Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Dichlorido-[*N*,*N*′-bis(2,6-dimethylphenyl)pentane-2,4-diiminato](indenyl)zirconium(IV) toluene hemisolvate

Emilie Verguet, Rose-Verla Fortuné, Paul O. Oguadinma and Frank Schaper*

Département de Chimie, Université de Montréal, CP 6128, Succ. Centre-ville, Montréal, Québec, Canada H3C 3J7
Correspondence e-mail: frank.schaper@umontreal.ca

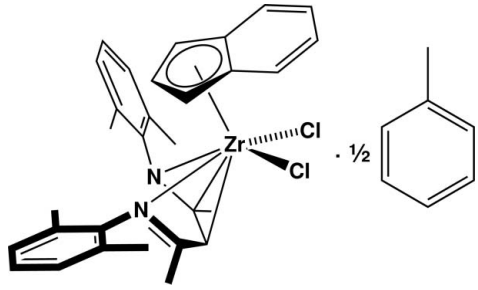
Received 26 August 2007; accepted 7 September 2007

Key indicators: single-crystal X-ray study; T = 150 K; mean σ(C–C) = 0.004 Å; disorder in solvent or counterion; R factor = 0.032; wR factor = 0.086; data-to-parameter ratio = 15.3.

The title compound, $[Zr(Cl)_2(C_{21}H_{25}N_2)(C_9H_7)]\cdot 0.5C_7H_8$, [bis(2,6-dimethylphenyl)nacnac](indenyl)$ZrCl_2$, where nacnac is the pentane-2,4-diiminate ligand, has pseudo-tetrahedral coordination geometry about the Zr center. The coordination mode of the nacnac ligand is intermediate between η^2- and η^5-coordination, with both N atoms and two C atoms clearly coordinated to the Zr center. The coordination is best described as an in-plane η^1-imine and η^3-enaminato coordination of the nacnac ligand. A toluene solvent molecule is present and is disordered about a twofold crystallographic axis.

Related literature

For a related mixed (indenyl)(nacnac)$ZrCl_2$ compound, see Rahim *et al.* (1998). For the analogous cyclopentadienyl compound, see Verguet *et al.* (2007). For comparable coordination of the nacnac ligand in five-coordinated complexes, see Basuli *et al.* (2004) [Cambridge Structural Database (Allen, 2002) refcodes FAPBUU, FAPCAP, FAPCEF and FABCIJ]. For Zr complexes containing η^2-coordinated nacnac, see: Kakaliou *et al.* (1999); Qian *et al.* (1999); Jin & Novak (2000); Franceschini *et al.* (2003); Hamaki *et al.* (2006). For Zr complexes containing η^5-like coordinated nacnac, see: Rahim *et al.* (1998); Vollmerhaus *et al.* (2000). For related literature, see: Faller *et al.* (1985); Fortuné *et al.* (2007); Lee *et al.* (1999).



Experimental

Crystal data

$[Zr(Cl)_2(C_{21}H_{25}N_2)(C_9H_7)]\cdot 0.5C_7H_8$
M_r = 628.77
Monoclinic, $C2/c$
a = 25.6719 (7) Å
b = 12.2509 (3) Å
c = 22.6278 (6) Å
β = 122.701 (1)°
V = 5988.6 (3) Å^3
Z = 8
Cu $K\alpha$ radiation
μ = 4.83 mm^{-1}
T = 150 (2) K
0.27 × 0.21 × 0.18 mm

Data collection

Bruker SMART 6000 diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.322, T_{max} = 0.419
36248 measured reflections
5814 independent reflections
5182 reflections with $I > 2\sigma(I)$
R_{int} = 0.036

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.032
$wR(F^2)$ = 0.086
S = 1.00
5814 reflections
380 parameters
42 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.48 e Å^{-3}
$\Delta\rho_{min}$ = −0.99 e Å^{-3}

Data collection: *APEX2* (Bruker, 2004); cell refinement: *APEX2*; data reduction: *APEX2*; 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: *UdMX* (local program).

The authors are grateful to the Natural Sciences and Engineering Research Council of Canada and the Ministère de l'Education du Québec for financial support.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: GG2042).

References

Allen, F. H. (2002). *Acta Cryst.* B**58**, 380–388.
Basuli, F., Kilgore, U. J., Brown, D., Huffman, J. C. & Mindiola, D. J. (2004). *Organometallics*, **23**, 6166–6175.
Bruker (1997). *SHELXTL*. Release 5.10. Bruker AXS Inc., Madison, Wisconsin, USA.
Bruker (2004). *APEX2*. Release 1.1.2.2. Bruker AXS Inc., Madison, Wisconsin, USA.
Faller, J. W., Crabtree, R. H. & Habib, A. (1985). *Organometallics*, **4**, 929–935.
Fortuné, R.-V., Verguet, E., Oguadinma, P. O. & Schaper, F. (2007). *Acta Cryst.* E. In the press.

 doi:10.1107/S1600536807043966

Franceschini, P. L., Morstein, M., Berke, H. & Schmalle, H. W. (2003). *Inorg. Chem.* **42**, 7273–7282.
Hamaki, H., Takeda, N. & Tokitoh, N. (2006). *Organometallics*, **25**, 2457–2464.
Jin, X. & Novak, B. M. (2000). *Macromolecules*, **33**, 6205–6207.
Kakaliou, L., Scanlon, W. J., Qian, B., Baek, S. W., Smith, M. R. & Motry, D. H. (1999). *Inorg. Chem.* **38**, 5964–5977.
Lee, L. W. M., Piers, W. E., Elsegood, M. R. J., Clegg, W. & Parvez, M. (1999). *Organometallics*, **18**, 2947–2949.
Qian, B., Scanlon, W. J., Smith, M. R. & Motry, D. H. (1999). *Organometallics*, **18**, 1693–1698.
Rahim, M., Taylor, N. J., Xin, S. & Collins, S. (1998). *Organometallics*, **17**, 1315–1323.
Sheldrick, G. M. (1996). *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Verguet, E., Oguadinma, P. O. & Schaper, F. (2007). *Acta Cryst.* E**63**, m2541.
Vollmerhaus, R., Rahim, M., Tomaszewski, R., Xin, S., Taylor, N. J. & Collins, S. (2000). *Organometallics*, **19**, 2161–2169.

supplementary materials

Acta Cryst. (2007). E**63**, m2539-m2540 [**doi:10.1107/S1600536807043966**]

Dichlorido-[*N*,*N*'-bis(2,6-dimethylphenyl)pentane-2,4-diiminato](indenyl)zirconium(IV) toluene hemisolvate

E. Verguet, R.-V. Fortuné, P. O. Oguadinma and F. Schaper

Comment

The title compound was synthesized by ligand metathesis starting from [bis(2,6-dimethylphenyl)nacnac]$ZrCl_3$(THF) ("nacnac" = pentane-2,4-diiminato) and indenyl lithium. Layering of a toluene solution with hexane yielded crystals in sufficient quality for X-ray analysis.

Coordination of the nacnac ligand to group 4 metals differs strongly depending on the compound composition, the nature of the nacnac ligand and the metal center. An in-plane η^2-coordination is often observed in octahedral coordinated compounds (Kakaliou *et al.*, 1999; Qian *et al.*; 1999; Jin & Novak, 2000; Franceschini *et al.*, 2003; Hamaki *et al.*, 2006). With sterically less encumbered nacnac ligands, such as *N*,*N*'-diphenyl nacnac, and in particular in the presence of a second, η^5-coordinated ligand such as cyclopentadienyl or indenyl, a cyclopentadienyl-like η^5-coordination has been observed (Rahim *et al.*, 1998; Vollmerhaus *et al.*, 2000). One example of such is (Ind)(*N*,*N*'-diphenyl-nacnac)$ZrCl_2$, which differs from the title compound (I) only by the lack of the 2,6-methyl substituents on the N-bonded phenyl rings (Rahim *et al.*, 1998).

In contrast to these, the nacnac ligand adopts in (I), an intermediate, distorted coordination mode. The coordination of N1 and the carbon atoms C2 and C3 can be described as an η^3-coordinated enamide, as evidenced by Zr—C distances of 2.617 (2) and 2.616 (2) Å, respectively, and an angle ⟨ (C1,C2,Zr) of 140.7 (2)°. The Zr—C4 distance of 2.825 (2) Å, however, is significantly elongated in comparison to C2 and C3 and the methyl substituent at C4 is orientated away from the metal center with a bond angle ⟨ (C5,C4,Zr) of 169.5 (2)°, indicating that the N lone pair, but not the C═N-bond is coordinated to the Zr center. (While we cannot completely exclude a π-coordination of C4 to the metal, the elongated Zr—C4 distance makes this improbable.) The coordination of the nacnac ligand can be thus broken down into two parts, an η^3-enaminato coordination of C2, C3 and N1 and an η^1-imine coordination of C4 and N2.

The planar coordination of the enaminato-moiety and the in-plane coordination of the imine-moiety results in a folding of the ligand backbone, which reduces its electron delocalization. The least-square planes through N1, C1–C3 and N2, C3–C5 display an angle of 41°. Bond distances observed in the ligand backbone agree with a slight separation of the π-system into an enaminato- and an imine-moiety. The proposed imine bond N2═C4 is shorter than the so-assigned enamine bond N1═C2 (1.303 (3) and 1.352 (3) Å, respectively). The C2—C3 distance of 1.394 (3) Å is comparable to the N—C distances, while the C3—C4 distance is significantly elongated to 1.454 (3) Å and can be assigned a higher single-bond character.

The coordination of the nacnac ligand observed here differs from the earlier described η^2 or η^5-coordination (*see above*) and from those observed, for example, in scandium complexes, where a placement of the Sc center outside of the ligand plane was ascribed to steric reasons without any significant coordination of the carbon atoms to the metal center (Lee *et al.*, 1999). A comparable coordination, however, was observed for the nacnac ligand in the five-coordinated complexes reported by Basuli *et al.* (2004) (CSD-codes: FAPBUU, FAPCAP, FAPCEF & FABCIJ). Their coordination was described simply

as "sandwich-like". Not surprisingly, the analogous compound in which indenyl is replaced by cyclopentadienyl is nearly isostructural (Verguet *et al.*, 2007).

The indenyl ligand displays only a very slight deviation from ideal η^5-coordination (ΔM–C = 0.11 Å and Ω = 4°, Faller *et al.*, 1985).

Experimental

All operations were carried out under N_2 atmosphere. Solvents have been dried by standard methods and de-oxygenized.

30 ml of toluene were added to a mixture of 0.5 g (0.87 mmol) (nacnac)$ZrCl_3$(THF) (Fortuné *et al.*, 2007) and 0.115 g indenyl lithium (0.96 mmol). After two days of stirring at room temperature, the obtained suspension is filtered and the precipitate washed with 8 ml of toluene. The volume of the combined filtrates was reduced to *ca* 10 ml and layered with 10 ml of hexane. After two weeks the product was isolated by decantation of the solvent as yellow microcrystals, 0.213 g (42%).

NMR ^{1}H (300 MHz, C_6D_6), δ p.p.m.: 7.13–7.30 (*m*), 6.70 (br s, 1H), 6.46 (br s, 2H), 5.67 (s, 1H), 2.63 (s, 6H), 2.07 (s, 6H), 1.97 (s, 6H).

Refinement

The H atoms were generated geometrically (C—H 0.93 to 0.98, N—H 0.86 and O—H 0.82 Å) and were included in the refinement in the riding model approximation, their temperature factors were set to 1.5 times those of the equivalent isotropic temperature factors of the parent site (methyl) and 1.2 times for others.

Figures

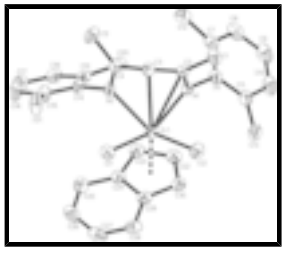


Fig. 1. *ORTEP* view of the title compound (I). Displacement ellipsoids are shown at 50% probability levels. Hydrogen atoms and the solvent molecule are omitted for clarity.

Dichlorido-[*N*,*N*'-bis(2,6-dimethylphenyl)pentane-2,4- diiminato](indenyl)zirconium(IV) toluene hemisolvate

Crystal data

$[Zr(Cl)_2(C_{21}H_{25}N_2)(C_9H_7)]\cdot 0.5C_7H_8$	F_{000} = 2600
M_r = 628.77	D_x = 1.395 Mg m^{-3}
Monoclinic, *C*2/*c*	Cu *K*α radiation λ = 1.54178 Å
Hall symbol: -C 2yc	Cell parameters from 16709 reflections
a = 25.6719 (7) Å	θ = 4.1–71.5º
b = 12.2509 (3) Å	μ = 4.83 mm^{-1}

c = 22.6278 (6) Å
β = 122.7010 (10)º
V = 5988.6 (3) Å^3
Z = 8

T = 150 (2) K
Hexagonal prism, yellow
0.27 × 0.21 × 0.18 mm

Data collection

Bruker SMART 6000 diffractometer
Radiation source: Rotating Anode
Monochromator: Montel 200 optics
Detector resolution: 5.5 pixels mm^{-1}
T = 150(2) K
ω scans
Absorption correction: multi-scan (SADABS; Sheldrick,1996)
T_{min} = 0.322, T_{max} = 0.419
36248 measured reflections

5814 independent reflections
5182 reflections with $I > 2\sigma(I)$
R_{int} = 0.036
θ_{max} = 71.8º
θ_{min} = 4.1º
h = −31→31
k = −15→14
l = −27→27

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.032
$wR(F^2)$ = 0.086
S = 1.00
5814 reflections
380 parameters
42 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 /[$\sigma^2(F_o^2)$ + (0.0655P)^2]
where P = (F_o^2 + 2F_c^2)/3
$(\Delta/\sigma)_{max}$ = 0.003
$\Delta\rho_{max}$ = 0.48 e Å^{-3}
$\Delta\rho_{min}$ = −0.99 e Å^{-3}
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. Half a molecule of toluene cocrystallized with the compound. The toluene was found disordered around a C2 axis. The disorder was resolved and the molecule refined isotropically with half occupancy and strong SIMU restraints.

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

	x	y	z	U_{iso}*/U_{eq}	Occ. (<1)
Zr	0.143188 (7)	0.483751 (13)	0.008416 (9)	0.01843 (7)	

Cl1	0.03687 (2)	0.47259 (4)	−0.09714 (3)	0.02579 (12)
Cl2	0.12545 (3)	0.68593 (4)	−0.00659 (3)	0.03025 (13)
N1	0.19716 (8)	0.51001 (13)	0.12184 (9)	0.0207 (4)
N2	0.11907 (8)	0.32659 (13)	0.04335 (9)	0.0204 (3)
C1	0.14769 (10)	0.64130 (18)	0.16091 (12)	0.0303 (5)
H1A	0.1793	0.6329	0.2110	0.045*
H1B	0.1071	0.6511	0.1546	0.045*
H1C	0.1573	0.7053	0.1425	0.045*
C2	0.14666 (10)	0.54086 (17)	0.12195 (11)	0.0213 (4)
C3	0.09133 (10)	0.48371 (16)	0.08108 (12)	0.0226 (4)
H3	0.0518	0.5251	0.0617	0.027*
C4	0.08729 (9)	0.36697 (17)	0.06765 (11)	0.0221 (4)
C5	0.04803 (11)	0.30251 (18)	0.08539 (14)	0.0323 (5)
H5A	0.0496	0.2251	0.0756	0.048*
H5B	0.0052	0.3284	0.0570	0.048*
H5C	0.0636	0.3118	0.1353	0.048*
C6	0.25771 (10)	0.52759 (17)	0.18412 (12)	0.0242 (4)
C7	0.27341 (11)	0.46406 (18)	0.24365 (12)	0.0277 (5)
C8	0.33397 (12)	0.4680 (2)	0.30195 (13)	0.0358 (6)
H8	0.3455	0.4229	0.3414	0.043*
C9	0.37739 (12)	0.5363 (2)	0.30332 (14)	0.0419 (6)
H9	0.4187	0.5367	0.3430	0.050*
C10	0.36058 (10)	0.6040 (2)	0.24692 (13)	0.0391 (6)
H10	0.3902	0.6533	0.2493	0.047*
C11	0.30077 (10)	0.60146 (19)	0.18634 (12)	0.0290 (5)
C12	0.22623 (11)	0.3966 (2)	0.24793 (12)	0.0324 (5)
H12A	0.2473	0.3378	0.2822	0.049*
H12B	0.1966	0.3651	0.2017	0.049*
H12C	0.2042	0.4432	0.2626	0.049*
C13	0.28577 (11)	0.6822 (2)	0.12911 (14)	0.0358 (5)
H13A	0.2997	0.7551	0.1496	0.054*
H13B	0.2410	0.6833	0.0950	0.054*
H13C	0.3069	0.6608	0.1055	0.054*
C14	0.12040 (10)	0.21030 (16)	0.03269 (11)	0.0232 (4)
C15	0.17576 (10)	0.15317 (17)	0.07763 (11)	0.0238 (4)
C16	0.17834 (12)	0.04197 (19)	0.06504 (13)	0.0295 (5)
H16	0.2157	0.0028	0.0942	0.035*
C17	0.12726 (14)	−0.01187 (19)	0.01081 (15)	0.0387 (6)
H17	0.1298	−0.0871	0.0026	0.046*
C18	0.07303 (12)	0.0442 (2)	−0.03091 (14)	0.0380 (6)
H18	0.0378	0.0063	−0.0669	0.046*
C19	0.06834 (11)	0.15637 (18)	−0.02168 (13)	0.0307 (5)
C20	0.23056 (10)	0.20341 (18)	0.14176 (12)	0.0283 (5)
H20A	0.2290	0.1860	0.1831	0.042*
H20B	0.2296	0.2828	0.1359	0.042*
H20C	0.2688	0.1742	0.1481	0.042*
C21	0.00696 (12)	0.2117 (2)	−0.07102 (15)	0.0465 (7)
H21A	0.0119	0.2909	−0.0641	0.070*
H21B	−0.0238	0.1858	−0.0613	0.070*

H21C	−0.0069	0.1942	−0.1197	0.070*	
C22	0.24844 (10)	0.45664 (19)	0.03229 (12)	0.0273 (5)	
H22	0.2828	0.4709	0.0784	0.033*	
C23	0.21781 (10)	0.35619 (17)	0.00798 (12)	0.0252 (4)	
H23	0.2261	0.2922	0.0354	0.030*	
C24	0.17205 (10)	0.36687 (18)	−0.06511 (11)	0.0244 (4)	
C25	0.13063 (11)	0.29092 (19)	−0.11733 (13)	0.0309 (5)	
H25	0.1287	0.2174	−0.1054	0.037*	
C26	0.09397 (12)	0.3268 (2)	−0.18478 (14)	0.0383 (6)	
H26	0.0667	0.2767	−0.2202	0.046*	
C27	0.09525 (12)	0.4366 (2)	−0.20382 (13)	0.0381 (6)	
H27	0.0689	0.4582	−0.2515	0.046*	
C28	0.13362 (12)	0.5117 (2)	−0.15509 (13)	0.0316 (5)	
H28	0.1337	0.5853	−0.1682	0.038*	
C29	0.17358 (11)	0.47757 (17)	−0.08417 (12)	0.0250 (5)	
C30	0.21977 (10)	0.53284 (16)	−0.02299 (12)	0.0265 (5)	
H30	0.2297	0.6082	−0.0198	0.032*	
C31	0.50653 (10)	0.57281 (16)	0.26223 (12)	0.0489 (14)	0.50
C32	0.47229 (10)	0.61465 (16)	0.19443 (12)	0.051 (2)	0.50
H32	0.4540	0.5658	0.1557	0.062*	0.50
C33	0.4645 (5)	0.7226 (9)	0.1824 (5)	0.056 (3)	0.50
H33	0.4387	0.7487	0.1357	0.067*	0.50
C34	0.4928 (5)	0.7944 (6)	0.2360 (4)	0.047 (2)	0.50
H34	0.4888	0.8706	0.2266	0.057*	0.50
C35	0.5272 (4)	0.7581 (6)	0.3039 (5)	0.0307 (17)	0.50
H35	0.5452	0.8091	0.3415	0.037*	0.50
C36	0.5356 (3)	0.6497 (6)	0.3179 (4)	0.0341 (14)	0.50
H36	0.5611	0.6251	0.3650	0.041*	0.50
C37	0.5191 (5)	0.4517 (6)	0.2769 (5)	0.091 (3)	0.50
H37A	0.4873	0.4191	0.2827	0.137*	0.50
H37B	0.5599	0.4411	0.3200	0.137*	0.50
H37C	0.5183	0.4165	0.2375	0.137*	0.50

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zr	0.01806 (11)	0.01647 (11)	0.02401 (11)	0.00228 (6)	0.01350 (8)	−0.00109 (6)
Cl1	0.0198 (2)	0.0313 (3)	0.0267 (3)	0.00414 (19)	0.0128 (2)	−0.00094 (19)
Cl2	0.0332 (3)	0.0180 (2)	0.0404 (3)	0.0040 (2)	0.0205 (2)	0.0020 (2)
N1	0.0185 (8)	0.0204 (8)	0.0241 (9)	−0.0002 (7)	0.0121 (7)	−0.0022 (7)
N2	0.0178 (8)	0.0164 (8)	0.0266 (9)	0.0010 (6)	0.0117 (7)	−0.0013 (6)
C1	0.0284 (11)	0.0281 (11)	0.0362 (12)	0.0015 (9)	0.0187 (10)	−0.0098 (9)
C2	0.0225 (10)	0.0197 (9)	0.0253 (10)	0.0032 (8)	0.0154 (8)	0.0010 (8)
C3	0.0224 (11)	0.0197 (10)	0.0308 (11)	0.0019 (8)	0.0177 (9)	−0.0018 (8)
C4	0.0167 (9)	0.0206 (10)	0.0284 (10)	0.0019 (8)	0.0119 (8)	0.0004 (8)
C5	0.0314 (12)	0.0254 (11)	0.0514 (15)	−0.0005 (9)	0.0299 (11)	0.0002 (10)
C6	0.0204 (10)	0.0254 (11)	0.0282 (11)	0.0012 (8)	0.0140 (9)	−0.0066 (8)
C7	0.0267 (11)	0.0291 (11)	0.0277 (11)	0.0054 (9)	0.0149 (10)	−0.0051 (9)

C8	0.0308 (13)	0.0418 (14)	0.0290 (12)	0.0090 (11)	0.0122 (10)	−0.0049 (10)
C9	0.0233 (12)	0.0507 (16)	0.0379 (14)	0.0031 (11)	0.0076 (10)	−0.0112 (12)
C10	0.0233 (12)	0.0450 (15)	0.0452 (15)	−0.0065 (11)	0.0160 (11)	−0.0149 (12)
C11	0.0235 (10)	0.0310 (11)	0.0349 (12)	−0.0034 (9)	0.0175 (10)	−0.0096 (9)
C12	0.0355 (12)	0.0351 (12)	0.0294 (11)	0.0058 (10)	0.0194 (10)	0.0028 (10)
C13	0.0324 (12)	0.0359 (13)	0.0433 (14)	−0.0128 (10)	0.0232 (11)	−0.0089 (11)
C14	0.0247 (10)	0.0171 (9)	0.0308 (11)	0.0010 (8)	0.0169 (9)	−0.0021 (8)
C15	0.0269 (10)	0.0222 (10)	0.0294 (11)	0.0043 (9)	0.0199 (9)	0.0031 (8)
C16	0.0388 (13)	0.0233 (10)	0.0379 (13)	0.0081 (10)	0.0282 (11)	0.0047 (9)
C17	0.0564 (17)	0.0199 (11)	0.0538 (17)	0.0012 (11)	0.0389 (15)	−0.0034 (10)
C18	0.0416 (14)	0.0249 (11)	0.0466 (15)	−0.0080 (11)	0.0233 (12)	−0.0125 (11)
C19	0.0279 (11)	0.0230 (11)	0.0376 (12)	−0.0006 (9)	0.0153 (10)	−0.0042 (9)
C20	0.0261 (11)	0.0308 (11)	0.0292 (11)	0.0075 (9)	0.0156 (9)	0.0037 (9)
C21	0.0266 (12)	0.0334 (13)	0.0524 (16)	−0.0044 (11)	0.0036 (11)	−0.0094 (12)
C22	0.0208 (10)	0.0353 (12)	0.0315 (11)	0.0038 (9)	0.0177 (9)	−0.0025 (9)
C23	0.0259 (10)	0.0252 (10)	0.0329 (11)	0.0072 (9)	0.0215 (9)	0.0000 (9)
C24	0.0241 (10)	0.0262 (11)	0.0313 (11)	0.0037 (9)	0.0204 (9)	−0.0020 (9)
C25	0.0313 (11)	0.0290 (11)	0.0419 (13)	0.0001 (10)	0.0259 (11)	−0.0074 (10)
C26	0.0308 (12)	0.0481 (15)	0.0394 (14)	−0.0040 (11)	0.0212 (11)	−0.0168 (11)
C27	0.0342 (13)	0.0554 (16)	0.0285 (12)	0.0078 (12)	0.0194 (11)	0.0007 (11)
C28	0.0327 (13)	0.0357 (12)	0.0351 (13)	0.0073 (10)	0.0240 (11)	0.0058 (10)
C29	0.0250 (11)	0.0274 (11)	0.0319 (12)	0.0039 (8)	0.0214 (10)	0.0000 (8)
C30	0.0260 (11)	0.0267 (11)	0.0350 (12)	−0.0004 (9)	0.0219 (10)	−0.0026 (9)
C31	0.071 (3)	0.033 (2)	0.067 (4)	−0.014 (3)	0.053 (3)	−0.012 (3)
C32	0.051 (4)	0.073 (6)	0.038 (3)	−0.025 (4)	0.030 (3)	−0.027 (4)
C33	0.041 (4)	0.084 (7)	0.031 (4)	−0.001 (6)	0.012 (3)	0.011 (5)
C34	0.035 (5)	0.055 (3)	0.044 (7)	0.012 (4)	0.016 (5)	0.028 (3)
C35	0.034 (4)	0.022 (3)	0.038 (5)	0.003 (2)	0.020 (4)	0.006 (2)
C36	0.039 (3)	0.023 (3)	0.036 (3)	−0.008 (2)	0.017 (2)	0.004 (2)
C37	0.122 (7)	0.043 (3)	0.130 (7)	−0.008 (4)	0.081 (6)	−0.007 (4)

Geometric parameters (Å, °)

Zr—N1	2.1836 (18)	C15—C20	1.503 (3)
Zr—N2	2.2900 (17)	C16—C17	1.386 (4)
Zr—C22	2.475 (2)	C16—H16	0.9500
Zr—Cl1	2.4758 (5)	C17—C18	1.372 (4)
Zr—C23	2.4763 (19)	C17—H17	0.9500
Zr—C30	2.498 (2)	C18—C19	1.404 (3)
Zr—Cl2	2.5081 (5)	C18—H18	0.9500
Zr—C24	2.588 (2)	C19—C21	1.513 (3)
Zr—C29	2.602 (2)	C20—H20A	0.9800
Zr—C3	2.616 (2)	C20—H20B	0.9800
Zr—C2	2.617 (2)	C20—H20C	0.9800
Zr—C4	2.825 (2)	C21—H21A	0.9800
N1—C2	1.352 (3)	C21—H21B	0.9800
N1—C6	1.443 (3)	C21—H21C	0.9800
N2—C4	1.303 (3)	C22—C23	1.403 (3)
N2—C14	1.448 (2)	C22—C30	1.408 (3)

C1—C2	1.506 (3)	C22—H22	0.9500
C1—H1A	0.9800	C23—C24	1.426 (3)
C1—H1B	0.9800	C23—H23	0.9500
C1—H1C	0.9800	C24—C25	1.427 (3)
C2—C3	1.394 (3)	C24—C29	1.430 (3)
C3—C4	1.454 (3)	C25—C26	1.362 (4)
C3—H3	1.0000	C25—H25	0.9500
C4—C5	1.496 (3)	C26—C27	1.418 (4)
C5—H5A	0.9800	C26—H26	0.9500
C5—H5B	0.9800	C27—C28	1.364 (4)
C5—H5C	0.9800	C27—H27	0.9500
C6—C11	1.408 (3)	C28—C29	1.422 (3)
C6—C7	1.413 (3)	C28—H28	0.9500
C7—C8	1.394 (3)	C29—C30	1.417 (3)
C7—C12	1.512 (3)	C30—H30	0.9500
C8—C9	1.381 (4)	C31—C32	1.3900
C8—H8	0.9500	C31—C36	1.419 (7)
C9—C10	1.381 (4)	C31—C37	1.517 (7)
C9—H9	0.9500	C32—C33	1.343 (12)
C10—C11	1.401 (3)	C32—H32	0.9500
C10—H10	0.9500	C33—C34	1.350 (11)
C11—C13	1.505 (3)	C33—H33	0.9500
C12—H12A	0.9800	C34—C35	1.368 (11)
C12—H12B	0.9800	C34—H34	0.9500
C12—H12C	0.9800	C35—C36	1.355 (9)
C13—H13A	0.9800	C35—H35	0.9500
C13—H13B	0.9800	C36—H36	0.9500
C13—H13C	0.9800	C37—H37A	0.9800
C14—C19	1.400 (3)	C37—H37B	0.9800
C14—C15	1.408 (3)	C37—H37C	0.9800
C15—C16	1.401 (3)		
N1—Zr—N2	80.58 (6)	C8—C9—C10	119.8 (2)
N1—Zr—C22	80.71 (7)	C8—C9—H9	120.1
N2—Zr—C22	106.18 (7)	C10—C9—H9	120.1
N1—Zr—Cl1	144.17 (5)	C9—C10—C11	121.4 (2)
N2—Zr—Cl1	85.63 (4)	C9—C10—H10	119.3
C22—Zr—Cl1	135.05 (5)	C11—C10—H10	119.3
N1—Zr—C23	95.55 (7)	C10—C11—C6	118.2 (2)
N2—Zr—C23	79.91 (7)	C10—C11—C13	117.6 (2)
C22—Zr—C23	32.92 (7)	C6—C11—C13	124.1 (2)
Cl1—Zr—C23	114.41 (5)	C7—C12—H12A	109.5
N1—Zr—C30	101.64 (7)	C7—C12—H12B	109.5
N2—Zr—C30	134.56 (6)	H12A—C12—H12B	109.5
C22—Zr—C30	32.89 (7)	C7—C12—H12C	109.5
Cl1—Zr—C30	111.45 (5)	H12A—C12—H12C	109.5
C23—Zr—C30	54.65 (7)	H12B—C12—H12C	109.5
N1—Zr—Cl2	88.12 (5)	C11—C13—H13A	109.5
N2—Zr—Cl2	144.48 (4)	C11—C13—H13B	109.5
C22—Zr—Cl2	105.01 (6)	H13A—C13—H13B	109.5

Cl1—Zr—Cl2	84.204 (18)	C11—C13—H13C	109.5
C23—Zr—Cl2	134.99 (5)	H13A—C13—H13C	109.5
C30—Zr—Cl2	80.62 (5)	H13B—C13—H13C	109.5
N1—Zr—C24	128.09 (7)	C19—C14—C15	120.80 (19)
N2—Zr—C24	88.94 (6)	C19—C14—N2	120.89 (19)
C22—Zr—C24	53.71 (7)	C15—C14—N2	118.30 (19)
Cl1—Zr—C24	84.18 (5)	C16—C15—C14	118.5 (2)
C23—Zr—C24	32.61 (7)	C16—C15—C20	118.2 (2)
C30—Zr—C24	53.68 (7)	C14—C15—C20	123.16 (19)
Cl2—Zr—C24	123.60 (5)	C17—C16—C15	121.1 (2)
N1—Zr—C29	132.44 (7)	C17—C16—H16	119.4
N2—Zr—C29	120.54 (6)	C15—C16—H16	119.4
C22—Zr—C29	53.48 (7)	C18—C17—C16	119.6 (2)
Cl1—Zr—C29	82.85 (5)	C18—C17—H17	120.2
C23—Zr—C29	53.80 (7)	C16—C17—H17	120.2
C30—Zr—C29	32.18 (7)	C17—C18—C19	121.6 (2)
Cl2—Zr—C29	91.79 (5)	C17—C18—H18	119.2
C24—Zr—C29	31.99 (6)	C19—C18—H18	119.2
N1—Zr—C3	58.43 (7)	C14—C19—C18	118.3 (2)
N2—Zr—C3	57.21 (6)	C14—C19—C21	123.8 (2)
C22—Zr—C3	136.82 (7)	C18—C19—C21	117.9 (2)
Cl1—Zr—C3	86.34 (5)	C15—C20—H20A	109.5
C23—Zr—C3	131.29 (7)	C15—C20—H20B	109.5
C30—Zr—C3	157.65 (7)	H20A—C20—H20B	109.5
Cl2—Zr—C3	88.19 (4)	C15—C20—H20C	109.5
C24—Zr—C3	145.45 (6)	H20A—C20—H20C	109.5
C29—Zr—C3	169.13 (7)	H20B—C20—H20C	109.5
N1—Zr—C2	31.06 (6)	C19—C21—H21A	109.5
N2—Zr—C2	76.00 (6)	C19—C21—H21B	109.5
C22—Zr—C2	111.56 (7)	H21A—C21—H21B	109.5
Cl1—Zr—C2	113.38 (5)	C19—C21—H21C	109.5
C23—Zr—C2	123.81 (7)	H21A—C21—H21C	109.5
C30—Zr—C2	126.88 (7)	H21B—C21—H21C	109.5
Cl2—Zr—C2	77.08 (5)	C23—C22—C30	108.7 (2)
C24—Zr—C2	155.38 (7)	C23—C22—Zr	73.59 (12)
C29—Zr—C2	158.77 (7)	C30—C22—Zr	74.47 (12)
C3—Zr—C2	30.90 (6)	C23—C22—H22	125.7
N1—Zr—C4	71.30 (6)	C30—C22—H22	125.7
N2—Zr—C4	27.01 (6)	Zr—C22—H22	118.2
C22—Zr—C4	127.08 (7)	C22—C23—C24	108.1 (2)
Cl1—Zr—C4	81.48 (4)	C22—C23—Zr	73.49 (12)
C23—Zr—C4	105.94 (7)	C24—C23—Zr	78.02 (12)
C30—Zr—C4	159.45 (6)	C22—C23—H23	126.0
Cl2—Zr—C4	117.57 (4)	C24—C23—H23	126.0
C24—Zr—C4	114.83 (7)	Zr—C23—H23	114.8
C29—Zr—C4	144.83 (6)	C23—C24—C25	132.8 (2)
C3—Zr—C4	30.70 (6)	C23—C24—C29	107.3 (2)
C2—Zr—C4	54.99 (6)	C25—C24—C29	119.9 (2)
C2—N1—C6	119.00 (18)	C23—C24—Zr	69.37 (11)

C2—N1—Zr	92.48 (13)	C25—C24—Zr	123.30 (14)
C6—N1—Zr	146.58 (14)	C29—C24—Zr	74.52 (12)
C4—N2—C14	121.34 (17)	C26—C25—C24	118.2 (2)
C4—N2—Zr	100.03 (13)	C26—C25—H25	120.9
C14—N2—Zr	137.26 (13)	C24—C25—H25	120.9
C2—C1—H1A	109.5	C25—C26—C27	122.1 (2)
C2—C1—H1B	109.5	C25—C26—H26	119.0
H1A—C1—H1B	109.5	C27—C26—H26	119.0
C2—C1—H1C	109.5	C28—C27—C26	121.3 (2)
H1A—C1—H1C	109.5	C28—C27—H27	119.3
H1B—C1—H1C	109.5	C26—C27—H27	119.3
N1—C2—C3	119.52 (18)	C27—C28—C29	118.7 (2)
N1—C2—C1	121.07 (19)	C27—C28—H28	120.7
C3—C2—C1	119.23 (18)	C29—C28—H28	120.7
N1—C2—Zr	56.46 (11)	C30—C29—C28	132.4 (2)
C3—C2—Zr	74.47 (12)	C30—C29—C24	107.7 (2)
C1—C2—Zr	140.69 (15)	C28—C29—C24	119.9 (2)
C2—C3—C4	124.38 (19)	C30—C29—Zr	69.89 (12)
C2—C3—Zr	74.62 (12)	C28—C29—Zr	123.55 (15)
C4—C3—Zr	82.64 (12)	C24—C29—Zr	73.49 (12)
C2—C3—H3	117.8	C22—C30—C29	108.12 (18)
C4—C3—H3	117.8	C22—C30—Zr	72.64 (12)
Zr—C3—H3	117.8	C29—C30—Zr	77.93 (12)
N2—C4—C3	118.12 (19)	C22—C30—H30	125.9
N2—C4—C5	125.40 (19)	C29—C30—H30	125.9
C3—C4—C5	116.45 (18)	Zr—C30—H30	115.6
N2—C4—Zr	52.96 (11)	C32—C31—C36	116.8 (3)
C3—C4—Zr	66.66 (12)	C32—C31—C37	122.4 (4)
C5—C4—Zr	169.51 (15)	C36—C31—C37	120.5 (5)
C4—C5—H5A	109.5	C33—C32—C31	121.5 (4)
C4—C5—H5B	109.5	C33—C32—H32	119.3
H5A—C5—H5B	109.5	C31—C32—H32	119.3
C4—C5—H5C	109.5	C32—C33—C34	120.8 (8)
H5A—C5—H5C	109.5	C32—C33—H33	119.6
H5B—C5—H5C	109.5	C34—C33—H33	119.6
C11—C6—C7	120.4 (2)	C33—C34—C35	120.3 (6)
C11—C6—N1	122.8 (2)	C33—C34—H34	119.9
C7—C6—N1	116.81 (19)	C35—C34—H34	119.9
C8—C7—C6	118.8 (2)	C36—C35—C34	120.4 (9)
C8—C7—C12	118.7 (2)	C36—C35—H35	119.8
C6—C7—C12	122.4 (2)	C34—C35—H35	119.8
C9—C8—C7	121.1 (3)	C35—C36—C31	120.2 (7)
C9—C8—H8	119.5	C35—C36—H36	119.9
C7—C8—H8	119.5	C31—C36—H36	119.9
N2—Zr—N1—C2	−78.47 (12)	C15—C16—C17—C18	−0.6 (4)
C22—Zr—N1—C2	173.26 (13)	C16—C17—C18—C19	2.2 (4)
Cl1—Zr—N1—C2	−9.68 (16)	C15—C14—C19—C18	−1.0 (4)
C23—Zr—N1—C2	−157.25 (12)	N2—C14—C19—C18	177.9 (2)
C30—Zr—N1—C2	147.74 (12)	C15—C14—C19—C21	178.7 (2)

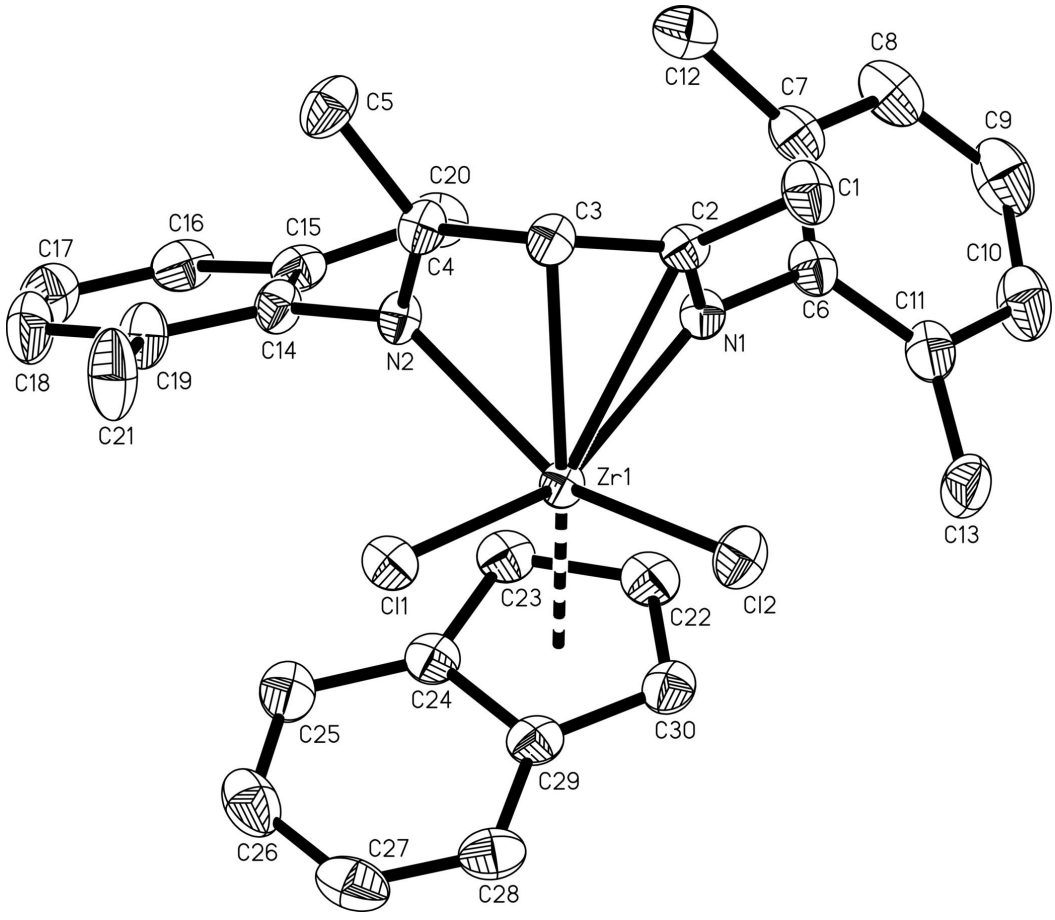
Cl2—Zr—N1—C2	67.72 (12)	N2—C14—C19—C21	−2.5 (4)
C24—Zr—N1—C2	−159.62 (11)	C17—C18—C19—C14	−1.4 (4)
C29—Zr—N1—C2	158.42 (11)	C17—C18—C19—C21	179.0 (3)
C3—Zr—N1—C2	−21.32 (11)	N1—Zr—C22—C23	115.65 (14)
C4—Zr—N1—C2	−52.28 (12)	N2—Zr—C22—C23	38.37 (14)
N2—Zr—N1—C6	120.3 (2)	Cl1—Zr—C22—C23	−61.91 (16)
C22—Zr—N1—C6	12.1 (2)	C30—Zr—C22—C23	−115.34 (19)
Cl1—Zr—N1—C6	−170.9 (2)	Cl2—Zr—C22—C23	−158.84 (12)
C23—Zr—N1—C6	41.6 (2)	C24—Zr—C22—C23	−37.92 (12)
C30—Zr—N1—C6	−13.5 (3)	C29—Zr—C22—C23	−77.95 (14)
Cl2—Zr—N1—C6	−93.5 (2)	C3—Zr—C22—C23	97.39 (15)
C24—Zr—N1—C6	39.2 (3)	C2—Zr—C22—C23	119.38 (13)
C29—Zr—N1—C6	−2.8 (3)	C4—Zr—C22—C23	57.72 (15)
C3—Zr—N1—C6	177.5 (3)	N1—Zr—C22—C30	−129.00 (14)
C2—Zr—N1—C6	−161.2 (3)	N2—Zr—C22—C30	153.71 (12)
C4—Zr—N1—C6	146.5 (3)	Cl1—Zr—C22—C30	53.43 (16)
N1—Zr—N2—C4	67.03 (13)	C23—Zr—C22—C30	115.34 (19)
C22—Zr—N2—C4	144.41 (13)	Cl2—Zr—C22—C30	−43.50 (13)
Cl1—Zr—N2—C4	−79.78 (12)	C24—Zr—C22—C30	77.43 (14)
C23—Zr—N2—C4	164.45 (14)	C29—Zr—C22—C30	37.39 (12)
C30—Zr—N2—C4	164.14 (12)	C3—Zr—C22—C30	−147.27 (12)
Cl2—Zr—N2—C4	−6.12 (17)	C2—Zr—C22—C30	−125.27 (13)
C24—Zr—N2—C4	−164.03 (13)	C4—Zr—C22—C30	173.06 (11)
C29—Zr—N2—C4	−158.83 (12)	C30—C22—C23—C24	4.3 (2)
C3—Zr—N2—C4	8.67 (12)	Zr—C22—C23—C24	71.07 (14)
C2—Zr—N2—C4	35.63 (13)	C30—C22—C23—Zr	−66.79 (14)
N1—Zr—N2—C14	−127.1 (2)	N1—Zr—C23—C22	−63.35 (14)
C22—Zr—N2—C14	−49.7 (2)	N2—Zr—C23—C22	−142.73 (14)
Cl1—Zr—N2—C14	86.1 (2)	Cl1—Zr—C23—C22	136.81 (12)
C23—Zr—N2—C14	−29.7 (2)	C30—Zr—C23—C22	36.99 (13)
C30—Zr—N2—C14	−30.0 (2)	Cl2—Zr—C23—C22	29.53 (16)
Cl2—Zr—N2—C14	159.74 (16)	C24—Zr—C23—C22	113.19 (19)
C24—Zr—N2—C14	1.8 (2)	C29—Zr—C23—C22	76.92 (14)
C29—Zr—N2—C14	7.0 (2)	C3—Zr—C23—C22	−115.41 (14)
C3—Zr—N2—C14	174.5 (2)	C2—Zr—C23—C22	−77.25 (15)
C2—Zr—N2—C14	−158.5 (2)	C4—Zr—C23—C22	−135.46 (13)
C4—Zr—N2—C14	165.9 (3)	N1—Zr—C23—C24	−176.54 (13)
C6—N1—C2—C3	−149.8 (2)	N2—Zr—C23—C24	104.08 (13)
Zr—N1—C2—C3	41.9 (2)	C22—Zr—C23—C24	−113.19 (19)
C6—N1—C2—C1	35.1 (3)	Cl1—Zr—C23—C24	23.62 (14)
Zr—N1—C2—C1	−133.18 (18)	C30—Zr—C23—C24	−76.19 (14)
C6—N1—C2—Zr	168.3 (2)	Cl2—Zr—C23—C24	−83.65 (14)
N2—Zr—C2—N1	94.99 (12)	C29—Zr—C23—C24	−36.26 (12)
C22—Zr—C2—N1	−7.15 (14)	C3—Zr—C23—C24	131.40 (12)
Cl1—Zr—C2—N1	173.85 (10)	C2—Zr—C23—C24	169.56 (12)
C23—Zr—C2—N1	27.60 (15)	C4—Zr—C23—C24	111.35 (13)
C30—Zr—C2—N1	−40.81 (15)	C22—C23—C24—C25	175.2 (2)
Cl2—Zr—C2—N1	−108.40 (12)	Zr—C23—C24—C25	−116.8 (2)
C24—Zr—C2—N1	41.1 (2)	C22—C23—C24—C29	−2.6 (2)

C29—Zr—C2—N1	−48.6 (2)	Zr—C23—C24—C29	65.43 (14)
C3—Zr—C2—N1	142.91 (19)	C22—C23—C24—Zr	−67.99 (14)
C4—Zr—C2—N1	113.84 (13)	N1—Zr—C24—C23	4.38 (16)
N1—Zr—C2—C3	−142.91 (19)	N2—Zr—C24—C23	−72.77 (13)
N2—Zr—C2—C3	−47.92 (12)	C22—Zr—C24—C23	38.30 (13)
C22—Zr—C2—C3	−150.06 (12)	Cl1—Zr—C24—C23	−158.48 (13)
Cl1—Zr—C2—C3	30.93 (13)	C30—Zr—C24—C23	79.43 (14)
C23—Zr—C2—C3	−115.32 (13)	Cl2—Zr—C24—C23	122.44 (12)
C30—Zr—C2—C3	176.27 (11)	C29—Zr—C24—C23	115.71 (19)
Cl2—Zr—C2—C3	108.69 (12)	C3—Zr—C24—C23	−83.63 (17)
C24—Zr—C2—C3	−101.77 (18)	C2—Zr—C24—C23	−21.2 (2)
C29—Zr—C2—C3	168.53 (17)	C4—Zr—C24—C23	−80.68 (13)
C4—Zr—C2—C3	−29.08 (11)	N1—Zr—C24—C25	132.76 (18)
N1—Zr—C2—C1	99.7 (3)	N2—Zr—C24—C25	55.62 (19)
N2—Zr—C2—C1	−165.4 (2)	C22—Zr—C24—C25	166.7 (2)
C22—Zr—C2—C1	92.5 (2)	Cl1—Zr—C24—C25	−30.10 (18)
Cl1—Zr—C2—C1	−86.5 (2)	C23—Zr—C24—C25	128.4 (3)
C23—Zr—C2—C1	127.3 (2)	C30—Zr—C24—C25	−152.2 (2)
C30—Zr—C2—C1	58.8 (3)	Cl2—Zr—C24—C25	−109.17 (18)
Cl2—Zr—C2—C1	−8.7 (2)	C29—Zr—C24—C25	−115.9 (2)
C24—Zr—C2—C1	140.8 (2)	C3—Zr—C24—C25	44.8 (2)
C29—Zr—C2—C1	51.1 (3)	C2—Zr—C24—C25	107.2 (2)
C3—Zr—C2—C1	−117.4 (3)	C4—Zr—C24—C25	47.7 (2)
C4—Zr—C2—C1	−146.5 (3)	N1—Zr—C24—C29	−111.33 (14)
N1—C2—C3—C4	34.3 (3)	N2—Zr—C24—C29	171.53 (13)
C1—C2—C3—C4	−150.6 (2)	C22—Zr—C24—C29	−77.41 (14)
Zr—C2—C3—C4	69.6 (2)	Cl1—Zr—C24—C29	85.81 (13)
N1—C2—C3—Zr	−35.28 (17)	C23—Zr—C24—C29	−115.71 (19)
C1—C2—C3—Zr	139.88 (19)	C30—Zr—C24—C29	−36.28 (13)
N1—Zr—C3—C2	21.42 (11)	Cl2—Zr—C24—C29	6.74 (15)
N2—Zr—C3—C2	121.06 (14)	C3—Zr—C24—C29	160.66 (14)
C22—Zr—C3—C2	42.71 (16)	C2—Zr—C24—C29	−136.88 (17)
Cl1—Zr—C3—C2	−151.79 (12)	C4—Zr—C24—C29	163.61 (12)
C23—Zr—C3—C2	88.54 (14)	C23—C24—C25—C26	−176.7 (2)
C30—Zr—C3—C2	−7.9 (2)	C29—C24—C25—C26	0.9 (3)
Cl2—Zr—C3—C2	−67.48 (12)	Zr—C24—C25—C26	91.4 (2)
C24—Zr—C3—C2	134.01 (13)	C24—C25—C26—C27	−1.1 (3)
C29—Zr—C3—C2	−157.5 (3)	C25—C26—C27—C28	0.1 (4)
C4—Zr—C3—C2	128.76 (19)	C26—C27—C28—C29	1.0 (4)
N1—Zr—C3—C4	−107.34 (13)	C27—C28—C29—C30	176.8 (2)
N2—Zr—C3—C4	−7.71 (11)	C27—C28—C29—C24	−1.2 (3)
C22—Zr—C3—C4	−86.05 (15)	C27—C28—C29—Zr	−90.5 (2)
Cl1—Zr—C3—C4	79.45 (12)	C23—C24—C29—C30	−0.1 (2)
C23—Zr—C3—C4	−40.22 (16)	C25—C24—C29—C30	−178.21 (18)
C30—Zr—C3—C4	−136.62 (17)	Zr—C24—C29—C30	61.92 (14)
Cl2—Zr—C3—C4	163.76 (12)	C23—C24—C29—C28	178.34 (19)
C24—Zr—C3—C4	5.24 (19)	C25—C24—C29—C28	0.2 (3)
C29—Zr—C3—C4	73.7 (4)	Zr—C24—C29—C28	−119.6 (2)
C2—Zr—C3—C4	−128.76 (19)	C23—C24—C29—Zr	−62.03 (13)

C14—N2—C4—C3	176.21 (19)	C25—C24—C29—Zr	119.86 (18)
Zr—N2—C4—C3	−15.0 (2)	N1—Zr—C29—C30	−19.93 (16)
C14—N2—C4—C5	−1.7 (3)	N2—Zr—C29—C30	−126.30 (12)
Zr—N2—C4—C5	167.14 (19)	C22—Zr—C29—C30	−38.26 (12)
C14—N2—C4—Zr	−168.8 (2)	Cl1—Zr—C29—C30	153.08 (12)
C2—C3—C4—N2	−52.7 (3)	C23—Zr—C29—C30	−79.46 (14)
Zr—C3—C4—N2	12.98 (18)	Cl2—Zr—C29—C30	69.15 (12)
C2—C3—C4—C5	125.4 (2)	C24—Zr—C29—C30	−116.46 (19)
Zr—C3—C4—C5	−168.95 (17)	C3—Zr—C29—C30	158.9 (3)
C2—C3—C4—Zr	−65.6 (2)	C2—Zr—C29—C30	11.7 (2)
N1—Zr—C4—N2	−106.47 (13)	C4—Zr—C29—C30	−142.85 (12)
C22—Zr—C4—N2	−44.47 (16)	N1—Zr—C29—C28	−148.19 (17)
Cl1—Zr—C4—N2	97.14 (12)	N2—Zr—C29—C28	105.43 (18)
C23—Zr—C4—N2	−15.93 (14)	C22—Zr—C29—C28	−166.5 (2)
C30—Zr—C4—N2	−33.7 (3)	Cl1—Zr—C29—C28	24.82 (18)
Cl2—Zr—C4—N2	175.99 (11)	C23—Zr—C29—C28	152.3 (2)
C24—Zr—C4—N2	17.65 (15)	C30—Zr—C29—C28	−128.3 (2)
C29—Zr—C4—N2	32.68 (18)	Cl2—Zr—C29—C28	−59.11 (19)
C3—Zr—C4—N2	−165.6 (2)	C24—Zr—C29—C28	115.3 (2)
C2—Zr—C4—N2	−136.36 (15)	C3—Zr—C29—C28	30.6 (4)
N1—Zr—C4—C3	59.15 (12)	C2—Zr—C29—C28	−116.6 (2)
N2—Zr—C4—C3	165.6 (2)	C4—Zr—C29—C28	88.9 (2)
C22—Zr—C4—C3	121.16 (13)	N1—Zr—C29—C24	96.53 (14)
Cl1—Zr—C4—C3	−97.23 (12)	N2—Zr—C29—C24	−9.85 (15)
C23—Zr—C4—C3	149.70 (13)	C22—Zr—C29—C24	78.19 (14)
C30—Zr—C4—C3	131.9 (2)	Cl1—Zr—C29—C24	−90.46 (13)
Cl2—Zr—C4—C3	−18.38 (13)	C23—Zr—C29—C24	36.99 (12)
C24—Zr—C4—C3	−176.73 (12)	C30—Zr—C29—C24	116.46 (19)
C29—Zr—C4—C3	−161.69 (13)	Cl2—Zr—C29—C24	−174.39 (12)
C2—Zr—C4—C3	29.27 (12)	C3—Zr—C29—C24	−84.7 (4)
N1—Zr—C4—C5	168.7 (8)	C2—Zr—C29—C24	128.14 (18)
N2—Zr—C4—C5	−84.8 (8)	C4—Zr—C29—C24	−26.39 (19)
C22—Zr—C4—C5	−129.3 (8)	C23—C22—C30—C29	−4.4 (2)
Cl1—Zr—C4—C5	12.3 (8)	Zr—C22—C30—C29	−70.56 (15)
C23—Zr—C4—C5	−100.8 (8)	C23—C22—C30—Zr	66.21 (14)
C30—Zr—C4—C5	−118.5 (8)	C28—C29—C30—C22	−175.5 (2)
Cl2—Zr—C4—C5	91.1 (8)	C24—C29—C30—C22	2.7 (2)
C24—Zr—C4—C5	−67.2 (8)	Zr—C29—C30—C22	66.98 (14)
C29—Zr—C4—C5	−52.2 (8)	C28—C29—C30—Zr	117.6 (2)
C3—Zr—C4—C5	109.5 (8)	C24—C29—C30—Zr	−64.27 (14)
C2—Zr—C4—C5	138.8 (8)	N1—Zr—C30—C22	51.54 (14)
C2—N1—C6—C11	−113.5 (2)	N2—Zr—C30—C22	−36.65 (17)
Zr—N1—C6—C11	44.9 (3)	Cl1—Zr—C30—C22	−142.44 (12)
C2—N1—C6—C7	68.5 (2)	C23—Zr—C30—C22	−37.03 (13)
Zr—N1—C6—C7	−133.1 (2)	Cl2—Zr—C30—C22	137.64 (13)
C11—C6—C7—C8	−6.2 (3)	C24—Zr—C30—C22	−77.53 (14)
N1—C6—C7—C8	171.90 (19)	C29—Zr—C30—C22	−113.58 (18)
C11—C6—C7—C12	170.5 (2)	C3—Zr—C30—C22	76.7 (2)
N1—C6—C7—C12	−11.4 (3)	C2—Zr—C30—C22	71.68 (14)

C6—C7—C8—C9	3.0 (3)	C4—Zr—C30—C22	−15.9 (3)
C12—C7—C8—C9	−173.8 (2)	N1—Zr—C30—C29	165.12 (12)
C7—C8—C9—C10	1.6 (4)	N2—Zr—C30—C29	76.93 (15)
C8—C9—C10—C11	−3.1 (4)	C22—Zr—C30—C29	113.58 (18)
C9—C10—C11—C6	−0.1 (3)	Cl1—Zr—C30—C29	−28.85 (13)
C9—C10—C11—C13	176.9 (2)	C23—Zr—C30—C29	76.56 (13)
C7—C6—C11—C10	4.7 (3)	Cl2—Zr—C30—C29	−108.78 (12)
N1—C6—C11—C10	−173.3 (2)	C24—Zr—C30—C29	36.06 (11)
C7—C6—C11—C13	−172.1 (2)	C3—Zr—C30—C29	−169.71 (16)
N1—C6—C11—C13	9.9 (3)	C2—Zr—C30—C29	−174.74 (11)
C4—N2—C14—C19	71.3 (3)	C4—Zr—C30—C29	97.6 (2)
Zr—N2—C14—C19	−92.4 (3)	C36—C31—C32—C33	−3.4 (8)
C4—N2—C14—C15	−109.9 (2)	C37—C31—C32—C33	−176.3 (9)
Zr—N2—C14—C15	86.5 (3)	C31—C32—C33—C34	3.9 (14)
C19—C14—C15—C16	2.4 (3)	C32—C33—C34—C35	−4(2)
N2—C14—C15—C16	−176.45 (19)	C33—C34—C35—C36	3(2)
C19—C14—C15—C20	−172.6 (2)	C34—C35—C36—C31	−2.9 (14)
N2—C14—C15—C20	8.5 (3)	C32—C31—C36—C35	2.9 (9)
C14—C15—C16—C17	−1.6 (3)	C37—C31—C36—C35	176.0 (9)
C20—C15—C16—C17	173.7 (2)		

Fig. 1


C12
C8
C7
C5
C9
C20
C1
C3
C2
C16
C15
C10
C17
C4
C6
C11
C14
N2
N1
C18
C19
C21
Zr1
C13
Cl1
C23
C22
Cl2
C24
C25
C30
C29
C26
C27
C28