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

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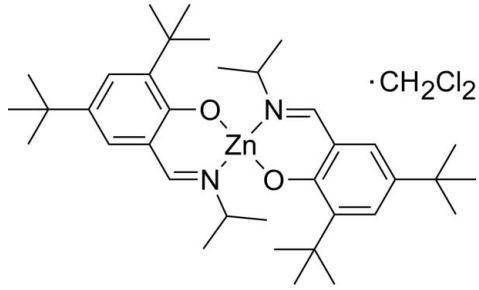
In the title compound, $[Zn(C_{18}H_{28}NO)_2]\cdot CH_2Cl_2$, the Zn^{II} atom is *N*,*O*-chelated by two crystallographically independent salicylaldehyde imine ligands, leading to a distorted tetrahedral coordination sphere. The dihedral angle between the planes of the two metallacycles is 88.69 (6)°. 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, $P2_1/n$
a = 13.6653 (17) Å
b = 14.6674 (18) Å
c = 19.663 (2) Å
β = 104.807 (2)°
V = 3810.4 (8) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.82 mm^{-1}
T = 173 K
0.42 × 0.41 × 0.26 mm

2.2. Data collection

Bruker APEXII area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2007)
T_{min} = 0.725, T_{max} = 0.816
22339 measured reflections
8281 independent reflections
6513 reflections with $I > 2\sigma(I)$
R_{int} = 0.024

2.3. Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.036
$wR(F^2)$ = 0.101
S = 1.03
8281 reflections
413 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.52 e Å^{-3}
$\Delta\rho_{min}$ = −0.37 e Å^{-3}

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C4—H4*A*···O1	0.98	2.37	3.018 (3)	123
C5—H5*C*···O1	0.98	2.32	2.967 (3)	123
C23—H23*C*···O2	0.98	2.35	2.994 (3)	122
C24—H24*A*···O2	0.98	2.33	2.986 (3)	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

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

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supporting information

Acta Cryst. (2014). E**70**, m390–m391 [doi:10.1107/S1600536814022636]

Crystal structure of bis{2,4-di-*tert*-butyl-6-[(isopropylimino)methyl]phenolato-κ^2N,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 salicylaldehyde-imine 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 CH_3 [U_{iso}(H)= 1.5U_{eq}(C)].

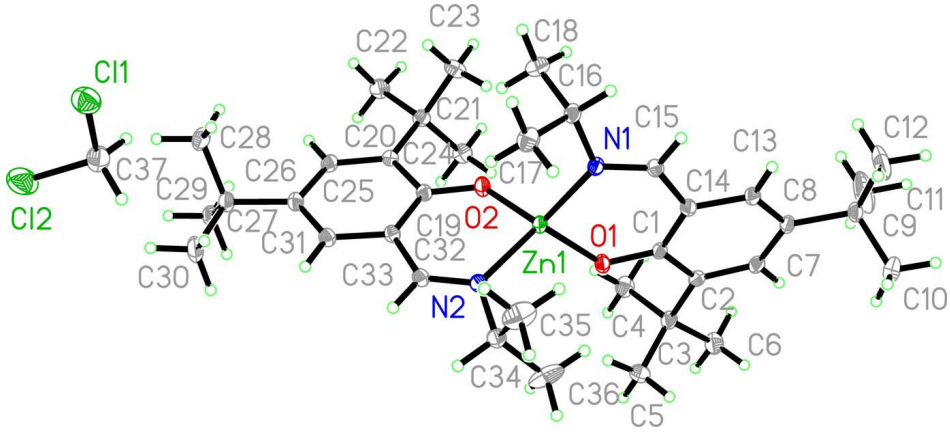

Figure 1

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

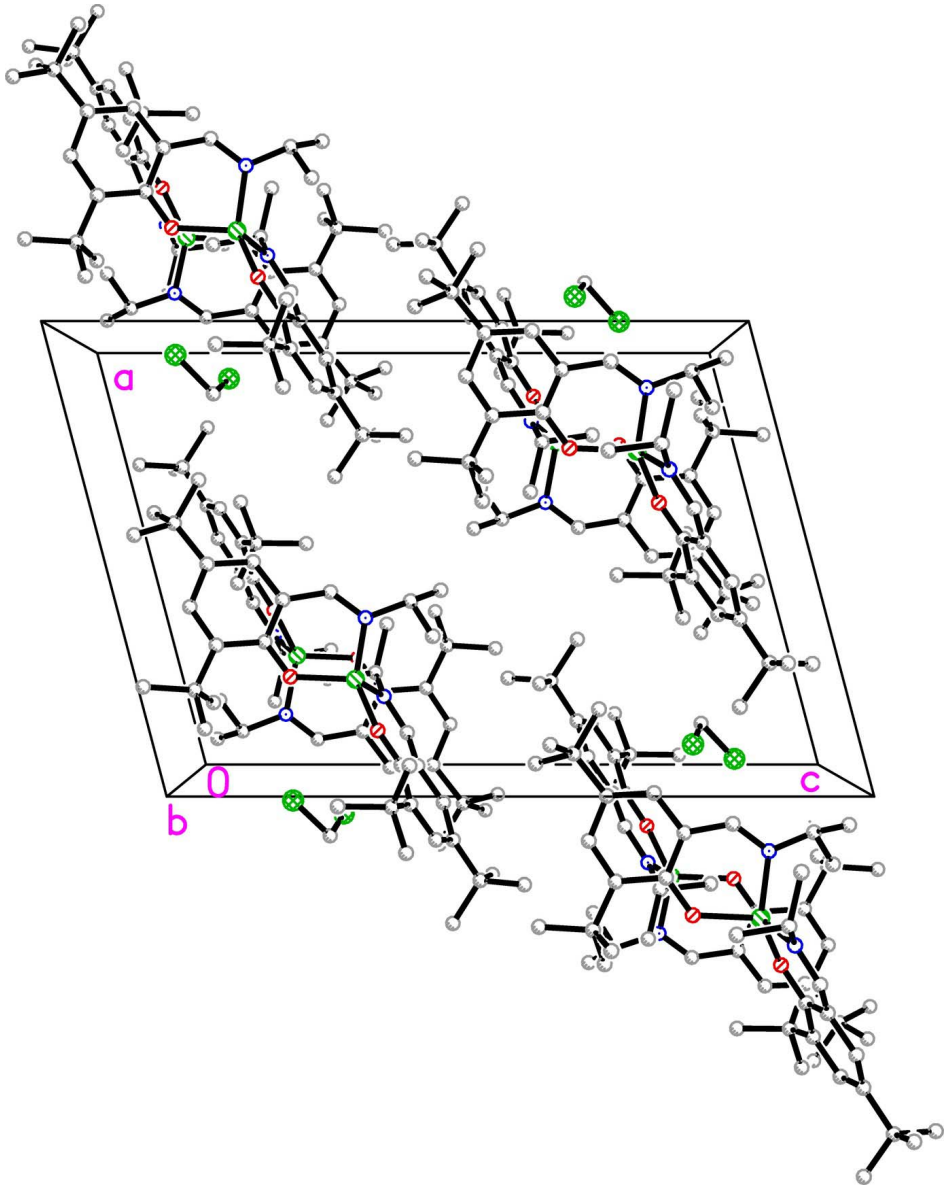

Figure 2

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

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

Crystal data

$[Zn(C_{18}H_{28}NO)_2]\cdot CH_2Cl_2$
$M_r = 699.12$
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
$a = 13.6653\ (17)$ Å
$b = 14.6674\ (18)$ Å
$c = 19.663\ (2)$ Å
$\beta = 104.807\ (2)°$
$V = 3810.4\ (8)$ Å^3
$Z = 4$
$F(000) = 1496$
$D_x = 1.219$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 5049 reflections
$\theta = 2.1–27.0°$
$\mu = 0.82$ mm^{-1}
$T = 173$ K
Block, light-green
0.42 × 0.41 × 0.26 mm

Data collection

Bruker APEXII area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2007)
T_{min} = 0.725, T_{max} = 0.816
22339 measured reflections
8281 independent reflections
6513 reflections with $I > 2\sigma(I)$
R_{int} = 0.024
θ_{max} = 27.1°, θ_{min} = 1.8°
h = −17→8
k = −18→18
l = −25→25

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.036
$wR(F^2)$ = 0.101
S = 1.02
8281 reflections
413 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0501P)^2 + 2.0294P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.52 e Å^{-3}
$\Delta\rho_{min}$ = −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 (Å²)

	x	y	z	U_{iso}*/U_{eq}
Zn1	0.231421 (16)	0.615892 (14)	0.299369 (11)	0.02227 (7)
O1	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)
O2	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)

C16	0.23887 (15)	0.40931 (13)	0.32679 (11)	0.0276 (4)
H16	0.2070	0.3606	0.3496	0.033*
C18	0.22391 (19)	0.38570 (15)	0.24970 (12)	0.0389 (5)
H18A	0.1513	0.3822	0.2268	0.058*
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 (5)
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)	0.68492 (13)	0.29838 (10)	0.0242 (4)
H33	0.4907	0.7113	0.3202	0.029*
C34	0.40723 (16)	0.69940 (14)	0.41395 (10)	0.0295 (4)
H34	0.4714	0.7344	0.4183	0.035*
C23	0.17481 (18)	0.50939 (14)	0.07091 (11)	0.0355 (5)
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 (4)
Cl1	0.91415 (5)	0.39983 (5)	0.22012 (4)	0.05363 (17)
Cl2	0.95759 (7)	0.56715 (6)	0.15546 (4)	0.0742 (3)
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*
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*
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 (5)
H17A	0.3823	0.4626	0.3422	0.057*
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 (Å²)

	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)
O1	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)
O2	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, º)

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
O1—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
O2—C19	1.303 (2)	C8—C9	1.532 (3)
C1—C14	1.425 (3)	C9—C11	1.508 (4)
C1—C2	1.438 (3)	C9—C12	1.513 (3)
C19—C32	1.418 (3)	C9—C10	1.517 (3)
C19—C20	1.444 (3)	C26—C27	1.535 (3)
C2—C7	1.382 (3)	C4—H4A	0.9800
C2—C3	1.538 (3)	C4—H4B	0.9800
C7—C8	1.409 (3)	C4—H4C	0.9800
C7—H7	0.9500	C35—H35A	0.9800
C14—C13	1.415 (3)	C35—H35B	0.9800
C14—C15	1.447 (3)	C35—H35C	0.9800
C13—C8	1.372 (3)	C17—H17A	0.9800
C13—H13	0.9500	C17—H17B	0.9800
C15—H15	0.9500	C17—H17C	0.9800
C21—C22	1.531 (3)	C5—H5A	0.9800
C21—C20	1.535 (3)	C5—H5B	0.9800
C21—C24	1.536 (3)	C5—H5C	0.9800
C21—C23	1.538 (3)	C30—C27	1.526 (3)
C16—C17	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	C37—H37A	0.9900
C24—H24A	0.9800	C37—H37B	0.9900
C24—H24B	0.9800	C29—H29A	0.9800
C24—H24C	0.9800	C29—H29B	0.9800
C33—C32	1.445 (3)	C29—H29C	0.9800
C33—H33	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
C23—H23B	0.9800	C36—H36C	0.9800
C23—H23C	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
C6—H6A	0.9800	C11—H11A	0.9800
C6—H6B	0.9800	C11—H11B	0.9800
C6—H6C	0.9800	C11—H11C	0.9800
O1—Zn1—O2	111.62 (6)	H22B—C22—H22C	109.5
O1—Zn1—N1	96.67 (6)	C20—C25—C26	124.69 (17)

O2—Zn1—N1	115.89 (6)	C20—C25—H25	117.7
O1—Zn1—N2	114.73 (6)	C26—C25—H25	117.7
O2—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)
C33—N2—C34	117.05 (16)	C11—C9—C12	108.7 (3)
C33—N2—Zn1	118.72 (13)	C11—C9—C10	109.8 (3)
C34—N2—Zn1	124.10 (12)	C12—C9—C10	107.2 (2)
C15—N1—C16	117.05 (16)	C11—C9—C8	109.53 (18)
C15—N1—Zn1	119.19 (13)	C12—C9—C8	112.46 (17)
C16—N1—Zn1	123.36 (12)	C10—C9—C8	109.12 (19)
C19—O2—Zn1	127.14 (12)	C31—C26—C25	116.67 (17)
O1—C1—C14	122.61 (17)	C31—C26—C27	123.65 (18)
O1—C1—C2	119.85 (17)	C25—C26—C27	119.68 (17)
C14—C1—C2	117.53 (16)	C3—C4—H4A	109.5
O2—C19—C32	122.75 (17)	C3—C4—H4B	109.5
O2—C19—C20	119.47 (17)	H4A—C4—H4B	109.5
C32—C19—C20	117.78 (16)	C3—C4—H4C	109.5
C7—C2—C1	118.41 (17)	H4A—C4—H4C	109.5
C7—C2—C3	121.52 (17)	H4B—C4—H4C	109.5
C1—C2—C3	120.05 (16)	C34—C35—H35A	109.5
C2—C7—C8	124.90 (18)	C34—C35—H35B	109.5
C2—C7—H7	117.6	H35A—C35—H35B	109.5
C8—C7—H7	117.6	C34—C35—H35C	109.5
C13—C14—C1	120.40 (17)	H35A—C35—H35C	109.5
C13—C14—C15	114.75 (16)	H35B—C35—H35C	109.5
C1—C14—C15	124.70 (16)	C16—C17—H17A	109.5
C8—C13—C14	122.49 (17)	C16—C17—H17B	109.5
C8—C13—H13	118.8	H17A—C17—H17B	109.5
C14—C13—H13	118.8	C16—C17—H17C	109.5
N1—C15—C14	129.42 (17)	H17A—C17—H17C	109.5
N1—C15—H15	115.3	H17B—C17—H17C	109.5
C14—C15—H15	115.3	C3—C5—H5A	109.5
C22—C21—C20	112.22 (17)	C3—C5—H5B	109.5
C22—C21—C24	107.39 (17)	H5A—C5—H5B	109.5
C20—C21—C24	110.06 (16)	C3—C5—H5C	109.5
C22—C21—C23	106.78 (17)	H5A—C5—H5C	109.5
C20—C21—C23	110.21 (16)	H5B—C5—H5C	109.5
C24—C21—C23	110.09 (18)	C27—C30—H30A	109.5
N1—C16—C17	110.34 (17)	C27—C30—H30B	109.5
N1—C16—C18	109.12 (16)	H30A—C30—H30B	109.5
C17—C16—C18	111.04 (18)	C27—C30—H30C	109.5
N1—C16—H16	108.8	H30A—C30—H30C	109.5
C17—C16—H16	108.8	H30B—C30—H30C	109.5
C18—C16—H16	108.8	C30—C27—C28	108.68 (19)
C16—C18—H18A	109.5	C30—C27—C26	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
C32—C33—H33	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)	C27—C29—H29C	109.5
N2—C34—H34	108.3	H29A—C29—H29C	109.5
C36—C34—H34	108.3	H29B—C29—H29C	109.5
C35—C34—H34	108.3	C27—C28—H28A	109.5
C21—C23—H23A	109.5	C27—C28—H28B	109.5
C21—C23—H23B	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)	C34—C36—H36B	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
C3—C6—H6A	109.5	C9—C10—H10B	109.5
C3—C6—H6B	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)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C4—H4*A*···O1	0.98	2.37	3.018 (3)	123
C5—H5*C*···O1	0.98	2.32	2.967 (3)	123
C23—H23*C*···O2	0.98	2.35	2.994 (3)	122
C24—H24*A*···O2	0.98	2.33	2.986 (3)	124