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Di-μ-chloro-bis[(*N*-*tert*-butylimido)chlorobis(pyridine-κN)titanium(IV)] perdeuterobenzene disolvate

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Key indicators

Single-crystal X-ray study
T = 150 K
Mean σ(C–C) = 0.003 Å
Disorder in main residue
R factor = 0.030
wR factor = 0.036
Data-to-parameter ratio = 15.6

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

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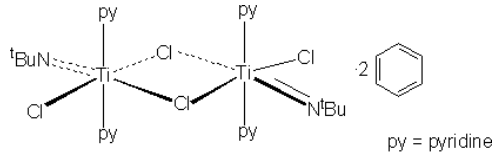
The title compound, $[Ti_2(C_4H_9N)_2Cl_2(C_5H_5N)_4]\cdot 2C_6D_6$, possesses a dinuclear structure featuring two six-coordinate pseudo-octahedral titanium(IV) centres with bridging Cl atoms. The complex is located on a crystallographic inversion centre.

Comment

Over the last 15 years, the chemistry of titanium–imido complexes has received considerable attention (Wigley, 1994). It has been shown that these complexes can be utilized in a wide variety of stoichiometric and sometimes catalytic coupling reactions with unsaturated substrates (Gade & Mountford, 2001, and references therein). A general entry point to new titanium–imido chemistry is gained *via* the readily prepared synthons $[Ti(NR)Cl_2(py)_3]$ (R = ^{t}Bu or aryl) (Mountford, 1997). During the course of our studies, we reported that prolonged exposure of $[Ti(N^tBu)Cl_2(py)_3]$ to vacuum results in the loss of the *trans* pyridine ligand (Blake *et al.*, 1997). We report here the solid-state structure of $[Ti_2(\mu\text{-}Cl)_2(N^tBu)_2Cl_2(py)_4]$ crystallized as its perdeuterobenzene disolvate, (I).



(I)

Molecules of (I) adopt a dinuclear structure in the solid state, possessing crystallographically imposed C_i molecular symmetry. The solid-state structure is entirely consistent with the previously reported solution ^{1}H and ^{13}C NMR data (Blake *et al.*, 1997). The two pseudo-octahedral six-coordinate titanium(IV) centres are bridged by two Cl atoms. The bridging Cl—Ti bond lengths [Ti1—Cl2 = 2.4600 (4) Å and Ti1—Cl2A = 2.7438 (4) Å] are longer than the terminal Ti—Cl bond length [Ti1—Cl1 = 2.3898 (4) Å]. The bridging Cl—Ti bond distance of the Cl atom *trans* to the imido group is considerably longer than the bridging Ti—Cl bond distance of the Cl atom *cis* to the imido group [difference between Ti1—Cl2 and Ti1—Cl2^i = 0.2838 (6) Å; symmetry code as in Table 1]. This is a reflection of the strong *trans* influence exercised by the imido group. The near linearity of the Ti═N^{t}Bu linkage [Ti1═N1—C1 = 170.9 (2)°] is consistent with the imido ligand acting as a four-electron donor to the titanium centre (Wigley, 1994).

The structure of (I) is closely related to that of the corresponding titanium–imido species $[Ti_2(\mu\text{-}Cl)_2(N\text{-}2\text{-}PhC_6H_4)_2Cl_2(py)_4]$ and $[Ti_2(\mu\text{-}Cl)_2(N\text{-}2\text{-}tBuC_6H_4)_2Cl_2(py)_4]$, synthe-

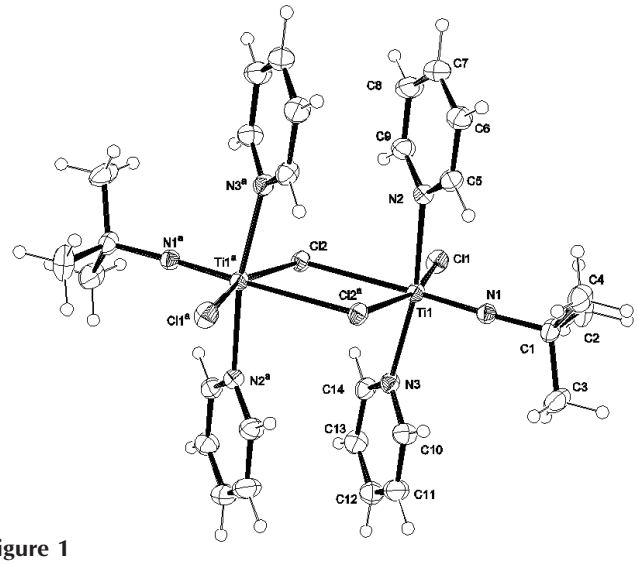


Figure 1
View of the molecular structure of (I). The displacement parameters are drawn at the 20% probability level and H atoms have been omitted for clarity. The solvent of crystallization has been omitted and the minor orientation of the disordered *tert*-butyl group is not shown. Atoms carrying the suffix *A* are related to their counterparts by the symmetry code $(1 - x, 1 - y, 1 - z)$.

sized by Nielson and co-workers (Nielson *et al.*, 2001), and the bond lengths and angles around $Ti_2(\mu\text{-Cl})_2$ are similar in all three compounds.

Experimental

The title compound was prepared according to the previously described procedure (Blake *et al.*, 1997) and authenticated by comparison of its solution ^{1}H NMR spectrum with that previously reported. Crystallization from C_6D_6 afforded crystals of (I) as air-sensitive yellow blocks.

Crystal data

$[Ti_2(C_4H_9N)_2Cl_2(C_5H_5N)_4]\cdot 2C_6D_6$
$M_r = 864.58$
Triclinic, $P\overline{1}$
$a = 8.0662$ (2) Å
$b = 11.0937$ (2) Å
$c = 12.7589$ (3) Å
$\alpha = 101.6259$ (9)°
$\beta = 90.1675$ (10)°
$\gamma = 103.4005$ (11)°
$V = 1086.37$ (4) Å^3
$Z = 1$
$D_x = 1.321$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 18502 reflections
$\theta = 5$–28°
$\mu = 0.65$ mm^{-1}
$T = 150$ K
Prism, pale orange
0.30 × 0.12 × 0.08 mm

Data collection

Nonius KappaCCD diffractometer
ω scans
Absorption correction: multi-scan (*DENZO*/*SCALEPACK*; Otwinowski & Minor, 1997)
$T_{min} = 0.82$, $T_{max} = 0.95$
18502 measured reflections
4933 independent reflections
3925 reflections with $I > 0$
$R_{int} = 0.028$
$\theta_{max} = 27.4°$
$h = -10 \rightarrow 10$
$k = -14 \rightarrow 14$
$l = -16 \rightarrow 16$

Refinement

Refinement on F
$R = 0.030$
$wR = 0.037$
$S = 1.03$
3925 reflections
252 parameters
H-atom parameters constrained
Weighting scheme: see text
$(\Delta/\sigma)_{max} = 0.019$
$\Delta\rho_{max} = 0.24$ e Å^{-3}
$\Delta\rho_{min} = -0.42$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Ti1—Cl1	2.3898 (4)	C5—C6	1.384 (2)
Ti1—Cl2	2.7438 (4)	C6—C7	1.380 (3)
Ti1—Cl2^{i}	2.4600 (4)	C7—C8	1.381 (3)
Ti1—N1	1.6921 (12)	C8—C9	1.386 (2)
Ti1—N2	2.2355 (12)	N3—C10	1.345 (2)
Ti1—N3	2.2316 (12)	N3—C14	1.3416 (19)
N1—C1	1.442 (4)	C10—C11	1.384 (2)
N1—C51	1.435 (19)	C11—C12	1.383 (3)
C1—C2	1.533 (5)	C12—C13	1.374 (3)
C1—C3	1.523 (4)	C13—C14	1.387 (2)
C1—C4	1.531 (5)	C15—C16	1.379 (3)
C51—C52	1.532 (15)	C15—C20	1.386 (3)
C51—C53	1.544 (14)	C16—C17	1.384 (3)
C51—C54	1.549 (14)	C17—C18	1.387 (3)
N2—C5	1.3387 (19)	C18—C19	1.384 (3)
N2—C9	1.343 (2)	C19—C20	1.381 (3)
Cl1—Ti1—Cl2	84.062 (14)	N1—C51—C54	109.4 (10)
Cl1—Ti1—Cl2^{i}	161.860 (17)	C52—C51—C53	110.3 (10)
Cl2—Ti1—Cl2^{i}	77.891 (13)	C52—C51—C54	109.9 (10)
Cl1—Ti1—N1	99.89 (4)	C53—C51—C54	110.1 (10)
Cl2—Ti1—N1	176.05 (4)	Ti1—N2—C5	118.15 (10)
Cl2^{i}—Ti1—N1	98.15 (4)	Ti1—N2—C9	124.02 (11)
Cl1—Ti1—N2	88.47 (3)	C5—N2—C9	117.82 (13)
Cl2—Ti1—N2	84.25 (3)	N2—C5—C6	123.11 (14)
Cl2^{i}—Ti1—N2	87.92 (3)	C5—C6—C7	118.72 (15)
N1—Ti1—N2	95.69 (5)	C6—C7—C8	118.77 (15)
Cl1—Ti1—N3	90.60 (3)	C7—C8—C9	119.22 (16)
Cl2—Ti1—N3	84.89 (3)	N2—C9—C8	122.36 (16)
Cl2^{i}—Ti1—N3	89.63 (3)	Ti1—N3—C10	120.12 (10)
N1—Ti1—N3	95.13 (5)	Ti1—N3—C14	122.11 (10)
N2—Ti1—N3	169.14 (4)	C10—N3—C14	117.52 (13)
Ti1—Cl2—Ti1^{i}	102.109 (13)	N3—C10—C11	122.96 (15)
Ti1—N1—C1	170.9 (2)	C10—C11—C12	118.93 (16)
Ti1—N1—C51	177.3 (6)	C11—C12—C13	118.57 (15)
N1—C1—C2	107.1 (3)	C12—C13—C14	119.46 (15)
N1—C1—C3	110.4 (3)	N3—C14—C13	122.53 (15)
C2—C1—C3	109.5 (3)	C16—C15—C20	119.88 (17)
N1—C1—C4	110.5 (3)	C15—C16—C17	120.09 (17)
C2—C1—C4	109.7 (3)	C16—C17—C18	120.11 (17)
C3—C1—C4	109.6 (3)	C17—C18—C19	119.68 (18)
N1—C51—C52	107.5 (10)	C18—C19—C20	120.12 (17)
N1—C51—C53	109.7 (10)	C15—C20—C19	120.12 (16)

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

All H atoms were positioned geometrically after each cycle of refinement. A three-term Chebychev polynomial weighting scheme was applied: $w = \{1 - [\Delta F/2\sigma(F)]^2\}^2/[1.08T_0(x) + 0.471T_1(x) + 0.742T_2(x)]$, where $x = F_{calc}/F_{max}$ (Prince, 1983; Watkin, 1994).

Data collection: *COLLECT* (Nonius, 2000); cell refinement: *DENZO*; data reduction: *DENZO* (Otwinowski & Minor, 1997); program(s) used to solve structure: *SIR*92 (Altomare *et al.*, 1999); program(s) used to refine structure: *CRYSTALS* (Betteridge *et al.*, 2003); molecular graphics: *CAMERON* (Watkin *et al.*, 1996); software used to prepare material for publication: *CRYSTALS*.

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supporting information

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$h = -10\rightarrow 10$
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$l = -16\rightarrow 16$

Refinement

Refinement on F
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.030$
$wR(F^2) = 0.037$
$S = 1.03$
3925 reflections
252 parameters
18 restraints
Primary atom site location: structure-invariant direct methods
Hydrogen site location: inferred from neighbouring sites
H-atom parameters not refined
Method, part 1, Chebychev polynomial (Watkin, 1994; *P*rince, 1983): [*w*eight] = 1/[A_0*T_0(x) + A_1*T_1(x) ··· + A_{n-1}]*T_{n-1}(x)], where A_i are the Chebychev coefficients listed below and x = F /Fmax. Method = Robust Weighting (*P*rince, 1983): W = [*w*eight] [1-(δF/6σF)^2]^2, where A_i are 1.08, 0.471 and 0.742
$(\Delta/\sigma)_{max} = 0.019$
$\Delta\rho_{max} = 0.24$ e Å^{-3}
$\Delta\rho_{min} = -0.42$ e Å^{-3}

Special details

Refinement. Geometric similarity restraints were applied to the C—C bond lengths (su 0.02 Å) and to the N—C—C anf C—C—C angles (su 2 °) of the disordered *tert*-butyl group C1—C54

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

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Ti1	0.43947 (3)	0.34292 (2)	0.38142 (2)	0.0233	
Cl1	0.17225 (5)	0.19292 (3)	0.37618 (3)	0.0339	
Cl2	0.32610 (4)	0.46699 (3)	0.56528 (3)	0.0255	
N1	0.52165 (15)	0.27465 (11)	0.26924 (9)	0.0254	
C1	0.5693 (5)	0.1994 (4)	0.1735 (3)	0.0307	0.809 (4)
C2	0.4143 (3)	0.0898 (2)	0.1323 (2)	0.0525	0.809 (4)
C3	0.7195 (3)	0.1464 (3)	0.19845 (19)	0.0477	0.809 (4)
C4	0.6164 (3)	0.2788 (2)	0.08804 (18)	0.0446	0.809 (4)
C51	0.5840 (19)	0.2164 (14)	0.1713 (14)	0.029 (5)*	0.191 (4)
C52	0.7583 (14)	0.3004 (11)	0.1564 (9)	0.055 (3)*	0.191 (4)
C53	0.4583 (13)	0.2062 (10)	0.0767 (8)	0.049 (3)*	0.191 (4)
C54	0.6034 (13)	0.0830 (9)	0.1798 (8)	0.042 (2)*	0.191 (4)
N2	0.30669 (16)	0.45794 (12)	0.30055 (10)	0.0268	
C5	0.38806 (19)	0.51368 (14)	0.22522 (12)	0.0296	
C6	0.3185 (2)	0.58732 (16)	0.17030 (14)	0.0358	
C7	0.1568 (2)	0.60320 (18)	0.19304 (15)	0.0410	
C8	0.0706 (2)	0.5450 (2)	0.26971 (16)	0.0449	
C9	0.1494 (2)	0.47387 (17)	0.32227 (13)	0.0356	
N3	0.55548 (16)	0.24758 (11)	0.49062 (10)	0.0263	
C10	0.7165 (2)	0.23462 (16)	0.47862 (13)	0.0334	
C11	0.7896 (2)	0.16493 (18)	0.53581 (15)	0.0398	
C12	0.6941 (2)	0.10617 (16)	0.60917 (14)	0.0384	
C13	0.5309 (2)	0.12131 (16)	0.62389 (13)	0.0362	
C14	0.4651 (2)	0.19185 (14)	0.56331 (12)	0.0311	
C15	0.8876 (2)	0.85413 (18)	0.23135 (14)	0.0402	
C16	0.9838 (2)	0.91397 (17)	0.15920 (17)	0.0438	
C17	0.9803 (3)	0.85268 (18)	0.05314 (16)	0.0464	
C18	0.8794 (3)	0.73109 (18)	0.01894 (15)	0.0442	
C19	0.7829 (2)	0.67129 (17)	0.09149 (16)	0.0423	
C20	0.7871 (2)	0.73249 (18)	0.19742 (15)	0.0414	
H21	0.4425	0.0352	0.0656	0.0577*	0.8087
H22	0.3837	0.0382	0.1883	0.0577*	0.8087
H23	0.3155	0.1246	0.1162	0.0577*	0.8087
H31	0.7510	0.0945	0.1313	0.0639*	0.8087
H32	0.8192	0.2179	0.2281	0.0639*	0.8087
H33	0.6871	0.0920	0.2524	0.0639*	0.8087
H41	0.6491	0.2253	0.0222	0.0577*	0.8087
H42	0.7147	0.3521	0.1162	0.0577*	0.8087
H43	0.5162	0.3110	0.0699	0.0577*	0.8087
H521	0.8054	0.2623	0.0887	0.0661*	0.1913
H522	0.8381	0.3068	0.2185	0.0661*	0.1913

H523	0.7452	0.3868	0.1525	0.0661*	0.1913
H531	0.5022	0.1657	0.0086	0.0588*	0.1913
H532	0.4474	0.2929	0.0716	0.0588*	0.1913
H533	0.3441	0.1536	0.0885	0.0588*	0.1913
H541	0.6468	0.0423	0.1116	0.0507*	0.1913
H542	0.6859	0.0907	0.2408	0.0507*	0.1913
H543	0.4899	0.0298	0.1924	0.0507*	0.1913
H51	0.5047	0.5015	0.2078	0.0357*	
H61	0.3841	0.6282	0.1152	0.0442*	
H71	0.1030	0.6559	0.1547	0.0520*	
H81	−0.0472	0.5541	0.2871	0.0579*	
H91	0.0870	0.4329	0.3784	0.0448*	
H101	0.7865	0.2773	0.4260	0.0415*	
H111	0.9096	0.1572	0.5243	0.0499*	
H121	0.7428	0.0538	0.6506	0.0478*	
H131	0.4600	0.0818	0.6778	0.0449*	
H141	0.3458	0.2015	0.5743	0.0383*	
H151	0.8903	0.8984	0.3080	0.0483*	
H161	1.0562	1.0018	0.1836	0.0520*	
H171	1.0506	0.8961	0.0011	0.0581*	
H181	0.8764	0.6869	−0.0578	0.0537*	
H191	0.7101	0.5836	0.0672	0.0501*	
H201	0.7176	0.6889	0.2497	0.0502*	

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ti1	0.02586 (13)	0.02258 (13)	0.02260 (13)	0.00782 (9)	0.00395 (9)	0.00503 (9)
Cl1	0.03041 (18)	0.02812 (18)	0.0398 (2)	0.00298 (14)	0.00431 (14)	0.00353 (14)
Cl2	0.02641 (16)	0.02532 (16)	0.02501 (16)	0.00652 (12)	0.00611 (12)	0.00525 (12)
N1	0.0295 (6)	0.0243 (6)	0.0238 (6)	0.0085 (5)	0.0023 (5)	0.0057 (5)
C1	0.0395 (17)	0.0289 (14)	0.0258 (14)	0.0128 (10)	0.0090 (9)	0.0054 (10)
C2	0.0590 (15)	0.0445 (13)	0.0409 (12)	0.0024 (11)	0.0088 (11)	−0.0101 (10)
C3	0.0593 (16)	0.0582 (15)	0.0420 (12)	0.0391 (13)	0.0223 (11)	0.0194 (11)
C4	0.0609 (14)	0.0504 (13)	0.0329 (11)	0.0261 (11)	0.0192 (10)	0.0176 (9)
N2	0.0280 (6)	0.0272 (6)	0.0258 (6)	0.0088 (5)	0.0005 (5)	0.0042 (5)
C5	0.0304 (7)	0.0269 (7)	0.0319 (7)	0.0073 (6)	0.0020 (6)	0.0067 (6)
C6	0.0396 (9)	0.0348 (8)	0.0359 (8)	0.0099 (7)	0.0014 (7)	0.0127 (7)
C7	0.0441 (9)	0.0440 (9)	0.0420 (9)	0.0203 (8)	−0.0017 (7)	0.0138 (7)
C8	0.0391 (9)	0.0596 (11)	0.0461 (10)	0.0269 (9)	0.0056 (8)	0.0166 (9)
C9	0.0335 (8)	0.0459 (9)	0.0325 (8)	0.0164 (7)	0.0058 (6)	0.0119 (7)
N3	0.0310 (6)	0.0243 (6)	0.0247 (6)	0.0082 (5)	0.0038 (5)	0.0057 (5)
C10	0.0310 (7)	0.0379 (8)	0.0348 (8)	0.0095 (6)	0.0045 (6)	0.0139 (7)
C11	0.0366 (8)	0.0474 (10)	0.0407 (9)	0.0173 (7)	0.0024 (7)	0.0133 (8)
C12	0.0481 (10)	0.0349 (8)	0.0364 (8)	0.0148 (7)	−0.0005 (7)	0.0116 (7)
C13	0.0463 (9)	0.0318 (8)	0.0342 (8)	0.0096 (7)	0.0077 (7)	0.0147 (6)
C14	0.0369 (8)	0.0287 (7)	0.0302 (7)	0.0108 (6)	0.0086 (6)	0.0086 (6)
C15	0.0360 (8)	0.0453 (9)	0.0395 (9)	0.0149 (7)	0.0035 (7)	0.0036 (7)

C16	0.0397 (9)	0.0329 (8)	0.0573 (11)	0.0083 (7)	0.0040 (8)	0.0068 (8)
C17	0.0509 (10)	0.0437 (10)	0.0507 (11)	0.0148 (8)	0.0145 (9)	0.0195 (8)
C18	0.0520 (11)	0.0449 (10)	0.0374 (9)	0.0176 (8)	0.0029 (8)	0.0056 (7)
C19	0.0371 (9)	0.0389 (9)	0.0492 (10)	0.0070 (7)	0.0009 (7)	0.0073 (8)
C20	0.0347 (8)	0.0462 (10)	0.0445 (10)	0.0088 (7)	0.0080 (7)	0.0134 (8)

Geometric parameters (Å, º)

Ti1—Cl1	2.3898 (4)	C5—H51	1.000
Ti1—Cl2	2.7438 (4)	C6—C7	1.380 (3)
Ti1—Cl2^{i}	2.4600 (4)	C6—H61	1.000
Ti1—N1	1.6921 (12)	C7—C8	1.381 (3)
Ti1—N2	2.2355 (12)	C7—H71	1.000
Ti1—N3	2.2316 (12)	C8—C9	1.386 (2)
N1—C1	1.442 (4)	C8—H81	1.000
N1—C51	1.435 (19)	C9—H91	1.000
C1—C2	1.533 (5)	N3—C10	1.345 (2)
C1—C3	1.523 (4)	N3—C14	1.3416 (19)
C1—C4	1.531 (5)	C10—C11	1.384 (2)
C2—H21	1.000	C10—H101	1.000
C2—H22	1.000	C11—C12	1.383 (3)
C2—H23	1.000	C11—H111	1.000
C2—H533	1.216	C12—C13	1.374 (3)
C3—H31	1.000	C12—H121	1.000
C3—H32	1.000	C13—C14	1.387 (2)
C3—H33	1.000	C13—H131	1.000
C4—H41	1.000	C14—H141	1.000
C4—H42	1.000	C15—C16	1.379 (3)
C4—H43	1.000	C15—C20	1.386 (3)
C51—C52	1.532 (15)	C15—H151	1.000
C51—C53	1.544 (14)	C16—C17	1.384 (3)
C51—C54	1.549 (14)	C16—H161	1.000
C52—H521	1.000	C17—C18	1.387 (3)
C52—H522	1.000	C17—H171	1.000
C52—H523	1.000	C18—C19	1.384 (3)
C53—H531	1.000	C18—H181	1.000
C53—H532	1.000	C19—C20	1.381 (3)
C53—H533	1.000	C19—H191	1.000
C54—H541	1.000	C20—H201	1.000
C54—H542	1.000	H23—H533	0.542
C54—H543	1.000	H33—H542	0.145
N2—C5	1.3387 (19)	H42—H523	0.554
N2—C9	1.343 (2)	H43—H532	0.547
C5—C6	1.384 (2)		

Cl1—Ti1—Cl2	84.062 (14)	C51—C54—H541	109.468
Cl1—Ti1—Cl2^{i}	161.860 (17)	C51—C54—H542	109.463
Cl2—Ti1—Cl2^{i}	77.891 (13)	C51—C54—H543	109.468

Cl1—Ti1—N1	99.89 (4)	H541—C54—H542	109.477
Cl2—Ti1—N1	176.05 (4)	H541—C54—H543	109.476
Cl2^{i}—Ti1—N1	98.15 (4)	H542—C54—H543	109.476
Cl1—Ti1—N2	88.47 (3)	Ti1—N2—C5	118.15 (10)
Cl2—Ti1—N2	84.25 (3)	Ti1—N2—C9	124.02 (11)
Cl2^{i}—Ti1—N2	87.92 (3)	C5—N2—C9	117.82 (13)
N1—Ti1—N2	95.69 (5)	N2—C5—C6	123.11 (14)
Cl1—Ti1—N3	90.60 (3)	N2—C5—H51	118.445
Cl2—Ti1—N3	84.89 (3)	C6—C5—H51	118.446
Cl2^{i}—Ti1—N3	89.63 (3)	C5—C6—C7	118.72 (15)
N1—Ti1—N3	95.13 (5)	C5—C6—H61	120.641
N2—Ti1—N3	169.14 (4)	C7—C6—H61	120.641
Ti1—Cl2—Ti1^{i}	102.109 (13)	C6—C7—C8	118.77 (15)
Ti1—N1—C1	170.9 (2)	C6—C7—H71	120.617
Ti1—N1—C51	177.3 (6)	C8—C7—H71	120.617
N1—C1—C2	107.1 (3)	C7—C8—C9	119.22 (16)
N1—C1—C3	110.4 (3)	C7—C8—H81	120.392
C2—C1—C3	109.5 (3)	C9—C8—H81	120.392
N1—C1—C4	110.5 (3)	N2—C9—C8	122.36 (16)
C2—C1—C4	109.7 (3)	N2—C9—H91	118.821
C3—C1—C4	109.6 (3)	C8—C9—H91	118.821
C1—C2—H21	109.467	Ti1—N3—C10	120.12 (10)
C1—C2—H22	109.466	Ti1—N3—C14	122.11 (10)
H21—C2—H22	109.476	C10—N3—C14	117.52 (13)
C1—C2—H23	109.467	N3—C10—C11	122.96 (15)
H21—C2—H23	109.476	N3—C10—H101	118.519
H22—C2—H23	109.476	C11—C10—H101	118.519
C1—C3—H31	109.466	C10—C11—C12	118.93 (16)
C1—C3—H32	109.470	C10—C11—H111	120.536
H31—C3—H32	109.476	C12—C11—H111	120.536
C1—C3—H33	109.464	C11—C12—C13	118.57 (15)
H31—C3—H33	109.476	C11—C12—H121	120.715
H32—C3—H33	109.476	C13—C12—H121	120.715
C1—C4—H41	109.466	C12—C13—C14	119.46 (15)
C1—C4—H42	109.469	C12—C13—H131	120.269
H41—C4—H42	109.476	C14—C13—H131	120.268
C1—C4—H43	109.465	N3—C14—C13	122.53 (15)
H41—C4—H43	109.476	N3—C14—H141	118.735
H42—C4—H43	109.476	C13—C14—H141	118.735
N1—C51—C52	107.5 (10)	C16—C15—C20	119.88 (17)
N1—C51—C53	109.7 (10)	C16—C15—H151	120.058
N1—C51—C54	109.4 (10)	C20—C15—H151	120.058
C52—C51—C53	110.3 (10)	C15—C16—C17	120.09 (17)
C52—C51—C54	109.9 (10)	C15—C16—H161	119.954
C53—C51—C54	110.1 (10)	C17—C16—H161	119.954
C51—C52—H521	109.467	C16—C17—C18	120.11 (17)
C51—C52—H522	109.462	C16—C17—H171	119.945
H521—C52—H522	109.477	C18—C17—H171	119.945

C51—C52—H523	109.468	C17—C18—C19	119.68 (18)
H521—C52—H523	109.477	C17—C18—H181	120.162
H522—C52—H523	109.477	C19—C18—H181	120.162
C51—C53—H531	109.468	C18—C19—C20	120.12 (17)
C51—C53—H532	109.467	C18—C19—H191	119.942
C51—C53—H533	109.468	C20—C19—H191	119.942
H531—C53—H532	109.475	C15—C20—C19	120.12 (16)
H531—C53—H533	109.476	C15—C20—H201	119.939
H532—C53—H533	109.474	C19—C20—H201	119.939

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