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Dichlorido(η^5-cyclopentadienyl)[*N*-(2,6-dimethylphenyl)-*N*′-({(2,6-dimethylphenyl)[imino(phenyl)methyl-κN]amino}-dimethylsilyl)benzamidinato-$\kappa^2 N,N'$]-zirconium(IV) dichloromethane solvate

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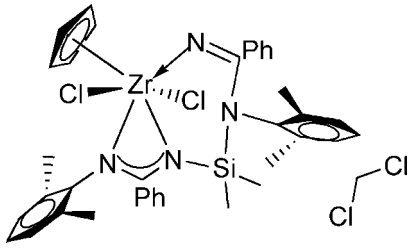
Key indicators: single-crystal X-ray study; T = 213 K; mean σ(C–C) = 0.006 Å; R factor = 0.042; wR factor = 0.102; data-to-parameter ratio = 15.2.

The Zr^{IV} atom in the title half-sandwich organometallic zirconium(IV) compound, $[Zr(C_5H_5)(C_{32}H_{35}N_4Si)Cl_2]\cdot CH_2Cl_2$, is *N*,*N*′,*N*″-chelated by the silyl-linked imino-amidinato monoanion in the first example of such an organozirconium derivative. The three *N*-donor atoms along with a Cl atom form a square, above and below which are the cyclopentadieny ring and the second Cl atom. The coordination geometry is octahedral.

Related literature

For related compounds and their applications, see: Gómez *et al.* (1995); Terasawa *et al.* (2005). For other organometallic compounds with similar bis(amidinate) ligands, see: Hill *et al.* (2006); Li *et al.* (2003). For the mechanism of the *N*-donor ligand rearrangement, see: Bai *et al.* (2006).



Experimental

Crystal data

$[Zr(C_5H_5)(C_{32}H_{35}N_4Si)Cl_2]\cdot CH_2Cl_2$
M_r = 815.87
Triclinic, $P\overline{1}$
a = 9.5134 (13) Å
b = 15.206 (2) Å
c = 15.369 (2) Å
α = 115.042 (2)°
β = 103.692 (2)°
γ = 92.069 (2)°
V = 1933.5 (4) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.62 mm^{-1}
T = 213 (2) K
0.50 × 0.30 × 0.30 mm

Data collection

Bruker SMART CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.605, T_{max} = 0.835
7987 measured reflections
6657 independent reflections
6186 reflections with $I > 2\sigma(I)$
R_{int} = 0.017

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.102
S = 1.09
6657 reflections
437 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.71 e Å^{-3}
$\Delta\rho_{min}$ = −0.49 e Å^{-3}

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL/PC* (Sheldrick, 1999); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: NG2353).

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supplementary materials

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Dichlorido(η^5-cyclopentadienyl)[*N*-(2,6-dimethylphenyl)-*N*'-({(2,6-dimethylphenyl)[imino(phenyl)methyl-κN]amino}dimethylsilyl)benzamidinato-$\kappa^2 N,N'$]zirconium(IV) dichloromethane solvate

J. Li and S.-D. Bai

Comment

The growing interest of the organometallic compounds incorporated with the dianionic linked bis(amidinate) ligands (Hill *et al.*, 2006; Li *et al.*, 2003) and widely applications of the half-sandwich compounds (Terasawa *et al.*, 2005) attracted us to the subject.

The title compound is the first half-sandwich compound with the silyl-linked-imino-amidinato ligand. It was obtained from the reaction of $ZrCl_3(C_5H_5)$ with $[SiMe_2\{NC(Ph)N(2,6\text{-}Me_2Ph)Li\}_2]$. The *N*-donor ligand coordinates to Zr center in tridentate mode, which is not the same as that in the lithium substrate. It results from an interesting rearrangement process (Bai *et al.*, 2006). In the molecular structure of the title compound, the amidinate moiety binds the metal center with N—Zr—N angle of 59.66 (9)°, slightly smaller than the corresponding value in the related $\{Zr(C_5H_5)[C(Ph)(NSiMe_3)_2]Cl_2\}$(Gómez *et al.*,1995). On one end of the amidinate unit, the pendant imino group coordinates the metal center and contributes the six-membered ring configuration, Zr1—N2—Si1—N3—C26—N4. The three Zr—N bonds are slightly longer than 2.2 Å in the normal range and they are coplanar. The angle between the $[ZrN_3]$ plane and the pentagon plane of the cyclopentadienyl is 88.9°, indicating the perpendicular relationship between them. Such situation is very special and rare because the cyclopentadienyl is usually on the side of amidinate ligand in most cases. In the title compound, the distance of Zr—$Cp_{centroid}$ is 2.225 Å, also in the $[ZrN_3]$ plane. Two Cl atoms are separated by the *N*-donor ligand. Thus, it displays the distorted octahedral geometry around the Zr ion.

Experimental

$ZrCl_3(C_5H_5)$ (0.46 g, 1.75 mmol) was added into the solution of $[SiMe_2\{NC(Ph)N(2,6\text{-}Me_2Ph)Li\}_2]$ (1.75 mmol) in THF (20 ml) at 273 K. The reaction mixture was warmed to room temperature and kept stirring for 12 h. It was dried in vacuum to remove all volatiles and the residue was extracted with CH_2Cl_2 (25 ml). Concentration of the filtrate under reduced pressure gave the title compound as colorless crystals (yield 0.86 g, 60%). CHN analysis, calculated for $C_{37}H_{40}Cl_2N_4SiZr$ (730.96): C 60.80, H 5.52, N 7.66%; found: C 60.33, H 5.17, N 7.37%. Spectroscopic analysis: ^{1}H NMR (300 MHz, $CDCl_3$, δ, p.p.m.): 7.37–6.93 (*m*, 16H; phenyls), 6.50 (*s*, 5H; Cp), 2.56–2.45 (*m*, 12H; methyls), 0.50 (*s*, 6H; $SiMe_2$); ^{13}C NMR (75 MHz, $CDCl_3$, δ, p.p.m.): 180.5, 177.1 (N—C—N), 147.8–120.5 (phenyls), 23.3, 22.6 (methyls), 7.7, 5.2 ($SiMe_2$).

Refinement

All H atoms were initially located in a difference Fourier map. The methyl H atoms were then constrained to an ideal geometry, with C—H distances of 0.96Å and U_{iso}(H) = 1.2U_{eq}(C), but each group was allowed to rotate freely about its

C–C bond. The other H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms, with C–H distances in the range 0.93Å and U_{iso}(H) = 1.2U_{eq}(C).

Figures

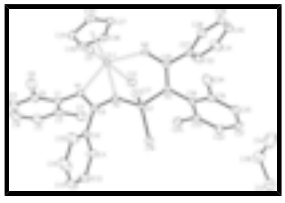


Fig. 1. **Figure 1**. Molecular structure of the title compound, showing the atom-lebelling scheme and 30% probability displacement ellipsoids. H atoms are not shown.

Dichlorido(η^5-cyclopentadienyl)[*N*-(2,6-dimethylphenyl)-*N*'- ({(2,6-dimethylphenyl)[imino(phenyl)methyl-κ*N*]amino}dimethylsilyl)benzamidinato-κ^2*N*,*N*']zirconium(IV) dichloromethane monosolvate

Crystal data

$[Zr(C_5H_5)(C_{32}H_{35}N_4Si)Cl_2]\cdot CH_2Cl_2$	$Z = 2$
$M_r = 815.87$	$F_{000} = 840$
Triclinic, $P\bar{1}$	$D_x = 1.401$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation λ = 0.71073 Å
$a = 9.5134$ (13) Å	Cell parameters from 6394 reflections
$b = 15.206$ (2) Å	θ = 2.2–27.7º
$c = 15.369$ (2) Å	μ = 0.62 mm^{-1}
α = 115.042 (2)º	$T = 213$ (2) K
β = 103.692 (2)º	Prism, colorless
γ = 92.069 (2)º	0.50 × 0.30 × 0.30 mm
$V = 1933.5$ (4) Å^3	

Data collection

Bruker Smart CCD-detector diffractometer	6657 independent reflections
Radiation source: fine-focus sealed tube	6186 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.017$
$T = 213(2)$ K	$\theta_{max} = 25.0$º
φ and ω scan	$\theta_{min} = 1.5$º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$h = -10\rightarrow11$
$T_{min} = 0.605$, $T_{max} = 0.835$	$k = -18\rightarrow11$
7987 measured reflections	$l = -18\rightarrow18$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.042$

$wR(F^2) = 0.102$

$S = 1.09$

6657 reflections

437 parameters

Primary atom site location: structure-invariant direct methods

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0435P)^2 + 1.5172P]$ where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} = 0.001$

$\Delta\rho_{max} = 0.71$ e Å^{-3}

$\Delta\rho_{min} = -0.49$ 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. 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}
Zr1	−0.10953 (3)	0.17095 (2)	0.14783 (2)	0.02311 (10)
Si1	0.25585 (8)	0.26176 (6)	0.31212 (6)	0.02434 (18)
Cl1	0.04791 (8)	0.16067 (6)	0.03096 (6)	0.03238 (18)
Cl2	−0.16730 (9)	0.19957 (6)	0.30950 (6)	0.0372 (2)
N1	−0.1045 (3)	0.32972 (18)	0.18845 (19)	0.0303 (6)
N2	0.0881 (3)	0.27996 (17)	0.25785 (18)	0.0250 (5)
N3	0.2134 (3)	0.15896 (17)	0.33685 (18)	0.0253 (5)
N4	0.0322 (3)	0.06850 (18)	0.18635 (18)	0.0273 (5)
H4A	0.0274	0.0126	0.1352	0.033*
C1	−0.1864 (3)	0.4020 (2)	0.1722 (3)	0.0365 (8)
C2	−0.2740 (4)	0.4472 (2)	0.2348 (3)	0.0446 (9)
C3	−0.3541 (5)	0.5162 (3)	0.2178 (4)	0.0646 (12)
H3A	−0.4124	0.5479	0.2599	0.078*
C4	−0.3494 (5)	0.5385 (3)	0.1411 (4)	0.0762 (15)
H4B	−0.4033	0.5857	0.1311	0.091*
C5	−0.2660 (5)	0.4922 (3)	0.0791 (4)	0.0683 (13)
H5A	−0.2650	0.5069	0.0257	0.082*
C6	−0.1822 (4)	0.4234 (3)	0.0931 (3)	0.0489 (9)
C7	−0.2843 (4)	0.4238 (3)	0.3191 (3)	0.0571 (11)
H7A	−0.3657	0.4509	0.3436	0.086*
H7B	−0.1941	0.4523	0.3728	0.086*
H7C	−0.2998	0.3531	0.2952	0.086*

C8	−0.0910 (5)	0.3759 (3)	0.0237 (3)	0.0675 (12)
H8A	0.0120	0.3976	0.0601	0.101*
H8B	−0.1128	0.3944	−0.0306	0.101*
H8C	−0.1129	0.3051	−0.0032	0.101*
C9	0.0321 (3)	0.3547 (2)	0.2486 (2)	0.0253 (6)
C10	0.1137 (3)	0.4568 (2)	0.2996 (2)	0.0283 (7)
C11	0.1057 (4)	0.5217 (3)	0.3922 (3)	0.0462 (9)
H11A	0.0457	0.5024	0.4236	0.055*
C12	0.1856 (5)	0.6157 (3)	0.4402 (3)	0.0629 (12)
H12A	0.1794	0.6597	0.5039	0.075*
C13	0.2720 (5)	0.6442 (3)	0.3958 (4)	0.0630 (13)
H13A	0.3254	0.7081	0.4284	0.076*
C14	0.2820 (5)	0.5804 (4)	0.3036 (4)	0.0735 (14)
H14A	0.3422	0.6005	0.2729	0.088*
C15	0.2036 (5)	0.4858 (3)	0.2550 (3)	0.0575 (11)
H15A	0.2119	0.4418	0.1920	0.069*
C16	0.3602 (4)	0.3661 (2)	0.4316 (2)	0.0357 (7)
H16A	0.3002	0.3852	0.4778	0.054*
H16B	0.3865	0.4212	0.4194	0.054*
H16C	0.4483	0.3465	0.4603	0.054*
C17	0.3718 (3)	0.2264 (2)	0.2254 (2)	0.0337 (7)
H17A	0.3181	0.1718	0.1625	0.051*
H17B	0.4599	0.2071	0.2545	0.051*
H17C	0.3982	0.2819	0.2137	0.051*
C18	0.3032 (3)	0.1606 (2)	0.4293 (2)	0.0305 (7)
C19	0.4297 (3)	0.1167 (2)	0.4282 (3)	0.0357 (8)
C20	0.5108 (4)	0.1183 (3)	0.5179 (3)	0.0467 (10)
H20A	0.5952	0.0880	0.5190	0.056*
C21	0.4692 (4)	0.1633 (3)	0.6040 (3)	0.0510 (10)
H21A	0.5247	0.1627	0.6631	0.061*
C22	0.3473 (4)	0.2091 (3)	0.6050 (3)	0.0472 (9)
H22A	0.3213	0.2408	0.6650	0.057*
C23	0.2618 (4)	0.2089 (2)	0.5173 (2)	0.0359 (8)
C24	0.4833 (4)	0.0687 (3)	0.3373 (3)	0.0485 (9)
H24A	0.4066	0.0591	0.2784	0.073*
H24B	0.5095	0.0056	0.3309	0.073*
H24C	0.5686	0.1104	0.3437	0.073*
C25	0.1288 (4)	0.2592 (3)	0.5212 (3)	0.0443 (9)
H25A	0.0443	0.2125	0.5069	0.066*
H25B	0.1118	0.2845	0.4719	0.066*
H25C	0.1444	0.3131	0.5873	0.066*
C26	0.1199 (3)	0.0764 (2)	0.2700 (2)	0.0246 (6)
C27	0.1091 (3)	−0.0107 (2)	0.2926 (2)	0.0285 (7)
C28	0.1635 (4)	−0.0944 (2)	0.2420 (3)	0.0406 (8)
H28A	0.2149	−0.0961	0.1962	0.049*
C29	0.1429 (4)	−0.1763 (3)	0.2584 (3)	0.0489 (9)
H29A	0.1816	−0.2329	0.2244	0.059*
C30	0.0667 (5)	−0.1750 (3)	0.3236 (3)	0.0515 (10)
H30A	0.0533	−0.2304	0.3350	0.062*

C31	0.0099 (5)	−0.0925 (3)	0.3722 (3)	0.0644 (12)
H31A	−0.0440	−0.0919	0.4164	0.077*
C32	0.0308 (5)	−0.0100 (3)	0.3573 (3)	0.0529 (10)
H32A	−0.0084	0.0464	0.3914	0.063*
C33	−0.2591 (3)	0.0458 (3)	−0.0229 (2)	0.0394 (8)
H33A	−0.2200	0.0066	−0.0795	0.047*
C34	−0.3107 (4)	0.1349 (3)	−0.0057 (3)	0.0410 (8)
H34A	−0.3160	0.1688	−0.0488	0.049*
C35	−0.3781 (3)	0.1577 (2)	0.0716 (2)	0.0375 (8)
H35A	−0.4375	0.2111	0.0927	0.045*
C36	−0.3691 (3)	0.0831 (2)	0.1009 (2)	0.0367 (8)
H36A	−0.4184	0.0754	0.1477	0.044*
C37	−0.2939 (3)	0.0147 (2)	0.0438 (2)	0.0359 (8)
H37A	−0.2816	−0.0499	0.0432	0.043*
C38	0.2517 (5)	0.2429 (4)	0.9050 (4)	0.0799 (15)
H38A	0.1779	0.2089	0.9198	0.096*
H38B	0.2009	0.2773	0.8686	0.096*
Cl3	0.37352 (15)	0.32951 (10)	1.01815 (10)	0.0853 (4)
Cl4	0.3398 (2)	0.15686 (15)	0.82979 (12)	0.1207 (6)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zr1	0.02140 (16)	0.02120 (16)	0.02449 (16)	0.00268 (11)	0.00554 (11)	0.00857 (12)
Si1	0.0224 (4)	0.0229 (4)	0.0267 (4)	0.0012 (3)	0.0054 (3)	0.0111 (3)
Cl1	0.0329 (4)	0.0351 (4)	0.0304 (4)	0.0038 (3)	0.0122 (3)	0.0141 (3)
Cl2	0.0362 (4)	0.0421 (5)	0.0303 (4)	0.0029 (4)	0.0140 (3)	0.0112 (4)
N1	0.0273 (13)	0.0236 (13)	0.0353 (15)	0.0047 (11)	0.0033 (11)	0.0113 (11)
N2	0.0245 (12)	0.0225 (13)	0.0268 (13)	0.0030 (10)	0.0060 (10)	0.0105 (11)
N3	0.0258 (13)	0.0259 (13)	0.0256 (13)	0.0036 (11)	0.0051 (10)	0.0136 (11)
N4	0.0295 (13)	0.0233 (13)	0.0240 (13)	0.0064 (11)	0.0058 (11)	0.0064 (11)
C1	0.0304 (17)	0.0236 (16)	0.046 (2)	0.0035 (14)	−0.0015 (15)	0.0134 (15)
C2	0.0344 (19)	0.0292 (18)	0.055 (2)	0.0071 (15)	0.0028 (17)	0.0094 (17)
C3	0.048 (2)	0.042 (2)	0.088 (3)	0.0205 (19)	0.010 (2)	0.017 (2)
C4	0.063 (3)	0.051 (3)	0.110 (4)	0.024 (2)	0.003 (3)	0.041 (3)
C5	0.076 (3)	0.049 (3)	0.083 (3)	0.018 (2)	0.003 (3)	0.042 (3)
C6	0.052 (2)	0.037 (2)	0.058 (2)	0.0065 (17)	0.0030 (19)	0.0266 (19)
C7	0.047 (2)	0.048 (2)	0.068 (3)	0.0167 (19)	0.024 (2)	0.013 (2)
C8	0.093 (3)	0.062 (3)	0.067 (3)	0.021 (3)	0.026 (3)	0.044 (2)
C9	0.0291 (16)	0.0240 (15)	0.0245 (15)	0.0038 (13)	0.0104 (13)	0.0108 (13)
C10	0.0249 (15)	0.0261 (16)	0.0336 (17)	0.0040 (13)	0.0040 (13)	0.0153 (14)
C11	0.049 (2)	0.037 (2)	0.040 (2)	−0.0009 (17)	0.0145 (17)	0.0055 (16)
C12	0.056 (3)	0.035 (2)	0.060 (3)	0.003 (2)	0.004 (2)	−0.0066 (19)
C13	0.046 (2)	0.029 (2)	0.094 (4)	−0.0032 (18)	−0.006 (2)	0.023 (2)
C14	0.063 (3)	0.062 (3)	0.108 (4)	−0.011 (2)	0.026 (3)	0.050 (3)
C15	0.065 (3)	0.050 (2)	0.059 (3)	−0.006 (2)	0.029 (2)	0.020 (2)
C16	0.0368 (18)	0.0310 (17)	0.0324 (18)	−0.0023 (14)	0.0014 (14)	0.0126 (14)
C17	0.0301 (16)	0.0360 (18)	0.0394 (19)	0.0074 (14)	0.0139 (14)	0.0185 (15)

C18	0.0321 (16)	0.0277 (16)	0.0334 (17)	−0.0024 (13)	0.0013 (14)	0.0198 (14)
C19	0.0295 (17)	0.0282 (17)	0.047 (2)	−0.0034 (14)	−0.0003 (15)	0.0210 (16)
C20	0.0348 (19)	0.037 (2)	0.065 (3)	−0.0026 (16)	−0.0084 (18)	0.0314 (19)
C21	0.060 (2)	0.044 (2)	0.041 (2)	−0.0063 (19)	−0.0112 (19)	0.0256 (19)
C22	0.060 (2)	0.046 (2)	0.036 (2)	−0.0011 (19)	0.0030 (17)	0.0240 (17)
C23	0.0445 (19)	0.0331 (18)	0.0299 (17)	−0.0018 (15)	0.0061 (15)	0.0168 (15)
C24	0.038 (2)	0.046 (2)	0.066 (3)	0.0140 (17)	0.0141 (18)	0.029 (2)
C25	0.056 (2)	0.047 (2)	0.0344 (19)	0.0099 (18)	0.0192 (17)	0.0183 (17)
C26	0.0256 (15)	0.0238 (15)	0.0256 (15)	0.0055 (12)	0.0115 (12)	0.0096 (13)
C27	0.0277 (15)	0.0274 (16)	0.0278 (16)	−0.0013 (13)	0.0018 (13)	0.0135 (13)
C28	0.051 (2)	0.0344 (19)	0.047 (2)	0.0122 (16)	0.0224 (17)	0.0225 (17)
C29	0.062 (2)	0.0311 (19)	0.059 (2)	0.0126 (18)	0.019 (2)	0.0237 (18)
C30	0.071 (3)	0.037 (2)	0.053 (2)	−0.0006 (19)	0.010 (2)	0.0309 (19)
C31	0.095 (3)	0.051 (3)	0.072 (3)	0.010 (2)	0.048 (3)	0.037 (2)
C32	0.075 (3)	0.037 (2)	0.063 (3)	0.0140 (19)	0.042 (2)	0.0252 (19)
C33	0.0268 (17)	0.042 (2)	0.0306 (18)	−0.0044 (15)	0.0067 (14)	−0.0004 (15)
C34	0.0341 (18)	0.047 (2)	0.0369 (19)	−0.0032 (16)	−0.0034 (15)	0.0218 (17)
C35	0.0233 (16)	0.0363 (19)	0.0408 (19)	0.0061 (14)	0.0025 (14)	0.0092 (15)
C36	0.0231 (16)	0.043 (2)	0.0351 (18)	−0.0068 (14)	0.0048 (14)	0.0123 (16)
C37	0.0250 (16)	0.0281 (17)	0.0423 (19)	−0.0022 (13)	−0.0010 (14)	0.0101 (15)
C38	0.065 (3)	0.101 (4)	0.084 (4)	−0.011 (3)	0.013 (3)	0.057 (3)
Cl3	0.0939 (9)	0.0799 (9)	0.0864 (9)	0.0132 (7)	0.0027 (7)	0.0525 (8)
Cl4	0.1454 (15)	0.1500 (16)	0.0749 (10)	0.0516 (13)	0.0290 (10)	0.0562 (11)

Geometric parameters (Å, °)

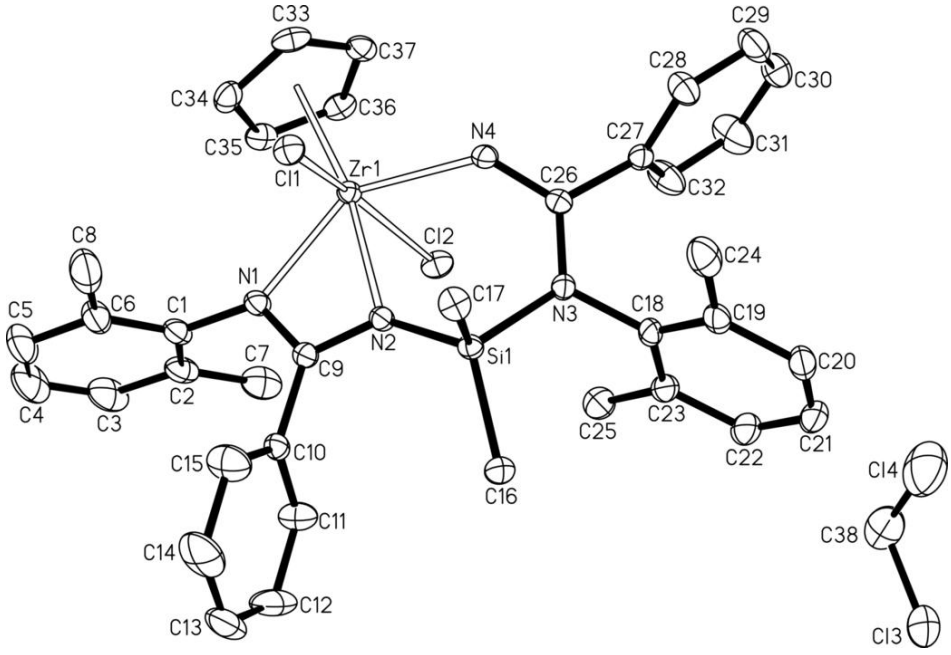
Zr1—N1	2.219 (2)	C15—H15A	0.9400
Zr1—N2	2.245 (2)	C16—H16A	0.9700
Zr1—N4	2.270 (2)	C16—H16B	0.9700
Zr1—C34	2.495 (3)	C16—H16C	0.9700
Zr1—C35	2.508 (3)	C17—H17A	0.9700
Zr1—C33	2.518 (3)	C17—H17B	0.9700
Zr1—Cl2	2.5326 (9)	C17—H17C	0.9700
Zr1—C37	2.536 (3)	C18—C19	1.397 (4)
Zr1—C36	2.550 (3)	C18—C23	1.397 (5)
Zr1—Cl1	2.5588 (8)	C19—C20	1.401 (5)
Zr1—C9	2.664 (3)	C19—C24	1.499 (5)
Si1—N2	1.708 (2)	C20—C21	1.370 (6)
Si1—N3	1.811 (2)	C20—H20A	0.9400
Si1—C17	1.847 (3)	C21—C22	1.374 (5)
Si1—C16	1.853 (3)	C21—H21A	0.9400
N1—C9	1.336 (4)	C22—C23	1.399 (5)
N1—C1	1.442 (4)	C22—H22A	0.9400
N2—C9	1.319 (4)	C23—C25	1.502 (5)
N3—C26	1.348 (4)	C24—H24A	0.9700
N3—C18	1.465 (4)	C24—H24B	0.9700
N4—C26	1.310 (4)	C24—H24C	0.9700
N4—H4A	0.8700	C25—H25A	0.9700
C1—C6	1.394 (5)	C25—H25B	0.9700

C1—C2	1.399 (5)	C25—H25C	0.9700
C2—C3	1.394 (5)	C26—C27	1.510 (4)
C2—C7	1.504 (6)	C27—C32	1.374 (5)
C3—C4	1.368 (7)	C27—C28	1.376 (4)
C3—H3A	0.9400	C28—C29	1.387 (5)
C4—C5	1.366 (7)	C28—H28A	0.9400
C4—H4B	0.9400	C29—C30	1.363 (5)
C5—C6	1.394 (5)	C29—H29A	0.9400
C5—H5A	0.9400	C30—C31	1.368 (6)
C6—C8	1.498 (6)	C30—H30A	0.9400
C7—H7A	0.9700	C31—C32	1.384 (5)
C7—H7B	0.9700	C31—H31A	0.9400
C7—H7C	0.9700	C32—H32A	0.9400
C8—H8A	0.9700	C33—C37	1.394 (5)
C8—H8B	0.9700	C33—C34	1.398 (5)
C8—H8C	0.9700	C33—H33A	0.9900
C9—C10	1.491 (4)	C34—C35	1.405 (5)
C10—C11	1.368 (5)	C34—H34A	0.9900
C10—C15	1.380 (5)	C35—C36	1.384 (5)
C11—C12	1.389 (5)	C35—H35A	0.9900
C11—H11A	0.9400	C36—C37	1.393 (5)
C12—C13	1.348 (6)	C36—H36A	0.9900
C12—H12A	0.9400	C37—H37A	0.9900
C13—C14	1.366 (7)	C38—Cl4	1.735 (6)
C13—H13A	0.9400	C38—Cl3	1.760 (5)
C14—C15	1.390 (6)	C38—H38A	0.9800
C14—H14A	0.9400	C38—H38B	0.9800
N1—Zr1—N2	59.62 (9)	C10—C11—H11A	119.7
N1—Zr1—N4	139.71 (9)	C12—C11—H11A	119.7
N2—Zr1—N4	80.10 (9)	C13—C12—C11	120.2 (4)
N1—Zr1—C34	88.49 (10)	C13—C12—H12A	119.9
N2—Zr1—C34	143.15 (10)	C11—C12—H12A	119.9
N4—Zr1—C34	129.52 (11)	C12—C13—C14	120.0 (4)
N1—Zr1—C35	84.59 (10)	C12—C13—H13A	120.0
N2—Zr1—C35	142.10 (10)	C14—C13—H13A	120.0
N4—Zr1—C35	133.95 (10)	C13—C14—C15	120.4 (4)
C34—Zr1—C35	32.61 (11)	C13—C14—H14A	119.8
N1—Zr1—C33	119.47 (11)	C15—C14—H14A	119.8
N2—Zr1—C33	154.74 (10)	C10—C15—C14	119.7 (4)
N4—Zr1—C33	97.16 (10)	C10—C15—H15A	120.2
C34—Zr1—C33	32.37 (11)	C14—C15—H15A	120.2
C35—Zr1—C33	53.48 (11)	Si1—C16—H16A	109.5
N1—Zr1—Cl2	89.79 (7)	Si1—C16—H16B	109.5
N2—Zr1—Cl2	80.36 (6)	H16A—C16—H16B	109.5
N4—Zr1—Cl2	81.87 (6)	Si1—C16—H16C	109.5
C34—Zr1—Cl2	120.44 (9)	H16A—C16—H16C	109.5
C35—Zr1—Cl2	88.01 (8)	H16B—C16—H16C	109.5
C33—Zr1—Cl2	124.38 (8)	Si1—C17—H17A	109.5
N1—Zr1—C37	137.10 (10)	Si1—C17—H17B	109.5

N2—Zr1—C37	162.75 (9)	H17A—C17—H17B	109.5
N4—Zr1—C37	82.98 (10)	Si1—C17—H17C	109.5
C34—Zr1—C37	53.26 (11)	H17A—C17—H17C	109.5
C35—Zr1—C37	52.94 (11)	H17B—C17—H17C	109.5
C33—Zr1—C37	32.02 (11)	C19—C18—C23	121.8 (3)
Cl2—Zr1—C37	93.98 (8)	C19—C18—N3	119.4 (3)
N1—Zr1—C36	111.93 (10)	C23—C18—N3	118.7 (3)
N2—Zr1—C36	152.26 (10)	C18—C19—C20	117.6 (3)
N4—Zr1—C36	103.14 (10)	C18—C19—C24	124.0 (3)
C34—Zr1—C36	53.18 (11)	C20—C19—C24	118.4 (3)
C35—Zr1—C36	31.75 (11)	C21—C20—C19	121.1 (3)
C33—Zr1—C36	52.94 (11)	C21—C20—H20A	119.5
Cl2—Zr1—C36	72.98 (8)	C19—C20—H20A	119.5
C37—Zr1—C36	31.79 (11)	C20—C21—C22	120.8 (3)
N1—Zr1—Cl1	88.80 (7)	C20—C21—H21A	119.6
N2—Zr1—Cl1	79.85 (6)	C22—C21—H21A	119.6
N4—Zr1—Cl1	84.96 (6)	C21—C22—C23	120.3 (4)
C34—Zr1—Cl1	81.65 (9)	C21—C22—H22A	119.8
C35—Zr1—Cl1	113.88 (8)	C23—C22—H22A	119.8
C33—Zr1—Cl1	74.90 (8)	C18—C23—C22	118.3 (3)
Cl2—Zr1—Cl1	157.82 (3)	C18—C23—C25	122.9 (3)
C37—Zr1—Cl1	102.06 (8)	C22—C23—C25	118.8 (3)
C36—Zr1—Cl1	127.71 (8)	C19—C24—H24A	109.5
N1—Zr1—C9	30.03 (9)	C19—C24—H24B	109.5
N2—Zr1—C9	29.63 (8)	H24A—C24—H24B	109.5
N4—Zr1—C9	109.73 (9)	C19—C24—H24C	109.5
C34—Zr1—C9	116.25 (10)	H24A—C24—H24C	109.5
C35—Zr1—C9	114.06 (10)	H24B—C24—H24C	109.5
C33—Zr1—C9	142.91 (10)	C23—C25—H25A	109.5
Cl2—Zr1—C9	85.40 (6)	C23—C25—H25B	109.5
C37—Zr1—C9	166.99 (10)	H25A—C25—H25B	109.5
C36—Zr1—C9	137.36 (10)	C23—C25—H25C	109.5
Cl1—Zr1—C9	82.35 (6)	H25A—C25—H25C	109.5
N2—Si1—N3	103.52 (11)	H25B—C25—H25C	109.5
N2—Si1—C17	111.54 (13)	N4—C26—N3	123.0 (3)
N3—Si1—C17	108.83 (13)	N4—C26—C27	117.3 (3)
N2—Si1—C16	115.46 (14)	N3—C26—C27	119.6 (2)
N3—Si1—C16	108.36 (13)	C32—C27—C28	119.3 (3)
C17—Si1—C16	108.82 (15)	C32—C27—C26	119.3 (3)
C9—N1—C1	121.6 (2)	C28—C27—C26	121.1 (3)
C9—N1—Zr1	93.77 (17)	C27—C28—C29	120.2 (3)
C1—N1—Zr1	144.60 (19)	C27—C28—H28A	119.9
C9—N2—Si1	135.7 (2)	C29—C28—H28A	119.9
C9—N2—Zr1	93.08 (17)	C30—C29—C28	120.3 (4)
Si1—N2—Zr1	130.28 (13)	C30—C29—H29A	119.8
C26—N3—C18	118.4 (2)	C28—C29—H29A	119.8
C26—N3—Si1	124.02 (19)	C29—C30—C31	119.5 (3)
C18—N3—Si1	116.92 (19)	C29—C30—H30A	120.3
C26—N4—Zr1	133.0 (2)	C31—C30—H30A	120.3

C26—N4—H4A	113.5	C30—C31—C32	120.8 (4)
Zr1—N4—H4A	113.5	C30—C31—H31A	119.6
C6—C1—C2	120.8 (3)	C32—C31—H31A	119.6
C6—C1—N1	120.4 (3)	C27—C32—C31	119.8 (4)
C2—C1—N1	118.8 (3)	C27—C32—H32A	120.1
C3—C2—C1	118.4 (4)	C31—C32—H32A	120.1
C3—C2—C7	119.4 (4)	C37—C33—C34	107.8 (3)
C1—C2—C7	122.2 (3)	C37—C33—Zr1	74.68 (19)
C4—C3—C2	121.2 (4)	C34—C33—Zr1	72.90 (19)
C4—C3—H3A	119.4	C37—C33—H33A	125.8
C2—C3—H3A	119.4	C34—C33—H33A	125.8
C5—C4—C3	119.8 (4)	Zr1—C33—H33A	125.8
C5—C4—H4B	120.1	C33—C34—C35	107.6 (3)
C3—C4—H4B	120.1	C33—C34—Zr1	74.73 (18)
C4—C5—C6	121.6 (4)	C35—C34—Zr1	74.18 (18)
C4—C5—H5A	119.2	C33—C34—H34A	125.7
C6—C5—H5A	119.2	C35—C34—H34A	125.7
C1—C6—C5	118.2 (4)	Zr1—C34—H34A	125.7
C1—C6—C8	122.5 (3)	C36—C35—C34	108.2 (3)
C5—C6—C8	119.3 (4)	C36—C35—Zr1	75.81 (18)
C2—C7—H7A	109.5	C34—C35—Zr1	73.21 (18)
C2—C7—H7B	109.5	C36—C35—H35A	125.5
H7A—C7—H7B	109.5	C34—C35—H35A	125.5
C2—C7—H7C	109.5	Zr1—C35—H35A	125.5
H7A—C7—H7C	109.5	C35—C36—C37	108.1 (3)
H7B—C7—H7C	109.5	C35—C36—Zr1	72.43 (18)
C6—C8—H8A	109.5	C37—C36—Zr1	73.54 (18)
C6—C8—H8B	109.5	C35—C36—H36A	125.7
H8A—C8—H8B	109.5	C37—C36—H36A	125.7
C6—C8—H8C	109.5	Zr1—C36—H36A	125.7
H8A—C8—H8C	109.5	C36—C37—C33	108.3 (3)
H8B—C8—H8C	109.5	C36—C37—Zr1	74.66 (18)
N2—C9—N1	113.4 (3)	C33—C37—Zr1	73.30 (18)
N2—C9—C10	123.3 (3)	C36—C37—H37A	125.5
N1—C9—C10	123.3 (3)	C33—C37—H37A	125.5
N2—C9—Zr1	57.29 (15)	Zr1—C37—H37A	125.5
N1—C9—Zr1	56.21 (15)	Cl4—C38—Cl3	112.5 (3)
C10—C9—Zr1	176.7 (2)	Cl4—C38—H38A	109.1
C11—C10—C15	119.0 (3)	Cl3—C38—H38A	109.1
C11—C10—C9	121.2 (3)	Cl4—C38—H38B	109.1
C15—C10—C9	119.8 (3)	Cl3—C38—H38B	109.1
C10—C11—C12	120.6 (4)	H38A—C38—H38B	107.8

Fig. 1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Cl4
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Cl3