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Coordination variety of phenyltetrazolato and dimethylamido ligands in dimeric Ti, Zr, and Ta complexes

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Three structurally diverse 5-phenyltetrazolato (Tz) Ti, Zr, and Ta complexes, namely, $(C_2H_8N)[Ti_2(C_7H_5N_4)_5(C_2H_6N)_4]\cdot 1.45C_6H_6$ or $(Me_2NH_2)[Ti_2(NMe_2)_4(2,3\text{-}\mu\text{-Tz})_3(2\text{-}\eta^1\text{-Tz})_2]\cdot 1.45C_6H_6$, (**1**·$1.45C_6H_6$), $[Zr_2(C_7H_5N_4)_6(C_2H_6N)_2(C_2H_7N)_2]\cdot 1.12C_6H_6\cdot 0.382CH_2Cl_2$ or $[Zr_2(Me_2NH)_2(NMe_2)_2(2,3\text{-}\mu\text{-Tz})_3(2\text{-}\eta^1\text{-Tz})_2(1,2\text{-}\eta^2\text{-Tz})]\cdot 1.12C_6H_6\cdot 0.38CH_2Cl_2$ (**2**·$1.12C_6H_6\cdot 0.38CH_2Cl_2$), and $(C_2H_8N)_2[Ta_2(C_7H_5N_4)_8(C_2H_6N)_2O]\cdot 0.25C_7H_8$ or $(Me_2NH_2)_2[Ta_2(NMe_2)_2(2,3\text{-}\mu\text{-Tz})_2(2\text{-}\eta^1\text{-Tz})_6O]\cdot 0.25C_7H_8$ (**3**·$0.25C_7H_8$), where TzH is 5-phenyl-1*H*-tetrazole, have been synthesized and structurally characterized. All three complexes are dinuclear; the Ti center in **1** is six-coordinate, whereas the Zr and Ta atoms in **2** and **3** are seven-coordinate. The coordination environments of the Ti centers in **1** are similar, and so are the ligations of the Ta centers in **3**. In contrast, the two Zr centers in **2** bear a different number of ligands, one of which is a bidentate η^2-5-phenyltetrazolato ligand that has not been observed previously for *d*-block elements. The dimethylamido ligand, present in the starting materials, remained unchanged, or was converted to dimethylamine and dimethylammonium during the synthesis. Dimethylamine coordinates as a neutral ligand, whereas dimethylammonium is retained as a hydrogen-bonded entity bridging Tz ligands.

1. Introduction

Since the discovery of a facile synthesis of stable complexes of *d*-block elements with η^2-coordinated pyrazoles (Guzei *et al.*, 1997), we have been interested in the preparation of transition-metal complexes with similarly coordinated 5-substituted tetrazoles. Tetrazolato (tz) ligands, with their four N-atom lone pairs, display a wide variety of coordination modes (Massi *et al.*, 2018; Aromí *et al.*, 2011) from monodentate to polydentate, engaging multiple metal centers in coordination clusters or polymers. We were interested in isolating discrete complexes of Ti, Zr, and Ta with a tz ligand that would display either 1,2-η^2 or 2,3-η^2 coordination, because such coordination by nonbridging tz ligands has not been reported for the *d*-block elements. The 1,2-η^2 coordination by a nonbridging tz ligand has been reported for Ba (Kobrsi *et al.*, 2005), Cs (Hernández-Arganis *et al.*, 2018), K (Kobrsi *et al.*, 2006; Zheng *et al.*, 2003; Hu *et al.*, 2005), Sm (Evans *et al.*, 1988), and actinides U and Th (Browne *et al.*, 2016), whereas the 2,3-η^2 coordination by a nonbridging tz ligand has only been reported for Ba (Kobrsi *et al.*, 2005).

The multidentate nature of the 5-phenyltetrazolato (Tz) ligand selected for these studies promotes dimerization; thus, all three complexes reported herein are dimeric, and only the Zr complex contains a desired 1,2-η^2 coordination (Fig. 1). To the best of our knowledge, this is the first structural report of a *d*-block element with a 1,2-η^2 coordination of a nonbridging tz

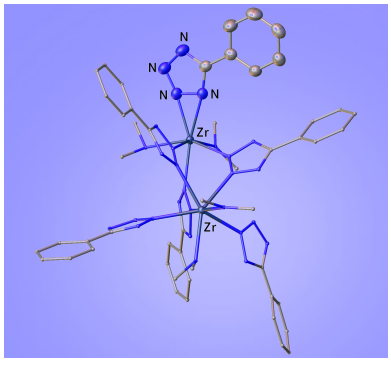


Table 1
Experimental details.

Experiments were carried out with Mo $K\alpha$ radiation using a Bruker SMART APEX CCD area-detector diffractometer. Absorption was corrected for by multi-scan methods (*SADABS*; Krause *et al.*, 2015).

	1	**2**	**3**
Crystal data			
Chemical formula	$(C_2H_8N)[Ti_2(C_7H_5N_4)_5(C_2H_6N)_4]\cdot 1.45C_6H_6$	$[Zr_2(C_7H_5N_4)_6(C_2H_6N)_2(C_2H_7N)_2]\cdot 1.118C_6H_6\cdot 0.382CH_2Cl_2$	$(C_2H_8N)_2[Ta_2(C_7H_5N_4)_8(C_2H_6N)_2O]\cdot 0.25C_7H_8$
M_r	1043.95	1351.41	1742.47
Crystal system, space group	Monoclinic, $P2_1/c$	Triclinic, $P\overline{1}$	Monoclinic, $P2_1/n$
Temperature (K)	100	100	105
a, b, c (Å)	11.6292 (9), 22.6611 (17), 22.3631 (17)	13.9631 (5), 16.7619 (6), 27.3054 (9)	22.5131 (8), 25.5101 (9), 26.7165 (9)
α, β, γ (°)	90, 93.857 (1), 90	86.902 (1), 81.154 (1), 89.969 (1)	90, 101.3830 (4), 90
V (Å^3)	5880.0 (8)	6305.3 (4)	15041.8 (9)
Z	4	4	8
μ (mm^{-1})	0.32	0.43	2.98
Crystal size (mm)	0.4 × 0.3 × 0.2	0.4 × 0.3 × 0.2	0.39 × 0.32 × 0.24
Data collection			
T_{min}, T_{max}	0.576, 0.745	0.578, 0.745	0.4, 0.5
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	46383, 11558, 8907	70012, 25682, 20488	173076, 29545, 25534
R_{int}	0.042	0.040	0.030
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.617	0.626	0.617
Refinement			
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.050, 0.142, 1.09	0.039, 0.103, 1.01	0.027, 0.068, 1.09
No. of reflections	11558	25682	29545
No. of parameters	826	1671	1915
No. of restraints	898	67	79
H-atom treatment	H-atom parameters constrained	H atoms treated by a mixture of independent and constrained refinement	H-atom parameters constrained
$\Delta\rho_{max}, \Delta\rho_{min}$ (e Å^{-3})	0.53, −0.42	0.78, −0.98	2.48, −1.24

Computer programs: *APEX3* (Bruker, 2018), *SAINT* (Bruker, 2018), *SHELXS* (Sheldrick, 2008), *olex2.solve* (Bourhis *et al.*, 2015), *SHELXT* (Sheldrick, 2015*a*), *SHELXL2018* (Sheldrick, 2015*b*), *SHELXL* (Sheldrick, 2008), and *OLEX2* (Dolomanov *et al.*, 2009).

ligand. In all three complexes, Tz moieties are involved in hydrogen-bonding interactions. Interestingly, the fate of the dimethylamido ligands present in the starting materials $Ti(NMe_2)_4$, $Zr(NMe_2)_4$, and $Ta(NMe_2)_5$ is different in the three synthetic reactions, as they are either retained or converted to either dimethylamine or dimethylammonium. In the cases of Ti and Ta, the final products contain amido ligands and dimethylammonium cations; in the Zr case, some groups remain amido, whereas some become coordinated dimethylamines. The dimethylamine is coordinated as a neutral ligand and dimethylammonium is retained as a hydrogen-bonded entity bridging Tz ligands. Numerous metal complexes with $[Me_2NH_x]^n$, where x = 0, 1, or 2, and n = −1, 0, or +1, respectively, have been reported in the Cambridge Structural Database (CSD; Groom *et al.*, 2016).

Herein we report three related, but diverse, crystal structures of dinuclear complexes, namely, dimethylammonium tris(μ-5-phenyltetrazolato-κ^2N^2:N^3)bis[bis(dimethylamido)(5-phenyltetrazolato-κN^2)titanium(IV)] benzene 1.45-solvate, $(Me_2NH_2)[Ti_2(NMe_2)_4(2,3\text{-}\mu\text{-Tz})_3(2\text{-}\eta^1\text{-Tz})_2]\cdot 1.45C_6H_6$, (**1**·1.45-$C_6H_6$), bis(dimethylamido)-1$\kappa N$,2$\kappa N$-bis(dimethylamine)-1$\kappa N$,-2$\kappa N$-tris($\mu$-5-phenyltetrazolato-1:2$\kappa^2N^2$:$N^3$)tris(5-phenyltetrazolato)-1κ^2N^2;2κ^2N^2,N^3-dizirconium(IV)]–benzene–dichloromethane (1/1.12/0.38), $[Zr_2(Me_2NH)_2(NMe_2)_2(2,3\text{-}\mu\text{-Tz})_3(2\text{-}\eta^1\text{-Tz})_2(1,2\text{-}\eta^2\text{-Tz})]\cdot 1.12C_6H_6\cdot 0.38CH_2Cl_2$ (**2**·1.12C_6H_6·0.38CH_2-Cl_2), and bis(dimethylammonium) μ-oxido-bis(μ-5-phenyltetrazolato-κ^2N^2:N^3)bis[(dimethylamido)tris(5-phenyltetrazolato-κN^2)-tantalum(V)] toluene 0.25-solvate, $(Me_2NH_2)_2[Ta_2(NMe_2)_2(2,3\text{-}\mu\text{-Tz})_2(2\text{-}\eta^1\text{-Tz})_6O]\cdot 0.25C_7H_8$ (**3**·0.25C_7H_8). The Zr and Ta complexes crystallize with two symmetry-independent molecules in the asymmetric unit; the second symmetry-independent molecules are labelled in a similar fashion with '*A*' as the label suffix.

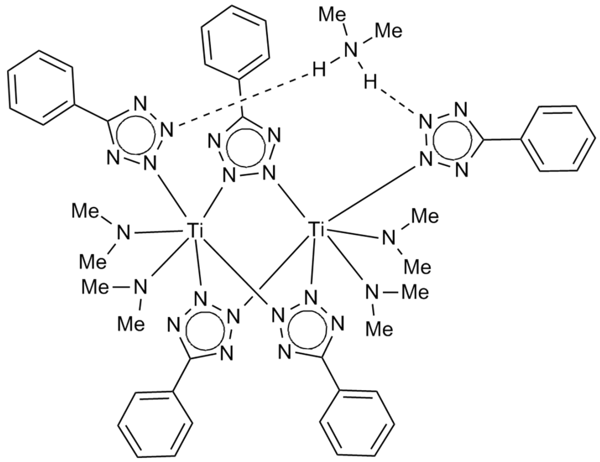
2. Experimental

2.1. Synthesis and crystallization

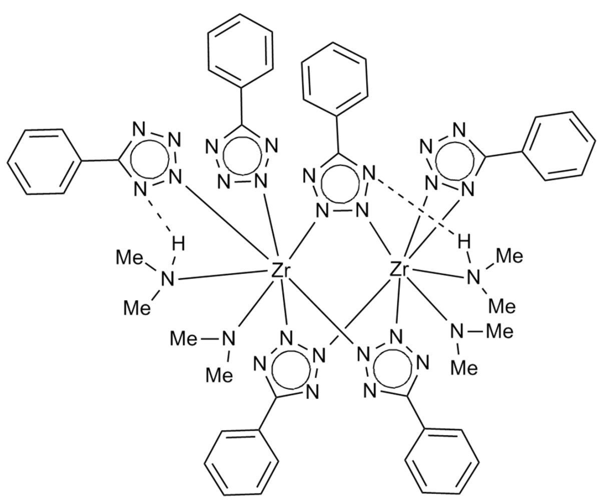
Complex **1** was prepared and crystallized according to a published procedure (Guzei, 1997). Complexes **2** and **3** were prepared in a similar manner and crystallized from CH_2Cl_2/benzene and toluene, respectively. Adventitious oxygen became incorporated in Ta complex **3**; no further attempts were made to repeat its synthesis.

2.2. Refinement

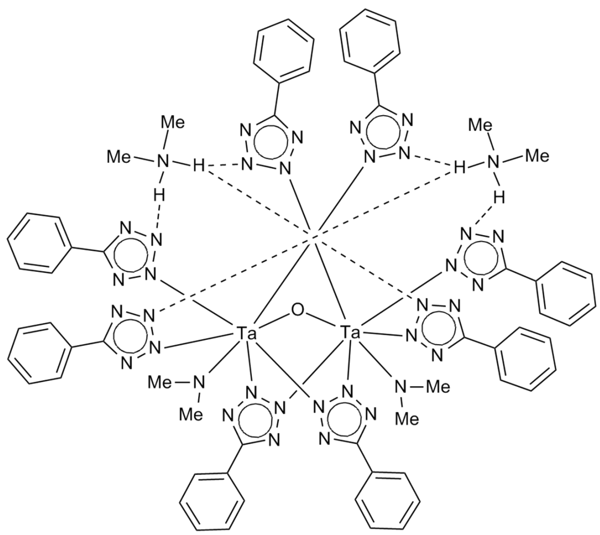
Crystal data, data collection and structure refinement details are summarized in Table 1. The diffraction data collections were performed by standard techniques on Bruker area-detector single-crystal diffractometers at 100 K with



$\mathbf{1}\cdot1.45C_6H_6$
(*a*)



$\mathbf{2}\cdot1.12(C_6H_6)\cdot0.38(CH_2Cl_2)$
(*b*)



$\mathbf{3}\cdot0.25C_7H_8$
(*c*)

Figure 1
The Ti, Zr, and Ta complexes (*a*) **1**, (*b*) **2**, and (*c*) **3**, shown with their formulae.

APEX3 (Bruker, 2018), the data were scaled with *SADABS* (Krause *et al.*, 2015), and the structures solved with *SHELXS* and *SHELXT* (Sheldrick, 2015*a*), and refined with *SHELXL* (Sheldrick, 2015*b*) and *OLEX2* (Dolomanov *et al.*, 2009).

Compound $\mathbf{1}\cdot1.45C_6H_6$ crystallizes with a monoanionic dinuclear titanium complex, a dimethylammonium cation, and ~1.45 molecules of benzene solvent in the asymmetric unit. The phenyl (Ph) rings at C12 and C26 are disordered over two positions, with major component contributions of 60.6 (13) and 77 (3)%, respectively. The Ph ring at C19 is disordered over three positions in a 43.4 (3):35.6 (3):21.0 (3) ratio. The disordered rings were refined with an idealized geometry and atomic displacement parameter restraints. The dimethylammonium cation is disordered over two positions, with the major component present 54.3 (15)% of the time. The fully occupied solvent molecule appeared to be benzene disordered over several positions. The other solvent molecule was disordered over a crystallographic inversion center. A significant amount of time was invested in identifying and refining the disordered molecules. Bond-length restraints were applied to model the molecules but the resulting isotropic displacement coefficients suggested the molecules were mobile. In addition, the refinement was computationally unstable. The SQUEEZE option (Spek, 2015) of *PLATON* (Spek, 2020) was used to correct the diffraction data for diffuse scattering effects and to identify the solvate molecule. *PLATON* calculated the upper limit of volume that can be occupied by the solvent to be 910 Å^3, or 15.5% of the unit-cell volume. The program calculated 246 electrons in the unit cell for the diffuse species. This approximately corresponds to one molecule of benzene (42 e^-) and 0.45 molecules of either benzene or CH_2Cl_2 (19 e^-) in the asymmetric unit. All derived results in the tables are based on the known contents. No data are given for the diffusely scattering species. This complex proved to be challenging to characterize and several data sets were collected on crystals isolated from several different syntheses.

Compound **2** crystallizes with two symmetry-independent dinuclear complexes in the asymmetric unit and several molecules of crystallization solvents. The solvent molecules occupy three different sites: (i) one fully occupied molecule of benzene; (ii) a site shared by benzene and CH_2Cl_2 in a 64.3 (2):35.7 (2) ratio; (iii) a site shared by CH_2Cl_2/benzene-(orientation #1)/benzene(orientation #2) in a 40.6 (2):35.7 (2): 23.7 (2) ratio. The asymmetric unit content is $\mathbf{2}_2$.(benzene)$_{2.24}$-$(CH_2Cl_2)_{0.76}$. The disordered benzene molecules were refined with idealized geometries and atomic displacement parameter restraints. Atoms C19*S*–C24*S* of the 23.7%-occupied benzene molecule were refined with identical isotropic atomic displacement parameters. The 40.6%-occupied dichloromethane molecule was refined with geometrical restraints.

Compound **3** crystallizes with two symmetry-independent molecules of the dinuclear dianioninc Ta complex, four dimethylammonium cations, and half a molecule of toluene solvent in the asymmetric unit. The toluene molecule is disordered over a crystallographic inversion center and was refined with an idealized geometry (Guzei, 2014). The Ph ring at atom C52 is disordered over two positions, with the major

Table 2
Ligand composition of complexes **1**–**3**.

	Compound			
	1	**2**		**3**
Charge	−1	0	0	−2
Ligand	Metal center			
	Ti	Zr1	Zr2	Ta
NMe_2	2	1	1	1
$HNMe_2$	0	1	1	0
μ-Tz	3	3	3	2
η^1-Tz terminal	1	2	0	3
η^2-Tz terminal	0	0	1	0
μ-oxo	0	0	0	1
Number of hydrogen-bonded $Me_2NH_2^+$	1	0	0	2

component occupied 52 (2)% of the time. The disordered Ph rings were refined with an idealized geometry and atomic displacement parameter restraints.

3. Results and discussion

The three complexes reported herein exemplify the remarkable structural diversity of dinuclear complexes of metals from periods IV, V, and VI with Tz and dimethylamido ligands (Table 2). These complexes possess different charges: the titanium complex is anionic, the tantalum complex dianionic, and the zirconium complex neutral. The charges are balanced by an appropriate number of dimethylammonium cations that form N—H···N interactions with Tz ligands residing on different metal atoms. All metal centers bear dimethylamido ligands, but in addition the Zr centers bind to a neutral dimethylamine. Each metal is also ligated by two or three bridging μ-η^1(N2):η^1(N3) Tz ligands. The Ti, Zr, and Ta centers are further coordinated to terminal η^1(N2) Tz ligands; interestingly, the titanium centers bear one such ligand,

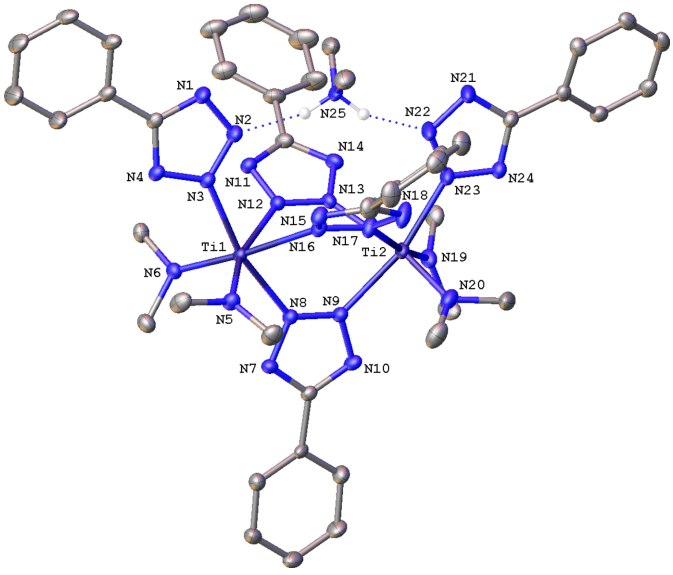


Figure 2
A molecular drawing of **1**, shown with 30% probability displacement ellipsoids. Minor disorder components and H atoms not participating in hydrogen bonds have been omitted.

Table 3
Selected bond lengths (Å) for **1**.

Ti1—N3	2.1534 (19)	Ti2—N9	2.1970 (19)
Ti1—N5	1.892 (2)	Ti2—N13	2.2404 (19)
Ti1—N6	1.893 (2)	Ti2—N17	2.266 (2)
Ti1—N8	2.1967 (18)	Ti2—N19	1.901 (2)
Ti1—N12	2.2592 (19)	Ti2—N20	1.890 (2)
Ti1—N16	2.294 (2)	Ti2—N23	2.151 (2)

zirconium zero or two, and tantalum three. Strikingly, one Zr center does not bear terminal Tz ligands and instead features an η^2(N1,N2) Tz moiety. The tantalum complex also contains a μ-oxo bridge, apparently due to a serendipitous incorporation of adventitious oxygen into the reaction mixture.

In the monoanionic dinuclear complex **1**, the two six-coordinate Ti centers are separated by 4.2668 (6) Å (Fig. 2). Each Ti atom is ligated by two NMe_2 ligands, three μ-η^1(N2):η^1(N3) Tz ligands, and one terminal η^1(N2) Tz moiety. The charge is balanced by a dimethylammonium cation that forms a hydrogen bond to each terminal Tz ligand. The four Ti—NMe_2 distances (Table 3) average 1.894 (5) Å and are in excellent agreement with the literature value of 1.91 (2) Å obtained by averaging 84 Ti—NMe_2 bonds observed in 44 complexes reported in the CSD. The Ti—N(terminal Tz) bond lengths in **1** are very similar and expectedly longer at an average of 2.152 (2) Å. There is only one Ti complex with a monodentate η^1(N2)-Tz ligand reported to the CSD, *i.e.* tris(3,5-di-*tert*-butylpyrazolato)(5-phenyltetrazolato)titanium(IV) (Yélamos

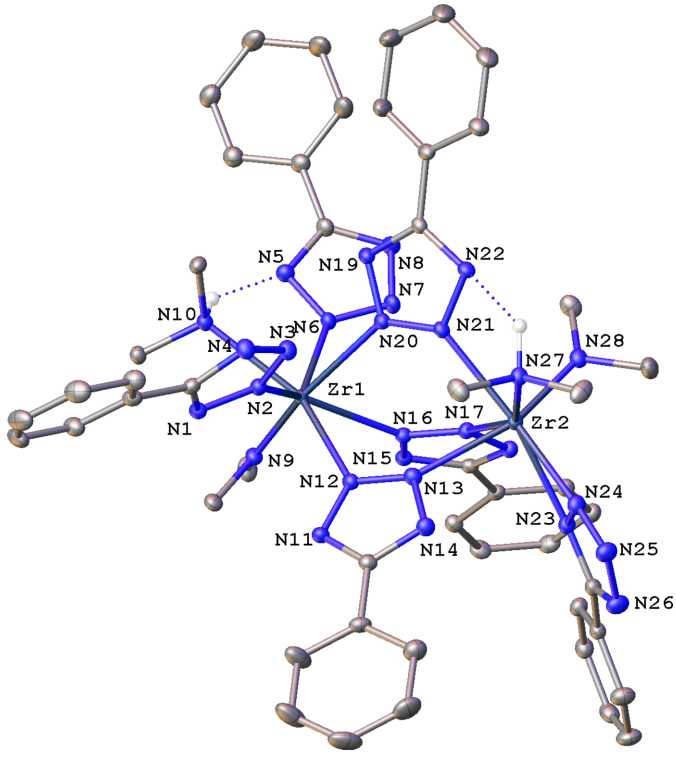


Figure 3
A molecular drawing of **2a**, shown with 30% probability displacement ellipsoids. All H atoms not participating in hydrogen bonds have been omitted.

Table 4
Hydrogen-bond geometry (Å, °) for **1**.

D—H···A	D—H	H···A	D···A	D—H···A
N25—H25C···N22	0.91	1.89	2.742 (7)	156
N25—H25D···N2	0.91	1.97	2.864 (8)	169
N25A—H25E···N22	0.91	2.00	2.847 (8)	154
N25A—H25F···N2	0.91	1.82	2.690 (8)	160

et al., 2001), and one with a neutral η^1(N2)-TzH ligand, $[TiCl_4(PhCN_4H)_2]$ (Hill *et al.*, 2004). The Ti—N(Tz) and Ti—N(TzH) distances in these were determined to be 2.104 Å (low precision room-temperature data set), with an average of 2.272 (7) Å. Predictably, the Ti—N(bridging Tz) bonds in **1** are even longer, and fall into two groups because the composition of the outer coordination sphere differs among the three bridging Tz ligands. Complex **1** may be described as pseudo-C_{2v}-symmetrical, with one mirror plane roughly containing both terminal and one bridging Tz ligands. The Ti—N bond distances to the bridging N8-tetrazolato ligand in the mirror plane are shorter [average 2.1970 (19) Å] than the other four Ti—N bridging distances [average 2.26 (2) Å], and the difference is statistically significant. This disparity can be explained by the relative location of these ligands. Atoms N8 and N9 of the bridging ligand in the mirror plane are *trans* to tz rings, whereas the ligated N atoms in the other bridging ligands are *trans* to π-electron-donating NMe_2 units. The charge-assisted hydrogen bonds between the $[H_2NMe_2]^+$ cation and the Tz ligands are asymmetrical, with D···A and D—H···A parameters of 2.690 (8)/160 and 2.847 (8) Å/154° for one position of the disordered cation, and 2.742 (7)/156 and 2.864 (8) Å/169° for the other (Table 4).

The dinuclear Zr complex **2** (Fig. 3) crystallizes with two symmetry-independent complexes designated hereafter **2a**, with atoms Zr1 and Zr2, and **2b**, with atoms Zr1A and Zr2A in the asymmetric unit. Complexes **2a** and **2b** are the only neutral ones in this series. They possess identical compositions, but a superposition of the two molecules clearly illustrates their conformational differences (Fig. 4). In the following discussion we will focus on Zr1 complex **2a** and provide data for **2b** as necessary. The two Zr atoms in **2a** are seven-coordinate, but have different coordination environments: Zr1 is ligated by a NMe_2, $HNMe_2$, three bridging μ-η^1(N2):η^1(N3) Tz ligands, and two terminal η^1(N2) Tz ligands; Zr2 is ligated similarly, except that the two terminal Tz ligands are replaced by one bidentate η^2(N1,N2) Tz fragment. The Zr···Zr separations in **2a** and **2b** are 4.5230 (3) and 4.5492 (3) Å, respectively, the latter being ∼0.27 Å longer than the Ti···Ti distance in **1**.

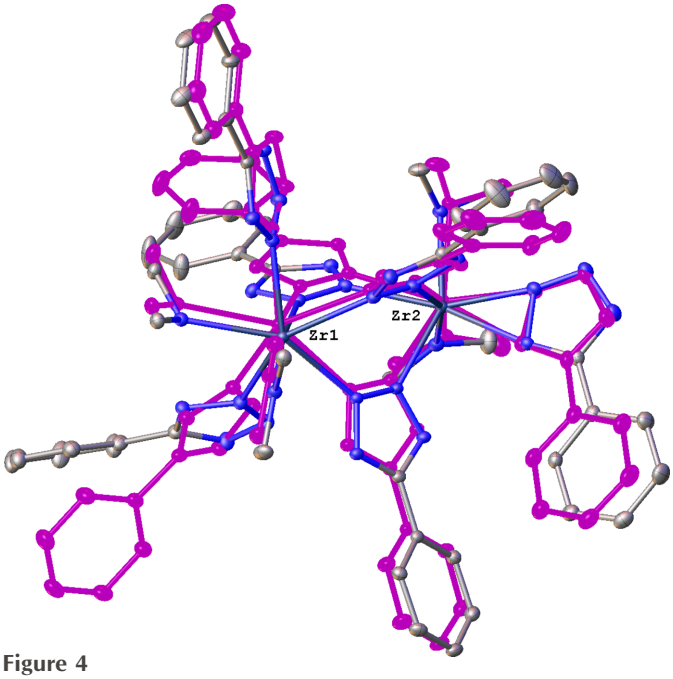


Figure 4
Superposition of **2a** and **2b**. All H atoms have been omitted. Complex **2b** is shown in monochrome.

The η^2(N1,N2) ligation mode of a nonbridging tz ring in Zr complex **2** is particularly exciting because it is the first structural report of a *d*-block element with this coordination mode. Based on a CSD search, such a coordination has been reported only for metals with atomic radii ≥ 1.75 Å (Slater, 1964), *i.e.* Ba with 5-(dimethylamino)tz (Kobrsi *et al.*, 2005), Cs with (1-phenyl-5-thione)tz (Hernández-Arganis *et al.*, 2018), K with 5-(pyrrolidin-1-yl)tz, 5-^{t}Butz (Kobrsi *et al.*, 2006), Tz (Zheng *et al.*, 2003), and losartanide (Hu *et al.*, 2005), Sm with 1,5-pentamethylene-tetrazole (Evans *et al.*, 1988), and actinides U and Th with 5-Metz (Browne *et al.*, 2016). A bridging μ-η^1(N3):η^2(N1,N2) tz ring has been observed in dimeric complexes of Dy, Gd, Ho, Y, and Yb, and polydentate η^2(N1, N2) tetrazolato ligands have been reported for the alkali metals Na, K, Cs, and Rb. The only example with an η^2(N2,N3) tz ligand has been reported for another large-atomic-radius-atom Ba (Kobrsi *et al.*, 2005). The atomic radius of Zr (1.55 Å) is noticeably smaller than the atomic radii of the elements listed above, but larger than those of Ti (1.40 Å) or Ta (1.45 Å), thus a large soft metal center is not a prerequisite for the formation of an η^2-tetrazolato complex.

In order to better understand the bidentate coordination mode of the tetrazolato ligand, a series of density functional theory (DFT) minimizations were performed on a model complex $Zr(Tz)Cl_3$ at the B3LYP/SDD level of theory. In these complexes, with largely ionic metal–ligand bonding, the complex with the 2,3-η^2 ligand is 0.34 kcal mol^{-1} more stable than the 1,2-η^2 analogue. Similar results were reported for model complexes trichloro[(1,2-η)-5-methyltetrazolato]titanium(IV) and trichloro[(2,3-η)-5-methyltetrazolato]titanium(IV), with the latter being more stable by less than 0.8 kcal mol^{-1} (Yélamos *et al.*, 2001). This is in slight contrast to the expectation based on the natural atomic charges computed for a free Tz^- anion: this analysis indicated that the N atoms in the 1- and 4-positions are more nucleophilic (by −0.21) than the 2- and 3-position N atoms, which means that a pair of adjacent atoms 1 and 2 (or 3 and 4) carries a larger combined negative charge than a combination of atoms 2 and 3, and that should favour the 1,2-η^2 binding mode.

Steric considerations may play a decisive role when several ligand arrangements are similar in energy. The different coordination environments of the metal centers in **2** deserve a special scrutiny with the use of *G*-parameters that are based

Table 5
Selected bond lengths (Å) for **2**.

Zr1—N2	2.2935 (18)	Zr1*A*—N2*A*	2.2856 (19)
Zr1—N6	2.3340 (19)	Zr1*A*—N6*A*	2.3073 (19)
Zr1—N9	1.9798 (19)	Zr1*A*—N9*A*	1.987 (2)
Zr1—N10	2.4073 (19)	Zr1*A*—N10*A*	2.4095 (19)
Zr1—N12	2.3829 (18)	Zr1*A*—N12*A*	2.3907 (18)
Zr1—N16	2.3741 (18)	Zr1*A*—N16*A*	2.3651 (19)
Zr1—N20	2.3699 (19)	Zr1*A*—N20*A*	2.3822 (19)
Zr2—N13	2.3115 (19)	Zr2*A*—N13*A*	2.2969 (18)
Zr2—N17	2.3085 (17)	Zr2*A*—N17*A*	2.336 (2)
Zr2—N21	2.3227 (18)	Zr2*A*—N21*A*	2.3166 (19)
Zr2—N23	2.3027 (19)	Zr2*A*—N23*A*	2.290 (2)
Zr2—N24	2.2238 (19)	Zr2*A*—N24*A*	2.214 (2)
Zr2—N27	2.3218 (19)	Zr2*A*—N27*A*	2.3145 (19)
Zr2—N28	1.975 (2)	Zr2*A*—N28*A*	1.989 (2)

on ligand solid angles (Guzei & Wendt, 2006). The *G*-parameter describes ligand steric effects and represents the percentage of the metal coordination sphere shielded by a given ligand. In the model complex Zr(1,2-η^2-Tz)Cl_3 (Fig. 5), the bidentate ligand shields the metal to the extent of 21.0 (2)%, and in Zr(2,3-η^2-Tz)Cl_3, the corresponding parameter is 20.2 (2)%. The small difference between these values is not as counterintuitive as it may seem based on the position of the Ph ring, because the metal centers are primarily shielded by the ligated N atoms. The coordination environment of the metals in these model complexes is not crowded because the four ligands shield no more than 62% of the metal; thus, sterics is unlikely to explain the computational results. Either bidentate coordination mode of Tz is viable for zirconium and the rationale for the observed 1,2-η^2 coordination may be found in the crystal packing forces.

Steric considerations become more complicated for experimentally observed geometries because the *G*-parameters may change depending on ligand conformations and orientations relative to the metal center. *G*-Parameters become smaller with increasing metal–ligand distances. Overall, atom Zr1 is shielded by seven ligands to an extent of 85% and atom Zr2 is shielded similarly up to 84% by six ligands. The *G*-parameters for the two terminal η^1-Tz ligands on atom Zr1 add up to 22%, whereas the sole η^2-Tz ligand on Zr2 shields 18% of the zirconium coordination sphere.

We note that the bond distances between the three bridging Tz ligands and Zr1 are slightly longer than those to Zr2; these ligands approach Zr2 closer and shield it by an additional 1% each. Consequently, the overall difference in the Zr1 and Zr2 *G*-parameters is only 1% (85 *versus* 84%).

Whereas the Zr—NMe_2 distances to each metal center are similar (Table 5), the Zr—$NHMe_2$ bond lengths are statistically significantly different. This distance to the seven-ligand-bearing Zr1 center is longer at 2.4073 (19) Å than to the six-ligand-ligated Zr2 atom at 2.3218 (19) Å. Both distances fall in the 2.308–2.574 Å range observed for Zr—$NHMe_2$ distances computed for 50 such bonds in 37 complexes reported to the CSD. The $HNMe_2$ ligands occupy different positions in the coordination spheres of each metal, as can be readily illustrated by the Zr···Zr—$NHMe_2$ angles. The Zr1···Zr2—$NHMe_2$ and Zr2···Zr1—$NHMe_2$ angles span the range 107.65 (5)–145.45 (5)°. The dimethylamine ligands participate

Table 6
Hydrogen-bond geometry (Å, °) for **2**.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N10—H10···N5	0.85 (2)	1.96 (2)	2.732 (3)	151 (2)
N27—H27···N22	0.84 (2)	2.35 (2)	2.965 (3)	130 (2)
N10*A*—H10*B*···N5*A*	0.85 (2)	2.16 (2)	2.902 (3)	145 (2)
N27*A*—H27*A*···N22*A*	0.85 (2)	2.33 (2)	2.940 (3)	129 (2)

in intramolecular hydrogen-bonding interactions (Table 6). The $HNMe_2$ ligand on the seven-ligand-bearing Zr1 center forms an N—H···N hydrogen bond to a terminal Tz ligand, whereas the $HNMe_2$ ligand on the six-ligand-ligated Zr2 atom forms a hydrogen bond to a bridging tz ring.

The Zr—N(bridging) distances to Zr1 and Zr2 are dissimilar, and the difference is statistically significant. These bond distances to the seven-ligand-bearing Zr1 center [average 2.376 (7) Å] are longer than the respective bonds to Zr2 [average 2.314 (7) Å], a behaviour also observed for the dimethylamine ligands. Bond distances are expected to be longer for metals with higher coordination numbers, but, in this case, the formal coordination number is the same and the two metals differ only in the number of ligands.

The Zr1—N(terminal Tz) distances are expectedly longer than Zr2—N(bidentate Tz). The coordination mode of the η^2(N1,N2)Tz may be described as 'slipped', with the Zr2—N23 distance to the N atom closest to the Ph ring being noticeably longer [2.3027 (19) Å] than the Zr2—N24 bond to the N atom in the second ring position [2.2238 (19) Å]. The difference can be rationalized in terms of the steric requirement of the Ph ring that does not allow a closer approach of N23 to Zr2.

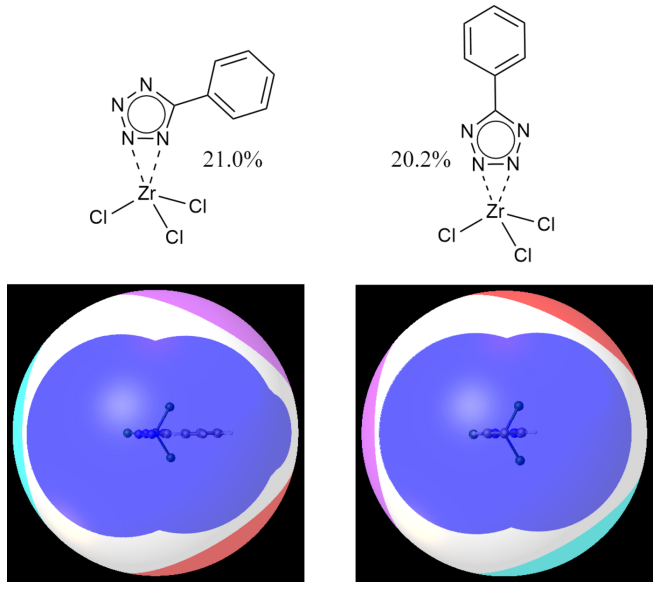


Figure 5
Model zirconium(IV) complexes used to evaluate the stability of the two coordination modes of the Tz ligand. The numbers are the *G*-parameters for the Tz ligands. The bottom figures illustrate how the bidentate ligands shield the metal – the colored portions of the sphere are ligands' 'shadows' on a 12 Å sphere they would cast if the metal were replaced with a light source. The view is from the position of the Tz ligand down toward the metal. The shadow is blue for the Tz ligand, and red, fuchsia, and turquoise for the Cl atoms.

The structure of **3**·0.5C_7H_8 appears to be the first example of a structurally characterized Ta complex bearing a tz ligand. In the structure, there are two symmetry-independent dinuclear Ta complexes (**3a** and **3b**), with an identical composition and very similar geometries about the metal centers (Fig. 6). The complexes differ mainly in the positions and conformations of the Tz ligands (Fig. 7). Each Ta center is seven-coordinated, with the coordination sphere comprised of an NMe_2 ligand, two bridging and three η^2(N2)-terminal Tz ligands, and a bridging oxo ligand (Table 7). The two bridging Tz ligand rings connect the Ta centers in the same μ-η^1(N2):η^1(N3) arrangement observed for corresponding ligands in **1** and **2**. The Ta···Ta separation averages 3.645 (2) Å for the two complexes, and is the shortest metal–metal distance in this series by a large margin, undoubtedly due to the presence of the oxo bridge. The metal–ligand bond distances fall into three well-separated ranges: the Ta—NMe_2 and Ta—O bond lengths are similar at ∼1.93 Å, the Ta—N(terminal Tz) are longer at ∼2.21 Å, and Ta—N(bridging Tz) are the longest at ∼2.27 Å. The complex exhibits a very approximate C_{2v} symmetry, with atoms Ta1, O1, and Ta2 defining one of the mirror planes. The dihedral angles between the tz-ring planes of the bridging ligands are 78.53 (10) and 75.43 (10)° in **3a** and **3b**, respectively, which is substantially smaller than the ideal 120° angle that could be expected between three bridging ligands.

Two dimethylammonium cations complete the second coordination sphere of each complex in a notable fashion by

Table 7
Selected bond lengths (Å) for **3**.

Ta1—O1	1.938 (2)	Ta1*A*—O1*A*	1.932 (2)
Ta1—N2	2.204 (3)	Ta1*A*—N2*A*	2.204 (3)
Ta1—N6	2.202 (3)	Ta1*A*—N6*A*	2.210 (3)
Ta1—N10	2.213 (3)	Ta1*A*—N10*A*	2.211 (3)
Ta1—N13	1.924 (3)	Ta1*A*—N13*A*	1.929 (3)
Ta1—N15	2.265 (3)	Ta1*A*—N19*A*	2.280 (3)
Ta1—N19	2.283 (3)	Ta1*A*—N15*A*	2.249 (3)
Ta2—O1	1.921 (2)	Ta2*A*—O1*A*	1.932 (2)
Ta2—N16	2.280 (3)	Ta2*A*—N20*A*	2.269 (3)
Ta2—N20	2.281 (3)	Ta2*A*—N16*A*	2.273 (3)
Ta2—N23	2.204 (3)	Ta2*A*—N23*A*	2.217 (3)
Ta2—N27	2.218 (3)	Ta2*A*—N27*A*	2.215 (3)
Ta2—N31	2.194 (3)	Ta2*A*—N31*A*	2.211 (3)
Ta2—N34	1.928 (3)	Ta2*A*—N34*A*	1.928 (3)

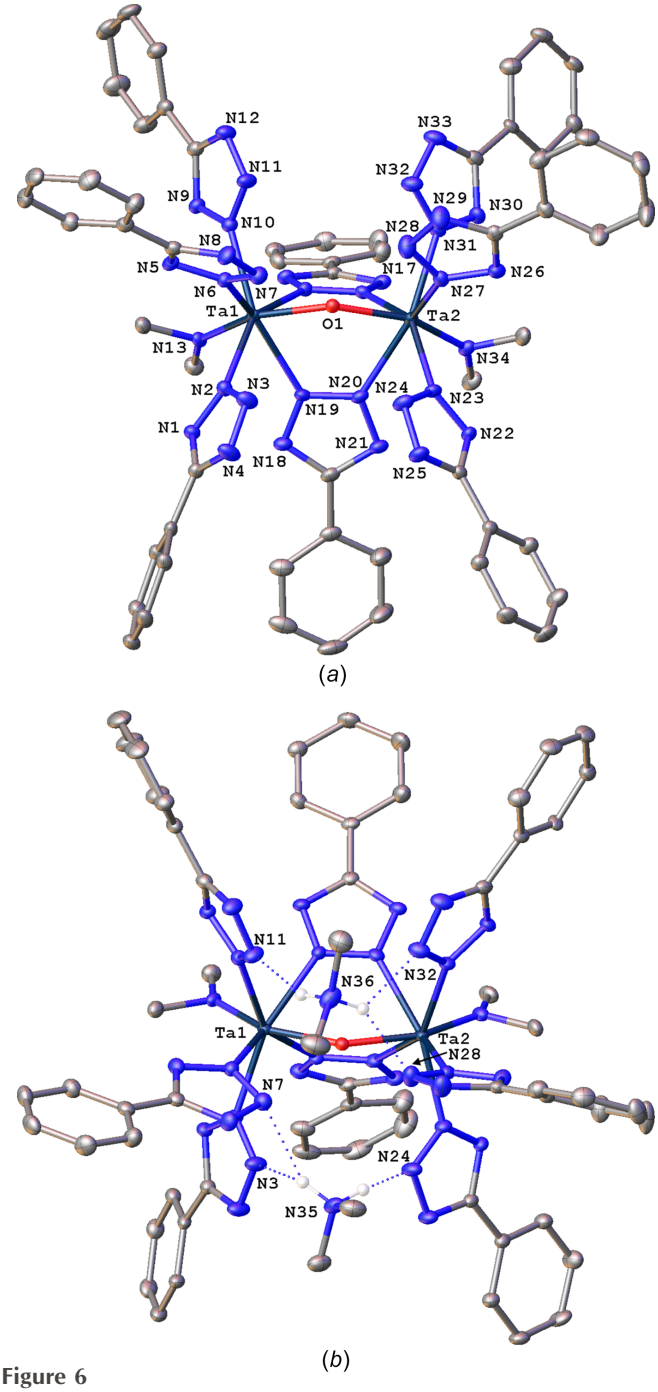


Figure 6
(*a*) A molecular drawing of **3a**, shown with 40% probability displacement ellipsoids. All H atoms and minor disorder components have been omitted. (*b*) Hydrogen-bonding interactions between two H_2NMe_2 cations and dianionic Ta complex **3a**.

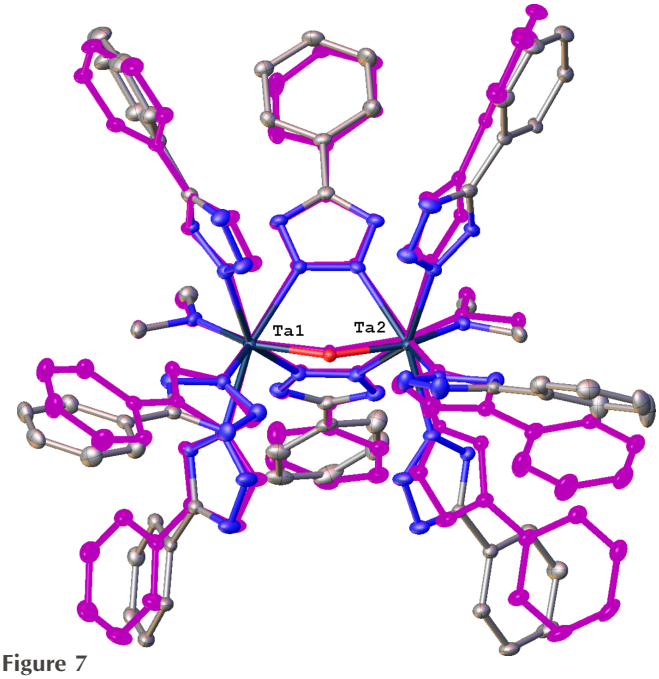


Figure 7
Superposition of **3a** and **3b**. All H atoms and minor disorder components have been omitted. Complex **3b** is shown in monochrome.

Table 8
Hydrogen-bond geometry (Å, °) for **3**.

D—H···A	D—H	H···A	D···A	D—H···A
N35—H35B···N24	0.91	2.00	2.875 (4)	161
N35—H35C···N3	0.91	2.46	3.031 (4)	121
N35—H35C···N7	0.91	2.12	2.943 (4)	150
N36—H36B···N11	0.91	1.98	2.836 (4)	156
N36—H36C···N28	0.91	2.17	2.978 (5)	148
N36—H36C···N32	0.91	2.44	3.085 (4)	128
N35A—H35D···N3A	0.91	2.05	2.867 (4)	149
N35A—H35E···N24A	0.91	2.33	2.994 (4)	130
N35A—H35E···N28A	0.91	2.20	2.954 (4)	140
N36A—H36D···N7A	0.91	2.23	2.961 (4)	137
N36A—H36D···N11A	0.91	2.34	2.981 (4)	127
N36A—H36E···N32A	0.91	1.95	2.828 (4)	161

forming a total of six charge-assisted hydrogen-bonding interactions. One $[H_2NMe_2]^+$ forms one hydrogen bond to a terminal Tz ligand on one Ta atom, and a bifurcated N—H···N(Tz) hydrogen bond with its second acidic proton to two Tz ligands from the other Ta center (Table 8). These three hydrogen-bonding interactions involve three of the six terminal Tz moieties. The other $[H_2NMe_2]^+$ cation forms similar interactions with the three remaining Tz ligands, but the connectivity of the single and bifurcated hydrogen bonds is reversed relative to the Ta centers. The single N—H···N hydrogen bonds average 2.85 (2) Å, with the D—H···A angles in the range 149–161°. The bifurcated bonds are appreciably longer, with an average of 2.99 (5) Å, and their suboptimal D—H···A angles span the range 121–150°. Whereas there are no Ta–tz complexes and no closely related seven-coordinated Ta complexes with Ta—O—Ta bridges reported to the CSD, there are 164 complexes with a Ta—NMe_2 fragment. In these, the Ta—N distances in the four-, five-, six-, seven-, eight-, and nine-coordinate complexes averaged 1.98 (3), 1.98 (3), 2.00 (5), 2.01 (3), 1.970 (15), and 1.990 (6) Å, respectively. The differences among these values are not statistically significant, and the expected trend of metal–ligand distance elongation with the increase in the metal coordination number is absent. The Ta—NMe_2 distances in **3a** and **3b** are much shorter at 1.93 Å, and are among the shortest bond lengths of this type reported to the CSD. This is probably a result of the dianionic nature of the complexes.

4. Conclusions

This work expands the number of structurally characterized complexes of Ti, Zr, and Ta with tetrazolato ligands. All three complexes are dinuclear; the Ti center in **1** is six-coordinate, whereas the Zr and Ta atoms in **2** and **3** are seven-coordinate. The coordination environments of the Ti centers **1** and Ta centers in **3** are similar; however, the two Zr centers in **2** bear a different number of ligands, one of which is a bidentate 1,2-η^2-Tz ligand, not previously observed for *d*-block elements. The starting materials for the chemical reactions leading to the isolation of **1–3** involved dimethylamido ligands that were (*a*) retained in the products, (*b*) converted to dimethylamine eliminated from the reaction mixture by gas evolution, (*c*) converted to dimethylamine and retained as a neutral ligand, and (*d*) converted to dimethylammonium and retained as a hydrogen-bonded entity bridging Tz ligands. These relatively large metal complexes crystallize with solvent-accessible voids in their lattices that are indeed occupied by ordered and disordered solvent molecules. The refinement of the disordered solvent molecules presented certain challenges but was accomplished by standard techniques.

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supporting information

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Coordination variety of phenyltetrazolato and dimethylamido ligands in dimeric Ti, Zr, and Ta complexes

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Computing details

Bis(dimethylammonium) tris(*μ*-5-phenyltetrazolato-*κ*^{2}*N*^{2}:*N*^{3})bis[bis(dimethylamido)(5-phenyltetrazolato-*κN*^{2})titanium] benzene 1.45-solvate (1)

Crystal data

$(C_2H_8N)[Ti_2(C_7H_5N_4)_5(C_2H_6N)_4]\cdot 1.45C_6H_6$
M_r = 1043.95
Monoclinic, $P2_1/c$
a = 11.6292 (9) Å
b = 22.6611 (17) Å
c = 22.3631 (17) Å
β = 93.857 (1)°
V = 5880.0 (8) Å^3
Z = 4
$F(000)$ = 2184
D_x = 1.179 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 22219 reflections
θ = 2.2–26.4°
μ = 0.32 mm^{-1}
T = 100 K
Block, brown
0.4 × 0.3 × 0.2 mm

Data collection

Bruker SMART APEX CCD area detector diffractometer
Radiation source: sealed tube
Graphite monochromator
Detector resolution: 8 pixels mm^{-1}
ω and φ scans
Absorption correction: multi-scan (SADABS; Bruker, 2018)
T_{min} = 0.576, T_{max} = 0.745
46383 measured reflections
11558 independent reflections
8907 reflections with $I > 2\sigma(I)$
R_{int} = 0.042
θ_{max} = 26.0°, θ_{min} = 1.8°
h = −14→14
k = −27→27
l = −27→27

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.050
$wR(F^2)$ = 0.142
S = 1.09
11558 reflections
826 parameters
898 restraints
Primary atom site location: structure-invariant direct methods
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0726P)^2 + 2.6632P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.53 e Å^{-3}
$\Delta\rho_{min}$ = −0.41 e Å^{-3}

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}	Occ. (<1)
Ti1	0.74516 (3)	0.20237 (2)	0.62569 (2)	0.02525 (11)	
Ti2	0.56820 (4)	0.29739 (2)	0.75626 (2)	0.02952 (12)	
N1	0.76100 (19)	0.02299 (8)	0.68243 (9)	0.0363 (5)	
N2	0.73530 (18)	0.08001 (9)	0.68754 (9)	0.0362 (5)	
N3	0.76913 (16)	0.10915 (8)	0.64050 (9)	0.0294 (4)	
N4	0.81803 (16)	0.07150 (8)	0.60321 (9)	0.0299 (4)	
N5	0.89897 (17)	0.22772 (9)	0.61966 (9)	0.0349 (5)	
N6	0.70669 (17)	0.18977 (8)	0.54308 (9)	0.0307 (4)	
N7	0.71383 (17)	0.33132 (8)	0.58545 (8)	0.0298 (4)	
N8	0.68922 (16)	0.29481 (8)	0.62947 (8)	0.0280 (4)	
N9	0.63051 (16)	0.32360 (8)	0.66955 (8)	0.0284 (4)	
N10	0.61479 (17)	0.37954 (8)	0.65171 (9)	0.0327 (4)	
N11	0.50202 (16)	0.14395 (8)	0.63901 (9)	0.0303 (4)	
N12	0.56788 (16)	0.18867 (8)	0.65889 (8)	0.0269 (4)	
N13	0.51682 (16)	0.21748 (8)	0.70183 (8)	0.0279 (4)	
N14	0.41627 (18)	0.19155 (9)	0.71021 (10)	0.0370 (5)	
N15	0.88137 (18)	0.18841 (9)	0.75326 (9)	0.0349 (5)	
N16	0.78387 (17)	0.21064 (8)	0.72730 (9)	0.0305 (4)	
N17	0.72863 (18)	0.24070 (9)	0.76779 (9)	0.0365 (5)	
N18	0.7888 (2)	0.23883 (10)	0.82038 (10)	0.0482 (6)	
N19	0.42108 (19)	0.33433 (9)	0.74992 (9)	0.0382 (5)	
N20	0.6561 (2)	0.35954 (9)	0.79243 (10)	0.0448 (5)	
N21	0.5049 (2)	0.18095 (9)	0.89978 (9)	0.0456 (6)	
N22	0.5435 (3)	0.19430 (9)	0.84678 (10)	0.0521 (7)	
N23	0.52220 (19)	0.25073 (9)	0.83493 (9)	0.0360 (5)	
N24	0.46968 (17)	0.27568 (8)	0.88041 (9)	0.0312 (4)	
N25	0.6039 (10)	0.0924 (3)	0.7906 (3)	0.0421 (19)	0.543 (15)
H25C	0.582194	0.130080	0.798267	0.051*	0.543 (15)
H25D	0.641010	0.092679	0.756107	0.051*	0.543 (15)
C44	0.6849 (11)	0.0717 (3)	0.8404 (4)	0.069 (3)	0.543 (15)
H44A	0.649715	0.077216	0.878653	0.104*	0.543 (15)
H44B	0.756490	0.094517	0.840620	0.104*	0.543 (15)
H44C	0.701810	0.029796	0.834852	0.104*	0.543 (15)
C45	0.5001 (11)	0.0553 (4)	0.7821 (4)	0.064 (2)	0.543 (15)
H45A	0.522744	0.013678	0.780946	0.096*	0.543 (15)
H45B	0.457705	0.065860	0.744228	0.096*	0.543 (15)
H45C	0.450783	0.061673	0.815331	0.096*	0.543 (15)
N25A	0.6630 (10)	0.0979 (4)	0.7979 (4)	0.035 (2)	0.457 (15)
H25E	0.644591	0.134792	0.810156	0.042*	0.457 (15)

H25F	0.680836	0.100582	0.758960	0.042*	0.457 (15)
C44A	0.7669 (10)	0.0776 (3)	0.8344 (3)	0.047 (2)	0.457 (15)
H44D	0.758615	0.087108	0.876658	0.071*	0.457 (15)
H44E	0.835248	0.097490	0.820777	0.071*	0.457 (15)
H44F	0.775375	0.034842	0.829911	0.071*	0.457 (15)
C45A	0.5606 (11)	0.0599 (4)	0.8007 (5)	0.047 (3)	0.457 (15)
H45D	0.578049	0.020376	0.785915	0.070*	0.457 (15)
H45E	0.496347	0.076824	0.775824	0.070*	0.457 (15)
H45F	0.539454	0.057114	0.842308	0.070*	0.457 (15)
C1	0.81178 (19)	0.01926 (10)	0.63002 (11)	0.0289 (5)	
C2	0.8566 (2)	−0.03605 (10)	0.60636 (12)	0.0342 (5)	
C3	0.8650 (2)	−0.08629 (10)	0.64193 (13)	0.0417 (6)	
H3	0.838645	−0.085132	0.681218	0.050*	
C4	0.9111 (2)	−0.13801 (11)	0.62100 (14)	0.0462 (7)	
H4	0.916066	−0.172097	0.645763	0.055*	
C5	0.9495 (3)	−0.13989 (12)	0.56437 (15)	0.0527 (8)	
H5	0.981003	−0.175331	0.549708	0.063*	
C6	0.9423 (3)	−0.08998 (13)	0.52871 (16)	0.0676 (10)	
H6	0.970093	−0.091086	0.489739	0.081*	
C7	0.8947 (3)	−0.03829 (12)	0.54941 (14)	0.0541 (8)	
H7	0.888527	−0.004460	0.524314	0.065*	
C8	0.9758 (2)	0.19549 (12)	0.58311 (14)	0.0471 (7)	
H8A	1.009743	0.222692	0.555124	0.071*	
H8B	0.932476	0.164744	0.560539	0.071*	
H8C	1.037305	0.177238	0.608956	0.071*	
C9	0.9601 (2)	0.27473 (13)	0.65306 (14)	0.0482 (7)	
H9A	1.019299	0.257484	0.681073	0.072*	
H9B	0.905505	0.297357	0.675461	0.072*	
H9C	0.996715	0.300926	0.625094	0.072*	
C10	0.6296 (2)	0.14369 (11)	0.51734 (11)	0.0366 (6)	
H10A	0.572147	0.161536	0.488801	0.055*	
H10B	0.590555	0.124243	0.549459	0.055*	
H10C	0.674742	0.114519	0.496582	0.055*	
C11	0.7545 (2)	0.22302 (12)	0.49464 (12)	0.0418 (6)	
H11A	0.794190	0.195942	0.468745	0.063*	
H11B	0.809432	0.252337	0.511619	0.063*	
H11C	0.692131	0.243089	0.471058	0.063*	
C12	0.6664 (2)	0.38283 (9)	0.60019 (10)	0.0290 (5)	
C13	0.6743 (4)	0.43560 (18)	0.56075 (18)	0.0289 (16)	0.606 (13)
C14	0.7432 (6)	0.43690 (13)	0.51233 (19)	0.0395 (15)	0.606 (13)
H14	0.785660	0.402854	0.502425	0.047*	0.606 (13)
C15	0.7500 (8)	0.48802 (15)	0.47840 (17)	0.0445 (17)	0.606 (13)
H15	0.797129	0.488910	0.445302	0.053*	0.606 (13)
C16	0.6880 (6)	0.53784 (15)	0.4929 (2)	0.0502 (19)	0.606 (13)
H16	0.692614	0.572773	0.469693	0.060*	0.606 (13)
C17	0.6191 (4)	0.53653 (19)	0.5413 (3)	0.0513 (19)	0.606 (13)
H17	0.576630	0.570580	0.551208	0.062*	0.606 (13)
C18	0.6122 (4)	0.4854 (2)	0.5752 (3)	0.0417 (17)	0.606 (13)

H18	0.565160	0.484524	0.608332	0.050*	0.606 (13)
C13A	0.6623 (6)	0.4392 (2)	0.5691 (3)	0.032 (3)	0.394 (13)
C14A	0.6798 (10)	0.43762 (18)	0.5082 (3)	0.039 (2)	0.394 (13)
H14A	0.695518	0.401156	0.489430	0.047*	0.394 (13)
C15A	0.6744 (12)	0.4894 (2)	0.4748 (2)	0.044 (3)	0.394 (13)
H15A	0.686352	0.488334	0.433232	0.053*	0.394 (13)
C16A	0.6515 (8)	0.54275 (19)	0.5023 (3)	0.043 (2)	0.394 (13)
H16A	0.647732	0.578139	0.479484	0.051*	0.394 (13)
C17A	0.6340 (8)	0.5443 (2)	0.5632 (4)	0.049 (3)	0.394 (13)
H17A	0.618279	0.580766	0.581934	0.059*	0.394 (13)
C18A	0.6394 (9)	0.4925 (3)	0.5965 (3)	0.036 (2)	0.394 (13)
H18A	0.627446	0.493589	0.638133	0.043*	0.394 (13)
C19	0.4092 (2)	0.14691 (10)	0.67089 (11)	0.0342 (5)	
C20	0.3063 (9)	0.1090 (6)	0.6666 (7)	0.043 (3)	0.434 (3)
C21	0.3064 (7)	0.0584 (6)	0.6315 (6)	0.045 (3)	0.434 (3)
H21	0.372689	0.048389	0.611001	0.054*	0.434 (3)
C22	0.2094 (9)	0.0224 (4)	0.6262 (5)	0.055 (3)	0.434 (3)
H22	0.209441	−0.012166	0.602207	0.066*	0.434 (3)
C23	0.1124 (7)	0.0370 (4)	0.6562 (5)	0.059 (3)	0.434 (3)
H23	0.046119	0.012439	0.652589	0.071*	0.434 (3)
C24	0.1124 (9)	0.0876 (5)	0.6913 (6)	0.071 (3)	0.434 (3)
H24	0.046044	0.097598	0.711765	0.085*	0.434 (3)
C25	0.2093 (12)	0.1236 (5)	0.6965 (8)	0.063 (3)	0.434 (3)
H25	0.209292	0.158153	0.720559	0.076*	0.434 (3)
C20A	0.3103 (11)	0.1074 (7)	0.6553 (7)	0.038 (3)	0.356 (3)
C21A	0.3177 (8)	0.0635 (7)	0.6123 (6)	0.039 (3)	0.356 (3)
H21A	0.383866	0.060955	0.589799	0.047*	0.356 (3)
C22A	0.2282 (10)	0.0233 (5)	0.6024 (5)	0.051 (3)	0.356 (3)
H22A	0.233231	−0.006753	0.572992	0.062*	0.356 (3)
C23A	0.1313 (8)	0.0269 (5)	0.6354 (5)	0.061 (4)	0.356 (3)
H23A	0.070165	−0.000550	0.628535	0.073*	0.356 (3)
C24A	0.1239 (9)	0.0708 (6)	0.6783 (6)	0.067 (3)	0.356 (3)
H24A	0.057732	0.073360	0.700886	0.080*	0.356 (3)
C25A	0.2134 (12)	0.1111 (6)	0.6883 (7)	0.052 (3)	0.356 (3)
H25A	0.208367	0.141068	0.717695	0.063*	0.356 (3)
C20B	0.3157 (11)	0.1033 (7)	0.6750 (8)	0.039 (4)	0.210 (3)
C21B	0.2851 (15)	0.0673 (9)	0.6261 (8)	0.045 (4)	0.210 (3)
H21B	0.329554	0.067873	0.591969	0.053*	0.210 (3)
C22B	0.1895 (15)	0.0307 (8)	0.6271 (8)	0.054 (4)	0.210 (3)
H22B	0.168551	0.006116	0.593719	0.065*	0.210 (3)
C23B	0.1245 (11)	0.0299 (7)	0.6771 (8)	0.074 (5)	0.210 (3)
H23B	0.059106	0.004819	0.677768	0.089*	0.210 (3)
C24B	0.1551 (11)	0.0658 (7)	0.7259 (7)	0.083 (5)	0.210 (3)
H24B	0.110663	0.065278	0.760069	0.099*	0.210 (3)
C25B	0.2507 (11)	0.1025 (6)	0.7249 (7)	0.067 (4)	0.210 (3)
H25B	0.271665	0.127035	0.758321	0.080*	0.210 (3)
C26	0.8816 (2)	0.20654 (11)	0.81012 (11)	0.0399 (6)	
C27	0.9669 (6)	0.1895 (3)	0.8593 (2)	0.0351 (15)	0.77 (3)

C28	1.0814 (5)	0.1834 (3)	0.8460 (3)	0.0444 (13)	0.77 (3)
H28	1.102169	0.187630	0.805888	0.053*	0.77 (3)
C29	1.1654 (5)	0.1711 (3)	0.8915 (4)	0.0532 (16)	0.77 (3)
H29	1.243668	0.166952	0.882391	0.064*	0.77 (3)
C30	1.1350 (6)	0.1649 (2)	0.9502 (3)	0.0491 (16)	0.77 (3)
H30	1.192496	0.156546	0.981262	0.059*	0.77 (3)
C31	1.0206 (7)	0.1710 (4)	0.9635 (2)	0.0515 (17)	0.77 (3)
H31	0.999824	0.166818	1.003630	0.062*	0.77 (3)
C32	0.9365 (7)	0.1833 (4)	0.9180 (2)	0.0440 (17)	0.77 (3)
H32	0.858323	0.187496	0.927128	0.053*	0.77 (3)
C27A	0.9879 (11)	0.1984 (9)	0.8493 (7)	0.025 (3)	0.23 (3)
C28A	1.0937 (12)	0.1801 (11)	0.8305 (9)	0.047 (4)	0.23 (3)
H28A	1.106165	0.178782	0.788982	0.056*	0.23 (3)
C29A	1.1814 (11)	0.1636 (10)	0.8725 (12)	0.051 (4)	0.23 (3)
H29A	1.253693	0.151088	0.859734	0.061*	0.23 (3)
C30A	1.1632 (16)	0.1655 (7)	0.9333 (11)	0.044 (4)	0.23 (3)
H30A	1.223047	0.154212	0.962035	0.053*	0.23 (3)
C31A	1.057 (2)	0.1838 (7)	0.9521 (8)	0.043 (4)	0.23 (3)
H31A	1.044871	0.185031	0.993584	0.051*	0.23 (3)
C32A	0.9697 (17)	0.2002 (7)	0.9100 (7)	0.032 (3)	0.23 (3)
H32A	0.897341	0.212726	0.922832	0.039*	0.23 (3)
C33	0.3098 (2)	0.30692 (12)	0.75896 (13)	0.0452 (7)	
H33A	0.277215	0.324416	0.794146	0.068*	
H33B	0.320483	0.264426	0.765300	0.068*	
H33C	0.257233	0.313542	0.723503	0.068*	
C34	0.4053 (3)	0.39726 (12)	0.73812 (15)	0.0553 (8)	
H34A	0.368944	0.415700	0.771719	0.083*	
H34B	0.355879	0.402649	0.701261	0.083*	
H34C	0.480370	0.415695	0.733442	0.083*	
C35	0.6108 (3)	0.39493 (13)	0.84034 (13)	0.0600 (9)	
H35A	0.662632	0.391692	0.876604	0.090*	
H35B	0.534132	0.380466	0.848729	0.090*	
H35C	0.605400	0.436319	0.827759	0.090*	
C36	0.7728 (3)	0.37658 (14)	0.78161 (16)	0.0591 (8)	
H36A	0.774019	0.418186	0.769707	0.089*	
H36B	0.800774	0.352126	0.749494	0.089*	
H36C	0.822549	0.370973	0.818289	0.089*	
C37	0.4609 (2)	0.23168 (10)	0.91961 (10)	0.0309 (5)	
C38	0.40735 (19)	0.23783 (10)	0.97704 (10)	0.0295 (5)	
C39	0.4304 (2)	0.19653 (11)	1.02244 (11)	0.0340 (5)	
H39	0.483056	0.165231	1.016964	0.041*	
C40	0.3760 (2)	0.20130 (12)	1.07596 (11)	0.0373 (6)	
H40	0.391651	0.173256	1.107022	0.045*	
C41	0.2993 (2)	0.24693 (12)	1.08378 (12)	0.0406 (6)	
H41	0.260817	0.249598	1.119831	0.049*	
C42	0.2786 (2)	0.28863 (11)	1.03920 (12)	0.0404 (6)	
H42	0.227303	0.320416	1.045154	0.048*	
C43	0.3320 (2)	0.28430 (10)	0.98602 (11)	0.0339 (5)	

H43	0.317407	0.313053	0.955546	0.041*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ti1	0.0254 (2)	0.0215 (2)	0.0296 (2)	0.00267 (16)	0.00727 (16)	−0.00238 (16)
Ti2	0.0371 (2)	0.0234 (2)	0.0287 (2)	0.00878 (17)	0.00751 (18)	−0.00126 (16)
N1	0.0452 (12)	0.0255 (10)	0.0395 (11)	0.0056 (9)	0.0114 (10)	−0.0026 (8)
N2	0.0449 (13)	0.0267 (10)	0.0380 (11)	0.0080 (9)	0.0111 (9)	−0.0013 (9)
N3	0.0306 (10)	0.0238 (9)	0.0343 (11)	0.0031 (8)	0.0065 (8)	−0.0029 (8)
N4	0.0278 (10)	0.0234 (9)	0.0393 (11)	0.0027 (8)	0.0086 (8)	−0.0031 (8)
N5	0.0279 (10)	0.0323 (11)	0.0452 (12)	−0.0003 (8)	0.0082 (9)	−0.0038 (9)
N6	0.0316 (11)	0.0298 (10)	0.0317 (10)	0.0048 (8)	0.0093 (8)	−0.0001 (8)
N7	0.0331 (11)	0.0247 (10)	0.0322 (10)	0.0001 (8)	0.0064 (8)	0.0032 (8)
N8	0.0283 (10)	0.0238 (9)	0.0328 (10)	0.0033 (8)	0.0080 (8)	−0.0007 (8)
N9	0.0293 (10)	0.0232 (9)	0.0334 (10)	0.0027 (8)	0.0074 (8)	−0.0005 (8)
N10	0.0329 (11)	0.0216 (9)	0.0445 (12)	0.0035 (8)	0.0087 (9)	0.0005 (8)
N11	0.0298 (10)	0.0253 (10)	0.0363 (11)	−0.0003 (8)	0.0055 (8)	−0.0019 (8)
N12	0.0285 (10)	0.0236 (9)	0.0294 (10)	0.0017 (7)	0.0069 (8)	−0.0003 (7)
N13	0.0307 (10)	0.0269 (9)	0.0272 (10)	0.0042 (8)	0.0099 (8)	0.0024 (8)
N14	0.0382 (12)	0.0322 (11)	0.0427 (12)	0.0024 (9)	0.0170 (9)	0.0045 (9)
N15	0.0354 (11)	0.0307 (10)	0.0377 (11)	0.0087 (9)	−0.0047 (9)	−0.0048 (9)
N16	0.0310 (10)	0.0254 (10)	0.0350 (11)	0.0066 (8)	0.0011 (8)	−0.0034 (8)
N17	0.0414 (12)	0.0339 (11)	0.0334 (11)	0.0128 (9)	−0.0040 (9)	−0.0084 (9)
N18	0.0565 (15)	0.0464 (13)	0.0396 (12)	0.0242 (11)	−0.0136 (11)	−0.0179 (10)
N19	0.0464 (13)	0.0329 (11)	0.0367 (11)	0.0171 (9)	0.0132 (10)	0.0027 (9)
N20	0.0616 (15)	0.0307 (11)	0.0413 (12)	0.0049 (10)	−0.0015 (11)	−0.0069 (9)
N21	0.0788 (17)	0.0303 (11)	0.0289 (11)	0.0099 (11)	0.0141 (11)	0.0006 (9)
N22	0.100 (2)	0.0281 (11)	0.0300 (11)	0.0193 (12)	0.0181 (12)	0.0036 (9)
N23	0.0528 (13)	0.0271 (10)	0.0290 (10)	0.0103 (9)	0.0088 (9)	−0.0022 (8)
N24	0.0345 (11)	0.0274 (10)	0.0324 (10)	0.0037 (8)	0.0073 (8)	−0.0039 (8)
N25	0.069 (6)	0.028 (3)	0.031 (3)	0.006 (4)	0.015 (4)	0.000 (2)
C44	0.086 (9)	0.044 (3)	0.076 (5)	0.010 (4)	−0.010 (4)	0.009 (3)
C45	0.090 (7)	0.047 (4)	0.054 (5)	−0.006 (4)	−0.003 (4)	0.013 (3)
N25A	0.054 (5)	0.019 (3)	0.034 (3)	0.004 (4)	0.014 (4)	−0.003 (2)
C44A	0.054 (6)	0.037 (3)	0.051 (4)	0.005 (3)	0.007 (3)	0.004 (3)
C45A	0.064 (7)	0.034 (4)	0.044 (5)	−0.001 (5)	0.020 (5)	−0.004 (4)
C1	0.0231 (11)	0.0243 (11)	0.0401 (13)	0.0002 (9)	0.0075 (10)	−0.0033 (9)
C2	0.0305 (13)	0.0231 (11)	0.0504 (15)	−0.0002 (9)	0.0122 (11)	−0.0038 (10)
C3	0.0414 (15)	0.0259 (12)	0.0605 (17)	0.0023 (11)	0.0235 (13)	0.0034 (12)
C4	0.0455 (16)	0.0229 (12)	0.073 (2)	0.0034 (11)	0.0225 (14)	0.0068 (12)
C5	0.0575 (18)	0.0273 (13)	0.077 (2)	0.0080 (12)	0.0314 (16)	−0.0080 (13)
C6	0.103 (3)	0.0346 (15)	0.071 (2)	0.0136 (17)	0.047 (2)	−0.0046 (15)
C7	0.083 (2)	0.0271 (13)	0.0564 (18)	0.0120 (14)	0.0319 (16)	0.0005 (12)
C8	0.0315 (14)	0.0386 (15)	0.073 (2)	0.0040 (11)	0.0162 (13)	−0.0062 (13)
C9	0.0368 (15)	0.0445 (16)	0.0636 (19)	−0.0095 (12)	0.0047 (13)	−0.0083 (14)
C10	0.0373 (14)	0.0418 (14)	0.0310 (13)	0.0032 (11)	0.0033 (10)	−0.0040 (11)
C11	0.0464 (16)	0.0431 (14)	0.0370 (14)	0.0054 (12)	0.0122 (12)	0.0037 (11)

C12	0.0296 (12)	0.0234 (11)	0.0343 (12)	−0.0011 (9)	0.0030 (10)	−0.0010 (9)
C13	0.041 (4)	0.019 (3)	0.026 (3)	−0.003 (3)	−0.001 (2)	−0.003 (2)
C14	0.049 (4)	0.035 (2)	0.035 (2)	−0.001 (2)	0.011 (3)	−0.0024 (18)
C15	0.063 (5)	0.036 (2)	0.037 (2)	−0.010 (2)	0.016 (3)	0.0005 (18)
C16	0.078 (5)	0.032 (3)	0.041 (3)	−0.005 (3)	0.002 (3)	0.007 (2)
C17	0.074 (4)	0.025 (3)	0.056 (5)	0.010 (3)	0.012 (4)	0.003 (3)
C18	0.055 (4)	0.032 (3)	0.039 (3)	0.007 (3)	0.011 (3)	−0.001 (2)
C13A	0.023 (5)	0.033 (5)	0.041 (5)	−0.002 (4)	0.011 (4)	0.004 (4)
C14A	0.057 (7)	0.023 (3)	0.037 (4)	0.006 (3)	0.002 (4)	−0.003 (2)
C15A	0.059 (8)	0.035 (4)	0.038 (4)	0.001 (4)	0.003 (4)	0.004 (3)
C16A	0.050 (6)	0.018 (3)	0.059 (6)	0.001 (3)	0.002 (4)	0.014 (3)
C17A	0.063 (6)	0.023 (4)	0.065 (6)	−0.001 (4)	0.024 (5)	0.001 (3)
C18A	0.042 (5)	0.024 (3)	0.044 (5)	−0.001 (3)	0.014 (4)	−0.002 (3)
C19	0.0326 (13)	0.0268 (12)	0.0445 (14)	0.0014 (10)	0.0122 (11)	0.0038 (10)
C20	0.039 (6)	0.037 (6)	0.055 (7)	−0.008 (5)	0.009 (5)	0.009 (5)
C21	0.026 (5)	0.040 (5)	0.069 (7)	0.000 (4)	0.000 (4)	0.008 (5)
C22	0.034 (5)	0.039 (5)	0.091 (8)	−0.006 (4)	0.005 (5)	0.005 (5)
C23	0.033 (4)	0.050 (5)	0.096 (9)	−0.005 (4)	0.010 (5)	0.015 (5)
C24	0.044 (5)	0.057 (6)	0.116 (9)	−0.003 (4)	0.032 (5)	0.010 (5)
C25	0.045 (5)	0.048 (5)	0.101 (8)	−0.008 (4)	0.036 (5)	0.001 (5)
C20A	0.033 (6)	0.035 (6)	0.046 (7)	0.001 (5)	0.008 (4)	0.014 (4)
C21A	0.024 (5)	0.033 (5)	0.059 (7)	−0.010 (4)	−0.001 (4)	0.011 (5)
C22A	0.027 (5)	0.050 (5)	0.076 (8)	−0.008 (4)	−0.001 (5)	0.012 (5)
C23A	0.032 (6)	0.060 (7)	0.092 (8)	−0.018 (5)	0.014 (6)	0.018 (5)
C24A	0.034 (5)	0.074 (8)	0.094 (7)	−0.011 (6)	0.021 (5)	0.007 (7)
C25A	0.040 (6)	0.053 (6)	0.066 (7)	−0.006 (5)	0.014 (5)	0.009 (5)
C20B	0.022 (7)	0.026 (7)	0.068 (9)	0.000 (6)	0.006 (6)	0.011 (6)
C21B	0.021 (7)	0.037 (8)	0.076 (9)	0.005 (6)	0.007 (7)	0.004 (8)
C22B	0.030 (8)	0.035 (7)	0.095 (9)	−0.008 (6)	−0.007 (7)	0.010 (7)
C23B	0.044 (9)	0.075 (10)	0.104 (11)	−0.020 (8)	0.006 (7)	0.012 (9)
C24B	0.056 (8)	0.093 (10)	0.102 (10)	−0.026 (7)	0.027 (8)	0.008 (8)
C25B	0.045 (8)	0.072 (9)	0.086 (9)	−0.018 (7)	0.028 (7)	−0.003 (7)
C26	0.0448 (15)	0.0326 (13)	0.0406 (14)	0.0104 (11)	−0.0092 (12)	−0.0095 (11)
C27	0.040 (2)	0.025 (3)	0.039 (3)	0.003 (2)	−0.008 (2)	−0.008 (2)
C28	0.040 (3)	0.054 (3)	0.038 (2)	−0.005 (2)	−0.006 (2)	−0.006 (2)
C29	0.036 (2)	0.072 (3)	0.051 (4)	−0.002 (2)	−0.005 (2)	−0.017 (3)
C30	0.048 (3)	0.049 (3)	0.048 (3)	0.003 (2)	−0.017 (3)	−0.005 (2)
C31	0.055 (3)	0.060 (3)	0.038 (2)	0.002 (3)	−0.005 (2)	−0.010 (2)
C32	0.043 (3)	0.046 (4)	0.042 (2)	0.006 (3)	−0.006 (2)	−0.012 (2)
C27A	0.032 (6)	0.013 (6)	0.031 (6)	−0.004 (5)	−0.001 (5)	0.000 (5)
C28A	0.025 (6)	0.065 (10)	0.049 (7)	0.002 (6)	−0.003 (5)	−0.005 (8)
C29A	0.038 (7)	0.059 (9)	0.054 (9)	0.003 (6)	−0.012 (6)	−0.019 (8)
C30A	0.041 (7)	0.042 (7)	0.046 (8)	−0.006 (6)	−0.018 (7)	−0.014 (7)
C31A	0.050 (8)	0.042 (7)	0.034 (6)	−0.008 (7)	−0.010 (6)	−0.005 (5)
C32A	0.034 (6)	0.024 (6)	0.040 (6)	−0.010 (5)	0.005 (5)	−0.004 (5)
C33	0.0415 (15)	0.0443 (15)	0.0508 (16)	0.0159 (12)	0.0103 (12)	−0.0038 (12)
C34	0.0580 (19)	0.0404 (15)	0.071 (2)	0.0264 (14)	0.0309 (16)	0.0139 (14)
C35	0.106 (3)	0.0385 (16)	0.0374 (15)	−0.0158 (16)	0.0174 (16)	−0.0089 (12)

C36	0.0516 (19)	0.0499 (18)	0.074 (2)	0.0017 (14)	−0.0085 (16)	−0.0216 (16)
C37	0.0333 (13)	0.0282 (12)	0.0312 (12)	0.0027 (10)	0.0019 (10)	−0.0025 (10)
C38	0.0266 (12)	0.0309 (12)	0.0312 (12)	−0.0049 (9)	0.0026 (9)	−0.0061 (9)
C39	0.0302 (12)	0.0403 (14)	0.0316 (12)	0.0019 (10)	0.0018 (10)	−0.0020 (10)
C40	0.0363 (14)	0.0461 (15)	0.0292 (12)	−0.0108 (11)	0.0004 (10)	0.0002 (11)
C41	0.0358 (14)	0.0490 (15)	0.0386 (14)	−0.0154 (12)	0.0149 (11)	−0.0118 (12)
C42	0.0333 (14)	0.0359 (14)	0.0536 (16)	−0.0055 (11)	0.0152 (12)	−0.0069 (12)
C43	0.0317 (13)	0.0306 (12)	0.0398 (14)	−0.0046 (10)	0.0057 (10)	0.0000 (10)

Geometric parameters (Å, º)

Ti1—N3	2.1534 (19)	C17—H17	0.9500
Ti1—N5	1.892 (2)	C17—C18	1.3900
Ti1—N6	1.893 (2)	C18—H18	0.9500
Ti1—N8	2.1967 (18)	C13A—C14A	1.3900
Ti1—N12	2.2592 (19)	C13A—C18A	1.3900
Ti1—N16	2.294 (2)	C14A—H14A	0.9500
Ti2—N9	2.1970 (19)	C14A—C15A	1.3900
Ti2—N13	2.2404 (19)	C15A—H15A	0.9500
Ti2—N17	2.266 (2)	C15A—C16A	1.3900
Ti2—N19	1.901 (2)	C16A—H16A	0.9500
Ti2—N20	1.890 (2)	C16A—C17A	1.3900
Ti2—N23	2.151 (2)	C17A—H17A	0.9500
N1—N2	1.333 (3)	C17A—C18A	1.3900
N1—C1	1.350 (3)	C18A—H18A	0.9500
N2—N3	1.324 (3)	C19—C20	1.471 (5)
N3—N4	1.346 (3)	C19—C20A	1.481 (6)
N4—C1	1.331 (3)	C19—C20B	1.477 (7)
N5—C8	1.449 (3)	C20—C21	1.3900
N5—C9	1.459 (3)	C20—C25	1.3900
N6—C10	1.468 (3)	C21—H21	0.9500
N6—C11	1.460 (3)	C21—C22	1.3900
N7—N8	1.332 (3)	C22—H22	0.9500
N7—C12	1.342 (3)	C22—C23	1.3900
N8—N9	1.333 (2)	C23—H23	0.9500
N9—N10	1.338 (3)	C23—C24	1.3900
N10—C12	1.337 (3)	C24—H24	0.9500
N11—N12	1.329 (3)	C24—C25	1.3900
N11—C19	1.335 (3)	C25—H25	0.9500
N12—N13	1.333 (2)	C20A—C21A	1.3900
N13—N14	1.333 (3)	C20A—C25A	1.3900
N14—C19	1.339 (3)	C21A—H21A	0.9500
N15—N16	1.337 (3)	C21A—C22A	1.3900
N15—C26	1.336 (3)	C22A—H22A	0.9500
N16—N17	1.332 (3)	C22A—C23A	1.3900
N17—N18	1.328 (3)	C23A—H23A	0.9500
N18—C26	1.337 (3)	C23A—C24A	1.3900
N19—C33	1.461 (4)	C24A—H24A	0.9500

N19—C34	1.460 (3)	C24A—C25A	1.3900
N20—C35	1.464 (3)	C25A—H25A	0.9500
N20—C36	1.447 (4)	C20B—C21B	1.3900
N21—N22	1.330 (3)	C20B—C25B	1.3900
N21—C37	1.345 (3)	C21B—H21B	0.9500
N22—N23	1.326 (3)	C21B—C22B	1.3900
N23—N24	1.346 (3)	C22B—H22B	0.9500
N24—C37	1.336 (3)	C22B—C23B	1.3900
N25—H25C	0.9100	C23B—H23B	0.9500
N25—H25D	0.9100	C23B—C24B	1.3900
N25—C44	1.485 (10)	C24B—H24B	0.9500
N25—C45	1.472 (10)	C24B—C25B	1.3900
C44—H44A	0.9800	C25B—H25B	0.9500
C44—H44B	0.9800	C26—C27	1.482 (4)
C44—H44C	0.9800	C26—C27A	1.477 (7)
C45—H45A	0.9800	C27—C28	1.3900
C45—H45B	0.9800	C27—C32	1.3900
C45—H45C	0.9800	C28—H28	0.9500
N25A—H25E	0.9100	C28—C29	1.3900
N25A—H25F	0.9100	C29—H29	0.9500
N25A—C44A	1.486 (10)	C29—C30	1.3900
N25A—C45A	1.474 (11)	C30—H30	0.9500
C44A—H44D	0.9800	C30—C31	1.3900
C44A—H44E	0.9800	C31—H31	0.9500
C44A—H44F	0.9800	C31—C32	1.3900
C45A—H45D	0.9800	C32—H32	0.9500
C45A—H45E	0.9800	C27A—C28A	1.3900
C45A—H45F	0.9800	C27A—C32A	1.3900
C1—C2	1.470 (3)	C28A—H28A	0.9500
C2—C3	1.389 (3)	C28A—C29A	1.3900
C2—C7	1.377 (4)	C29A—H29A	0.9500
C3—H3	0.9500	C29A—C30A	1.3900
C3—C4	1.383 (3)	C30A—H30A	0.9500
C4—H4	0.9500	C30A—C31A	1.3900
C4—C5	1.372 (4)	C31A—H31A	0.9500
C5—H5	0.9500	C31A—C32A	1.3900
C5—C6	1.383 (4)	C32A—H32A	0.9500
C6—H6	0.9500	C33—H33A	0.9800
C6—C7	1.388 (4)	C33—H33B	0.9800
C7—H7	0.9500	C33—H33C	0.9800
C8—H8A	0.9800	C34—H34A	0.9800
C8—H8B	0.9800	C34—H34B	0.9800
C8—H8C	0.9800	C34—H34C	0.9800
C9—H9A	0.9800	C35—H35A	0.9800
C9—H9B	0.9800	C35—H35B	0.9800
C9—H9C	0.9800	C35—H35C	0.9800
C10—H10A	0.9800	C36—H36A	0.9800
C10—H10B	0.9800	C36—H36B	0.9800

C10—H10C	0.9800	C36—H36C	0.9800
C11—H11A	0.9800	C37—C38	1.471 (3)
C11—H11B	0.9800	C38—C39	1.394 (3)
C11—H11C	0.9800	C38—C43	1.393 (3)
C12—C13	1.492 (3)	C39—H39	0.9500
C12—C13A	1.453 (5)	C39—C40	1.395 (3)
C13—C14	1.3900	C40—H40	0.9500
C13—C18	1.3900	C40—C41	1.385 (4)
C14—H14	0.9500	C41—H41	0.9500
C14—C15	1.3900	C41—C42	1.383 (4)
C15—H15	0.9500	C42—H42	0.9500
C15—C16	1.3900	C42—C43	1.382 (3)
C16—H16	0.9500	C43—H43	0.9500
C16—C17	1.3900		

N3—Ti1—N8	164.82 (7)	C15—C16—C17	120.0
N3—Ti1—N12	85.77 (7)	C17—C16—H16	120.0
N3—Ti1—N16	85.01 (7)	C16—C17—H17	120.0
N5—Ti1—N3	101.28 (8)	C16—C17—C18	120.0
N5—Ti1—N6	97.98 (9)	C18—C17—H17	120.0
N5—Ti1—N8	89.83 (8)	C13—C18—H18	120.0
N5—Ti1—N12	162.38 (8)	C17—C18—C13	120.0
N5—Ti1—N16	85.55 (8)	C17—C18—H18	120.0
N6—Ti1—N3	91.25 (8)	C14A—C13A—C12	116.4 (4)
N6—Ti1—N8	97.48 (8)	C14A—C13A—C18A	120.0
N6—Ti1—N12	97.99 (8)	C18A—C13A—C12	123.6 (4)
N6—Ti1—N16	175.31 (8)	C13A—C14A—H14A	120.0
N8—Ti1—N12	80.75 (7)	C13A—C14A—C15A	120.0
N8—Ti1—N16	85.58 (7)	C15A—C14A—H14A	120.0
N12—Ti1—N16	78.95 (7)	C14A—C15A—H15A	120.0
N9—Ti2—N13	80.25 (7)	C14A—C15A—C16A	120.0
N9—Ti2—N17	86.32 (7)	C16A—C15A—H15A	120.0
N13—Ti2—N17	77.94 (7)	C15A—C16A—H16A	120.0
N19—Ti2—N9	99.42 (8)	C17A—C16A—C15A	120.0
N19—Ti2—N13	96.29 (8)	C17A—C16A—H16A	120.0
N19—Ti2—N17	171.14 (9)	C16A—C17A—H17A	120.0
N19—Ti2—N23	90.31 (8)	C16A—C17A—C18A	120.0
N20—Ti2—N9	88.58 (9)	C18A—C17A—H17A	120.0
N20—Ti2—N13	162.12 (9)	C13A—C18A—H18A	120.0
N20—Ti2—N17	87.51 (9)	C17A—C18A—C13A	120.0
N20—Ti2—N19	99.30 (10)	C17A—C18A—H18A	120.0
N20—Ti2—N23	99.98 (9)	N11—C19—N14	111.9 (2)
N23—Ti2—N9	165.88 (7)	N11—C19—C20	128.2 (6)
N23—Ti2—N13	88.58 (7)	N11—C19—C20A	119.2 (6)
N23—Ti2—N17	82.90 (8)	N11—C19—C20B	128.6 (7)
N2—N1—C1	104.42 (19)	N14—C19—C20	119.9 (6)
N3—N2—N1	109.57 (18)	N14—C19—C20A	128.6 (6)
N2—N3—Ti1	124.69 (14)	N14—C19—C20B	118.6 (7)

N2—N3—N4	109.68 (17)	C21—C20—C19	119.2 (9)
N4—N3—Ti1	125.62 (14)	C21—C20—C25	120.0
C1—N4—N3	104.27 (18)	C25—C20—C19	120.8 (9)
C8—N5—Ti1	120.62 (17)	C20—C21—H21	120.0
C8—N5—C9	111.0 (2)	C22—C21—C20	120.0
C9—N5—Ti1	128.03 (17)	C22—C21—H21	120.0
C10—N6—Ti1	126.00 (15)	C21—C22—H22	120.0
C11—N6—Ti1	124.70 (17)	C23—C22—C21	120.0
C11—N6—C10	109.2 (2)	C23—C22—H22	120.0
N8—N7—C12	104.28 (17)	C22—C23—H23	120.0
N7—N8—Ti1	119.02 (13)	C22—C23—C24	120.0
N7—N8—N9	109.76 (17)	C24—C23—H23	120.0
N9—N8—Ti1	131.21 (14)	C23—C24—H24	120.0
N8—N9—Ti2	132.47 (14)	C25—C24—C23	120.0
N8—N9—N10	109.22 (17)	C25—C24—H24	120.0
N10—N9—Ti2	118.22 (14)	C20—C25—H25	120.0
C12—N10—N9	104.46 (17)	C24—C25—C20	120.0
N12—N11—C19	104.57 (18)	C24—C25—H25	120.0
N11—N12—Ti1	120.87 (13)	C21A—C20A—C19	120.8 (9)
N11—N12—N13	109.87 (17)	C21A—C20A—C25A	120.0
N13—N12—Ti1	129.04 (14)	C25A—C20A—C19	118.9 (9)
N12—N13—Ti2	132.19 (14)	C20A—C21A—H21A	120.0
N14—N13—Ti2	118.97 (14)	C22A—C21A—C20A	120.0
N14—N13—N12	108.83 (18)	C22A—C21A—H21A	120.0
N13—N14—C19	104.86 (18)	C21A—C22A—H22A	120.0
C26—N15—N16	104.17 (19)	C23A—C22A—C21A	120.0
N15—N16—Ti1	120.23 (14)	C23A—C22A—H22A	120.0
N17—N16—Ti1	130.05 (15)	C22A—C23A—H23A	120.0
N17—N16—N15	109.33 (18)	C22A—C23A—C24A	120.0
N16—N17—Ti2	130.06 (15)	C24A—C23A—H23A	120.0
N18—N17—Ti2	119.97 (15)	C23A—C24A—H24A	120.0
N18—N17—N16	109.65 (19)	C25A—C24A—C23A	120.0
N17—N18—C26	104.4 (2)	C25A—C24A—H24A	120.0
C33—N19—Ti2	127.09 (16)	C20A—C25A—H25A	120.0
C34—N19—Ti2	123.05 (19)	C24A—C25A—C20A	120.0
C34—N19—C33	109.8 (2)	C24A—C25A—H25A	120.0
C35—N20—Ti2	120.7 (2)	C21B—C20B—C19	119.6 (10)
C36—N20—Ti2	127.85 (18)	C21B—C20B—C25B	120.0
C36—N20—C35	111.3 (2)	C25B—C20B—C19	120.0 (10)
N22—N21—C37	105.0 (2)	C20B—C21B—H21B	120.0
N23—N22—N21	109.12 (19)	C20B—C21B—C22B	120.0
N22—N23—Ti2	125.74 (15)	C22B—C21B—H21B	120.0
N22—N23—N24	110.03 (19)	C21B—C22B—H22B	120.0
N24—N23—Ti2	124.21 (14)	C23B—C22B—C21B	120.0
C37—N24—N23	103.93 (18)	C23B—C22B—H22B	120.0
H25C—N25—H25D	107.8	C22B—C23B—H23B	120.0
C44—N25—H25C	109.0	C22B—C23B—C24B	120.0
C44—N25—H25D	109.0	C24B—C23B—H23B	120.0

C45—N25—H25C	109.0	C23B—C24B—H24B	120.0
C45—N25—H25D	109.0	C25B—C24B—C23B	120.0
C45—N25—C44	113.0 (6)	C25B—C24B—H24B	120.0
N25—C44—H44A	109.5	C20B—C25B—H25B	120.0
N25—C44—H44B	109.5	C24B—C25B—C20B	120.0
N25—C44—H44C	109.5	C24B—C25B—H25B	120.0
H44A—C44—H44B	109.5	N15—C26—N18	112.4 (2)
H44A—C44—H44C	109.5	N15—C26—C27	125.8 (3)
H44B—C44—H44C	109.5	N15—C26—C27A	118.2 (8)
N25—C45—H45A	109.5	N18—C26—C27	121.6 (3)
N25—C45—H45B	109.5	N18—C26—C27A	128.3 (8)
N25—C45—H45C	109.5	C28—C27—C26	118.0 (4)
H45A—C45—H45B	109.5	C28—C27—C32	120.0
H45A—C45—H45C	109.5	C32—C27—C26	121.8 (4)
H45B—C45—H45C	109.5	C27—C28—H28	120.0
H25E—N25A—H25F	107.5	C27—C28—C29	120.0
C44A—N25A—H25E	108.5	C29—C28—H28	120.0
C44A—N25A—H25F	108.5	C28—C29—H29	120.0
C45A—N25A—H25E	108.5	C28—C29—C30	120.0
C45A—N25A—H25F	108.5	C30—C29—H29	120.0
C45A—N25A—C44A	115.1 (7)	C29—C30—H30	120.0
N25A—C44A—H44D	109.5	C31—C30—C29	120.0
N25A—C44A—H44E	109.5	C31—C30—H30	120.0
N25A—C44A—H44F	109.5	C30—C31—H31	120.0
H44D—C44A—H44E	109.5	C30—C31—C32	120.0
H44D—C44A—H44F	109.5	C32—C31—H31	120.0
H44E—C44A—H44F	109.5	C27—C32—H32	120.0
N25A—C45A—H45D	109.5	C31—C32—C27	120.0
N25A—C45A—H45E	109.5	C31—C32—H32	120.0
N25A—C45A—H45F	109.5	C28A—C27A—C26	125.5 (10)
H45D—C45A—H45E	109.5	C28A—C27A—C32A	120.0
H45D—C45A—H45F	109.5	C32A—C27A—C26	113.5 (9)
H45E—C45A—H45F	109.5	C27A—C28A—H28A	120.0
N1—C1—C2	123.5 (2)	C29A—C28A—C27A	120.0
N4—C1—N1	112.07 (19)	C29A—C28A—H28A	120.0
N4—C1—C2	124.4 (2)	C28A—C29A—H29A	120.0
C3—C2—C1	120.4 (2)	C30A—C29A—C28A	120.0
C7—C2—C1	120.6 (2)	C30A—C29A—H29A	120.0
C7—C2—C3	119.0 (2)	C29A—C30A—H30A	120.0
C2—C3—H3	119.5	C29A—C30A—C31A	120.0
C4—C3—C2	121.0 (2)	C31A—C30A—H30A	120.0
C4—C3—H3	119.5	C30A—C31A—H31A	120.0
C3—C4—H4	120.1	C32A—C31A—C30A	120.0
C5—C4—C3	119.8 (2)	C32A—C31A—H31A	120.0
C5—C4—H4	120.1	C27A—C32A—H32A	120.0
C4—C5—H5	120.1	C31A—C32A—C27A	120.0
C4—C5—C6	119.7 (2)	C31A—C32A—H32A	120.0
C6—C5—H5	120.1	N19—C33—H33A	109.5

C5—C6—H6	119.7	N19—C33—H33B	109.5
C5—C6—C7	120.5 (3)	N19—C33—H33C	109.5
C7—C6—H6	119.7	H33A—C33—H33B	109.5
C2—C7—C6	120.0 (3)	H33A—C33—H33C	109.5
C2—C7—H7	120.0	H33B—C33—H33C	109.5
C6—C7—H7	120.0	N19—C34—H34A	109.5
N5—C8—H8A	109.5	N19—C34—H34B	109.5
N5—C8—H8B	109.5	N19—C34—H34C	109.5
N5—C8—H8C	109.5	H34A—C34—H34B	109.5
H8A—C8—H8B	109.5	H34A—C34—H34C	109.5
H8A—C8—H8C	109.5	H34B—C34—H34C	109.5
H8B—C8—H8C	109.5	N20—C35—H35A	109.5
N5—C9—H9A	109.5	N20—C35—H35B	109.5
N5—C9—H9B	109.5	N20—C35—H35C	109.5
N5—C9—H9C	109.5	H35A—C35—H35B	109.5
H9A—C9—H9B	109.5	H35A—C35—H35C	109.5
H9A—C9—H9C	109.5	H35B—C35—H35C	109.5
H9B—C9—H9C	109.5	N20—C36—H36A	109.5
N6—C10—H10A	109.5	N20—C36—H36B	109.5
N6—C10—H10B	109.5	N20—C36—H36C	109.5
N6—C10—H10C	109.5	H36A—C36—H36B	109.5
H10A—C10—H10B	109.5	H36A—C36—H36C	109.5
H10A—C10—H10C	109.5	H36B—C36—H36C	109.5
H10B—C10—H10C	109.5	N21—C37—C38	124.2 (2)
N6—C11—H11A	109.5	N24—C37—N21	112.0 (2)
N6—C11—H11B	109.5	N24—C37—C38	123.9 (2)
N6—C11—H11C	109.5	C39—C38—C37	120.0 (2)
H11A—C11—H11B	109.5	C43—C38—C37	120.3 (2)
H11A—C11—H11C	109.5	C43—C38—C39	119.7 (2)
H11B—C11—H11C	109.5	C38—C39—H39	120.1
N7—C12—C13	120.6 (3)	C38—C39—C40	119.8 (2)
N7—C12—C13A	130.3 (3)	C40—C39—H39	120.1
N10—C12—N7	112.27 (19)	C39—C40—H40	120.0
N10—C12—C13	127.1 (3)	C41—C40—C39	120.0 (2)
N10—C12—C13A	117.4 (3)	C41—C40—H40	120.0
C14—C13—C12	122.6 (3)	C40—C41—H41	119.9
C14—C13—C18	120.0	C42—C41—C40	120.1 (2)
C18—C13—C12	117.3 (3)	C42—C41—H41	119.9
C13—C14—H14	120.0	C41—C42—H42	119.8
C13—C14—C15	120.0	C43—C42—C41	120.3 (2)
C15—C14—H14	120.0	C43—C42—H42	119.8
C14—C15—H15	120.0	C38—C43—H43	119.9
C16—C15—C14	120.0	C42—C43—C38	120.1 (2)
C16—C15—H15	120.0	C42—C43—H43	119.9
C15—C16—H16	120.0		

Ti1—N3—N4—C1	−178.70 (15)	N18—C26—C27—C28	−148.5 (4)
Ti1—N8—N9—Ti2	5.1 (3)	N18—C26—C27—C32	27.4 (5)

Ti1—N8—N9—N10	−178.59 (15)	N18—C26—C27A—C28A	−159.1 (8)
Ti1—N12—N13—Ti2	6.7 (3)	N18—C26—C27A—C32A	32.0 (15)
Ti1—N12—N13—N14	−174.66 (15)	N19—Ti2—N20—C35	41.5 (2)
Ti1—N16—N17—Ti2	0.9 (3)	N19—Ti2—N20—C36	−142.7 (2)
Ti1—N16—N17—N18	−172.50 (17)	N21—N22—N23—Ti2	178.79 (18)
Ti2—N9—N10—C12	176.63 (15)	N21—N22—N23—N24	0.5 (3)
Ti2—N13—N14—C19	178.54 (15)	N21—C37—C38—C39	20.1 (4)
Ti2—N17—N18—C26	−174.34 (18)	N21—C37—C38—C43	−158.9 (2)
Ti2—N23—N24—C37	−178.31 (17)	N22—N21—C37—N24	0.8 (3)
N1—N2—N3—Ti1	178.75 (15)	N22—N21—C37—C38	179.6 (2)
N1—N2—N3—N4	0.1 (3)	N22—N23—N24—C37	0.0 (3)
N1—C1—C2—C3	−10.2 (4)	N23—Ti2—N20—C35	−50.4 (2)
N1—C1—C2—C7	172.1 (3)	N23—Ti2—N20—C36	125.3 (2)
N2—N1—C1—N4	0.0 (3)	N23—N24—C37—N21	−0.5 (3)
N2—N1—C1—C2	179.0 (2)	N23—N24—C37—C38	−179.3 (2)
N2—N3—N4—C1	0.0 (2)	N24—C37—C38—C39	−161.3 (2)
N3—Ti1—N5—C8	46.1 (2)	N24—C37—C38—C43	19.7 (4)
N3—Ti1—N5—C9	−126.9 (2)	C1—N1—N2—N3	−0.1 (3)
N3—Ti1—N6—C10	44.08 (19)	C1—C2—C3—C4	−177.5 (2)
N3—Ti1—N6—C11	−132.57 (19)	C1—C2—C7—C6	176.7 (3)
N3—N4—C1—N1	0.0 (3)	C2—C3—C4—C5	0.2 (4)
N3—N4—C1—C2	−178.9 (2)	C3—C2—C7—C6	−1.0 (5)
N4—C1—C2—C3	168.5 (2)	C3—C4—C5—C6	0.2 (5)
N4—C1—C2—C7	−9.1 (4)	C4—C5—C6—C7	−1.0 (6)
N5—Ti1—N6—C10	145.65 (19)	C5—C6—C7—C2	1.4 (6)
N5—Ti1—N6—C11	−31.0 (2)	C7—C2—C3—C4	0.2 (4)
N6—Ti1—N5—C8	−46.8 (2)	C12—N7—N8—Ti1	178.60 (14)
N6—Ti1—N5—C9	140.2 (2)	C12—N7—N8—N9	−0.8 (2)
N7—N8—N9—Ti2	−175.61 (15)	C12—C13—C14—C15	−177.9 (4)
N7—N8—N9—N10	0.7 (2)	C12—C13—C18—C17	178.0 (4)
N7—C12—C13—C14	−9.2 (5)	C12—C13A—C14A—C15A	178.4 (6)
N7—C12—C13—C18	172.9 (3)	C12—C13A—C18A—C17A	−178.2 (6)
N7—C12—C13A—C14A	20.4 (7)	C13—C14—C15—C16	0.0
N7—C12—C13A—C18A	−161.3 (5)	C14—C13—C18—C17	0.0
N8—Ti1—N5—C8	−144.4 (2)	C14—C15—C16—C17	0.0
N8—Ti1—N5—C9	42.7 (2)	C15—C16—C17—C18	0.0
N8—Ti1—N6—C10	−123.46 (18)	C16—C17—C18—C13	0.0
N8—Ti1—N6—C11	59.88 (19)	C18—C13—C14—C15	0.0
N8—N7—C12—N10	0.6 (3)	C13A—C14A—C15A—C16A	0.0
N8—N7—C12—C13	−179.2 (3)	C14A—C13A—C18A—C17A	0.0
N8—N7—C12—C13A	−178.7 (4)	C14A—C15A—C16A—C17A	0.0
N8—N9—N10—C12	−0.3 (2)	C15A—C16A—C17A—C18A	0.0
N9—Ti2—N20—C35	140.9 (2)	C16A—C17A—C18A—C13A	0.0
N9—Ti2—N20—C36	−43.4 (2)	C18A—C13A—C14A—C15A	0.0
N9—N10—C12—N7	−0.2 (3)	C19—N11—N12—Ti1	175.55 (15)
N9—N10—C12—C13	179.6 (3)	C19—N11—N12—N13	0.5 (2)
N9—N10—C12—C13A	179.2 (3)	C19—C20—C21—C22	−179.1 (13)
N10—C12—C13—C14	170.9 (4)	C19—C20—C25—C24	179.1 (13)

N10—C12—C13—C18	−7.0 (5)	C19—C20A—C21A—C22A	173.9 (15)
N10—C12—C13A—C14A	−158.9 (5)	C19—C20A—C25A—C24A	−174.0 (15)
N10—C12—C13A—C18A	19.4 (7)	C19—C20B—C21B—C22B	−173.1 (15)
N11—N12—N13—Ti2	−178.75 (15)	C19—C20B—C25B—C24B	173.1 (15)
N11—N12—N13—N14	−0.1 (2)	C20—C21—C22—C23	0.0
N11—C19—C20—C21	9.3 (15)	C21—C20—C25—C24	0.0
N11—C19—C20—C25	−169.8 (6)	C21—C22—C23—C24	0.0
N11—C19—C20A—C21A	6.6 (13)	C22—C23—C24—C25	0.0
N11—C19—C20A—C25A	−179.4 (6)	C23—C24—C25—C20	0.0
N11—C19—C20B—C21B	−30.6 (13)	C25—C20—C21—C22	0.0
N11—C19—C20B—C25B	156.3 (8)	C20A—C21A—C22A—C23A	0.0
N12—Ti1—N5—C8	158.3 (2)	C21A—C20A—C25A—C24A	0.0
N12—Ti1—N5—C9	−14.6 (4)	C21A—C22A—C23A—C24A	0.0
N12—Ti1—N6—C10	−41.82 (19)	C22A—C23A—C24A—C25A	0.0
N12—Ti1—N6—C11	141.53 (18)	C23A—C24A—C25A—C20A	0.0
N12—N11—C19—N14	−0.7 (3)	C25A—C20A—C21A—C22A	0.0
N12—N11—C19—C20	178.4 (9)	C20B—C21B—C22B—C23B	0.0
N12—N11—C19—C20A	172.9 (9)	C21B—C20B—C25B—C24B	0.0
N12—N11—C19—C20B	−169.3 (10)	C21B—C22B—C23B—C24B	0.0
N12—N13—N14—C19	−0.3 (2)	C22B—C23B—C24B—C25B	0.0
N13—Ti2—N20—C35	−168.1 (2)	C23B—C24B—C25B—C20B	0.0
N13—Ti2—N20—C36	7.7 (4)	C25B—C20B—C21B—C22B	0.0
N13—N14—C19—N11	0.6 (3)	C26—N15—N16—Ti1	173.39 (16)
N13—N14—C19—C20	−178.5 (8)	C26—N15—N16—N17	−0.2 (3)
N13—N14—C19—C20A	−172.2 (10)	C26—C27—C28—C29	176.0 (6)
N13—N14—C19—C20B	170.5 (9)	C26—C27—C32—C31	−175.8 (6)
N14—C19—C20—C21	−171.7 (6)	C26—C27A—C28A—C29A	−168.2 (15)
N14—C19—C20—C25	9.2 (11)	C26—C27A—C32A—C31A	169.5 (14)
N14—C19—C20A—C21A	179.0 (6)	C27—C28—C29—C30	0.0
N14—C19—C20A—C25A	−7.0 (13)	C28—C27—C32—C31	0.0
N14—C19—C20B—C21B	161.4 (8)	C28—C29—C30—C31	0.0
N14—C19—C20B—C25B	−11.7 (15)	C29—C30—C31—C32	0.0
N15—N16—N17—Ti2	173.61 (16)	C30—C31—C32—C27	0.0
N15—N16—N17—N18	0.2 (3)	C32—C27—C28—C29	0.0
N15—C26—C27—C28	37.5 (8)	C27A—C28A—C29A—C30A	0.0
N15—C26—C27—C32	−146.6 (5)	C28A—C27A—C32A—C31A	0.0
N15—C26—C27A—C28A	8.6 (14)	C28A—C29A—C30A—C31A	0.0
N15—C26—C27A—C32A	−160.2 (9)	C29A—C30A—C31A—C32A	0.0
N16—Ti1—N5—C8	130.1 (2)	C30A—C31A—C32A—C27A	0.0
N16—Ti1—N5—C9	−42.9 (2)	C32A—C27A—C28A—C29A	0.0
N16—N15—C26—N18	0.1 (3)	C37—N21—N22—N23	−0.8 (3)
N16—N15—C26—C27	174.6 (5)	C37—C38—C39—C40	−177.6 (2)
N16—N15—C26—C27A	−169.5 (9)	C37—C38—C43—C42	177.6 (2)
N16—N17—N18—C26	−0.2 (3)	C38—C39—C40—C41	0.1 (4)
N17—Ti2—N20—C35	−132.8 (2)	C39—C38—C43—C42	−1.4 (4)
N17—Ti2—N20—C36	42.9 (2)	C39—C40—C41—C42	−1.6 (4)
N17—N18—C26—N15	0.1 (3)	C40—C41—C42—C43	1.6 (4)
N17—N18—C26—C27	−174.7 (5)	C41—C42—C43—C38	−0.1 (4)

N17—N18—C26—C27A	168.4 (10)	C43—C38—C39—C40	1.4 (3)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N25—H25*C*···N22	0.91	1.89	2.742 (7)	156
N25—H25*D*···N2	0.91	1.97	2.864 (8)	169
N25*A*—H25*E*···N22	0.91	2.00	2.847 (8)	154
N25*A*—H25*F*···N2	0.91	1.82	2.690 (8)	160

Bis(dimethylamido)-1κN,2κN-bis(dimethylamine)-1κN,2κN-tris(μ-5-phenyltetrazolato-1:2κ^2N^2:N^3)tris(5-phenyltetrazolato)-1κ^2N^2;2κ^2N^2,N^3- dizirconium(III)]–benzene–dichloromethane (1/1.12/0.38) (2)

Crystal data

$[Zr_2(C_7H_5N_4)_6(C_2H_6N)_2(C_2H_7N)_2]\cdot1.118C_6H_6\cdot0.382CH_2Cl_2$
M_r = 1351.41
Triclinic, $P\overline{1}$
a = 13.9631 (5) Å
b = 16.7619 (6) Å
c = 27.3054 (9) Å
α = 86.902 (1)°
β = 81.154 (1)°
γ = 89.969 (1)°
V = 6305.3 (4) Å^3
Z = 4
$F(000)$ = 2780
D_x = 1.424 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 7364 reflections
θ = 2.3–26.4°
μ = 0.43 mm^{-1}
T = 100 K
Block, black
0.4 × 0.3 × 0.2 mm

Data collection

Bruker SMART APEX CCD area detector diffractometer
φ and ω scans
Absorption correction: multi-scan (SADABS; Bruker, 2018)
T_{min} = 0.578, T_{max} = 0.745
70012 measured reflections
25682 independent reflections
20488 reflections with $I > 2\sigma(I)$
R_{int} = 0.040
θ_{max} = 26.4°, θ_{min} = 1.6°
h = −17→17
k = −20→20
l = −34→34

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.103
S = 1.01
25682 reflections
1671 parameters
67 restraints
Primary atom site location: dual
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0515P)^2 + 3.6611P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.002
$\Delta\rho_{max}$ = 0.78 e Å^{-3}
$\Delta\rho_{min}$ = −0.98 e Å^{-3}

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}	Occ. (<1)
Zr1	0.61268 (2)	0.30119 (2)	0.47371 (2)	0.01542 (6)	
Zr2	0.34460 (2)	0.20179 (2)	0.42388 (2)	0.01759 (6)	
N1	0.62854 (13)	0.22073 (11)	0.58320 (7)	0.0208 (4)	
N2	0.60391 (13)	0.20746 (11)	0.53866 (7)	0.0192 (4)	
N3	0.58410 (14)	0.13076 (11)	0.53494 (7)	0.0234 (4)	
N4	0.59644 (14)	0.09241 (11)	0.57734 (7)	0.0247 (4)	
N5	0.80075 (14)	0.31034 (12)	0.38630 (7)	0.0229 (4)	
N6	0.70385 (13)	0.31597 (11)	0.39458 (7)	0.0199 (4)	
N7	0.66779 (14)	0.30315 (12)	0.35321 (7)	0.0241 (4)	
N8	0.74034 (14)	0.28880 (13)	0.31795 (7)	0.0280 (5)	
N9	0.63792 (14)	0.41426 (11)	0.48542 (7)	0.0210 (4)	
N10	0.77681 (14)	0.27429 (11)	0.48624 (7)	0.0201 (4)	
H10	0.8031 (17)	0.2918 (15)	0.4576 (7)	0.024*	
N11	0.41333 (13)	0.31161 (11)	0.55967 (7)	0.0217 (4)	
N12	0.44930 (13)	0.28982 (11)	0.51454 (7)	0.0194 (4)	
N13	0.38227 (14)	0.25117 (11)	0.49607 (7)	0.0216 (4)	
N14	0.30044 (14)	0.24728 (11)	0.52818 (7)	0.0230 (4)	
N15	0.52088 (13)	0.42456 (11)	0.39744 (7)	0.0184 (4)	
N16	0.50747 (13)	0.35138 (10)	0.41900 (7)	0.0174 (4)	
N17	0.43992 (13)	0.31375 (11)	0.39964 (7)	0.0179 (4)	
N18	0.40824 (13)	0.36086 (11)	0.36503 (7)	0.0191 (4)	
N19	0.65646 (13)	0.14180 (11)	0.41511 (7)	0.0206 (4)	
N20	0.58099 (13)	0.18582 (11)	0.43214 (7)	0.0192 (4)	
N21	0.50045 (13)	0.15249 (11)	0.42243 (7)	0.0187 (4)	
N22	0.52220 (13)	0.08542 (11)	0.39893 (7)	0.0202 (4)	
N23	0.21105 (13)	0.28332 (11)	0.42890 (7)	0.0211 (4)	
N24	0.18528 (14)	0.20888 (11)	0.44746 (7)	0.0232 (4)	
N25	0.09398 (14)	0.20583 (12)	0.46739 (8)	0.0286 (5)	
N26	0.05718 (14)	0.27850 (13)	0.46227 (8)	0.0300 (5)	
N27	0.32391 (14)	0.07081 (11)	0.45608 (7)	0.0210 (4)	
H27	0.3670 (16)	0.0447 (14)	0.4388 (9)	0.025*	
N28	0.36740 (14)	0.18038 (11)	0.35261 (7)	0.0226 (4)	
C1	0.62307 (16)	0.14830 (13)	0.60612 (8)	0.0205 (5)	
C2	0.64476 (17)	0.13144 (14)	0.65660 (9)	0.0245 (5)	
C3	0.68779 (19)	0.18972 (15)	0.68025 (9)	0.0294 (6)	
H3	0.703395	0.240413	0.663675	0.035*	
C4	0.7082 (2)	0.17444 (17)	0.72797 (10)	0.0363 (6)	
H4	0.737349	0.214607	0.744162	0.044*	
C5	0.6858 (2)	0.10033 (18)	0.75192 (10)	0.0396 (7)	
H5	0.699961	0.089655	0.784565	0.048*	
C6	0.6433 (2)	0.04215 (17)	0.72872 (10)	0.0386 (7)	
H6	0.628119	−0.008528	0.745401	0.046*	
C7	0.62236 (18)	0.05710 (15)	0.68105 (9)	0.0298 (6)	
H7	0.592866	0.016792	0.665115	0.036*	
C8	0.82114 (17)	0.29256 (14)	0.33908 (8)	0.0236 (5)	

C9	0.91872 (18)	0.27617 (15)	0.31423 (9)	0.0266 (5)
C10	0.9320 (2)	0.22943 (19)	0.27315 (10)	0.0391 (7)
H10A	0.877308	0.209749	0.260602	0.047*
C11	1.0243 (2)	0.2115 (2)	0.25055 (11)	0.0468 (8)
H11	1.032876	0.179091	0.222761	0.056*
C12	1.1038 (2)	0.24065 (19)	0.26823 (10)	0.0414 (7)
H12	1.167278	0.228665	0.252458	0.050*
C13	1.09133 (19)	0.28737 (18)	0.30897 (10)	0.0368 (6)
H13	1.146295	0.307683	0.320991	0.044*
C14	0.99937 (18)	0.30453 (15)	0.33219 (10)	0.0302 (6)
H14	0.991163	0.335800	0.360515	0.036*
C15	0.61138 (17)	0.42062 (14)	0.53901 (9)	0.0253 (5)
H15A	0.556837	0.457340	0.545566	0.038*
H15B	0.666914	0.440987	0.552688	0.038*
H15C	0.592614	0.367799	0.554675	0.038*
C16	0.6714 (2)	0.48938 (15)	0.45970 (10)	0.0322 (6)
H16A	0.688532	0.481604	0.424122	0.048*
H16B	0.728414	0.508270	0.472702	0.048*
H16C	0.619724	0.529058	0.464893	0.048*
C17	0.81005 (17)	0.19055 (14)	0.49107 (9)	0.0240 (5)
H17A	0.784073	0.167261	0.524132	0.036*
H17B	0.881037	0.189648	0.486494	0.036*
H17C	0.787000	0.159430	0.465770	0.036*
C18	0.81420 (16)	0.32087 (14)	0.52359 (9)	0.0230 (5)
H18A	0.807665	0.378037	0.515320	0.034*
H18B	0.882684	0.308321	0.523833	0.034*
H18C	0.777100	0.307216	0.556439	0.034*
C19	0.32131 (16)	0.28518 (13)	0.56707 (9)	0.0222 (5)
C20	0.24926 (17)	0.29685 (15)	0.61158 (9)	0.0273 (5)
C21	0.2758 (2)	0.33139 (18)	0.65243 (11)	0.0449 (8)
H21	0.340865	0.348642	0.651736	0.054*
C22	0.2078 (3)	0.3409 (2)	0.69446 (13)	0.0580 (10)
H22	0.226500	0.364496	0.722445	0.070*
C23	0.1142 (2)	0.31654 (19)	0.69568 (13)	0.0534 (9)
H23	0.067624	0.323399	0.724376	0.064*
C24	0.0873 (2)	0.28183 (19)	0.65500 (12)	0.0465 (8)
H24	0.022110	0.264904	0.655945	0.056*
C25	0.15409 (19)	0.27145 (17)	0.61302 (11)	0.0376 (6)
H25	0.135124	0.247138	0.585340	0.045*
C26	0.45857 (16)	0.42866 (13)	0.36455 (8)	0.0184 (4)
C27	0.44358 (15)	0.49932 (13)	0.33280 (8)	0.0193 (5)
C28	0.39002 (16)	0.49213 (14)	0.29410 (8)	0.0222 (5)
H28	0.364471	0.441574	0.288319	0.027*
C29	0.37408 (17)	0.55839 (14)	0.26418 (9)	0.0258 (5)
H29	0.337534	0.553296	0.237888	0.031*
C30	0.41116 (18)	0.63209 (15)	0.27240 (9)	0.0273 (5)
H30	0.400530	0.677472	0.251598	0.033*
C31	0.46386 (18)	0.63978 (14)	0.31100 (9)	0.0261 (5)

H31	0.488549	0.690593	0.316902	0.031*
C32	0.48054 (16)	0.57368 (13)	0.34089 (9)	0.0218 (5)
H32	0.517370	0.579034	0.367040	0.026*
C33	0.61834 (16)	0.08062 (13)	0.39496 (8)	0.0184 (4)
C34	0.67460 (17)	0.01661 (14)	0.36960 (8)	0.0225 (5)
C35	0.77428 (19)	0.02168 (17)	0.35880 (11)	0.0397 (7)
H35	0.807664	0.066366	0.368220	0.048*
C36	0.8254 (2)	−0.0390 (2)	0.33407 (14)	0.0563 (10)
H36	0.894143	−0.036073	0.327002	0.068*
C37	0.7778 (2)	−0.10332 (19)	0.31972 (13)	0.0502 (8)
H37	0.813340	−0.144104	0.302299	0.060*
C38	0.6789 (2)	−0.10855 (16)	0.33056 (11)	0.0379 (7)
H38	0.645919	−0.153221	0.320852	0.046*
C39	0.62687 (19)	−0.04890 (15)	0.35562 (10)	0.0293 (5)
H39	0.558279	−0.052895	0.363264	0.035*
C40	0.12978 (16)	0.32573 (14)	0.43856 (9)	0.0225 (5)
C41	0.11764 (17)	0.41034 (14)	0.42446 (9)	0.0234 (5)
C42	0.03013 (19)	0.44829 (16)	0.43942 (10)	0.0342 (6)
H42	−0.021270	0.419545	0.459662	0.041*
C43	0.0174 (2)	0.52724 (17)	0.42509 (11)	0.0384 (7)
H43	−0.042829	0.552410	0.435179	0.046*
C44	0.09181 (19)	0.56970 (15)	0.39622 (10)	0.0313 (6)
H44	0.083071	0.624206	0.386593	0.038*
C45	0.17932 (18)	0.53285 (15)	0.38124 (9)	0.0285 (5)
H45	0.230731	0.562235	0.361440	0.034*
C46	0.19222 (17)	0.45358 (14)	0.39496 (9)	0.0253 (5)
H46	0.252195	0.428424	0.384222	0.030*
C47	0.22943 (18)	0.03270 (15)	0.45250 (11)	0.0339 (6)
H47A	0.177429	0.059708	0.473496	0.051*
H47B	0.230662	−0.023785	0.463684	0.051*
H47C	0.217838	0.037037	0.417962	0.051*
C48	0.3456 (2)	0.05685 (15)	0.50735 (9)	0.0310 (6)
H48A	0.410200	0.078238	0.509243	0.047*
H48B	0.343922	−0.000647	0.516161	0.047*
H48C	0.297158	0.083740	0.530521	0.047*
C49	0.2814 (2)	0.15562 (18)	0.33299 (11)	0.0402 (7)
H49A	0.291653	0.102347	0.320083	0.060*
H49B	0.269383	0.193745	0.306165	0.060*
H49C	0.225463	0.154119	0.359524	0.060*
C50	0.45123 (19)	0.18986 (16)	0.31334 (9)	0.0310 (6)
H50A	0.436490	0.229191	0.287723	0.047*
H50B	0.466121	0.138440	0.298565	0.047*
H50C	0.507229	0.208300	0.327420	0.047*
Zr1A	0.37957 (2)	0.70314 (2)	0.04253 (2)	0.01696 (6)
Zr2A	0.64966 (2)	0.80361 (2)	0.09192 (2)	0.01925 (6)
N1A	0.36150 (14)	0.77776 (11)	−0.06673 (7)	0.0221 (4)
N2A	0.38650 (13)	0.79473 (11)	−0.02306 (7)	0.0217 (4)
N3A	0.41342 (14)	0.87049 (11)	−0.02291 (7)	0.0238 (4)

N4A	0.40542 (15)	0.90441 (12)	−0.06726 (7)	0.0253 (4)
N5A	0.20531 (14)	0.64040 (12)	0.12747 (7)	0.0235 (4)
N6A	0.28677 (14)	0.68526 (11)	0.11991 (7)	0.0215 (4)
N7A	0.31114 (14)	0.70497 (12)	0.16280 (7)	0.0251 (4)
N8A	0.24647 (14)	0.67307 (12)	0.19905 (7)	0.0252 (4)
N9A	0.36279 (14)	0.59105 (12)	0.02498 (8)	0.0271 (5)
N10A	0.21364 (14)	0.72782 (12)	0.03220 (7)	0.0230 (4)
H10B	0.1874 (17)	0.7119 (15)	0.0611 (7)	0.028*
N11A	0.47335 (14)	0.58276 (11)	0.12085 (7)	0.0230 (4)
N12A	0.48419 (13)	0.65560 (11)	0.09910 (7)	0.0207 (4)
N13A	0.55103 (13)	0.69500 (11)	0.11788 (7)	0.0204 (4)
N14A	0.58527 (13)	0.64884 (11)	0.15251 (7)	0.0218 (4)
N15A	0.57138 (14)	0.68622 (11)	−0.04041 (7)	0.0231 (4)
N16A	0.54249 (13)	0.71614 (11)	0.00336 (7)	0.0207 (4)
N17A	0.61683 (14)	0.74946 (11)	0.01917 (7)	0.0225 (4)
N18A	0.69654 (14)	0.74154 (12)	−0.01383 (7)	0.0238 (4)
N19A	0.34077 (14)	0.86992 (11)	0.09398 (7)	0.0216 (4)
N20A	0.41367 (13)	0.82036 (11)	0.08255 (7)	0.0198 (4)
N21A	0.49519 (13)	0.85353 (11)	0.09094 (7)	0.0196 (4)
N22A	0.47646 (14)	0.92570 (11)	0.10816 (7)	0.0213 (4)
N23A	0.77778 (14)	0.71751 (12)	0.08384 (7)	0.0234 (4)
N24A	0.80739 (14)	0.79207 (12)	0.06710 (7)	0.0253 (4)
N25A	0.89672 (15)	0.79183 (14)	0.04436 (8)	0.0334 (5)
N26A	0.92812 (15)	0.71682 (14)	0.04562 (9)	0.0354 (5)
N27A	0.67541 (15)	0.93016 (12)	0.05386 (8)	0.0244 (4)
H27A	0.6310 (16)	0.9604 (14)	0.0670 (10)	0.029*
N28A	0.63770 (15)	0.82844 (12)	0.16301 (8)	0.0281 (5)
C1A	0.37409 (16)	0.84700 (13)	−0.09319 (8)	0.0202 (5)
C21A	0.51900 (18)	0.43569 (15)	0.17568 (10)	0.0299 (6)
H21A	0.482113	0.430854	0.149499	0.036*
C2A	0.35484 (17)	0.85862 (15)	−0.14460 (9)	0.0243 (5)
C3A	0.31896 (18)	0.79562 (16)	−0.16750 (10)	0.0302 (6)
H3A	0.306680	0.745332	−0.149869	0.036*
C4A	0.3010 (2)	0.80564 (18)	−0.21580 (10)	0.0368 (6)
H4A	0.275770	0.762408	−0.231124	0.044*
C5A	0.3195 (2)	0.87799 (19)	−0.24179 (10)	0.0418 (7)
H5A	0.307811	0.884380	−0.275138	0.050*
C6A	0.3550 (2)	0.94122 (18)	−0.21960 (10)	0.0406 (7)
H6A	0.367136	0.991202	−0.237602	0.049*
C7A	0.37299 (19)	0.93208 (16)	−0.17083 (9)	0.0312 (6)
H7A	0.397509	0.975675	−0.155544	0.037*
C8A	0.18268 (16)	0.63352 (13)	0.17671 (8)	0.0216 (5)
C9A	0.10072 (17)	0.58678 (14)	0.20418 (9)	0.0232 (5)
C10A	0.10237 (18)	0.55922 (15)	0.25292 (9)	0.0271 (5)
H10C	0.155284	0.572952	0.268998	0.033*
C11A	0.02767 (19)	0.51193 (15)	0.27831 (9)	0.0306 (6)
H11A	0.029839	0.492910	0.311535	0.037*
C12A	−0.0499 (2)	0.49240 (16)	0.25541 (10)	0.0341 (6)

H12A	−0.100673	0.459258	0.272646	0.041*
C13A	−0.0536 (2)	0.52101 (17)	0.20758 (10)	0.0362 (6)
H13A	−0.107957	0.508779	0.192213	0.043*
C14A	0.02166 (19)	0.56767 (16)	0.18156 (10)	0.0311 (6)
H14A	0.019086	0.586488	0.148340	0.037*
C15A	0.33493 (19)	0.51583 (14)	0.05217 (10)	0.0309 (6)
H15D	0.387914	0.477565	0.045879	0.046*
H15E	0.276807	0.494639	0.041229	0.046*
H15F	0.321248	0.524436	0.087771	0.046*
C16A	0.38255 (19)	0.58051 (16)	−0.02858 (10)	0.0328 (6)
H16D	0.397973	0.632451	−0.046268	0.049*
H16E	0.325264	0.557511	−0.039371	0.049*
H16F	0.437627	0.544526	−0.035899	0.049*
C17A	0.17900 (18)	0.81114 (15)	0.02603 (10)	0.0293 (6)
H17D	0.203433	0.844212	0.050009	0.044*
H17E	0.107975	0.811461	0.031756	0.044*
H17F	0.202769	0.832661	−0.007734	0.044*
C18A	0.17712 (17)	0.67913 (14)	−0.00470 (9)	0.0270 (5)
H18D	0.213647	0.692573	−0.037714	0.041*
H18E	0.108260	0.690248	−0.004885	0.041*
H18F	0.185254	0.622325	0.004062	0.041*
C19A	0.53665 (16)	0.58033 (14)	0.15330 (8)	0.0217 (5)
C20A	0.55593 (17)	0.50953 (14)	0.18418 (9)	0.0240 (5)
C22A	0.5357 (2)	0.36906 (16)	0.20516 (11)	0.0360 (6)
H22A	0.509589	0.318653	0.199486	0.043*
C23A	0.59041 (19)	0.37576 (16)	0.24297 (10)	0.0335 (6)
H23A	0.600926	0.330100	0.263572	0.040*
C24A	0.62965 (18)	0.44862 (15)	0.25077 (9)	0.0301 (6)
H24A	0.668468	0.452830	0.276209	0.036*
C25A	0.61248 (17)	0.51586 (15)	0.22145 (9)	0.0254 (5)
H25A	0.639370	0.566076	0.226882	0.030*
C26A	0.66635 (17)	0.70236 (13)	−0.05005 (8)	0.0216 (5)
C27A	0.73017 (18)	0.67617 (14)	−0.09393 (9)	0.0262 (5)
C28A	0.8295 (2)	0.67398 (18)	−0.09588 (10)	0.0390 (7)
H28A	0.858220	0.691142	−0.068844	0.047*
C29A	0.8871 (2)	0.6467 (2)	−0.13739 (11)	0.0497 (8)
H29A	0.955572	0.645890	−0.138982	0.060*
C30A	0.8459 (2)	0.62070 (18)	−0.17630 (11)	0.0485 (8)
H30A	0.885906	0.600877	−0.204287	0.058*
C31A	0.7469 (2)	0.62320 (18)	−0.17502 (11)	0.0444 (7)
H31A	0.718526	0.605926	−0.202127	0.053*
C32A	0.6894 (2)	0.65118 (16)	−0.13376 (10)	0.0346 (6)
H32A	0.621172	0.653314	−0.132700	0.042*
C33A	0.38131 (16)	0.93432 (13)	0.10943 (8)	0.0201 (5)
C34A	0.32784 (17)	1.00600 (13)	0.12636 (8)	0.0222 (5)
C35A	0.2296 (2)	1.01144 (17)	0.12761 (11)	0.0402 (7)
H35A	0.194593	0.968197	0.117579	0.048*
C36A	0.1810 (2)	1.07999 (18)	0.14348 (12)	0.0439 (7)

H36A	0.112902	1.083376	0.144313	0.053*	
C37A	0.2308 (2)	1.14256 (15)	0.15792 (10)	0.0342 (6)	
H37A	0.197420	1.189515	0.168451	0.041*	
C38A	0.3289 (2)	1.13745 (16)	0.15717 (13)	0.0452 (8)	
H38A	0.363446	1.180879	0.167324	0.054*	
C39A	0.3782 (2)	1.06897 (15)	0.14161 (12)	0.0383 (7)	
H39A	0.446164	1.065362	0.141430	0.046*	
C40A	0.85429 (17)	0.67146 (15)	0.06976 (9)	0.0258 (5)	
C41A	0.85979 (17)	0.58503 (15)	0.07928 (9)	0.0268 (5)	
C42A	0.94231 (19)	0.54378 (17)	0.05985 (10)	0.0349 (6)	
H42A	0.994610	0.571691	0.039765	0.042*	
C43A	0.9483 (2)	0.46300 (18)	0.06963 (11)	0.0394 (7)	
H43A	1.005177	0.435365	0.056590	0.047*	
C44A	0.8722 (2)	0.42134 (17)	0.09833 (10)	0.0360 (6)	
H44A	0.876692	0.365294	0.104741	0.043*	
C45A	0.78982 (19)	0.46150 (16)	0.11761 (10)	0.0341 (6)	
H45A	0.737339	0.433206	0.137290	0.041*	
C46A	0.78399 (18)	0.54318 (16)	0.10813 (10)	0.0315 (6)	
H46A	0.727393	0.570811	0.121560	0.038*	
C47A	0.76743 (19)	0.96858 (16)	0.06143 (11)	0.0370 (6)	
H47D	0.772408	0.965700	0.096891	0.056*	
H47E	0.768283	1.024653	0.049177	0.056*	
H47F	0.822330	0.940722	0.043216	0.056*	
C48A	0.6656 (2)	0.93651 (16)	0.00038 (10)	0.0358 (6)	
H48D	0.716534	0.905255	−0.018410	0.054*	
H48E	0.671755	0.992624	−0.011802	0.054*	
H48F	0.601933	0.915820	−0.003919	0.054*	
C49A	0.7266 (2)	0.83834 (19)	0.18419 (11)	0.0434 (7)	
H49D	0.734186	0.792635	0.207185	0.065*	
H49E	0.723058	0.887626	0.202101	0.065*	
H49F	0.782328	0.841379	0.157488	0.065*	
C50A	0.5533 (2)	0.82403 (17)	0.20201 (10)	0.0367 (6)	
H50D	0.494760	0.815381	0.187230	0.055*	
H50E	0.547571	0.874161	0.219072	0.055*	
H50F	0.561024	0.779594	0.225881	0.055*	
Cl1	0.9285 (3)	1.1746 (2)	0.11598 (13)	0.0669 (10)	0.357 (2)
Cl2	1.0097 (3)	1.0617 (2)	0.04681 (14)	0.0539 (9)	0.357 (2)
C25S	1.0205 (7)	1.1567 (6)	0.0675 (4)	0.046 (2)	0.357 (2)
H25B	1.017704	1.196837	0.039794	0.056*	0.357 (2)
H25C	1.084110	1.162264	0.078817	0.056*	0.357 (2)
Cl3	1.0223 (2)	0.79436 (19)	0.14804 (13)	0.0590 (9)	0.406 (2)
Cl4	1.0338 (3)	0.8803 (3)	0.23589 (13)	0.0950 (15)	0.406 (2)
C26S	1.0943 (6)	0.8270 (7)	0.1895 (4)	0.066 (3)	0.406 (2)
H26A	1.123951	0.779886	0.204610	0.079*	0.406 (2)
H26B	1.147494	0.860559	0.170973	0.079*	0.406 (2)
C1S	0.0684 (2)	−0.09231 (18)	0.39313 (12)	0.0429 (7)	
H1S	0.086158	−0.146729	0.397141	0.052*	
C2S	0.0093 (2)	−0.05709 (19)	0.43123 (11)	0.0407 (7)	

H2S	−0.014096	−0.087279	0.461119	0.049*	
C3S	−0.0151 (2)	0.02124 (19)	0.42557 (12)	0.0435 (7)	
H3S	−0.055299	0.045857	0.451685	0.052*	
C4S	0.0184 (2)	0.06485 (19)	0.38206 (15)	0.0526 (9)	
H4S	0.001858	0.119581	0.378283	0.063*	
C5S	0.0759 (2)	0.0288 (2)	0.34410 (12)	0.0540 (9)	
H5S	0.097930	0.058458	0.313819	0.065*	
C6S	0.1015 (2)	−0.0497 (2)	0.34990 (12)	0.0480 (8)	
H6S	0.142055	−0.074367	0.323914	0.058*	
C7S	0.9702 (4)	1.1481 (2)	0.07599 (17)	0.0587 (17)	0.643 (2)
H7S	0.980292	1.196289	0.055897	0.070*	0.643 (2)
C8S	1.0034 (3)	1.0762 (3)	0.05692 (12)	0.064 (3)	0.643 (2)
H8S	1.036185	1.075226	0.023792	0.077*	0.643 (2)
C9S	0.9886 (3)	1.0056 (2)	0.08633 (14)	0.0489 (12)	0.643 (2)
H9S	1.011290	0.956472	0.073294	0.059*	0.643 (2)
C10S	0.9406 (2)	1.0070 (2)	0.13480 (13)	0.0542 (13)	0.643 (2)
H10S	0.930502	0.958779	0.154901	0.065*	0.643 (2)
C11S	0.9074 (3)	1.0789 (3)	0.15388 (12)	0.0531 (13)	0.643 (2)
H11S	0.874610	1.079842	0.187007	0.064*	0.643 (2)
C12S	0.9222 (3)	1.1494 (2)	0.12447 (18)	0.070 (3)	0.643 (2)
H12S	0.899503	1.198597	0.137506	0.083*	0.643 (2)
C13S	0.9655 (5)	0.9447 (3)	0.21569 (18)	0.0416 (19)	0.357 (2)
H13S	0.941996	0.987281	0.235680	0.050*	0.357 (2)
C14S	0.9531 (4)	0.9463 (3)	0.16610 (19)	0.0399 (19)	0.357 (2)
H14S	0.921088	0.990028	0.152208	0.048*	0.357 (2)
C15S	0.9876 (4)	0.8840 (3)	0.13685 (16)	0.0382 (19)	0.357 (2)
H15S	0.979083	0.885119	0.102958	0.046*	0.357 (2)
C16S	1.0344 (5)	0.8201 (3)	0.1572 (2)	0.052 (4)	0.357 (2)
H16S	1.057985	0.777462	0.137180	0.063*	0.357 (2)
C17S	1.0469 (5)	0.8184 (3)	0.2068 (2)	0.039 (2)	0.357 (2)
H17S	1.078894	0.774713	0.220652	0.047*	0.357 (2)
C18S	1.0124 (6)	0.8807 (4)	0.23601 (17)	0.039 (3)	0.357 (2)
H18S	1.020900	0.879622	0.269903	0.047*	0.357 (2)
C19S	0.9980 (10)	0.8603 (8)	0.2339 (4)	0.071 (2)*	0.237 (2)
H19S	0.983326	0.888421	0.263431	0.085*	0.237 (2)
C20S	1.0894 (9)	0.8676 (8)	0.2055 (5)	0.071 (2)*	0.237 (2)
H20S	1.137241	0.900686	0.215588	0.085*	0.237 (2)
C21S	1.1109 (7)	0.8265 (9)	0.1624 (5)	0.071 (2)*	0.237 (2)
H21S	1.173341	0.831460	0.142946	0.085*	0.237 (2)
C22S	1.0409 (10)	0.7781 (9)	0.1476 (4)	0.071 (2)*	0.237 (2)
H22S	1.055526	0.749970	0.118145	0.085*	0.237 (2)
C23S	0.9494 (8)	0.7708 (7)	0.1761 (5)	0.071 (2)*	0.237 (2)
H23S	0.901612	0.737704	0.165988	0.085*	0.237 (2)
C24S	0.9280 (7)	0.8119 (8)	0.2192 (4)	0.071 (2)*	0.237 (2)
H24S	0.865510	0.806929	0.238631	0.085*	0.237 (2)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zr1	0.01761 (11)	0.01427 (11)	0.01456 (11)	−0.00046 (8)	−0.00293 (8)	−0.00102 (8)
Zr2	0.01791 (11)	0.01568 (11)	0.01906 (12)	−0.00183 (8)	−0.00321 (8)	0.00110 (8)
N1	0.0238 (10)	0.0195 (10)	0.0190 (10)	0.0019 (8)	−0.0030 (8)	0.0000 (8)
N2	0.0199 (9)	0.0197 (10)	0.0179 (10)	−0.0003 (7)	−0.0030 (7)	0.0005 (7)
N3	0.0271 (10)	0.0204 (10)	0.0226 (11)	−0.0037 (8)	−0.0047 (8)	0.0026 (8)
N4	0.0306 (11)	0.0203 (10)	0.0234 (11)	−0.0033 (8)	−0.0059 (8)	0.0032 (8)
N5	0.0228 (10)	0.0252 (11)	0.0199 (10)	−0.0013 (8)	−0.0010 (8)	−0.0004 (8)
N6	0.0209 (10)	0.0221 (10)	0.0171 (10)	−0.0006 (8)	−0.0037 (7)	−0.0020 (8)
N7	0.0252 (10)	0.0311 (11)	0.0166 (10)	0.0003 (8)	−0.0045 (8)	−0.0024 (8)
N8	0.0253 (11)	0.0384 (12)	0.0199 (11)	0.0036 (9)	−0.0009 (8)	−0.0055 (9)
N9	0.0238 (10)	0.0169 (10)	0.0230 (10)	−0.0004 (8)	−0.0052 (8)	−0.0024 (8)
N10	0.0220 (10)	0.0206 (10)	0.0176 (10)	−0.0018 (8)	−0.0032 (8)	−0.0006 (8)
N11	0.0209 (10)	0.0243 (10)	0.0193 (10)	0.0012 (8)	−0.0009 (8)	−0.0033 (8)
N12	0.0214 (10)	0.0191 (10)	0.0177 (10)	0.0017 (7)	−0.0034 (7)	−0.0005 (7)
N13	0.0249 (10)	0.0195 (10)	0.0193 (10)	−0.0010 (8)	−0.0012 (8)	0.0012 (8)
N14	0.0231 (10)	0.0234 (10)	0.0219 (11)	−0.0024 (8)	−0.0018 (8)	0.0008 (8)
N15	0.0201 (9)	0.0160 (9)	0.0185 (10)	0.0004 (7)	−0.0019 (7)	0.0008 (7)
N16	0.0194 (9)	0.0151 (9)	0.0173 (9)	−0.0002 (7)	−0.0019 (7)	0.0009 (7)
N17	0.0189 (9)	0.0159 (9)	0.0186 (10)	−0.0006 (7)	−0.0033 (7)	0.0021 (7)
N18	0.0213 (10)	0.0182 (10)	0.0172 (10)	0.0002 (7)	−0.0028 (7)	0.0024 (7)
N19	0.0231 (10)	0.0197 (10)	0.0202 (10)	0.0026 (8)	−0.0057 (8)	−0.0028 (8)
N20	0.0213 (10)	0.0186 (10)	0.0180 (10)	0.0010 (7)	−0.0048 (7)	0.0002 (7)
N21	0.0220 (10)	0.0158 (9)	0.0184 (10)	−0.0023 (7)	−0.0034 (7)	−0.0010 (7)
N22	0.0244 (10)	0.0153 (9)	0.0213 (10)	0.0002 (7)	−0.0041 (8)	−0.0023 (7)
N23	0.0211 (10)	0.0199 (10)	0.0226 (10)	−0.0024 (8)	−0.0048 (8)	0.0009 (8)
N24	0.0228 (10)	0.0206 (10)	0.0261 (11)	−0.0040 (8)	−0.0043 (8)	0.0012 (8)
N25	0.0231 (11)	0.0275 (11)	0.0336 (12)	−0.0024 (8)	0.0004 (9)	0.0010 (9)
N26	0.0226 (10)	0.0284 (12)	0.0370 (13)	−0.0009 (9)	0.0017 (9)	−0.0009 (9)
N27	0.0215 (10)	0.0183 (10)	0.0230 (11)	−0.0019 (8)	−0.0036 (8)	0.0012 (8)
N28	0.0267 (10)	0.0179 (10)	0.0236 (11)	−0.0020 (8)	−0.0058 (8)	0.0004 (8)
C1	0.0190 (11)	0.0207 (12)	0.0210 (12)	0.0021 (9)	−0.0017 (9)	0.0018 (9)
C2	0.0266 (12)	0.0251 (12)	0.0207 (12)	0.0055 (10)	−0.0012 (9)	0.0002 (10)
C3	0.0389 (15)	0.0270 (13)	0.0228 (13)	0.0072 (11)	−0.0062 (11)	−0.0012 (10)
C4	0.0501 (17)	0.0375 (16)	0.0241 (14)	0.0139 (13)	−0.0109 (12)	−0.0112 (11)
C5	0.0525 (18)	0.0486 (18)	0.0172 (13)	0.0188 (14)	−0.0050 (12)	0.0013 (12)
C6	0.0491 (17)	0.0377 (16)	0.0266 (15)	0.0101 (13)	−0.0018 (12)	0.0093 (12)
C7	0.0343 (14)	0.0287 (14)	0.0246 (13)	0.0018 (11)	−0.0013 (10)	0.0054 (10)
C8	0.0267 (12)	0.0271 (13)	0.0168 (12)	0.0002 (10)	−0.0030 (9)	−0.0006 (9)
C9	0.0286 (13)	0.0310 (14)	0.0193 (12)	0.0047 (10)	−0.0016 (10)	0.0000 (10)
C10	0.0303 (14)	0.062 (2)	0.0260 (14)	0.0050 (13)	−0.0055 (11)	−0.0115 (13)
C11	0.0390 (16)	0.077 (2)	0.0253 (15)	0.0158 (15)	−0.0040 (12)	−0.0189 (15)
C12	0.0308 (14)	0.068 (2)	0.0244 (14)	0.0133 (14)	−0.0003 (11)	−0.0034 (13)
C13	0.0301 (14)	0.0504 (18)	0.0296 (15)	0.0027 (12)	−0.0047 (11)	0.0001 (13)
C14	0.0324 (14)	0.0317 (14)	0.0265 (14)	0.0002 (11)	−0.0046 (11)	−0.0010 (11)
C15	0.0273 (12)	0.0222 (12)	0.0273 (13)	0.0009 (10)	−0.0055 (10)	−0.0067 (10)

C16	0.0398 (15)	0.0215 (13)	0.0374 (15)	−0.0085 (11)	−0.0144 (12)	0.0031 (11)
C17	0.0218 (12)	0.0229 (12)	0.0288 (13)	0.0036 (9)	−0.0076 (10)	−0.0041 (10)
C18	0.0221 (12)	0.0247 (12)	0.0230 (12)	−0.0010 (9)	−0.0052 (9)	−0.0039 (9)
C19	0.0231 (12)	0.0199 (12)	0.0230 (12)	0.0011 (9)	−0.0019 (9)	−0.0017 (9)
C20	0.0242 (12)	0.0256 (13)	0.0299 (14)	0.0046 (10)	0.0036 (10)	−0.0037 (10)
C21	0.0390 (16)	0.0505 (19)	0.0416 (18)	−0.0133 (14)	0.0116 (13)	−0.0213 (14)
C22	0.059 (2)	0.064 (2)	0.046 (2)	−0.0138 (17)	0.0161 (16)	−0.0310 (17)
C23	0.0473 (19)	0.0483 (19)	0.055 (2)	0.0007 (15)	0.0262 (16)	−0.0159 (16)
C24	0.0222 (14)	0.056 (2)	0.056 (2)	0.0024 (13)	0.0082 (13)	−0.0007 (16)
C25	0.0299 (14)	0.0440 (17)	0.0373 (16)	0.0011 (12)	0.0000 (12)	−0.0033 (13)
C26	0.0200 (11)	0.0180 (11)	0.0163 (11)	0.0015 (9)	0.0001 (8)	−0.0004 (9)
C27	0.0181 (11)	0.0205 (11)	0.0183 (12)	0.0020 (9)	−0.0004 (9)	0.0016 (9)
C28	0.0221 (12)	0.0218 (12)	0.0224 (12)	−0.0006 (9)	−0.0026 (9)	0.0001 (9)
C29	0.0247 (12)	0.0292 (13)	0.0232 (13)	0.0021 (10)	−0.0044 (10)	0.0021 (10)
C30	0.0304 (13)	0.0245 (13)	0.0247 (13)	0.0059 (10)	−0.0003 (10)	0.0066 (10)
C31	0.0331 (13)	0.0168 (12)	0.0273 (13)	−0.0015 (10)	−0.0017 (10)	0.0002 (10)
C32	0.0232 (12)	0.0220 (12)	0.0196 (12)	−0.0019 (9)	−0.0012 (9)	−0.0005 (9)
C33	0.0225 (11)	0.0170 (11)	0.0160 (11)	0.0004 (9)	−0.0045 (9)	0.0002 (8)
C34	0.0270 (12)	0.0215 (12)	0.0200 (12)	0.0061 (9)	−0.0067 (9)	−0.0026 (9)
C35	0.0280 (14)	0.0404 (16)	0.0558 (19)	0.0068 (12)	−0.0143 (13)	−0.0271 (14)
C36	0.0302 (16)	0.064 (2)	0.082 (3)	0.0179 (15)	−0.0168 (16)	−0.0430 (19)
C37	0.0458 (18)	0.0438 (18)	0.069 (2)	0.0206 (14)	−0.0223 (16)	−0.0329 (16)
C38	0.0453 (17)	0.0255 (14)	0.0466 (18)	0.0060 (12)	−0.0143 (13)	−0.0144 (12)
C39	0.0327 (14)	0.0235 (13)	0.0328 (14)	0.0035 (10)	−0.0071 (11)	−0.0059 (10)
C40	0.0210 (11)	0.0256 (12)	0.0211 (12)	−0.0004 (9)	−0.0028 (9)	−0.0044 (9)
C41	0.0246 (12)	0.0253 (12)	0.0213 (12)	0.0009 (9)	−0.0057 (9)	−0.0046 (9)
C42	0.0289 (14)	0.0333 (15)	0.0379 (16)	0.0045 (11)	0.0036 (11)	−0.0028 (12)
C43	0.0333 (15)	0.0363 (16)	0.0451 (17)	0.0135 (12)	−0.0023 (12)	−0.0080 (13)
C44	0.0429 (15)	0.0240 (13)	0.0295 (14)	0.0064 (11)	−0.0123 (11)	−0.0059 (10)
C45	0.0319 (13)	0.0263 (13)	0.0288 (14)	−0.0009 (10)	−0.0097 (11)	−0.0008 (10)
C46	0.0216 (12)	0.0284 (13)	0.0264 (13)	0.0016 (10)	−0.0050 (10)	−0.0015 (10)
C47	0.0257 (13)	0.0202 (13)	0.0556 (18)	−0.0052 (10)	−0.0094 (12)	0.0073 (12)
C48	0.0484 (16)	0.0225 (13)	0.0221 (13)	−0.0022 (11)	−0.0069 (11)	0.0045 (10)
C49	0.0321 (15)	0.0516 (18)	0.0414 (17)	0.0023 (13)	−0.0129 (12)	−0.0205 (14)
C50	0.0365 (14)	0.0312 (14)	0.0238 (13)	−0.0066 (11)	0.0003 (11)	−0.0001 (10)
Zr1A	0.01933 (11)	0.01475 (11)	0.01675 (12)	−0.00050 (8)	−0.00290 (8)	−0.00006 (8)
Zr2A	0.01831 (11)	0.01878 (12)	0.02023 (12)	−0.00096 (8)	−0.00181 (8)	−0.00063 (8)
N1A	0.0230 (10)	0.0208 (10)	0.0223 (11)	−0.0006 (8)	−0.0028 (8)	−0.0013 (8)
N2A	0.0230 (10)	0.0193 (10)	0.0228 (11)	−0.0008 (8)	−0.0034 (8)	−0.0001 (8)
N3A	0.0310 (11)	0.0209 (10)	0.0190 (10)	−0.0033 (8)	−0.0033 (8)	0.0024 (8)
N4A	0.0341 (11)	0.0216 (10)	0.0202 (10)	−0.0023 (8)	−0.0050 (8)	0.0025 (8)
N5A	0.0251 (10)	0.0242 (10)	0.0208 (11)	−0.0012 (8)	−0.0021 (8)	−0.0013 (8)
N6A	0.0239 (10)	0.0213 (10)	0.0195 (10)	−0.0006 (8)	−0.0037 (8)	−0.0008 (8)
N7A	0.0269 (11)	0.0290 (11)	0.0199 (11)	−0.0036 (8)	−0.0053 (8)	0.0000 (8)
N8A	0.0275 (11)	0.0275 (11)	0.0203 (11)	−0.0016 (8)	−0.0036 (8)	0.0006 (8)
N9A	0.0261 (11)	0.0213 (10)	0.0360 (12)	0.0017 (8)	−0.0102 (9)	−0.0048 (9)
N10A	0.0243 (10)	0.0257 (11)	0.0183 (10)	−0.0004 (8)	−0.0025 (8)	0.0034 (8)
N11A	0.0248 (10)	0.0194 (10)	0.0244 (11)	0.0002 (8)	−0.0041 (8)	0.0029 (8)

N12A	0.0221 (10)	0.0172 (9)	0.0226 (10)	0.0000 (8)	−0.0034 (8)	0.0011 (8)
N13A	0.0215 (10)	0.0206 (10)	0.0189 (10)	0.0014 (8)	−0.0030 (8)	0.0024 (8)
N14A	0.0226 (10)	0.0203 (10)	0.0221 (10)	0.0018 (8)	−0.0034 (8)	0.0034 (8)
N15A	0.0261 (10)	0.0221 (10)	0.0206 (11)	0.0004 (8)	−0.0023 (8)	−0.0018 (8)
N16A	0.0242 (10)	0.0193 (10)	0.0181 (10)	0.0008 (8)	−0.0020 (8)	−0.0010 (8)
N17A	0.0235 (10)	0.0224 (10)	0.0205 (10)	−0.0013 (8)	−0.0001 (8)	−0.0004 (8)
N18A	0.0253 (10)	0.0240 (10)	0.0210 (10)	−0.0015 (8)	−0.0005 (8)	−0.0006 (8)
N19A	0.0233 (10)	0.0215 (10)	0.0199 (10)	0.0040 (8)	−0.0034 (8)	−0.0011 (8)
N20A	0.0206 (9)	0.0197 (10)	0.0191 (10)	0.0009 (8)	−0.0031 (7)	0.0000 (8)
N21A	0.0237 (10)	0.0162 (9)	0.0184 (10)	−0.0011 (7)	−0.0013 (8)	−0.0010 (7)
N22A	0.0247 (10)	0.0162 (10)	0.0221 (10)	−0.0003 (8)	−0.0013 (8)	−0.0004 (8)
N23A	0.0218 (10)	0.0273 (11)	0.0217 (10)	0.0002 (8)	−0.0047 (8)	−0.0024 (8)
N24A	0.0230 (10)	0.0272 (11)	0.0255 (11)	−0.0025 (8)	−0.0037 (8)	−0.0010 (8)
N25A	0.0219 (11)	0.0398 (13)	0.0361 (13)	−0.0011 (9)	0.0028 (9)	−0.0003 (10)
N26A	0.0264 (11)	0.0380 (13)	0.0398 (14)	0.0035 (10)	0.0010 (10)	−0.0021 (10)
N27A	0.0254 (11)	0.0210 (10)	0.0251 (11)	−0.0028 (8)	0.0018 (8)	−0.0009 (8)
N28A	0.0351 (12)	0.0259 (11)	0.0222 (11)	−0.0014 (9)	−0.0009 (9)	−0.0008 (8)
C1A	0.0193 (11)	0.0208 (12)	0.0198 (12)	0.0008 (9)	−0.0006 (9)	−0.0001 (9)
C21A	0.0334 (14)	0.0254 (13)	0.0323 (14)	−0.0003 (10)	−0.0106 (11)	0.0031 (11)
C2A	0.0247 (12)	0.0291 (13)	0.0185 (12)	0.0017 (10)	−0.0009 (9)	−0.0029 (10)
C3A	0.0326 (14)	0.0317 (14)	0.0269 (14)	0.0015 (11)	−0.0051 (11)	−0.0056 (11)
C4A	0.0403 (16)	0.0453 (17)	0.0271 (15)	0.0043 (13)	−0.0079 (12)	−0.0149 (12)
C5A	0.0455 (17)	0.061 (2)	0.0195 (14)	0.0090 (14)	−0.0066 (12)	−0.0062 (13)
C6A	0.0524 (18)	0.0445 (17)	0.0233 (14)	0.0025 (14)	−0.0034 (12)	0.0061 (12)
C7A	0.0385 (15)	0.0324 (14)	0.0221 (13)	−0.0022 (11)	−0.0040 (11)	0.0006 (10)
C8A	0.0261 (12)	0.0195 (11)	0.0188 (12)	0.0026 (9)	−0.0025 (9)	−0.0009 (9)
C9A	0.0276 (12)	0.0204 (12)	0.0205 (12)	−0.0003 (9)	0.0004 (9)	−0.0035 (9)
C10A	0.0295 (13)	0.0290 (13)	0.0222 (13)	−0.0020 (10)	−0.0020 (10)	−0.0022 (10)
C11A	0.0387 (15)	0.0291 (14)	0.0221 (13)	−0.0030 (11)	0.0012 (11)	−0.0011 (10)
C12A	0.0374 (15)	0.0314 (14)	0.0307 (15)	−0.0107 (11)	0.0041 (11)	−0.0046 (11)
C13A	0.0337 (15)	0.0410 (16)	0.0345 (16)	−0.0110 (12)	−0.0048 (12)	−0.0074 (12)
C14A	0.0374 (14)	0.0344 (14)	0.0222 (13)	−0.0081 (11)	−0.0067 (11)	−0.0011 (11)
C15A	0.0333 (14)	0.0194 (12)	0.0409 (16)	−0.0009 (10)	−0.0082 (11)	−0.0026 (11)
C16A	0.0327 (14)	0.0274 (14)	0.0397 (16)	−0.0044 (11)	−0.0105 (12)	0.0008 (11)
C17A	0.0265 (13)	0.0297 (14)	0.0344 (15)	0.0069 (10)	−0.0106 (11)	−0.0084 (11)
C18A	0.0228 (12)	0.0250 (13)	0.0340 (14)	−0.0027 (10)	−0.0062 (10)	−0.0030 (10)
C19A	0.0215 (11)	0.0220 (12)	0.0211 (12)	0.0025 (9)	−0.0019 (9)	0.0010 (9)
C20A	0.0227 (12)	0.0230 (12)	0.0251 (13)	0.0030 (9)	−0.0017 (9)	0.0035 (10)
C22A	0.0415 (16)	0.0236 (13)	0.0441 (17)	0.0009 (11)	−0.0124 (13)	0.0040 (12)
C23A	0.0391 (15)	0.0282 (14)	0.0322 (15)	0.0084 (11)	−0.0065 (11)	0.0094 (11)
C24A	0.0304 (13)	0.0350 (14)	0.0249 (13)	0.0061 (11)	−0.0063 (10)	0.0030 (11)
C25A	0.0269 (12)	0.0253 (13)	0.0235 (13)	0.0032 (10)	−0.0028 (10)	0.0011 (10)
C26A	0.0264 (12)	0.0169 (11)	0.0208 (12)	0.0012 (9)	−0.0014 (9)	−0.0009 (9)
C27A	0.0327 (13)	0.0196 (12)	0.0241 (13)	0.0036 (10)	0.0023 (10)	0.0000 (10)
C28A	0.0340 (15)	0.0561 (19)	0.0262 (14)	0.0110 (13)	−0.0040 (11)	0.0015 (13)
C29A	0.0386 (17)	0.068 (2)	0.0385 (18)	0.0253 (15)	0.0031 (13)	0.0069 (15)
C30A	0.067 (2)	0.0395 (17)	0.0324 (17)	0.0182 (15)	0.0127 (15)	−0.0022 (13)
C31A	0.062 (2)	0.0388 (17)	0.0293 (16)	−0.0066 (14)	0.0055 (14)	−0.0111 (12)

C32A	0.0424 (16)	0.0304 (14)	0.0293 (15)	−0.0091 (12)	0.0031 (12)	−0.0091 (11)
C33A	0.0252 (12)	0.0190 (11)	0.0151 (11)	0.0007 (9)	−0.0009 (9)	0.0018 (9)
C34A	0.0293 (12)	0.0196 (12)	0.0163 (12)	0.0043 (9)	−0.0004 (9)	0.0011 (9)
C35A	0.0363 (15)	0.0374 (16)	0.0528 (19)	0.0117 (12)	−0.0179 (13)	−0.0224 (14)
C36A	0.0355 (16)	0.0447 (18)	0.056 (2)	0.0209 (13)	−0.0160 (14)	−0.0208 (15)
C37A	0.0465 (16)	0.0230 (13)	0.0298 (14)	0.0116 (11)	0.0046 (12)	−0.0012 (11)
C38A	0.0422 (17)	0.0196 (14)	0.070 (2)	−0.0014 (12)	0.0068 (15)	−0.0105 (13)
C39A	0.0274 (14)	0.0234 (14)	0.061 (2)	−0.0012 (11)	0.0053 (13)	−0.0091 (13)
C40A	0.0197 (12)	0.0338 (14)	0.0247 (13)	0.0040 (10)	−0.0045 (9)	−0.0050 (10)
C41A	0.0253 (12)	0.0331 (14)	0.0239 (13)	0.0057 (10)	−0.0079 (10)	−0.0065 (10)
C42A	0.0314 (14)	0.0413 (16)	0.0315 (15)	0.0109 (12)	−0.0023 (11)	−0.0063 (12)
C43A	0.0370 (15)	0.0473 (18)	0.0342 (16)	0.0177 (13)	−0.0040 (12)	−0.0093 (13)
C44A	0.0453 (16)	0.0329 (15)	0.0346 (15)	0.0105 (12)	−0.0181 (13)	−0.0108 (12)
C45A	0.0328 (14)	0.0328 (15)	0.0386 (16)	0.0030 (11)	−0.0111 (12)	−0.0039 (12)
C46A	0.0279 (13)	0.0332 (14)	0.0340 (15)	0.0083 (11)	−0.0053 (11)	−0.0058 (11)
C47A	0.0282 (14)	0.0276 (14)	0.0529 (18)	−0.0076 (11)	0.0006 (12)	0.0003 (12)
C48A	0.0554 (18)	0.0248 (13)	0.0247 (14)	−0.0030 (12)	0.0014 (12)	0.0016 (10)
C49A	0.0457 (17)	0.0542 (19)	0.0311 (16)	−0.0053 (14)	−0.0043 (13)	−0.0134 (13)
C50A	0.0453 (16)	0.0364 (15)	0.0255 (14)	−0.0032 (12)	0.0039 (12)	−0.0021 (11)
Cl1	0.077 (2)	0.0678 (19)	0.0477 (17)	0.0210 (15)	0.0134 (15)	0.0055 (15)
Cl2	0.061 (2)	0.0524 (16)	0.0445 (15)	−0.0176 (14)	0.0021 (13)	−0.0008 (13)
C25S	0.048 (6)	0.051 (6)	0.040 (5)	0.011 (5)	−0.010 (5)	−0.002 (4)
Cl3	0.0656 (19)	0.0556 (18)	0.0608 (16)	0.0213 (14)	−0.0219 (13)	−0.0144 (14)
Cl4	0.077 (2)	0.157 (4)	0.057 (2)	0.022 (2)	−0.0135 (16)	−0.049 (2)
C26S	0.044 (6)	0.079 (8)	0.078 (8)	0.021 (5)	−0.008 (5)	−0.035 (7)
C1S	0.0385 (16)	0.0365 (16)	0.058 (2)	0.0031 (13)	−0.0189 (14)	−0.0094 (14)
C2S	0.0341 (15)	0.0507 (19)	0.0380 (17)	−0.0108 (13)	−0.0093 (12)	0.0028 (14)
C3S	0.0302 (15)	0.055 (2)	0.0495 (19)	0.0025 (13)	−0.0126 (13)	−0.0191 (15)
C4S	0.0496 (19)	0.0336 (17)	0.084 (3)	−0.0050 (14)	−0.0389 (19)	−0.0006 (17)
C5S	0.0379 (17)	0.082 (3)	0.0431 (19)	−0.0263 (17)	−0.0168 (14)	0.0194 (18)
C6S	0.0308 (15)	0.075 (2)	0.0408 (18)	−0.0004 (15)	−0.0075 (13)	−0.0202 (17)
C7S	0.042 (3)	0.068 (4)	0.070 (4)	0.005 (3)	−0.027 (3)	0.010 (3)
C8S	0.049 (5)	0.083 (5)	0.066 (5)	−0.007 (4)	−0.029 (4)	0.008 (4)
C9S	0.039 (3)	0.054 (3)	0.059 (3)	−0.001 (2)	−0.022 (2)	−0.016 (2)
C10S	0.043 (3)	0.062 (3)	0.061 (3)	−0.014 (2)	−0.022 (2)	0.006 (2)
C11S	0.033 (2)	0.081 (3)	0.045 (3)	−0.005 (2)	0.000 (2)	−0.012 (2)
C12S	0.028 (3)	0.096 (6)	0.085 (5)	0.005 (3)	−0.011 (3)	−0.005 (4)
C13S	0.050 (4)	0.033 (3)	0.039 (4)	0.005 (3)	0.003 (3)	0.000 (3)
C14S	0.034 (4)	0.040 (5)	0.044 (5)	−0.005 (3)	−0.002 (3)	0.005 (4)
C15S	0.041 (4)	0.042 (5)	0.030 (4)	−0.013 (4)	−0.003 (3)	0.000 (3)
C16S	0.050 (7)	0.048 (8)	0.054 (9)	−0.008 (6)	0.007 (6)	−0.005 (6)
C17S	0.046 (5)	0.034 (4)	0.037 (5)	0.008 (3)	−0.001 (4)	−0.002 (3)
C18S	0.060 (6)	0.031 (4)	0.023 (5)	0.010 (4)	0.002 (4)	0.000 (3)

Geometric parameters (Å, º)

Zr1—N2	2.2935 (18)	N10A—C18A	1.479 (3)
Zr1—N6	2.3340 (19)	N11A—N12A	1.327 (3)

Zr1—N9	1.9798 (19)	N11A—C19A	1.343 (3)
Zr1—N10	2.4073 (19)	N12A—N13A	1.325 (3)
Zr1—N12	2.3829 (18)	N13A—N14A	1.335 (3)
Zr1—N16	2.3741 (18)	N14A—C19A	1.332 (3)
Zr1—N20	2.3699 (19)	N15A—N16A	1.326 (3)
Zr2—N13	2.3115 (19)	N15A—C26A	1.337 (3)
Zr2—N17	2.3085 (17)	N16A—N17A	1.319 (3)
Zr2—N21	2.3227 (18)	N17A—N18A	1.331 (3)
Zr2—N23	2.3027 (19)	N18A—C26A	1.336 (3)
Zr2—N24	2.2238 (19)	N19A—N20A	1.324 (3)
Zr2—N27	2.3218 (19)	N19A—C33A	1.337 (3)
Zr2—N28	1.975 (2)	N20A—N21A	1.324 (3)
N1—N2	1.343 (3)	N21A—N22A	1.333 (3)
N1—C1	1.332 (3)	N22A—C33A	1.332 (3)
N2—N3	1.328 (3)	N23A—N24A	1.350 (3)
N3—N4	1.328 (3)	N23A—C40A	1.338 (3)
N4—C1	1.343 (3)	N24A—N25A	1.305 (3)
N5—N6	1.341 (3)	N25A—N26A	1.332 (3)
N5—C8	1.327 (3)	N26A—C40A	1.347 (3)
N6—N7	1.333 (3)	N27A—H27A	0.849 (16)
N7—N8	1.317 (3)	N27A—C47A	1.485 (3)
N8—C8	1.347 (3)	N27A—C48A	1.486 (3)
N9—C15	1.463 (3)	N28A—C49A	1.461 (3)
N9—C16	1.449 (3)	N28A—C50A	1.461 (3)
N10—H10	0.847 (16)	C1A—C2A	1.472 (3)
N10—C17	1.484 (3)	C21A—H21A	0.9500
N10—C18	1.474 (3)	C21A—C20A	1.386 (3)
N11—N12	1.328 (3)	C21A—C22A	1.382 (3)
N11—C19	1.341 (3)	C2A—C3A	1.388 (3)
N12—N13	1.316 (3)	C2A—C7A	1.394 (3)
N13—N14	1.328 (3)	C3A—H3A	0.9500
N14—C19	1.336 (3)	C3A—C4A	1.381 (4)
N15—N16	1.332 (2)	C4A—H4A	0.9500
N15—C26	1.342 (3)	C4A—C5A	1.376 (4)
N16—N17	1.325 (2)	C5A—H5A	0.9500
N17—N18	1.326 (2)	C5A—C6A	1.377 (4)
N18—C26	1.335 (3)	C6A—H6A	0.9500
N19—N20	1.325 (3)	C6A—C7A	1.393 (4)
N19—C33	1.338 (3)	C7A—H7A	0.9500
N20—N21	1.325 (2)	C8A—C9A	1.470 (3)
N21—N22	1.336 (3)	C9A—C10A	1.389 (3)
N22—C33	1.333 (3)	C9A—C14A	1.391 (3)
N23—N24	1.349 (3)	C10A—H10C	0.9500
N23—C40	1.338 (3)	C10A—C11A	1.384 (3)
N24—N25	1.307 (3)	C11A—H11A	0.9500
N25—N26	1.331 (3)	C11A—C12A	1.379 (4)
N26—C40	1.348 (3)	C12A—H12A	0.9500
N27—H27	0.843 (16)	C12A—C13A	1.375 (4)

N27—C47	1.485 (3)	C13A—H13A	0.9500
N27—C48	1.484 (3)	C13A—C14A	1.390 (4)
N28—C49	1.457 (3)	C14A—H14A	0.9500
N28—C50	1.463 (3)	C15A—H15D	0.9800
C1—C2	1.469 (3)	C15A—H15E	0.9800
C2—C3	1.386 (4)	C15A—H15F	0.9800
C2—C7	1.394 (3)	C16A—H16D	0.9800
C3—H3	0.9500	C16A—H16E	0.9800
C3—C4	1.387 (4)	C16A—H16F	0.9800
C4—H4	0.9500	C17A—H17D	0.9800
C4—C5	1.385 (4)	C17A—H17E	0.9800
C5—H5	0.9500	C17A—H17F	0.9800
C5—C6	1.374 (4)	C18A—H18D	0.9800
C6—H6	0.9500	C18A—H18E	0.9800
C6—C7	1.387 (4)	C18A—H18F	0.9800
C7—H7	0.9500	C19A—C20A	1.467 (3)
C8—C9	1.459 (3)	C20A—C25A	1.389 (3)
C9—C10	1.392 (4)	C22A—H22A	0.9500
C9—C14	1.389 (3)	C22A—C23A	1.385 (4)
C10—H10A	0.9500	C23A—H23A	0.9500
C10—C11	1.380 (4)	C23A—C24A	1.379 (4)
C11—H11	0.9500	C24A—H24A	0.9500
C11—C12	1.377 (4)	C24A—C25A	1.389 (3)
C12—H12	0.9500	C25A—H25A	0.9500
C12—C13	1.384 (4)	C26A—C27A	1.466 (3)
C13—H13	0.9500	C27A—C28A	1.380 (4)
C13—C14	1.379 (4)	C27A—C32A	1.386 (4)
C14—H14	0.9500	C28A—H28A	0.9500
C15—H15A	0.9800	C28A—C29A	1.384 (4)
C15—H15B	0.9800	C29A—H29A	0.9500
C15—H15C	0.9800	C29A—C30A	1.374 (5)
C16—H16A	0.9800	C30A—H30A	0.9500
C16—H16B	0.9800	C30A—C31A	1.378 (5)
C16—H16C	0.9800	C31A—H31A	0.9500
C17—H17A	0.9800	C31A—C32A	1.383 (4)
C17—H17B	0.9800	C32A—H32A	0.9500
C17—H17C	0.9800	C33A—C34A	1.472 (3)
C18—H18A	0.9800	C34A—C35A	1.370 (4)
C18—H18B	0.9800	C34A—C39A	1.386 (4)
C18—H18C	0.9800	C35A—H35A	0.9500
C19—C20	1.475 (3)	C35A—C36A	1.390 (4)
C20—C21	1.384 (4)	C36A—H36A	0.9500
C20—C25	1.390 (4)	C36A—C37A	1.367 (4)
C21—H21	0.9500	C37A—H37A	0.9500
C21—C22	1.389 (4)	C37A—C38A	1.369 (4)
C22—H22	0.9500	C38A—H38A	0.9500
C22—C23	1.365 (5)	C38A—C39A	1.391 (4)
C23—H23	0.9500	C39A—H39A	0.9500

C23—C24	1.382 (5)	C40A—C41A	1.462 (4)
C24—H24	0.9500	C41A—C42A	1.392 (3)
C24—C25	1.381 (4)	C41A—C46A	1.385 (4)
C25—H25	0.9500	C42A—H42A	0.9500
C26—C27	1.464 (3)	C42A—C43A	1.371 (4)
C27—C28	1.396 (3)	C43A—H43A	0.9500
C27—C32	1.391 (3)	C43A—C44A	1.384 (4)
C28—H28	0.9500	C44A—H44A	0.9500
C28—C29	1.381 (3)	C44A—C45A	1.380 (4)
C29—H29	0.9500	C45A—H45A	0.9500
C29—C30	1.382 (3)	C45A—C46A	1.384 (4)
C30—H30	0.9500	C46A—H46A	0.9500
C30—C31	1.386 (3)	C47A—H47D	0.9800
C31—H31	0.9500	C47A—H47E	0.9800
C31—C32	1.381 (3)	C47A—H47F	0.9800
C32—H32	0.9500	C48A—H48D	0.9800
C33—C34	1.470 (3)	C48A—H48E	0.9800
C34—C35	1.379 (4)	C48A—H48F	0.9800
C34—C39	1.386 (3)	C49A—H49D	0.9800
C35—H35	0.9500	C49A—H49E	0.9800
C35—C36	1.388 (4)	C49A—H49F	0.9800
C36—H36	0.9500	C50A—H50D	0.9800
C36—C37	1.373 (4)	C50A—H50E	0.9800
C37—H37	0.9500	C50A—H50F	0.9800
C37—C38	1.368 (4)	Cl1—C25S	1.736 (11)
C38—H38	0.9500	Cl2—C25S	1.732 (11)
C38—C39	1.384 (4)	C25S—H25B	0.9900
C39—H39	0.9500	C25S—H25C	0.9900
C40—C41	1.466 (3)	Cl3—C26S	1.735 (7)
C41—C42	1.392 (3)	Cl4—C26S	1.705 (7)
C41—C46	1.392 (3)	C26S—H26A	0.9900
C42—H42	0.9500	C26S—H26B	0.9900
C42—C43	1.379 (4)	C1S—H1S	0.9500
C43—H43	0.9500	C1S—C2S	1.383 (4)
C43—C44	1.377 (4)	C1S—C6S	1.363 (5)
C44—H44	0.9500	C2S—H2S	0.9500
C44—C45	1.384 (4)	C2S—C3S	1.363 (4)
C45—H45	0.9500	C3S—H3S	0.9500
C45—C46	1.380 (3)	C3S—C4S	1.378 (5)
C46—H46	0.9500	C4S—H4S	0.9500
C47—H47A	0.9800	C4S—C5S	1.376 (5)
C47—H47B	0.9800	C5S—H5S	0.9500
C47—H47C	0.9800	C5S—C6S	1.372 (5)
C48—H48A	0.9800	C6S—H6S	0.9500
C48—H48B	0.9800	C7S—H7S	0.9500
C48—H48C	0.9800	C7S—C8S	1.3900
C49—H49A	0.9800	C7S—C12S	1.3900
C49—H49B	0.9800	C8S—H8S	0.9500

C49—H49C	0.9800	C8S—C9S	1.3900
C50—H50A	0.9800	C9S—H9S	0.9500
C50—H50B	0.9800	C9S—C10S	1.3900
C50—H50C	0.9800	C10S—H10S	0.9500
Zr1A—N2A	2.2856 (19)	C10S—C11S	1.3900
Zr1A—N6A	2.3073 (19)	C11S—H11S	0.9500
Zr1A—N9A	1.987 (2)	C11S—C12S	1.3900
Zr1A—N10A	2.4095 (19)	C12S—H12S	0.9500
Zr1A—N12A	2.3907 (18)	C13S—H13S	0.9500
Zr1A—N16A	2.3651 (19)	C13S—C14S	1.3900
Zr1A—N20A	2.3822 (19)	C13S—C18S	1.3900
Zr2A—N13A	2.2969 (18)	C14S—H14S	0.9500
Zr2A—N17A	2.336 (2)	C14S—C15S	1.3900
Zr2A—N21A	2.3166 (19)	C15S—H15S	0.9500
Zr2A—N23A	2.290 (2)	C15S—C16S	1.3900
Zr2A—N24A	2.214 (2)	C16S—H16S	0.9500
Zr2A—N27A	2.3145 (19)	C16S—C17S	1.3900
Zr2A—N28A	1.989 (2)	C17S—H17S	0.9500
N1A—N2A	1.338 (3)	C17S—C18S	1.3900
N1A—C1A	1.330 (3)	C18S—H18S	0.9500
N2A—N3A	1.325 (3)	C19S—H19S	0.9500
N3A—N4A	1.330 (3)	C19S—C20S	1.3900
N4A—C1A	1.337 (3)	C19S—C24S	1.3900
N5A—N6A	1.347 (3)	C20S—H20S	0.9500
N5A—C8A	1.332 (3)	C20S—C21S	1.3900
N6A—N7A	1.327 (3)	C21S—H21S	0.9500
N7A—N8A	1.323 (3)	C21S—C22S	1.3900
N8A—C8A	1.348 (3)	C22S—H22S	0.9500
N9A—C15A	1.450 (3)	C22S—C23S	1.3900
N9A—C16A	1.466 (3)	C23S—H23S	0.9500
N10A—H10B	0.847 (16)	C23S—C24S	1.3900
N10A—C17A	1.487 (3)	C24S—H24S	0.9500

N2—Zr1—N6	134.97 (7)	C1A—N1A—N2A	103.40 (18)
N2—Zr1—N10	73.39 (6)	N1A—N2A—Zr1A	123.14 (14)
N2—Zr1—N12	70.76 (6)	N3A—N2A—Zr1A	125.37 (15)
N2—Zr1—N16	136.58 (6)	N3A—N2A—N1A	111.47 (18)
N2—Zr1—N20	80.56 (6)	N2A—N3A—N4A	107.23 (18)
N6—Zr1—N10	75.26 (6)	N3A—N4A—C1A	106.12 (18)
N6—Zr1—N12	141.40 (6)	C8A—N5A—N6A	103.64 (18)
N6—Zr1—N16	72.74 (6)	N5A—N6A—Zr1A	121.77 (14)
N6—Zr1—N20	73.79 (6)	N7A—N6A—Zr1A	126.71 (14)
N9—Zr1—N2	119.12 (7)	N7A—N6A—N5A	110.71 (18)
N9—Zr1—N6	90.53 (7)	N8A—N7A—N6A	108.19 (18)
N9—Zr1—N10	87.31 (7)	N7A—N8A—C8A	105.85 (19)
N9—Zr1—N12	99.17 (7)	C15A—N9A—Zr1A	135.77 (17)
N9—Zr1—N16	86.27 (7)	C15A—N9A—C16A	110.9 (2)
N9—Zr1—N20	160.32 (7)	C16A—N9A—Zr1A	113.32 (15)

N12—Zr1—N10	141.97 (6)	Zr1A—N10A—H10B	97.7 (18)
N16—Zr1—N10	147.26 (6)	C17A—N10A—Zr1A	120.15 (14)
N16—Zr1—N12	70.77 (6)	C17A—N10A—H10B	104.6 (18)
N20—Zr1—N10	99.73 (6)	C18A—N10A—Zr1A	114.89 (15)
N20—Zr1—N12	86.62 (6)	C18A—N10A—H10B	109.3 (18)
N20—Zr1—N16	77.86 (6)	C18A—N10A—C17A	108.66 (18)
N13—Zr2—N21	79.81 (7)	N12A—N11A—C19A	104.34 (18)
N13—Zr2—N27	94.79 (7)	N11A—N12A—Zr1A	121.09 (14)
N17—Zr2—N13	74.01 (6)	N13A—N12A—Zr1A	129.15 (14)
N17—Zr2—N21	77.41 (6)	N13A—N12A—N11A	109.39 (17)
N17—Zr2—N27	151.53 (6)	N12A—N13A—Zr2A	135.17 (14)
N23—Zr2—N13	89.81 (7)	N12A—N13A—N14A	110.03 (17)
N23—Zr2—N17	88.12 (6)	N14A—N13A—Zr2A	112.03 (13)
N23—Zr2—N21	164.03 (6)	C19A—N14A—N13A	103.92 (18)
N23—Zr2—N27	118.47 (7)	N16A—N15A—C26A	104.48 (18)
N24—Zr2—N13	94.29 (7)	N15A—N16A—Zr1A	121.02 (14)
N24—Zr2—N17	122.35 (7)	N17A—N16A—Zr1A	129.28 (14)
N24—Zr2—N21	157.26 (7)	N17A—N16A—N15A	109.69 (18)
N24—Zr2—N23	34.62 (6)	N16A—N17A—Zr2A	137.44 (15)
N24—Zr2—N27	83.88 (7)	N16A—N17A—N18A	109.70 (18)
N27—Zr2—N21	74.84 (6)	N18A—N17A—Zr2A	112.34 (14)
N28—Zr2—N13	155.40 (7)	N17A—N18A—C26A	104.23 (18)
N28—Zr2—N17	84.68 (7)	N20A—N19A—C33A	104.74 (18)
N28—Zr2—N21	83.74 (7)	N19A—N20A—Zr1A	116.80 (14)
N28—Zr2—N23	101.82 (7)	N21A—N20A—Zr1A	133.03 (14)
N28—Zr2—N24	107.64 (8)	N21A—N20A—N19A	109.55 (18)
N28—Zr2—N27	98.43 (7)	N20A—N21A—Zr2A	132.39 (14)
C1—N1—N2	103.28 (18)	N20A—N21A—N22A	109.38 (18)
N1—N2—Zr1	124.70 (14)	N22A—N21A—Zr2A	117.53 (14)
N3—N2—Zr1	123.62 (14)	C33A—N22A—N21A	104.56 (18)
N3—N2—N1	111.29 (17)	N24A—N23A—Zr2A	69.52 (12)
N2—N3—N4	107.58 (18)	C40A—N23A—Zr2A	168.90 (17)
N3—N4—C1	105.93 (18)	C40A—N23A—N24A	104.53 (19)
C8—N5—N6	104.20 (18)	N23A—N24A—Zr2A	75.64 (12)
N5—N6—Zr1	122.93 (13)	N25A—N24A—Zr2A	168.83 (17)
N7—N6—Zr1	123.18 (14)	N25A—N24A—N23A	110.8 (2)
N7—N6—N5	110.12 (18)	N24A—N25A—N26A	108.0 (2)
N8—N7—N6	108.37 (18)	N25A—N26A—C40A	106.9 (2)
N7—N8—C8	105.84 (19)	Zr2A—N27A—H27A	108.1 (19)
C15—N9—Zr1	105.05 (14)	C47A—N27A—Zr2A	114.18 (15)
C16—N9—Zr1	142.02 (17)	C47A—N27A—H27A	105.0 (18)
C16—N9—C15	112.93 (19)	C47A—N27A—C48A	109.9 (2)
Zr1—N10—H10	95.9 (17)	C48A—N27A—Zr2A	115.15 (15)
C17—N10—Zr1	119.92 (13)	C48A—N27A—H27A	103.3 (19)
C17—N10—H10	105.3 (18)	C49A—N28A—Zr2A	118.14 (17)
C18—N10—Zr1	116.27 (14)	C50A—N28A—Zr2A	130.06 (18)
C18—N10—H10	108.6 (18)	C50A—N28A—C49A	110.7 (2)
C18—N10—C17	108.88 (17)	N1A—C1A—N4A	111.8 (2)

N12—N11—C19	104.57 (18)	N1A—C1A—C2A	123.8 (2)
N11—N12—Zr1	127.83 (14)	N4A—C1A—C2A	124.4 (2)
N13—N12—Zr1	122.40 (14)	C20A—C21A—H21A	119.9
N13—N12—N11	109.37 (17)	C22A—C21A—H21A	119.9
N12—N13—Zr2	143.33 (15)	C22A—C21A—C20A	120.2 (2)
N12—N13—N14	110.20 (18)	C3A—C2A—C1A	119.8 (2)
N14—N13—Zr2	105.68 (13)	C3A—C2A—C7A	119.4 (2)
N13—N14—C19	104.20 (18)	C7A—C2A—C1A	120.8 (2)
N16—N15—C26	104.27 (17)	C2A—C3A—H3A	119.8
N15—N16—Zr1	120.39 (13)	C4A—C3A—C2A	120.3 (3)
N17—N16—Zr1	129.65 (13)	C4A—C3A—H3A	119.8
N17—N16—N15	109.33 (16)	C3A—C4A—H4A	119.9
N16—N17—Zr2	134.22 (13)	C5A—C4A—C3A	120.2 (3)
N16—N17—N18	110.00 (17)	C5A—C4A—H4A	119.9
N18—N17—Zr2	114.01 (13)	C4A—C5A—H5A	119.9
N17—N18—C26	104.36 (17)	C4A—C5A—C6A	120.2 (3)
N20—N19—C33	104.64 (18)	C6A—C5A—H5A	119.9
N19—N20—Zr1	117.06 (13)	C5A—C6A—H6A	119.9
N21—N20—Zr1	133.38 (14)	C5A—C6A—C7A	120.2 (3)
N21—N20—N19	109.53 (17)	C7A—C6A—H6A	119.9
N20—N21—Zr2	131.62 (14)	C2A—C7A—H7A	120.2
N20—N21—N22	109.52 (17)	C6A—C7A—C2A	119.6 (3)
N22—N21—Zr2	117.40 (13)	C6A—C7A—H7A	120.2
C33—N22—N21	104.26 (18)	N5A—C8A—N8A	111.6 (2)
N24—N23—Zr2	69.49 (11)	N5A—C8A—C9A	125.1 (2)
C40—N23—Zr2	171.55 (16)	N8A—C8A—C9A	123.2 (2)
C40—N23—N24	104.30 (18)	C10A—C9A—C8A	120.2 (2)
N23—N24—Zr2	75.89 (11)	C10A—C9A—C14A	119.0 (2)
N25—N24—Zr2	170.93 (16)	C14A—C9A—C8A	120.8 (2)
N25—N24—N23	111.00 (18)	C9A—C10A—H10C	119.7
N24—N25—N26	107.97 (18)	C11A—C10A—C9A	120.7 (2)
N25—N26—C40	106.70 (19)	C11A—C10A—H10C	119.7
Zr2—N27—H27	105.1 (18)	C10A—C11A—H11A	120.0
C47—N27—Zr2	115.91 (14)	C12A—C11A—C10A	120.0 (2)
C47—N27—H27	106.9 (18)	C12A—C11A—H11A	120.0
C48—N27—Zr2	115.04 (14)	C11A—C12A—H12A	120.1
C48—N27—H27	103.6 (18)	C13A—C12A—C11A	119.9 (2)
C48—N27—C47	109.16 (19)	C13A—C12A—H12A	120.1
C49—N28—Zr2	114.57 (16)	C12A—C13A—H13A	119.7
C49—N28—C50	111.3 (2)	C12A—C13A—C14A	120.5 (2)
C50—N28—Zr2	133.88 (16)	C14A—C13A—H13A	119.7
N1—C1—N4	111.9 (2)	C9A—C14A—H14A	120.0
N1—C1—C2	124.0 (2)	C13A—C14A—C9A	119.9 (2)
N4—C1—C2	124.0 (2)	C13A—C14A—H14A	120.0
C3—C2—C1	119.9 (2)	N9A—C15A—H15D	109.5
C3—C2—C7	119.6 (2)	N9A—C15A—H15E	109.5
C7—C2—C1	120.5 (2)	N9A—C15A—H15F	109.5
C2—C3—H3	119.8	H15D—C15A—H15E	109.5

C2—C3—C4	120.3 (2)	H15D—C15A—H15F	109.5
C4—C3—H3	119.8	H15E—C15A—H15F	109.5
C3—C4—H4	120.2	N9A—C16A—H16D	109.5
C5—C4—C3	119.7 (3)	N9A—C16A—H16E	109.5
C5—C4—H4	120.2	N9A—C16A—H16F	109.5
C4—C5—H5	119.8	H16D—C16A—H16E	109.5
C6—C5—C4	120.4 (2)	H16D—C16A—H16F	109.5
C6—C5—H5	119.8	H16E—C16A—H16F	109.5
C5—C6—H6	119.9	N10A—C17A—H17D	109.5
C5—C6—C7	120.3 (3)	N10A—C17A—H17E	109.5
C7—C6—H6	119.9	N10A—C17A—H17F	109.5
C2—C7—H7	120.1	H17D—C17A—H17E	109.5
C6—C7—C2	119.8 (3)	H17D—C17A—H17F	109.5
C6—C7—H7	120.1	H17E—C17A—H17F	109.5
N5—C8—N8	111.5 (2)	N10A—C18A—H18D	109.5
N5—C8—C9	123.7 (2)	N10A—C18A—H18E	109.5
N8—C8—C9	124.8 (2)	N10A—C18A—H18F	109.5
C10—C9—C8	120.1 (2)	H18D—C18A—H18E	109.5
C14—C9—C8	120.6 (2)	H18D—C18A—H18F	109.5
C14—C9—C10	119.2 (2)	H18E—C18A—H18F	109.5
C9—C10—H10A	119.8	N11A—C19A—C20A	124.8 (2)
C11—C10—C9	120.3 (3)	N14A—C19A—N11A	112.32 (19)
C11—C10—H10A	119.8	N14A—C19A—C20A	122.8 (2)
C10—C11—H11	119.9	C21A—C20A—C19A	120.0 (2)
C12—C11—C10	120.1 (3)	C21A—C20A—C25A	119.7 (2)
C12—C11—H11	119.9	C25A—C20A—C19A	120.3 (2)
C11—C12—H12	120.0	C21A—C22A—H22A	120.0
C11—C12—C13	120.0 (3)	C21A—C22A—C23A	120.0 (2)
C13—C12—H12	120.0	C23A—C22A—H22A	120.0
C12—C13—H13	119.9	C22A—C23A—H23A	120.0
C14—C13—C12	120.2 (3)	C24A—C23A—C22A	120.1 (2)
C14—C13—H13	119.9	C24A—C23A—H23A	120.0
C9—C14—H14	119.9	C23A—C24A—H24A	120.0
C13—C14—C9	120.1 (3)	C23A—C24A—C25A	120.1 (2)
C13—C14—H14	119.9	C25A—C24A—H24A	120.0
N9—C15—H15A	109.5	C20A—C25A—C24A	119.9 (2)
N9—C15—H15B	109.5	C20A—C25A—H25A	120.1
N9—C15—H15C	109.5	C24A—C25A—H25A	120.1
H15A—C15—H15B	109.5	N15A—C26A—C27A	123.7 (2)
H15A—C15—H15C	109.5	N18A—C26A—N15A	111.9 (2)
H15B—C15—H15C	109.5	N18A—C26A—C27A	124.4 (2)
N9—C16—H16A	109.5	C28A—C27A—C26A	121.5 (2)
N9—C16—H16B	109.5	C28A—C27A—C32A	119.4 (2)
N9—C16—H16C	109.5	C32A—C27A—C26A	119.1 (2)
H16A—C16—H16B	109.5	C27A—C28A—H28A	120.1
H16A—C16—H16C	109.5	C27A—C28A—C29A	119.7 (3)
H16B—C16—H16C	109.5	C29A—C28A—H28A	120.1
N10—C17—H17A	109.5	C28A—C29A—H29A	119.8

N10—C17—H17B	109.5	C30A—C29A—C28A	120.4 (3)
N10—C17—H17C	109.5	C30A—C29A—H29A	119.8
H17A—C17—H17B	109.5	C29A—C30A—H30A	119.8
H17A—C17—H17C	109.5	C29A—C30A—C31A	120.5 (3)
H17B—C17—H17C	109.5	C31A—C30A—H30A	119.8
N10—C18—H18A	109.5	C30A—C31A—H31A	120.4
N10—C18—H18B	109.5	C30A—C31A—C32A	119.1 (3)
N10—C18—H18C	109.5	C32A—C31A—H31A	120.4
H18A—C18—H18B	109.5	C27A—C32A—H32A	119.6
H18A—C18—H18C	109.5	C31A—C32A—C27A	120.8 (3)
H18B—C18—H18C	109.5	C31A—C32A—H32A	119.6
N11—C19—C20	125.7 (2)	N19A—C33A—C34A	124.5 (2)
N14—C19—N11	111.6 (2)	N22A—C33A—N19A	111.8 (2)
N14—C19—C20	122.7 (2)	N22A—C33A—C34A	123.7 (2)
C21—C20—C19	120.7 (2)	C35A—C34A—C33A	121.4 (2)
C21—C20—C25	119.5 (2)	C35A—C34A—C39A	119.5 (2)
C25—C20—C19	119.8 (2)	C39A—C34A—C33A	119.1 (2)
C20—C21—H21	119.9	C34A—C35A—H35A	119.9
C20—C21—C22	120.2 (3)	C34A—C35A—C36A	120.2 (3)
C22—C21—H21	119.9	C36A—C35A—H35A	119.9
C21—C22—H22	119.9	C35A—C36A—H36A	119.8
C23—C22—C21	120.2 (3)	C37A—C36A—C35A	120.3 (3)
C23—C22—H22	119.9	C37A—C36A—H36A	119.8
C22—C23—H23	120.1	C36A—C37A—H37A	120.1
C22—C23—C24	119.7 (3)	C36A—C37A—C38A	119.9 (3)
C24—C23—H23	120.1	C38A—C37A—H37A	120.1
C23—C24—H24	119.6	C37A—C38A—H38A	119.9
C25—C24—C23	120.8 (3)	C37A—C38A—C39A	120.3 (3)
C25—C24—H24	119.6	C39A—C38A—H38A	119.9
C20—C25—H25	120.3	C34A—C39A—C38A	119.8 (3)
C24—C25—C20	119.5 (3)	C34A—C39A—H39A	120.1
C24—C25—H25	120.3	C38A—C39A—H39A	120.1
N15—C26—C27	124.95 (19)	N23A—C40A—N26A	109.8 (2)
N18—C26—N15	112.05 (18)	N23A—C40A—C41A	126.3 (2)
N18—C26—C27	123.0 (2)	N26A—C40A—C41A	123.9 (2)
C28—C27—C26	119.4 (2)	C42A—C41A—C40A	120.2 (2)
C32—C27—C26	121.3 (2)	C46A—C41A—C40A	120.8 (2)
C32—C27—C28	119.4 (2)	C46A—C41A—C42A	119.0 (2)
C27—C28—H28	119.9	C41A—C42A—H42A	119.9
C29—C28—C27	120.1 (2)	C43A—C42A—C41A	120.2 (3)
C29—C28—H28	119.9	C43A—C42A—H42A	119.9
C28—C29—H29	119.9	C42A—C43A—H43A	119.7
C28—C29—C30	120.2 (2)	C42A—C43A—C44A	120.6 (3)
C30—C29—H29	119.9	C44A—C43A—H43A	119.7
C29—C30—H30	120.0	C43A—C44A—H44A	120.1
C29—C30—C31	120.0 (2)	C45A—C44A—C43A	119.8 (3)
C31—C30—H30	120.0	C45A—C44A—H44A	120.1
C30—C31—H31	119.9	C44A—C45A—H45A	120.1

C32—C31—C30	120.1 (2)	C44A—C45A—C46A	119.7 (3)
C32—C31—H31	119.9	C46A—C45A—H45A	120.1
C27—C32—H32	119.9	C41A—C46A—H46A	119.6
C31—C32—C27	120.2 (2)	C45A—C46A—C41A	120.7 (2)
C31—C32—H32	119.9	C45A—C46A—H46A	119.6
N19—C33—C34	124.9 (2)	N27A—C47A—H47D	109.5
N22—C33—N19	112.1 (2)	N27A—C47A—H47E	109.5
N22—C33—C34	123.1 (2)	N27A—C47A—H47F	109.5
C35—C34—C33	120.7 (2)	H47D—C47A—H47E	109.5
C35—C34—C39	119.6 (2)	H47D—C47A—H47F	109.5
C39—C34—C33	119.6 (2)	H47E—C47A—H47F	109.5
C34—C35—H35	120.3	N27A—C48A—H48D	109.5
C34—C35—C36	119.5 (3)	N27A—C48A—H48E	109.5
C36—C35—H35	120.3	N27A—C48A—H48F	109.5
C35—C36—H36	119.6	H48D—C48A—H48E	109.5
C37—C36—C35	120.7 (3)	H48D—C48A—H48F	109.5
C37—C36—H36	119.6	H48E—C48A—H48F	109.5
C36—C37—H37	120.1	N28A—C49A—H49D	109.5
C38—C37—C36	119.9 (3)	N28A—C49A—H49E	109.5
C38—C37—H37	120.1	N28A—C49A—H49F	109.5
C37—C38—H38	119.9	H49D—C49A—H49E	109.5
C37—C38—C39	120.2 (3)	H49D—C49A—H49F	109.5
C39—C38—H38	119.9	H49E—C49A—H49F	109.5
C34—C39—H39	119.9	N28A—C50A—H50D	109.5
C38—C39—C34	120.2 (2)	N28A—C50A—H50E	109.5
C38—C39—H39	119.9	N28A—C50A—H50F	109.5
N23—C40—N26	110.0 (2)	H50D—C50A—H50E	109.5
N23—C40—C41	126.4 (2)	H50D—C50A—H50F	109.5
N26—C40—C41	123.5 (2)	H50E—C50A—H50F	109.5
C42—C41—C40	120.3 (2)	Cl1—C25S—H25B	109.5
C46—C41—C40	120.8 (2)	Cl1—C25S—H25C	109.5
C46—C41—C42	118.9 (2)	Cl2—C25S—Cl1	110.9 (6)
C41—C42—H42	119.7	Cl2—C25S—H25B	109.5
C43—C42—C41	120.6 (2)	Cl2—C25S—H25C	109.5
C43—C42—H42	119.7	H25B—C25S—H25C	108.0
C42—C43—H43	119.9	Cl3—C26S—H26A	108.7
C44—C43—C42	120.2 (3)	Cl3—C26S—H26B	108.7
C44—C43—H43	119.9	Cl4—C26S—Cl3	114.2 (5)
C43—C44—H44	120.1	Cl4—C26S—H26A	108.7
C43—C44—C45	119.9 (2)	Cl4—C26S—H26B	108.7
C45—C44—H44	120.1	H26A—C26S—H26B	107.6
C44—C45—H45	119.9	C2S—C1S—H1S	119.7
C46—C45—C44	120.3 (2)	C6S—C1S—H1S	119.7
C46—C45—H45	119.9	C6S—C1S—C2S	120.7 (3)
C41—C46—H46	119.9	C1S—C2S—H2S	120.2
C45—C46—C41	120.2 (2)	C3S—C2S—C1S	119.5 (3)
C45—C46—H46	119.9	C3S—C2S—H2S	120.2
N27—C47—H47A	109.5	C2S—C3S—H3S	119.9

N27—C47—H47B	109.5	C2S—C3S—C4S	120.2 (3)
N27—C47—H47C	109.5	C4S—C3S—H3S	119.9
H47A—C47—H47B	109.5	C3S—C4S—H4S	120.1
H47A—C47—H47C	109.5	C5S—C4S—C3S	119.8 (3)
H47B—C47—H47C	109.5	C5S—C4S—H4S	120.1
N27—C48—H48A	109.5	C4S—C5S—H5S	119.9
N27—C48—H48B	109.5	C6S—C5S—C4S	120.2 (3)
N27—C48—H48C	109.5	C6S—C5S—H5S	119.9
H48A—C48—H48B	109.5	C1S—C6S—C5S	119.7 (3)
H48A—C48—H48C	109.5	C1S—C6S—H6S	120.2
H48B—C48—H48C	109.5	C5S—C6S—H6S	120.2
N28—C49—H49A	109.5	C8S—C7S—H7S	120.0
N28—C49—H49B	109.5	C8S—C7S—C12S	120.0
N28—C49—H49C	109.5	C12S—C7S—H7S	120.0
H49A—C49—H49B	109.5	C7S—C8S—H8S	120.0
H49A—C49—H49C	109.5	C7S—C8S—C9S	120.0
H49B—C49—H49C	109.5	C9S—C8S—H8S	120.0
N28—C50—H50A	109.5	C8S—C9S—H9S	120.0
N28—C50—H50B	109.5	C10S—C9S—C8S	120.0
N28—C50—H50C	109.5	C10S—C9S—H9S	120.0
H50A—C50—H50B	109.5	C9S—C10S—H10S	120.0
H50A—C50—H50C	109.5	C9S—C10S—C11S	120.0
H50B—C50—H50C	109.5	C11S—C10S—H10S	120.0
N2A—Zr1A—N6A	135.77 (7)	C10S—C11S—H11S	120.0
N2A—Zr1A—N10A	74.36 (7)	C10S—C11S—C12S	120.0
N2A—Zr1A—N12A	137.39 (6)	C12S—C11S—H11S	120.0
N2A—Zr1A—N16A	71.45 (6)	C7S—C12S—H12S	120.0
N2A—Zr1A—N20A	80.57 (7)	C11S—C12S—C7S	120.0
N6A—Zr1A—N10A	72.87 (7)	C11S—C12S—H12S	120.0
N6A—Zr1A—N12A	72.47 (7)	C14S—C13S—H13S	120.0
N6A—Zr1A—N16A	141.64 (7)	C14S—C13S—C18S	120.0
N6A—Zr1A—N20A	76.90 (6)	C18S—C13S—H13S	120.0
N9A—Zr1A—N2A	114.04 (8)	C13S—C14S—H14S	120.0
N9A—Zr1A—N6A	94.15 (8)	C15S—C14S—C13S	120.0
N9A—Zr1A—N10A	88.78 (7)	C15S—C14S—H14S	120.0
N9A—Zr1A—N12A	88.63 (7)	C14S—C15S—H15S	120.0
N9A—Zr1A—N16A	95.60 (8)	C14S—C15S—C16S	120.0
N9A—Zr1A—N20A	164.65 (7)	C16S—C15S—H15S	120.0
N12A—Zr1A—N10A	144.95 (6)	C15S—C16S—H16S	120.0
N16A—Zr1A—N10A	144.23 (6)	C17S—C16S—C15S	120.0
N16A—Zr1A—N12A	70.78 (6)	C17S—C16S—H16S	120.0
N16A—Zr1A—N20A	84.41 (6)	C16S—C17S—H17S	120.0
N20A—Zr1A—N10A	100.20 (7)	C16S—C17S—C18S	120.0
N20A—Zr1A—N12A	76.85 (6)	C18S—C17S—H17S	120.0
N13A—Zr2A—N17A	74.78 (7)	C13S—C18S—H18S	120.0
N13A—Zr2A—N21A	76.58 (6)	C17S—C18S—C13S	120.0
N13A—Zr2A—N27A	151.06 (7)	C17S—C18S—H18S	120.0
N21A—Zr2A—N17A	80.90 (7)	C20S—C19S—H19S	120.0

N23A—Zr2A—N13A	87.66 (7)	C20S—C19S—C24S	120.0
N23A—Zr2A—N17A	83.96 (7)	C24S—C19S—H19S	120.0
N23A—Zr2A—N21A	160.50 (7)	C19S—C20S—H20S	120.0
N23A—Zr2A—N27A	117.29 (7)	C19S—C20S—C21S	120.0
N24A—Zr2A—N13A	122.34 (7)	C21S—C20S—H20S	120.0
N24A—Zr2A—N17A	90.66 (7)	C20S—C21S—H21S	120.0
N24A—Zr2A—N21A	156.60 (7)	C22S—C21S—C20S	120.0
N24A—Zr2A—N23A	34.83 (7)	C22S—C21S—H21S	120.0
N24A—Zr2A—N27A	82.91 (7)	C21S—C22S—H22S	120.0
N27A—Zr2A—N17A	92.54 (7)	C23S—C22S—C21S	120.0
N27A—Zr2A—N21A	75.76 (7)	C23S—C22S—H22S	120.0
N28A—Zr2A—N13A	86.95 (8)	C22S—C23S—H23S	120.0
N28A—Zr2A—N17A	160.63 (8)	C22S—C23S—C24S	120.0
N28A—Zr2A—N21A	88.76 (8)	C24S—C23S—H23S	120.0
N28A—Zr2A—N23A	101.97 (8)	C19S—C24S—H24S	120.0
N28A—Zr2A—N24A	104.79 (8)	C23S—C24S—C19S	120.0
N28A—Zr2A—N27A	100.78 (8)	C23S—C24S—H24S	120.0

Zr1—N2—N3—N4	172.54 (14)	Zr2A—N24A—N25A—N26A	−123.9 (9)
Zr1—N6—N7—N8	−158.33 (15)	N1A—N2A—N3A—N4A	0.4 (3)
Zr1—N12—N13—Zr2	−18.5 (3)	N1A—C1A—C2A—C3A	1.8 (4)
Zr1—N12—N13—N14	174.03 (13)	N1A—C1A—C2A—C7A	−177.6 (2)
Zr1—N16—N17—Zr2	26.3 (3)	N2A—N1A—C1A—N4A	0.0 (2)
Zr1—N16—N17—N18	−170.36 (14)	N2A—N1A—C1A—C2A	−179.5 (2)
Zr1—N20—N21—Zr2	16.6 (3)	N2A—N3A—N4A—C1A	−0.4 (2)
Zr1—N20—N21—N22	−177.97 (14)	N3A—N4A—C1A—N1A	0.3 (3)
Zr2—N13—N14—C19	−172.49 (14)	N3A—N4A—C1A—C2A	179.8 (2)
Zr2—N17—N18—C26	166.46 (14)	N4A—C1A—C2A—C3A	−177.6 (2)
Zr2—N21—N22—C33	167.53 (13)	N4A—C1A—C2A—C7A	3.0 (4)
Zr2—N23—N24—N25	173.82 (19)	N5A—N6A—N7A—N8A	0.3 (3)
N1—N2—N3—N4	−0.5 (2)	N5A—C8A—C9A—C10A	156.5 (2)
N1—C1—C2—C3	−10.5 (4)	N5A—C8A—C9A—C14A	−21.9 (4)
N1—C1—C2—C7	169.5 (2)	N6A—N5A—C8A—N8A	0.7 (3)
N2—N1—C1—N4	0.1 (2)	N6A—N5A—C8A—C9A	−177.4 (2)
N2—N1—C1—C2	179.4 (2)	N6A—N7A—N8A—C8A	0.1 (2)
N2—N3—N4—C1	0.5 (2)	N7A—N8A—C8A—N5A	−0.5 (3)
N3—N4—C1—N1	−0.4 (3)	N7A—N8A—C8A—C9A	177.6 (2)
N3—N4—C1—C2	−179.6 (2)	N8A—C8A—C9A—C10A	−21.4 (4)
N4—C1—C2—C3	168.7 (2)	N8A—C8A—C9A—C14A	160.3 (2)
N4—C1—C2—C7	−11.3 (4)	N11A—N12A—N13A—Zr2A	158.69 (16)
N5—N6—N7—N8	0.3 (2)	N11A—N12A—N13A—N14A	−0.2 (2)
N5—C8—C9—C10	155.0 (3)	N11A—C19A—C20A—C21A	10.1 (4)
N5—C8—C9—C14	−22.7 (4)	N11A—C19A—C20A—C25A	−171.0 (2)
N6—N5—C8—N8	1.3 (3)	N12A—N11A—C19A—N14A	0.4 (3)
N6—N5—C8—C9	−176.4 (2)	N12A—N11A—C19A—C20A	−175.9 (2)
N6—N7—N8—C8	0.5 (3)	N12A—N13A—N14A—C19A	0.4 (2)
N7—N8—C8—N5	−1.2 (3)	N13A—N14A—C19A—N11A	−0.5 (3)
N7—N8—C8—C9	176.5 (2)	N13A—N14A—C19A—C20A	175.9 (2)

N8—C8—C9—C10	−22.4 (4)	N14A—C19A—C20A—C21A	−165.9 (2)
N8—C8—C9—C14	159.8 (2)	N14A—C19A—C20A—C25A	13.0 (4)
N11—N12—N13—Zr2	168.14 (18)	N15A—N16A—N17A—Zr2A	−171.18 (16)
N11—N12—N13—N14	0.7 (2)	N15A—N16A—N17A—N18A	−0.5 (2)
N11—C19—C20—C21	−6.1 (4)	N15A—C26A—C27A—C28A	−161.6 (2)
N11—C19—C20—C25	175.3 (2)	N15A—C26A—C27A—C32A	16.8 (3)
N12—N11—C19—N14	0.7 (2)	N16A—N15A—C26A—N18A	−0.4 (2)
N12—N11—C19—C20	−178.0 (2)	N16A—N15A—C26A—C27A	176.6 (2)
N12—N13—N14—C19	−0.2 (2)	N16A—N17A—N18A—C26A	0.3 (2)
N13—N14—C19—N11	−0.3 (2)	N17A—N18A—C26A—N15A	0.1 (2)
N13—N14—C19—C20	178.5 (2)	N17A—N18A—C26A—C27A	−176.8 (2)
N14—C19—C20—C21	175.3 (3)	N18A—C26A—C27A—C28A	15.0 (4)
N14—C19—C20—C25	−3.3 (4)	N18A—C26A—C27A—C32A	−166.7 (2)
N15—N16—N17—Zr2	−163.00 (15)	N19A—N20A—N21A—Zr2A	170.00 (14)
N15—N16—N17—N18	0.4 (2)	N19A—N20A—N21A—N22A	0.1 (2)
N15—C26—C27—C28	168.6 (2)	N19A—C33A—C34A—C35A	0.3 (4)
N15—C26—C27—C32	−12.3 (3)	N19A—C33A—C34A—C39A	179.9 (2)
N16—N15—C26—N18	−0.4 (2)	N20A—N19A—C33A—N22A	−0.4 (2)
N16—N15—C26—C27	177.5 (2)	N20A—N19A—C33A—C34A	−179.8 (2)
N16—N17—N18—C26	−0.6 (2)	N20A—N21A—N22A—C33A	−0.3 (2)
N17—N18—C26—N15	0.6 (2)	N21A—N22A—C33A—N19A	0.5 (2)
N17—N18—C26—C27	−177.3 (2)	N21A—N22A—C33A—C34A	179.9 (2)
N18—C26—C27—C28	−13.7 (3)	N22A—C33A—C34A—C35A	−179.1 (2)
N18—C26—C27—C32	165.4 (2)	N22A—C33A—C34A—C39A	0.5 (3)
N19—N20—N21—Zr2	−165.14 (14)	N23A—N24A—N25A—N26A	0.0 (3)
N19—N20—N21—N22	0.3 (2)	N23A—C40A—C41A—C42A	176.1 (2)
N19—C33—C34—C35	−9.1 (4)	N23A—C40A—C41A—C46A	−4.7 (4)
N19—C33—C34—C39	172.0 (2)	N24A—N23A—C40A—N26A	0.5 (3)
N20—N19—C33—N22	0.1 (2)	N24A—N23A—C40A—C41A	179.5 (2)
N20—N19—C33—C34	177.9 (2)	N24A—N25A—N26A—C40A	0.3 (3)
N20—N21—N22—C33	−0.3 (2)	N25A—N26A—C40A—N23A	−0.5 (3)
N21—N22—C33—N19	0.1 (2)	N25A—N26A—C40A—C41A	−179.6 (2)
N21—N22—C33—C34	−177.77 (19)	N26A—C40A—C41A—C42A	−4.9 (4)
N22—C33—C34—C35	168.5 (2)	N26A—C40A—C41A—C46A	174.3 (2)
N22—C33—C34—C39	−10.4 (3)	C1A—N1A—N2A—Zr1A	178.62 (14)
N23—N24—N25—N26	0.2 (3)	C1A—N1A—N2A—N3A	−0.2 (2)
N23—C40—C41—C42	−176.3 (2)	C1A—C2A—C3A—C4A	−179.7 (2)
N23—C40—C41—C46	5.3 (4)	C1A—C2A—C7A—C6A	179.4 (2)
N24—N23—C40—N26	0.1 (3)	C21A—C20A—C25A—C24A	−1.6 (4)
N24—N23—C40—C41	−177.8 (2)	C21A—C22A—C23A—C24A	−1.0 (4)
N24—N25—N26—C40	−0.1 (3)	C2A—C3A—C4A—C5A	0.7 (4)
N25—N26—C40—N23	0.0 (3)	C3A—C2A—C7A—C6A	0.0 (4)
N25—N26—C40—C41	178.0 (2)	C3A—C4A—C5A—C6A	−0.8 (4)
N26—C40—C41—C42	6.0 (4)	C4A—C5A—C6A—C7A	0.5 (4)
N26—C40—C41—C46	−172.4 (2)	C5A—C6A—C7A—C2A	−0.1 (4)
C1—N1—N2—Zr1	−172.68 (14)	C7A—C2A—C3A—C4A	−0.3 (4)
C1—N1—N2—N3	0.3 (2)	C8A—N5A—N6A—Zr1A	169.77 (14)
C1—C2—C3—C4	179.7 (2)	C8A—N5A—N6A—N7A	−0.6 (2)

C1—C2—C7—C6	−180.0 (2)	C8A—C9A—C10A—C11A	−176.9 (2)
C2—C3—C4—C5	0.4 (4)	C8A—C9A—C14A—C13A	177.7 (2)
C3—C2—C7—C6	0.0 (4)	C9A—C10A—C11A—C12A	−0.7 (4)
C3—C4—C5—C6	−0.3 (4)	C10A—C9A—C14A—C13A	−0.6 (4)
C4—C5—C6—C7	0.0 (4)	C10A—C11A—C12A—C13A	−1.0 (4)
C5—C6—C7—C2	0.1 (4)	C11A—C12A—C13A—C14A	1.8 (4)
C7—C2—C3—C4	−0.2 (4)	C12A—C13A—C14A—C9A	−1.0 (4)
C8—N5—N6—Zr1	157.72 (15)	C14A—C9A—C10A—C11A	1.5 (4)
C8—N5—N6—N7	−1.0 (2)	C19A—N11A—N12A—Zr1A	−173.70 (14)
C8—C9—C10—C11	−177.8 (3)	C19A—N11A—N12A—N13A	−0.1 (2)
C8—C9—C14—C13	178.7 (2)	C19A—C20A—C25A—C24A	179.5 (2)
C9—C10—C11—C12	−0.7 (5)	C20A—C21A—C22A—C23A	−0.8 (4)
C10—C9—C14—C13	1.0 (4)	C22A—C21A—C20A—C19A	−179.0 (2)
C10—C11—C12—C13	0.5 (5)	C22A—C21A—C20A—C25A	2.1 (4)
C11—C12—C13—C14	0.4 (4)	C22A—C23A—C24A—C25A	1.5 (4)
C12—C13—C14—C9	−1.2 (4)	C23A—C24A—C25A—C20A	−0.2 (4)
C14—C9—C10—C11	0.0 (4)	C26A—N15A—N16A—Zr1A	−178.14 (14)
C19—N11—N12—Zr1	−173.71 (14)	C26A—N15A—N16A—N17A	0.5 (2)
C19—N11—N12—N13	−0.8 (2)	C26A—C27A—C28A—C29A	178.1 (3)
C19—C20—C21—C22	−179.0 (3)	C26A—C27A—C32A—C31A	−177.5 (2)
C19—C20—C25—C24	179.3 (3)	C27A—C28A—C29A—C30A	−0.9 (5)
C20—C21—C22—C23	−0.2 (5)	C28A—C27A—C32A—C31A	0.9 (4)
C21—C20—C25—C24	0.7 (4)	C28A—C29A—C30A—C31A	1.5 (5)
C21—C22—C23—C24	0.4 (6)	C29A—C30A—C31A—C32A	−0.9 (5)
C22—C23—C24—C25	0.0 (5)	C30A—C31A—C32A—C27A	−0.3 (4)
C23—C24—C25—C20	−0.5 (5)	C32A—C27A—C28A—C29A	−0.2 (4)
C25—C20—C21—C22	−0.3 (5)	C33A—N19A—N20A—Zr1A	−171.93 (13)
C26—N15—N16—Zr1	171.73 (13)	C33A—N19A—N20A—N21A	0.2 (2)
C26—N15—N16—N17	0.0 (2)	C33A—C34A—C35A—C36A	−179.6 (3)
C26—C27—C28—C29	179.2 (2)	C33A—C34A—C39A—C38A	179.3 (3)
C26—C27—C32—C31	−178.8 (2)	C34A—C35A—C36A—C37A	0.1 (5)
C27—C28—C29—C30	0.1 (4)	C35A—C34A—C39A—C38A	−1.1 (4)
C28—C27—C32—C31	0.3 (3)	C35A—C36A—C37A—C38A	−0.6 (5)
C28—C29—C30—C31	−0.5 (4)	C36A—C37A—C38A—C39A	0.2 (5)
C29—C30—C31—C32	0.9 (4)	C37A—C38A—C39A—C34A	0.6 (5)
C30—C31—C32—C27	−0.8 (4)	C39A—C34A—C35A—C36A	0.8 (4)
C32—C27—C28—C29	0.0 (3)	C40A—N23A—N24A—Zr2A	170.16 (17)
C33—N19—N20—Zr1	178.37 (13)	C40A—N23A—N24A—N25A	−0.3 (3)
C33—N19—N20—N21	−0.2 (2)	C40A—C41A—C42A—C43A	178.6 (2)
C33—C34—C35—C36	−178.9 (3)	C40A—C41A—C46A—C45A	−179.2 (2)
C33—C34—C39—C38	178.3 (2)	C41A—C42A—C43A—C44A	0.8 (4)
C34—C35—C36—C37	0.9 (5)	C42A—C41A—C46A—C45A	0.0 (4)
C35—C34—C39—C38	−0.6 (4)	C42A—C43A—C44A—C45A	−0.5 (4)
C35—C36—C37—C38	−1.1 (6)	C43A—C44A—C45A—C46A	−0.1 (4)
C36—C37—C38—C39	0.5 (5)	C44A—C45A—C46A—C41A	0.3 (4)
C37—C38—C39—C34	0.4 (4)	C46A—C41A—C42A—C43A	−0.5 (4)
C39—C34—C35—C36	0.0 (4)	C1S—C2S—C3S—C4S	0.4 (4)
C40—N23—N24—Zr2	−173.99 (16)	C2S—C1S—C6S—C5S	0.0 (4)

C40—N23—N24—N25	−0.2 (2)	C2S—C3S—C4S—C5S	0.6 (4)
C40—C41—C42—C43	−178.2 (2)	C3S—C4S—C5S—C6S	−1.3 (4)
C40—C41—C46—C45	178.9 (2)	C4S—C5S—C6S—C1S	1.0 (4)
C41—C42—C43—C44	−0.7 (4)	C6S—C1S—C2S—C3S	−0.7 (4)
C42—C41—C46—C45	0.5 (4)	C7S—C8S—C9S—C10S	0.0
C42—C43—C44—C45	0.5 (4)	C8S—C7S—C12S—C11S	0.0
C43—C44—C45—C46	0.3 (4)	C8S—C9S—C10S—C11S	0.0
C44—C45—C46—C41	−0.8 (4)	C9S—C10S—C11S—C12S	0.0
C46—C41—C42—C43	0.2 (4)	C10S—C11S—C12S—C7S	0.0
Zr1A—N2A—N3A—N4A	−178.42 (14)	C12S—C7S—C8S—C9S	0.0
Zr1A—N6A—N7A—N8A	−169.47 (14)	C13S—C14S—C15S—C16S	0.0
Zr1A—N12A—N13A—Zr2A	−28.4 (3)	C14S—C13S—C18S—C17S	0.0
Zr1A—N12A—N13A—N14A	172.70 (14)	C14S—C15S—C16S—C17S	0.0
Zr1A—N16A—N17A—Zr2A	7.3 (3)	C15S—C16S—C17S—C18S	0.0
Zr1A—N16A—N17A—N18A	178.01 (14)	C16S—C17S—C18S—C13S	0.0
Zr1A—N20A—N21A—Zr2A	−19.6 (3)	C18S—C13S—C14S—C15S	0.0
Zr1A—N20A—N21A—N22A	170.46 (14)	C19S—C20S—C21S—C22S	0.0
Zr2A—N13A—N14A—C19A	−163.67 (14)	C20S—C19S—C24S—C23S	0.0
Zr2A—N17A—N18A—C26A	173.46 (14)	C20S—C21S—C22S—C23S	0.0
Zr2A—N21A—N22A—C33A	−171.94 (13)	C21S—C22S—C23S—C24S	0.0
Zr2A—N23A—N24A—N25A	−170.44 (19)	C22S—C23S—C24S—C19S	0.0
Zr2A—N23A—C40A—N26A	56.7 (9)	C24S—C19S—C20S—C21S	0.0
Zr2A—N23A—C40A—C41A	−124.2 (8)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N10—H10···N5	0.85 (2)	1.96 (2)	2.732 (3)	151 (2)
N27—H27···N22	0.84 (2)	2.35 (2)	2.965 (3)	130 (2)
N10*A*—H10*B*···N5*A*	0.85 (2)	2.16 (2)	2.902 (3)	145 (2)
N27*A*—H27*A*···N22*A*	0.85 (2)	2.33 (2)	2.940 (3)	129 (2)

μ-Oxido-bis(μ-5-phenyltetrazolato-κ^2N^2:N^3)\ bis[(dimethylamido)tris(5-phenyltetrazolato-κN^2)tantalum(V)] toluene 0.25-solvate (3)

Crystal data

$(C_2H_8N)_2[Ta_2(C_7H_5N_4)_8(C_2H_6N)_2O]\cdot 0.25C_7H_8$	$F(000) = 6964$
$M_r = 1742.47$	$D_x = 1.539$ Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
$a = 22.5131$ (8) Å	Cell parameters from 91158 reflections
$b = 25.5101$ (9) Å	$\theta = 2.3$–$29.1°$
$c = 26.7165$ (9) Å	$\mu = 2.98$ mm^{-1}
$\beta = 101.3830$ (4)°	$T = 105$ K
$V = 15041.8$ (9) Å^3	Block, yellow
$Z = 8$	0.39 × 0.32 × 0.24 mm

Data collection

Bruker SMART APEX CCD area detector diffractometer
Radiation source: sealed tube
Graphite monochromator
Detector resolution: 8 pixels mm^{-1}
ω and φ scans
Absorption correction: multi-scan (SADABS; Bruker, 2018)
T_{min} = 0.4, T_{max} = 0.5
173076 measured reflections
29545 independent reflections
25534 reflections with $I > 2\sigma(I)$
R_{int} = 0.030
θ_{max} = 26.0°, θ_{min} = 1.8°
h = −27→27
k = −31→30
l = −32→32

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.027
$wR(F^2)$ = 0.068
S = 1.09
29545 reflections
1915 parameters
79 restraints
Primary atom site location: dual
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0298P)^2 + 35.7711P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.007
$\Delta\rho_{max}$ = 2.48 e Å^{-3}
$\Delta\rho_{min}$ = −1.24 e Å^{-3}

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}	Occ. (<1)
Ta1	0.78099 (2)	0.94792 (2)	0.79238 (2)	0.01469 (3)	
Ta2	0.74252 (2)	0.91178 (2)	0.65793 (2)	0.01519 (3)	
O1	0.76194 (9)	0.90565 (8)	0.73102 (8)	0.0153 (4)	
N1	0.67073 (12)	0.98108 (11)	0.84250 (11)	0.0193 (6)	
N2	0.69683 (12)	0.94095 (11)	0.82225 (10)	0.0185 (6)	
N3	0.65957 (13)	0.89992 (12)	0.81262 (13)	0.0275 (7)	
N4	0.60817 (13)	0.91288 (12)	0.82675 (13)	0.0292 (7)	
N5	0.80972 (12)	0.87098 (12)	0.88725 (11)	0.0213 (6)	
N6	0.78700 (12)	0.87496 (11)	0.83714 (10)	0.0180 (6)	
N7	0.76471 (13)	0.82945 (12)	0.81798 (11)	0.0242 (6)	
N8	0.77283 (14)	0.79436 (12)	0.85588 (11)	0.0256 (7)	
N9	0.92147 (12)	0.96424 (11)	0.83791 (11)	0.0197 (6)	
N10	0.87845 (12)	0.92979 (11)	0.81737 (10)	0.0185 (6)	
N11	0.90236 (13)	0.88290 (12)	0.81292 (12)	0.0251 (6)	
N12	0.96129 (13)	0.88549 (12)	0.83045 (12)	0.0260 (7)	
N13	0.79424 (12)	1.01515 (11)	0.82530 (10)	0.0184 (6)	
N14	0.86383 (12)	1.02821 (11)	0.74126 (11)	0.0182 (6)	
N15	0.82675 (12)	0.98755 (11)	0.73422 (10)	0.0167 (6)	
N16	0.81155 (12)	0.97630 (11)	0.68477 (10)	0.0176 (6)	
N17	0.83841 (12)	1.00968 (11)	0.65811 (11)	0.0193 (6)	

N18	0.67607 (12)	1.03450 (11)	0.74570 (11)	0.0203 (6)
N19	0.70844 (12)	0.99327 (11)	0.73745 (11)	0.0186 (6)
N20	0.69345 (12)	0.97906 (11)	0.68876 (11)	0.0188 (6)
N21	0.65025 (12)	1.01033 (11)	0.66414 (11)	0.0211 (6)
N22	0.60300 (12)	0.90994 (11)	0.60742 (10)	0.0190 (6)
N23	0.64588 (12)	0.89017 (11)	0.64458 (11)	0.0191 (6)
N24	0.62186 (12)	0.86451 (12)	0.67870 (12)	0.0247 (6)
N25	0.56221 (12)	0.86681 (12)	0.66476 (11)	0.0243 (6)
N26	0.72941 (13)	0.79831 (12)	0.60770 (11)	0.0236 (6)
N27	0.73978 (12)	0.82504 (11)	0.65197 (10)	0.0196 (6)
N28	0.76376 (15)	0.79373 (12)	0.69040 (12)	0.0301 (7)
N29	0.76860 (16)	0.74581 (12)	0.67199 (12)	0.0304 (7)
N30	0.84918 (12)	0.90238 (12)	0.59743 (11)	0.0211 (6)
N31	0.82797 (12)	0.88601 (11)	0.63810 (11)	0.0187 (6)
N32	0.86789 (13)	0.85609 (12)	0.66852 (12)	0.0246 (6)
N33	0.91654 (13)	0.85224 (12)	0.64756 (12)	0.0266 (7)
N34	0.72447 (12)	0.95314 (12)	0.59642 (11)	0.0205 (6)
N35	0.64569 (13)	0.79255 (12)	0.76311 (12)	0.0268 (7)
H35B	0.644289	0.810440	0.733436	0.032*
H35C	0.673368	0.808615	0.787768	0.032*
N36	0.88190 (14)	0.78445 (12)	0.76317 (13)	0.0311 (7)
H36B	0.880419	0.812398	0.784064	0.037*
H36C	0.856117	0.791043	0.733061	0.037*
C1	0.61626 (14)	0.96213 (13)	0.84464 (12)	0.0195 (7)
C2	0.56820 (14)	0.99352 (14)	0.86073 (12)	0.0204 (7)
C3	0.57101 (15)	1.04780 (14)	0.85999 (13)	0.0224 (7)
H3	0.605487	1.064580	0.851707	0.027*
C4	0.52421 (16)	1.07772 (15)	0.87116 (14)	0.0268 (8)
H4	0.526494	1.114895	0.870540	0.032*
C5	0.47382 (16)	1.05329 (16)	0.88331 (14)	0.0297 (8)
H5	0.441234	1.073736	0.890492	0.036*
C6	0.47103 (16)	0.99914 (16)	0.88496 (14)	0.0281 (8)
H6	0.436768	0.982611	0.893902	0.034*
C7	0.51796 (15)	0.96864 (15)	0.87366 (13)	0.0229 (7)
H7	0.515877	0.931468	0.874707	0.028*
C8	0.80033 (14)	0.82073 (14)	0.89758 (13)	0.0205 (7)
C9	0.81943 (15)	0.79595 (14)	0.94777 (13)	0.0220 (7)
C10	0.84377 (16)	0.82556 (15)	0.99044 (14)	0.0269 (8)
H10	0.847272	0.862496	0.987526	0.032*
C11	0.86302 (17)	0.80141 (16)	1.03735 (14)	0.0297 (8)
H11	0.879622	0.821912	1.066435	0.036*
C12	0.85821 (17)	0.74792 (16)	1.04203 (14)	0.0294 (8)
H12	0.871647	0.731461	1.074163	0.035*
C13	0.83370 (18)	0.71835 (16)	0.99966 (15)	0.0321 (9)
H13	0.830140	0.681445	1.002815	0.039*
C14	0.81423 (17)	0.74206 (15)	0.95251 (15)	0.0293 (8)
H14	0.797376	0.721452	0.923569	0.035*
C15	0.97205 (15)	0.93540 (14)	0.84566 (13)	0.0206 (7)

C16	1.03290 (15)	0.95550 (15)	0.86742 (13)	0.0232 (7)
C17	1.08101 (16)	0.92040 (16)	0.88275 (14)	0.0270 (8)
H17	1.074405	0.883665	0.879632	0.032*
C18	1.13812 (17)	0.93985 (18)	0.90245 (16)	0.0370 (10)
H18	1.170866	0.916180	0.912583	0.044*
C19	1.14842 (18)	0.99319 (19)	0.90767 (17)	0.0405 (10)
H19	1.187814	1.006031	0.921638	0.049*
C20	1.10103 (18)	1.02764 (18)	0.89243 (18)	0.0412 (10)
H20	1.107822	1.064323	0.895995	0.049*
C21	1.04357 (17)	1.00893 (16)	0.87193 (16)	0.0323 (9)
H21	1.011337	1.032886	0.860920	0.039*
C22	0.79369 (17)	1.07116 (14)	0.81602 (14)	0.0264 (8)
H22A	0.783033	1.077766	0.779200	0.040*
H22B	0.833925	1.085695	0.829656	0.040*
H22C	0.763752	1.087872	0.832926	0.040*
C23	0.80943 (15)	1.00180 (14)	0.88000 (13)	0.0232 (7)
H23A	0.849431	1.016029	0.894945	0.035*
H23B	0.809954	0.963609	0.883998	0.035*
H23C	0.778992	1.016896	0.897425	0.035*
C24	0.87044 (14)	1.04135 (13)	0.69410 (13)	0.0184 (7)
C25	0.90677 (14)	1.08673 (13)	0.68413 (13)	0.0184 (7)
C26	0.93104 (15)	1.12008 (13)	0.72404 (13)	0.0207 (7)
H26	0.923833	1.113508	0.757328	0.025*
C27	0.96558 (15)	1.16271 (14)	0.71565 (14)	0.0235 (7)
H27	0.982144	1.185327	0.743111	0.028*
C28	0.97604 (16)	1.17244 (15)	0.66709 (15)	0.0284 (8)
H28	0.999347	1.202053	0.661258	0.034*
C29	0.95277 (18)	1.13933 (16)	0.62717 (15)	0.0333 (9)
H29	0.960339	1.145994	0.594010	0.040*
C30	0.91817 (17)	1.09614 (15)	0.63557 (14)	0.0282 (8)
H30	0.902382	1.073135	0.608205	0.034*
C31	0.64054 (14)	1.04421 (14)	0.70026 (13)	0.0217 (7)
C32	0.59486 (15)	1.08617 (14)	0.69033 (14)	0.0237 (7)
C33	0.57201 (16)	1.10708 (14)	0.73043 (16)	0.0291 (8)
H33	0.588194	1.096473	0.764481	0.035*
C34	0.52532 (17)	1.14364 (15)	0.72083 (18)	0.0351 (10)
H34	0.509163	1.157565	0.748302	0.042*
C35	0.50252 (17)	1.15966 (16)	0.67173 (19)	0.0402 (11)
H35	0.470269	1.184292	0.665319	0.048*
C36	0.5263 (2)	1.14006 (17)	0.63149 (18)	0.0433 (11)
H36	0.511366	1.152142	0.597715	0.052*
C37	0.57202 (18)	1.10279 (16)	0.64060 (16)	0.0355 (9)
H37	0.587716	1.088625	0.612990	0.043*
C38	0.55178 (14)	0.89463 (13)	0.62075 (12)	0.0178 (7)
C39	0.49076 (14)	0.90553 (13)	0.59108 (13)	0.0186 (7)
C40	0.44038 (15)	0.88391 (14)	0.60693 (13)	0.0224 (7)
H40	0.445709	0.861700	0.636017	0.027*
C41	0.38281 (16)	0.89509 (15)	0.57996 (15)	0.0274 (8)

H41	0.348535	0.881153	0.591161	0.033*	
C42	0.37463 (16)	0.92630 (16)	0.53694 (15)	0.0318 (9)	
H42	0.334881	0.933811	0.518715	0.038*	
C43	0.42458 (17)	0.94672 (16)	0.52033 (15)	0.0313 (9)	
H43	0.419141	0.967458	0.490231	0.038*	
C44	0.48232 (16)	0.93674 (15)	0.54779 (14)	0.0249 (8)	
H44	0.516422	0.951400	0.536885	0.030*	
C45	0.74726 (14)	0.74971 (13)	0.62146 (13)	0.0192 (7)	
C46	0.74600 (15)	0.70509 (13)	0.58607 (13)	0.0208 (7)	
C47	0.7125 (2)	0.70717 (16)	0.53689 (15)	0.0351 (9)	
H47	0.690199	0.737956	0.525375	0.042*	
C48	0.7111 (2)	0.66473 (17)	0.50403 (16)	0.0455 (12)	
H48	0.687092	0.666204	0.470546	0.055*	
C49	0.7445 (2)	0.62057 (16)	0.52016 (15)	0.0354 (9)	
H49	0.743775	0.591558	0.497748	0.042*	
C50	0.77918 (17)	0.61839 (15)	0.56893 (16)	0.0315 (9)	
H50	0.802537	0.587982	0.579812	0.038*	
C51	0.78007 (16)	0.66019 (15)	0.60199 (15)	0.0276 (8)	
H51	0.803844	0.658387	0.635532	0.033*	
C52	0.90386 (15)	0.88046 (13)	0.60430 (13)	0.0204 (7)	
C53	0.9427 (3)	0.8923 (3)	0.5670 (3)	0.019 (2)	0.52 (2)
C54	0.9259 (3)	0.9295 (4)	0.5288 (3)	0.021 (2)	0.52 (2)
H54	0.887547	0.946301	0.524891	0.025*	0.52 (2)
C55	0.9651 (4)	0.9423 (4)	0.49653 (19)	0.027 (2)	0.52 (2)
H55	0.953581	0.967788	0.470493	0.032*	0.52 (2)
C56	1.0212 (4)	0.9178 (4)	0.5023 (3)	0.029 (2)	0.52 (2)
H56	1.047996	0.926523	0.480240	0.034*	0.52 (2)
C57	1.0380 (4)	0.8805 (3)	0.5404 (4)	0.029 (2)	0.52 (2)
H57	1.076378	0.863769	0.544384	0.034*	0.52 (2)
C58	0.9988 (4)	0.8678 (3)	0.5727 (4)	0.030 (2)	0.52 (2)
H58	1.010344	0.842280	0.598781	0.036*	0.52 (2)
C53B	0.9510 (3)	0.8850 (4)	0.5731 (3)	0.020 (3)	0.48 (2)
C54B	0.9369 (3)	0.9145 (4)	0.5286 (3)	0.022 (2)	0.48 (2)
H54B	0.897605	0.929155	0.518458	0.027*	0.48 (2)
C55B	0.9804 (4)	0.9227 (5)	0.4990 (2)	0.027 (3)	0.48 (2)
H55B	0.970809	0.942903	0.468650	0.032*	0.48 (2)
C56B	1.0380 (4)	0.9013 (5)	0.5139 (3)	0.029 (3)	0.48 (2)
H56B	1.067720	0.906895	0.493711	0.035*	0.48 (2)
C57B	1.0521 (3)	0.8718 (3)	0.5584 (4)	0.032 (3)	0.48 (2)
H57B	1.091428	0.857139	0.568580	0.038*	0.48 (2)
C58B	1.0086 (3)	0.8636 (3)	0.5880 (4)	0.022 (2)	0.48 (2)
H58B	1.018224	0.843390	0.618389	0.027*	0.48 (2)
C59	0.71463 (17)	1.00705 (15)	0.57857 (14)	0.0274 (8)	
H59A	0.734067	1.012550	0.549249	0.041*	
H59B	0.732159	1.031147	0.606118	0.041*	
H59C	0.671039	1.013698	0.568363	0.041*	
C60	0.71215 (16)	0.91489 (15)	0.55483 (13)	0.0248 (8)	
H60A	0.670427	0.919182	0.536036	0.037*	

H60B	0.717506	0.879371	0.568976	0.037*
H60C	0.740281	0.920507	0.531638	0.037*
C61	0.58513 (17)	0.79503 (16)	0.77741 (16)	0.0328 (9)
H61A	0.554712	0.779433	0.750158	0.049*
H61B	0.574552	0.831696	0.782251	0.049*
H61C	0.586231	0.775604	0.809221	0.049*
C62	0.66572 (18)	0.73832 (16)	0.75659 (18)	0.0370 (10)
H62A	0.668548	0.719123	0.788751	0.056*
H62B	0.705518	0.738896	0.746953	0.056*
H62C	0.636391	0.720926	0.729742	0.056*
C63	0.8606 (2)	0.73747 (17)	0.7866 (2)	0.0443 (11)
H63A	0.859754	0.707533	0.763499	0.066*
H63B	0.819812	0.743784	0.792929	0.066*
H63C	0.888240	0.729879	0.819022	0.066*
C64	0.94420 (19)	0.77971 (17)	0.75350 (17)	0.0371 (9)
H64A	0.972817	0.775694	0.786045	0.056*
H64B	0.954343	0.811300	0.736076	0.056*
H64C	0.946674	0.748989	0.731984	0.056*
Ta1A	0.26714 (2)	0.72176 (2)	0.71402 (2)	0.01344 (3)
Ta2A	0.29513 (2)	0.74260 (2)	0.85171 (2)	0.01326 (3)
O1A	0.27922 (9)	0.75693 (8)	0.77928 (8)	0.0142 (4)
N1A	0.13400 (12)	0.70670 (11)	0.65006 (10)	0.0184 (6)
N2A	0.16996 (12)	0.73609 (11)	0.68461 (11)	0.0199 (6)
N3A	0.14053 (13)	0.77740 (12)	0.69751 (12)	0.0275 (7)
N4A	0.08356 (13)	0.77494 (13)	0.67209 (13)	0.0303 (7)
N5A	0.23949 (12)	0.81042 (11)	0.62773 (10)	0.0194 (6)
N6A	0.25839 (12)	0.79982 (11)	0.67745 (10)	0.0192 (6)
N7A	0.26897 (14)	0.84346 (12)	0.70444 (12)	0.0278 (7)
N8A	0.25557 (15)	0.88409 (12)	0.67244 (12)	0.0288 (7)
N9A	0.38677 (12)	0.70156 (11)	0.66938 (10)	0.0175 (6)
N10A	0.35469 (12)	0.73677 (11)	0.69102 (10)	0.0168 (6)
N11A	0.38599 (13)	0.78081 (11)	0.70247 (12)	0.0241 (6)
N12A	0.43915 (13)	0.77517 (12)	0.68886 (12)	0.0248 (6)
N13A	0.25854 (12)	0.65860 (10)	0.67350 (10)	0.0162 (5)
N18A	0.17617 (12)	0.63601 (11)	0.75149 (10)	0.0180 (6)
N19A	0.21718 (11)	0.67334 (11)	0.76438 (10)	0.0164 (5)
N20A	0.22933 (12)	0.67997 (10)	0.81466 (10)	0.0167 (6)
N21A	0.19661 (12)	0.64639 (11)	0.83615 (11)	0.0192 (6)
N14A	0.36445 (12)	0.63040 (10)	0.75573 (10)	0.0170 (6)
N15A	0.33665 (11)	0.67364 (10)	0.76658 (10)	0.0153 (5)
N16A	0.34704 (12)	0.68041 (10)	0.81706 (10)	0.0166 (5)
N17A	0.38166 (12)	0.64206 (11)	0.84009 (10)	0.0182 (6)
N22A	0.18552 (12)	0.73668 (11)	0.90947 (10)	0.0186 (6)
N23A	0.20570 (12)	0.75949 (11)	0.87101 (10)	0.0177 (6)
N24A	0.16173 (13)	0.78632 (13)	0.84101 (13)	0.0298 (7)
N25A	0.11198 (13)	0.78163 (13)	0.86037 (13)	0.0307 (7)
N26A	0.32430 (12)	0.85444 (11)	0.90694 (10)	0.0196 (6)
N27A	0.29329 (12)	0.82800 (11)	0.86626 (10)	0.0180 (6)

N28A	0.26022 (13)	0.86109 (12)	0.83374 (11)	0.0251 (6)
N29A	0.26961 (13)	0.90938 (11)	0.85203 (12)	0.0248 (6)
N30A	0.43523 (12)	0.75290 (11)	0.90586 (10)	0.0174 (6)
N31A	0.39034 (11)	0.76951 (10)	0.86839 (10)	0.0155 (5)
N32A	0.40948 (12)	0.80781 (12)	0.84174 (11)	0.0226 (6)
N33A	0.46722 (12)	0.81703 (12)	0.86116 (11)	0.0236 (6)
N34A	0.30935 (12)	0.69495 (11)	0.90885 (10)	0.0171 (6)
N35A	0.14406 (13)	0.86915 (11)	0.76003 (11)	0.0231 (6)
H35D	0.154847	0.846480	0.737079	0.028*
H35E	0.165763	0.860689	0.791452	0.028*
N36A	0.38820 (13)	0.88081 (12)	0.76051 (12)	0.0259 (7)
H36D	0.365967	0.863438	0.733412	0.031*
H36E	0.388013	0.861240	0.788963	0.031*
C1A	0.08082 (15)	0.73124 (13)	0.64343 (13)	0.0202 (7)
C2A	0.02598 (15)	0.71488 (13)	0.60712 (13)	0.0206 (7)
C3A	0.02972 (16)	0.68132 (14)	0.56685 (13)	0.0237 (7)
H3A	0.067878	0.667574	0.563286	0.028*
C4A	−0.02221 (17)	0.66786 (15)	0.53183 (14)	0.0281 (8)
H4A	−0.019619	0.645068	0.504224	0.034*
C5A	−0.07799 (17)	0.68786 (15)	0.53732 (15)	0.0308 (9)
H5A	−0.113588	0.678452	0.513546	0.037*
C6A	−0.08192 (16)	0.72116 (15)	0.57696 (16)	0.0326 (9)
H6A	−0.120201	0.734810	0.580292	0.039*
C7A	−0.03028 (16)	0.73500 (15)	0.61219 (15)	0.0270 (8)
H7A	−0.033190	0.758006	0.639561	0.032*
C8A	0.23703 (15)	0.86233 (14)	0.62615 (13)	0.0210 (7)
C9A	0.21752 (15)	0.89393 (14)	0.57955 (14)	0.0238 (7)
C10A	0.21072 (14)	0.87161 (14)	0.53135 (13)	0.0229 (7)
H10A	0.219301	0.835462	0.528007	0.028*
C11A	0.19141 (16)	0.90192 (16)	0.48800 (14)	0.0298 (8)
H11A	0.187230	0.886509	0.455124	0.036*
C12A	0.17826 (18)	0.95440 (17)	0.49252 (15)	0.0342 (9)
H12A	0.164128	0.974883	0.462865	0.041*
C13A	0.1858 (2)	0.97693 (17)	0.54033 (16)	0.0405 (10)
H13A	0.177471	1.013174	0.543428	0.049*
C14A	0.2053 (2)	0.94704 (16)	0.58403 (16)	0.0357 (9)
H14A	0.210396	0.962811	0.616810	0.043*
C15A	0.43839 (14)	0.72680 (13)	0.66868 (12)	0.0183 (7)
C16A	0.48935 (15)	0.70549 (14)	0.64756 (12)	0.0205 (7)
C17A	0.53079 (16)	0.74017 (15)	0.63326 (15)	0.0279 (8)
H17A	0.526119	0.776843	0.637310	0.033*
C18A	0.57896 (17)	0.72121 (16)	0.61308 (16)	0.0319 (9)
H18A	0.607160	0.744969	0.603379	0.038*
C19A	0.58592 (17)	0.66808 (16)	0.60711 (15)	0.0316 (9)
H19A	0.618737	0.655231	0.593108	0.038*
C20A	0.54523 (19)	0.63356 (17)	0.62148 (17)	0.0375 (10)
H20A	0.550157	0.596920	0.617404	0.045*
C21A	0.49685 (17)	0.65217 (15)	0.64197 (15)	0.0295 (8)

H21A	0.469109	0.628226	0.652070	0.035*
C22A	0.25478 (16)	0.60210 (13)	0.67613 (13)	0.0228 (7)
H22D	0.263403	0.590988	0.711948	0.034*
H22E	0.284448	0.586328	0.658299	0.034*
H22F	0.213940	0.590686	0.659922	0.034*
C23A	0.25146 (15)	0.67814 (14)	0.62072 (12)	0.0209 (7)
H23D	0.284994	0.665252	0.605634	0.031*
H23E	0.251723	0.716551	0.620919	0.031*
H23F	0.212962	0.665587	0.600516	0.031*
C31A	0.16464 (14)	0.61984 (13)	0.79628 (13)	0.0186 (7)
C32A	0.12045 (15)	0.57897 (13)	0.80175 (13)	0.0202 (7)
C33A	0.08205 (15)	0.55939 (13)	0.75887 (14)	0.0225 (7)
H33A	0.086103	0.570649	0.725816	0.027*
C34A	0.03751 (16)	0.52318 (14)	0.76432 (15)	0.0260 (8)
H34A	0.011033	0.509769	0.734975	0.031*
C35A	0.03181 (16)	0.50673 (14)	0.81247 (16)	0.0283 (8)
H35A	0.000916	0.482483	0.816103	0.034*
C36A	0.07049 (19)	0.52521 (16)	0.85504 (16)	0.0355 (9)
H36A	0.067049	0.512993	0.887937	0.043*
C37A	0.11467 (18)	0.56177 (16)	0.85006 (15)	0.0330 (9)
H37A	0.140934	0.575053	0.879585	0.040*
C24A	0.39164 (14)	0.61164 (13)	0.80118 (12)	0.0177 (7)
C25A	0.42659 (15)	0.56266 (13)	0.80780 (13)	0.0197 (7)
C30A	0.4372 (2)	0.53736 (15)	0.85475 (15)	0.0341 (9)
H30A	0.421512	0.551642	0.882339	0.041*
C29A	0.4705 (2)	0.49138 (16)	0.86147 (15)	0.0398 (10)
H29A	0.477236	0.473901	0.893491	0.048*
C28A	0.49391 (17)	0.47089 (14)	0.82141 (15)	0.0296 (8)
H28A	0.517831	0.439945	0.826238	0.036*
C27A	0.48240 (15)	0.49559 (14)	0.77435 (14)	0.0242 (7)
H27A	0.497901	0.481094	0.746775	0.029*
C26A	0.44857 (14)	0.54115 (13)	0.76712 (13)	0.0205 (7)
H26A	0.440368	0.557690	0.734627	0.025*
C38A	0.12797 (15)	0.75121 (13)	0.90228 (13)	0.0192 (7)
C39A	0.08618 (15)	0.73592 (14)	0.93581 (13)	0.0222 (7)
C40A	0.03213 (17)	0.76313 (16)	0.93421 (16)	0.0303 (8)
H40A	0.021798	0.791631	0.911249	0.036*
C41A	−0.00674 (18)	0.74835 (18)	0.96645 (18)	0.0393 (10)
H41A	−0.043615	0.766801	0.965420	0.047*
C42A	0.00833 (19)	0.70690 (19)	0.99990 (16)	0.0393 (10)
H42A	−0.018244	0.696943	1.021793	0.047*
C43A	0.06179 (18)	0.67998 (18)	1.00159 (15)	0.0355 (9)
H43A	0.071860	0.651434	1.024541	0.043*
C44A	0.10100 (16)	0.69446 (15)	0.96983 (14)	0.0267 (8)
H44A	0.137981	0.676028	0.971340	0.032*
C45A	0.30932 (14)	0.90431 (13)	0.89672 (12)	0.0169 (6)
C46A	0.33240 (14)	0.94901 (13)	0.92958 (13)	0.0190 (7)
C51A	0.31297 (16)	0.99956 (14)	0.91548 (14)	0.0256 (8)

H51A	0.284160	1.005199	0.884822	0.031*	
C50A	0.33554 (19)	1.04177 (15)	0.94603 (16)	0.0333 (9)	
H50A	0.321667	1.076146	0.936267	0.040*	
C49A	0.37789 (19)	1.03455 (15)	0.99045 (15)	0.0333 (9)	
H49A	0.393391	1.063665	1.011123	0.040*	
C48A	0.39740 (19)	0.98431 (16)	1.00437 (15)	0.0334 (9)	
H48A	0.426540	0.978875	1.034872	0.040*	
C47A	0.37489 (17)	0.94183 (14)	0.97430 (14)	0.0257 (8)	
H47A	0.388641	0.907488	0.984359	0.031*	
C52A	0.48212 (15)	0.78308 (13)	0.90026 (12)	0.0181 (7)	
C53A	0.54360 (14)	0.78027 (13)	0.93194 (13)	0.0199 (7)	
C58A	0.58885 (16)	0.81337 (15)	0.92083 (14)	0.0268 (8)	
H58A	0.579671	0.837497	0.893297	0.032*	
C57A	0.64684 (17)	0.81102 (17)	0.94981 (16)	0.0343 (9)	
H57A	0.677356	0.833570	0.942030	0.041*	
C56A	0.66094 (16)	0.77606 (17)	0.99014 (15)	0.0329 (9)	
H56A	0.700987	0.774418	1.009752	0.040*	
C55A	0.61601 (17)	0.74341 (16)	1.00168 (15)	0.0300 (8)	
H55A	0.625272	0.719757	1.029597	0.036*	
C54A	0.55746 (16)	0.74526 (14)	0.97245 (14)	0.0245 (8)	
H54A	0.527028	0.722595	0.980210	0.029*	
C59A	0.31041 (17)	0.64000 (14)	0.92362 (14)	0.0250 (8)	
H59D	0.350514	0.631164	0.943588	0.037*	
H59E	0.301788	0.618065	0.892924	0.037*	
H59F	0.279657	0.633769	0.944280	0.037*	
C60A	0.32171 (15)	0.73029 (13)	0.95311 (12)	0.0200 (7)	
H60D	0.291769	0.724323	0.974610	0.030*	
H60E	0.319186	0.766742	0.941294	0.030*	
H60F	0.362430	0.723389	0.972948	0.030*	
C61A	0.07900 (16)	0.86250 (15)	0.76007 (14)	0.0276 (8)	
H61D	0.066119	0.889048	0.782209	0.041*	
H61E	0.071987	0.827473	0.772804	0.041*	
H61F	0.055674	0.866563	0.725221	0.041*	
C62A	0.16001 (17)	0.92300 (16)	0.74715 (18)	0.0378 (10)	
H62D	0.135590	0.932971	0.713970	0.057*	
H62E	0.203086	0.924437	0.745512	0.057*	
H62F	0.151936	0.947298	0.773421	0.057*	
C63A	0.35920 (18)	0.93188 (17)	0.76607 (17)	0.0361 (9)	
H63D	0.383836	0.951506	0.794253	0.054*	
H63E	0.318693	0.926070	0.773309	0.054*	
H63F	0.355828	0.951920	0.734344	0.054*	
C64A	0.45147 (16)	0.88582 (15)	0.75288 (15)	0.0277 (8)	
H64D	0.452140	0.907292	0.722588	0.042*	
H64E	0.467745	0.850938	0.748128	0.042*	
H64F	0.476311	0.902523	0.782898	0.042*	
C1S	1.0077 (4)	1.1023 (2)	1.0167 (4)	0.065 (3)*	0.5
H1SA	0.967672	1.118836	1.008921	0.098*	0.5
H1SB	1.025923	1.107962	1.052736	0.098*	0.5

H1SC	1.033730	1.117785	0.995226	0.098*	0.5
C2S	1.0013 (3)	1.0443 (2)	1.0062 (3)	0.073 (3)*	0.5
C3S	0.9442 (3)	1.0215 (3)	0.9891 (3)	0.060 (3)*	0.5
H3S	0.909175	1.043135	0.983254	0.072*	0.5
C4S	0.9381 (4)	0.9676 (3)	0.9804 (4)	0.077 (4)*	0.5
H4S	0.899009	0.952906	0.968850	0.093*	0.5
C5S	0.9891 (5)	0.9354 (2)	0.9888 (4)	0.096 (5)*	0.5
H5S	0.985033	0.898684	0.982984	0.115*	0.5
C6S	1.0463 (5)	0.9575 (3)	1.0057 (5)	0.103 (5)*	0.5
H6S	1.081330	0.935763	1.011393	0.124*	0.5
C7S	1.0522 (3)	1.0114 (3)	1.0143 (4)	0.105 (5)*	0.5
H7S	1.091347	1.025998	1.025764	0.127*	0.5

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ta1	0.01097 (6)	0.01775 (7)	0.01564 (6)	0.00017 (5)	0.00330 (5)	0.00109 (5)
Ta2	0.01086 (6)	0.01959 (7)	0.01530 (7)	−0.00063 (5)	0.00306 (5)	0.00148 (5)
O1	0.0135 (10)	0.0175 (11)	0.0151 (11)	−0.0009 (8)	0.0035 (8)	0.0003 (9)
N1	0.0151 (13)	0.0231 (15)	0.0205 (14)	0.0003 (11)	0.0057 (11)	−0.0015 (12)
N2	0.0168 (13)	0.0202 (15)	0.0193 (14)	−0.0017 (11)	0.0058 (11)	−0.0011 (11)
N3	0.0198 (15)	0.0264 (17)	0.0386 (18)	−0.0044 (12)	0.0114 (13)	−0.0051 (14)
N4	0.0201 (15)	0.0281 (17)	0.0428 (19)	−0.0041 (12)	0.0147 (14)	−0.0086 (14)
N5	0.0173 (14)	0.0271 (16)	0.0188 (14)	0.0026 (11)	0.0019 (11)	0.0047 (12)
N6	0.0164 (13)	0.0197 (14)	0.0176 (14)	−0.0006 (11)	0.0027 (11)	0.0005 (11)
N7	0.0241 (15)	0.0248 (16)	0.0234 (15)	0.0007 (12)	0.0037 (12)	0.0029 (12)
N8	0.0267 (16)	0.0268 (16)	0.0216 (15)	0.0012 (13)	0.0008 (12)	0.0072 (13)
N9	0.0152 (13)	0.0234 (15)	0.0199 (14)	−0.0011 (11)	0.0022 (11)	0.0014 (12)
N10	0.0171 (13)	0.0199 (14)	0.0186 (14)	0.0010 (11)	0.0037 (11)	0.0020 (11)
N11	0.0154 (14)	0.0258 (16)	0.0327 (17)	0.0018 (12)	0.0018 (12)	−0.0040 (13)
N12	0.0174 (14)	0.0268 (17)	0.0337 (17)	0.0028 (12)	0.0044 (12)	−0.0038 (13)
N13	0.0149 (13)	0.0203 (15)	0.0204 (14)	−0.0026 (11)	0.0043 (11)	−0.0063 (11)
N14	0.0128 (13)	0.0203 (15)	0.0216 (14)	−0.0023 (11)	0.0036 (11)	0.0022 (11)
N15	0.0139 (13)	0.0191 (14)	0.0174 (13)	−0.0014 (10)	0.0033 (10)	−0.0015 (11)
N16	0.0134 (13)	0.0206 (15)	0.0201 (14)	0.0013 (11)	0.0066 (11)	0.0014 (11)
N17	0.0142 (13)	0.0220 (15)	0.0222 (14)	−0.0008 (11)	0.0045 (11)	0.0051 (12)
N18	0.0162 (13)	0.0191 (14)	0.0259 (15)	0.0033 (11)	0.0052 (11)	0.0043 (12)
N19	0.0126 (13)	0.0216 (15)	0.0214 (14)	0.0037 (11)	0.0033 (11)	−0.0022 (11)
N20	0.0125 (13)	0.0212 (15)	0.0219 (14)	0.0010 (11)	0.0011 (11)	0.0043 (12)
N21	0.0140 (13)	0.0218 (15)	0.0265 (15)	0.0019 (11)	0.0012 (11)	0.0031 (12)
N22	0.0133 (13)	0.0258 (15)	0.0171 (14)	−0.0004 (11)	0.0013 (11)	−0.0002 (11)
N23	0.0115 (13)	0.0228 (15)	0.0228 (14)	0.0004 (11)	0.0030 (11)	0.0009 (12)
N24	0.0147 (14)	0.0298 (17)	0.0291 (16)	−0.0019 (12)	0.0033 (12)	0.0092 (13)
N25	0.0136 (14)	0.0312 (17)	0.0277 (16)	−0.0017 (12)	0.0028 (12)	0.0065 (13)
N26	0.0188 (14)	0.0263 (16)	0.0248 (15)	0.0036 (12)	0.0025 (12)	−0.0033 (13)
N27	0.0166 (13)	0.0242 (15)	0.0192 (14)	−0.0029 (11)	0.0064 (11)	−0.0010 (12)
N28	0.0402 (19)	0.0256 (17)	0.0244 (16)	−0.0065 (14)	0.0060 (14)	−0.0008 (13)
N29	0.0423 (19)	0.0212 (16)	0.0273 (17)	−0.0046 (14)	0.0058 (14)	0.0007 (13)

N30	0.0179 (14)	0.0274 (16)	0.0197 (14)	−0.0029 (12)	0.0080 (11)	−0.0010 (12)
N31	0.0137 (13)	0.0224 (15)	0.0209 (14)	−0.0002 (11)	0.0060 (11)	0.0005 (12)
N32	0.0196 (14)	0.0227 (16)	0.0331 (17)	0.0035 (12)	0.0090 (13)	0.0070 (13)
N33	0.0206 (15)	0.0235 (16)	0.0385 (18)	0.0044 (12)	0.0126 (13)	0.0034 (14)
N34	0.0147 (13)	0.0284 (16)	0.0184 (14)	−0.0005 (11)	0.0032 (11)	0.0055 (12)
N35	0.0210 (15)	0.0283 (17)	0.0289 (16)	−0.0055 (12)	−0.0001 (12)	0.0079 (13)
N36	0.0291 (17)	0.0228 (17)	0.0376 (19)	0.0039 (13)	−0.0026 (14)	−0.0030 (14)
C1	0.0163 (16)	0.0241 (18)	0.0182 (16)	−0.0012 (13)	0.0039 (13)	−0.0012 (13)
C2	0.0153 (16)	0.0310 (19)	0.0148 (16)	−0.0009 (13)	0.0024 (12)	−0.0039 (14)
C3	0.0187 (16)	0.0299 (19)	0.0191 (17)	−0.0004 (14)	0.0050 (13)	−0.0017 (14)
C4	0.0264 (19)	0.028 (2)	0.0258 (19)	0.0044 (15)	0.0050 (15)	−0.0045 (15)
C5	0.0206 (18)	0.043 (2)	0.0267 (19)	0.0072 (16)	0.0060 (15)	−0.0098 (17)
C6	0.0183 (17)	0.043 (2)	0.0243 (18)	−0.0039 (15)	0.0075 (14)	−0.0080 (16)
C7	0.0174 (16)	0.032 (2)	0.0205 (17)	−0.0055 (14)	0.0060 (13)	−0.0046 (15)
C8	0.0156 (16)	0.0246 (18)	0.0223 (17)	0.0014 (13)	0.0063 (13)	0.0018 (14)
C9	0.0170 (16)	0.0275 (19)	0.0227 (17)	0.0014 (13)	0.0069 (13)	0.0034 (14)
C10	0.0284 (19)	0.029 (2)	0.0243 (19)	0.0020 (15)	0.0067 (15)	0.0038 (15)
C11	0.032 (2)	0.039 (2)	0.0181 (18)	0.0048 (17)	0.0043 (15)	0.0019 (16)
C12	0.0283 (19)	0.040 (2)	0.0199 (18)	0.0065 (16)	0.0050 (15)	0.0110 (16)
C13	0.034 (2)	0.029 (2)	0.033 (2)	0.0008 (16)	0.0035 (17)	0.0119 (17)
C14	0.029 (2)	0.031 (2)	0.0257 (19)	−0.0025 (16)	0.0005 (15)	0.0042 (16)
C15	0.0161 (16)	0.0258 (19)	0.0202 (17)	0.0013 (13)	0.0044 (13)	0.0030 (14)
C16	0.0180 (17)	0.033 (2)	0.0193 (17)	0.0009 (14)	0.0049 (13)	0.0025 (15)
C17	0.0190 (17)	0.032 (2)	0.0288 (19)	0.0016 (15)	0.0024 (14)	0.0028 (16)
C18	0.0157 (18)	0.054 (3)	0.038 (2)	0.0057 (17)	−0.0014 (16)	0.009 (2)
C19	0.0187 (19)	0.058 (3)	0.042 (2)	−0.0070 (18)	−0.0017 (17)	0.005 (2)
C20	0.027 (2)	0.037 (2)	0.057 (3)	−0.0079 (18)	0.0011 (19)	−0.001 (2)
C21	0.0210 (18)	0.033 (2)	0.041 (2)	0.0008 (15)	0.0014 (16)	0.0032 (18)
C22	0.0270 (19)	0.0230 (19)	0.030 (2)	−0.0012 (15)	0.0073 (15)	−0.0023 (15)
C23	0.0207 (17)	0.0268 (19)	0.0224 (18)	−0.0009 (14)	0.0049 (14)	−0.0057 (15)
C24	0.0117 (15)	0.0208 (17)	0.0227 (17)	0.0015 (12)	0.0033 (13)	0.0012 (13)
C25	0.0107 (14)	0.0188 (17)	0.0252 (17)	0.0005 (12)	0.0023 (13)	0.0041 (13)
C26	0.0226 (17)	0.0206 (17)	0.0208 (17)	0.0016 (13)	0.0085 (14)	0.0019 (14)
C27	0.0213 (17)	0.0188 (17)	0.0303 (19)	0.0002 (13)	0.0047 (14)	−0.0010 (14)
C28	0.0258 (19)	0.0247 (19)	0.036 (2)	−0.0051 (15)	0.0094 (16)	0.0087 (16)
C29	0.038 (2)	0.038 (2)	0.0243 (19)	−0.0088 (18)	0.0079 (17)	0.0085 (17)
C30	0.0273 (19)	0.032 (2)	0.0243 (19)	−0.0054 (15)	0.0026 (15)	0.0024 (16)
C31	0.0129 (15)	0.0247 (18)	0.0265 (18)	−0.0007 (13)	0.0016 (13)	0.0033 (14)
C32	0.0146 (16)	0.0203 (18)	0.035 (2)	−0.0022 (13)	0.0023 (14)	0.0037 (15)
C33	0.0232 (18)	0.0223 (19)	0.044 (2)	0.0000 (14)	0.0115 (16)	0.0077 (17)
C34	0.0258 (19)	0.022 (2)	0.063 (3)	−0.0015 (15)	0.0213 (19)	0.0016 (19)
C35	0.0189 (19)	0.027 (2)	0.070 (3)	0.0054 (15)	−0.0027 (19)	0.002 (2)
C36	0.040 (2)	0.036 (2)	0.045 (3)	0.0147 (19)	−0.011 (2)	−0.001 (2)
C37	0.032 (2)	0.035 (2)	0.036 (2)	0.0088 (17)	−0.0013 (17)	−0.0007 (18)
C38	0.0141 (15)	0.0203 (17)	0.0194 (16)	−0.0011 (12)	0.0042 (12)	−0.0041 (13)
C39	0.0150 (15)	0.0205 (17)	0.0202 (16)	−0.0001 (13)	0.0037 (13)	−0.0036 (13)
C40	0.0174 (16)	0.0264 (19)	0.0235 (17)	−0.0017 (13)	0.0044 (13)	−0.0011 (14)
C41	0.0151 (16)	0.033 (2)	0.034 (2)	−0.0046 (14)	0.0066 (15)	−0.0013 (16)

C42	0.0154 (17)	0.038 (2)	0.038 (2)	−0.0034 (15)	−0.0052 (15)	0.0055 (18)
C43	0.0248 (19)	0.039 (2)	0.028 (2)	0.0001 (16)	0.0008 (15)	0.0110 (17)
C44	0.0183 (17)	0.031 (2)	0.0251 (18)	−0.0026 (14)	0.0044 (14)	0.0025 (15)
C45	0.0156 (15)	0.0214 (18)	0.0219 (17)	−0.0039 (13)	0.0068 (13)	0.0001 (13)
C46	0.0214 (17)	0.0205 (17)	0.0228 (17)	−0.0037 (13)	0.0095 (14)	0.0003 (14)
C47	0.048 (2)	0.026 (2)	0.029 (2)	0.0104 (18)	0.0011 (18)	0.0016 (16)
C48	0.077 (3)	0.034 (2)	0.021 (2)	0.009 (2)	−0.001 (2)	−0.0020 (17)
C49	0.055 (3)	0.025 (2)	0.029 (2)	0.0017 (18)	0.0143 (19)	−0.0052 (16)
C50	0.028 (2)	0.023 (2)	0.044 (2)	0.0058 (15)	0.0086 (17)	0.0022 (17)
C51	0.0235 (18)	0.027 (2)	0.031 (2)	−0.0007 (15)	0.0021 (15)	0.0039 (16)
C52	0.0171 (15)	0.0195 (16)	0.0260 (17)	−0.0030 (12)	0.0073 (13)	−0.0052 (13)
C53	0.016 (3)	0.020 (4)	0.022 (4)	0.000 (3)	0.008 (3)	−0.008 (3)
C54	0.016 (3)	0.030 (4)	0.019 (3)	0.003 (3)	0.008 (2)	−0.005 (3)
C55	0.025 (4)	0.034 (4)	0.023 (3)	−0.002 (3)	0.008 (3)	−0.005 (3)
C56	0.022 (4)	0.035 (4)	0.032 (4)	0.002 (3)	0.015 (3)	−0.007 (3)
C57	0.018 (3)	0.030 (4)	0.041 (4)	0.003 (3)	0.012 (3)	−0.006 (3)
C58	0.025 (4)	0.027 (4)	0.038 (4)	0.002 (3)	0.005 (3)	0.001 (3)
C53B	0.017 (4)	0.020 (4)	0.023 (4)	−0.004 (3)	0.005 (3)	−0.005 (3)
C54B	0.015 (3)	0.026 (4)	0.026 (4)	0.004 (3)	0.005 (3)	−0.007 (3)
C55B	0.026 (4)	0.033 (4)	0.022 (3)	−0.001 (3)	0.007 (3)	−0.002 (3)
C56B	0.022 (4)	0.037 (4)	0.030 (4)	0.000 (3)	0.009 (3)	−0.006 (3)
C57B	0.020 (4)	0.041 (4)	0.035 (4)	0.003 (3)	0.004 (3)	−0.005 (3)
C58B	0.017 (3)	0.024 (4)	0.027 (4)	0.002 (3)	0.007 (3)	−0.006 (3)
C59	0.0250 (18)	0.034 (2)	0.0232 (18)	−0.0006 (15)	0.0053 (15)	0.0121 (16)
C60	0.0232 (18)	0.036 (2)	0.0162 (17)	−0.0011 (15)	0.0054 (14)	0.0038 (15)
C61	0.0253 (19)	0.029 (2)	0.045 (2)	−0.0055 (16)	0.0090 (17)	−0.0051 (18)
C62	0.029 (2)	0.033 (2)	0.053 (3)	−0.0013 (17)	0.0161 (19)	0.0060 (19)
C63	0.037 (2)	0.036 (2)	0.065 (3)	0.0051 (19)	0.022 (2)	0.007 (2)
C64	0.037 (2)	0.032 (2)	0.042 (2)	0.0052 (18)	0.0095 (19)	0.0071 (18)
Ta1A	0.01206 (6)	0.01466 (7)	0.01334 (6)	0.00030 (5)	0.00184 (5)	0.00029 (5)
Ta2A	0.01178 (6)	0.01450 (7)	0.01351 (6)	0.00023 (5)	0.00254 (5)	−0.00019 (5)
O1A	0.0135 (10)	0.0173 (11)	0.0117 (10)	−0.0019 (8)	0.0021 (8)	−0.0012 (9)
N1A	0.0155 (13)	0.0216 (15)	0.0176 (14)	−0.0024 (11)	0.0021 (11)	0.0005 (11)
N2A	0.0170 (14)	0.0193 (15)	0.0205 (14)	0.0005 (11)	−0.0032 (11)	−0.0050 (11)
N3A	0.0180 (15)	0.0305 (17)	0.0321 (17)	0.0008 (12)	0.0001 (13)	−0.0079 (14)
N4A	0.0174 (15)	0.0339 (18)	0.0365 (18)	0.0043 (13)	−0.0020 (13)	−0.0088 (14)
N5A	0.0185 (14)	0.0214 (15)	0.0180 (14)	0.0000 (11)	0.0032 (11)	0.0026 (11)
N6A	0.0192 (14)	0.0190 (15)	0.0191 (14)	0.0000 (11)	0.0035 (11)	0.0006 (11)
N7A	0.0304 (17)	0.0234 (16)	0.0275 (16)	−0.0005 (13)	0.0005 (13)	0.0012 (13)
N8A	0.0364 (18)	0.0215 (16)	0.0265 (16)	0.0008 (13)	0.0010 (14)	0.0045 (13)
N9A	0.0152 (13)	0.0203 (14)	0.0179 (14)	−0.0003 (11)	0.0050 (11)	−0.0009 (11)
N10A	0.0185 (14)	0.0170 (14)	0.0155 (13)	−0.0013 (11)	0.0054 (11)	−0.0001 (11)
N11A	0.0216 (15)	0.0221 (16)	0.0311 (17)	−0.0046 (12)	0.0108 (13)	−0.0064 (13)
N12A	0.0196 (15)	0.0255 (16)	0.0319 (17)	−0.0062 (12)	0.0114 (13)	−0.0048 (13)
N13A	0.0139 (13)	0.0176 (14)	0.0168 (13)	−0.0009 (10)	0.0026 (10)	−0.0039 (11)
N18A	0.0156 (13)	0.0184 (14)	0.0202 (14)	−0.0013 (11)	0.0040 (11)	−0.0002 (11)
N19A	0.0125 (12)	0.0182 (14)	0.0182 (14)	−0.0013 (10)	0.0027 (10)	−0.0001 (11)
N20A	0.0147 (13)	0.0164 (14)	0.0191 (14)	−0.0012 (10)	0.0033 (11)	0.0011 (11)

N21A	0.0185 (14)	0.0177 (14)	0.0233 (15)	−0.0029 (11)	0.0087 (11)	0.0007 (11)
N14A	0.0167 (13)	0.0164 (14)	0.0185 (14)	0.0030 (10)	0.0053 (11)	0.0012 (11)
N15A	0.0140 (13)	0.0168 (14)	0.0155 (13)	0.0010 (10)	0.0039 (10)	−0.0017 (11)
N16A	0.0132 (13)	0.0172 (14)	0.0196 (14)	0.0014 (10)	0.0039 (11)	−0.0003 (11)
N17A	0.0168 (13)	0.0165 (14)	0.0203 (14)	0.0029 (11)	0.0015 (11)	0.0014 (11)
N22A	0.0161 (13)	0.0229 (15)	0.0174 (14)	−0.0014 (11)	0.0049 (11)	−0.0014 (11)
N23A	0.0162 (13)	0.0185 (14)	0.0194 (14)	−0.0001 (11)	0.0056 (11)	0.0019 (11)
N24A	0.0187 (15)	0.0352 (18)	0.0380 (18)	0.0060 (13)	0.0113 (13)	0.0153 (15)
N25A	0.0183 (15)	0.0373 (19)	0.0398 (19)	0.0058 (13)	0.0137 (14)	0.0154 (15)
N26A	0.0212 (14)	0.0185 (15)	0.0192 (14)	−0.0009 (11)	0.0047 (11)	−0.0029 (11)
N27A	0.0151 (13)	0.0207 (15)	0.0174 (14)	0.0014 (11)	0.0012 (11)	0.0028 (11)
N28A	0.0241 (15)	0.0215 (16)	0.0262 (16)	0.0012 (12)	−0.0035 (12)	0.0008 (12)
N29A	0.0249 (15)	0.0187 (15)	0.0290 (16)	0.0019 (12)	0.0009 (13)	−0.0014 (12)
N30A	0.0150 (13)	0.0186 (14)	0.0185 (14)	0.0015 (10)	0.0031 (11)	−0.0022 (11)
N31A	0.0129 (13)	0.0157 (14)	0.0171 (13)	0.0007 (10)	0.0012 (10)	0.0000 (11)
N32A	0.0169 (14)	0.0264 (16)	0.0246 (15)	−0.0022 (12)	0.0040 (12)	0.0064 (12)
N33A	0.0145 (14)	0.0273 (16)	0.0284 (16)	−0.0036 (12)	0.0023 (12)	0.0034 (13)
N34A	0.0170 (13)	0.0174 (14)	0.0163 (13)	0.0022 (11)	0.0021 (10)	0.0022 (11)
N35A	0.0195 (14)	0.0224 (15)	0.0263 (16)	0.0060 (12)	0.0019 (12)	−0.0018 (12)
N36A	0.0268 (16)	0.0245 (16)	0.0250 (16)	−0.0057 (12)	0.0020 (13)	0.0035 (13)
C1A	0.0157 (16)	0.0198 (17)	0.0243 (17)	−0.0002 (13)	0.0022 (13)	−0.0005 (14)
C2A	0.0180 (16)	0.0194 (17)	0.0230 (17)	−0.0026 (13)	0.0006 (13)	0.0055 (14)
C3A	0.0218 (17)	0.0223 (18)	0.0261 (18)	−0.0044 (14)	0.0025 (14)	0.0043 (14)
C4A	0.031 (2)	0.027 (2)	0.0236 (18)	−0.0091 (15)	−0.0005 (15)	0.0010 (15)
C5A	0.0250 (19)	0.026 (2)	0.034 (2)	−0.0092 (15)	−0.0127 (16)	0.0083 (16)
C6A	0.0163 (17)	0.028 (2)	0.049 (2)	−0.0006 (15)	−0.0046 (16)	0.0054 (18)
C7A	0.0195 (17)	0.0253 (19)	0.034 (2)	0.0006 (14)	−0.0005 (15)	−0.0009 (16)
C8A	0.0174 (16)	0.0232 (18)	0.0217 (17)	−0.0004 (13)	0.0020 (13)	0.0029 (14)
C9A	0.0180 (16)	0.0270 (19)	0.0254 (18)	−0.0032 (14)	0.0021 (14)	0.0071 (15)
C10A	0.0141 (16)	0.0265 (19)	0.0280 (19)	−0.0023 (13)	0.0037 (14)	0.0055 (15)
C11A	0.0204 (18)	0.045 (2)	0.0234 (19)	−0.0051 (16)	0.0031 (14)	0.0065 (17)
C12A	0.030 (2)	0.043 (2)	0.026 (2)	−0.0045 (17)	−0.0020 (16)	0.0150 (18)
C13A	0.052 (3)	0.026 (2)	0.039 (2)	−0.0001 (19)	−0.005 (2)	0.0108 (18)
C14A	0.050 (3)	0.026 (2)	0.027 (2)	0.0003 (18)	−0.0011 (18)	0.0029 (16)
C15A	0.0157 (15)	0.0236 (18)	0.0153 (15)	−0.0018 (13)	0.0018 (12)	0.0019 (13)
C16A	0.0169 (16)	0.0295 (19)	0.0151 (16)	−0.0015 (13)	0.0032 (13)	−0.0017 (14)
C17A	0.0245 (18)	0.027 (2)	0.034 (2)	−0.0002 (15)	0.0101 (16)	0.0001 (16)
C18A	0.0206 (18)	0.040 (2)	0.038 (2)	−0.0050 (16)	0.0133 (16)	0.0044 (18)
C19A	0.0219 (18)	0.041 (2)	0.036 (2)	0.0058 (16)	0.0146 (16)	0.0040 (18)
C20A	0.037 (2)	0.031 (2)	0.051 (3)	0.0043 (17)	0.022 (2)	0.0018 (19)
C21A	0.0254 (19)	0.029 (2)	0.038 (2)	−0.0013 (15)	0.0161 (16)	0.0010 (17)
C22A	0.0242 (18)	0.0224 (18)	0.0226 (17)	−0.0042 (14)	0.0063 (14)	−0.0029 (14)
C23A	0.0218 (17)	0.0225 (18)	0.0177 (16)	−0.0011 (13)	0.0018 (13)	−0.0037 (13)
C31A	0.0163 (16)	0.0190 (17)	0.0203 (16)	0.0009 (13)	0.0031 (13)	−0.0015 (13)
C32A	0.0192 (16)	0.0170 (17)	0.0261 (18)	−0.0001 (13)	0.0085 (14)	0.0010 (14)
C33A	0.0204 (17)	0.0179 (17)	0.0295 (19)	0.0006 (13)	0.0054 (14)	0.0009 (14)
C34A	0.0191 (17)	0.0221 (18)	0.035 (2)	−0.0010 (14)	0.0014 (15)	−0.0029 (15)
C35A	0.0208 (18)	0.0191 (18)	0.048 (2)	−0.0050 (14)	0.0136 (16)	0.0018 (16)

C36A	0.041 (2)	0.035 (2)	0.034 (2)	−0.0132 (18)	0.0136 (18)	0.0042 (18)
C37A	0.037 (2)	0.034 (2)	0.028 (2)	−0.0149 (17)	0.0060 (17)	−0.0006 (17)
C24A	0.0153 (15)	0.0204 (17)	0.0175 (16)	0.0003 (12)	0.0032 (12)	−0.0012 (13)
C25A	0.0175 (16)	0.0199 (17)	0.0206 (17)	0.0033 (13)	0.0012 (13)	−0.0007 (13)
C30A	0.052 (3)	0.028 (2)	0.0219 (19)	0.0158 (18)	0.0056 (17)	−0.0024 (16)
C29A	0.061 (3)	0.030 (2)	0.023 (2)	0.019 (2)	−0.0030 (19)	0.0030 (17)
C28A	0.0253 (19)	0.0195 (18)	0.039 (2)	0.0077 (14)	−0.0067 (16)	−0.0046 (16)
C27A	0.0173 (16)	0.0229 (18)	0.032 (2)	0.0004 (13)	0.0047 (14)	−0.0058 (15)
C26A	0.0165 (16)	0.0224 (18)	0.0230 (17)	0.0012 (13)	0.0049 (13)	0.0004 (14)
C38A	0.0186 (16)	0.0184 (17)	0.0210 (17)	−0.0039 (13)	0.0053 (13)	−0.0010 (13)
C39A	0.0160 (16)	0.0298 (19)	0.0223 (17)	−0.0060 (14)	0.0075 (13)	−0.0052 (15)
C40A	0.0232 (18)	0.031 (2)	0.039 (2)	−0.0012 (15)	0.0127 (16)	0.0012 (17)
C41A	0.025 (2)	0.048 (3)	0.051 (3)	0.0014 (18)	0.0217 (19)	0.001 (2)
C42A	0.030 (2)	0.061 (3)	0.032 (2)	−0.006 (2)	0.0177 (17)	0.005 (2)
C43A	0.028 (2)	0.052 (3)	0.028 (2)	−0.0056 (18)	0.0070 (16)	0.0097 (18)
C44A	0.0180 (17)	0.036 (2)	0.0256 (19)	−0.0022 (15)	0.0043 (14)	0.0023 (16)
C45A	0.0146 (15)	0.0179 (17)	0.0191 (16)	0.0000 (12)	0.0059 (12)	−0.0001 (13)
C46A	0.0169 (16)	0.0201 (17)	0.0216 (17)	−0.0018 (13)	0.0075 (13)	−0.0012 (13)
C51A	0.0241 (18)	0.0231 (19)	0.0273 (19)	0.0021 (14)	−0.0009 (15)	−0.0004 (15)
C50A	0.040 (2)	0.0177 (19)	0.039 (2)	0.0015 (16)	0.0004 (18)	−0.0018 (16)
C49A	0.045 (2)	0.025 (2)	0.027 (2)	−0.0055 (17)	0.0011 (17)	−0.0093 (16)
C48A	0.041 (2)	0.032 (2)	0.0241 (19)	−0.0028 (17)	−0.0016 (17)	−0.0008 (16)
C47A	0.033 (2)	0.0195 (18)	0.0241 (18)	0.0022 (15)	0.0035 (15)	0.0018 (14)
C52A	0.0173 (16)	0.0184 (17)	0.0191 (16)	0.0020 (12)	0.0050 (13)	−0.0030 (13)
C53A	0.0145 (16)	0.0231 (18)	0.0222 (17)	0.0029 (13)	0.0039 (13)	−0.0070 (14)
C58A	0.0190 (17)	0.034 (2)	0.0266 (19)	−0.0005 (15)	0.0030 (14)	0.0000 (16)
C57A	0.0190 (18)	0.042 (2)	0.042 (2)	−0.0050 (16)	0.0040 (16)	−0.0070 (19)
C56A	0.0148 (17)	0.046 (2)	0.035 (2)	0.0058 (16)	−0.0034 (15)	−0.0085 (18)
C55A	0.0238 (19)	0.037 (2)	0.027 (2)	0.0098 (16)	0.0015 (15)	−0.0023 (16)
C54A	0.0187 (17)	0.0268 (19)	0.0279 (19)	0.0044 (14)	0.0043 (14)	−0.0049 (15)
C59A	0.0297 (19)	0.0217 (18)	0.0236 (18)	0.0002 (14)	0.0054 (15)	0.0047 (14)
C60A	0.0247 (17)	0.0223 (18)	0.0129 (15)	−0.0017 (13)	0.0039 (13)	0.0012 (13)
C61A	0.0210 (18)	0.032 (2)	0.0292 (19)	0.0041 (15)	0.0028 (15)	0.0056 (16)
C62A	0.0205 (19)	0.033 (2)	0.059 (3)	0.0019 (16)	0.0059 (18)	0.009 (2)
C63A	0.029 (2)	0.037 (2)	0.044 (2)	−0.0023 (17)	0.0137 (18)	−0.0044 (19)
C64A	0.0247 (18)	0.0238 (19)	0.034 (2)	−0.0031 (14)	0.0037 (15)	−0.0020 (16)

Geometric parameters (Å, º)

Ta1—O1	1.938 (2)	Ta1A—N6A	2.210 (3)
Ta1—N2	2.204 (3)	Ta1A—N10A	2.211 (3)
Ta1—N6	2.202 (3)	Ta1A—N13A	1.929 (3)
Ta1—N10	2.213 (3)	Ta1A—N19A	2.280 (3)
Ta1—N13	1.924 (3)	Ta1A—N15A	2.249 (3)
Ta1—N15	2.265 (3)	Ta2A—O1A	1.932 (2)
Ta1—N19	2.283 (3)	Ta2A—N20A	2.269 (3)
Ta2—O1	1.921 (2)	Ta2A—N16A	2.273 (3)
Ta2—N16	2.280 (3)	Ta2A—N23A	2.217 (3)

Ta2—N20	2.281 (3)	Ta2A—N27A	2.215 (3)
Ta2—N23	2.204 (3)	Ta2A—N31A	2.211 (3)
Ta2—N27	2.218 (3)	Ta2A—N34A	1.928 (3)
Ta2—N31	2.194 (3)	N1A—N2A	1.332 (4)
Ta2—N34	1.928 (3)	N1A—C1A	1.332 (4)
N1—N2	1.346 (4)	N2A—N3A	1.326 (4)
N1—C1	1.330 (4)	N3A—N4A	1.329 (4)
N2—N3	1.334 (4)	N4A—C1A	1.347 (5)
N3—N4	1.328 (4)	N5A—N6A	1.340 (4)
N4—C1	1.344 (5)	N5A—C8A	1.326 (4)
N5—N6	1.339 (4)	N6A—N7A	1.322 (4)
N5—C8	1.337 (5)	N7A—N8A	1.339 (4)
N6—N7	1.327 (4)	N8A—C8A	1.345 (5)
N7—N8	1.337 (4)	N9A—N10A	1.352 (4)
N8—C8	1.343 (5)	N9A—C15A	1.332 (4)
N9—N10	1.342 (4)	N10A—N11A	1.329 (4)
N9—C15	1.337 (4)	N11A—N12A	1.326 (4)
N10—N11	1.327 (4)	N12A—C15A	1.345 (5)
N11—N12	1.319 (4)	N13A—C22A	1.447 (4)
N12—C15	1.344 (5)	N13A—C23A	1.474 (4)
N13—C22	1.450 (5)	N18A—N19A	1.324 (4)
N13—C23	1.473 (4)	N18A—C31A	1.339 (4)
N14—N15	1.321 (4)	N19A—N20A	1.328 (4)
N14—C24	1.340 (4)	N20A—N21A	1.331 (4)
N15—N16	1.329 (4)	N21A—C31A	1.345 (4)
N16—N17	1.330 (4)	N14A—N15A	1.328 (4)
N17—C24	1.350 (4)	N14A—C24A	1.336 (4)
N18—N19	1.323 (4)	N15A—N16A	1.334 (4)
N18—C31	1.339 (4)	N16A—N17A	1.324 (4)
N19—N20	1.328 (4)	N17A—C24A	1.351 (4)
N20—N21	1.328 (4)	N22A—N23A	1.336 (4)
N21—C31	1.345 (5)	N22A—C38A	1.325 (4)
N22—N23	1.339 (4)	N23A—N24A	1.333 (4)
N22—C38	1.331 (4)	N24A—N25A	1.329 (4)
N23—N24	1.322 (4)	N25A—C38A	1.351 (5)
N24—N25	1.322 (4)	N26A—N27A	1.351 (4)
N25—C38	1.354 (4)	N26A—C45A	1.331 (4)
N26—N27	1.345 (4)	N27A—N28A	1.329 (4)
N26—C45	1.332 (4)	N28A—N29A	1.327 (4)
N27—N28	1.329 (4)	N29A—C45A	1.349 (4)
N28—N29	1.330 (4)	N30A—N31A	1.343 (4)
N29—C45	1.344 (5)	N30A—C52A	1.339 (4)
N30—N31	1.337 (4)	N31A—N32A	1.330 (4)
N30—C52	1.331 (4)	N32A—N33A	1.322 (4)
N31—N32	1.328 (4)	N33A—C52A	1.348 (4)
N32—N33	1.328 (4)	N34A—C59A	1.455 (4)
N33—C52	1.343 (5)	N34A—C60A	1.469 (4)
N34—C59	1.458 (5)	N35A—H35D	0.9100

N34—C60	1.464 (5)	N35A—H35E	0.9100
N35—H35B	0.9100	N35A—C61A	1.475 (4)
N35—H35C	0.9100	N35A—C62A	1.477 (5)
N35—C61	1.488 (5)	N36A—H36D	0.9100
N35—C62	1.476 (5)	N36A—H36E	0.9100
N36—H36B	0.9100	N36A—C63A	1.478 (5)
N36—H36C	0.9100	N36A—C64A	1.484 (5)
N36—C63	1.475 (5)	C1A—C2A	1.472 (5)
N36—C64	1.480 (5)	C2A—C3A	1.390 (5)
C1—C2	1.477 (5)	C2A—C7A	1.398 (5)
C2—C3	1.386 (5)	C3A—H3A	0.9500
C2—C7	1.398 (5)	C3A—C4A	1.389 (5)
C3—H3	0.9500	C4A—H4A	0.9500
C3—C4	1.380 (5)	C4A—C5A	1.390 (6)
C4—H4	0.9500	C5A—H5A	0.9500
C4—C5	1.388 (5)	C5A—C6A	1.374 (6)
C5—H5	0.9500	C6A—H6A	0.9500
C5—C6	1.384 (6)	C6A—C7A	1.389 (5)
C6—H6	0.9500	C7A—H7A	0.9500
C6—C7	1.392 (5)	C8A—C9A	1.475 (5)
C7—H7	0.9500	C9A—C10A	1.389 (5)
C8—C9	1.468 (5)	C9A—C14A	1.392 (5)
C9—C10	1.387 (5)	C10A—H10A	0.9500
C9—C14	1.388 (5)	C10A—C11A	1.389 (5)
C10—H10	0.9500	C11A—H11A	0.9500
C10—C11	1.387 (5)	C11A—C12A	1.381 (6)
C11—H11	0.9500	C12A—H12A	0.9500
C11—C12	1.376 (6)	C12A—C13A	1.380 (6)
C12—H12	0.9500	C13A—H13A	0.9500
C12—C13	1.381 (6)	C13A—C14A	1.391 (5)
C13—H13	0.9500	C14A—H14A	0.9500
C13—C14	1.388 (5)	C15A—C16A	1.479 (5)
C14—H14	0.9500	C16A—C17A	1.393 (5)
C15—C16	1.471 (5)	C16A—C21A	1.382 (5)
C16—C17	1.403 (5)	C17A—H17A	0.9500
C16—C21	1.385 (5)	C17A—C18A	1.390 (5)
C17—H17	0.9500	C18A—H18A	0.9500
C17—C18	1.382 (5)	C18A—C19A	1.377 (6)
C18—H18	0.9500	C19A—H19A	0.9500
C18—C19	1.383 (6)	C19A—C20A	1.379 (6)
C19—H19	0.9500	C20A—H20A	0.9500
C19—C20	1.380 (6)	C20A—C21A	1.395 (5)
C20—H20	0.9500	C21A—H21A	0.9500
C20—C21	1.386 (5)	C22A—H22D	0.9800
C21—H21	0.9500	C22A—H22E	0.9800
C22—H22A	0.9800	C22A—H22F	0.9800
C22—H22B	0.9800	C23A—H23D	0.9800
C22—H22C	0.9800	C23A—H23E	0.9800

C23—H23A	0.9800	C23A—H23F	0.9800
C23—H23B	0.9800	C31A—C32A	1.468 (5)
C23—H23C	0.9800	C32A—C33A	1.385 (5)
C24—C25	1.472 (4)	C32A—C37A	1.394 (5)
C25—C26	1.389 (5)	C33A—H33A	0.9500
C25—C30	1.392 (5)	C33A—C34A	1.392 (5)
C26—H26	0.9500	C34A—H34A	0.9500
C26—C27	1.381 (5)	C34A—C35A	1.383 (5)
C27—H27	0.9500	C35A—H35A	0.9500
C27—C28	1.386 (5)	C35A—C36A	1.372 (6)
C28—H28	0.9500	C36A—H36A	0.9500
C28—C29	1.380 (6)	C36A—C37A	1.389 (5)
C29—H29	0.9500	C37A—H37A	0.9500
C29—C30	1.393 (5)	C24A—C25A	1.468 (5)
C30—H30	0.9500	C25A—C30A	1.389 (5)
C31—C32	1.472 (5)	C25A—C26A	1.393 (5)
C32—C33	1.384 (5)	C30A—H30A	0.9500
C32—C37	1.393 (5)	C30A—C29A	1.385 (5)
C33—H33	0.9500	C29A—H29A	0.9500
C33—C34	1.391 (5)	C29A—C28A	1.385 (6)
C34—H34	0.9500	C28A—H28A	0.9500
C34—C35	1.373 (6)	C28A—C27A	1.384 (5)
C35—H35	0.9500	C27A—H27A	0.9500
C35—C36	1.386 (7)	C27A—C26A	1.382 (5)
C36—H36	0.9500	C26A—H26A	0.9500
C36—C37	1.387 (5)	C38A—C39A	1.474 (5)
C37—H37	0.9500	C39A—C40A	1.394 (5)
C38—C39	1.471 (4)	C39A—C44A	1.391 (5)
C39—C40	1.400 (5)	C40A—H40A	0.9500
C39—C44	1.386 (5)	C40A—C41A	1.396 (5)
C40—H40	0.9500	C41A—H41A	0.9500
C40—C41	1.383 (5)	C41A—C42A	1.383 (6)
C41—H41	0.9500	C42A—H42A	0.9500
C41—C42	1.380 (5)	C42A—C43A	1.379 (6)
C42—H42	0.9500	C43A—H43A	0.9500
C42—C43	1.389 (5)	C43A—C44A	1.390 (5)
C43—H43	0.9500	C44A—H44A	0.9500
C43—C44	1.384 (5)	C45A—C46A	1.470 (5)
C44—H44	0.9500	C46A—C51A	1.390 (5)
C45—C46	1.476 (5)	C46A—C47A	1.388 (5)
C46—C47	1.381 (5)	C51A—H51A	0.9500
C46—C51	1.397 (5)	C51A—C50A	1.386 (5)
C47—H47	0.9500	C50A—H50A	0.9500
C47—C48	1.390 (6)	C50A—C49A	1.380 (6)
C48—H48	0.9500	C49A—H49A	0.9500
C48—C49	1.376 (6)	C49A—C48A	1.382 (6)
C49—H49	0.9500	C48A—H48A	0.9500
C49—C50	1.381 (6)	C48A—C47A	1.384 (5)

C50—H50	0.9500	C47A—H47A	0.9500
C50—C51	1.382 (5)	C52A—C53A	1.475 (4)
C51—H51	0.9500	C53A—C58A	1.399 (5)
C52—C53	1.482 (4)	C53A—C54A	1.390 (5)
C52—C53B	1.478 (4)	C58A—H58A	0.9500
C53—C54	1.3900	C58A—C57A	1.382 (5)
C53—C58	1.3900	C57A—H57A	0.9500
C54—H54	0.9500	C57A—C56A	1.386 (6)
C54—C55	1.3900	C56A—H56A	0.9500
C55—H55	0.9500	C56A—C55A	1.391 (6)
C55—C56	1.3900	C55A—H55A	0.9500
C56—H56	0.9500	C55A—C54A	1.394 (5)
C56—C57	1.3900	C54A—H54A	0.9500
C57—H57	0.9500	C59A—H59D	0.9800
C57—C58	1.3900	C59A—H59E	0.9800
C58—H58	0.9500	C59A—H59F	0.9800
C53B—C54B	1.3900	C60A—H60D	0.9800
C53B—C58B	1.3900	C60A—H60E	0.9800
C54B—H54B	0.9500	C60A—H60F	0.9800
C54B—C55B	1.3900	C61A—H61D	0.9800
C55B—H55B	0.9500	C61A—H61E	0.9800
C55B—C56B	1.3900	C61A—H61F	0.9800
C56B—H56B	0.9500	C62A—H62D	0.9800
C56B—C57B	1.3900	C62A—H62E	0.9800
C57B—H57B	0.9500	C62A—H62F	0.9800
C57B—C58B	1.3900	C63A—H63D	0.9800
C58B—H58B	0.9500	C63A—H63E	0.9800
C59—H59A	0.9800	C63A—H63F	0.9800
C59—H59B	0.9800	C64A—H64D	0.9800
C59—H59C	0.9800	C64A—H64E	0.9800
C60—H60A	0.9800	C64A—H64F	0.9800
C60—H60B	0.9800	C1S—H1SA	0.9800
C60—H60C	0.9800	C1S—H1SB	0.9800
C61—H61A	0.9800	C1S—H1SC	0.9800
C61—H61B	0.9800	C1S—C2S	1.5076
C61—H61C	0.9800	C2S—C3S	1.4025
C62—H62A	0.9800	C2S—C7S	1.4023
C62—H62B	0.9800	C3S—H3S	0.9500
C62—H62C	0.9800	C3S—C4S	1.3964
C63—H63A	0.9800	C4S—H4S	0.9500
C63—H63B	0.9800	C4S—C5S	1.3961
C63—H63C	0.9800	C5S—H5S	0.9500
C64—H64A	0.9800	C5S—C6S	1.3967
C64—H64B	0.9800	C6S—H6S	0.9500
C64—H64C	0.9800	C6S—C7S	1.3962
Ta1A—O1A	1.932 (2)	C7S—H7S	0.9500
Ta1A—N2A	2.204 (3)		

O1—Ta1—N2	101.48 (9)	O1A—Ta1A—N10A	101.30 (9)
O1—Ta1—N6	88.21 (10)	O1A—Ta1A—N19A	73.56 (9)
O1—Ta1—N10	100.35 (10)	O1A—Ta1A—N15A	74.54 (9)
O1—Ta1—N15	73.91 (9)	N2A—Ta1A—N6A	72.38 (10)
O1—Ta1—N19	74.19 (9)	N2A—Ta1A—N10A	138.48 (10)
N2—Ta1—N10	138.26 (10)	N2A—Ta1A—N19A	74.32 (10)
N2—Ta1—N15	145.54 (10)	N2A—Ta1A—N15A	146.34 (10)
N2—Ta1—N19	73.53 (10)	N6A—Ta1A—N10A	74.19 (10)
N6—Ta1—N2	72.55 (10)	N6A—Ta1A—N19A	137.55 (10)
N6—Ta1—N10	73.05 (10)	N6A—Ta1A—N15A	139.30 (10)
N6—Ta1—N15	139.68 (10)	N10A—Ta1A—N19A	145.96 (10)
N6—Ta1—N19	137.46 (10)	N10A—Ta1A—N15A	73.71 (10)
N10—Ta1—N15	75.06 (10)	N13A—Ta1A—O1A	151.05 (10)
N10—Ta1—N19	147.23 (10)	N13A—Ta1A—N2A	87.48 (11)
N13—Ta1—O1	150.60 (11)	N13A—Ta1A—N6A	120.93 (11)
N13—Ta1—N2	88.46 (11)	N13A—Ta1A—N10A	89.13 (10)
N13—Ta1—N6	121.19 (11)	N13A—Ta1A—N19A	82.66 (11)
N13—Ta1—N10	89.62 (11)	N13A—Ta1A—N15A	82.82 (10)
N13—Ta1—N15	82.25 (11)	N15A—Ta1A—N19A	72.51 (9)
N13—Ta1—N19	82.46 (11)	O1A—Ta2A—N20A	73.75 (9)
N15—Ta1—N19	72.39 (10)	O1A—Ta2A—N16A	74.50 (9)
O1—Ta2—N16	74.62 (9)	O1A—Ta2A—N23A	101.46 (9)
O1—Ta2—N20	73.95 (9)	O1A—Ta2A—N27A	89.05 (9)
O1—Ta2—N23	99.41 (10)	O1A—Ta2A—N31A	97.12 (9)
O1—Ta2—N27	89.39 (10)	N20A—Ta2A—N16A	71.02 (9)
O1—Ta2—N31	100.74 (10)	N23A—Ta2A—N20A	72.16 (10)
O1—Ta2—N34	151.45 (11)	N23A—Ta2A—N16A	142.55 (10)
N16—Ta2—N20	72.06 (9)	N27A—Ta2A—N20A	137.39 (10)
N23—Ta2—N16	145.21 (10)	N27A—Ta2A—N16A	141.90 (10)
N23—Ta2—N20	73.37 (10)	N27A—Ta2A—N23A	73.66 (10)
N23—Ta2—N27	74.12 (10)	N31A—Ta2A—N20A	146.12 (10)
N27—Ta2—N16	138.60 (10)	N31A—Ta2A—N16A	75.10 (10)
N27—Ta2—N20	140.16 (10)	N31A—Ta2A—N23A	141.41 (10)
N31—Ta2—N16	73.54 (10)	N31A—Ta2A—N27A	73.15 (10)
N31—Ta2—N20	145.35 (10)	N34A—Ta2A—O1A	151.80 (10)
N31—Ta2—N23	140.38 (10)	N34A—Ta2A—N20A	83.89 (11)
N31—Ta2—N27	72.37 (10)	N34A—Ta2A—N16A	82.19 (11)
N34—Ta2—N16	83.62 (11)	N34A—Ta2A—N23A	87.41 (11)
N34—Ta2—N20	81.97 (11)	N34A—Ta2A—N27A	119.15 (11)
N34—Ta2—N23	87.92 (11)	N34A—Ta2A—N31A	91.91 (11)
N34—Ta2—N27	119.12 (11)	Ta1A—O1A—Ta2A	141.38 (12)
N34—Ta2—N31	90.32 (11)	C1A—N1A—N2A	103.6 (3)
Ta2—O1—Ta1	141.47 (12)	N1A—N2A—Ta1A	125.3 (2)
C1—N1—N2	102.7 (3)	N3A—N2A—Ta1A	123.4 (2)
N1—N2—Ta1	124.0 (2)	N3A—N2A—N1A	111.2 (3)
N3—N2—Ta1	123.1 (2)	N2A—N3A—N4A	108.1 (3)
N3—N2—N1	111.5 (3)	N3A—N4A—C1A	105.1 (3)
N4—N3—N2	107.5 (3)	C8A—N5A—N6A	103.7 (3)

N3—N4—C1	105.6 (3)	N5A—N6A—Ta1A	127.1 (2)
C8—N5—N6	103.6 (3)	N7A—N6A—Ta1A	121.8 (2)
N5—N6—Ta1	125.3 (2)	N7A—N6A—N5A	111.0 (3)
N7—N6—Ta1	123.5 (2)	N6A—N7A—N8A	108.1 (3)
N7—N6—N5	111.1 (3)	N7A—N8A—C8A	104.9 (3)
N6—N7—N8	108.0 (3)	C15A—N9A—N10A	103.1 (3)
N7—N8—C8	105.3 (3)	N9A—N10A—Ta1A	125.8 (2)
C15—N9—N10	103.1 (3)	N11A—N10A—Ta1A	122.9 (2)
N9—N10—Ta1	125.4 (2)	N11A—N10A—N9A	110.9 (3)
N11—N10—Ta1	123.9 (2)	N12A—N11A—N10A	108.1 (3)
N11—N10—N9	110.8 (3)	N11A—N12A—C15A	105.6 (3)
N12—N11—N10	108.7 (3)	C22A—N13A—Ta1A	143.6 (2)
N11—N12—C15	105.3 (3)	C22A—N13A—C23A	112.8 (3)
C22—N13—Ta1	143.6 (2)	C23A—N13A—Ta1A	103.6 (2)
C22—N13—C23	112.9 (3)	N19A—N18A—C31A	103.7 (3)
C23—N13—Ta1	103.4 (2)	N18A—N19A—Ta1A	129.5 (2)
N15—N14—C24	104.3 (3)	N18A—N19A—N20A	110.4 (3)
N14—N15—Ta1	127.8 (2)	N20A—N19A—Ta1A	120.06 (19)
N14—N15—N16	110.0 (3)	N19A—N20A—Ta2A	121.2 (2)
N16—N15—Ta1	121.5 (2)	N19A—N20A—N21A	109.5 (3)
N15—N16—Ta2	119.6 (2)	N21A—N20A—Ta2A	129.3 (2)
N15—N16—N17	109.8 (3)	N20A—N21A—C31A	103.7 (3)
N17—N16—Ta2	130.4 (2)	N15A—N14A—C24A	104.5 (3)
N16—N17—C24	103.7 (3)	N14A—N15A—Ta1A	128.1 (2)
N19—N18—C31	104.3 (3)	N14A—N15A—N16A	109.4 (2)
N18—N19—Ta1	130.1 (2)	N16A—N15A—Ta1A	121.48 (19)
N18—N19—N20	109.8 (3)	N15A—N16A—Ta2A	120.03 (19)
N20—N19—Ta1	120.2 (2)	N17A—N16A—Ta2A	129.0 (2)
N19—N20—Ta2	120.8 (2)	N17A—N16A—N15A	110.1 (3)
N21—N20—Ta2	129.3 (2)	N16A—N17A—C24A	103.8 (3)
N21—N20—N19	109.9 (3)	C38A—N22A—N23A	103.8 (3)
N20—N21—C31	103.7 (3)	N22A—N23A—Ta2A	123.8 (2)
C38—N22—N23	103.1 (3)	N24A—N23A—Ta2A	124.1 (2)
N22—N23—Ta2	124.7 (2)	N24A—N23A—N22A	111.2 (3)
N24—N23—Ta2	122.5 (2)	N25A—N24A—N23A	107.6 (3)
N24—N23—N22	111.4 (3)	N24A—N25A—C38A	105.5 (3)
N23—N24—N25	108.3 (3)	C45A—N26A—N27A	104.0 (3)
N24—N25—C38	105.1 (3)	N26A—N27A—Ta2A	127.4 (2)
C45—N26—N27	103.8 (3)	N28A—N27A—Ta2A	122.5 (2)
N26—N27—Ta2	124.5 (2)	N28A—N27A—N26A	110.0 (3)
N28—N27—Ta2	122.9 (2)	N29A—N28A—N27A	108.7 (3)
N28—N27—N26	110.4 (3)	N28A—N29A—C45A	105.5 (3)
N27—N28—N29	108.5 (3)	C52A—N30A—N31A	103.2 (3)
N28—N29—C45	105.3 (3)	N30A—N31A—Ta2A	127.5 (2)
C52—N30—N31	103.0 (3)	N32A—N31A—Ta2A	121.6 (2)
N30—N31—Ta2	125.0 (2)	N32A—N31A—N30A	110.8 (3)
N32—N31—Ta2	123.0 (2)	N33A—N32A—N31A	108.5 (3)
N32—N31—N30	111.7 (3)	N32A—N33A—C52A	105.3 (3)

N31—N32—N33	107.4 (3)	C59A—N34A—Ta2A	144.4 (2)
N32—N33—C52	105.7 (3)	C59A—N34A—C60A	112.5 (3)
C59—N34—Ta2	142.0 (2)	C60A—N34A—Ta2A	103.0 (2)
C59—N34—C60	112.8 (3)	H35D—N35A—H35E	107.7
C60—N34—Ta2	105.0 (2)	C61A—N35A—H35D	108.9
H35B—N35—H35C	107.8	C61A—N35A—H35E	108.9
C61—N35—H35B	109.0	C61A—N35A—C62A	113.2 (3)
C61—N35—H35C	109.0	C62A—N35A—H35D	108.9
C62—N35—H35B	109.0	C62A—N35A—H35E	108.9
C62—N35—H35C	109.0	H36D—N36A—H36E	107.8
C62—N35—C61	112.8 (3)	C63A—N36A—H36D	108.9
H36B—N36—H36C	107.7	C63A—N36A—H36E	108.9
C63—N36—H36B	108.8	C63A—N36A—C64A	113.1 (3)
C63—N36—H36C	108.8	C64A—N36A—H36D	108.9
C63—N36—C64	113.9 (3)	C64A—N36A—H36E	108.9
C64—N36—H36B	108.8	N1A—C1A—N4A	112.0 (3)
C64—N36—H36C	108.8	N1A—C1A—C2A	124.7 (3)
N1—C1—N4	112.7 (3)	N4A—C1A—C2A	123.2 (3)
N1—C1—C2	123.4 (3)	C3A—C2A—C1A	120.9 (3)
N4—C1—C2	123.7 (3)	C3A—C2A—C7A	119.7 (3)
C3—C2—C1	120.0 (3)	C7A—C2A—C1A	119.4 (3)
C3—C2—C7	119.9 (3)	C2A—C3A—H3A	119.9
C7—C2—C1	120.0 (3)	C4A—C3A—C2A	120.1 (3)
C2—C3—H3	119.7	C4A—C3A—H3A	119.9
C4—C3—C2	120.7 (3)	C3A—C4A—H4A	120.1
C4—C3—H3	119.7	C3A—C4A—C5A	119.7 (4)
C3—C4—H4	120.1	C5A—C4A—H4A	120.1
C3—C4—C5	119.8 (4)	C4A—C5A—H5A	119.8
C5—C4—H4	120.1	C6A—C5A—C4A	120.4 (3)
C4—C5—H5	120.0	C6A—C5A—H5A	119.8
C6—C5—C4	120.0 (3)	C5A—C6A—H6A	119.8
C6—C5—H5	120.0	C5A—C6A—C7A	120.4 (4)
C5—C6—H6	119.7	C7A—C6A—H6A	119.8
C5—C6—C7	120.7 (3)	C2A—C7A—H7A	120.2
C7—C6—H6	119.7	C6A—C7A—C2A	119.6 (4)
C2—C7—H7	120.5	C6A—C7A—H7A	120.2
C6—C7—C2	119.0 (3)	N5A—C8A—N8A	112.3 (3)
C6—C7—H7	120.5	N5A—C8A—C9A	125.2 (3)
N5—C8—N8	112.0 (3)	N8A—C8A—C9A	122.5 (3)
N5—C8—C9	124.9 (3)	C10A—C9A—C8A	121.2 (3)
N8—C8—C9	123.1 (3)	C10A—C9A—C14A	119.4 (3)
C10—C9—C8	120.9 (3)	C14A—C9A—C8A	119.3 (3)
C10—C9—C14	119.4 (3)	C9A—C10A—H10A	119.9
C14—C9—C8	119.7 (3)	C9A—C10A—C11A	120.3 (4)
C9—C10—H10	119.9	C11A—C10A—H10A	119.9
C11—C10—C9	120.2 (4)	C10A—C11A—H11A	119.9
C11—C10—H10	119.9	C12A—C11A—C10A	120.3 (4)
C10—C11—H11	119.8	C12A—C11A—H11A	119.9

C12—C11—C10	120.4 (4)	C11A—C12A—H12A	120.2
C12—C11—H11	119.8	C13A—C12A—C11A	119.7 (4)
C11—C12—H12	120.2	C13A—C12A—H12A	120.2
C11—C12—C13	119.5 (3)	C12A—C13A—H13A	119.7
C13—C12—H12	120.2	C12A—C13A—C14A	120.6 (4)
C12—C13—H13	119.7	C14A—C13A—H13A	119.7
C12—C13—C14	120.6 (4)	C9A—C14A—H14A	120.1
C14—C13—H13	119.7	C13A—C14A—C9A	119.8 (4)
C9—C14—C13	119.8 (4)	C13A—C14A—H14A	120.1
C9—C14—H14	120.1	N9A—C15A—N12A	112.3 (3)
C13—C14—H14	120.1	N9A—C15A—C16A	124.9 (3)
N9—C15—N12	112.2 (3)	N12A—C15A—C16A	122.7 (3)
N9—C15—C16	124.6 (3)	C17A—C16A—C15A	118.9 (3)
N12—C15—C16	123.2 (3)	C21A—C16A—C15A	121.6 (3)
C17—C16—C15	119.9 (3)	C21A—C16A—C17A	119.5 (3)
C21—C16—C15	120.6 (3)	C16A—C17A—H17A	119.9
C21—C16—C17	119.5 (3)	C18A—C17A—C16A	120.1 (4)
C16—C17—H17	120.4	C18A—C17A—H17A	119.9
C18—C17—C16	119.3 (4)	C17A—C18A—H18A	119.9
C18—C17—H17	120.4	C19A—C18A—C17A	120.2 (4)
C17—C18—H18	119.4	C19A—C18A—H18A	119.9
C17—C18—C19	121.1 (4)	C18A—C19A—H19A	120.0
C19—C18—H18	119.4	C18A—C19A—C20A	120.0 (4)
C18—C19—H19	120.3	C20A—C19A—H19A	120.0
C20—C19—C18	119.5 (4)	C19A—C20A—H20A	119.8
C20—C19—H19	120.3	C19A—C20A—C21A	120.3 (4)
C19—C20—H20	119.9	C21A—C20A—H20A	119.8
C19—C20—C21	120.3 (4)	C16A—C21A—C20A	119.9 (4)
C21—C20—H20	119.9	C16A—C21A—H21A	120.0
C16—C21—C20	120.4 (4)	C20A—C21A—H21A	120.0
C16—C21—H21	119.8	N13A—C22A—H22D	109.5
C20—C21—H21	119.8	N13A—C22A—H22E	109.5
N13—C22—H22A	109.5	N13A—C22A—H22F	109.5
N13—C22—H22B	109.5	H22D—C22A—H22E	109.5
N13—C22—H22C	109.5	H22D—C22A—H22F	109.5
H22A—C22—H22B	109.5	H22E—C22A—H22F	109.5
H22A—C22—H22C	109.5	N13A—C23A—H23D	109.5
H22B—C22—H22C	109.5	N13A—C23A—H23E	109.5
N13—C23—H23A	109.5	N13A—C23A—H23F	109.5
N13—C23—H23B	109.5	H23D—C23A—H23E	109.5
N13—C23—H23C	109.5	H23D—C23A—H23F	109.5
H23A—C23—H23B	109.5	H23E—C23A—H23F	109.5
H23A—C23—H23C	109.5	N18A—C31A—N21A	112.6 (3)
H23B—C23—H23C	109.5	N18A—C31A—C32A	124.2 (3)
N14—C24—N17	112.1 (3)	N21A—C31A—C32A	123.1 (3)
N14—C24—C25	122.4 (3)	C33A—C32A—C31A	119.9 (3)
N17—C24—C25	125.4 (3)	C33A—C32A—C37A	119.7 (3)
C26—C25—C24	119.4 (3)	C37A—C32A—C31A	120.3 (3)

C26—C25—C30	119.5 (3)	C32A—C33A—H33A	120.1
C30—C25—C24	121.0 (3)	C32A—C33A—C34A	119.9 (3)
C25—C26—H26	119.8	C34A—C33A—H33A	120.1
C27—C26—C25	120.4 (3)	C33A—C34A—H34A	120.0
C27—C26—H26	119.8	C35A—C34A—C33A	120.0 (3)
C26—C27—H27	120.1	C35A—C34A—H34A	120.0
C26—C27—C28	119.9 (3)	C34A—C35A—H35A	119.8
C28—C27—H27	120.1	C36A—C35A—C34A	120.4 (3)
C27—C28—H28	119.8	C36A—C35A—H35A	119.8
C29—C28—C27	120.3 (3)	C35A—C36A—H36A	120.0
C29—C28—H28	119.8	C35A—C36A—C37A	120.0 (4)
C28—C29—H29	120.0	C37A—C36A—H36A	120.0
C28—C29—C30	119.9 (4)	C32A—C37A—H37A	120.0
C30—C29—H29	120.0	C36A—C37A—C32A	120.0 (4)
C25—C30—C29	119.9 (3)	C36A—C37A—H37A	120.0
C25—C30—H30	120.1	N14A—C24A—N17A	112.2 (3)
C29—C30—H30	120.1	N14A—C24A—C25A	123.6 (3)
N18—C31—N21	112.3 (3)	N17A—C24A—C25A	124.2 (3)
N18—C31—C32	124.7 (3)	C30A—C25A—C24A	119.8 (3)
N21—C31—C32	123.0 (3)	C30A—C25A—C26A	119.9 (3)
C33—C32—C31	119.6 (3)	C26A—C25A—C24A	120.4 (3)
C33—C32—C37	119.8 (3)	C25A—C30A—H30A	119.9
C37—C32—C31	120.4 (3)	C29A—C30A—C25A	120.2 (4)
C32—C33—H33	120.0	C29A—C30A—H30A	119.9
C32—C33—C34	119.9 (4)	C30A—C29A—H29A	120.0
C34—C33—H33	120.0	C30A—C29A—C28A	119.9 (4)
C33—C34—H34	119.9	C28A—C29A—H29A	120.0
C35—C34—C33	120.1 (4)	C29A—C28A—H28A	120.1
C35—C34—H34	119.9	C27A—C28A—C29A	119.9 (3)
C34—C35—H35	119.8	C27A—C28A—H28A	120.1
C34—C35—C36	120.3 (4)	C28A—C27A—H27A	119.7
C36—C35—H35	119.8	C26A—C27A—C28A	120.6 (3)
C35—C36—H36	120.1	C26A—C27A—H27A	119.7
C35—C36—C37	119.9 (4)	C25A—C26A—H26A	120.2
C37—C36—H36	120.1	C27A—C26A—C25A	119.6 (3)
C32—C37—H37	120.1	C27A—C26A—H26A	120.2
C36—C37—C32	119.8 (4)	N22A—C38A—N25A	112.0 (3)
C36—C37—H37	120.1	N22A—C38A—C39A	124.1 (3)
N22—C38—N25	112.1 (3)	N25A—C38A—C39A	123.9 (3)
N22—C38—C39	124.5 (3)	C40A—C39A—C38A	120.5 (3)
N25—C38—C39	123.4 (3)	C44A—C39A—C38A	119.9 (3)
C40—C39—C38	119.3 (3)	C44A—C39A—C40A	119.6 (3)
C44—C39—C38	121.2 (3)	C39A—C40A—H40A	120.1
C44—C39—C40	119.5 (3)	C39A—C40A—C41A	119.7 (4)
C39—C40—H40	120.2	C41A—C40A—H40A	120.1
C41—C40—C39	119.6 (3)	C40A—C41A—H41A	119.9
C41—C40—H40	120.2	C42A—C41A—C40A	120.1 (4)
C40—C41—H41	119.7	C42A—C41A—H41A	119.9

C42—C41—C40	120.7 (3)	C41A—C42A—H42A	119.9
C42—C41—H41	119.7	C43A—C42A—C41A	120.2 (4)
C41—C42—H42	120.0	C43A—C42A—H42A	119.9
C41—C42—C43	119.9 (3)	C42A—C43A—H43A	119.9
C43—C42—H42	120.0	C42A—C43A—C44A	120.2 (4)
C42—C43—H43	120.1	C44A—C43A—H43A	119.9
C44—C43—C42	119.8 (3)	C39A—C44A—H44A	119.9
C44—C43—H43	120.1	C43A—C44A—C39A	120.1 (4)
C39—C44—H44	119.7	C43A—C44A—H44A	119.9
C43—C44—C39	120.5 (3)	N26A—C45A—N29A	111.7 (3)
C43—C44—H44	119.7	N26A—C45A—C46A	125.0 (3)
N26—C45—N29	112.0 (3)	N29A—C45A—C46A	123.3 (3)
N26—C45—C46	125.0 (3)	C51A—C46A—C45A	120.2 (3)
N29—C45—C46	122.9 (3)	C47A—C46A—C45A	120.9 (3)
C47—C46—C45	121.2 (3)	C47A—C46A—C51A	118.9 (3)
C47—C46—C51	119.0 (3)	C46A—C51A—H51A	119.9
C51—C46—C45	119.8 (3)	C50A—C51A—C46A	120.1 (3)
C46—C47—H47	119.6	C50A—C51A—H51A	119.9
C46—C47—C48	120.7 (4)	C51A—C50A—H50A	119.5
C48—C47—H47	119.6	C49A—C50A—C51A	120.9 (4)
C47—C48—H48	120.1	C49A—C50A—H50A	119.5
C49—C48—C47	119.8 (4)	C50A—C49A—H49A	120.5
C49—C48—H48	120.1	C50A—C49A—C48A	119.0 (4)
C48—C49—H49	120.0	C48A—C49A—H49A	120.5
C48—C49—C50	120.0 (4)	C49A—C48A—H48A	119.7
C50—C49—H49	120.0	C49A—C48A—C47A	120.6 (4)
C49—C50—H50	119.8	C47A—C48A—H48A	119.7
C49—C50—C51	120.4 (4)	C46A—C47A—H47A	119.7
C51—C50—H50	119.8	C48A—C47A—C46A	120.5 (3)
C46—C51—H51	120.0	C48A—C47A—H47A	119.7
C50—C51—C46	120.0 (3)	N30A—C52A—N33A	112.1 (3)
C50—C51—H51	120.0	N30A—C52A—C53A	125.4 (3)
N30—C52—N33	112.2 (3)	N33A—C52A—C53A	122.5 (3)
N30—C52—C53	118.3 (4)	C58A—C53A—C52A	119.3 (3)
N30—C52—C53B	129.6 (5)	C54A—C53A—C52A	121.3 (3)
N33—C52—C53	129.4 (5)	C54A—C53A—C58A	119.5 (3)
N33—C52—C53B	118.2 (5)	C53A—C58A—H58A	119.9
C54—C53—C52	121.3 (5)	C57A—C58A—C53A	120.1 (4)
C54—C53—C58	120.0	C57A—C58A—H58A	119.9
C58—C53—C52	118.5 (5)	C58A—C57A—H57A	119.7
C53—C54—H54	120.0	C58A—C57A—C56A	120.6 (4)
C53—C54—C55	120.0	C56A—C57A—H57A	119.7
C55—C54—H54	120.0	C57A—C56A—H56A	120.3
C54—C55—H55	120.0	C57A—C56A—C55A	119.5 (3)
C56—C55—C54	120.0	C55A—C56A—H56A	120.3
C56—C55—H55	120.0	C56A—C55A—H55A	119.9
C55—C56—H56	120.0	C56A—C55A—C54A	120.3 (4)
C55—C56—C57	120.0	C54A—C55A—H55A	119.9

C57—C56—H56	120.0	C53A—C54A—C55A	120.0 (4)
C56—C57—H57	120.0	C53A—C54A—H54A	120.0
C58—C57—C56	120.0	C55A—C54A—H54A	120.0
C58—C57—H57	120.0	N34A—C59A—H59D	109.5
C53—C58—H58	120.0	N34A—C59A—H59E	109.5
C57—C58—C53	120.0	N34A—C59A—H59F	109.5
C57—C58—H58	120.0	H59D—C59A—H59E	109.5
C54B—C53B—C52	117.1 (5)	H59D—C59A—H59F	109.5
C54B—C53B—C58B	120.0	H59E—C59A—H59F	109.5
C58B—C53B—C52	122.8 (5)	N34A—C60A—H60D	109.5
C53B—C54B—H54B	120.0	N34A—C60A—H60E	109.5
C53B—C54B—C55B	120.0	N34A—C60A—H60F	109.5
C55B—C54B—H54B	120.0	H60D—C60A—H60E	109.5
C54B—C55B—H55B	120.0	H60D—C60A—H60F	109.5
C56B—C55B—C54B	120.0	H60E—C60A—H60F	109.5
C56B—C55B—H55B	120.0	N35A—C61A—H61D	109.5
C55B—C56B—H56B	120.0	N35A—C61A—H61E	109.5
C55B—C56B—C57B	120.0	N35A—C61A—H61F	109.5
C57B—C56B—H56B	120.0	H61D—C61A—H61E	109.5
C56B—C57B—H57B	120.0	H61D—C61A—H61F	109.5
C58B—C57B—C56B	120.0	H61E—C61A—H61F	109.5
C58B—C57B—H57B	120.0	N35A—C62A—H62D	109.5
C53B—C58B—H58B	120.0	N35A—C62A—H62E	109.5
C57B—C58B—C53B	120.0	N35A—C62A—H62F	109.5
C57B—C58B—H58B	120.0	H62D—C62A—H62E	109.5
N34—C59—H59A	109.5	H62D—C62A—H62F	109.5
N34—C59—H59B	109.5	H62E—C62A—H62F	109.5
N34—C59—H59C	109.5	N36A—C63A—H63D	109.5
H59A—C59—H59B	109.5	N36A—C63A—H63E	109.5
H59A—C59—H59C	109.5	N36A—C63A—H63F	109.5
H59B—C59—H59C	109.5	H63D—C63A—H63E	109.5
N34—C60—H60A	109.5	H63D—C63A—H63F	109.5
N34—C60—H60B	109.5	H63E—C63A—H63F	109.5
N34—C60—H60C	109.5	N36A—C64A—H64D	109.5
H60A—C60—H60B	109.5	N36A—C64A—H64E	109.5
H60A—C60—H60C	109.5	N36A—C64A—H64F	109.5
H60B—C60—H60C	109.5	H64D—C64A—H64E	109.5
N35—C61—H61A	109.5	H64D—C64A—H64F	109.5
N35—C61—H61B	109.5	H64E—C64A—H64F	109.5
N35—C61—H61C	109.5	H1SA—C1S—H1SB	109.5
H61A—C61—H61B	109.5	H1SA—C1S—H1SC	109.5
H61A—C61—H61C	109.5	H1SB—C1S—H1SC	109.5
H61B—C61—H61C	109.5	C2S—C1S—H1SA	109.5
N35—C62—H62A	109.5	C2S—C1S—H1SB	109.5
N35—C62—H62B	109.5	C2S—C1S—H1SC	109.5
N35—C62—H62C	109.5	C3S—C2S—C1S	121.0
H62A—C62—H62B	109.5	C7S—C2S—C1S	120.9
H62A—C62—H62C	109.5	C7S—C2S—C3S	118.1

H62B—C62—H62C	109.5	C2S—C3S—H3S	119.5
N36—C63—H63A	109.5	C4S—C3S—C2S	121.1
N36—C63—H63B	109.5	C4S—C3S—H3S	119.5
N36—C63—H63C	109.5	C3S—C4S—H4S	119.9
H63A—C63—H63B	109.5	C5S—C4S—C3S	120.1
H63A—C63—H63C	109.5	C5S—C4S—H4S	119.9
H63B—C63—H63C	109.5	C4S—C5S—H5S	120.3
N36—C64—H64A	109.5	C4S—C5S—C6S	119.4
N36—C64—H64B	109.5	C6S—C5S—H5S	120.3
N36—C64—H64C	109.5	C5S—C6S—H6S	119.9
H64A—C64—H64B	109.5	C7S—C6S—C5S	120.1
H64A—C64—H64C	109.5	C7S—C6S—H6S	119.9
H64B—C64—H64C	109.5	C2S—C7S—H7S	119.5
O1A—Ta1A—N2A	101.40 (9)	C6S—C7S—C2S	121.1
O1A—Ta1A—N6A	87.99 (10)	C6S—C7S—H7S	119.5

Ta1—N2—N3—N4	−167.1 (2)	C55B—C56B—C57B—C58B	0.0
Ta1—N6—N7—N8	−176.3 (2)	C56B—C57B—C58B—C53B	0.0
Ta1—N10—N11—N12	178.9 (2)	C58B—C53B—C54B—C55B	0.0
Ta1—N15—N16—Ta2	−4.2 (3)	Ta1A—N2A—N3A—N4A	178.2 (2)
Ta1—N15—N16—N17	171.25 (19)	Ta1A—N6A—N7A—N8A	−175.3 (2)
Ta1—N19—N20—Ta2	−2.9 (3)	Ta1A—N10A—N11A—N12A	172.6 (2)
Ta1—N19—N20—N21	179.4 (2)	Ta1A—N19A—N20A—Ta2A	3.9 (3)
Ta2—N16—N17—C24	174.9 (2)	Ta1A—N19A—N20A—N21A	−177.70 (19)
Ta2—N20—N21—C31	−176.9 (2)	Ta1A—N15A—N16A—Ta2A	−1.0 (3)
Ta2—N23—N24—N25	167.2 (2)	Ta1A—N15A—N16A—N17A	169.22 (19)
Ta2—N27—N28—N29	−164.6 (2)	Ta2A—N20A—N21A—C31A	178.1 (2)
Ta2—N31—N32—N33	−173.9 (2)	Ta2A—N16A—N17A—C24A	169.0 (2)
N1—N2—N3—N4	−0.2 (4)	Ta2A—N23A—N24A—N25A	170.1 (2)
N1—C1—C2—C3	19.1 (5)	Ta2A—N27A—N28A—N29A	−178.3 (2)
N1—C1—C2—C7	−164.9 (3)	Ta2A—N31A—N32A—N33A	177.6 (2)
N2—N1—C1—N4	−0.1 (4)	N1A—N2A—N3A—N4A	1.5 (4)
N2—N1—C1—C2	−175.1 (3)	N1A—C1A—C2A—C3A	−18.4 (5)
N2—N3—N4—C1	0.1 (4)	N1A—C1A—C2A—C7A	164.0 (3)
N3—N4—C1—N1	0.0 (4)	N2A—N1A—C1A—N4A	1.1 (4)
N3—N4—C1—C2	174.9 (3)	N2A—N1A—C1A—C2A	177.7 (3)
N4—C1—C2—C3	−155.3 (3)	N2A—N3A—N4A—C1A	−0.8 (4)
N4—C1—C2—C7	20.7 (5)	N3A—N4A—C1A—N1A	−0.2 (4)
N5—N6—N7—N8	−0.2 (4)	N3A—N4A—C1A—C2A	−176.9 (3)
N5—C8—C9—C10	7.0 (5)	N4A—C1A—C2A—C3A	157.9 (4)
N5—C8—C9—C14	−171.7 (3)	N4A—C1A—C2A—C7A	−19.6 (5)
N6—N5—C8—N8	−0.1 (4)	N5A—N6A—N7A—N8A	1.5 (4)
N6—N5—C8—C9	177.7 (3)	N5A—C8A—C9A—C10A	−12.4 (5)
N6—N7—N8—C8	0.1 (4)	N5A—C8A—C9A—C14A	167.2 (4)
N7—N8—C8—N5	0.0 (4)	N6A—N5A—C8A—N8A	2.1 (4)
N7—N8—C8—C9	−177.8 (3)	N6A—N5A—C8A—C9A	−178.9 (3)
N8—C8—C9—C10	−175.4 (3)	N6A—N7A—N8A—C8A	−0.1 (4)
N8—C8—C9—C14	5.9 (5)	N7A—N8A—C8A—N5A	−1.3 (4)

N9—N10—N11—N12	0.1 (4)
N9—C15—C16—C17	168.1 (3)
N9—C15—C16—C21	−13.3 (5)
N10—N9—C15—N12	0.4 (4)
N10—N9—C15—C16	179.4 (3)
N10—N11—N12—C15	0.1 (4)
N11—N12—C15—N9	−0.3 (4)
N11—N12—C15—C16	−179.3 (3)
N12—C15—C16—C17	−13.0 (5)
N12—C15—C16—C21	165.6 (4)
N14—N15—N16—Ta2	−175.65 (19)
N14—N15—N16—N17	−0.2 (3)
N14—C24—C25—C26	−5.7 (5)
N14—C24—C25—C30	173.0 (3)
N15—N14—C24—N17	−0.2 (4)
N15—N14—C24—C25	177.5 (3)
N15—N16—N17—C24	0.1 (3)
N16—N17—C24—N14	0.0 (4)
N16—N17—C24—C25	−177.5 (3)
N17—C24—C25—C26	171.6 (3)
N17—C24—C25—C30	−9.7 (5)
N18—N19—N20—Ta2	176.91 (19)
N18—N19—N20—N21	−0.8 (4)
N18—C31—C32—C33	−21.4 (5)
N18—C31—C32—C37	162.3 (4)
N19—N18—C31—N21	−0.3 (4)
N19—N18—C31—C32	178.4 (3)
N19—N20—N21—C31	0.6 (3)
N20—N21—C31—N18	−0.2 (4)
N20—N21—C31—C32	−178.9 (3)
N21—C31—C32—C33	157.2 (3)
N21—C31—C32—C37	−19.1 (5)
N22—N23—N24—N25	0.0 (4)
N22—C38—C39—C40	175.1 (3)
N22—C38—C39—C44	−4.9 (5)
N23—N22—C38—N25	0.6 (4)
N23—N22—C38—C39	−178.4 (3)
N23—N24—N25—C38	0.4 (4)
N24—N25—C38—N22	−0.6 (4)
N24—N25—C38—C39	178.4 (3)
N25—C38—C39—C40	−3.8 (5)
N25—C38—C39—C44	176.3 (3)
N26—N27—N28—N29	−0.9 (4)
N26—C45—C46—C47	−15.9 (5)
N26—C45—C46—C51	162.9 (3)
N27—N26—C45—N29	−0.7 (4)
N27—N26—C45—C46	−178.9 (3)
N27—N28—N29—C45	0.5 (4)
N7A—N8A—C8A—C9A	179.7 (3)
N8A—C8A—C9A—C10A	166.4 (3)
N8A—C8A—C9A—C14A	−14.0 (5)
N9A—N10A—N11A—N12A	−0.4 (4)
N9A—C15A—C16A—C17A	158.5 (3)
N9A—C15A—C16A—C21A	−21.8 (5)
N10A—N9A—C15A—N12A	0.2 (4)
N10A—N9A—C15A—C16A	−178.8 (3)
N10A—N11A—N12A—C15A	0.5 (4)
N11A—N12A—C15A—N9A	−0.4 (4)
N11A—N12A—C15A—C16A	178.6 (3)
N12A—C15A—C16A—C17A	−20.4 (5)
N12A—C15A—C16A—C21A	159.3 (3)
N18A—N19A—N20A—Ta2A	−177.79 (19)
N18A—N19A—N20A—N21A	0.6 (3)
N18A—C31A—C32A—C33A	−8.4 (5)
N18A—C31A—C32A—C37A	175.1 (3)
N19A—N18A—C31A—N21A	0.8 (4)
N19A—N18A—C31A—C32A	178.7 (3)
N19A—N20A—N21A—C31A	−0.1 (3)
N20A—N21A—C31A—N18A	−0.4 (4)
N20A—N21A—C31A—C32A	−178.4 (3)
N21A—C31A—C32A—C33A	169.3 (3)
N21A—C31A—C32A—C37A	−7.2 (5)
N14A—N15A—N16A—Ta2A	−170.18 (19)
N14A—N15A—N16A—N17A	0.1 (3)
N14A—C24A—C25A—C30A	−159.8 (3)
N14A—C24A—C25A—C26A	19.4 (5)
N15A—N14A—C24A—N17A	−0.1 (4)
N15A—N14A—C24A—C25A	178.0 (3)
N15A—N16A—N17A—C24A	−0.1 (3)
N16A—N17A—C24A—N14A	0.2 (4)
N16A—N17A—C24A—C25A	−177.9 (3)
N17A—C24A—C25A—C30A	18.1 (5)
N17A—C24A—C25A—C26A	−162.7 (3)
N22A—N23A—N24A—N25A	0.7 (4)
N22A—C38A—C39A—C40A	162.9 (3)
N22A—C38A—C39A—C44A	−16.3 (5)
N23A—N22A—C38A—N25A	0.7 (4)
N23A—N22A—C38A—C39A	−179.5 (3)
N23A—N24A—N25A—C38A	−0.2 (4)
N24A—N25A—C38A—N22A	−0.3 (4)
N24A—N25A—C38A—C39A	179.9 (3)
N25A—C38A—C39A—C40A	−17.3 (5)
N25A—C38A—C39A—C44A	163.5 (4)
N26A—N27A—N28A—N29A	0.9 (4)
N26A—C45A—C46A—C51A	−179.1 (3)
N26A—C45A—C46A—C47A	2.6 (5)

N28—N29—C45—N26	0.1 (4)
N28—N29—C45—C46	178.4 (3)
N29—C45—C46—C47	166.0 (4)
N29—C45—C46—C51	−15.2 (5)
N30—N31—N32—N33	−0.3 (4)
N30—C52—C53—C54	6.9 (7)
N30—C52—C53—C58	−177.3 (4)
N30—C52—C53B—C54B	−2.8 (8)
N30—C52—C53B—C58B	173.6 (4)
N31—N30—C52—N33	−0.7 (4)
N31—N30—C52—C53	−177.2 (4)
N31—N30—C52—C53B	−177.8 (5)
N31—N32—N33—C52	−0.2 (4)
N32—N33—C52—N30	0.6 (4)
N32—N33—C52—C53	176.5 (5)
N32—N33—C52—C53B	178.0 (5)
N33—C52—C53—C54	−168.8 (5)
N33—C52—C53—C58	7.0 (8)
N33—C52—C53B—C54B	−179.8 (4)
N33—C52—C53B—C58B	−3.4 (7)
C1—N1—N2—Ta1	167.0 (2)
C1—N1—N2—N3	0.1 (4)
C1—C2—C3—C4	175.0 (3)
C1—C2—C7—C6	−175.2 (3)
C2—C3—C4—C5	0.0 (5)
C3—C2—C7—C6	0.8 (5)
C3—C4—C5—C6	1.0 (6)
C4—C5—C6—C7	−1.1 (6)
C5—C6—C7—C2	0.2 (5)
C7—C2—C3—C4	−1.0 (5)
C8—N5—N6—Ta1	176.3 (2)
C8—N5—N6—N7	0.2 (3)
C8—C9—C10—C11	−178.4 (3)
C8—C9—C14—C13	178.3 (3)
C9—C10—C11—C12	0.0 (6)
C10—C9—C14—C13	−0.4 (6)
C10—C11—C12—C13	−0.4 (6)
C11—C12—C13—C14	0.3 (6)
C12—C13—C14—C9	0.1 (6)
C14—C9—C10—C11	0.4 (5)
C15—N9—N10—Ta1	−179.0 (2)
C15—N9—N10—N11	−0.3 (3)
C15—C16—C17—C18	179.1 (3)
C15—C16—C21—C20	−179.9 (4)
C16—C17—C18—C19	0.6 (6)
C17—C16—C21—C20	−1.4 (6)
C17—C18—C19—C20	−0.7 (7)
C18—C19—C20—C21	−0.1 (7)
N27A—N26A—C45A—N29A	1.2 (4)
N27A—N26A—C45A—C46A	−179.0 (3)
N27A—N28A—N29A—C45A	−0.2 (4)
N28A—N29A—C45A—N26A	−0.7 (4)
N28A—N29A—C45A—C46A	179.6 (3)
N29A—C45A—C46A—C51A	0.7 (5)
N29A—C45A—C46A—C47A	−177.6 (3)
N30A—N31A—N32A—N33A	0.0 (4)
N30A—C52A—C53A—C58A	178.2 (3)
N30A—C52A—C53A—C54A	−1.5 (5)
N31A—N30A—C52A—N33A	0.1 (4)
N31A—N30A—C52A—C53A	−179.3 (3)
N31A—N32A—N33A—C52A	0.0 (4)
N32A—N33A—C52A—N30A	−0.1 (4)
N32A—N33A—C52A—C53A	179.3 (3)
N33A—C52A—C53A—C58A	−1.1 (5)
N33A—C52A—C53A—C54A	179.2 (3)
C1A—N1A—N2A—Ta1A	−178.2 (2)
C1A—N1A—N2A—N3A	−1.5 (4)
C1A—C2A—C3A—C4A	−177.6 (3)
C1A—C2A—C7A—C6A	177.7 (3)
C2A—C3A—C4A—C5A	−0.3 (5)
C3A—C2A—C7A—C6A	0.1 (5)
C3A—C4A—C5A—C6A	0.5 (6)
C4A—C5A—C6A—C7A	−0.4 (6)
C5A—C6A—C7A—C2A	0.1 (6)
C7A—C2A—C3A—C4A	0.0 (5)
C8A—N5A—N6A—Ta1A	174.4 (2)
C8A—N5A—N6A—N7A	−2.2 (4)
C8A—C9A—C10A—C11A	179.0 (3)
C8A—C9A—C14A—C13A	−178.7 (4)
C9A—C10A—C11A—C12A	−0.6 (5)
C10A—C9A—C14A—C13A	0.9 (6)
C10A—C11A—C12A—C13A	1.5 (6)
C11A—C12A—C13A—C14A	−1.2 (7)
C12A—C13A—C14A—C9A	0.0 (7)
C14A—C9A—C10A—C11A	−0.6 (5)
C15A—N9A—N10A—Ta1A	−172.6 (2)
C15A—N9A—N10A—N11A	0.1 (3)
C15A—C16A—C17A—C18A	−179.7 (3)
C15A—C16A—C21A—C20A	179.5 (4)
C16A—C17A—C18A—C19A	0.0 (6)
C17A—C16A—C21A—C20A	−0.9 (6)
C17A—C18A—C19A—C20A	−0.4 (6)
C18A—C19A—C20A—C21A	0.1 (7)
C19A—C20A—C21A—C16A	0.5 (6)
C21A—C16A—C17A—C18A	0.6 (6)
C31A—N18A—N19A—Ta1A	177.3 (2)

C19—C20—C21—C16	1.2 (7)
C21—C16—C17—C18	0.5 (6)
C24—N14—N15—Ta1	−170.5 (2)
C24—N14—N15—N16	0.2 (3)
C24—C25—C26—C27	179.6 (3)
C24—C25—C30—C29	−179.9 (3)
C25—C26—C27—C28	0.2 (5)
C26—C25—C30—C29	−1.2 (5)
C26—C27—C28—C29	−0.9 (6)
C27—C28—C29—C30	0.5 (6)
C28—C29—C30—C25	0.5 (6)
C30—C25—C26—C27	0.9 (5)
C31—N18—N19—Ta1	−179.6 (2)
C31—N18—N19—N20	0.7 (3)
C31—C32—C33—C34	−174.7 (3)
C31—C32—C37—C36	176.0 (4)
C32—C33—C34—C35	−1.0 (6)
C33—C32—C37—C36	−0.3 (6)
C33—C34—C35—C36	−0.8 (6)
C34—C35—C36—C37	2.2 (7)
C35—C36—C37—C32	−1.6 (7)
C37—C32—C33—C34	1.6 (5)
C38—N22—N23—Ta2	−167.2 (2)
C38—N22—N23—N24	−0.3 (4)
C38—C39—C40—C41	178.3 (3)
C38—C39—C44—C43	−179.9 (3)
C39—C40—C41—C42	1.5 (6)
C40—C39—C44—C43	0.2 (5)
C40—C41—C42—C43	0.1 (6)
C41—C42—C43—C44	−1.6 (6)
C42—C43—C44—C39	1.5 (6)
C44—C39—C40—C41	−1.7 (5)
C45—N26—N27—Ta2	164.3 (2)
C45—N26—N27—N28	1.0 (4)
C45—C46—C47—C48	−179.3 (4)
C45—C46—C51—C50	−179.8 (3)
C46—C47—C48—C49	−1.6 (7)
C47—C46—C51—C50	−1.0 (5)
C47—C48—C49—C50	0.3 (7)
C48—C49—C50—C51	0.7 (7)
C49—C50—C51—C46	−0.3 (6)
C51—C46—C47—C48	1.9 (6)
C52—N30—N31—Ta2	174.1 (2)
C52—N30—N31—N32	0.6 (4)
C52—C53—C54—C55	175.7 (7)
C52—C53—C58—C57	−175.8 (7)
C52—C53B—C54B—C55B	176.5 (7)
C52—C53B—C58B—C57B	−176.3 (7)
C31A—N18A—N19A—N20A	−0.8 (3)
C31A—C32A—C33A—C34A	−175.8 (3)
C31A—C32A—C37A—C36A	176.4 (4)
C32A—C33A—C34A—C35A	−0.2 (5)
C33A—C32A—C37A—C36A	−0.1 (6)
C33A—C34A—C35A—C36A	−1.1 (6)
C34A—C35A—C36A—C37A	1.8 (6)
C35A—C36A—C37A—C32A	−1.2 (6)
C37A—C32A—C33A—C34A	0.8 (5)
C24A—N14A—N15A—Ta1A	−168.2 (2)
C24A—N14A—N15A—N16A	0.0 (3)
C24A—C25A—C30A—C29A	−179.5 (4)
C24A—C25A—C26A—C27A	178.7 (3)
C25A—C30A—C29A—C28A	0.8 (7)
C30A—C25A—C26A—C27A	−2.0 (5)
C30A—C29A—C28A—C27A	−2.0 (7)
C29A—C28A—C27A—C26A	1.2 (6)
C28A—C27A—C26A—C25A	0.8 (5)
C26A—C25A—C30A—C29A	1.2 (6)
C38A—N22A—N23A—Ta2A	−170.3 (2)
C38A—N22A—N23A—N24A	−0.9 (4)
C38A—C39A—C40A—C41A	−179.6 (4)
C38A—C39A—C44A—C43A	179.9 (3)
C39A—C40A—C41A—C42A	0.1 (7)
C40A—C39A—C44A—C43A	0.7 (6)
C40A—C41A—C42A—C43A	0.0 (7)
C41A—C42A—C43A—C44A	0.3 (7)
C42A—C43A—C44A—C39A	−0.6 (6)
C44A—C39A—C40A—C41A	−0.4 (6)
C45A—N26A—N27A—Ta2A	177.9 (2)
C45A—N26A—N27A—N28A	−1.3 (3)
C45A—C46A—C51A—C50A	−178.9 (3)
C45A—C46A—C47A—C48A	178.5 (3)
C46A—C51A—C50A—C49A	0.7 (6)
C51A—C46A—C47A—C48A	0.1 (5)
C51A—C50A—C49A—C48A	−0.4 (7)
C50A—C49A—C48A—C47A	0.0 (6)
C49A—C48A—C47A—C46A	0.1 (6)
C47A—C46A—C51A—C50A	−0.5 (5)
C52A—N30A—N31A—Ta2A	−177.4 (2)
C52A—N30A—N31A—N32A	−0.1 (3)
C52A—C53A—C58A—C57A	−179.5 (3)
C52A—C53A—C54A—C55A	179.9 (3)
C53A—C58A—C57A—C56A	−0.1 (6)
C58A—C53A—C54A—C55A	0.1 (5)
C58A—C57A—C56A—C55A	−0.5 (6)
C57A—C56A—C55A—C54A	1.0 (6)
C56A—C55A—C54A—C53A	−0.8 (5)

C53—C54—C55—C56	0.0	C54A—C53A—C58A—C57A	0.3 (5)
C54—C53—C58—C57	0.0	C1S—C2S—C3S—C4S	−178.6
C54—C55—C56—C57	0.0	C1S—C2S—C7S—C6S	178.6
C55—C56—C57—C58	0.0	C2S—C3S—C4S—C5S	−0.1
C56—C57—C58—C53	0.0	C3S—C2S—C7S—C6S	−0.2
C58—C53—C54—C55	0.0	C3S—C4S—C5S—C6S	−0.1
C53B—C54B—C55B—C56B	0.0	C4S—C5S—C6S—C7S	0.1
C54B—C53B—C58B—C57B	0.0	C5S—C6S—C7S—C2S	0.0
C54B—C55B—C56B—C57B	0.0	C7S—C2S—C3S—C4S	0.2

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N35—H35*B*···N24	0.91	2.00	2.875 (4)	161
N35—H35*C*···N3	0.91	2.46	3.031 (4)	121
N35—H35*C*···N7	0.91	2.12	2.943 (4)	150
N36—H36*B*···N11	0.91	1.98	2.836 (4)	156
N36—H36*C*···N28	0.91	2.17	2.978 (5)	148
N36—H36*C*···N32	0.91	2.44	3.085 (4)	128
N35*A*—H35*D*···N3*A*	0.91	2.05	2.867 (4)	149
N35*A*—H35*E*···N24*A*	0.91	2.33	2.994 (4)	130
N35*A*—H35*E*···N28*A*	0.91	2.20	2.954 (4)	140
N36*A*—H36*D*···N7*A*	0.91	2.23	2.961 (4)	137
N36*A*—H36*D*···N11*A*	0.91	2.34	2.981 (4)	127
N36*A*—H36*E*···N32*A*	0.91	1.95	2.828 (4)	161