.41395 (10) 0.0225 (13)C34 0.4723 (16) 0.69940 (14) 0.41395 (10) 0.0255 (12)C33 0.17481 (18) 0.50939 (14) 0.07091 (11) 0.0355 (12)C23 0.17481 (18) 0.50939 (14) 0.07091 (11) 0.053^* H23B 0.1114 0.4926 0.0370 0.053^* C3 -0.03675 (15) 0.81732 (13) 0.30842 (11) 0.0278 (2)C11 0.91415 (5) 0.39983 (5) 0.22012 (4) 0.07363 C12 0.95759 (7) 0.56715 (6) 0.15546 (4) 0.0742 (7)C6 -0.13092 (18) 0.87132 (14) 0.31363 (14) 0.0397 (7)H6A -0.1917 0.8419 0.2846 0.060^* H6B -0.1264 0.9337 0.2969 0.666^* H6B -0.1347 0.8728 0.3627 0.0216 (C)C31 0.49349 (15) 0.68533 (13) 0.19565 (10) 0.02255 (13)H220 0.2649 0.5561 -0.02269 (11) 0.0354 C22 0.21423 (18) 0.60298 (16) -0.02269 (11) 0.0354 H22C 0.2629 0.5561 -0.03577 0.054^* H220 0.2629 0.567561 -0.0279 0.054^* <td>H24B</td> <td>0.0604</td> <td>0.6569</td> <td>0.0260</td> <td>0.050*</td>	H24B	0.0604	0.6569	0.0260	0.050*
C33 $0.42696 (14)$ $0.68492 (13)$ $0.29838 (10)$ $0.0242 (4)$ H33 0.4907 0.7113 0.3202 0.0298 C34 $0.40723 (16)$ $0.69940 (14)$ $0.41395 (10)$ $0.0295 (4)$ H34 0.4714 0.7344 $0.41395 (10)$ $0.0258 (4)$ C23 $0.17481 (18)$ $0.50939 (14)$ $0.07091 (11)$ 0.0358 C23 $0.17481 (18)$ $0.50939 (14)$ $0.07091 (11)$ $0.0358 (10) (11)$ C3 0.2276 0.4654 0.0681 $0.0538 (10) (11) (11) (11) (11) (11) (11) (11)$	H24C	0.1444	0.7354	0.0444	0.050*
H33 0.4907 0.7113 0.3202 0.029^* C34 $0.40723 (16)$ $0.69940 (14)$ $0.41395 (10)$ $0.0295 (20)$ H34 0.4714 0.7344 $0.41335 (10)$ $0.0255 (20)$ C23 $0.17481 (18)$ $0.50939 (14)$ $0.07091 (11)$ $0.0355 (20)$ H23A 0.2276 0.4654 0.0681 0.053^* H23B 0.1114 0.4926 0.0370 0.053^* H23C 0.1648 0.5089 0.1185 0.053^* C3 $-0.03675 (15)$ $0.81732 (13)$ $0.30842 (11)$ $0.0278 (20)$ C11 $0.91415 (5)$ $0.39983 (5)$ $0.22012 (4)$ 0.05363 C12 $0.95759 (7)$ $0.56715 (6)$ $0.15546 (4)$ $0.0742 (2)$ C6 $-0.13092 (18)$ $0.87132 (14)$ $0.31363 (14)$ $0.397 (2)$ H6A -0.1917 0.8419 0.2846 0.060^* H6B -0.1264 0.9337 0.2969 0.060^* C20 $0.30799 (14)$ $0.63163 (12)$ $0.1553 (10)$ $0.0255 (13)$ C21 $0.21423 (18)$ $0.60298 (16)$ $-0.02269 (11)$ 0.314^* C22 $0.21423 (18)$ $0.60298 (16)$ $-0.02264 (10) (13)^*$ C23 $0.39349 (15)$ $0.64874 (13)$ $0.08192 (10)$ 0.0254^* C25 $0.39349 (15)$ $0.64874 (13)$ $0.08192 (10)$ 0.0254^* C25 $0.39349 (15)$ $0.5675 (14)$ $0.40596 (11)$ $0.0244 (29)$ C25 $0.39349 (15)$ $0.56725 (14)$ $0.40596 (11)$ <	C33	0.42696 (14)	0.68492 (13)	0.29838 (10)	0.0242 (4)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	H33	0.4907	0.7113	0.3202	0.029*
H34 0.4714 0.7344 0.4183 0.035^* C23 0.17481 (18) 0.50939 (14) 0.07091 (11) 0.0355 (19)H23A 0.2276 0.4654 0.0681 0.053^* H23B 0.1114 0.4926 0.0370 0.053^* H23C 0.1648 0.5089 0.1185 0.053^* C3 -0.03675 (15) 0.81732 (13) 0.30842 (11) 0.0278 (20)C11 0.91415 (5) 0.39983 (5) 0.22012 (4) 0.05363 C12 0.95759 (7) 0.56715 (6) 0.15546 (4) 0.0742 (2)C6 -0.13092 (18) 0.87132 (14) 0.31363 (14) 0.0397 (20)H6A -0.1917 0.8419 0.28464 0.606^* H6B -0.1264 0.9337 0.2969 0.606^* H6C -0.1347 0.8728 0.3627 0.606^* C20 0.30799 (14) 0.6163163 (12) 0.10503 (9) 0.0216 (2)C31 0.49349 (15) 0.68533 (13) 0.19565 (10) 0.0255 (4)H31 0.5554 0.7049 0.2264 0.031^* C22 0.21423 (18) 0.60298 (16) -0.02269 (11) 0.0361 (2)H22B 0.1476 0.5888 -0.0537 0.054^* C25 0.39349 (15) 0.64874 (13) 0.08192 (10) 0.0225 (2)C25 0.39349 (15) 0.59650 (13) 0.38169 (10) 0.0244 (2)C26 0.48822 (15) 0.67477 (13) 0.12575 (10) 0.0288 (2)<	C34	0.40723 (16)	0.69940 (14)	0.41395 (10)	0.0295 (4)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	H34	0.4714	0.7344	0.4183	0.035*
H23A 0.2276 0.4654 0.0681 0.053^* H23B 0.1114 0.4926 0.0370 0.053^* H23C 0.1648 0.5089 0.1185 0.053^* C3 $-0.03675(15)$ $0.81732(13)$ $0.30842(11)$ $0.0278(6)$ C11 $0.91415(5)$ $0.3998(5)$ $0.22012(4)$ 0.05363 C2 $0.95759(7)$ $0.56715(6)$ $0.15546(4)$ $0.0742(5)$ C6 $-0.13092(18)$ $0.87132(14)$ $0.31363(14)$ $0.0397(5)$ H6A -0.1917 0.8419 0.2846 0.060^* H6B -0.1264 0.9337 0.2969 0.060^* H6C -0.1347 0.8728 0.3627 0.060^* C20 $0.30799(14)$ $0.63163(12)$ $0.10503(9)$ $0.0216(6)$ C31 $0.49349(15)$ $0.68533(13)$ $0.19565(10)$ $0.0225(6)$ H31 0.5554 0.7049 0.2264 0.031^* C22 $0.21423(18)$ $0.60298(16)$ $-0.02269(11)$ $0.0361(5)$ H22B 0.1476 0.5888 -0.0537 0.054^* H22B 0.1476 0.5888 -0.0537 0.054^* C25 $0.39349(15)$ $0.64874(13)$ $0.8192(10)$ $0.0225(6)$ H25 0.3882 0.6425 0.0330 0.031^* C3 $-0.02791(15)$ $0.5675(14)$ $0.40596(11)$ $0.0284(6)$ C4 $-0.0358(18)$ $0.81635(15)$ $0.23040(11)$ $0.0366(6)$ H4A 0.0233 0.7816 0.2025 <td< td=""><td>C23</td><td>0.17481 (18)</td><td>0.50939 (14)</td><td>0.07091 (11)</td><td>0.0355 (5)</td></td<>	C23	0.17481 (18)	0.50939 (14)	0.07091 (11)	0.0355 (5)
H23B 0.1114 0.4926 0.0370 0.053^* H23C 0.1648 0.5089 0.1185 0.053^* C3 $-0.03675(15)$ $0.81732(13)$ $0.30842(11)$ $0.0278(6)$ C11 $0.91415(5)$ $0.39983(5)$ $0.22012(4)$ 0.05363 C12 $0.95759(7)$ $0.56715(6)$ $0.15546(4)$ $0.0742(3)$ C6 $-0.13092(18)$ $0.87132(14)$ $0.31363(14)$ $0.0397(3)$ H6A -0.1917 0.8419 0.2846 0.060^* H6B -0.1264 0.9337 0.2969 0.060^* H6C -0.1347 0.8728 0.3627 0.060^* C20 $0.30799(14)$ $0.63163(12)$ $0.10503(9)$ $0.0216(6)$ C31 $0.49349(15)$ $0.68533(13)$ $0.19565(10)$ $0.0255(6)$ H31 0.5554 0.7049 0.2264 0.031^* C22 $0.21423(18)$ 0.6625 -0.0354 0.054^* H22B 0.1476 0.5888 -0.0537 0.054^* H22B 0.1476 0.5888 -0.0537 0.054^* H22C 0.2629 0.5561 -0.0279 0.054^* C4 $-0.12791(15)$ $0.56725(14)$ $0.40596(11)$ $0.0284(6)$ C5 $0.39349(15)$ $0.67477(13)$ $0.12575(10)$ $0.0228(6)$ C4 $-0.03558(18)$ $0.81635(15)$ $0.23040(11)$ 0.054^* C4 $-0.03558(18)$ $0.81635(15)$ $0.23040(11)$ 0.054^* C4 -0.0316 0.8790 0.2141 </td <td>H23A</td> <td>0.2276</td> <td>0.4654</td> <td>0.0681</td> <td>0.053*</td>	H23A	0.2276	0.4654	0.0681	0.053*
H23C 0.1648 0.5089 0.1185 0.053^* C3 $-0.03675(15)$ $0.81732(13)$ $0.30842(11)$ $0.0278(2)$ C11 $0.91415(5)$ $0.39983(5)$ $0.22012(4)$ 0.05363 C12 $0.95759(7)$ $0.56715(6)$ $0.15546(4)$ $0.0742(7)$ C6 $-0.13092(18)$ $0.87132(14)$ $0.31363(14)$ $0.0397(7)$ H6A -0.1917 0.8419 0.2846 0.060^* H6B -0.1264 0.9337 0.2969 0.060^* H6C -0.1347 0.8728 0.3627 0.060^* C20 $0.30799(14)$ $0.63163(12)$ $0.10503(9)$ $0.0216(6)$ C31 $0.49349(15)$ $0.68533(13)$ $0.19565(10)$ $0.0255(6)$ H31 0.5554 0.7049 0.2264 0.031^* C22 $0.21423(18)$ $0.60298(16)$ $-0.02269(11)$ $0.0361(2)$ H22B 0.1476 0.5888 -0.0537 0.054^* H22C 0.2629 0.5561 -0.0279 0.54^* H22C 0.2629 0.5561 -0.0279 0.054^* C25 $0.39349(15)$ $0.64474(13)$ $0.8192(10)$ $0.0225(6)$ C4 $-0.3558(18)$ $0.81635(15)$ $0.23040(11)$ $0.0284(6)$ C4 -0.0357 $0.5477(13)$ $0.12575(10)$ $0.0284(7)$ C4 $-0.0358(18)$ $0.81635(15)$ 0.2249 0.054^* C4 $-0.0358(18)$ $0.81635(15)$ 0.2249 0.054^* C4 -0.03577 0.7876	H23B	0.1114	0.4926	0.0370	0.053*
C3 $-0.03675(15)$ $0.81732(13)$ $0.30842(11)$ $0.0278(4)$ C11 $0.91415(5)$ $0.39983(5)$ $0.22012(4)$ 0.05363 C12 $0.95759(7)$ $0.56715(6)$ $0.15546(4)$ $0.0742(7)$ C6 $-0.13092(18)$ $0.87132(14)$ $0.31363(14)$ $0.0397(7)$ H6A -0.1917 0.8419 0.2846 $0.060*$ H6B -0.1264 0.9337 0.2969 $0.660*$ C20 $0.30799(14)$ $0.63163(12)$ $0.10503(9)$ $0.0216(6)$ C31 $0.49349(15)$ $0.68533(13)$ $0.19565(10)$ $0.0225(6)$ H31 0.5554 0.7049 0.2264 $0.031*$ C22 $0.21423(18)$ $0.60298(16)$ $-0.02269(11)$ $0.0364*$ H22A 0.2368 0.6625 -0.0354 $0.054*$ H22B 0.1476 0.5888 -0.05377 $0.054*$ H22C 0.2629 0.5561 -0.0279 $0.054*$ H22C 0.2629 0.5561 -0.0279 $0.054*$ C25 $0.39349(15)$ $0.64874(13)$ $0.08192(10)$ $0.0255(6)$ C4 $-0.12791(15)$ $0.59650(13)$ $0.38169(10)$ $0.0244(6)$ C26 $0.48822(15)$ $0.67477(13)$ $0.12575(10)$ $0.0258(6)$ C4 $-0.03558(18)$ $0.81635(15)$ $0.23040(11)$ $0.0360(5)$ H4A 0.0233 0.7818 0.2249 $0.054*$ H4B -0.0316 0.8790 0.2141 $0.054*$ H4A 0.0233 $0.61854(19)$ <t< td=""><td>H23C</td><td>0.1648</td><td>0.5089</td><td>0.1185</td><td>0.053*</td></t<>	H23C	0.1648	0.5089	0.1185	0.053*
Cl1 0.91415 (5) 0.39983 (5) 0.22012 (4) 0.05363 Cl2 0.95759 (7) 0.56715 (6) 0.15546 (4) 0.0742 (5)C6 -0.13092 (18) 0.87132 (14) 0.31363 (14) 0.0397 (5)H6A -0.1917 0.8419 0.2846 0.060^* H6B -0.1264 0.9337 0.2969 0.060^* H6C -0.1347 0.8728 0.3627 0.060^* C20 0.30799 (14) 0.63163 (12) 0.10503 (9) 0.0216 (4)C31 0.49349 (15) 0.68533 (13) 0.19565 (10) 0.0255 (4)H31 0.5554 0.7049 0.2264 0.031^* C22 0.21423 (18) 0.60298 (16) -0.02269 (11) 0.0361 (5)H22A 0.2368 0.6625 -0.0354 0.054^* H22B 0.1476 0.5888 -0.0537 0.054^* H22C 0.2629 0.5561 -0.0279 0.054^* H22S 0.39349 (15) 0.64874 (13) 0.08192 (10) 0.0255 (4)L25 0.3882 0.6425 0.0330 0.31^* C26 0.48822 (15) 0.67477 (13) 0.12575 (10) 0.0258 (6)C4 -0.0356 (15) 0.23040 (11) 0.0360 (2)C4 -0.0316 0.8790 0.2141 0.054^* H4B -0.0316 0.8790 0.2141 0.054^* C4 -0.0356 (15) 0.23040 (11) 0.0258 (6)C4 -0.0356 (15) 0.2249 0.054^* <	C3	-0.03675 (15)	0.81732 (13)	0.30842 (11)	0.0278 (4)
Cl2 $0.95759(7)$ $0.56715(6)$ $0.15546(4)$ $0.0742(5)$ C6 $-0.13092(18)$ $0.87132(14)$ $0.31363(14)$ $0.0397(5)$ H6A -0.1917 0.8419 0.2846 0.060^* H6B -0.1264 0.9337 0.2969 0.060^* H6C -0.1347 0.8728 0.3627 0.060^* C20 $0.30799(14)$ $0.63163(12)$ $0.10503(9)$ $0.0216(6)$ C31 $0.49349(15)$ $0.68533(13)$ $0.19565(10)$ $0.0225(6)$ H31 0.5554 0.7049 0.2264 0.031^* C22 $0.21423(18)$ $0.60298(16)$ $-0.02269(11)$ $0.0361(5)$ H22A 0.2368 0.6625 -0.0354 0.054^* H22B 0.1476 0.5888 -0.0537 0.054^* H22C 0.2629 0.5561 -0.0279 0.054^* H22C 0.2629 0.5561 -0.0279 0.054^* C25 $0.39349(15)$ $0.64874(13)$ $0.8192(10)$ $0.0225(6)$ H25 0.3882 0.6425 0.0330 0.031^* C8 $-0.12791(15)$ $0.59650(13)$ $0.38169(10)$ $0.0244(6)$ C9 $-0.22116(15)$ $0.57725(14)$ $0.40596(11)$ $0.0258(6)$ C4 $-0.0358(18)$ $0.81635(15)$ $0.23040(11)$ 0.0364^* H4B -0.0316 0.8790 0.2141 0.054^* C35 $0.4302(3)$ $0.61854(19)$ $0.46227(13)$ $0.0565(13)$ H4B -0.0316 0.8799 0.4479	Cl1	0.91415 (5)	0.39983 (5)	0.22012 (4)	0.05363 (17)
C6 $-0.13092(18)$ $0.87132(14)$ $0.31363(14)$ $0.0397(2)$ H6A -0.1917 0.8419 0.2846 0.060^* H6B -0.1264 0.9337 0.2969 0.660^* H6C -0.1347 0.8728 0.3627 0.060^* C20 $0.30799(14)$ $0.63163(12)$ $0.10503(9)$ $0.0216(6)$ C31 $0.49349(15)$ $0.68533(13)$ $0.19565(10)$ $0.0225(6)$ H31 0.5554 0.7049 0.2264 0.031^* C22 $0.21423(18)$ $0.60298(16)$ $-0.02269(11)$ $0.0361(5)$ H22A 0.2368 0.6625 -0.0354 0.054^* H22B 0.1476 0.5888 -0.0537 0.054^* H22C 0.2629 0.5561 -0.0279 0.054^* H22C 0.2629 0.5561 -0.0279 0.054^* H25 0.3882 0.6425 0.0330 0.031^* C8 $-0.12791(15)$ $0.59650(13)$ $0.38169(10)$ $0.0244(6)$ C9 $-0.22116(15)$ $0.56725(14)$ $0.40596(11)$ $0.0284(6)$ C4 $-0.03558(18)$ $0.81635(15)$ $0.23040(11)$ $0.0366(5)$ H4B -0.0316 0.8790 0.2141 0.054^* H4B -0.0316 0.8790 0.2141 0.054^* H4B -0.0316 0.8790 0.2141 0.054^* H4B -0.0316 0.8790 0.2141 0.058^* H35B 0.4589 0.6395 0.5106 0.085^* H35B	C12	0.95759 (7)	0.56715 (6)	0.15546 (4)	0.0742 (3)
H6A -0.1917 0.8419 0.2846 0.060^* H6B -0.1264 0.9337 0.2969 0.060^* H6C -0.1347 0.8728 0.3627 0.060^* C20 $0.30799 (14)$ $0.63163 (12)$ $0.10503 (9)$ $0.0216 (20)$ C31 $0.49349 (15)$ $0.68533 (13)$ $0.19565 (10)$ $0.0225 (20)$ H31 0.5554 0.7049 0.2264 0.031^* C22 $0.21423 (18)$ $0.60298 (16)$ $-0.02269 (11)$ $0.0361 (20)$ H22A 0.2368 0.6625 -0.0354 0.054^* H22B 0.1476 0.5888 -0.0537 0.054^* H22C 0.2629 0.5561 -0.0279 0.054^* H22C 0.2629 0.56761 -0.0279 0.054^* H22C 0.2629 $0.59650 (13)$ $0.38169 (10)$ $0.0224 (20)$ C35 0.3882 0.6425 0.0330 0.031^* C4 $-0.12791 (15)$ $0.59650 (13)$ $0.38169 (10)$ $0.0244 (20)$ C56 $0.48822 (15)$ $0.67477 (13)$ $0.12575 (10)$ $0.0228 (20)$ C4 $-0.03558 (18)$ $0.81635 (15)$ $0.23040 (11)$ $0.0360 (20)$ H4B -0.0316 0.8790 0.2141 0.054^* H4B -0.0316 0.8790 0.2141 0.054^* H4C -0.0977 0.7876 0.2025 0.054^* C35 $0.4302 (3)$ $0.61854 (19)$ $0.46227 (13)$ $0.0566 (20)$ H4B -0.0316 0.8799 <t< td=""><td>C6</td><td>-0.13092 (18)</td><td>0.87132 (14)</td><td>0.31363 (14)</td><td>0.0397 (5)</td></t<>	C6	-0.13092 (18)	0.87132 (14)	0.31363 (14)	0.0397 (5)
H6B -0.1264 0.9337 0.2969 0.060^* H6C -0.1347 0.8728 0.3627 0.060^* C20 $0.30799(14)$ $0.63163(12)$ $0.10503(9)$ $0.0216(6)$ C31 $0.49349(15)$ $0.68533(13)$ $0.19565(10)$ $0.0255(6)$ H31 0.5554 0.7049 0.2264 0.031^* C22 $0.21423(18)$ $0.60298(16)$ $-0.02269(11)$ $0.0361(5)$ H22A 0.2368 0.6625 -0.0354 0.054^* H22B 0.1476 0.5888 -0.0537 0.054^* H22C 0.2629 0.5561 -0.0279 0.054^* H22C 0.2629 0.5561 -0.0279 0.054^* H25 $0.39349(15)$ $0.64874(13)$ $0.8192(10)$ $0.0225(6)$ H25 0.3882 0.6425 0.0330 0.031^* C8 $-0.12791(15)$ $0.59650(13)$ $0.38169(10)$ $0.0244(6)$ C9 $-0.22116(15)$ $0.56725(14)$ $0.40596(11)$ $0.0284(6)$ C4 $-0.03558(18)$ $0.81635(15)$ $0.23040(11)$ $0.0360(5)$ H4A 0.0233 0.7818 0.2249 0.654^* H4B -0.0316 0.8790 0.2141 0.054^* H4C -0.0977 0.7876 0.2025 0.054^* H35B 0.4589 0.6395 0.5106 0.085^* H35B 0.4589 0.6395 0.5106 0.085^* H35B 0.4589 0.6395 0.5106 0.0857^* H47A<	H6A	-0.1917	0.8419	0.2846	0.060*
H6C -0.1347 0.8728 0.3627 0.060^* C20 $0.30799(14)$ $0.63163(12)$ $0.10503(9)$ $0.0216(6)$ C31 $0.49349(15)$ $0.68533(13)$ $0.19565(10)$ $0.0255(6)$ H31 0.5554 0.7049 0.2264 0.031^* C22 $0.21423(18)$ $0.60298(16)$ $-0.02269(11)$ $0.0361(5)$ H22A 0.2368 0.6625 -0.0354 0.054^* H22B 0.1476 0.5888 -0.0537 0.054^* H22C 0.2629 0.5561 -0.0279 0.054^* C25 $0.39349(15)$ $0.64874(13)$ $0.08192(10)$ $0.0225(6)$ H25 0.3882 0.6425 0.0330 0.031^* C8 $-0.12791(15)$ $0.59650(13)$ $0.38169(10)$ $0.0244(6)$ C9 $-0.22116(15)$ $0.56725(14)$ $0.40596(11)$ $0.0284(6)$ C4 $-0.03558(18)$ $0.81635(15)$ $0.23040(11)$ $0.0360(5)$ H4B -0.0316 0.8790 0.2141 0.054^* H4B -0.0316 0.8790 0.2141 0.054^* H4C -0.0977 0.7876 0.2025 0.054^* C35 $0.4302(3)$ $0.61854(19)$ $0.46227(13)$ $0.0566(6)$ H35B 0.4589 0.6395 0.5106 0.085^* H35B 0.4589 0.6395 0.5106 0.085^* H35C 0.4790 0.5789 0.4479 $0.0816(1)$ H17A 0.3823 0.4626 0.3422 0.057^* </td <td>H6B</td> <td>-0.1264</td> <td>0.9337</td> <td>0.2969</td> <td>0.060*</td>	H6B	-0.1264	0.9337	0.2969	0.060*
C20 $0.30799 (14)$ $0.63163 (12)$ $0.10503 (9)$ $0.0216 (20)$ C31 $0.49349 (15)$ $0.68533 (13)$ $0.19565 (10)$ $0.0255 (20)$ H31 0.5554 0.7049 0.2264 $0.031*$ C22 $0.21423 (18)$ $0.60298 (16)$ $-0.02269 (11)$ $0.0361 (20)$ H22A 0.2368 0.6625 -0.0354 $0.054*$ H22B 0.1476 0.5888 -0.0537 $0.054*$ H22C 0.2629 0.5561 -0.0279 $0.054*$ C25 $0.39349 (15)$ $0.64874 (13)$ $0.08192 (10)$ $0.0255 (20)$ H25 0.3882 0.6425 0.0330 $0.031*$ C8 $-0.12791 (15)$ $0.59650 (13)$ $0.38169 (10)$ $0.0284 (20)$ C26 $0.48822 (15)$ $0.67477 (13)$ $0.12575 (10)$ $0.0288 (20)$ C4 $-0.03558 (18)$ $0.81635 (15)$ $0.23040 (11)$ $0.0360 (20)$ H4B -0.0316 0.8790 0.2141 $0.054*$ H4C -0.0977 0.7876 0.2025 $0.054*$ C35 $0.4302 (3)$ $0.61854 (19)$ $0.46227 (13)$ $0.0566 (20)$ H35B 0.4589 0.6395 0.5106 $0.085*$ H35C 0.4790 0.5789 0.4479 $0.085*$ H35C 0.4790 0.5789 0.4479 $0.085*$ H35B 0.4523 0.4626 0.3422 $0.057*$ H17A 0.3823 0.4626 0.3422 $0.057*$	H6C	-0.1347	0.8728	0.3627	0.060*
C31 $0.49349(15)$ $0.68533(13)$ $0.19565(10)$ $0.0255(6)$ H31 0.5554 0.7049 0.2264 $0.031*$ C22 $0.21423(18)$ $0.60298(16)$ $-0.02269(11)$ $0.0361(5)$ H22A 0.2368 0.6625 -0.0354 $0.054*$ H22B 0.1476 0.5888 -0.0537 $0.054*$ H22C 0.2629 0.5561 -0.0279 $0.054*$ C25 $0.39349(15)$ $0.64874(13)$ $0.08192(10)$ $0.0255(2)$ H25 0.3882 0.6425 0.0330 $0.031*$ C8 $-0.12791(15)$ $0.59650(13)$ $0.38169(10)$ $0.0224(2)$ C26 $0.48822(15)$ $0.67477(13)$ $0.12575(10)$ $0.0284(2)$ C26 $0.48822(15)$ $0.67477(13)$ $0.12575(10)$ $0.0284(2)$ C4 $-0.03558(18)$ $0.81635(15)$ $0.23040(11)$ $0.054*$ H4B -0.0316 0.8790 0.2141 $0.054*$ H4C -0.0977 0.7876 0.2025 $0.054*$ C35 $0.4302(3)$ $0.61854(19)$ $0.46227(13)$ $0.0566(3)$ H35B 0.4589 0.6395 0.5106 $0.085*$ H35C 0.4790 0.5789 0.4479 $0.085*$ C17 $0.35026(17)$ 0.4626 0.3422 $0.057*$ H17A 0.3823 0.4626 0.3422 $0.057*$	C20	0.30799 (14)	0.63163 (12)	0.10503 (9)	0.0216 (4)
H31 0.5554 0.7049 0.2264 0.031^* C22 $0.21423 (18)$ $0.60298 (16)$ $-0.02269 (11)$ $0.0361 (2)$ H22A 0.2368 0.6625 -0.0354 0.054^* H22B 0.1476 0.5888 -0.0537 0.054^* H22C 0.2629 0.5561 -0.0279 0.054^* C25 $0.39349 (15)$ $0.64874 (13)$ $0.08192 (10)$ $0.0255 (2)$ H25 0.3882 0.6425 0.0330 0.031^* C8 $-0.12791 (15)$ $0.59650 (13)$ $0.38169 (10)$ $0.0244 (2)$ C26 $0.48822 (15)$ $0.67477 (13)$ $0.12575 (10)$ $0.0258 (2)$ C26 $0.48822 (15)$ $0.67477 (13)$ $0.12575 (10)$ $0.0258 (2)$ C4 $-0.03558 (18)$ $0.81635 (15)$ $0.23040 (11)$ $0.0360 (2)$ H4A 0.0233 0.7818 0.2249 0.054^* H4B -0.0316 0.8790 0.2141 0.054^* H4C -0.0977 0.7876 0.2025 0.054^* H35B 0.4589 0.6395 0.5106 0.085^* H35B 0.4589 0.6395 0.5106 0.085^* H35C 0.4790 0.5789 0.4479 0.085^* C17 $0.35026 (17)$ $0.41501 (16)$ 0.3422 0.057^* H17A 0.3823 0.4626 0.3422 0.057^*	C31	0.49349 (15)	0.68533 (13)	0.19565 (10)	0.0255 (4)
C22 $0.21423 (18)$ $0.60298 (16)$ $-0.02269 (11)$ $0.0361 (2)$ H22A 0.2368 0.6625 -0.0354 $0.054*$ H22B 0.1476 0.5888 -0.0537 $0.054*$ H22C 0.2629 0.5561 -0.0279 $0.054*$ C25 $0.39349 (15)$ $0.64874 (13)$ $0.08192 (10)$ $0.0255 (2)$ H25 0.3882 0.6425 0.0330 $0.031*$ C8 $-0.12791 (15)$ $0.59650 (13)$ $0.38169 (10)$ $0.0244 (2)$ C26 $0.48822 (15)$ $0.67477 (13)$ $0.12575 (10)$ $0.0258 (2)$ C4 $-0.03558 (18)$ $0.81635 (15)$ $0.23040 (11)$ $0.0360 (2)$ H4B -0.0316 0.8790 0.2141 $0.054*$ H4B -0.0316 0.8790 0.2141 $0.054*$ H4C -0.0977 0.7876 0.2025 $0.054*$ H4B 0.3677 0.5845 0.4599 $0.085*$ H35B 0.4589 0.6395 0.5106 $0.085*$ H35C 0.4790 0.5789 0.4479 $0.085*$ H17A 0.3823 0.4626 0.3422 $0.057*$	H31	0.5554	0.7049	0.2264	0.031*
H22A 0.2368 0.6625 -0.0354 0.054^* H22B 0.1476 0.5888 -0.0537 0.054^* H22C 0.2629 0.5561 -0.0279 0.054^* C25 $0.39349 (15)$ $0.64874 (13)$ $0.08192 (10)$ $0.0255 (20)$ H25 0.3882 0.6425 0.0330 0.031^* C8 $-0.12791 (15)$ $0.59650 (13)$ $0.38169 (10)$ $0.0244 (20)$ C9 $-0.22116 (15)$ $0.56725 (14)$ $0.40596 (11)$ $0.0284 (20)$ C26 $0.48822 (15)$ $0.67477 (13)$ $0.12575 (10)$ $0.0258 (20)$ C4 $-0.03558 (18)$ $0.81635 (15)$ $0.23040 (11)$ $0.0360 (20)$ H4A 0.0233 0.7818 0.2249 0.054^* H4B -0.0316 0.8790 0.2141 0.054^* H4C -0.0977 0.7876 0.2025 0.054^* H35B $0.4302 (3)$ $0.61854 (19)$ $0.46227 (13)$ $0.0566 (20)$ H35B 0.4589 0.6395 0.5106 0.085^* H35B 0.4589 0.6395 0.5106 0.085^* H35C 0.4790 0.5789 0.4479 0.085^* H17A 0.3823 0.4626 0.3422 0.057^*	C22	0.21423 (18)	0.60298 (16)	-0.02269 (11)	0.0361 (5)
H22B 0.1476 0.5888 -0.0537 $0.054*$ H22C 0.2629 0.5561 -0.0279 $0.054*$ C25 $0.39349(15)$ $0.64874(13)$ $0.08192(10)$ $0.0255(4)$ H25 0.3882 0.6425 0.0330 $0.031*$ C8 $-0.12791(15)$ $0.59650(13)$ $0.38169(10)$ $0.0244(4)$ C9 $-0.22116(15)$ $0.56725(14)$ $0.40596(11)$ $0.0284(4)$ C26 $0.48822(15)$ $0.67477(13)$ $0.12575(10)$ $0.0258(4)$ C4 $-0.03558(18)$ $0.81635(15)$ $0.23040(11)$ $0.0360(5)$ H4A 0.0233 0.7818 0.2249 $0.054*$ H4B -0.0316 0.8790 0.2141 $0.054*$ H4C -0.0977 0.7876 0.2025 $0.054*$ H35B $0.4302(3)$ $0.61854(19)$ $0.46227(13)$ $0.0566(6)$ H35A 0.3677 0.5845 0.4599 $0.085*$ H35B 0.4589 0.6395 0.5106 $0.085*$ H35C 0.4790 0.5789 0.4479 $0.085*$ C17 $0.35026(17)$ $0.41501(16)$ $0.36411(12)$ $0.0381(5)$ H17A 0.3823 0.4626 0.3422 $0.057*$	H22A	0.2368	0.6625	-0.0354	0.054*
H22C 0.2629 0.5561 -0.0279 0.054^* C25 $0.39349 (15)$ $0.64874 (13)$ $0.08192 (10)$ $0.0255 (4)$ H25 0.3882 0.6425 0.0330 0.031^* C8 $-0.12791 (15)$ $0.59650 (13)$ $0.38169 (10)$ $0.0244 (4)$ C9 $-0.22116 (15)$ $0.56725 (14)$ $0.40596 (11)$ $0.0284 (4)$ C26 $0.48822 (15)$ $0.67477 (13)$ $0.12575 (10)$ $0.0258 (4)$ C4 $-0.03558 (18)$ $0.81635 (15)$ $0.23040 (11)$ $0.0360 (2)$ H4A 0.0233 0.7818 0.2249 0.054^* H4B -0.0316 0.8790 0.2141 0.054^* H4C -0.0977 0.7876 0.2025 0.054^* H35A 0.3677 0.5845 0.4599 0.085^* H35B 0.4589 0.6395 0.5106 0.085^* H35B 0.4589 0.5789 0.4479 0.085^* C17 $0.35026 (17)$ $0.41501 (16)$ 0.3422 0.057^* H17A 0.3823 0.4626 0.3422 0.057^*	H22B	0.1476	0.5888	-0.0537	0.054*
C25 $0.39349 (15)$ $0.64874 (13)$ $0.08192 (10)$ $0.0255 (4)$ H25 0.3882 0.6425 0.0330 $0.031*$ C8 $-0.12791 (15)$ $0.59650 (13)$ $0.38169 (10)$ $0.0244 (4)$ C9 $-0.22116 (15)$ $0.56725 (14)$ $0.40596 (11)$ $0.0288 (4)$ C26 $0.48822 (15)$ $0.67477 (13)$ $0.12575 (10)$ $0.0258 (4)$ C4 $-0.03558 (18)$ $0.81635 (15)$ $0.23040 (11)$ $0.0360 (5)$ H4A 0.0233 0.7818 0.2249 $0.054*$ H4B -0.0316 0.8790 0.2141 $0.054*$ H4C -0.0977 0.7876 0.2025 $0.054*$ C35 $0.4302 (3)$ $0.61854 (19)$ $0.46227 (13)$ $0.0566 (6)$ H35A 0.3677 0.5845 0.4599 $0.085*$ H35B 0.4589 0.6395 0.5106 $0.085*$ H35C 0.4790 0.5789 0.4479 $0.085*$ C17 $0.35026 (17)$ $0.41501 (16)$ $0.36411 (12)$ $0.0381 (2)$ H17A 0.3823 0.4626 0.3422 $0.057*$	H22C	0.2629	0.5561	-0.0279	0.054*
H25 0.3882 0.6425 0.0330 0.031^* C8 $-0.12791(15)$ $0.59650(13)$ $0.38169(10)$ $0.0244(4)$ C9 $-0.22116(15)$ $0.56725(14)$ $0.40596(11)$ $0.0284(4)$ C26 $0.48822(15)$ $0.67477(13)$ $0.12575(10)$ $0.0258(4)$ C4 $-0.03558(18)$ $0.81635(15)$ $0.23040(11)$ $0.0360(5)$ H4A 0.0233 0.7818 0.2249 0.054^* H4B -0.0316 0.8790 0.2141 0.054^* H4C -0.0977 0.7876 0.2025 0.054^* C35 $0.4302(3)$ $0.61854(19)$ $0.46227(13)$ $0.0566(8)$ H35A 0.3677 0.5845 0.4599 0.085^* H35B 0.4589 0.6395 0.5106 0.085^* H35C 0.4790 0.5789 0.4479 0.085^* C17 $0.35026(17)$ $0.41501(16)$ $0.36411(12)$ $0.0381(6)$ H17A 0.3823 0.4626 0.3422 0.057^*	C25	0.39349 (15)	0.64874 (13)	0.08192 (10)	0.0255 (4)
C8 $-0.12791(15)$ $0.59650(13)$ $0.38169(10)$ $0.0244(4)$ C9 $-0.22116(15)$ $0.56725(14)$ $0.40596(11)$ $0.0284(4)$ C26 $0.48822(15)$ $0.67477(13)$ $0.12575(10)$ $0.0258(4)$ C4 $-0.03558(18)$ $0.81635(15)$ $0.23040(11)$ $0.0360(2)$ H4A 0.0233 0.7818 0.2249 $0.054*$ H4B -0.0316 0.8790 0.2141 $0.054*$ H4C -0.0977 0.7876 0.2025 $0.054*$ C35 $0.4302(3)$ $0.61854(19)$ $0.46227(13)$ $0.0566(6)$ H35A 0.3677 0.5845 0.4599 $0.085*$ H35B 0.4589 0.6395 0.5106 $0.085*$ H35C 0.4790 0.5789 0.4479 $0.085*$ H17A 0.3823 0.4626 0.3422 $0.057*$	H25	0.3882	0.6425	0.0330	0.031*
C9-0.22116 (15)0.56725 (14)0.40596 (11)0.0284 (4)C260.48822 (15)0.67477 (13)0.12575 (10)0.0258 (4)C4-0.03558 (18)0.81635 (15)0.23040 (11)0.0360 (5)H4A0.02330.78180.22490.054*H4B-0.03160.87900.21410.054*H4C-0.09770.78760.20250.054*C350.4302 (3)0.61854 (19)0.46227 (13)0.0566 (5)H35B0.45890.63950.51060.085*H35C0.47900.57890.44790.085*C170.35026 (17)0.41501 (16)0.36411 (12)0.0381 (5)H17A0.38230.46260.34220.057*	C8	-0.12791 (15)	0.59650 (13)	0.38169 (10)	0.0244 (4)
C260.48822 (15)0.67477 (13)0.12575 (10)0.0258 (4)C4-0.03558 (18)0.81635 (15)0.23040 (11)0.0360 (4)H4A0.02330.78180.22490.054*H4B-0.03160.87900.21410.054*H4C-0.09770.78760.20250.054*C350.4302 (3)0.61854 (19)0.46227 (13)0.0566 (6)H35A0.36770.58450.45990.085*H35B0.45890.63950.51060.085*H35C0.47900.57890.44790.085*C170.35026 (17)0.41501 (16)0.36411 (12)0.0381 (2)H17A0.38230.46260.34220.057*	C9	-0.22116 (15)	0.56725 (14)	0.40596 (11)	0.0284 (4)
C4-0.03558 (18)0.81635 (15)0.23040 (11)0.0360 (3)H4A0.02330.78180.22490.054*H4B-0.03160.87900.21410.054*H4C-0.09770.78760.20250.054*C350.4302 (3)0.61854 (19)0.46227 (13)0.0566 (3)H35A0.36770.58450.45990.085*H35B0.45890.63950.51060.085*H35C0.47900.57890.44790.085*C170.35026 (17)0.41501 (16)0.36411 (12)0.0381 (3)H17A0.38230.46260.34220.057*	C26	0.48822 (15)	0.67477 (13)	0.12575 (10)	0.0258 (4)
H4A0.02330.78180.22490.054*H4B-0.03160.87900.21410.054*H4C-0.09770.78760.20250.054*C350.4302 (3)0.61854 (19)0.46227 (13)0.0566 (3)H35A0.36770.58450.45990.085*H35B0.45890.63950.51060.085*H35C0.47900.57890.44790.085*C170.35026 (17)0.41501 (16)0.36411 (12)0.0381 (2)H17A0.38230.46260.34220.057*	C4	-0.03558 (18)	0.81635 (15)	0.23040 (11)	0.0360 (5)
H4B-0.03160.87900.21410.054*H4C-0.09770.78760.20250.054*C350.4302 (3)0.61854 (19)0.46227 (13)0.0566 (3)H35A0.36770.58450.45990.085*H35B0.45890.63950.51060.085*H35C0.47900.57890.44790.085*C170.35026 (17)0.41501 (16)0.36411 (12)0.0381 (2)H17A0.38230.46260.34220.057*	H4A	0.0233	0.7818	0.2249	0.054*
H4C-0.09770.78760.20250.054*C350.4302 (3)0.61854 (19)0.46227 (13)0.0566 (3)H35A0.36770.58450.45990.085*H35B0.45890.63950.51060.085*H35C0.47900.57890.44790.085*C170.35026 (17)0.41501 (16)0.36411 (12)0.0381 (3)H17A0.38230.46260.34220.057*	H4B	-0.0316	0.8790	0.2141	0.054*
C350.4302 (3)0.61854 (19)0.46227 (13)0.0566 (3)H35A0.36770.58450.45990.085*H35B0.45890.63950.51060.085*H35C0.47900.57890.44790.085*C170.35026 (17)0.41501 (16)0.36411 (12)0.0381 (3)H17A0.38230.46260.34220.057*	H4C	-0.0977	0.7876	0.2025	0.054*
H35A0.36770.58450.45990.085*H35B0.45890.63950.51060.085*H35C0.47900.57890.44790.085*C170.35026 (17)0.41501 (16)0.36411 (12)0.0381 (2000)H17A0.38230.46260.34220.057*H17D0.28270.25620.26050.057*	C35	0.4302 (3)	0.61854 (19)	0.46227 (13)	0.0566 (8)
H35B0.45890.63950.51060.085*H35C0.47900.57890.44790.085*C170.35026 (17)0.41501 (16)0.36411 (12)0.0381 (12)H17A0.38230.46260.34220.057*H17D0.28270.25620.26050.057*	H35A	0.3677	0.5845	0.4599	0.085*
H35C0.47900.57890.44790.085*C170.35026 (17)0.41501 (16)0.36411 (12)0.0381 (300)H17A0.38230.46260.34220.057*U17D0.28270.25620.26050.057*	H35B	0.4589	0.6395	0.5106	0.085*
C170.35026 (17)0.41501 (16)0.36411 (12)0.0381 (30)H17A0.38230.46260.34220.057*U17D0.28270.25620.26050.057*	H35C	0.4790	0.5789	0.4479	0.085*
H17A 0.3823 0.4626 0.3422 0.057*	C17	0.35026 (17)	0.41501 (16)	0.36411 (12)	0.0381 (5)
U17D 0.2227 0.2562 0.2605 0.057*	H17A	0.3823	0.4626	0.3422	0.057*
n1/b 0.382/ 0.3502 0.3003 0.05/*	H17B	0.3827	0.3562	0.3605	0.057*

H17C	0.3579	0.4299	0.4138	0.057*
C5	0.05595 (18)	0.86917 (14)	0.35161 (12)	0.0374 (5)
H5A	0.0538	0.8711	0.4010	0.056*
H5B	0.0555	0.9315	0.3335	0.056*
H5C	0.1178	0.8380	0.3479	0.056*
C30	0.67305 (17)	0.72050 (19)	0.14855 (12)	0.0439 (6)
H30A	0.6591	0.7790	0.1683	0.066*
H30B	0.7289	0.7279	0.1262	0.066*
H30C	0.6917	0.6752	0.1863	0.066*
C27	0.57872 (15)	0.68851 (14)	0.09393 (11)	0.0295 (4)
C32	0.40933 (14)	0.66789 (13)	0.22385 (9)	0.0230 (4)
C37	0.87357 (19)	0.51175 (18)	0.19483 (13)	0.0437 (6)
H37A	0.8058	0.5096	0.1614	0.052*
H37B	0.8678	0.5466	0.2368	0.052*
C29	0.55214 (17)	0.76021 (15)	0.03504 (12)	0.0358 (5)
H29A	0.5363	0.8183	0.0545	0.054*
H29B	0.4933	0.7396	-0.0015	0.054*
H29C	0.6099	0.7685	0.0146	0.054*
C28	0.60274 (19)	0.59837 (15)	0.06249 (13)	0.0398 (5)
H28A	0.6606	0.6068	0.0422	0.060*
H28B	0.5437	0.5786	0.0256	0.060*
H28C	0.6193	0.5519	0.0995	0.060*
C36	0.3316 (2)	0.7614 (2)	0.43351 (13)	0.0629 (9)
H36A	0.3173	0.8129	0.4007	0.094*
H36B	0.3590	0.7841	0.4815	0.094*
H36C	0.2688	0.7277	0.4311	0.094*
C10	-0.2250 (3)	0.6212 (2)	0.47101 (18)	0.0754 (11)
H10A	-0.2275	0.6865	0.4601	0.113*
H10B	-0.1645	0.6081	0.5089	0.113*
H10C	-0.2856	0.6040	0.4860	0.113*
C12	-0.2184 (2)	0.46734 (19)	0.4255 (2)	0.0779 (11)
H12A	-0.2801	0.4516	0.4397	0.117*
H12B	-0.1591	0.4555	0.4646	0.117*
H12C	-0.2143	0.4303	0.3849	0.117*
C11	-0.3154 (2)	0.5852 (3)	0.34809 (19)	0.0842 (12)
H11A	-0.3750	0.5660	0.3635	0.126*
H11B	-0.3123	0.5506	0.3060	0.126*
H11C	-0.3203	0.6504	0.3371	0.126*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn1	0.02082 (12)	0.02398 (12)	0.02386 (12)	-0.00122 (9)	0.00912 (9)	0.00045 (8)
01	0.0244 (7)	0.0247 (7)	0.0362 (7)	-0.0010 (5)	0.0151 (6)	0.0008 (6)
N2	0.0242 (8)	0.0261 (8)	0.0197 (7)	-0.0019 (7)	0.0038 (6)	0.0007 (6)
N1	0.0239 (8)	0.0229 (8)	0.0248 (8)	0.0020 (6)	0.0098 (7)	0.0011 (6)
02	0.0219 (7)	0.0388 (8)	0.0227 (7)	-0.0043 (6)	0.0069 (5)	-0.0003 (6)
C1	0.0219 (9)	0.0256 (9)	0.0192 (8)	-0.0018 (7)	0.0067 (7)	-0.0016 (7)

C19	0.0215 (9)	0.0208 (9)	0.0246 (9)	0.0003 (7)	0.0061 (7)	0.0019 (7)
C2	0.0261 (10)	0.0232 (9)	0.0221 (9)	0.0012 (8)	0.0075 (8)	-0.0015 (7)
C7	0.0241 (10)	0.0260 (9)	0.0267 (9)	0.0033 (8)	0.0092 (8)	-0.0021 (8)
C14	0.0214 (9)	0.0249 (9)	0.0226 (9)	0.0001 (7)	0.0064 (7)	-0.0004 (7)
C13	0.0268 (10)	0.0243 (9)	0.0234 (9)	-0.0007 (8)	0.0089 (8)	0.0018 (7)
C15	0.0264 (10)	0.0223 (9)	0.0233 (9)	-0.0011 (7)	0.0076 (8)	0.0028 (7)
C21	0.0268 (10)	0.0279 (10)	0.0230 (9)	-0.0014 (8)	0.0035 (8)	-0.0007 (8)
C16	0.0266 (10)	0.0233 (9)	0.0365 (11)	0.0045 (8)	0.0149 (9)	0.0039 (8)
C18	0.0449 (13)	0.0316 (11)	0.0401 (12)	0.0075 (10)	0.0108 (10)	-0.0073 (9)
C24	0.0287 (11)	0.0368 (11)	0.0313 (10)	0.0033 (9)	0.0020 (9)	0.0015 (9)
C33	0.0216 (9)	0.0266 (9)	0.0236 (9)	-0.0022 (8)	0.0043 (8)	0.0012 (7)
C34	0.0287 (11)	0.0395 (11)	0.0191 (9)	-0.0070 (9)	0.0039 (8)	-0.0025 (8)
C23	0.0374 (12)	0.0312 (11)	0.0344 (11)	-0.0091 (9)	0.0026 (9)	-0.0014 (9)
C3	0.0294 (11)	0.0239 (9)	0.0332 (10)	0.0031 (8)	0.0133 (9)	0.0020 (8)
Cl1	0.0483 (4)	0.0510 (4)	0.0571 (4)	-0.0032 (3)	0.0053 (3)	-0.0029 (3)
Cl2	0.0979 (6)	0.0661 (5)	0.0702 (5)	-0.0349 (4)	0.0430 (5)	-0.0148 (4)
C6	0.0418 (13)	0.0267 (11)	0.0575 (15)	0.0087 (9)	0.0253 (12)	0.0071 (10)
C20	0.0221 (9)	0.0211 (9)	0.0208 (8)	0.0005 (7)	0.0042 (7)	0.0008 (7)
C31	0.0221 (9)	0.0295 (10)	0.0243 (9)	-0.0024 (8)	0.0048 (8)	0.0009 (8)
C22	0.0363 (12)	0.0459 (13)	0.0236 (10)	-0.0045 (10)	0.0033 (9)	-0.0043 (9)
C25	0.0288 (10)	0.0283 (9)	0.0204 (9)	0.0001 (8)	0.0080 (8)	0.0006 (8)
C8	0.0233 (10)	0.0293 (10)	0.0227 (9)	-0.0002 (8)	0.0097 (8)	-0.0013 (7)
C9	0.0246 (10)	0.0299 (10)	0.0353 (11)	0.0005 (8)	0.0159 (9)	0.0018 (8)
C26	0.0250 (10)	0.0279 (10)	0.0267 (9)	-0.0002 (8)	0.0105 (8)	0.0023 (8)
C4	0.0406 (13)	0.0345 (11)	0.0354 (11)	0.0045 (10)	0.0142 (10)	0.0080 (9)
C35	0.079 (2)	0.0570 (16)	0.0265 (12)	0.0163 (15)	0.0008 (13)	0.0044 (11)
C17	0.0335 (12)	0.0380 (12)	0.0433 (13)	0.0112 (10)	0.0108 (10)	0.0025 (10)
C5	0.0428 (13)	0.0269 (11)	0.0440 (13)	-0.0043 (9)	0.0140 (11)	-0.0028 (9)
C30	0.0271 (12)	0.0695 (17)	0.0386 (12)	-0.0089 (11)	0.0146 (10)	-0.0034 (12)
C27	0.0255 (10)	0.0361 (11)	0.0295 (10)	-0.0017 (8)	0.0116 (8)	0.0005 (8)
C32	0.0224 (9)	0.0240 (9)	0.0229 (9)	-0.0010 (7)	0.0061 (7)	0.0017 (7)
C37	0.0384 (13)	0.0545 (15)	0.0381 (12)	0.0002 (11)	0.0093 (10)	-0.0028 (11)
C29	0.0393 (12)	0.0345 (11)	0.0385 (12)	-0.0044 (9)	0.0188 (10)	0.0030 (9)
C28	0.0398 (13)	0.0386 (12)	0.0483 (13)	0.0059 (10)	0.0244 (11)	0.0020 (10)
C36	0.076 (2)	0.0688 (19)	0.0339 (13)	0.0311 (16)	-0.0052 (13)	-0.0218 (13)
C10	0.091 (2)	0.082 (2)	0.078 (2)	-0.0284 (18)	0.067 (2)	-0.0262 (17)
C12	0.0624 (19)	0.0434 (15)	0.155 (3)	0.0052 (14)	0.077 (2)	0.0251 (18)
C11	0.0269 (14)	0.144 (3)	0.078 (2)	-0.0172 (17)	0.0057 (14)	0.044 (2)

Geometric parameters (Å, °)

Zn1—O1	1.9138 (13)	C20—C25	1.380 (3)	
Zn1—O2	1.9163 (13)	C31—C26	1.367 (3)	
Zn1—N1	2.0001 (15)	C31—C32	1.422 (3)	
Zn1—N2	2.0105 (16)	C31—H31	0.9500	
01—C1	1.302 (2)	C22—H22A	0.9800	
N2—C33	1.289 (2)	C22—H22B	0.9800	
N2—C34	1.483 (2)	C22—H22C	0.9800	

N1—C15	1.290 (2)	C25—C26	1.412 (3)
N1—C16	1.482 (2)	C25—H25	0.9500
Ω^2 —C19	1.303 (2)	C8—C9	1.532 (3)
C1-C14	1.425 (3)	C9—C11	1.508 (4)
C1-C2	1438(3)	<u>C9</u> C12	1 513 (3)
C_{19} C_{32}	1.138(3)	C9 - C10	1.515(3)
$C_{19} - C_{20}$	1.410(3) 1 444(3)	C^{26}	1.517(3) 1.535(3)
$C_{2}^{-}C_{7}^{7}$	1.111(3) 1.382(3)	C4 - H4A	0.9800
$C_2 - C_3$	1.532(3)	C4 - H4B	0.9800
$C_2 - C_3$	1.556(5) 1 409(3)	C4 - H4C	0.9800
С7—Н7	0.9500	C35_H35A	0.9800
$C_1 = C_1 $	1.415(3)	C35_H35R	0.9800
$C_{14} = C_{15}$	1.415(3) 1.447(3)	C35_H35C	0.9800
C_{14}	1.447(3) 1.372(3)	C17 H17A	0.9800
$C_{13} = C_{6}$	1.372 (3)	C17_H17R	0.9800
C15_H15	0.9300	C1/-H1/B	0.9800
C13—H13	0.9300		0.9800
$C_{21} - C_{22}$	1.551(5) 1.525(2)	C5—H5A	0.9800
$C_{21} - C_{20}$	1.535 (5)	C5—H5B	0.9800
$C_{21} - C_{24}$	1.536 (3)	CS—HSC	0.9800
C21—C23	1.538 (3)	C_{30} C_{27}	1.526 (3)
	1.514 (3)	C30—H30A	0.9800
C16—C18	1.517 (3)	C30—H30B	0.9800
C16—H16	1.0000	C30—H30C	0.9800
C18—H18A	0.9800	C27—C28	1.530 (3)
C18—H18B	0.9800	C27—C29	1.538 (3)
C18—H18C	0.9800	С37—Н37А	0.9900
C24—H24A	0.9800	С37—Н37В	0.9900
C24—H24B	0.9800	С29—Н29А	0.9800
C24—H24C	0.9800	C29—H29B	0.9800
C33—C32	1.445 (3)	С29—Н29С	0.9800
С33—Н33	0.9500	C28—H28A	0.9800
C34—C36	1.499 (3)	C28—H28B	0.9800
C34—C35	1.502 (3)	C28—H28C	0.9800
C34—H34	1.0000	C36—H36A	0.9800
C23—H23A	0.9800	C36—H36B	0.9800
С23—Н23В	0.9800	С36—Н36С	0.9800
С23—Н23С	0.9800	C10—H10A	0.9800
C3—C5	1.534 (3)	C10—H10B	0.9800
C3—C6	1.537 (3)	C10—H10C	0.9800
C3—C4	1.538 (3)	C12—H12A	0.9800
Cl1—C37	1.763 (3)	C12—H12B	0.9800
Cl2—C37	1.741 (3)	C12—H12C	0.9800
С6—Н6А	0.9800	C11—H11A	0.9800
С6—Н6В	0.9800	C11—H11B	0.9800
С6—Н6С	0.9800	C11—H11C	0.9800
		-	
01—Zn1—O2	111.62 (6)	H22B—C22—H22C	109.5
01—Zn1—N1	96.67 (6)	C20—C25—C26	124.69 (17)
	× /		()

O2—Zn1—N1	115.89 (6)	C20—C25—H25	117.7
01-Zn1-N2	114.73 (6)	C26—C25—H25	117.7
Ω_2 —Zn1—N2	96.21 (6)	C13—C8—C7	116.22 (17)
N1 - Zn1 - N2	122.59 (6)	C13—C8—C9	123.19 (17)
C1 - O1 - Zn1	127 12 (12)	C7—C8—C9	120.58(17)
$C_{33} = N^2 = C_{34}$	117.05 (16)	$C_{11} - C_{9} - C_{12}$	108.7(3)
$C_{33} = N_2 = Z_n 1$	118 72 (13)	$C_{11} - C_{9} - C_{10}$	109.8(3)
$C_{34} N_{2} Z_{n1}$	$124\ 10\ (12)$	C12 - C9 - C10	107.2(2)
C_{15} N1 $-C_{16}$	117.05(16)	$C_{11} - C_{9} - C_{8}$	107.2(2) 109.53(18)
C15 - N1 - 7n1	119 19 (13)	C12 - C9 - C8	112 46 (17)
C16 - N1 - 7n1	123 36 (12)	C10-C9-C8	109 12 (19)
C10 - 02 - 7n1	125.50(12) 127.14(12)	$C_{10} = C_{20} = C_{20}$	116.67(17)
$C_{1}^{-} = C_{2}^{-} = Z_{1}^{-} C_{1}^{-} $	127.14(12) 122.61(17)	$C_{31} = C_{20} = C_{23}$	123.65(18)
01 - 01 - 02	122.01(17) 110.85(17)	$C_{20} = C_{20} = C_{27}$	123.03(10) 110.68(17)
$C_1 = C_1 = C_2$	117.53 (16)	$C_{23} = C_{20} = C_{27}$	100.5
$C_1 + C_1 - C_2$	117.35(10) 122.75(17)	$C_3 = C_4 = H_4 R_1$	109.5
02 - C19 - C32	122.73(17) 110.47(17)	$C_3 - C_4 - H_4 D$	109.5
$C_{2} = C_{19} = C_{20}$	117.78 (16)	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	109.5
$C_{2}^{-} = C_{1}^{-} = C_{2}^{-} $	117.78(10) 118.41(17)		109.5
$C_{7} = C_{2} = C_{1}$	110.41(17) 121.52(17)	H4P C4 H4C	109.5
$C_{1} = C_{2} = C_{3}$	121.32(17) 120.05(16)	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	109.5
$C_1 = C_2 = C_3$	120.03(10) 124.00(18)	$C_{34} = C_{35} = H_{35R}$	109.5
$C_2 = C_7 = C_3$	117.6	$H_{254} = C_{35} = H_{35B}$	109.5
$C_2 = C_7 = H_7$	117.6	C_{24} C_{25} H_{25} H_{25}	109.5
C_{3} C_{14} $C_$	120 40 (17)	$H_{354} = C_{35} = H_{35C}$	109.5
C_{13} C_{14} C_{15}	120.40(17) 114.75(16)	H35B_C35_H35C	109.5
$C_{1} = C_{14} = C_{15}$	124.70(16)	$C_{16} C_{17} H_{17A}$	109.5
$C_{1}^{$	124.70(10) 122.40(17)	C16 C17 H17B	109.5
$C_{8} = C_{13} = C_{14}$	1122.49 (17)	H17A C17 H17B	109.5
C_{14} C_{13} H_{13}	118.8	C16 C17 H17C	109.5
N1 C15 C14	120 42 (17)	H_{17} C_{17} H_{17} C_{17}	109.5
N1_C15_H15	115.3	H17B_C17_H17C	109.5
C14 - C15 - H15	115.3	$C_3 - C_5 - H_5 \Delta$	109.5
C_{22} C_{21} C_{20}	112.22 (17)	C3_C5_H5B	109.5
$C_{22} = C_{21} = C_{20}$	107.39(17)	H5A_C5_H5B	109.5
$C_{22} = C_{21} = C_{24}$	110.06 (16)	C3_C5_H5C	109.5
$C_{20} = C_{21} = C_{24}$	106 78 (17)	H5A_C5_H5C	109.5
$C_{22} = C_{21} = C_{23}$	110.21(16)	H5B_C5_H5C	109.5
$C_{20} = C_{21} = C_{23}$	110.09 (18)	C_{27} C_{30} H_{30A}	109.5
$N_1 - C_{16} - C_{17}$	110.09(10) 110.34(17)	C27—C30—H30R	109.5
N1-C16-C18	109.12 (16)	$H_{30A} - C_{30} - H_{30B}$	109.5
C17 - C16 - C18	111 04 (18)	C_{27} C_{30} H_{30C}	109.5
N1-C16-H16	108.8	$H_{30A} - C_{30} - H_{30C}$	109.5
C17—C16—H16	108.8	H_{30B} C_{30} H_{30C}	109.5
C18—C16—H16	108.8	C_{30} $-C_{27}$ $-C_{28}$	108.68 (19)
C16—C18—H18A	109.5	C_{30} C_{27} C_{26}	112.16(17)
C16—C18—H18B	109.5	C28—C27—C26	109.24 (17)
H18A—C18—H18B	109.5	C30—C27—C29	108.32 (18)

C16—C18—H18C	109.5	C28—C27—C29	108.69 (17)
H18A—C18—H18C	109.5	C26—C27—C29	109.68 (17)
H18B—C18—H18C	109.5	C19—C32—C31	120.46 (16)
C21—C24—H24A	109.5	C19—C32—C33	124.51 (17)
C21—C24—H24B	109.5	C31—C32—C33	115.00 (17)
H24A—C24—H24B	109.5	Cl2—C37—Cl1	111.36 (14)
C21—C24—H24C	109.5	Cl2—C37—H37A	109.4
H24A—C24—H24C	109.5	Cl1—C37—H37A	109.4
H24B—C24—H24C	109.5	Cl2—C37—H37B	109.4
N2—C33—C32	129.84 (18)	Cl1—C37—H37B	109.4
N2—C33—H33	115.1	H37A—C37—H37B	108.0
С32—С33—Н33	115.1	C27—C29—H29A	109.5
N2-C34-C36	109.88 (17)	C27—C29—H29B	109.5
N2-C34-C35	110.76 (18)	H29A—C29—H29B	109.5
C36—C34—C35	111.3 (2)	С27—С29—Н29С	109.5
N2—C34—H34	108.3	H29A—C29—H29C	109.5
C36—C34—H34	108.3	H29B—C29—H29C	109.5
С35—С34—Н34	108.3	C27—C28—H28A	109.5
C21—C23—H23A	109.5	C27—C28—H28B	109.5
С21—С23—Н23В	109.5	H28A—C28—H28B	109.5
H23A—C23—H23B	109.5	C27—C28—H28C	109.5
C21—C23—H23C	109.5	H28A—C28—H28C	109.5
H23A—C23—H23C	109.5	H28B—C28—H28C	109.5
H23B—C23—H23C	109.5	C34—C36—H36A	109.5
C5—C3—C6	107.14 (17)	С34—С36—Н36В	109.5
C5—C3—C4	109.82 (17)	H36A—C36—H36B	109.5
C6—C3—C4	107.07 (18)	C34—C36—H36C	109.5
C5—C3—C2	111.19 (17)	H36A—C36—H36C	109.5
C6—C3—C2	111.92 (16)	H36B—C36—H36C	109.5
C4—C3—C2	109.58 (16)	C9—C10—H10A	109.5
С3—С6—Н6А	109.5	C9—C10—H10B	109.5
С3—С6—Н6В	109.5	H10A—C10—H10B	109.5
H6A—C6—H6B	109.5	C9—C10—H10C	109.5
C3—C6—H6C	109.5	H10A—C10—H10C	109.5
H6A—C6—H6C	109.5	H10B—C10—H10C	109.5
H6B—C6—H6C	109.5	C9—C12—H12A	109.5
C25—C20—C19	118.17 (17)	C9—C12—H12B	109.5
C25—C20—C21	121.55 (16)	H12A—C12—H12B	109.5
C19—C20—C21	120.28 (16)	C9—C12—H12C	109.5
C26—C31—C32	122.13 (18)	H12A—C12—H12C	109.5
C26—C31—H31	118.9	H12B—C12—H12C	109.5
C32—C31—H31	118.9	C9—C11—H11A	109.5
C21—C22—H22A	109.5	C9—C11—H11B	109.5
C21—C22—H22B	109.5	H11A—C11—H11B	109.5
H22A—C22—H22B	109.5	C9—C11—H11C	109.5
C21—C22—H22C	109.5	H11A—C11—H11C	109.5
H22A—C22—H22C	109.5	H11B—C11—H11C	109.5

O2—Zn1—O1—C1	117.19 (15)	Zn1—N2—C34—C35	72.3 (2)
N1—Zn1—O1—C1	-4.09 (16)	C7—C2—C3—C5	121.9 (2)
N2—Zn1—O1—C1	-134.71 (14)	C1—C2—C3—C5	-59.4 (2)
O1—Zn1—N2—C33	-122.85 (14)	C7—C2—C3—C6	2.1 (3)
O2—Zn1—N2—C33	-5.58 (15)	C1—C2—C3—C6	-179.21 (18)
N1—Zn1—N2—C33	120.64 (14)	C7—C2—C3—C4	-116.5 (2)
O1—Zn1—N2—C34	52.74 (16)	C1—C2—C3—C4	62.2 (2)
O2—Zn1—N2—C34	170.01 (15)	O2—C19—C20—C25	-177.27 (17)
N1—Zn1—N2—C34	-63.77 (16)	C32—C19—C20—C25	3.2 (3)
O1—Zn1—N1—C15	0.81 (15)	O2-C19-C20-C21	2.6 (3)
O2—Zn1—N1—C15	-117.16 (14)	C32—C19—C20—C21	-176.92 (16)
N2—Zn1—N1—C15	125.89 (14)	C22—C21—C20—C25	-1.1 (3)
O1—Zn1—N1—C16	173.28 (14)	C24—C21—C20—C25	-120.7(2)
O2—Zn1—N1—C16	55.31 (16)	C23—C21—C20—C25	117.7 (2)
N2—Zn1—N1—C16	-61.64 (16)	C22—C21—C20—C19	178.94 (17)
O1—Zn1—O2—C19	128.66 (15)	C24—C21—C20—C19	59.4 (2)
N1—Zn1—O2—C19	-122.00 (15)	C23—C21—C20—C19	-62.2 (2)
N2—Zn1—O2—C19	8.93 (16)	C19—C20—C25—C26	-1.3 (3)
Zn1—O1—C1—C14	7.0 (3)	C21—C20—C25—C26	178.82 (18)
Zn1—O1—C1—C2	-172.01 (12)	C14—C13—C8—C7	-0.2 (3)
Zn1—O2—C19—C32	-5.2 (3)	C14—C13—C8—C9	178.99 (18)
Zn1—O2—C19—C20	175.25 (12)	C2—C7—C8—C13	-0.9 (3)
O1—C1—C2—C7	-179.46 (17)	C2—C7—C8—C9	179.93 (18)
C14—C1—C2—C7	1.5 (3)	C13—C8—C9—C11	-123.5 (3)
O1—C1—C2—C3	1.8 (3)	C7—C8—C9—C11	55.6 (3)
C14—C1—C2—C3	-177.24 (16)	C13—C8—C9—C12	-2.5(3)
C1—C2—C7—C8	0.2 (3)	C7—C8—C9—C12	176.6 (2)
C3—C2—C7—C8	178.92 (18)	C13—C8—C9—C10	116.3 (3)
O1—C1—C14—C13	178.48 (17)	C7—C8—C9—C10	-64.6 (3)
C2-C1-C14-C13	-2.5 (3)	C32—C31—C26—C25	2.3 (3)
O1—C1—C14—C15	-6.2 (3)	C32—C31—C26—C27	-176.98 (18)
C2-C1-C14-C15	172.80 (17)	C20-C25-C26-C31	-1.5 (3)
C1—C14—C13—C8	1.9 (3)	C20—C25—C26—C27	177.80 (18)
C15—C14—C13—C8	-173.86 (17)	C31—C26—C27—C30	-3.3 (3)
C16—N1—C15—C14	-173.53 (18)	C25—C26—C27—C30	177.48 (19)
Zn1—N1—C15—C14	-0.6 (3)	C31—C26—C27—C28	117.3 (2)
C13—C14—C15—N1	178.47 (19)	C25—C26—C27—C28	-62.0 (2)
C1—C14—C15—N1	2.9 (3)	C31—C26—C27—C29	-123.7 (2)
C15—N1—C16—C17	-130.34 (19)	C25—C26—C27—C29	57.1 (2)
Zn1—N1—C16—C17	57.0 (2)	O2—C19—C32—C31	178.00 (17)
C15—N1—C16—C18	107.4 (2)	C20-C19-C32-C31	-2.5 (3)
Zn1—N1—C16—C18	-65.2 (2)	O2—C19—C32—C33	-4.2 (3)
C34—N2—C33—C32	-176.93 (19)	C20—C19—C32—C33	175.34 (17)
Zn1—N2—C33—C32	-1.0 (3)	C26—C31—C32—C19	-0.3 (3)
C33—N2—C34—C36	124.6 (2)	C26—C31—C32—C33	-178.31 (18)
Zn1—N2—C34—C36	-51.1 (2)	N2—C33—C32—C19	7.7 (3)
C33—N2—C34—C35	-112.0 (2)	N2-C33-C32-C31	-174.42 (19)
			(-)

	D—H	H···A	D···A	D—H···A
C4—H4 <i>A</i> …O1	0.98	2.37	3.018 (3)	123
C5—H5 <i>C</i> ···O1	0.98	2.32	2.967 (3)	123
C23—H23 <i>C</i> ···O2	0.98	2.35	2.994 (3)	122
C24—H24A…O2	0.98	2.33	2.986 (3)	124

Hydrogen-bond geometry (Å, °)