IUCrData

ISSN 2414-3146

[*N*-(2-Anilinoethyl)-*N*′-(trimethylsilyl)benzenecarboximidamidato-κ^3N,N',N''](benzonitrile-κN)trichloridozirconium(IV)

Wei Li,[a,b]* Shengdi Bai,[b] Feng Su,[c] Xine Duan[b] and Diansheng Liu[b]

[a]Institute of Molecular Science, Shanxi University, Taiyuan 030006, People's Republic of China, [b]Research Institute of Applied Chemistry, Shanxi University, Taiyuan 030006, People's Republic of China, and [c]Department of Chemistry, Changzhi University, Changzhi 046011, People's Republic of China. *Correspondence e-mail: dsliu@sxu.edu.cn

Received 2 March 2017
Accepted 9 March 2017

Edited by O. Blacque, University of Zürich, Switzerland

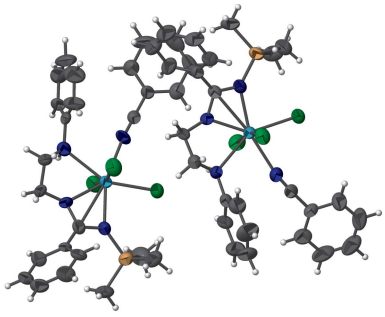
Keywords: crystal structure; zirconium complex; mononuclear structure; mixed ligands.

CCDC reference: 1536806

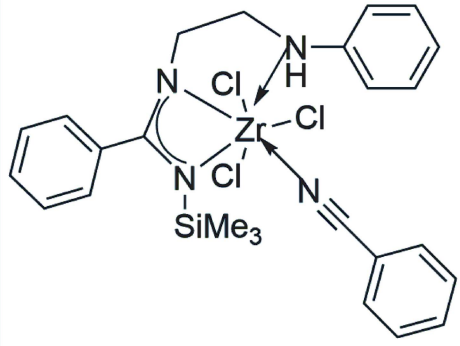
Structural data: full structural data are available from iucrdata.iucr.org

There are two independent molecules in the asymmetric unit of the title compound, $[Zr(C_{18}H_{24}N_3Si)Cl_3(C_7H_5N)]$, which are connected by an N—H···Cl hydrogen bond. The Zr atoms are seven-coordinate and possess a distorted pentagonal–bipyramidal geometry. In the crystal, molecules are connected by N—H···Cl hydrogen bonds, forming ribbons along [010].

3D view



Chemical scheme



Structure description

Nitrogen-based ligands have attracted much interest in organometallic chemistry and catalysis chemistry (Edelmann, 1995; Mack & Eisen, 1996). As the closest relatives of nitrogen-based ligands, amidinate ligands have attracted considerable attention due to their relatively simple synthesis and easy modification of steric and electronic requirements by varying the substituents on the nitrogen atom. A more sterically hindered amidinate is required, or amidinates that can give additional electronic stabilization to the highly electronically unsaturated metal atom are required. In the course of extending amidinate chemistry, we have explored a practical synthetic pathway to alkyl-ended amidinate and *ansa*-bis(amidinate) ligands (Bai *et al.*, 2013). They have been applied in the synthesis of Group 4 complexes, which are good catalysts for ethylene polymerization (Bai *et al.*, 2010). In our recent work, we have reported the synthesis and characterization of carbon chain-linked mixed amidinate-amido chelate complexes, and have described the different catalytic activities of the zirconium and titanium compounds toward ethylene polymerization (Li *et al.*, 2016, 2017).

There are two independent molecules in the asymmetric unit of the title compound. The Zr atoms are seven-coordinate and possess a distorted pentagonal–bipyramidal

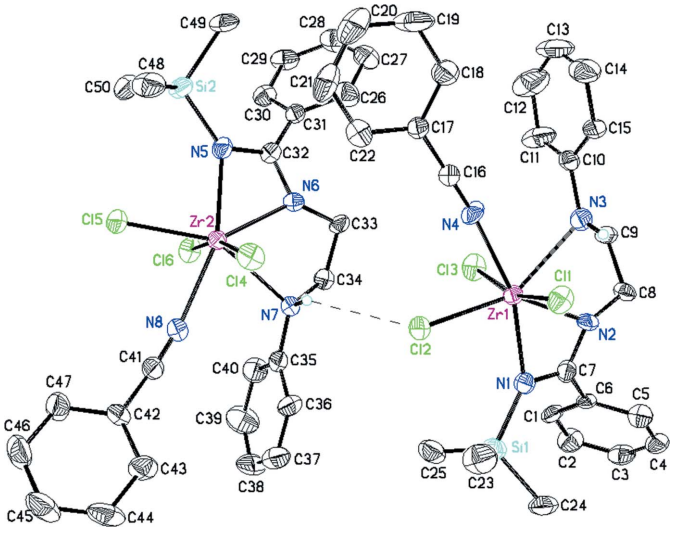


Figure 1
The molecular structures of the two independent molecules in the title compound, showing the atom labelling and with displacement ellipsoids drawn at 50% probability level.

geometry. The four non-bridging chloride ions (Cl1 and Cl3, Cl4 and Cl6) occupy the axial positions and form a near straight angle [Cl1—Zr1—Cl3 = 165.62 (13)°, Cl4—Zr2—Cl6 = 165.14 (12)°]. Atoms N1–N4/Cl2 and N5–N8/Cl5 form the equatorial planes, with r.m.s. deviations of 0.044 and 0.0508 Å, respectively. The Zr1—N1 and Zr1—N2 bond lengths compare well with those reported for amidinate zirconium complexes (Li *et al.*, 2016, 2017). Intramolecular N3—H3*A*···Cl1 and N7—H7*A*···Cl4 hydrogen bonds occur and the two independent molecules are linked by N7—H7*A*···Cl2 hydrogen bonds (Table 1 and Fig. 1). Weak intramolecular C–H···Cl interactions further stabilize the molecular structure.

In the crystal, the molecules are linked by N3—H3*A*···Cl5 interactions, forming ribbons along [010] (Table 1 and Fig. 2).

Synthesis and crystallization

The title compound was obtained unexpectedly during an attempt to synthesize a zirconium complex based on the ethylene-linked amidinate-amido ligand To a solution of

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C40—H40···Cl6	0.95	2.83	3.466 (16)	125
C34—H34*A*···Cl6	0.99	2.99	3.525 (13)	115
C9—H9*B*···Cl3	0.99	2.85	3.404 (13)	116
N7—H7*A*···Cl4	0.88	2.70	3.267 (10)	123
N7—H7*A*···Cl2	0.88	2.84	3.467 (10)	129
N3—H3*A*···Cl5^{i}	0.88	2.98	3.516 (10)	121
N3—H3*A*···Cl1	0.88	2.74	3.316 (11)	124

Symmetry code: (i) $x, y-1, z$.

Table 2
Experimental details.

Crystal data	
Chemical formula	$[Zr(C_{18}H_{24}N_3Si)Cl_3(C_7H_5N)]$
M_r	611.18
Crystal system, space group	Orthorhombic, $Pna2_1$
Temperature (K)	194
a, b, c (Å)	35.830 (2), 14.292 (9), 11.057 (6)
V (Å^3)	5662 (5)
Z	8
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.73
Crystal size (mm)	0.35 × 0.32 × 0.30
Data collection	
Diffractometer	Bruker SMART APEX CCD area detector
Absorption correction	Multi-scan *SADABS* (Bruker, 2012)
T_{min}, T_{max}	0.773, 0.802
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	29608, 9600, 5601
R_{int}	0.133
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.596
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.066, 0.194, 1.00
No. of reflections	9600
No. of parameters	571
No. of restraints	1
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	1.02, −0.80
Absolute structure	Flack x determined using 1602 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons *et al.*, 2013)
Absolute structure parameter	0.06 (6)

Computer programs: *APEX2* (Bruker, and *SAINT* (Bruker, 2012), *SHELXT* (Sheldrick, 2015*a*), *SHELXL* (Sheldrick, 2015*b*) and *SHELXTL* (Sheldrick, 2008).

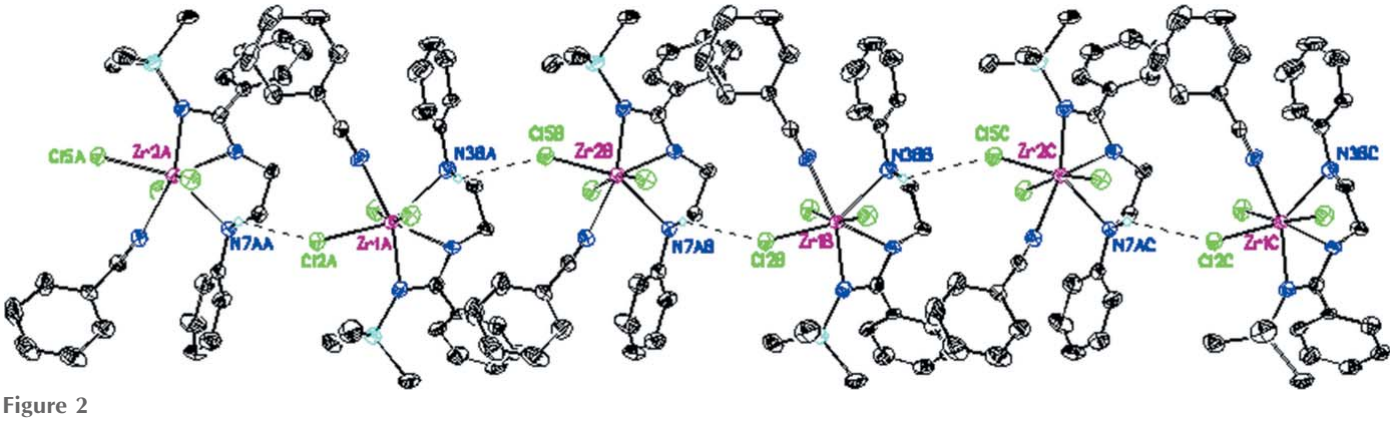


Figure 2
A partial view along the *c* axis of the crystal packing of the title compound. Hydrogen bonds are shown as dashed lines.

$PhNH(CH_2)_2NHSiMe_3$ (0.625 g, 3.00 mmol) in Et_2O (30 ml) at 273 K was added one equivalent of $LiBu^n$ and the reaction mixture was warmed to room temperature and stirred for a further 4 h. One equivalent PhCN was added at 195 K. The resulting mixture was warmed to room temperature and stirred for 12 h. Then one equivalent $ZrCl_4$ (0.699 g, 3 mmol) was added at 195 K. The resulting mixture was warmed to room temperature and stirred for 12 h. The volatiles were removed *in vacuo*, and the residue was extracted with 15 ml of dichloromethane and filtered. The filtrate was concentrated *in vacuo* to *ca* 10 ml and left at room temperature for one month to give colorless block-shaped crystals of the title compound in 36% yield.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

Funding information

Funding for this research was provided by: National Natural Science Foundation of China (award No. 21272142); the Natural Science Foundation of Shanxi Province (award No. 2015011015).

References

Bai, S.-D., Liu, R.-Q., Guan, F., Wang, T., Tong, H.-B., Guo, J.-P. & Liu, D.-S. (2013). *Mendeleev Commun.* **23**, 265–267.
Bai, S.-D., Tong, H.-B., Guo, J.-P., Zhou, M.-S., Liu, D.-S. & Yuan, S.-F. (2010). *Polyhedron*, **29**, 262–269.
Bruker (2012). *APEX2*, *SAINT* and *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
Edelmann, F. T. (1995). *Angew. Chem. Int. Ed. Engl.* **34**, 2466–2488.
Li, W., Bai, S.-D., Su, F., Yuan, S.-F., Duan, X.-E. & Liu, D.-S. (2017). *New J. Chem.* **41**, 661–670.
Li, W., Su, F., Yuan, S.-F., Duan, X.-E., Bai, S.-D. & Liu, D.-S. (2016). *RSC Adv.* **6**, 40741–40749.
Mack, H. & Eisen, M. S. (1996). *J. Organomet. Chem.* **525**, 81–87.
Parsons, S., Flack, H. D. & Wagner, T. (2013). *Acta Cryst.* B**69**, 249–259.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Sheldrick, G. M. (2015*a*). *Acta Cryst.* A**71**, 3–8.
Sheldrick, G. M. (2015*b*). *Acta Cryst.* C**71**, 3–8.

full crystallographic data

IUCrData (2017). **2**, x170380 [https://doi.org/10.1107/S2414314617003807]

[*N*-(2-Anilinoethyl)-*N*′-(trimethylsilyl)benzenecarboximidamidato-κ^3N,N',N''](benzonitrile-κN)trichloridozirconium(IV)

Wei Li, Shengdi Bai, Feng Su, Xine Duan and Diansheng Liu

[*N*-(2-Anilinoethyl)-*N*′-(trimethylsilyl)benzenecarboximidamidato-κ^3N,N',N''](benzonitrile-κN)trichloridozirconium(IV)

Crystal data

$[Zr(C_{18}H_{24}N_3Si)Cl_3(C_7H_5N)]$
M_r = 611.18
Orthorhombic, $Pna2_1$
a = 35.830 (2) Å
b = 14.292 (9) Å
c = 11.057 (6) Å
V = 5662 (5) Å^3
Z = 8
$F(000)$ = 2496
D_x = 1.434 Mg m^{-3}
D_m = 1.434 Mg m^{-3}
D_m measured by not measured
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 2629 reflections
θ = 2.2–28.5°
μ = 0.73 mm^{-1}
T = 194 K
Block, colorless
0.35 × 0.32 × 0.30 mm

Data collection

Bruker SMART APEX CCD area detector diffractometer
φ and ω scan
Absorption correction: multi-scan SADABS (Bruker, 2012)
T_{min} = 0.773, T_{max} = 0.802
29608 measured reflections
9600 independent reflections
5601 reflections with $I > 2\sigma(I)$
R_{int} = 0.133
θ_{max} = 25.1°, θ_{min} = 1.5°
h = −42→39
k = −13→17
l = −13→11

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.066
$wR(F^2)$ = 0.194
S = 1.00
9600 reflections
571 parameters
1 restraint
Hydrogen site location: mixed
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0852P)^2 + 0.8394P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 1.02 e Å^{-3}
$\Delta\rho_{min}$ = −0.80 e Å^{-3}
Absolute structure: Flack x determined using 1602 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons *et al.*, 2013)
Absolute structure parameter: 0.06 (6)

Special details

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

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Zr1	0.88588 (3)	0.41831 (7)	0.15136 (10)	0.0389 (3)
Zr2	0.85844 (3)	0.91156 (7)	0.25654 (10)	0.0372 (3)
Cl1	0.83935 (9)	0.3568 (2)	0.0148 (3)	0.0586 (9)
Cl2	0.88440 (9)	0.5773 (2)	0.0649 (3)	0.0547 (9)
Cl3	0.92042 (9)	0.4735 (2)	0.3257 (3)	0.0626 (10)
Cl4	0.81962 (9)	0.8434 (2)	0.0999 (3)	0.0575 (9)
Cl5	0.83063 (9)	1.0686 (2)	0.2387 (3)	0.0549 (9)
Cl6	0.90977 (9)	0.9766 (2)	0.3736 (3)	0.0544 (9)
N1	0.9333 (3)	0.4009 (6)	0.0270 (10)	0.049 (3)
N2	0.9162 (2)	0.2879 (6)	0.1474 (9)	0.046 (3)
N3	0.8622 (3)	0.2975 (7)	0.2951 (9)	0.051 (3)
H3A	0.8547	0.2684	0.2293	0.061*
N4	0.8335 (3)	0.4850 (6)	0.2414 (11)	0.052 (3)
N5	0.8207 (3)	0.8984 (6)	0.4144 (9)	0.047 (3)
N6	0.8566 (2)	0.7835 (6)	0.3559 (8)	0.036 (2)
N7	0.9046 (3)	0.7949 (6)	0.1871 (8)	0.043 (3)
H7A	0.8860	0.7641	0.1535	0.051*
N8	0.8870 (3)	0.9788 (7)	0.0859 (10)	0.052 (3)
Si1	0.95406 (11)	0.4573 (3)	−0.0973 (4)	0.0580 (11)
Si2	0.78585 (10)	0.9616 (3)	0.4884 (4)	0.0515 (10)
C1	1.01141 (16)	0.3356 (4)	0.1174 (5)	0.052 (4)
H1	1.0081	0.3989	0.1411	0.062*
C2	1.04686 (14)	0.2961 (5)	0.1181 (7)	0.070 (5)
H2	1.0678	0.3325	0.1423	0.084*
C3	1.05173 (17)	0.2034 (5)	0.0834 (9)	0.065 (4)
H3	1.0760	0.1764	0.0839	0.078*
C4	1.0212 (2)	0.1502 (4)	0.0480 (8)	0.061 (4)
H4	1.0245	0.0869	0.0243	0.074*
C5	0.98570 (19)	0.1897 (5)	0.0473 (8)	0.056 (4)
H5	0.9648	0.1533	0.0231	0.068*
C6	0.98082 (14)	0.2824 (5)	0.0820 (7)	0.041 (3)
C7	0.9437 (3)	0.3241 (8)	0.0806 (12)	0.047 (3)
C8	0.9185 (3)	0.2158 (8)	0.2356 (11)	0.049 (3)
H8A	0.9446	0.2072	0.2621	0.058*
H8B	0.9094	0.1559	0.2014	0.058*
C9	0.8948 (3)	0.2443 (9)	0.3392 (11)	0.052 (3)
H9A	0.8863	0.1882	0.3838	0.062*
H9B	0.9096	0.2837	0.3954	0.062*
C10	0.8357 (4)	0.3151 (8)	0.3911 (12)	0.060 (4)

C11	0.8451 (5)	0.3583 (12)	0.4938 (14)	0.086 (5)
H11	0.8698	0.3809	0.5055	0.104*
C12	0.8189 (6)	0.3694 (13)	0.5810 (16)	0.117 (7)
H12	0.8250	0.4002	0.6545	0.141*
C13	0.7826 (5)	0.3351 (13)	0.5624 (18)	0.114 (6)
H13	0.7646	0.3401	0.6251	0.136*
C14	0.7733 (4)	0.2958 (11)	0.4582 (18)	0.097 (6)
H14	0.7482	0.2768	0.4454	0.117*
C15	0.7990 (3)	0.2821 (9)	0.3685 (15)	0.063 (4)
H15	0.7926	0.2519	0.2948	0.076*
C16	0.8083 (3)	0.5232 (8)	0.2749 (11)	0.046 (3)
C17	0.77775 (18)	0.5721 (5)	0.3193 (7)	0.049 (3)
C18	0.7530 (2)	0.5264 (5)	0.3961 (8)	0.077 (5)
H18	0.7565	0.4621	0.4144	0.092*
C19	0.7231 (2)	0.5749 (8)	0.4459 (10)	0.107 (7)
H19	0.7062	0.5437	0.4983	0.129*
C20	0.7179 (3)	0.6690 (8)	0.4190 (11)	0.099 (6)
H20	0.6975	0.7021	0.4531	0.119*
C21	0.7427 (3)	0.7147 (5)	0.3423 (11)	0.093 (6)
H21	0.7391	0.7790	0.3240	0.112*
C22	0.7726 (2)	0.6662 (5)	0.2925 (8)	0.059 (4)
H22	0.7895	0.6975	0.2400	0.070*
C23	0.9156 (5)	0.4887 (12)	−0.2023 (14)	0.092 (6)
H23A	0.8976	0.4372	−0.2061	0.138*
H23B	0.9259	0.5002	−0.2831	0.138*
H23C	0.9031	0.5454	−0.1731	0.138*
C24	0.9847 (4)	0.3759 (11)	−0.1819 (13)	0.079 (5)
H24A	1.0080	0.3667	−0.1371	0.119*
H24B	0.9903	0.4022	−0.2617	0.119*
H24C	0.9720	0.3156	−0.1917	0.119*
C25	0.9795 (4)	0.5593 (10)	−0.0452 (13)	0.075 (5)
H25A	0.9653	0.5905	0.0188	0.113*
H25B	0.9832	0.6027	−0.1129	0.113*
H25C	1.0039	0.5399	−0.0136	0.113*
C26	0.82672 (16)	0.6878 (4)	0.5896 (6)	0.065 (4)
H26	0.8197	0.6488	0.5238	0.078*
C27	0.8262 (2)	0.6529 (5)	0.7069 (7)	0.079 (5)
H27	0.8188	0.5901	0.7214	0.095*
C28	0.8365 (2)	0.7100 (7)	0.8031 (6)	0.078 (5)
H28	0.8361	0.6862	0.8833	0.093*
C29	0.8473 (2)	0.8020 (6)	0.7819 (7)	0.063 (4)
H29	0.8543	0.8410	0.8476	0.075*
C30	0.8478 (2)	0.8369 (5)	0.6645 (8)	0.053 (4)
H30	0.8552	0.8997	0.6501	0.064*
C31	0.83752 (18)	0.7798 (5)	0.5684 (6)	0.043 (3)
C32	0.8372 (3)	0.8207 (8)	0.4468 (10)	0.039 (3)
C33	0.8826 (3)	0.7077 (8)	0.3604 (10)	0.044 (3)
H33A	0.8717	0.6510	0.3230	0.052*

H33B	0.8892	0.6932	0.4453	0.052*
C34	0.9161 (3)	0.7387 (8)	0.2920 (11)	0.052 (4)
H34A	0.9324	0.7764	0.3453	0.062*
H34B	0.9304	0.6834	0.2643	0.062*
C35	0.9367 (3)	0.8201 (8)	0.1140 (12)	0.050 (4)
C36	0.9352 (4)	0.7984 (9)	−0.0099 (12)	0.060 (4)
H36	0.9146	0.7664	−0.0443	0.073*
C37	0.9656 (5)	0.8262 (11)	−0.0799 (16)	0.092 (6)
H37	0.9660	0.8094	−0.1630	0.110*
C38	0.9941 (5)	0.8751 (12)	−0.0358 (17)	0.095 (6)
H38	1.0135	0.8969	−0.0874	0.115*
C39	0.9948 (5)	0.8938 (12)	0.088 (2)	0.111 (7)
H39	1.0156	0.9255	0.1223	0.133*
C40	0.9661 (4)	0.8671 (10)	0.1616 (16)	0.069 (4)
H40	0.9667	0.8814	0.2455	0.082*
C41	0.8919 (3)	1.0162 (8)	−0.0021 (13)	0.050 (3)
C42	0.89633 (19)	1.0673 (5)	−0.1091 (6)	0.043 (3)
C43	0.9081 (2)	1.0260 (5)	−0.2163 (7)	0.066 (4)
H43	0.9152	0.9620	−0.2173	0.079*
C44	0.9096 (3)	1.0785 (8)	−0.3221 (6)	0.091 (6)
H44	0.9177	1.0503	−0.3953	0.110*
C45	0.8993 (3)	1.1722 (7)	−0.3206 (7)	0.098 (6)
H45	0.9003	1.2081	−0.3929	0.118*
C46	0.8875 (3)	1.2135 (5)	−0.2134 (9)	0.096 (6)
H46	0.8804	1.2776	−0.2124	0.115*
C47	0.8860 (3)	1.1611 (5)	−0.1077 (7)	0.070 (5)
H47	0.8779	1.1893	−0.0344	0.084*
C48	0.7505 (4)	0.9971 (11)	0.3784 (14)	0.080 (5)
H48A	0.7627	1.0167	0.3033	0.119*
H48B	0.7359	1.0493	0.4112	0.119*
H48C	0.7338	0.9442	0.3617	0.119*
C49	0.7612 (3)	0.8871 (10)	0.6011 (13)	0.063 (4)
H49A	0.7581	0.8238	0.5684	0.094*
H49B	0.7366	0.9139	0.6184	0.094*
H49C	0.7758	0.8843	0.6759	0.094*
C50	0.8055 (4)	1.0640 (9)	0.5622 (14)	0.072 (5)
H50A	0.8268	1.0452	0.6120	0.108*
H50B	0.7864	1.0931	0.6135	0.108*
H50C	0.8137	1.1089	0.5008	0.108*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zr1	0.0321 (5)	0.0383 (5)	0.0464 (6)	0.0035 (5)	0.0039 (6)	−0.0009 (6)
Zr2	0.0410 (5)	0.0378 (5)	0.0327 (5)	0.0036 (5)	−0.0003 (6)	0.0024 (6)
Cl1	0.0488 (17)	0.0609 (19)	0.066 (2)	−0.0017 (16)	−0.0101 (18)	−0.0124 (17)
Cl2	0.0609 (19)	0.0439 (16)	0.059 (2)	0.0061 (15)	0.0060 (18)	0.0056 (15)
Cl3	0.056 (2)	0.062 (2)	0.069 (2)	−0.0013 (16)	−0.0176 (18)	−0.0050 (18)

Cl4	0.0555 (18)	0.069 (2)	0.0484 (19)	−0.0065 (16)	−0.0116 (17)	−0.0003 (16)
Cl5	0.0594 (18)	0.0466 (16)	0.059 (2)	0.0138 (14)	0.0064 (18)	0.0068 (16)
Cl6	0.0568 (18)	0.0536 (18)	0.0528 (19)	0.0002 (15)	−0.0157 (17)	−0.0079 (15)
N1	0.048 (6)	0.042 (6)	0.058 (7)	0.013 (5)	0.010 (5)	0.009 (5)
N2	0.036 (5)	0.048 (5)	0.054 (6)	−0.001 (4)	0.018 (6)	0.005 (5)
N3	0.046 (6)	0.048 (6)	0.059 (7)	0.004 (5)	0.003 (6)	0.000 (5)
N4	0.034 (5)	0.049 (5)	0.074 (7)	0.013 (4)	0.006 (6)	−0.010 (6)
N5	0.049 (6)	0.044 (6)	0.049 (6)	0.011 (5)	0.003 (5)	0.003 (5)
N6	0.038 (5)	0.045 (5)	0.025 (5)	0.000 (4)	−0.004 (4)	0.000 (4)
N7	0.046 (5)	0.037 (5)	0.045 (6)	−0.001 (4)	0.007 (5)	0.001 (4)
N8	0.055 (6)	0.043 (6)	0.057 (7)	−0.001 (5)	0.006 (6)	0.005 (5)
Si1	0.054 (2)	0.059 (2)	0.060 (2)	0.0059 (19)	0.015 (2)	0.011 (2)
Si2	0.0444 (19)	0.058 (2)	0.052 (2)	0.0124 (17)	0.0070 (19)	−0.0024 (18)
C1	0.046 (7)	0.059 (7)	0.051 (8)	0.003 (6)	0.015 (6)	−0.016 (6)
C2	0.042 (7)	0.085 (10)	0.082 (11)	0.000 (7)	0.001 (8)	−0.007 (8)
C3	0.044 (7)	0.089 (10)	0.062 (9)	0.018 (7)	0.009 (7)	0.007 (8)
C4	0.054 (8)	0.060 (8)	0.069 (9)	0.019 (7)	0.020 (8)	0.002 (7)
C5	0.044 (7)	0.063 (8)	0.062 (9)	0.018 (6)	−0.004 (7)	0.011 (7)
C6	0.033 (6)	0.043 (6)	0.047 (7)	0.007 (5)	0.020 (6)	0.003 (6)
C7	0.049 (7)	0.038 (6)	0.055 (8)	0.000 (6)	0.000 (7)	−0.006 (6)
C8	0.039 (6)	0.046 (6)	0.060 (8)	0.012 (5)	0.016 (6)	0.023 (6)
C9	0.055 (7)	0.053 (7)	0.048 (7)	0.009 (6)	0.019 (7)	0.009 (6)
C10	0.080 (9)	0.035 (6)	0.064 (8)	0.017 (6)	0.033 (8)	0.024 (6)
C11	0.085 (11)	0.121 (13)	0.053 (10)	0.027 (10)	0.023 (9)	0.002 (10)
C12	0.163 (17)	0.133 (15)	0.055 (10)	0.068 (13)	0.030 (12)	0.026 (10)
C13	0.103 (12)	0.133 (14)	0.104 (13)	0.049 (11)	0.072 (11)	0.050 (11)
C14	0.074 (11)	0.085 (11)	0.133 (15)	0.032 (8)	0.047 (11)	0.037 (11)
C15	0.044 (7)	0.049 (8)	0.096 (11)	0.008 (6)	0.035 (8)	0.001 (7)
C16	0.049 (7)	0.041 (6)	0.049 (8)	−0.001 (5)	0.005 (7)	−0.001 (6)
C17	0.039 (6)	0.042 (7)	0.064 (8)	0.001 (5)	0.011 (7)	−0.001 (6)
C18	0.064 (9)	0.067 (9)	0.100 (12)	0.018 (8)	0.024 (9)	0.020 (9)
C19	0.075 (11)	0.153 (17)	0.094 (13)	0.018 (11)	0.050 (10)	0.016 (12)
C20	0.062 (9)	0.101 (12)	0.134 (16)	0.046 (9)	−0.017 (11)	−0.022 (12)
C21	0.090 (11)	0.065 (9)	0.124 (15)	0.036 (8)	−0.017 (12)	−0.016 (10)
C22	0.056 (8)	0.060 (8)	0.060 (9)	−0.004 (7)	−0.009 (7)	0.006 (7)
C23	0.098 (12)	0.107 (13)	0.072 (11)	0.030 (10)	−0.001 (10)	0.016 (10)
C24	0.086 (11)	0.089 (11)	0.062 (9)	0.015 (9)	0.036 (8)	0.005 (8)
C25	0.085 (11)	0.078 (10)	0.064 (10)	0.003 (8)	0.012 (9)	0.023 (8)
C26	0.085 (10)	0.062 (8)	0.049 (8)	−0.002 (7)	−0.002 (8)	0.014 (7)
C27	0.098 (11)	0.076 (10)	0.063 (9)	−0.001 (9)	0.016 (9)	0.024 (8)
C28	0.083 (11)	0.103 (12)	0.047 (9)	0.007 (9)	0.002 (9)	0.027 (8)
C29	0.053 (8)	0.099 (10)	0.036 (8)	0.007 (7)	−0.004 (7)	0.006 (7)
C30	0.043 (6)	0.061 (8)	0.055 (8)	0.000 (6)	−0.002 (7)	−0.008 (7)
C31	0.034 (6)	0.042 (6)	0.053 (8)	0.005 (5)	0.004 (6)	0.001 (6)
C32	0.040 (6)	0.045 (6)	0.032 (6)	0.005 (5)	−0.007 (6)	−0.003 (5)
C33	0.059 (7)	0.044 (6)	0.027 (6)	0.015 (6)	0.005 (6)	0.000 (5)
C34	0.055 (7)	0.045 (7)	0.056 (8)	0.007 (6)	0.008 (7)	0.005 (6)
C35	0.050 (7)	0.038 (6)	0.062 (9)	0.005 (6)	0.012 (7)	0.001 (6)

C36	0.072 (9)	0.061 (8)	0.048 (8)	0.009 (7)	0.014 (8)	−0.007 (7)
C37	0.119 (13)	0.082 (11)	0.073 (11)	−0.010 (10)	0.042 (10)	−0.017 (9)
C38	0.079 (11)	0.098 (13)	0.109 (14)	0.002 (9)	0.057 (10)	0.015 (10)
C39	0.067 (10)	0.118 (14)	0.147 (18)	−0.035 (9)	0.032 (12)	0.006 (13)
C40	0.053 (8)	0.069 (8)	0.084 (10)	−0.005 (7)	0.004 (9)	−0.003 (9)
C41	0.044 (7)	0.040 (6)	0.067 (8)	−0.011 (5)	0.012 (7)	−0.004 (6)
C42	0.045 (7)	0.050 (7)	0.034 (6)	−0.013 (5)	−0.005 (6)	0.003 (6)
C43	0.080 (10)	0.075 (9)	0.041 (8)	−0.009 (8)	0.000 (8)	−0.010 (7)
C44	0.117 (13)	0.122 (14)	0.035 (9)	−0.028 (11)	0.012 (9)	0.004 (9)
C45	0.132 (15)	0.105 (13)	0.057 (10)	−0.015 (11)	0.001 (11)	0.034 (9)
C46	0.166 (18)	0.059 (9)	0.063 (11)	0.015 (10)	−0.010 (11)	0.019 (8)
C47	0.106 (12)	0.055 (8)	0.048 (8)	0.010 (8)	−0.007 (9)	0.001 (7)
C48	0.047 (8)	0.115 (13)	0.076 (10)	0.022 (8)	0.005 (8)	0.027 (9)
C49	0.038 (7)	0.090 (10)	0.061 (9)	0.010 (7)	0.016 (7)	0.003 (8)
C50	0.081 (10)	0.066 (9)	0.070 (10)	0.014 (8)	0.012 (9)	−0.009 (8)

Geometric parameters (Å, º)

Zr1—N2	2.159 (9)	C17—C22	1.3900
Zr1—N1	2.200 (10)	C18—C19	1.3900
Zr1—N4	2.328 (9)	C18—H18	0.9500
Zr1—Cl1	2.415 (4)	C19—C20	1.3900
Zr1—Cl3	2.422 (4)	C19—H19	0.9500
Zr1—Cl2	2.466 (3)	C20—C21	1.3900
Zr1—N3	2.496 (10)	C20—H20	0.9500
Zr1—C7	2.592 (12)	C21—C22	1.3900
Zr2—N6	2.135 (9)	C21—H21	0.9500
Zr2—N5	2.216 (10)	C22—H22	0.9500
Zr2—N8	2.351 (11)	C23—H23A	0.9800
Zr2—Cl4	2.426 (3)	C23—H23B	0.9800
Zr2—Cl6	2.433 (3)	C23—H23C	0.9800
Zr2—Cl5	2.464 (3)	C24—H24A	0.9800
Zr2—N7	2.470 (9)	C24—H24B	0.9800
Zr2—C32	2.587 (12)	C24—H24C	0.9800
N1—C7	1.303 (14)	C25—H25A	0.9800
N1—Si1	1.758 (11)	C25—H25B	0.9800
N2—C7	1.334 (14)	C25—H25C	0.9800
N2—C8	1.421 (14)	C26—C27	1.3900
N3—C10	1.446 (16)	C26—C31	1.3900
N3—C9	1.477 (15)	C26—H26	0.9500
N3—H3A	0.8800	C27—C28	1.3900
N4—C16	1.118 (14)	C27—H27	0.9500
N5—C32	1.309 (14)	C28—C29	1.3900
N5—Si2	1.744 (10)	C28—H28	0.9500
N6—C32	1.332 (14)	C29—C30	1.3900
N6—C33	1.430 (14)	C29—H29	0.9500
N7—C35	1.451 (15)	C30—C31	1.3900
N7—C34	1.471 (15)	C30—H30	0.9500

N7—H7A	0.8800	C31—C32	1.466 (13)
N8—C41	1.125 (16)	C33—C34	1.487 (16)
Si1—C25	1.814 (15)	C33—H33A	0.9900
Si1—C24	1.854 (15)	C33—H33B	0.9900
Si1—C23	1.856 (16)	C34—H34A	0.9900
Si2—C50	1.817 (15)	C34—H34B	0.9900
Si2—C48	1.829 (14)	C35—C40	1.356 (18)
Si2—C49	1.863 (14)	C35—C36	1.406 (18)
C1—C2	1.3900	C36—C37	1.39 (2)
C1—C6	1.3900	C36—H36	0.9500
C1—H1	0.9500	C37—C38	1.33 (2)
C2—C3	1.3900	C37—H37	0.9500
C2—H2	0.9500	C38—C39	1.40 (3)
C3—C4	1.3900	C38—H38	0.9500
C3—H3	0.9500	C39—C40	1.36 (2)
C4—C5	1.3900	C39—H39	0.9500
C4—H4	0.9500	C40—H40	0.9500
C5—C6	1.3900	C41—C42	1.399 (15)
C5—H5	0.9500	C42—C43	1.3900
C6—C7	1.458 (13)	C42—C47	1.3900
C8—C9	1.482 (16)	C43—C44	1.3900
C8—H8A	0.9900	C43—H43	0.9500
C8—H8B	0.9900	C44—C45	1.3900
C9—H9A	0.9900	C44—H44	0.9500
C9—H9B	0.9900	C45—C46	1.3900
C10—C11	1.34 (2)	C45—H45	0.9500
C10—C15	1.420 (18)	C46—C47	1.3900
C11—C12	1.36 (2)	C46—H46	0.9500
C11—H11	0.9500	C47—H47	0.9500
C12—C13	1.40 (3)	C48—H48A	0.9800
C12—H12	0.9500	C48—H48B	0.9800
C13—C14	1.32 (3)	C48—H48C	0.9800
C13—H13	0.9500	C49—H49A	0.9800
C14—C15	1.37 (2)	C49—H49B	0.9800
C14—H14	0.9500	C49—H49C	0.9800
C15—H15	0.9500	C50—H50A	0.9800
C16—C17	1.389 (13)	C50—H50B	0.9800
C17—C18	1.3900	C50—H50C	0.9800

N2—Zr1—N1	60.0 (3)	C13—C12—H12	120.1
N2—Zr1—N4	140.2 (3)	C14—C13—C12	120.5 (17)
N1—Zr1—N4	159.4 (4)	C14—C13—H13	119.7
N2—Zr1—Cl1	91.2 (3)	C12—C13—H13	119.7
N1—Zr1—Cl1	95.8 (3)	C13—C14—C15	121.5 (17)
N4—Zr1—Cl1	82.0 (3)	C13—C14—H14	119.2
N2—Zr1—Cl3	92.3 (3)	C15—C14—H14	119.2
N1—Zr1—Cl3	98.0 (3)	C14—C15—C10	116.7 (15)
N4—Zr1—Cl3	86.4 (3)	C14—C15—H15	121.7

Cl1—Zr1—Cl3	165.62 (13)	C10—C15—H15	121.7
N2—Zr1—Cl2	143.0 (3)	N4—C16—C17	178.0 (13)
N1—Zr1—Cl2	83.0 (3)	C16—C17—C18	118.8 (7)
N4—Zr1—Cl2	76.8 (3)	C16—C17—C22	121.1 (7)
Cl1—Zr1—Cl2	94.48 (12)	C18—C17—C22	120.0
Cl3—Zr1—Cl2	91.12 (12)	C17—C18—C19	120.0
N2—Zr1—N3	65.6 (3)	C17—C18—H18	120.0
N1—Zr1—N3	125.6 (3)	C19—C18—H18	120.0
N4—Zr1—N3	74.7 (3)	C20—C19—C18	120.0
Cl1—Zr1—N3	84.9 (3)	C20—C19—H19	120.0
Cl3—Zr1—N3	83.8 (3)	C18—C19—H19	120.0
Cl2—Zr1—N3	151.3 (2)	C19—C20—C21	120.0
N2—Zr1—C7	31.0 (3)	C19—C20—H20	120.0
N1—Zr1—C7	30.2 (4)	C21—C20—H20	120.0
N4—Zr1—C7	170.4 (4)	C20—C21—C22	120.0
Cl1—Zr1—C7	100.0 (3)	C20—C21—H21	120.0
Cl3—Zr1—C7	90.1 (3)	C22—C21—H21	120.0
Cl2—Zr1—C7	112.3 (3)	C21—C22—C17	120.0
N3—Zr1—C7	96.0 (3)	C21—C22—H22	120.0
N6—Zr2—N5	60.2 (3)	C17—C22—H22	120.0
N6—Zr2—N8	140.9 (3)	Si1—C23—H23A	109.5
N5—Zr2—N8	158.8 (3)	Si1—C23—H23B	109.5
N6—Zr2—Cl4	90.3 (2)	H23A—C23—H23B	109.5
N5—Zr2—Cl4	100.3 (3)	Si1—C23—H23C	109.5
N8—Zr2—Cl4	80.8 (3)	H23A—C23—H23C	109.5
N6—Zr2—Cl6	94.5 (2)	H23B—C23—H23C	109.5
N5—Zr2—Cl6	94.3 (3)	Si1—C24—H24A	109.5
N8—Zr2—Cl6	86.7 (3)	Si1—C24—H24B	109.5
Cl4—Zr2—Cl6	165.14 (12)	H24A—C24—H24B	109.5
N6—Zr2—Cl5	144.0 (3)	Si1—C24—H24C	109.5
N5—Zr2—Cl5	83.9 (2)	H24A—C24—H24C	109.5
N8—Zr2—Cl5	74.9 (2)	H24B—C24—H24C	109.5
Cl4—Zr2—Cl5	94.40 (12)	Si1—C25—H25A	109.5
Cl6—Zr2—Cl5	90.02 (12)	Si1—C25—H25B	109.5
N6—Zr2—N7	66.6 (3)	H25A—C25—H25B	109.5
N5—Zr2—N7	126.6 (3)	Si1—C25—H25C	109.5
N8—Zr2—N7	74.6 (3)	H25A—C25—H25C	109.5
Cl4—Zr2—N7	83.7 (2)	H25B—C25—H25C	109.5
Cl6—Zr2—N7	85.2 (2)	C27—C26—C31	120.0
Cl5—Zr2—N7	149.4 (2)	C27—C26—H26	120.0
N6—Zr2—C32	30.9 (3)	C31—C26—H26	120.0
N5—Zr2—C32	30.4 (3)	C26—C27—C28	120.0
N8—Zr2—C32	170.3 (4)	C26—C27—H27	120.0
Cl4—Zr2—C32	102.2 (3)	C28—C27—H27	120.0
Cl6—Zr2—C32	88.9 (3)	C27—C28—C29	120.0
Cl5—Zr2—C32	113.8 (3)	C27—C28—H28	120.0
N7—Zr2—C32	96.4 (3)	C29—C28—H28	120.0
C7—N1—Si1	128.5 (9)	C30—C29—C28	120.0

C7—N1—Zr1	91.8 (8)	C30—C29—H29	120.0
Si1—N1—Zr1	139.8 (5)	C28—C29—H29	120.0
C7—N2—C8	128.2 (9)	C31—C30—C29	120.0
C7—N2—Zr1	92.7 (7)	C31—C30—H30	120.0
C8—N2—Zr1	129.8 (7)	C29—C30—H30	120.0
C10—N3—C9	111.5 (10)	C30—C31—C26	120.0
C10—N3—Zr1	124.8 (7)	C30—C31—C32	118.0 (6)
C9—N3—Zr1	107.3 (7)	C26—C31—C32	122.0 (6)
C10—N3—H3A	119.3	N5—C32—N6	111.5 (10)
C9—N3—H3A	105.8	N5—C32—C31	126.4 (10)
Zr1—N3—H3A	84.5	N6—C32—C31	121.9 (9)
C16—N4—Zr1	172.9 (11)	N5—C32—Zr2	58.9 (6)
C32—N5—Si2	129.4 (9)	N6—C32—Zr2	55.5 (6)
C32—N5—Zr2	90.7 (7)	C31—C32—Zr2	160.7 (7)
Si2—N5—Zr2	139.7 (5)	N6—C33—C34	106.4 (9)
C32—N6—C33	128.0 (9)	N6—C33—H33A	110.4
C32—N6—Zr2	93.6 (7)	C34—C33—H33A	110.4
C33—N6—Zr2	130.3 (7)	N6—C33—H33B	110.4
C35—N7—C34	110.7 (9)	C34—C33—H33B	110.4
C35—N7—Zr2	122.4 (7)	H33A—C33—H33B	108.6
C34—N7—Zr2	108.1 (7)	N7—C34—C33	109.7 (10)
C35—N7—H7A	119.2	N7—C34—H34A	109.7
C34—N7—H7A	105.7	C33—C34—H34A	109.7
Zr2—N7—H7A	87.9	N7—C34—H34B	109.7
C41—N8—Zr2	163.2 (10)	C33—C34—H34B	109.7
N1—Si1—C25	109.5 (6)	H34A—C34—H34B	108.2
N1—Si1—C24	110.9 (6)	C40—C35—C36	121.0 (13)
C25—Si1—C24	111.5 (7)	C40—C35—N7	121.5 (12)
N1—Si1—C23	106.6 (6)	C36—C35—N7	117.4 (11)
C25—Si1—C23	112.2 (7)	C37—C36—C35	116.7 (14)
C24—Si1—C23	106.0 (7)	C37—C36—H36	121.6
N5—Si2—C50	110.5 (6)	C35—C36—H36	121.6
N5—Si2—C48	109.1 (6)	C38—C37—C36	123.1 (16)
C50—Si2—C48	110.1 (7)	C38—C37—H37	118.4
N5—Si2—C49	111.0 (5)	C36—C37—H37	118.4
C50—Si2—C49	110.1 (7)	C37—C38—C39	118.3 (16)
C48—Si2—C49	105.9 (6)	C37—C38—H38	120.9
C2—C1—C6	120.0	C39—C38—H38	120.9
C2—C1—H1	120.0	C40—C39—C38	121.0 (17)
C6—C1—H1	120.0	C40—C39—H39	119.5
C3—C2—C1	120.0	C38—C39—H39	119.5
C3—C2—H2	120.0	C35—C40—C39	119.7 (16)
C1—C2—H2	120.0	C35—C40—H40	120.2
C2—C3—C4	120.0	C39—C40—H40	120.2
C2—C3—H3	120.0	N8—C41—C42	176.2 (13)
C4—C3—H3	120.0	C43—C42—C47	120.0
C3—C4—C5	120.0	C43—C42—C41	122.3 (7)
C3—C4—H4	120.0	C47—C42—C41	117.6 (7)

C5—C4—H4	120.0	C42—C43—C44	120.0
C6—C5—C4	120.0	C42—C43—H43	120.0
C6—C5—H5	120.0	C44—C43—H43	120.0
C4—C5—H5	120.0	C45—C44—C43	120.0
C5—C6—C1	120.0	C45—C44—H44	120.0
C5—C6—C7	120.1 (6)	C43—C44—H44	120.0
C1—C6—C7	119.9 (6)	C46—C45—C44	120.0
N1—C7—N2	111.6 (10)	C46—C45—H45	120.0
N1—C7—C6	127.6 (10)	C44—C45—H45	120.0
N2—C7—C6	120.6 (10)	C47—C46—C45	120.0
N1—C7—Zr1	58.1 (6)	C47—C46—H46	120.0
N2—C7—Zr1	56.3 (6)	C45—C46—H46	120.0
C6—C7—Zr1	159.8 (8)	C46—C47—C42	120.0
N2—C8—C9	107.4 (9)	C46—C47—H47	120.0
N2—C8—H8A	110.2	C42—C47—H47	120.0
C9—C8—H8A	110.2	Si2—C48—H48A	109.5
N2—C8—H8B	110.2	Si2—C48—H48B	109.5
C9—C8—H8B	110.2	H48A—C48—H48B	109.5
H8A—C8—H8B	108.5	Si2—C48—H48C	109.5
N3—C9—C8	109.8 (10)	H48A—C48—H48C	109.5
N3—C9—H9A	109.7	H48B—C48—H48C	109.5
C8—C9—H9A	109.7	Si2—C49—H49A	109.5
N3—C9—H9B	109.7	Si2—C49—H49B	109.5
C8—C9—H9B	109.7	H49A—C49—H49B	109.5
H9A—C9—H9B	108.2	Si2—C49—H49C	109.5
C11—C10—C15	122.4 (14)	H49A—C49—H49C	109.5
C11—C10—N3	122.6 (13)	H49B—C49—H49C	109.5
C15—C10—N3	114.9 (12)	Si2—C50—H50A	109.5
C10—C11—C12	119.0 (17)	Si2—C50—H50B	109.5
C10—C11—H11	120.5	H50A—C50—H50B	109.5
C12—C11—H11	120.5	Si2—C50—H50C	109.5
C11—C12—C13	119.8 (19)	H50A—C50—H50C	109.5
C11—C12—H12	120.1	H50B—C50—H50C	109.5

C7—N1—Si1—C25	−104.3 (12)	C17—C18—C19—C20	0.0
Zr1—N1—Si1—C25	75.2 (10)	C18—C19—C20—C21	0.0
C7—N1—Si1—C24	19.2 (13)	C19—C20—C21—C22	0.0
Zr1—N1—Si1—C24	−161.3 (9)	C20—C21—C22—C17	0.0
C7—N1—Si1—C23	134.2 (12)	C16—C17—C22—C21	−177.2 (8)
Zr1—N1—Si1—C23	−46.3 (11)	C18—C17—C22—C21	0.0
C32—N5—Si2—C50	103.1 (12)	C31—C26—C27—C28	0.0
Zr2—N5—Si2—C50	−68.9 (10)	C26—C27—C28—C29	0.0
C32—N5—Si2—C48	−135.7 (11)	C27—C28—C29—C30	0.0
Zr2—N5—Si2—C48	52.3 (10)	C28—C29—C30—C31	0.0
C32—N5—Si2—C49	−19.4 (13)	C29—C30—C31—C26	0.0
Zr2—N5—Si2—C49	168.7 (8)	C29—C30—C31—C32	177.8 (7)
C6—C1—C2—C3	0.0	C27—C26—C31—C30	0.0
C1—C2—C3—C4	0.0	C27—C26—C31—C32	−177.7 (7)

C2—C3—C4—C5	0.0	Si2—N5—C32—N6	166.8 (8)
C3—C4—C5—C6	0.0	Zr2—N5—C32—N6	−18.3 (9)
C4—C5—C6—C1	0.0	Si2—N5—C32—C31	−17.2 (17)
C4—C5—C6—C7	179.7 (9)	Zr2—N5—C32—C31	157.6 (10)
C2—C1—C6—C5	0.0	Si2—N5—C32—Zr2	−174.8 (11)
C2—C1—C6—C7	−179.7 (9)	C33—N6—C32—N5	169.7 (10)
Si1—N1—C7—N2	−162.1 (9)	Zr2—N6—C32—N5	19.1 (10)
Zr1—N1—C7—N2	18.2 (10)	C33—N6—C32—C31	−6.5 (17)
Si1—N1—C7—C6	23.3 (19)	Zr2—N6—C32—C31	−157.1 (9)
Zr1—N1—C7—C6	−156.4 (11)	C33—N6—C32—Zr2	150.6 (12)
Si1—N1—C7—Zr1	179.7 (12)	C30—C31—C32—N5	−51.0 (13)
C8—N2—C7—N1	−167.3 (11)	C26—C31—C32—N5	126.8 (10)
Zr1—N2—C7—N1	−18.6 (11)	C30—C31—C32—N6	124.6 (9)
C8—N2—C7—C6	7.7 (18)	C26—C31—C32—N6	−57.7 (12)
Zr1—N2—C7—C6	156.4 (9)	C30—C31—C32—Zr2	49 (2)
C8—N2—C7—Zr1	−148.7 (14)	C26—C31—C32—Zr2	−133.7 (19)
C5—C6—C7—N1	−126.5 (11)	C32—N6—C33—C34	−132.6 (11)
C1—C6—C7—N1	53.2 (15)	Zr2—N6—C33—C34	7.4 (13)
C5—C6—C7—N2	59.4 (13)	C35—N7—C34—C33	−175.8 (9)
C1—C6—C7—N2	−121.0 (10)	Zr2—N7—C34—C33	47.6 (10)
C5—C6—C7—Zr1	134.3 (19)	N6—C33—C34—N7	−37.1 (12)
C1—C6—C7—Zr1	−46 (3)	C34—N7—C35—C40	−56.7 (14)
C7—N2—C8—C9	138.0 (12)	Zr2—N7—C35—C40	72.6 (14)
Zr1—N2—C8—C9	0.5 (14)	C34—N7—C35—C36	126.7 (12)
C10—N3—C9—C8	171.7 (10)	Zr2—N7—C35—C36	−104.0 (11)
Zr1—N3—C9—C8	−48.4 (11)	C40—C35—C36—C37	1 (2)
N2—C8—C9—N3	33.9 (13)	N7—C35—C36—C37	177.6 (12)
C9—N3—C10—C11	55.8 (16)	C35—C36—C37—C38	−3 (2)
Zr1—N3—C10—C11	−75.6 (15)	C36—C37—C38—C39	5 (3)
C9—N3—C10—C15	−123.5 (12)	C37—C38—C39—C40	−4 (3)
Zr1—N3—C10—C15	105.0 (11)	C36—C35—C40—C39	0 (2)
C15—C10—C11—C12	1 (2)	N7—C35—C40—C39	−176.6 (13)
N3—C10—C11—C12	−177.9 (13)	C38—C39—C40—C35	1 (3)
C10—C11—C12—C13	0 (3)	C47—C42—C43—C44	0.0
C11—C12—C13—C14	−3 (3)	C41—C42—C43—C44	175.6 (8)
C12—C13—C14—C15	4 (3)	C42—C43—C44—C45	0.0
C13—C14—C15—C10	−2 (2)	C43—C44—C45—C46	0.0
C11—C10—C15—C14	−1 (2)	C44—C45—C46—C47	0.0
N3—C10—C15—C14	178.8 (11)	C45—C46—C47—C42	0.0
C16—C17—C18—C19	177.3 (8)	C43—C42—C47—C46	0.0
C22—C17—C18—C19	0.0	C41—C42—C47—C46	−175.8 (8)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C40—H40···Cl6	0.95	2.83	3.466 (16)	125
C34—H34*A*···Cl6	0.99	2.99	3.525 (13)	115
C9—H9*B*···Cl3	0.99	2.85	3.404 (13)	116

N7—H7*A*···Cl4	0.88	2.70	3.267 (10)	123
N7—H7*A*···Cl2	0.88	2.84	3.467 (10)	129
N3—H3*A*···Cl5^{i}	0.88	2.98	3.516 (10)	121
N3—H3*A*···Cl1	0.88	2.74	3.316 (11)	124

Symmetry code: (i) x, $y-1$, z.