Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Dichloridobis{2-[(triphenylmethyl)amino]pyridine-κN}zinc(II)

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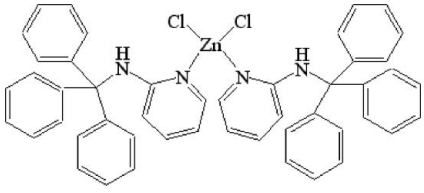
Received 12 July 2007; accepted 24 July 2007

Key indicators: single-crystal X-ray study; T = 273 K; mean σ(C–C) = 0.004 Å; R factor = 0.041; wR factor = 0.093; data-to-parameter ratio = 14.4.

In the title compound, $[ZnCl_2(C_{24}H_{20}N_2)_2]$, the Zn^{II} centre has a distorted tetrahedral geometry defined by two chloride ions and two N atoms of the pyridine rings of the monodentate 2-[(triphenylmethyl)amino]pyridine ligands. Long intramolecular N—H···Cl hydrogen bonds help to establish the three-dimensional architecture.

Related literature

For the isostructural cobalt(II) complex, see Fang *et al.* (2006).



Experimental

Crystal data

$[ZnCl_2(C_{24}H_{20}N_2)_2]$
M_r = 809.11
Monoclinic, $P2_1/n$
a = 10.0020 (11) Å
b = 22.806 (3) Å
c = 17.4859 (19) Å
β = 97.474 (2)°
V = 3954.8 (7) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.80 mm^{-1}
T = 273 (2) K
0.21 × 0.18 × 0.09 mm

Data collection

Bruker SMART APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2003)
T_{min} = 0.851, T_{max} = 0.932
20069 measured reflections
7154 independent reflections
4606 reflections with $I > 2\sigma(I)$
R_{int} = 0.048

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.093
S = 0.98
7154 reflections
496 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.26 e Å^{-3}
$\Delta\rho_{min}$ = −0.25 e Å^{-3}

Table 1
Selected bond lengths (Å).

Zn1—N1	2.069 (2)	Zn1—Cl1	2.2193 (8)
Zn1—N4	2.067 (2)	Zn1—Cl2	2.2218 (8)

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2B···Cl1	0.86	2.62	3.450 (2)	162
N3—H3B···Cl2	0.86	2.66	3.470 (2)	158

Data collection: *APEX2* (Bruker, 2005); cell refinement: *SAINT* (Bruker, 2005); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1997); software used to prepare material for publication: *SHELXTL*.

This work was supported by the Education Office Foundation of Liaoning Province (project No. 605 L207).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB2480).

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Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Sheldrick, G. M. (2003). *SADABS*. University of Göttingen, Germany.

 doi:10.1107/S1600536807036380

supplementary materials

Acta Cryst. (2007). E**63**, m2247 [**doi:10.1107/S1600536807036380**]

Dichloridobis{2-[(triphenylmethyl)amino]pyridine-κ*N*}zinc(II)

G.-N. Zhang, Y. Fang, C.-Y. Huang and W.-S. You

Comment

A new four-coordinated zinc complex (I) (Fig. 1) has been synthesized at room temperature, using 2-[*N*-(triphenylmethyl)imino]pyridyl as ligand. This complex is isomorphic with $CoCl_2(C_{24}H_{20}N_2)_2$ (Fang *et al.*, 2006) and exhibits approximate *C*2 local point symmetry. The Zn atom is tetrahedrally coordinated by atoms Cl1, Cl2, N1 and N4 (Table 1). Because of the large volume of the 2-[*N*-(triphenylmethyl)imino]pyridyl ligand, the formation of a four-coordinate complex is more possible rather than six-coordinate one. Long intramolecular N—H···Cl hydrogen bonds help to establish the three-dimensional architecture (Table 2).

As shown in Fig. 2, the complex molecules stack in the A—B—A—B sequence along the *b* axis.

Experimental

2-[*N*-(triphenylmethyl)imino]pyridine (0.03 g, 0.09 mmol) and $ZnCl_2$ (0.025 g, 7.5 mmol) were dissolved in 3 ml and 5 ml of THF, respectively, then mixed. The mixed solution was stirred about 10 minutes and covered with hexane (10 ml). After three weeks, colourless crystals of (I) were obtained.

Refinement

All H atoms were placed in calculated positions and allowed to ride during subsequent refinement, with C—H = 0.95 Å, N—H=0.88 Å and U_{iso}(H) = 1.2U_{eq}(C,*N*).

Figures

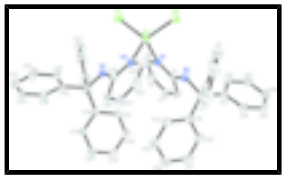

Fig. 1. Molecular structure of (I), showing displacement ellipsids at the 15% probability level. H atoms have been omitted.

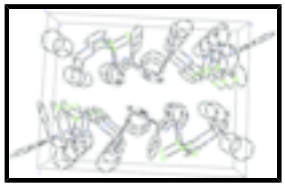

Fig. 2. View of the packing of (I) with the unit cell outlined along the *a* axis, showing the stacking of complex (I). H atoms have been omitted for clarity.

Dichloridobis{2-[(triphenylmethyl)amino]pyridine-κ*N*}zinc(II)

Crystal data

$[ZnCl_2(C_{24}H_{20}N_2)_2]$	$F_{000} = 1680$
$M_r = 809.11$	$D_x = 1.359$ Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
Hall symbol: -P 2yn	Cell parameters from 10562 reflections
$a = 10.0020$ (11) Å	$\theta = 1.0$–$25.3°$
$b = 22.806$ (3) Å	$\mu = 0.80$ mm^{-1}
$c = 17.4859$ (19) Å	$T = 273$ (2) K
$\beta = 97.474$ (2)°	Slab, colourless
$V = 3954.8$ (7) Å^3	0.21 × 0.18 × 0.09 mm
$Z = 4$	

Data collection

Bruker SMART APEXII CCD diffractometer	7154 independent reflections
Radiation source: fine-focus sealed tube	4606 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.048$
$T = 273$(2) K	$\theta_{max} = 25.3°$
CCD scans	$\theta_{min} = 2.1°$
Absorption correction: multi-scan (SADABS; Sheldrick, 2003)	$h = -11 \rightarrow 12$
$T_{min} = 0.851$, $T_{max} = 0.932$	$k = -27 \rightarrow 27$
20069 measured reflections	$l = -17 \rightarrow 20$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.041$	H-atom parameters constrained
$wR(F^2) = 0.093$	$w = 1/[\sigma^2(F_o^2) + (0.0382P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 0.98$	$(\Delta/\sigma)_{max} = 0.014$
7154 reflections	$\Delta\rho_{max} = 0.26$ e Å^{-3}
496 parameters	$\Delta\rho_{min} = -0.25$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

Special details

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

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

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Zn1	0.20829 (3)	0.184545 (14)	0.672517 (19)	0.04241 (12)
Cl1	0.38196 (8)	0.24000 (4)	0.65113 (5)	0.0688 (3)
Cl2	0.18386 (8)	0.10023 (3)	0.60858 (5)	0.0542 (2)
N1	0.0303 (2)	0.23186 (9)	0.65577 (13)	0.0397 (6)
N2	0.1226 (2)	0.31113 (9)	0.72501 (13)	0.0374 (5)
H2B	0.1983	0.2960	0.7169	0.045*
N3	0.0306 (2)	0.10933 (9)	0.77520 (13)	0.0409 (6)
H3B	0.0446	0.1069	0.7278	0.049*
N4	0.2199 (2)	0.16819 (9)	0.78946 (13)	0.0372 (6)
C1	0.0105 (3)	0.28327 (12)	0.69121 (16)	0.0371 (7)
C2	−0.1211 (3)	0.30574 (11)	0.69143 (17)	0.0425 (7)
H2A	−0.1350	0.3402	0.7178	0.051*
C3	−0.2278 (3)	0.27629 (13)	0.65236 (18)	0.0505 (8)
H3A	−0.3148	0.2906	0.6524	0.061*
C4	−0.2071 (3)	0.22538 (13)	0.61273 (18)	0.0546 (9)
H4A	−0.2788	0.2057	0.5847	0.065*
C5	−0.0785 (3)	0.20487 (12)	0.61586 (17)	0.0490 (8)
H5A	−0.0643	0.1706	0.5893	0.059*
C6	0.2808 (3)	0.36848 (11)	0.81083 (16)	0.0373 (7)
C7	0.3823 (3)	0.36604 (12)	0.76456 (19)	0.0494 (8)
H7A	0.3600	0.3615	0.7116	0.059*
C8	0.5154 (3)	0.37011 (14)	0.7951 (2)	0.0673 (10)
H8A	0.5826	0.3679	0.7631	0.081*
C9	0.5489 (4)	0.37745 (15)	0.8733 (3)	0.0763 (12)
H9A	0.6390	0.3790	0.8947	0.092*
C10	0.4501 (4)	0.38241 (16)	0.9193 (2)	0.0772 (11)
H10A	0.4727	0.3893	0.9718	0.093*
C11	0.3167 (3)	0.37737 (14)	0.88887 (19)	0.0594 (9)
H11A	0.2501	0.3800	0.9212	0.071*
C12	0.1315 (2)	0.36419 (11)	0.77412 (15)	0.0346 (6)
C13	0.1005 (3)	0.41989 (11)	0.72485 (17)	0.0372 (7)
C14	0.1290 (3)	0.47495 (12)	0.75785 (18)	0.0466 (8)
H14A	0.1653	0.4775	0.8095	0.056*

C15	0.1042 (3)	0.52547 (13)	0.7153 (2)	0.0568 (9)
H15A	0.1216	0.5617	0.7389	0.068*
C16	0.0545 (3)	0.52296 (15)	0.6390 (2)	0.0648 (10)
H16A	0.0383	0.5572	0.6105	0.078*
C17	0.0285 (3)	0.46927 (15)	0.6047 (2)	0.0625 (9)
H17A	−0.0056	0.4671	0.5527	0.075*
C18	0.0529 (3)	0.41828 (13)	0.64725 (17)	0.0477 (8)
H18A	0.0367	0.3822	0.6230	0.057*
C19	0.0425 (3)	0.35623 (11)	0.83840 (15)	0.0364 (7)
C20	−0.0364 (3)	0.39970 (12)	0.86408 (17)	0.0431 (7)
H20A	−0.0489	0.4347	0.8368	0.052*
C21	−0.0972 (3)	0.39191 (13)	0.92989 (18)	0.0497 (8)
H21A	−0.1481	0.4221	0.9471	0.060*
C22	−0.0835 (3)	0.34015 (14)	0.97023 (18)	0.0524 (8)
H22A	−0.1243	0.3352	1.0146	0.063*
C23	−0.0086 (3)	0.29585 (13)	0.94400 (18)	0.0508 (8)
H23A	0.0004	0.2603	0.9703	0.061*
C24	0.0530 (3)	0.30366 (12)	0.87916 (17)	0.0442 (7)
H24A	0.1030	0.2731	0.8620	0.053*
C25	0.1263 (3)	0.13813 (11)	0.82368 (16)	0.0364 (7)
C26	0.1330 (3)	0.13687 (12)	0.90385 (16)	0.0445 (7)
H26A	0.0680	0.1168	0.9270	0.053*
C27	0.2352 (3)	0.16520 (13)	0.94814 (18)	0.0522 (8)
H27A	0.2396	0.1647	1.0016	0.063*
C28	0.3319 (3)	0.19449 (13)	0.91378 (19)	0.0536 (8)
H28A	0.4028	0.2137	0.9433	0.064*
C29	0.3209 (3)	0.19459 (12)	0.83550 (18)	0.0463 (8)
H29A	0.3868	0.2140	0.8123	0.056*
C30	−0.0681 (3)	0.02180 (12)	0.83451 (16)	0.0400 (7)
C31	0.0595 (3)	0.00155 (13)	0.85977 (17)	0.0462 (8)
H31A	0.1338	0.0240	0.8514	0.055*
C32	0.0790 (3)	−0.05162 (13)	0.89734 (18)	0.0546 (8)
H32A	0.1661	−0.0643	0.9148	0.065*
C33	−0.0291 (3)	−0.08587 (13)	0.90904 (18)	0.0565 (9)
H33A	−0.0158	−0.1217	0.9343	0.068*
C34	−0.1571 (3)	−0.06679 (13)	0.88316 (19)	0.0582 (9)
H34A	−0.2310	−0.0897	0.8910	0.070*
C35	−0.1765 (3)	−0.01386 (13)	0.84577 (18)	0.0509 (8)
H35A	−0.2636	−0.0017	0.8277	0.061*
C36	−0.1688 (3)	0.12494 (12)	0.84274 (17)	0.0419 (7)
C37	−0.1913 (3)	0.18148 (13)	0.81464 (19)	0.0538 (8)
H37A	−0.1603	0.1922	0.7687	0.065*
C38	−0.2584 (3)	0.22170 (14)	0.8536 (2)	0.0623 (9)
H38A	−0.2753	0.2589	0.8329	0.075*
C39	−0.3011 (3)	0.20764 (16)	0.9228 (2)	0.0671 (10)
H39A	−0.3451	0.2353	0.9496	0.081*
C40	−0.2781 (3)	0.15248 (16)	0.9517 (2)	0.0650 (10)
H40A	−0.3066	0.1426	0.9985	0.078*
C41	−0.2128 (3)	0.11109 (14)	0.91195 (19)	0.0532 (8)

H41A	−0.1985	0.0736	0.9322	0.064*
C42	−0.0958 (3)	0.08155 (12)	0.79461 (16)	0.0394 (7)
C43	−0.1807 (3)	0.06963 (11)	0.71533 (17)	0.0423 (7)
C44	−0.3136 (3)	0.08702 (13)	0.69783 (19)	0.0541 (9)
H44A	−0.3559	0.1064	0.7348	0.065*
C45	−0.3841 (4)	0.07584 (15)	0.6259 (2)	0.0692 (11)
H45A	−0.4737	0.0875	0.6152	0.083*
C46	−0.3238 (4)	0.04807 (15)	0.5709 (2)	0.0692 (11)
H46A	−0.3710	0.0420	0.5221	0.083*
C47	−0.1932 (4)	0.02886 (14)	0.5873 (2)	0.0649 (10)
H47A	−0.1519	0.0095	0.5499	0.078*
C48	−0.1228 (3)	0.03851 (13)	0.66026 (19)	0.0528 (8)
H48A	−0.0357	0.0239	0.6721	0.063*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn1	0.0464 (2)	0.0439 (2)	0.0381 (2)	−0.00337 (16)	0.01008 (16)	−0.00190 (17)
Cl1	0.0696 (6)	0.0687 (6)	0.0756 (7)	−0.0228 (4)	0.0382 (5)	−0.0186 (5)
Cl2	0.0642 (5)	0.0505 (5)	0.0484 (5)	−0.0032 (4)	0.0099 (4)	−0.0093 (4)
N1	0.0435 (14)	0.0375 (14)	0.0366 (14)	−0.0042 (11)	−0.0007 (12)	0.0026 (11)
N2	0.0320 (12)	0.0382 (13)	0.0421 (15)	0.0016 (10)	0.0047 (11)	−0.0034 (11)
N3	0.0418 (14)	0.0481 (14)	0.0325 (14)	−0.0125 (11)	0.0037 (12)	0.0037 (11)
N4	0.0338 (13)	0.0437 (14)	0.0339 (14)	−0.0046 (10)	0.0040 (11)	−0.0021 (11)
C1	0.0396 (17)	0.0387 (17)	0.0316 (17)	−0.0053 (13)	−0.0001 (14)	0.0060 (13)
C2	0.0405 (17)	0.0397 (17)	0.0462 (19)	−0.0021 (13)	0.0015 (15)	0.0045 (14)
C3	0.0442 (18)	0.051 (2)	0.054 (2)	0.0028 (15)	−0.0018 (16)	0.0169 (17)
C4	0.053 (2)	0.050 (2)	0.055 (2)	−0.0096 (16)	−0.0170 (17)	0.0062 (17)
C5	0.060 (2)	0.0415 (17)	0.042 (2)	−0.0050 (15)	−0.0042 (17)	−0.0025 (14)
C6	0.0391 (16)	0.0345 (15)	0.0367 (18)	−0.0006 (12)	−0.0007 (15)	0.0022 (13)
C7	0.0423 (18)	0.055 (2)	0.051 (2)	−0.0072 (14)	0.0065 (16)	−0.0037 (16)
C8	0.0349 (19)	0.079 (3)	0.089 (3)	−0.0040 (16)	0.0102 (19)	−0.011 (2)
C9	0.041 (2)	0.083 (3)	0.096 (4)	−0.0061 (18)	−0.021 (2)	0.004 (2)
C10	0.064 (3)	0.103 (3)	0.058 (3)	−0.021 (2)	−0.018 (2)	0.010 (2)
C11	0.048 (2)	0.085 (2)	0.043 (2)	−0.0120 (17)	−0.0009 (17)	0.0030 (18)
C12	0.0348 (15)	0.0345 (15)	0.0336 (16)	−0.0008 (12)	0.0016 (13)	0.0007 (13)
C13	0.0318 (15)	0.0409 (17)	0.0395 (18)	0.0000 (12)	0.0063 (14)	0.0063 (14)
C14	0.0437 (17)	0.0458 (18)	0.050 (2)	−0.0049 (14)	0.0037 (16)	0.0049 (16)
C15	0.056 (2)	0.0392 (18)	0.078 (3)	0.0004 (15)	0.018 (2)	0.0093 (18)
C16	0.060 (2)	0.055 (2)	0.081 (3)	0.0056 (17)	0.014 (2)	0.034 (2)
C17	0.064 (2)	0.071 (2)	0.051 (2)	−0.0059 (19)	−0.0004 (18)	0.0243 (19)
C18	0.0515 (18)	0.0489 (19)	0.043 (2)	−0.0034 (14)	0.0059 (16)	0.0071 (15)
C19	0.0343 (15)	0.0396 (17)	0.0345 (17)	−0.0022 (12)	0.0012 (13)	0.0002 (13)
C20	0.0350 (16)	0.0444 (18)	0.049 (2)	0.0005 (13)	0.0031 (15)	0.0019 (15)
C21	0.0400 (17)	0.055 (2)	0.056 (2)	0.0013 (14)	0.0110 (16)	−0.0096 (17)
C22	0.0517 (19)	0.064 (2)	0.044 (2)	−0.0076 (16)	0.0143 (17)	−0.0004 (17)
C23	0.0554 (19)	0.0491 (19)	0.049 (2)	−0.0036 (15)	0.0095 (17)	0.0109 (16)
C24	0.0491 (18)	0.0412 (18)	0.0433 (19)	0.0042 (13)	0.0102 (15)	0.0036 (14)

C25	0.0347 (15)	0.0399 (16)	0.0340 (17)	0.0026 (13)	0.0027 (14)	0.0006 (14)
C26	0.0401 (17)	0.0575 (19)	0.0364 (18)	−0.0059 (14)	0.0064 (15)	0.0016 (15)
C27	0.0520 (19)	0.067 (2)	0.0356 (19)	−0.0007 (16)	−0.0001 (16)	−0.0035 (16)
C28	0.0408 (18)	0.068 (2)	0.049 (2)	−0.0108 (15)	−0.0044 (16)	−0.0067 (17)
C29	0.0360 (17)	0.0549 (19)	0.048 (2)	−0.0081 (14)	0.0073 (16)	−0.0021 (16)
C30	0.0383 (17)	0.0461 (17)	0.0352 (18)	−0.0029 (13)	0.0033 (14)	0.0050 (14)
C31	0.0430 (18)	0.0526 (19)	0.0440 (19)	−0.0016 (14)	0.0097 (15)	0.0052 (15)
C32	0.0482 (19)	0.063 (2)	0.053 (2)	0.0120 (16)	0.0060 (17)	0.0130 (17)
C33	0.070 (2)	0.0474 (19)	0.052 (2)	0.0038 (17)	0.0091 (19)	0.0158 (16)
C34	0.060 (2)	0.050 (2)	0.065 (2)	−0.0083 (16)	0.0096 (19)	0.0143 (18)
C35	0.0416 (18)	0.054 (2)	0.057 (2)	−0.0051 (14)	0.0049 (16)	0.0107 (16)
C36	0.0333 (15)	0.0499 (18)	0.0415 (19)	−0.0047 (13)	0.0017 (14)	0.0045 (15)
C37	0.058 (2)	0.0487 (19)	0.055 (2)	−0.0029 (16)	0.0099 (17)	0.0056 (17)
C38	0.062 (2)	0.048 (2)	0.076 (3)	0.0027 (17)	0.008 (2)	0.0046 (19)
C39	0.050 (2)	0.072 (3)	0.083 (3)	0.0022 (18)	0.020 (2)	−0.014 (2)
C40	0.060 (2)	0.081 (3)	0.057 (2)	0.0048 (19)	0.0203 (19)	0.005 (2)
C41	0.0489 (19)	0.059 (2)	0.052 (2)	0.0016 (15)	0.0086 (17)	0.0093 (17)
C42	0.0337 (15)	0.0467 (17)	0.0374 (18)	−0.0092 (13)	0.0033 (14)	0.0053 (14)
C43	0.0429 (18)	0.0388 (17)	0.0430 (19)	−0.0105 (13)	−0.0032 (15)	0.0079 (15)
C44	0.0473 (19)	0.060 (2)	0.052 (2)	−0.0035 (16)	−0.0071 (17)	0.0077 (16)
C45	0.057 (2)	0.074 (3)	0.071 (3)	−0.0073 (19)	−0.013 (2)	0.012 (2)
C46	0.078 (3)	0.067 (2)	0.055 (3)	−0.016 (2)	−0.021 (2)	0.011 (2)
C47	0.079 (3)	0.065 (2)	0.049 (2)	−0.0132 (19)	0.000 (2)	−0.0056 (18)
C48	0.055 (2)	0.0506 (19)	0.051 (2)	−0.0108 (15)	−0.0017 (18)	0.0010 (16)

Geometric parameters (Å, °)

Zn1—N1	2.069 (2)	C21—C22	1.373 (4)
Zn1—N4	2.067 (2)	C21—H21A	0.9300
Zn1—Cl1	2.2193 (8)	C22—C23	1.372 (4)
Zn1—Cl2	2.2218 (8)	C22—H22A	0.9300
N1—C1	1.353 (3)	C23—C24	1.371 (4)
N1—C5	1.361 (3)	C23—H23A	0.9300
N2—C1	1.356 (3)	C24—H24A	0.9300
N2—C12	1.480 (3)	C25—C26	1.395 (4)
N2—H2B	0.8600	C26—C27	1.362 (4)
N3—C25	1.362 (3)	C26—H26A	0.9300
N3—C42	1.492 (3)	C27—C28	1.376 (4)
N3—H3B	0.8600	C27—H27A	0.9300
N4—C29	1.349 (3)	C28—C29	1.359 (4)
N4—C25	1.360 (3)	C28—H28A	0.9300
C1—C2	1.413 (4)	C29—H29A	0.9300
C2—C3	1.366 (4)	C30—C31	1.375 (4)
C2—H2A	0.9300	C30—C35	1.389 (4)
C3—C4	1.381 (4)	C30—C42	1.540 (4)
C3—H3A	0.9300	C31—C32	1.381 (4)
C4—C5	1.363 (4)	C31—H31A	0.9300
C4—H4A	0.9300	C32—C33	1.371 (4)
C5—H5A	0.9300	C32—H32A	0.9300

C6—C7	1.378 (4)	C33—C34	1.372 (4)
C6—C11	1.380 (4)	C33—H33A	0.9300
C6—C12	1.551 (3)	C34—C35	1.374 (4)
C7—C8	1.372 (4)	C34—H34A	0.9300
C7—H7A	0.9300	C35—H35A	0.9300
C8—C9	1.376 (5)	C36—C41	1.377 (4)
C8—H8A	0.9300	C36—C37	1.388 (4)
C9—C10	1.358 (5)	C36—C42	1.542 (4)
C9—H9A	0.9300	C37—C38	1.369 (4)
C10—C11	1.375 (4)	C37—H37A	0.9300
C10—H10A	0.9300	C38—C39	1.372 (5)
C11—H11A	0.9300	C38—H38A	0.9300
C12—C19	1.532 (4)	C39—C40	1.364 (4)
C12—C13	1.543 (3)	C39—H39A	0.9300
C13—C18	1.379 (4)	C40—C41	1.385 (4)
C13—C14	1.396 (4)	C40—H40A	0.9300
C14—C15	1.376 (4)	C41—H41A	0.9300
C14—H14A	0.9300	C42—C43	1.552 (4)
C15—C16	1.364 (4)	C43—C44	1.382 (4)
C15—H15A	0.9300	C43—C48	1.383 (4)
C16—C17	1.374 (4)	C44—C45	1.383 (4)
C16—H16A	0.9300	C44—H44A	0.9300
C17—C18	1.385 (4)	C45—C46	1.357 (5)
C17—H17A	0.9300	C45—H45A	0.9300
C18—H18A	0.9300	C46—C47	1.372 (5)
C19—C20	1.379 (4)	C46—H46A	0.9300
C19—C24	1.392 (3)	C47—C48	1.392 (4)
C20—C21	1.381 (4)	C47—H47A	0.9300
C20—H20A	0.9300	C48—H48A	0.9300
N1—Zn1—N4	99.83 (9)	C21—C22—C23	118.9 (3)
N1—Zn1—Cl1	110.89 (7)	C21—C22—H22A	120.5
N4—Zn1—Cl1	108.97 (6)	C23—C22—H22A	120.5
N1—Zn1—Cl2	110.11 (7)	C24—C23—C22	120.3 (3)
N4—Zn1—Cl2	109.27 (6)	C24—C23—H23A	119.9
Cl1—Zn1—Cl2	116.46 (3)	C22—C23—H23A	119.9
C1—N1—C5	118.1 (2)	C23—C24—C19	121.6 (3)
C1—N1—Zn1	124.20 (17)	C23—C24—H24A	119.2
C5—N1—Zn1	116.90 (19)	C19—C24—H24A	119.2
C1—N2—C12	128.3 (2)	N4—C25—N3	116.0 (2)
C1—N2—H2B	115.9	N4—C25—C26	120.4 (2)
C12—N2—H2B	115.9	N3—C25—C26	123.6 (2)
C25—N3—C42	127.7 (2)	C27—C26—C25	119.7 (3)
C25—N3—H3B	116.2	C27—C26—H26A	120.1
C42—N3—H3B	116.2	C25—C26—H26A	120.1
C29—N4—C25	117.8 (2)	C26—C27—C28	120.0 (3)
C29—N4—Zn1	116.83 (18)	C26—C27—H27A	120.0
C25—N4—Zn1	124.95 (18)	C28—C27—H27A	120.0
N2—C1—N1	116.3 (2)	C29—C28—C27	118.1 (3)
N2—C1—C2	123.2 (3)	C29—C28—H28A	121.0

N1—C1—C2	120.5 (2)	C27—C28—H28A	121.0
C3—C2—C1	119.2 (3)	N4—C29—C28	123.9 (3)
C3—C2—H2A	120.4	N4—C29—H29A	118.1
C1—C2—H2A	120.4	C28—C29—H29A	118.1
C2—C3—C4	120.4 (3)	C31—C30—C35	117.8 (3)
C2—C3—H3A	119.8	C31—C30—C42	123.2 (2)
C4—C3—H3A	119.8	C35—C30—C42	119.0 (2)
C5—C4—C3	118.1 (3)	C32—C31—C30	121.1 (3)
C5—C4—H4A	121.0	C32—C31—H31A	119.5
C3—C4—H4A	121.0	C30—C31—H31A	119.5
C4—C5—N1	123.6 (3)	C33—C32—C31	120.4 (3)
C4—C5—H5A	118.2	C33—C32—H32A	119.8
N1—C5—H5A	118.2	C31—C32—H32A	119.8
C7—C6—C11	118.0 (3)	C32—C33—C34	119.4 (3)
C7—C6—C12	119.8 (2)	C32—C33—H33A	120.3
C11—C6—C12	122.1 (3)	C34—C33—H33A	120.3
C8—C7—C6	121.4 (3)	C33—C34—C35	120.2 (3)
C8—C7—H7A	119.3	C33—C34—H34A	119.9
C6—C7—H7A	119.3	C35—C34—H34A	119.9
C9—C8—C7	119.6 (3)	C34—C35—C30	121.1 (3)
C9—C8—H8A	120.2	C34—C35—H35A	119.4
C7—C8—H8A	120.2	C30—C35—H35A	119.4
C10—C9—C8	119.8 (3)	C41—C36—C37	117.9 (3)
C10—C9—H9A	120.1	C41—C36—C42	124.1 (3)
C8—C9—H9A	120.1	C37—C36—C42	118.0 (3)
C9—C10—C11	120.6 (3)	C38—C37—C36	120.9 (3)
C9—C10—H10A	119.7	C38—C37—H37A	119.5
C11—C10—H10A	119.7	C36—C37—H37A	119.5
C10—C11—C6	120.6 (3)	C37—C38—C39	120.7 (3)
C10—C11—H11A	119.7	C37—C38—H38A	119.6
C6—C11—H11A	119.7	C39—C38—H38A	119.6
N2—C12—C19	109.4 (2)	C40—C39—C38	119.0 (3)
N2—C12—C13	110.9 (2)	C40—C39—H39A	120.5
C19—C12—C13	114.4 (2)	C38—C39—H39A	120.5
N2—C12—C6	105.87 (19)	C39—C40—C41	120.7 (3)
C19—C12—C6	108.9 (2)	C39—C40—H40A	119.6
C13—C12—C6	106.9 (2)	C41—C40—H40A	119.6
C18—C13—C14	117.2 (3)	C36—C41—C40	120.7 (3)
C18—C13—C12	123.1 (2)	C36—C41—H41A	119.7
C14—C13—C12	119.6 (2)	C40—C41—H41A	119.7
C15—C14—C13	121.2 (3)	N3—C42—C30	111.8 (2)
C15—C14—H14A	119.4	N3—C42—C36	109.1 (2)
C13—C14—H14A	119.4	C30—C42—C36	113.0 (2)
C16—C15—C14	120.7 (3)	N3—C42—C43	104.6 (2)
C16—C15—H15A	119.6	C30—C42—C43	107.2 (2)
C14—C15—H15A	119.6	C36—C42—C43	110.9 (2)
C15—C16—C17	119.3 (3)	C44—C43—C48	118.1 (3)
C15—C16—H16A	120.4	C44—C43—C42	123.1 (3)
C17—C16—H16A	120.4	C48—C43—C42	118.8 (3)

C16—C17—C18	120.2 (3)	C43—C44—C45	120.7 (3)
C16—C17—H17A	119.9	C43—C44—H44A	119.7
C18—C17—H17A	119.9	C45—C44—H44A	119.7
C13—C18—C17	121.4 (3)	C46—C45—C44	120.6 (3)
C13—C18—H18A	119.3	C46—C45—H45A	119.7
C17—C18—H18A	119.3	C44—C45—H45A	119.7
C20—C19—C24	117.4 (3)	C45—C46—C47	120.0 (3)
C20—C19—C12	124.4 (2)	C45—C46—H46A	120.0
C24—C19—C12	117.7 (2)	C47—C46—H46A	120.0
C19—C20—C21	120.8 (3)	C46—C47—C48	119.7 (4)
C19—C20—H20A	119.6	C46—C47—H47A	120.2
C21—C20—H20A	119.6	C48—C47—H47A	120.2
C22—C21—C20	120.9 (3)	C43—C48—C47	120.7 (3)
C22—C21—H21A	119.6	C43—C48—H48A	119.6
C20—C21—H21A	119.6	C47—C48—H48A	119.6

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2B···Cl1	0.86	2.62	3.450 (2)	162
N3—H3B···Cl2	0.86	2.66	3.470 (2)	158

Fig. 1

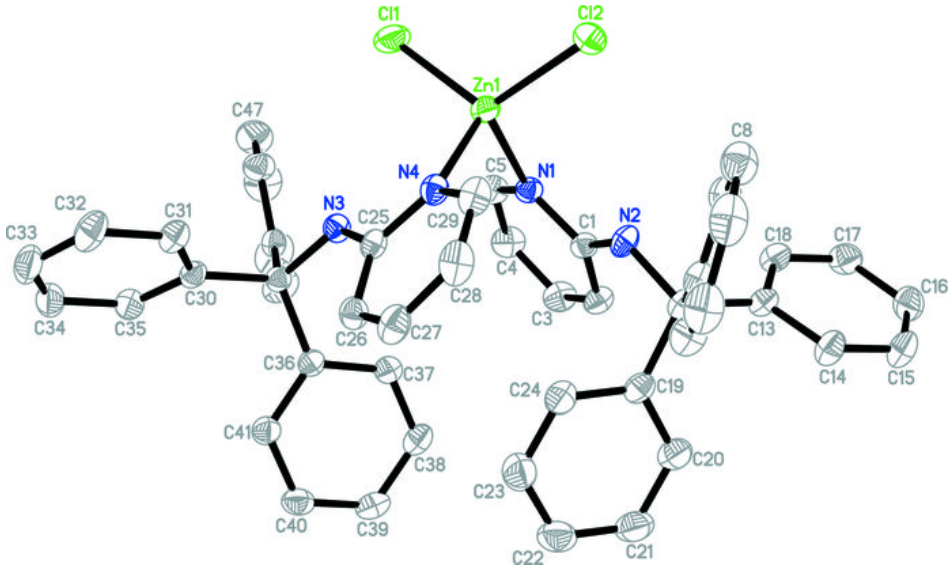
Cl1
Cl2
Zn1
C47
C8
N4
C5
N1
N3
C25
C29
C1
N2
C32
C31
C33
C4
C18
C17
C16
C30
C28
C3
C13
C34
C35
C26
C27
C14
C15
C36
C37
C24
C19
C41
C38
C20
C23
C40
C39
C22
C21

Fig. 2