Acta Cryst E CRYSTALLOGRAPHIC COMMUNICATIONS

ISSN 2056-9890

Crystal structure of tris(dimethylamido-κN)bis(dimethylamine-κN)zirconium(IV) iodide

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Received 5 August 2015
Accepted 11 December 2015

Edited by S. Parkin, University of Kentucky, USA

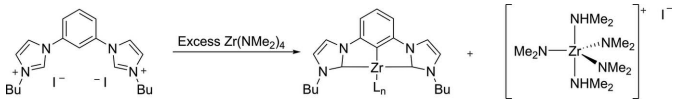
Keywords: crystal structure; zirconium; amido ligands; iodide; dimethylamine; N—H···I interactions

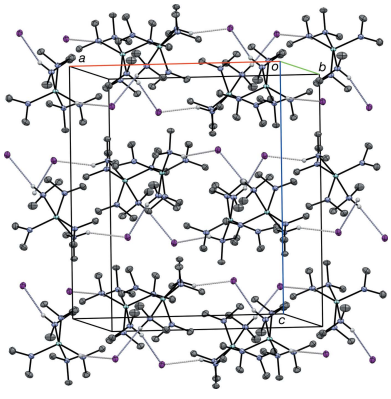
CCDC reference: 1037746
Supporting information: this article has supporting information at journals.iucr.org/e

Zirconium amides have become increasingly popular and useful due to their widespread use as precursors to other zirconium complexes and their use in the production of solid oxide fuel cells (SOFCs). Herein we report the molecular structure of tris(dimethylamido)bis(dimethylamine)zirconium(IV) iodide, $[Zr(C_2H_6N)_3(C_2H_7N)_2]I$. The bond lengths and bond angles are consistent with a slightly distorted trigonal–bipyramidal coordination geometry around the metal atom. N···I contacts of 3.6153 (15) and 3.5922 (14) Å are consistent with the presence of N—H···I interactions. These N—H···I interactions link the complex cations and iodide anions into extended chains that propagate parallel to the *a* axis.

1. Chemical context

Zirconium amide complexes are widely used in the synthesis of other zirconium complexes and solid oxide fuel cells (SOFCs). Additionally, many zirconium amide complexes are precatalysts for hydroamination/cyclization of unactivated aminoalkenes (Luconi *et al.*, 2013, Manna *et al.*, 2013 and references therein). Perhaps one of the most well known zirconium amide complexes is tetrakis(dimethylamido)-zirconium(IV). The title compound serendipitously formed from the reaction of an excess of tetrakis(dimethylamido)-zirconium(IV) and a bis(imidazolium) salt that we routinely perform, as illustrated in the Scheme below.





2. Structural commentary

The zirconium complex has a slightly distorted trigonal–bipyramidal geometry with three dimethamido ligands in equatorial positions and two dimethyamine ligands in axial positions (Fig. 1). Iodide provides a counterbalancing charge for the cationic zirconium complex. The Zr—amine bonds [Zr1—N1 and Zr1—N2, 2.3730 (13) and 2.3695 (14) Å, respectively] are significantly longer than those of the amide ligands [Zr1—N3 2.0249 (14), Zr1—N4 2.0393 (14), and Zr1—N5 2.0389 (14) Å]. The C—N bonds vary little, with the shortest and longest bond being only 0.026 (2) Å different [N1–C2 1.480 (2) and N3—C5 1.454 (2) Å]. The N1—Zr1—N2 angle of 172.83 (5)° and the N1—Zr1—N3 of 94.35 (5)° deviate slightly from the ideal angles of trigonal–bipyramidal geometry. The N3—Zr1—N5, N3—Zr1—N4, and N4—Zr1—N5 angles are close to 120° [116.76 (6), 120.99 (6), and

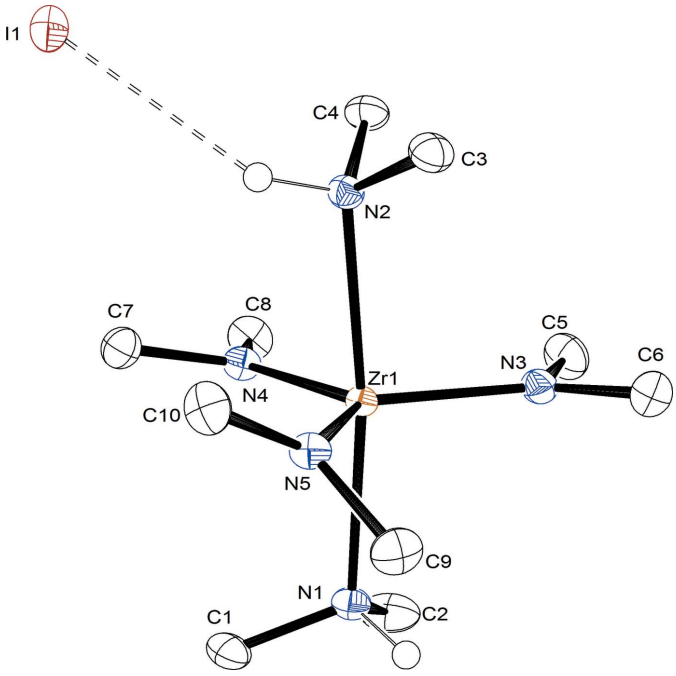


Figure 1
Displacement ellipsoid plot of the title compound. All hydrogens except the amine H atoms have been omitted for clarity. Ellipsoids are shown at the 50% probability level.

122.15 (6)°, respectively]. The C—N—Zr angles vary with the smallest and largest angles being almost 20° different [C10—N5—Zr1 135.34 (11) and C1—N1—Zr1 110.52 (10)°]. The amine nitrogen atoms (N1 and N2) are puckered in the structure [Zr1—N1—C1—C2 −124.71 (15) and Zr1—N2—C3—C4 127.27 (15)°]. This is in contrast to the amide ligands which are essentially coplanar with the metal [Zr1—N3—C5—C6 175.88 (19), Zr1—N4—C7—C8 174.05 (17), and Zr1—N5—C9—C10 −176.79 (17)°]. One amide ligand is twisted out of the plane by roughly 40° [C9—N5—Zr1—N3 −39.10 (13)°].

3. Supramolecular features

N···I contacts of 3.6153 (15) and 3.5922 (14) Å are consistent with the presence of N—H···I interactions (Table 1). The 'twist' of the second dimethylamido ligand away from the first is consistent with interaction with a symmetry-related I^- atom (H2—N2—N1—H1 − 114°; Fig. 2). The N—H···I interactions link the complex cations and iodide anions into extended chains that propagate parallel to the *a* axis.

4. Database survey

The synthesis or crystal structure of tris(dimethylamido)bis-(dimethylamine)zirconium(IV) iodide has not been reported as of 22 April 2015 based on a comprehensive WebCSD and Scifinder Scholar search. Similar compounds have been characterized crystallographically, for example tetrakis(dimethylamido)zirconium(IV) and its lithium dimethylamido adduct (Chisholm *et al.*, 1988) and several more zirconium-amide iodide complexes (Lehn & Hoffman, 2002).

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···I1^{i}	1.00	2.78	3.5922 (14)	138
N2—H2···I1	1.00	2.69	3.6153 (15)	138

Symmetry code: (i) $x-\frac{1}{2}, -y+\frac{3}{2}, -z+1$.

5. Synthesis and crystallization

1,3-Bis(3′-hexylimidazol-1′-yl)benzene diiodide (301 mg, 0.475 mmol), tetrakis(dimethylamido)zirconium(IV) (317 mg, 1.24 mmol) and dry toluene (2.8 mL) were combined in an inert atmosphere of Ar and heated at 383 K for 5 min in a sealed screw-cap vial. While heating, the reaction mixture became homogeneous. Upon cooling to room temperature, an oil formed. The top layer was removed and the oil was washed with toluene (3 × 3 mL). The toluene washings were combined and allowed to sit at room temperature. Colorless crystals formed after 2 months. The mother liquor was decanted and the crystals were covered with paratone oil after using a few crystals for ^{1}H NMR spectroscopy. ^{1}H NMR spectra of the samples indicated that 2-[1,3-bis(3′-hexyl-imidazol-2′-ylidene)phenylene](dimethylamido)diiodido-zirconium(IV) and 2-[1,3-bis(3′-hexyl-imidazol-2′-ylidene)-phenylene]bis(dimethylamido)iodidozirconium(IV) had

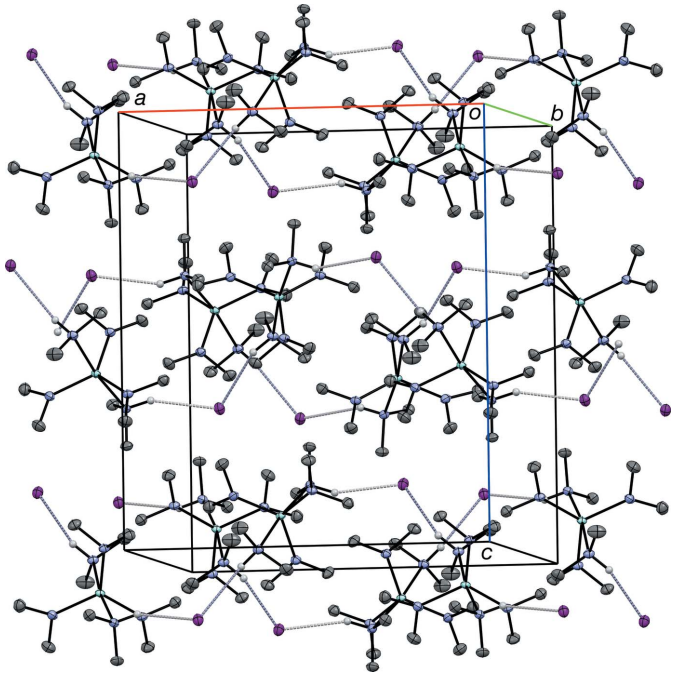


Figure 2
A packing plot of the unit cell viewed approximately down the *b* axis, illustrating the N—H···I interactions (grey dotted lines). All hydrogen atoms except the amine H atoms have been omitted for clarity. Displacement ellipsoids are shown at the 50% probability level.

Table 2
Experimental details.

Crystal data	
Chemical formula	$[Zr(C_2H_7N)_2(C_2H_6N)_3]I$
M_r	440.52
Crystal system, space group	Orthorhombic, *Pbca*
Temperature (K)	100
a, *b*, *c* (Å)	14.2425 (3), 15.4113 (3), 16.8537 (3)
V (Å^3)	3699.31 (12)
Z	8
Radiation type	Mo $K\alpha$
μ (mm^{-1})	2.26
Crystal size (mm)	0.2 × 0.1 × 0.1
Data collection	
Diffractometer	Bruker APEXII CCD
Absorption correction	Numerical (*SADABS*; Bruker, 2014)
T_{min}, T_{max}	0.656, 0.745
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	29665, 3620, 3319
R_{int}	0.027
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.617
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.015, 0.036, 1.07
No. of reflections	3620
No. of parameters	154
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.33, −0.34

Computer programs: *APEX2* and *SAINT* (Bruker, 2013), *SHELXS* and *SHELXL* (Sheldrick, 2008), *OLEX2* (Dolomanov *et al.*, 2009), *Mercury* (Macrae *et al.*, 2006) and *publCIF* (Westrip, 2010).

crystallized in the form of needles, which were not suitable for single-crystal X-ray diffraction. However, a suitable tablet-shaped crystal of tris(dimethylamido)bis(dimethylammine)-zirconium(IV) iodide was selected, mounted, and analyzed.

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. H atoms bonded to C and N atoms were placed at geometrically calculated positions and refined using a riding model: C—H = 0.98, N—H = 1.00 Å; U_{iso}(H) = 1.5U_{eq}(C) or 1.2U_{eq}(N).

Acknowledgements

The authors gratefully acknowledge Mississippi State University for financial support.

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supporting information

Acta Cryst. (2016). E**72**, 73-75 [doi:10.1107/S2056989015023919]

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Computing details

Data collection: *APEX2* (Bruker, 2013); cell refinement: *SAINT* (Bruker, 2013); data reduction: *SAINT* (Bruker, 2013); program(s) used to solve structure: *SHELXS* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL* (Sheldrick, 2008); molecular graphics: *OLEX2* (Dolomanov *et al.*, 2009) and *Mercury* (Macrae *et al.*, 2006); software used to prepare material for publication: *publCIF* (Westrip, 2010).

Tris(dimethylamido-κN)bis(dimethylamine-κN)zirconium(IV) iodide

Crystal data

$[Zr(C_2H_6N)_3(C_2H_7N)_2]I$
$M_r = 440.52$
Orthorhombic, *Pbca*
$a = 14.2425$ (3) Å
$b = 15.4113$ (3) Å
$c = 16.8537$ (3) Å
$V = 3699.31$ (12) Å^3
$Z = 8$
$F(000) = 1760$
$D_x = 1.582$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 9970 reflections
$\theta = 2.3$–$26.0°$
$\mu = 2.26$ mm^{-1}
$T = 100$ K
Tablet, colourless
0.2 × 0.1 × 0.1 mm

Data collection

Bruker APEXII CCD diffractometer
φ and ω scans
Absorption correction: numerical (SADABS; Bruker, 2014)
$T_{min} = 0.656$, $T_{max} = 0.745$
29665 measured reflections
3620 independent reflections
3319 reflections with $I > 2\sigma(I)$
$R_{int} = 0.027$
$\theta_{max} = 26.0°$, $\theta_{min} = 2.3°$
$h = -17 \rightarrow 17$
$k = -18 \rightarrow 19$
$l = -18 \rightarrow 20$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.015$
$wR(F^2) = 0.036$
$S = 1.07$
3620 reflections
154 parameters
0 restraints
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0158P)^2 + 1.6295P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.002$
$\Delta\rho_{max} = 0.33$ e Å^{-3}
$\Delta\rho_{min} = -0.34$ e Å^{-3}

Special details

Experimental. wR2(int) was 0.0590 before and 0.0411 after absorption correction. The ratio of minimum to maximum transmission is 0.8806. The $\lambda/2$ correction factor is 0.00150.

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}
C1	0.42535 (13)	0.59533 (12)	0.45204 (11)	0.0250 (4)
H1A	0.4484	0.6453	0.4219	0.037*
H1B	0.4754	0.5737	0.4867	0.037*
H1C	0.4062	0.5494	0.4153	0.037*
C2	0.30833 (15)	0.54710 (12)	0.54677 (12)	0.0314 (5)
H2A	0.2545	0.5655	0.5788	0.047*
H2B	0.2888	0.5010	0.5103	0.047*
H2C	0.3580	0.5253	0.5817	0.047*
C3	0.39168 (13)	0.94138 (11)	0.64365 (11)	0.0208 (4)
H3A	0.3892	0.9531	0.5865	0.031*
H3B	0.3277	0.9361	0.6644	0.031*
H3C	0.4240	0.9892	0.6706	0.031*
C4	0.44722 (13)	0.84138 (11)	0.74390 (10)	0.0210 (4)
H4A	0.4814	0.7871	0.7531	0.031*
H4B	0.4796	0.8891	0.7709	0.031*
H4C	0.3833	0.8360	0.7648	0.031*
C5	0.23350 (14)	0.69989 (13)	0.70093 (11)	0.0279 (4)
H5A	0.2871	0.6622	0.7130	0.042*
H5B	0.2214	0.7383	0.7461	0.042*
H5C	0.1779	0.6642	0.6908	0.042*
C6	0.17635 (12)	0.80851 (13)	0.61133 (12)	0.0260 (4)
H6A	0.1921	0.8427	0.5642	0.039*
H6B	0.1204	0.7735	0.6006	0.039*
H6C	0.1639	0.8476	0.6560	0.039*
C7	0.57938 (12)	0.68391 (12)	0.60513 (11)	0.0222 (4)
H7A	0.5755	0.7251	0.5609	0.033*
H7B	0.6177	0.7089	0.6477	0.033*
H7C	0.6081	0.6298	0.5867	0.033*
C8	0.48782 (14)	0.60495 (12)	0.70102 (11)	0.0249 (4)
H8A	0.4239	0.5941	0.7200	0.037*
H8B	0.5160	0.5503	0.6832	0.037*
H8C	0.5256	0.6294	0.7442	0.037*
C9	0.33176 (13)	0.81902 (12)	0.42983 (11)	0.0235 (4)
H9A	0.2804	0.7826	0.4495	0.035*
H9B	0.3103	0.8793	0.4258	0.035*
H9C	0.3515	0.7984	0.3774	0.035*
C10	0.48868 (13)	0.86737 (11)	0.45761 (11)	0.0233 (4)

H10A	0.5408	0.8630	0.4954	0.035*
H10B	0.5094	0.8471	0.4054	0.035*
H10C	0.4683	0.9279	0.4537	0.035*
N1	0.34417 (10)	0.62186 (9)	0.50068 (8)	0.0166 (3)
H1	0.2932	0.6412	0.4639	0.020*
N2	0.44334 (10)	0.85934 (9)	0.65782 (8)	0.0153 (3)
H2	0.5094	0.8692	0.6399	0.018*
N3	0.25455 (10)	0.75170 (9)	0.63104 (8)	0.0180 (3)
N4	0.48491 (10)	0.66602 (9)	0.63514 (8)	0.0162 (3)
N5	0.41111 (10)	0.81422 (9)	0.48479 (8)	0.0159 (3)
Zr1	0.38438 (2)	0.74109 (2)	0.58304 (2)	0.01200 (5)
I1	0.68609 (2)	0.92790 (2)	0.65905 (2)	0.02035 (4)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0281 (10)	0.0224 (10)	0.0244 (10)	0.0032 (8)	−0.0005 (8)	−0.0092 (8)
C2	0.0509 (14)	0.0178 (9)	0.0256 (11)	−0.0139 (9)	−0.0001 (9)	0.0003 (8)
C3	0.0240 (10)	0.0157 (8)	0.0228 (10)	0.0010 (7)	−0.0006 (8)	−0.0027 (7)
C4	0.0258 (10)	0.0226 (9)	0.0146 (9)	−0.0021 (7)	−0.0008 (7)	−0.0024 (7)
C5	0.0300 (11)	0.0307 (10)	0.0231 (10)	−0.0020 (8)	0.0079 (8)	0.0020 (8)
C6	0.0211 (10)	0.0283 (10)	0.0287 (11)	−0.0001 (8)	−0.0007 (8)	−0.0021 (8)
C7	0.0212 (10)	0.0229 (9)	0.0224 (10)	0.0000 (7)	−0.0011 (8)	0.0017 (7)
C8	0.0322 (11)	0.0215 (9)	0.0211 (10)	0.0050 (8)	−0.0011 (8)	0.0070 (8)
C9	0.0279 (10)	0.0207 (9)	0.0220 (10)	0.0016 (8)	−0.0057 (8)	0.0043 (7)
C10	0.0255 (10)	0.0208 (9)	0.0236 (10)	−0.0017 (7)	0.0052 (8)	0.0063 (7)
N1	0.0209 (8)	0.0144 (7)	0.0145 (7)	−0.0017 (6)	−0.0003 (6)	−0.0003 (6)
N2	0.0166 (7)	0.0154 (7)	0.0138 (7)	−0.0006 (6)	0.0009 (6)	−0.0006 (5)
N3	0.0177 (8)	0.0205 (8)	0.0157 (7)	−0.0025 (6)	0.0025 (6)	−0.0022 (6)
N4	0.0202 (8)	0.0147 (7)	0.0136 (7)	0.0011 (6)	−0.0014 (6)	0.0021 (6)
N5	0.0195 (8)	0.0137 (7)	0.0145 (7)	−0.0018 (6)	−0.0005 (6)	0.0013 (5)
Zr1	0.01412 (9)	0.01104 (8)	0.01085 (9)	−0.00094 (6)	0.00062 (6)	0.00062 (6)
I1	0.01689 (7)	0.02028 (7)	0.02389 (8)	0.00079 (4)	0.00159 (4)	0.00231 (4)

Geometric parameters (Å, º)

C1—H1A	0.9800	C7—H7A	0.9800
C1—H1B	0.9800	C7—H7B	0.9800
C1—H1C	0.9800	C7—H7C	0.9800
C1—N1	1.475 (2)	C7—N4	1.464 (2)
C2—H2A	0.9800	C8—H8A	0.9800
C2—H2B	0.9800	C8—H8B	0.9800
C2—H2C	0.9800	C8—H8C	0.9800
C2—N1	1.480 (2)	C8—N4	1.456 (2)
C3—H3A	0.9800	C9—H9A	0.9800
C3—H3B	0.9800	C9—H9B	0.9800
C3—H3C	0.9800	C9—H9C	0.9800
C3—N2	1.482 (2)	C9—N5	1.463 (2)

C4—H4A	0.9800	C10—H10A	0.9800
C4—H4B	0.9800	C10—H10B	0.9800
C4—H4C	0.9800	C10—H10C	0.9800
C4—N2	1.478 (2)	C10—N5	1.450 (2)
C5—H5A	0.9800	N1—H1	1.0000
C5—H5B	0.9800	N1—Zr1	2.3730 (13)
C5—H5C	0.9800	N2—H2	1.0000
C5—N3	1.454 (2)	N2—Zr1	2.3695 (14)
C6—H6A	0.9800	N3—Zr1	2.0249 (14)
C6—H6B	0.9800	N4—Zr1	2.0393 (14)
C6—H6C	0.9800	N5—Zr1	2.0389 (14)
C6—N3	1.455 (2)		

H1A—C1—H1B	109.5	N4—C8—H8B	109.5
H1A—C1—H1C	109.5	N4—C8—H8C	109.5
H1B—C1—H1C	109.5	H9A—C9—H9B	109.5
N1—C1—H1A	109.5	H9A—C9—H9C	109.5
N1—C1—H1B	109.5	H9B—C9—H9C	109.5
N1—C1—H1C	109.5	N5—C9—H9A	109.5
H2A—C2—H2B	109.5	N5—C9—H9B	109.5
H2A—C2—H2C	109.5	N5—C9—H9C	109.5
H2B—C2—H2C	109.5	H10A—C10—H10B	109.5
N1—C2—H2A	109.5	H10A—C10—H10C	109.5
N1—C2—H2B	109.5	H10B—C10—H10C	109.5
N1—C2—H2C	109.5	N5—C10—H10A	109.5
H3A—C3—H3B	109.5	N5—C10—H10B	109.5
H3A—C3—H3C	109.5	N5—C10—H10C	109.5
H3B—C3—H3C	109.5	C1—N1—C2	110.24 (14)
N2—C3—H3A	109.5	C1—N1—H1	107.9
N2—C3—H3B	109.5	C1—N1—Zr1	110.52 (10)
N2—C3—H3C	109.5	C2—N1—H1	107.9
H4A—C4—H4B	109.5	C2—N1—Zr1	112.27 (11)
H4A—C4—H4C	109.5	Zr1—N1—H1	107.9
H4B—C4—H4C	109.5	C3—N2—H2	106.8
N2—C4—H4A	109.5	C3—N2—Zr1	113.23 (10)
N2—C4—H4B	109.5	C4—N2—C3	109.66 (13)
N2—C4—H4C	109.5	C4—N2—H2	106.8
H5A—C5—H5B	109.5	C4—N2—Zr1	113.04 (10)
H5A—C5—H5C	109.5	Zr1—N2—H2	106.8
H5B—C5—H5C	109.5	C5—N3—C6	110.95 (14)
N3—C5—H5A	109.5	C5—N3—Zr1	117.87 (12)
N3—C5—H5B	109.5	C6—N3—Zr1	131.02 (12)
N3—C5—H5C	109.5	C7—N4—Zr1	112.94 (10)
H6A—C6—H6B	109.5	C8—N4—C7	111.04 (14)
H6A—C6—H6C	109.5	C8—N4—Zr1	135.64 (12)
H6B—C6—H6C	109.5	C9—N5—Zr1	113.45 (11)
N3—C6—H6A	109.5	C10—N5—C9	111.11 (14)
N3—C6—H6B	109.5	C10—N5—Zr1	135.34 (11)

N3—C6—H6C	109.5	N2—Zr1—N1	172.83 (5)
H7A—C7—H7B	109.5	N3—Zr1—N1	94.35 (5)
H7A—C7—H7C	109.5	N3—Zr1—N2	92.81 (5)
H7B—C7—H7C	109.5	N3—Zr1—N4	120.99 (6)
N4—C7—H7A	109.5	N3—Zr1—N5	116.76 (6)
N4—C7—H7B	109.5	N4—Zr1—N1	88.97 (5)
N4—C7—H7C	109.5	N4—Zr1—N2	87.62 (5)
H8A—C8—H8B	109.5	N5—Zr1—N1	89.88 (5)
H8A—C8—H8C	109.5	N5—Zr1—N2	86.60 (5)
H8B—C8—H8C	109.5	N5—Zr1—N4	122.15 (6)
N4—C8—H8A	109.5		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···I1^{i}	1.00	2.78	3.5922 (14)	138
N2—H2···I1	1.00	2.69	3.6153 (15)	138

Symmetry code: (i) $x-1/2, -y+3/2, -z+1$.