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

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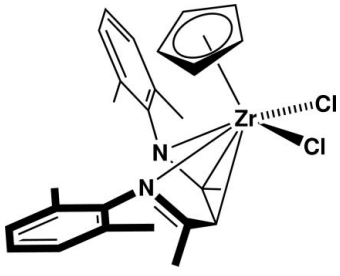
Key indicators: single-crystal X-ray study; T = 150 K; mean σ(C–C) = 0.004 Å; R factor = 0.042; wR factor = 0.103; data-to-parameter ratio = 15.9.

The title compound, $[Zr(Cl)_2(C_{21}H_{25}N_2)(C_5H_5)]$, [bis(2,6-dimethylphenyl)nacnac](cp)$ZrCl_2$, where nacnac is the pentane-2,4-diiminate ligand and cp is cyclopentadiene, 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 an η^3-enaminato coordination of the nacnac ligand.

Related literature

The title compound is almost isostructural with the indenyl complex (Verguet *et al.*, 2007) and its synthesis and structural discussion are closely related. For a related mixed (indenyl)(nacnac)$ZrCl_2$ compound, see Rahim *et al.* (1998). A comparable coordination of the nacnac ligand can be found in the five-coordinated complexes reported by 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 ligands, see: Rahim *et al.* (1998); Vollmerhaus *et al.* (2000). For related literature, see: Fortuné *et al.* (2007); Faller *et al.* (1985); Lee *et al.* (1999).



Experimental

Crystal data

$[Zr(Cl)_2(C_{21}H_{25}N_2)(C_5H_5)]$
M_r = 532.64
Triclinic, $P\overline{1}$
a = 10.0163 (3) Å
b = 10.5990 (4) Å
c = 13.1392 (5) Å
α = 73.803 (1)°
β = 78.869 (2)°
γ = 66.178 (1)°
V = 1220.27 (7) Å^3
Z = 2
Cu $K\alpha$ radiation
μ = 5.82 mm^{-1}
T = 150 K
0.30 × 0.26 × 0.12 mm

Data collection

Bruker SMART 6000 diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.27, T_{max} = 0.49
14734 measured reflections
4561 independent reflections
4541 reflections with $I > 2\sigma(I)$
R_{int} = 0.036

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.103
S = 1.13
4561 reflections
287 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.75 e Å^{-3}
$\Delta\rho_{min}$ = −1.59 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).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: GG2043).

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supplementary materials

Acta Cryst. (2007). E**63**, m2541 [**doi:10.1107/S1600536807043978**]

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

E. Verguet, 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 cyclopentadienyl sodium. 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 dependent 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).

In contrast to these, the nacnac ligand adopts in the title complex (I), an intermediate, distorted coordination mode. An analogous coordination mode has already been observed and described for the analogous complex (Verguet *et al.*, 2007), in which cyclopentadienyl was replaced by indenyl. The assignment of the coordination mode follows the same rational and we will point out in the following only shortly the necessary metrical data. The η^3-coordinated enamito-moiety C2, C3 and N1 displays short Zr—C2 and Zr—C3 distances of 2.616 (2) and 2.620 (2) Å, respectively compared to a Zr—C4 distance of 2.826 (2) Å for the η^1-coordinated imine-moiety. The C2═N1 bond is slighty longer than C4═N2 (1.354 (3) and 1.306 (3) Å, respectively). The metal center is nearly in the plane of the imine moiety (∢ (C5,C4,Zr) = 169.5 (2)°), while a more side-on coordination is observed for N1, C1–C3 (∢ (C1,C2,Zr) = 140.7 (2)°). An elongated C3—C4 distance in comparison with C2—C3 (1.462 (3) and 1.389 (3) Å, respectively) and a 44° angle between the least square planes through N1, C1–C3 and N2, C3–C5 agree with a slight loss of electron delocalization in the nacnac ligand.

Analogous to the corresponding indenyl complex (Verguet *et al.*, 2007), 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 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 plane of the nacnac ligand was ascribed to steric reasons without any significant coordination of the carbon atoms to the metal center (Lee *et al.*, 1999). However, a comparable nacnac coordination was observed in the five-coordinated complexes reported by Basuli *et al.* (2004) (CSD-codes: FAPBUU, FAPCAP, FAPCEF & FABCIJ), which was simply described as "sandwich-like".

The cyclopentadienyl ligand displays an ideal η^5-coordination ($\Delta M–C < 3\sigma$, 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 0.086 g NaCp (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, 0.15 g (32%).

NMR ^{1}H (300 MHz, C_6D_6), δ p.p.m.: 6.93–6.75 (m, 6H, CH [$C_6H_3Me_2$]), 6.33 (s, 5H, H [Cp]), 5.35 (s, 1H, CH [nacnac]), 2.66 (s, 12H, CH_3 [$C_6H_3Me_2$]), 1.59 (s, 6H, CH_3 [nacnac]). Elem. Anal. for $C_{26}H_{30}N_2Cl_2Zr$: clcd. C, 58.60%; H, 5.60%; N,5.30%. found C, 58.47%; H, 5.99%; N, 5.07%.

Refinement

The H atoms were generated geometrically (C—H 0.95 to 0.98 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

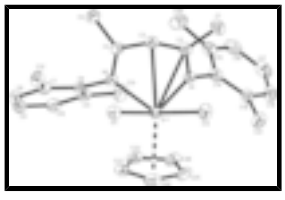


Fig. 1. *ORTEP* view of the title compound (I). Displacement ellipsoids are shown at the 50% probability level.

Dichlorido-[<it>*N*</it>,<it>*N*</it>'-bis(2,6-dimethylphenyl)pentane-2,4-diiminato](cyclopentadienyl)zirconium(IV)

Crystal data

$[Zr(Cl)_2(C_{21}H_{25}N_2)(C_5H_5)]$	$Z = 2$
$M_r = 532.64$	$F_{000} = 548$
Triclinic, $P\overline{1}$	$D_x = 1.450$ Mg m^{-3}
Hall symbol: -P 1	Cu $K\alpha$ radiation λ = 1.54178 Å
$a = 10.0163$ (3) Å	Cell parameters from 13439 reflections
$b = 10.5990$ (4) Å	θ = 3.5–71.3°
$c = 13.1392$ (5) Å	μ = 5.82 mm^{-1}
α = 73.803 (1)°	$T = 150$ K
β = 78.869 (2)°	Plate, colorless
γ = 66.178 (1)°	0.30 × 0.26 × 0.12 mm
$V = 1220.27$ (7) Å^3	

Data collection

Bruker SMART 6000 diffractometer
Radiation source: Rotating Anode
Monochromator: Montel 200 optics
Detector resolution: 5.5 pixels mm^{-1}
T = 150 K
ω scans
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)
T_{min} = 0.27, T_{max} = 0.49
14734 measured reflections
4561 independent reflections
4541 reflections with $I > 2\sigma(I)$
R_{int} = 0.036
θ_{max} = 71.8º
θ_{min} = 3.5º
$h = -12 \rightarrow 12$
$k = -12 \rightarrow 12$
$l = -16 \rightarrow 16$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.103
S = 1.13
4561 reflections
287 parameters
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
$w = 1/[\sigma^2(F_o^2) + (0.0762P)^2 + 0.4394P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.002
$\Delta\rho_{max}$ = 0.75 e $Å^{-3}$
$\Delta\rho_{min}$ = −1.59 e $Å^{-3}$
Extinction correction: SHELXL97 (Sheldrick, 1997), $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0309 (9)

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. Comments on CHECKCIF-errors: All geometrically accessible data was collected. A data completeness of 0.95 was due to geometrical constraints of the instrument (particularly severe for triclinic space groups) and could not be improved. Errors in the T_{max}/T_{min} ratio are probably due to inaccurate determination of crystal dimensions.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Zr1	0.308862 (17)	1.073009 (17)	0.252603 (12)	0.01780 (13)
Cl1	0.38706 (6)	1.24068 (6)	0.10173 (4)	0.02458 (16)
Cl2	0.57167 (6)	0.97220 (6)	0.29131 (5)	0.02741 (16)
N1	0.3069 (2)	0.8588 (2)	0.29919 (14)	0.0201 (4)

N2	0.1471 (2)	1.0924 (2)	0.14178 (15)	0.0188 (4)
C1	0.5300 (3)	0.6836 (3)	0.2257 (2)	0.0318 (5)
H1A	0.5924	0.6811	0.2758	0.048*
H1B	0.5862	0.6758	0.1563	0.048*
H1C	0.4963	0.6045	0.2527	0.048*
C2	0.3999 (2)	0.8209 (2)	0.21377 (19)	0.0224 (5)
C3	0.3805 (3)	0.9139 (2)	0.11475 (18)	0.0224 (5)
H3	0.4649	0.9149	0.0674	0.027*
C4	0.2365 (2)	1.0103 (2)	0.07984 (17)	0.0205 (4)
C5	0.2026 (3)	0.9982 (3)	−0.02249 (19)	0.0285 (5)
H5A	0.1018	1.0617	−0.0364	0.043*
H5B	0.2135	0.9004	−0.0170	0.043*
H5C	0.2704	1.0244	−0.0809	0.043*
C6	−0.0015 (2)	1.1825 (2)	0.11747 (18)	0.0198 (4)
C7	−0.0299 (3)	1.2987 (2)	0.02897 (19)	0.0242 (5)
C8	−0.1755 (3)	1.3857 (3)	0.0140 (2)	0.0285 (5)
H8	−0.1966	1.4641	−0.0452	0.034*
C9	−0.2902 (3)	1.3617 (3)	0.0825 (2)	0.0308 (5)
H9	−0.3883	1.4241	0.0711	0.037*
C10	−0.2614 (3)	1.2461 (3)	0.1679 (2)	0.0272 (5)
H10	−0.3405	1.2287	0.2144	0.033*
C11	−0.1171 (3)	1.1545 (2)	0.18677 (18)	0.0222 (4)
C12	0.0889 (3)	1.3325 (3)	−0.0499 (2)	0.0296 (5)
H12A	0.1084	1.2855	−0.1086	0.044*
H12B	0.1785	1.2990	−0.0144	0.044*
H12C	0.0569	1.4351	−0.0778	0.044*
C13	−0.0938 (3)	1.0269 (3)	0.2775 (2)	0.0306 (5)
H13A	−0.1544	1.0555	0.3414	0.046*
H13B	0.0097	0.9841	0.2914	0.046*
H13C	−0.1214	0.9578	0.2590	0.046*
C14	0.2780 (3)	0.7493 (2)	0.38273 (19)	0.0227 (5)
C15	0.1997 (3)	0.6783 (2)	0.3584 (2)	0.0272 (5)
C16	0.1606 (3)	0.5787 (3)	0.4393 (2)	0.0330 (6)
H16	0.1060	0.5320	0.4239	0.040*
C17	0.1999 (3)	0.5467 (3)	0.5414 (2)	0.0345 (6)
H17	0.1706	0.4802	0.5960	0.041*
C18	0.2819 (3)	0.6121 (3)	0.5633 (2)	0.0305 (5)
H18	0.3098	0.5888	0.6333	0.037*
C19	0.3249 (3)	0.7120 (2)	0.48493 (19)	0.0249 (5)
C20	0.1620 (3)	0.7018 (3)	0.2470 (2)	0.0368 (6)
H20A	0.2484	0.6487	0.2054	0.055*
H20B	0.1306	0.8028	0.2132	0.055*
H20C	0.0824	0.6690	0.2501	0.055*
C21	0.4278 (3)	0.7660 (3)	0.5126 (2)	0.0302 (5)
H21A	0.3766	0.8252	0.5643	0.045*
H21B	0.4618	0.8222	0.4481	0.045*
H21C	0.5120	0.6857	0.5436	0.045*
C22	0.0701 (3)	1.2031 (3)	0.3459 (2)	0.0298 (5)
H22	−0.0181	1.2071	0.3261	0.036*

C23	0.1387 (3)	1.3008 (3)	0.3012 (2)	0.0319 (6)
H23	0.1053	1.3824	0.2455	0.038*
C24	0.2652 (3)	1.2569 (3)	0.3532 (2)	0.0328 (6)
H24	0.3327	1.3034	0.3386	0.039*
C25	0.2746 (3)	1.1325 (3)	0.4306 (2)	0.0312 (5)
H25	0.3488	1.0806	0.4781	0.037*
C26	0.1550 (3)	1.0983 (3)	0.42522 (19)	0.0296 (5)
H26	0.1348	1.0183	0.4678	0.036*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zr1	0.01333 (16)	0.02266 (16)	0.01805 (16)	−0.00592 (10)	−0.00042 (9)	−0.00736 (9)
Cl1	0.0210 (3)	0.0266 (3)	0.0257 (3)	−0.0101 (2)	−0.0002 (2)	−0.0045 (2)
Cl2	0.0156 (3)	0.0351 (3)	0.0303 (3)	−0.0096 (2)	−0.0041 (2)	−0.0040 (2)
N1	0.0188 (9)	0.0235 (9)	0.0179 (9)	−0.0078 (7)	−0.0004 (7)	−0.0057 (7)
N2	0.0147 (9)	0.0238 (9)	0.0191 (8)	−0.0077 (7)	−0.0009 (7)	−0.0064 (7)
C1	0.0245 (12)	0.0291 (12)	0.0320 (13)	−0.0007 (10)	0.0008 (10)	−0.0086 (10)
C2	0.0183 (11)	0.0244 (11)	0.0251 (11)	−0.0066 (9)	−0.0009 (9)	−0.0091 (9)
C3	0.0183 (11)	0.0258 (11)	0.0214 (11)	−0.0062 (9)	0.0037 (9)	−0.0095 (9)
C4	0.0209 (11)	0.0240 (10)	0.0185 (10)	−0.0105 (9)	0.0013 (9)	−0.0065 (8)
C5	0.0293 (12)	0.0334 (12)	0.0230 (11)	−0.0075 (10)	−0.0039 (10)	−0.0117 (9)
C6	0.0175 (11)	0.0231 (10)	0.0207 (10)	−0.0064 (9)	−0.0040 (9)	−0.0080 (8)
C7	0.0255 (12)	0.0245 (11)	0.0249 (11)	−0.0091 (9)	−0.0068 (10)	−0.0066 (9)
C8	0.0301 (13)	0.0223 (11)	0.0322 (12)	−0.0049 (9)	−0.0120 (11)	−0.0057 (9)
C9	0.0202 (11)	0.0304 (12)	0.0407 (14)	0.0001 (9)	−0.0115 (11)	−0.0150 (11)
C10	0.0170 (11)	0.0358 (12)	0.0313 (12)	−0.0074 (10)	−0.0002 (10)	−0.0163 (10)
C11	0.0175 (10)	0.0289 (11)	0.0220 (11)	−0.0072 (9)	−0.0022 (9)	−0.0104 (9)
C12	0.0313 (13)	0.0307 (12)	0.0265 (11)	−0.0142 (10)	−0.0073 (10)	0.0013 (9)
C13	0.0211 (11)	0.0433 (14)	0.0252 (12)	−0.0142 (10)	0.0000 (10)	−0.0022 (10)
C14	0.0190 (11)	0.0225 (10)	0.0232 (11)	−0.0059 (9)	0.0028 (9)	−0.0058 (9)
C15	0.0240 (12)	0.0245 (11)	0.0319 (12)	−0.0071 (9)	−0.0012 (10)	−0.0085 (9)
C16	0.0280 (12)	0.0279 (12)	0.0427 (14)	−0.0114 (10)	0.0050 (11)	−0.0112 (11)
C17	0.0326 (14)	0.0251 (12)	0.0371 (14)	−0.0093 (10)	0.0089 (11)	−0.0041 (10)
C18	0.0270 (12)	0.0291 (12)	0.0243 (11)	−0.0035 (10)	0.0008 (10)	−0.0019 (9)
C19	0.0178 (10)	0.0240 (10)	0.0259 (11)	−0.0019 (8)	−0.0010 (9)	−0.0046 (9)
C20	0.0401 (15)	0.0432 (15)	0.0389 (14)	−0.0234 (13)	−0.0047 (12)	−0.0144 (12)
C21	0.0260 (12)	0.0394 (13)	0.0241 (11)	−0.0103 (10)	−0.0054 (10)	−0.0058 (10)
C22	0.0191 (11)	0.0438 (14)	0.0277 (12)	−0.0056 (10)	0.0018 (10)	−0.0219 (11)
C23	0.0310 (13)	0.0289 (12)	0.0307 (12)	−0.0002 (10)	−0.0008 (11)	−0.0168 (10)
C24	0.0317 (13)	0.0381 (14)	0.0368 (14)	−0.0139 (11)	0.0004 (11)	−0.0221 (12)
C25	0.0274 (12)	0.0445 (14)	0.0230 (11)	−0.0079 (11)	−0.0048 (10)	−0.0161 (10)
C26	0.0283 (12)	0.0400 (13)	0.0218 (11)	−0.0124 (11)	0.0044 (10)	−0.0139 (10)

Geometric parameters (Å, °)

Zr1—N1	2.1879 (19)	C10—H10	0.95
Zr1—N2	2.2944 (19)	C11—C13	1.503 (3)
Zr1—C26	2.500 (2)	C12—H12A	0.98

Zr1—C23	2.502 (2)	C12—H12B	0.98
Zr1—Cl1	2.5022 (5)	C12—H12C	0.98
Zr1—C24	2.503 (2)	C13—H13A	0.98
Zr1—C22	2.504 (2)	C13—H13B	0.98
Zr1—Cl2	2.5043 (5)	C13—H13C	0.98
Zr1—C25	2.514 (2)	C14—C19	1.406 (3)
Zr1—C2	2.616 (2)	C14—C15	1.412 (3)
Zr1—C3	2.620 (2)	C15—C16	1.393 (4)
Zr1—C4	2.826 (2)	C15—C20	1.511 (4)
N2—C4	1.306 (3)	C16—C17	1.383 (4)
N2—C6	1.447 (3)	C16—H16	0.95
N1—C2	1.354 (3)	C17—C18	1.378 (4)
N1—C14	1.440 (3)	C17—H17	0.95
C5—C4	1.499 (3)	C18—C19	1.399 (3)
C5—H5A	0.98	C18—H18	0.95
C5—H5B	0.98	C19—C21	1.503 (3)
C5—H5C	0.98	C20—H20A	0.98
C4—C3	1.462 (3)	C20—H20B	0.98
C3—C2	1.389 (3)	C20—H20C	0.98
C3—H3	0.95	C21—H21A	0.98
C2—C1	1.504 (3)	C21—H21B	0.98
C1—H1A	0.98	C21—H21C	0.98
C1—H1B	0.98	C22—C23	1.403 (4)
C1—H1C	0.98	C22—C26	1.406 (4)
C6—C11	1.406 (3)	C22—H22	0.95
C6—C7	1.413 (3)	C23—C24	1.404 (4)
C7—C8	1.393 (3)	C23—H23	0.95
C7—C12	1.510 (3)	C24—C25	1.404 (4)
C8—C9	1.379 (4)	C24—H24	0.95
C8—H8	0.95	C25—C26	1.404 (4)
C9—C10	1.384 (4)	C25—H25	0.95
C9—H9	0.95	C26—H26	0.95
C10—C11	1.402 (3)		
N1—Zr1—N2	79.32 (7)	C2—C1—H1A	109.5
N1—Zr1—C26	83.28 (8)	C2—C1—H1B	109.5
N2—Zr1—C26	103.18 (8)	H1A—C1—H1B	109.5
N1—Zr1—C23	132.68 (8)	C2—C1—H1C	109.5
N2—Zr1—C23	90.58 (8)	H1A—C1—H1C	109.5
C26—Zr1—C23	54.01 (9)	H1B—C1—H1C	109.5
N1—Zr1—Cl1	142.40 (5)	C11—C6—C7	120.8 (2)
N2—Zr1—Cl1	85.52 (5)	C11—C6—N2	118.1 (2)
C26—Zr1—Cl1	133.94 (6)	C7—C6—N2	121.0 (2)
C23—Zr1—Cl1	81.18 (7)	C8—C7—C6	117.9 (2)
N1—Zr1—C24	133.71 (8)	C8—C7—C12	118.7 (2)
N2—Zr1—C24	123.08 (8)	C6—C7—C12	123.5 (2)
C26—Zr1—C24	53.96 (9)	C9—C8—C7	122.1 (2)
C23—Zr1—C24	32.57 (9)	C9—C8—H8	118.9
Cl1—Zr1—C24	83.13 (7)	C7—C8—H8	118.9
N1—Zr1—C22	100.32 (8)	C8—C9—C10	119.6 (2)

N2—Zr1—C22	79.26 (7)	C8—C9—H9	120.2
C26—Zr1—C22	32.63 (9)	C10—C9—H9	120.2
C23—Zr1—C22	32.54 (9)	C9—C10—C11	120.8 (2)
Cl1—Zr1—C22	110.42 (7)	C9—C10—H10	119.6
C24—Zr1—C22	53.92 (9)	C11—C10—H10	119.6
N1—Zr1—Cl2	89.10 (5)	C10—C11—C6	118.7 (2)
N2—Zr1—Cl2	145.66 (5)	C10—C11—C13	118.1 (2)
C26—Zr1—Cl2	107.45 (6)	C6—C11—C13	123.1 (2)
C23—Zr1—Cl2	119.98 (7)	C7—C12—H12A	109.5
Cl1—Zr1—Cl2	84.333 (18)	C7—C12—H12B	109.5
C24—Zr1—Cl2	88.08 (7)	H12A—C12—H12B	109.5
C22—Zr1—Cl2	134.92 (6)	C7—C12—H12C	109.5
N1—Zr1—C25	101.61 (8)	H12A—C12—H12C	109.5
N2—Zr1—C25	132.79 (8)	H12B—C12—H12C	109.5
C26—Zr1—C25	32.52 (8)	C11—C13—H13A	109.5
C23—Zr1—C25	53.89 (9)	C11—C13—H13B	109.5
Cl1—Zr1—C25	113.76 (7)	H13A—C13—H13B	109.5
C24—Zr1—C25	32.49 (9)	C11—C13—H13C	109.5
C22—Zr1—C25	53.89 (8)	H13A—C13—H13C	109.5
Cl2—Zr1—C25	81.06 (6)	H13B—C13—H13C	109.5
N1—Zr1—C2	31.15 (7)	C19—C14—C15	120.1 (2)
N2—Zr1—C2	75.52 (7)	C19—C14—N1	122.6 (2)
C26—Zr1—C2	114.33 (8)	C15—C14—N1	117.3 (2)
C23—Zr1—C2	159.80 (9)	C16—C15—C14	118.9 (2)
Cl1—Zr1—C2	111.65 (5)	C16—C15—C20	118.7 (2)
C24—Zr1—C2	158.19 (9)	C14—C15—C20	122.4 (2)
C22—Zr1—C2	128.32 (8)	C17—C16—C15	121.3 (2)
Cl2—Zr1—C2	77.97 (5)	C17—C16—H16	119.4
C25—Zr1—C2	127.19 (8)	C15—C16—H16	119.4
N1—Zr1—C3	58.30 (7)	C18—C17—C16	119.5 (2)
N2—Zr1—C3	57.41 (7)	C18—C17—H17	120.3
C26—Zr1—C3	138.28 (8)	C16—C17—H17	120.3
C23—Zr1—C3	145.88 (8)	C17—C18—C19	121.6 (2)
Cl1—Zr1—C3	84.54 (5)	C17—C18—H18	119.2
C24—Zr1—C3	167.55 (9)	C19—C18—H18	119.2
C22—Zr1—C3	133.33 (8)	C18—C19—C14	118.5 (2)
Cl2—Zr1—C3	88.97 (5)	C18—C19—C21	117.9 (2)
C25—Zr1—C3	157.90 (8)	C14—C19—C21	123.5 (2)
C2—Zr1—C3	30.77 (7)	C15—C20—H20A	109.5
N1—Zr1—C4	70.63 (7)	C15—C20—H20B	109.5
N2—Zr1—C4	27.09 (7)	H20A—C20—H20B	109.5
C26—Zr1—C4	125.55 (7)	C15—C20—H20C	109.5
C23—Zr1—C4	115.63 (8)	H20A—C20—H20C	109.5
Cl1—Zr1—C4	80.25 (4)	H20B—C20—H20C	109.5
C24—Zr1—C4	146.60 (8)	C19—C21—H21A	109.5
C22—Zr1—C4	106.02 (7)	C19—C21—H21B	109.5
Cl2—Zr1—C4	118.61 (5)	H21A—C21—H21B	109.5
C25—Zr1—C4	157.86 (8)	C19—C21—H21C	109.5
C2—Zr1—C4	54.74 (7)	H21A—C21—H21C	109.5

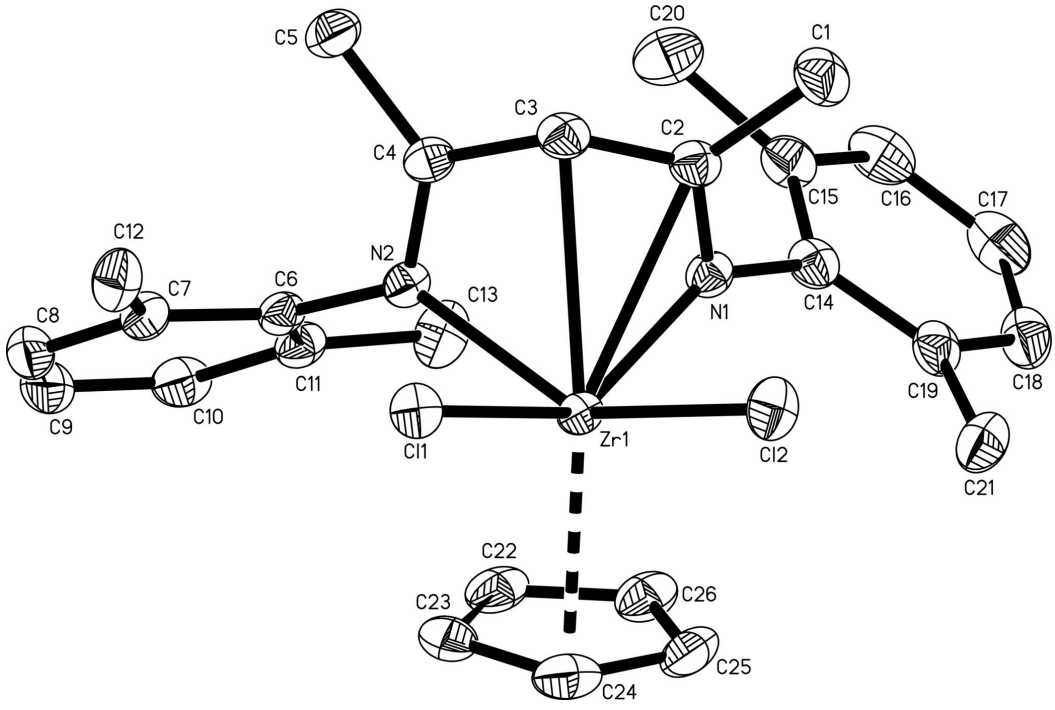
C3—Zr1—C4	30.85 (7)	H21B—C21—H21C	109.5
C4—N2—C6	121.83 (19)	C23—C22—C26	107.9 (2)
C4—N2—Zr1	99.75 (14)	C23—C22—Zr1	73.64 (14)
C6—N2—Zr1	137.20 (14)	C26—C22—Zr1	73.50 (14)
C2—N1—C14	118.35 (19)	C23—C22—H22	126
C2—N1—Zr1	92.15 (14)	C26—C22—H22	126
C14—N1—Zr1	147.43 (15)	Zr1—C22—H22	118.7
C4—C5—H5A	109.5	C22—C23—C24	108.0 (2)
C4—C5—H5B	109.5	C22—C23—Zr1	73.82 (14)
H5A—C5—H5B	109.5	C24—C23—Zr1	73.75 (14)
C4—C5—H5C	109.5	C22—C23—H23	126
H5A—C5—H5C	109.5	C24—C23—H23	126
H5B—C5—H5C	109.5	Zr1—C23—H23	118.4
N2—C4—C3	118.3 (2)	C23—C24—C25	108.1 (2)
N2—C4—C5	126.0 (2)	C23—C24—Zr1	73.68 (14)
C3—C4—C5	115.61 (19)	C25—C24—Zr1	74.20 (14)
N2—C4—Zr1	53.16 (11)	C23—C24—H24	125.9
C3—C4—Zr1	66.77 (12)	C25—C24—H24	125.9
C5—C4—Zr1	170.65 (16)	Zr1—C24—H24	118.1
C2—C3—C4	123.2 (2)	C24—C25—C26	107.9 (2)
C2—C3—Zr1	74.45 (13)	C24—C25—Zr1	73.31 (14)
C4—C3—Zr1	82.37 (13)	C26—C25—Zr1	73.16 (14)
C2—C3—H3	118.4	C24—C25—H25	126.1
C4—C3—H3	118.4	C26—C25—H25	126.1
Zr1—C3—H3	114.9	Zr1—C25—H25	119.3
N1—C2—C3	119.7 (2)	C25—C26—C22	108.1 (2)
N1—C2—C1	120.9 (2)	C25—C26—Zr1	74.32 (14)
C3—C2—C1	119.2 (2)	C22—C26—Zr1	73.87 (13)
N1—C2—Zr1	56.70 (11)	C25—C26—H26	126
C3—C2—Zr1	74.77 (13)	C22—C26—H26	126
C1—C2—Zr1	140.72 (17)	Zr1—C26—H26	117.8
N1—Zr1—N2—C4	−68.14 (14)	C12—C7—C8—C9	179.9 (2)
C26—Zr1—N2—C4	−148.56 (14)	C7—C8—C9—C10	−1.4 (4)
C23—Zr1—N2—C4	158.40 (14)	C8—C9—C10—C11	1.1 (4)
Cl1—Zr1—N2—C4	77.30 (13)	C9—C10—C11—C6	0.3 (3)
C24—Zr1—N2—C4	156.10 (14)	C9—C10—C11—C13	−176.9 (2)
C22—Zr1—N2—C4	−170.92 (15)	C7—C6—C11—C10	−1.5 (3)
Cl2—Zr1—N2—C4	4.16 (18)	N2—C6—C11—C10	176.1 (2)
C25—Zr1—N2—C4	−164.14 (14)	C7—C6—C11—C13	175.6 (2)
C2—Zr1—N2—C4	−36.43 (13)	N2—C6—C11—C13	−6.8 (3)
C3—Zr1—N2—C4	−9.08 (13)	C2—N1—C14—C19	112.3 (2)
N1—Zr1—N2—C6	125.2 (2)	Zr1—N1—C14—C19	−45.2 (4)
C26—Zr1—N2—C6	44.8 (2)	C2—N1—C14—C15	−67.5 (3)
C23—Zr1—N2—C6	−8.3 (2)	Zr1—N1—C14—C15	135.0 (2)
Cl1—Zr1—N2—C6	−89.4 (2)	C19—C14—C15—C16	4.7 (3)
C24—Zr1—N2—C6	−10.6 (2)	N1—C14—C15—C16	−175.5 (2)
C22—Zr1—N2—C6	22.4 (2)	C19—C14—C15—C20	−172.7 (2)
Cl2—Zr1—N2—C6	−162.52 (17)	N1—C14—C15—C20	7.0 (3)
C25—Zr1—N2—C6	29.2 (3)	C14—C15—C16—C17	−1.4 (4)

C2—Zr1—N2—C6	156.9 (2)	C20—C15—C16—C17	176.1 (2)
C3—Zr1—N2—C6	−175.8 (2)	C15—C16—C17—C18	−1.4 (4)
C4—Zr1—N2—C6	−166.7 (3)	C16—C17—C18—C19	0.9 (4)
N2—Zr1—N1—C2	79.63 (13)	C17—C18—C19—C14	2.3 (4)
C26—Zr1—N1—C2	−175.54 (14)	C17—C18—C19—C21	−173.4 (2)
C23—Zr1—N1—C2	160.44 (14)	C15—C14—C19—C18	−5.2 (3)
Cl1—Zr1—N1—C2	11.66 (17)	N1—C14—C19—C18	175.1 (2)
C24—Zr1—N1—C2	−154.33 (14)	C15—C14—C19—C21	170.3 (2)
C22—Zr1—N1—C2	156.51 (14)	N1—C14—C19—C21	−9.4 (3)
Cl2—Zr1—N1—C2	−67.85 (13)	N1—Zr1—C22—C23	174.62 (15)
C25—Zr1—N1—C2	−148.53 (14)	N2—Zr1—C22—C23	−108.45 (16)
C3—Zr1—N1—C2	21.50 (13)	C26—Zr1—C22—C23	114.9 (2)
C4—Zr1—N1—C2	53.02 (13)	Cl1—Zr1—C22—C23	−27.39 (16)
N2—Zr1—N1—C14	−120.1 (3)	C24—Zr1—C22—C23	37.20 (16)
C26—Zr1—N1—C14	−15.2 (3)	Cl2—Zr1—C22—C23	75.47 (17)
C23—Zr1—N1—C14	−39.2 (3)	C25—Zr1—C22—C23	77.71 (17)
Cl1—Zr1—N1—C14	172.0 (2)	C2—Zr1—C22—C23	−170.14 (14)
C24—Zr1—N1—C14	6.0 (3)	C3—Zr1—C22—C23	−129.61 (15)
C22—Zr1—N1—C14	−43.2 (3)	C4—Zr1—C22—C23	−112.74 (15)
Cl2—Zr1—N1—C14	92.5 (3)	N1—Zr1—C22—C26	59.68 (16)
C25—Zr1—N1—C14	11.8 (3)	N2—Zr1—C22—C26	136.61 (16)
C2—Zr1—N1—C14	160.3 (4)	C23—Zr1—C22—C26	−114.9 (2)
C3—Zr1—N1—C14	−178.2 (3)	Cl1—Zr1—C22—C26	−142.33 (14)
C4—Zr1—N1—C14	−146.7 (3)	C24—Zr1—C22—C26	−77.75 (17)
C6—N2—C4—C3	−174.92 (19)	Cl2—Zr1—C22—C26	−39.48 (19)
Zr1—N2—C4—C3	15.7 (2)	C25—Zr1—C22—C26	−37.24 (15)
C6—N2—C4—C5	1.0 (3)	C2—Zr1—C22—C26	74.91 (17)
Zr1—N2—C4—C5	−168.4 (2)	C3—Zr1—C22—C26	115.45 (16)
C6—N2—C4—Zr1	169.4 (2)	C4—Zr1—C22—C26	132.32 (15)
N1—Zr1—C4—N2	104.83 (14)	C26—C22—C23—C24	−0.3 (3)
C26—Zr1—C4—N2	38.63 (17)	Zr1—C22—C23—C24	−66.38 (17)
C23—Zr1—C4—N2	−24.10 (16)	C26—C22—C23—Zr1	66.04 (17)
Cl1—Zr1—C4—N2	−99.32 (13)	N1—Zr1—C23—C22	−7.2 (2)
C24—Zr1—C4—N2	−38.1 (2)	N2—Zr1—C23—C22	68.76 (15)
C22—Zr1—C4—N2	9.28 (15)	C26—Zr1—C23—C22	−37.18 (15)
Cl2—Zr1—C4—N2	−177.33 (12)	Cl1—Zr1—C23—C22	154.13 (15)
C25—Zr1—C4—N2	32.2 (3)	C24—Zr1—C23—C22	−114.8 (2)
C2—Zr1—C4—N2	135.23 (16)	Cl2—Zr1—C23—C22	−127.69 (14)
C3—Zr1—C4—N2	165.0 (2)	C25—Zr1—C23—C22	−77.70 (16)
N1—Zr1—C4—C3	−60.15 (13)	C2—Zr1—C23—C22	22.9 (3)
N2—Zr1—C4—C3	−165.0 (2)	C3—Zr1—C23—C22	87.8 (2)
C26—Zr1—C4—C3	−126.35 (14)	C4—Zr1—C23—C22	79.47 (16)
C23—Zr1—C4—C3	170.93 (13)	N1—Zr1—C23—C24	107.62 (17)
Cl1—Zr1—C4—C3	95.70 (12)	N2—Zr1—C23—C24	−176.42 (17)
C24—Zr1—C4—C3	156.96 (17)	C26—Zr1—C23—C24	77.64 (18)
C22—Zr1—C4—C3	−155.69 (13)	Cl1—Zr1—C23—C24	−91.05 (16)
Cl2—Zr1—C4—C3	17.70 (14)	C22—Zr1—C23—C24	114.8 (2)
C25—Zr1—C4—C3	−132.8 (2)	Cl2—Zr1—C23—C24	−12.87 (19)
C2—Zr1—C4—C3	−29.74 (13)	C25—Zr1—C23—C24	37.12 (16)

N2—C4—C3—C2	52.1 (3)	C2—Zr1—C23—C24	137.7 (2)
C5—C4—C3—C2	−124.2 (2)	C3—Zr1—C23—C24	−157.42 (17)
Zr1—C4—C3—C2	65.7 (2)	C4—Zr1—C23—C24	−165.71 (15)
N2—C4—C3—Zr1	−13.63 (19)	C22—C23—C24—C25	−0.3 (3)
C5—C4—C3—Zr1	170.06 (18)	Zr1—C23—C24—C25	−66.77 (18)
N1—Zr1—C3—C2	−21.75 (13)	C22—C23—C24—Zr1	66.43 (17)
N2—Zr1—C3—C2	−119.59 (15)	N1—Zr1—C24—C23	−104.21 (18)
C26—Zr1—C3—C2	−47.67 (19)	N2—Zr1—C24—C23	4.3 (2)
C23—Zr1—C3—C2	−142.33 (17)	C26—Zr1—C24—C23	−77.83 (18)
Cl1—Zr1—C3—C2	152.24 (13)	Cl1—Zr1—C24—C23	84.35 (16)
C24—Zr1—C3—C2	144.1 (4)	C22—Zr1—C24—C23	−37.16 (16)
C22—Zr1—C3—C2	−94.70 (16)	Cl2—Zr1—C24—C23	168.87 (16)
Cl2—Zr1—C3—C2	67.84 (13)	C25—Zr1—C24—C23	−114.8 (2)
C25—Zr1—C3—C2	5.1 (3)	C2—Zr1—C24—C23	−141.3 (2)
C4—Zr1—C3—C2	−127.6 (2)	C3—Zr1—C24—C23	92.5 (4)
N1—Zr1—C3—C4	105.90 (14)	C4—Zr1—C24—C23	23.9 (2)
N2—Zr1—C3—C4	8.06 (11)	N1—Zr1—C24—C25	10.6 (2)
C26—Zr1—C3—C4	79.97 (17)	N2—Zr1—C24—C25	119.10 (16)
C23—Zr1—C3—C4	−14.7 (2)	C26—Zr1—C24—C25	37.00 (15)
Cl1—Zr1—C3—C4	−80.11 (12)	C23—Zr1—C24—C25	114.8 (2)
C24—Zr1—C3—C4	−88.2 (4)	Cl1—Zr1—C24—C25	−160.82 (16)
C22—Zr1—C3—C4	32.95 (17)	C22—Zr1—C24—C25	77.67 (17)
Cl2—Zr1—C3—C4	−164.52 (12)	Cl2—Zr1—C24—C25	−76.30 (15)
C25—Zr1—C3—C4	132.7 (2)	C2—Zr1—C24—C25	−26.5 (3)
C2—Zr1—C3—C4	127.6 (2)	C3—Zr1—C24—C25	−152.7 (3)
C14—N1—C2—C3	149.3 (2)	C4—Zr1—C24—C25	138.68 (16)
Zr1—N1—C2—C3	−42.6 (2)	C23—C24—C25—C26	0.9 (3)
C14—N1—C2—C1	−34.8 (3)	Zr1—C24—C25—C26	−65.52 (17)
Zr1—N1—C2—C1	133.3 (2)	C23—C24—C25—Zr1	66.42 (17)
C14—N1—C2—Zr1	−168.1 (2)	N1—Zr1—C25—C24	−172.18 (15)
C4—C3—C2—N1	−33.8 (3)	N2—Zr1—C25—C24	−86.05 (18)
Zr1—C3—C2—N1	35.90 (19)	C26—Zr1—C25—C24	−115.2 (2)
C4—C3—C2—C1	150.2 (2)	C23—Zr1—C25—C24	−37.22 (16)
Zr1—C3—C2—C1	−140.1 (2)	Cl1—Zr1—C25—C24	20.88 (17)
C4—C3—C2—Zr1	−69.7 (2)	C22—Zr1—C25—C24	−77.80 (17)
N2—Zr1—C2—N1	−93.29 (14)	Cl2—Zr1—C25—C24	100.60 (15)
C26—Zr1—C2—N1	4.86 (16)	C2—Zr1—C25—C24	168.00 (14)
C23—Zr1—C2—N1	−45.5 (3)	C3—Zr1—C25—C24	164.76 (19)
Cl1—Zr1—C2—N1	−172.38 (11)	C4—Zr1—C25—C24	−105.3 (2)
C24—Zr1—C2—N1	57.4 (3)	N1—Zr1—C25—C26	−57.02 (17)
C22—Zr1—C2—N1	−29.99 (17)	N2—Zr1—C25—C26	29.1 (2)
Cl2—Zr1—C2—N1	108.76 (13)	C23—Zr1—C25—C26	77.95 (17)
C25—Zr1—C2—N1	39.93 (17)	Cl1—Zr1—C25—C26	136.04 (14)
C3—Zr1—C2—N1	−142.5 (2)	C24—Zr1—C25—C26	115.2 (2)
C4—Zr1—C2—N1	−112.63 (15)	C22—Zr1—C25—C26	37.37 (16)
N1—Zr1—C2—C3	142.5 (2)	Cl2—Zr1—C25—C26	−144.24 (16)
N2—Zr1—C2—C3	49.17 (13)	C2—Zr1—C25—C26	−76.83 (18)
C26—Zr1—C2—C3	147.32 (14)	C3—Zr1—C25—C26	−80.1 (3)
C23—Zr1—C2—C3	97.0 (3)	C4—Zr1—C25—C26	9.8 (3)

Cl1—Zr1—C2—C3	−29.92 (14)	C24—C25—C26—C22	−1.1 (3)
C24—Zr1—C2—C3	−160.1 (2)	Zr1—C25—C26—C22	−66.73 (17)
C22—Zr1—C2—C3	112.47 (15)	C24—C25—C26—Zr1	65.62 (17)
Cl2—Zr1—C2—C3	−108.78 (13)	C23—C22—C26—C25	0.9 (3)
C25—Zr1—C2—C3	−177.61 (13)	Zr1—C22—C26—C25	67.03 (17)
C4—Zr1—C2—C3	29.82 (12)	C23—C22—C26—Zr1	−66.13 (17)
N1—Zr1—C2—C1	−99.7 (3)	N1—Zr1—C26—C25	124.17 (16)
N2—Zr1—C2—C1	167.0 (3)	N2—Zr1—C26—C25	−158.49 (15)
C26—Zr1—C2—C1	−94.9 (3)	C23—Zr1—C26—C25	−77.53 (18)
C23—Zr1—C2—C1	−145.2 (3)	Cl1—Zr1—C26—C25	−61.92 (18)
Cl1—Zr1—C2—C1	87.9 (3)	C24—Zr1—C26—C25	−36.96 (16)
C24—Zr1—C2—C1	−42.3 (4)	C22—Zr1—C26—C25	−114.6 (2)
C22—Zr1—C2—C1	−129.7 (3)	Cl2—Zr1—C26—C25	37.24 (17)
Cl2—Zr1—C2—C1	9.0 (3)	C2—Zr1—C26—C25	121.64 (16)
C25—Zr1—C2—C1	−59.8 (3)	C3—Zr1—C26—C25	146.17 (15)
C3—Zr1—C2—C1	117.8 (3)	C4—Zr1—C26—C25	−175.47 (14)
C4—Zr1—C2—C1	147.7 (3)	N1—Zr1—C26—C22	−121.23 (16)
C4—N2—C6—C11	114.9 (2)	N2—Zr1—C26—C22	−43.89 (16)
Zr1—N2—C6—C11	−80.6 (3)	C23—Zr1—C26—C22	37.07 (15)
C4—N2—C6—C7	−67.5 (3)	Cl1—Zr1—C26—C22	52.68 (18)
Zr1—N2—C6—C7	97.0 (3)	C24—Zr1—C26—C22	77.64 (17)
C11—C6—C7—C8	1.2 (3)	Cl2—Zr1—C26—C22	151.84 (14)
N2—C6—C7—C8	−176.3 (2)	C25—Zr1—C26—C22	114.6 (2)
C11—C6—C7—C12	−178.5 (2)	C2—Zr1—C26—C22	−123.76 (15)
N2—C6—C7—C12	4.0 (3)	C3—Zr1—C26—C22	−99.23 (17)
C6—C7—C8—C9	0.2 (4)	C4—Zr1—C26—C22	−60.86 (17)

Fig. 1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