Electronic Supplementary Information (ESI)

Synthesis of Half-Titanocenes Containing 1,3-Imidazolidin-2-Iminato Ligands of type, $Cp^*TiCl_2[1,3\text{-}R_2(CH_2N)_2C{=}N]$: Highly Active Catalyst Precursors in Ethylene (Co)polymerisation

Kotohiro Nomura,[a,b]* *Srisuda Patamma,*[a] *Hideshi Matsuda,*[a] *Shohei Katao,*[b] *Ken Tsutsumi,*[a] *and Hiroya Fukuda,*[b b]

[a]Department of Chemistry, Tokyo Metropolitan University, 1-1 Minami Osawa, Hachioiji, Tokyo 192-0397, Japan, [b]Graduate School of Materials Science, Nara Institute of Science and Technology, 8916-5 Takayama, Ikoma, Nara 630-0101, Japan

Structure reports for complexes **1b-e** (CCDC1403201-1403204).

EMAIL: ktnomura@tmu.ac.jp

*Corresponding Author, tel.: +81-42-677-2547, fax: +81-42-677-2547, e-mail: ktnomura@tmu.ac.jp

X-ray Structure Report for $Cp^*TiCl_2[1,3\text{-}Cy_2(CH_2N)_2C{=}N]$ (**1b**).

Experimental

Data Collection

A yellow block crystal of $C_{25}H_{41}Cl_2N_3Ti$ having approximate dimensions of 0.65 x 0.55 x 0.40 mm was mounted on a glass fiber. All measurements were made on a Rigaku RAXIS RAPID imaging plate area detector with graphite monochromated Mo-Kα radiation.

Indexing was performed from 3 oscillations that were exposed for 40 seconds. The crystal-to-detector distance was 127.40 mm.

Cell constants and an orientation matrix for data collection corresponded to a primitive monoclinic cell with dimensions:

a = 8.5977(3) Å
b = 15.5686(4) Å β = 103.7144(8)^o
c = 20.0179(6) Å
V = 2603.07(13) Å^3

For Z = 4 and F.W. = 502.42, the calculated density is 1.282 g/cm^3. The systematic absences of:

h0l: l ± 2n
0k0: k ± 2n

uniquely determine the space group to be:

$P2_1/c$ (#14)

The data were collected at a temperature of -150 ± 1^{o}C to a maximum 2θ value of 54.9^o. A total of 74 oscillation images were collected. A sweep of data was done using ω scans from 130.0 to 190.0^o in 3.0^o step, at χ=45.0^o and ϕ = 0.0^o. The exposure rate was 30.0 [sec./^{o}]. A second sweep was performed using ω scans from 0.0 to 162.0^o in 3.0^o step, at χ=45.0^o and ϕ = 180.0^o. The exposure rate was 30.0 [sec./^{o}]. The crystal-to-detector distance was 127.40 mm. Readout was performed in

the 0.100 mm pixel mode.

Data Reduction

Of the 25348 reflections that were collected, 5923 were unique (R_{int} = 0.032); equivalent reflections were merged.

The linear absorption coefficient, μ, for Mo-Kα radiation is 5.512 cm^{-1}. An empirical absorption correction was applied which resulted in transmission factors ranging from 0.657 to 0.802. The data were corrected for Lorentz and polarization effects.

Structure Solution and Refinement

The structure was solved by direct methods[1] and expanded using Fourier techniques[2]. The non-hydrogen atoms were refined anisotropically. Hydrogen atoms were refined using the riding model. The final cycle of full-matrix least-squares refinement[3] on F^2 was based on 5923 observed reflections and 281 variable parameters and converged (largest parameter shift was 0.00 times its esd) with unweighted and weighted agreement factors of:

$$R1 = \Sigma \, ||Fo| - |Fc|| \, / \, \Sigma \, |Fo| = 0.0331$$

$$wR2 = [\, \Sigma \, (\, w \, (Fo^2 - Fc^2)^2 \,) / \, \Sigma \, w(Fo^2)^2]^{1/2} = 0.0750$$

The standard deviation of an observation of unit weight[4] was 1.10. Unit weights were used. The maximum and minimum peaks on the final difference Fourier map corresponded to 0.34 and -0.34 $e^-/Å^3$, respectively.

Neutral atom scattering factors were taken from Cromer and Waber[5]. Anomalous dispersion effects were included in Fcalc[6]; the values for Δf' and Δf'' were those of Creagh and McAuley[7]. The values for the mass attenuation coefficients are those of Creagh and Hubbell[8]. All calculations were performed using the CrystalStructure[9] crystallographic software package except for refinement, which was performed using SHELXL-97[10].

References

(1) SIR92: Altomare, A., Cascarano, G., Giacovazzo, C., Guagliardi, A., Burla, M., Polidori, G., and Camalli, M. (1994) J. Appl. Cryst., 27, 435.

(2) DIRDIF99: Beurskens, P.T., Admiraal, G., Beurskens, G., Bosman, W.P., de Gelder, R., Israel, R. and Smits, J.M.M.(1999). The DIRDIF-99 program system, Technical Report of the Crystallography Laboratory, University of Nijmegen, The Netherlands.

(3) Least Squares function minimized: (SHELXL97)

$\Sigma w(F_o^2-F_c^2)^2$ where w = Least Squares weights.

(4) Standard deviation of an observation of unit weight:

$[\Sigma w(F_o^2-F_c^2)^2/(N_o-N_v)]^{1/2}$

where: N_o = number of observations
N_v = number of variables

(5) Cromer, D. T. & Waber, J. T.; "International Tables for X-ray Crystallography", Vol. IV, The Kynoch Press, Birmingham, England, Table 2.2 A (1974).

(6) Ibers, J. A. & Hamilton, W. C.; Acta Crystallogr., 17, 781 (1964).

(7) Creagh, D. C. & McAuley, W.J .; "International Tables for Crystallography", Vol C, (A.J.C. Wilson, ed.), Kluwer Academic Publishers, Boston, Table 4.2.6.8, pages 219-222 (1992).

(8) Creagh, D. C. & Hubbell, J.H..; "International Tables for Crystallography", Vol C, (A.J.C. Wilson, ed.), Kluwer Academic Publishers, Boston, Table 4.2.4.3, pages 200-206 (1992).

(9) CrystalStructure 3.8: Crystal Structure Analysis Package, Rigaku and Rigaku Americas (2000-2007). 9009 New Trails Dr. The Woodlands TX 77381 USA.

(10) SHELX97: Sheldrick, G.M. (1997).

EXPERIMENTAL DETAILS

A. Crystal Data

Empirical Formula	$C_{25}H_{41}Cl_2N_3Ti$
Formula Weight	502.42
Crystal Color, Habit	yellow, block
Crystal Dimensions	0.65 X 0.55 X 0.40 mm
Crystal System	monoclinic
Lattice Type	Primitive
Indexing Images	3 oscillations @ 40.0 seconds
Detector Position	127.40 mm
Pixel Size	0.100 mm
Lattice Parameters	a = 8.5977(3) Å b = 15.5686(4) Å c = 20.0179(6) Å β = 103.7144(8) ^{o} V = 2603.07(13) Å^3
Space Group	$P2_1/c$ (#14)
Z value	4
D_{calc}	1.282 g/cm^3
F_{000}	1072.00
μ(MoKα)	5.512 cm^{-1}

B. Intensity Measurements

Diffractometer	Rigaku RAXIS-RAPID
Radiation	MoKα (λ = 0.71075 Å) graphite monochromated
Detector Aperture	280 mm x 256 mm
Data Images	74 exposures
ω oscillation Range (χ=45.0, ϕ=0.0)	130.0 - 190.0^{o}
Exposure Rate	30.0 sec./^{o}
ω oscillation Range (χ=45.0, ϕ=180.0)	0.0 - 162.0^{o}
Exposure Rate	30.0 sec./^{o}
Detector Position	127.40 mm
Pixel Size	0.100 mm
$2\theta_{max}$	54.9^{o}
No. of Reflections Measured	Total: 25348 Unique: 5923 (R_{int} = 0.032)
Corrections	Lorentz-polarization Absorption (trans. factors: 0.657 - 0.802)

C. Structure Solution and Refinement

Structure Solution	Direct Methods (SIR92)
Refinement	Full-matrix least-squares on F^2
Function Minimized	Σ w $(Fo^2 - Fc^2)^2$
Least Squares Weights	$w = 1/ [\sigma^2(Fo^2) + (0.0284 \cdot P)^2 + 1.6131 \cdot P]$ where $P = (Max(Fo^2,0) + 2Fc^2)/3$
$2\theta_{max}$ cutoff	54.9^o
Anomalous Dispersion	All non-hydrogen atoms
No. Observations (All reflections)	5923
No. Variables	281
Reflection/Parameter Ratio	21.08
Residuals: R1 (I>2.00σ(I))	0.0331
Residuals: R (All reflections)	0.0387
Residuals: wR2 (All reflections)	0.0750
Goodness of Fit Indicator	1.095
Max Shift/Error in Final Cycle	0.001
Maximum peak in Final Diff. Map	0.34 $e^-/Å^3$
Minimum peak in Final Diff. Map	-0.34 $e^-/Å^3$

Table 1. Atomic coordinates and B_{iso}/B_{eq}

atom	x	y	z	B_{eq}
Ti(1)	0.66692(3)	0.027061(14)	0.278692(11)	0.895(5)
Cl(1)	0.62341(4)	-0.06100(2)	0.182936(17)	1.455(6)
Cl(2)	0.83111(4)	-0.05538(2)	0.362405(18)	1.830(7)
N(1)	0.79655(14)	0.10641(7)	0.25785(6)	1.168(17)
N(2)	0.96764(14)	0.22765(7)	0.28193(6)	1.252(18)
N(3)	0.86556(16)	0.19285(8)	0.17303(6)	1.90(2)
C(1)	0.54132(17)	0.08735(9)	0.35989(7)	1.34(2)
C(2)	0.51416(17)	0.14343(8)	0.30246(7)	1.40(2)
C(3)	0.41925(16)	0.09900(9)	0.24518(7)	1.36(2)
C(4)	0.38131(16)	0.01663(8)	0.26836(7)	1.27(2)
C(5)	0.45731(16)	0.00916(9)	0.33863(7)	1.28(2)
C(6)	0.63456(19)	0.10820(11)	0.43155(8)	2.05(2)
C(7)	0.5669(2)	0.23512(9)	0.30235(9)	2.18(2)
C(8)	0.3610(2)	0.13320(10)	0.17337(8)	2.12(2)
C(9)	0.26875(18)	-0.04753(10)	0.22651(8)	1.87(2)
C(10)	0.4441(2)	-0.06621(10)	0.38370(8)	2.02(2)
C(11)	0.87143(16)	0.17183(8)	0.23879(7)	1.142(19)
C(12)	1.05967(18)	0.27931(9)	0.24371(7)	1.61(2)
C(13)	0.96450(18)	0.26819(9)	0.16889(7)	1.51(2)
C(14)	1.01992(16)	0.20937(8)	0.35557(7)	1.160(19)
C(15)	1.15012(18)	0.14062(9)	0.37187(7)	1.61(2)
C(16)	1.19157(19)	0.12041(9)	0.44883(7)	1.85(2)
C(17)	1.24218(19)	0.20124(10)	0.49162(7)	1.88(2)
C(18)	1.1147(2)	0.27100(10)	0.47356(7)	1.90(2)
C(19)	1.07254(19)	0.29135(9)	0.39640(7)	1.62(2)
C(20)	0.78004(17)	0.14142(9)	0.11474(7)	1.39(2)
C(21)	0.89145(19)	0.07685(10)	0.09257(8)	1.86(2)
C(22)	0.7994(2)	0.02122(10)	0.03344(8)	2.08(2)
C(23)	0.7124(2)	0.07658(11)	-0.02673(8)	2.17(2)
C(24)	0.60295(19)	0.14152(10)	-0.00416(8)	2.07(2)
C(25)	0.69479(18)	0.19773(9)	0.05485(7)	1.67(2)

$B_{eq} = 8/3\ \pi^2(U_{11}(aa^*)^2 + U_{22}(bb^*)^2 + U_{33}(cc^*)^2 + 2U_{12}(aa^*bb^*)\cos\gamma + 2U_{13}(aa^*cc^*)\cos\beta + 2U_{23}(bb^*cc^*)\cos\alpha)$

Table 2. Atomic coordinates and B_{iso} involving hydrogens/B_{eq}

atom	x	y	z	B_{eq}
H(1)	0.7127	0.1534	0.4296	2.46
H(2)	0.6906	0.0566	0.4528	2.46
H(3)	0.5611	0.1282	0.4589	2.46
H(4)	0.4830	0.2728	0.3115	2.62
H(5)	0.5868	0.2492	0.2574	2.62
H(6)	0.6655	0.2434	0.3382	2.62
H(7)	0.4233	0.1842	0.1675	2.55
H(8)	0.2476	0.1486	0.1655	2.55
H(9)	0.3741	0.0891	0.1402	2.55
H(10)	0.1595	-0.0359	0.2307	2.24
H(11)	0.3001	-0.1056	0.2434	2.24
H(12)	0.2732	-0.0431	0.1782	2.24
H(13)	0.3418	-0.0636	0.3972	2.42
H(14)	0.5323	-0.0647	0.4249	2.42
H(15)	0.4495	-0.1196	0.3584	2.42
H(16)	1.1703	0.2573	0.2502	1.93
H(17)	1.0636	0.3403	0.2579	1.93
H(18)	0.8976	0.3193	0.1527	1.81
H(19)	1.0366	0.2577	0.1378	1.81
H(20)	0.9250	0.1865	0.3706	1.39
H(21)	1.2470	0.1612	0.3581	1.93
H(22)	1.1122	0.0878	0.3454	1.93
H(23)	1.0972	0.0947	0.4615	2.22
H(24)	1.2797	0.0779	0.4591	2.22
H(25)	1.2604	0.1869	0.5411	2.26
H(26)	1.3441	0.2229	0.4832	2.26
H(27)	1.1542	0.3238	0.4997	2.28
H(28)	1.0171	0.2520	0.4874	2.28
H(29)	0.9851	0.3342	0.3860	1.95
H(30)	1.1670	0.3160	0.3831	1.95
H(31)	0.6960	0.1080	0.1305	1.67
H(32)	0.9411	0.0398	0.1320	2.23
H(33)	0.9781	0.1079	0.0778	2.23
H(34)	0.8748	-0.0177	0.0179	2.49
H(35)	0.7206	-0.0145	0.0498	2.49
H(36)	0.7920	0.1073	-0.0464	2.60
H(37)	0.6482	0.0393	-0.0630	2.60

Table 2. Atomic coordinates and B_{iso} involving hydrogens/B_{eq} (continued)

atom	x	y	z	B_{eq}
H(38)	0.5163	0.1107	0.0108	2.49
H(39)	0.5530	0.1785	-0.0437	2.49
H(40)	0.7743	0.2332	0.0387	2.00
H(41)	0.6195	0.2369	0.0703	2.00

$B_{eq} = 8/3\ \pi^2(U_{11}(aa^*)^2 + U_{22}(bb^*)^2 + U_{33}(cc^*)^2 + 2U_{12}(aa^*bb^*)\cos\gamma + 2U_{13}(aa^*cc^*)\cos\beta + 2U_{23}(bb^*cc^*)\cos\alpha)$

Table 3. Anisotropic displacement parameters

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Ti(1)	0.01192(12)	0.00936(11)	0.01314(11)	0.00018(8)	0.00377(8)	0.00059(8)
Cl(1)	0.02226(18)	0.01422(15)	0.01935(16)	-0.00259(12)	0.00605(12)	-0.00440(11)
Cl(2)	0.02558(19)	0.02377(17)	0.02039(17)	0.01090(13)	0.00586(13)	0.00732(13)
N(1)	0.0149(5)	0.0151(5)	0.0142(5)	-0.0023(4)	0.0030(4)	-0.0003(4)
N(2)	0.0163(5)	0.0165(5)	0.0140(5)	-0.0057(4)	0.0021(4)	0.0006(4)
N(3)	0.0329(7)	0.0240(6)	0.0138(5)	-0.0174(5)	0.0031(5)	0.0002(4)
C(1)	0.0145(6)	0.0186(6)	0.0194(6)	0.0013(5)	0.0070(5)	-0.0048(5)
C(2)	0.0148(6)	0.0129(6)	0.0269(7)	0.0025(4)	0.0077(5)	-0.0024(5)
C(3)	0.0133(6)	0.0169(6)	0.0218(6)	0.0039(4)	0.0050(5)	0.0019(5)
C(4)	0.0119(6)	0.0162(6)	0.0209(6)	0.0008(4)	0.0054(5)	-0.0010(5)
C(5)	0.0136(6)	0.0170(6)	0.0199(6)	0.0006(4)	0.0080(5)	0.0007(5)
C(6)	0.0236(7)	0.0337(8)	0.0209(7)	-0.0013(6)	0.0060(5)	-0.0101(6)
C(7)	0.0244(8)	0.0126(6)	0.0474(9)	0.0017(5)	0.0111(6)	-0.0026(6)
C(8)	0.0245(8)	0.0288(7)	0.0263(7)	0.0086(6)	0.0038(6)	0.0093(6)
C(9)	0.0170(7)	0.0243(7)	0.0290(7)	-0.0047(5)	0.0040(5)	-0.0051(5)
C(10)	0.0262(8)	0.0263(7)	0.0268(7)	-0.0015(6)	0.0116(6)	0.0073(5)
C(11)	0.0136(6)	0.0144(5)	0.0149(5)	-0.0010(4)	0.0026(4)	-0.0005(4)
C(12)	0.0223(7)	0.0225(6)	0.0161(6)	-0.0109(5)	0.0041(5)	0.0006(5)
C(13)	0.0214(7)	0.0179(6)	0.0173(6)	-0.0077(5)	0.0032(5)	0.0020(5)
C(14)	0.0138(6)	0.0166(6)	0.0134(5)	-0.0014(4)	0.0027(4)	-0.0003(4)
C(15)	0.0213(7)	0.0205(6)	0.0185(6)	0.0041(5)	0.0032(5)	-0.0016(5)
C(16)	0.0252(8)	0.0218(7)	0.0208(6)	0.0040(5)	0.0004(5)	0.0021(5)
C(17)	0.0235(7)	0.0285(7)	0.0165(6)	-0.0023(5)	-0.0014(5)	0.0005(5)
C(18)	0.0326(8)	0.0230(7)	0.0160(6)	0.0001(6)	0.0043(5)	-0.0045(5)
C(19)	0.0263(7)	0.0168(6)	0.0174(6)	-0.0000(5)	0.0028(5)	-0.0023(5)
C(20)	0.0198(7)	0.0190(6)	0.0129(5)	-0.0072(5)	0.0014(5)	-0.0003(4)
C(21)	0.0204(7)	0.0222(7)	0.0252(7)	0.0003(5)	-0.0004(5)	0.0027(5)
C(22)	0.0291(8)	0.0216(7)	0.0280(7)	-0.0006(6)	0.0066(6)	-0.0048(5)
C(23)	0.0333(9)	0.0320(8)	0.0166(6)	-0.0049(6)	0.0053(6)	-0.0061(5)
C(24)	0.0246(8)	0.0313(8)	0.0184(6)	0.0001(6)	-0.0038(5)	-0.0002(5)
C(25)	0.0224(7)	0.0205(6)	0.0187(6)	0.0018(5)	0.0013(5)	0.0006(5)

The general temperature factor expression: $\exp(-2\pi^2(a^{*2}U_{11}h^2 + b^{*2}U_{22}k^2 + c^{*2}U_{33}l^2 + 2a^*b^*U_{12}hk + 2a^*c^*U_{13}hl + 2b^*c^*U_{23}kl))$

Table 4. Bond lengths (Å)

atom	atom	distance	atom	atom	distance
Ti(1)	Cl(1)	2.3138(3)	Ti(1)	Cl(2)	2.3079(3)
Ti(1)	N(1)	1.7784(12)	Ti(1)	C(1)	2.3498(15)
Ti(1)	C(2)	2.3516(14)	Ti(1)	C(3)	2.3582(13)
Ti(1)	C(4)	2.4204(14)	Ti(1)	C(5)	2.4063(15)
N(1)	C(11)	1.3091(18)	N(2)	C(11)	1.3589(16)
N(2)	C(12)	1.465(2)	N(2)	C(14)	1.4635(17)
N(3)	C(11)	1.3457(18)	N(3)	C(13)	1.4628(19)
N(3)	C(20)	1.4617(17)	C(1)	C(2)	1.4182(19)
C(1)	C(5)	1.4279(19)	C(1)	C(6)	1.5035(19)
C(2)	C(3)	1.4197(17)	C(2)	C(7)	1.4980(19)
C(3)	C(4)	1.4276(19)	C(3)	C(8)	1.503(2)
C(4)	C(5)	1.4083(18)	C(4)	C(9)	1.5006(19)
C(5)	C(10)	1.501(2)	C(12)	C(13)	1.5368(18)
C(14)	C(15)	1.5271(19)	C(14)	C(19)	1.5252(18)
C(15)	C(16)	1.5294(19)	C(16)	C(17)	1.526(2)
C(17)	C(18)	1.524(2)	C(18)	C(19)	1.5336(19)
C(20)	C(21)	1.525(2)	C(20)	C(25)	1.5253(18)
C(21)	C(22)	1.528(2)	C(22)	C(23)	1.525(2)
C(23)	C(24)	1.521(2)	C(24)	C(25)	1.5305(19)

Table 5. Bond lengths involving hydrogens (Å)

atom	atom	distance	atom	atom	distance
C(6)	H(1)	0.980	C(6)	H(2)	0.980
C(6)	H(3)	0.980	C(7)	H(4)	0.980
C(7)	H(5)	0.980	C(7)	H(6)	0.980
C(8)	H(7)	0.980	C(8)	H(8)	0.980
C(8)	H(9)	0.980	C(9)	H(10)	0.980
C(9)	H(11)	0.980	C(9)	H(12)	0.980
C(10)	H(13)	0.980	C(10)	H(14)	0.980
C(10)	H(15)	0.980	C(12)	H(16)	0.990
C(12)	H(17)	0.990	C(13)	H(18)	0.990
C(13)	H(19)	0.990	C(14)	H(20)	1.000
C(15)	H(21)	0.990	C(15)	H(22)	0.990
C(16)	H(23)	0.990	C(16)	H(24)	0.990
C(17)	H(25)	0.990	C(17)	H(26)	0.990
C(18)	H(27)	0.990	C(18)	H(28)	0.990
C(19)	H(29)	0.990	C(19)	H(30)	0.990
C(20)	H(31)	1.000	C(21)	H(32)	0.990
C(21)	H(33)	0.990	C(22)	H(34)	0.990
C(22)	H(35)	0.990	C(23)	H(36)	0.990
C(23)	H(37)	0.990	C(24)	H(38)	0.990
C(24)	H(39)	0.990	C(25)	H(40)	0.990
C(25)	H(41)	0.990			

Table 6. Bond angles (°)

atom	atom	atom	angle	atom	atom	atom	angle
Cl(1)	Ti(1)	Cl(2)	102.881(14)	Cl(1)	Ti(1)	N(1)	101.80(4)
Cl(1)	Ti(1)	C(1)	143.05(3)	Cl(1)	Ti(1)	C(2)	129.48(3)
Cl(1)	Ti(1)	C(3)	95.05(3)	Cl(1)	Ti(1)	C(4)	85.87(3)
Cl(1)	Ti(1)	C(5)	110.57(3)	Cl(2)	Ti(1)	N(1)	104.31(3)
Cl(2)	Ti(1)	C(1)	91.27(3)	Cl(2)	Ti(1)	C(2)	123.80(3)
Cl(2)	Ti(1)	C(3)	145.72(3)	Cl(2)	Ti(1)	C(4)	117.27(3)
Cl(2)	Ti(1)	C(5)	88.57(3)	N(1)	Ti(1)	C(1)	107.53(5)
N(1)	Ti(1)	C(2)	85.61(5)	N(1)	Ti(1)	C(3)	100.21(5)
N(1)	Ti(1)	C(4)	134.92(4)	N(1)	Ti(1)	C(5)	141.49(5)
C(1)	Ti(1)	C(2)	35.11(4)	C(1)	Ti(1)	C(3)	58.33(4)
C(1)	Ti(1)	C(4)	57.49(4)	C(1)	Ti(1)	C(5)	34.92(4)
C(2)	Ti(1)	C(3)	35.09(4)	C(2)	Ti(1)	C(4)	57.66(4)
C(2)	Ti(1)	C(5)	57.87(4)	C(3)	Ti(1)	C(4)	34.73(4)
C(3)	Ti(1)	C(5)	57.61(4)	C(4)	Ti(1)	C(5)	33.93(4)
Ti(1)	N(1)	C(11)	170.98(10)	C(11)	N(2)	C(12)	110.00(11)
C(11)	N(2)	C(14)	120.74(11)	C(12)	N(2)	C(14)	123.92(10)
C(11)	N(3)	C(13)	111.28(10)	C(11)	N(3)	C(20)	122.87(12)
C(13)	N(3)	C(20)	125.68(11)	Ti(1)	C(1)	C(2)	72.51(8)
Ti(1)	C(1)	C(5)	74.71(8)	Ti(1)	C(1)	C(6)	121.18(10)
C(2)	C(1)	C(5)	107.99(11)	C(2)	C(1)	C(6)	126.06(12)
C(5)	C(1)	C(6)	125.88(13)	Ti(1)	C(2)	C(1)	72.37(8)
Ti(1)	C(2)	C(3)	72.71(7)	Ti(1)	C(2)	C(7)	123.37(11)
C(1)	C(2)	C(3)	107.90(11)	C(1)	C(2)	C(7)	126.59(12)
C(3)	C(2)	C(7)	125.41(12)	Ti(1)	C(3)	C(2)	72.20(7)
Ti(1)	C(3)	C(4)	75.01(7)	Ti(1)	C(3)	C(8)	120.93(10)
C(2)	C(3)	C(4)	107.88(11)	C(2)	C(3)	C(8)	126.67(12)
C(4)	C(3)	C(8)	125.38(11)	Ti(1)	C(4)	C(3)	70.25(7)
Ti(1)	C(4)	C(5)	72.49(7)	Ti(1)	C(4)	C(9)	126.82(10)
C(3)	C(4)	C(5)	108.13(11)	C(3)	C(4)	C(9)	125.68(11)
C(5)	C(4)	C(9)	126.00(12)	Ti(1)	C(5)	C(1)	70.38(8)
Ti(1)	C(5)	C(4)	73.58(8)	Ti(1)	C(5)	C(10)	124.25(10)
C(1)	C(5)	C(4)	108.02(11)	C(1)	C(5)	C(10)	126.33(11)
C(4)	C(5)	C(10)	125.57(12)	N(1)	C(11)	N(2)	125.43(12)
N(1)	C(11)	N(3)	124.56(11)	N(2)	C(11)	N(3)	110.01(12)
N(2)	C(12)	C(13)	102.62(11)	N(3)	C(13)	C(12)	102.56(11)
N(2)	C(14)	C(15)	112.71(11)	N(2)	C(14)	C(19)	110.99(10)
C(15)	C(14)	C(19)	111.27(10)	C(14)	C(15)	C(16)	110.08(12)

Table 6. Bond angles (°) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
C(15)	C(16)	C(17)	111.28(11)	C(16)	C(17)	C(18)	111.17(11)
C(17)	C(18)	C(19)	111.79(13)	C(14)	C(19)	C(18)	109.64(11)
N(3)	C(20)	C(21)	111.20(11)	N(3)	C(20)	C(25)	111.69(11)
C(21)	C(20)	C(25)	111.59(12)	C(20)	C(21)	C(22)	110.68(12)
C(21)	C(22)	C(23)	111.01(12)	C(22)	C(23)	C(24)	111.29(13)
C(23)	C(24)	C(25)	111.54(12)	C(20)	C(25)	C(24)	109.99(11)

Table 7. Bond angles involving hydrogens (^{o})

atom	atom	atom	angle	atom	atom	atom	angle
C(1)	C(6)	H(1)	109.5	C(1)	C(6)	H(2)	109.5
C(1)	C(6)	H(3)	109.5	H(1)	C(6)	H(2)	109.5
H(1)	C(6)	H(3)	109.5	H(2)	C(6)	H(3)	109.5
C(2)	C(7)	H(4)	109.5	C(2)	C(7)	H(5)	109.5
C(2)	C(7)	H(6)	109.5	H(4)	C(7)	H(5)	109.5
H(4)	C(7)	H(6)	109.5	H(5)	C(7)	H(6)	109.5
C(3)	C(8)	H(7)	109.5	C(3)	C(8)	H(8)	109.5
C(3)	C(8)	H(9)	109.5	H(7)	C(8)	H(8)	109.5
H(7)	C(8)	H(9)	109.5	H(8)	C(8)	H(9)	109.5
C(4)	C(9)	H(10)	109.5	C(4)	C(9)	H(11)	109.5
C(4)	C(9)	H(12)	109.5	H(10)	C(9)	H(11)	109.5
H(10)	C(9)	H(12)	109.5	H(11)	C(9)	H(12)	109.5
C(5)	C(10)	H(13)	109.5	C(5)	C(10)	H(14)	109.5
C(5)	C(10)	H(15)	109.5	H(13)	C(10)	H(14)	109.5
H(13)	C(10)	H(15)	109.5	H(14)	C(10)	H(15)	109.5
N(2)	C(12)	H(16)	111.2	N(2)	C(12)	H(17)	111.2
C(13)	C(12)	H(16)	111.2	C(13)	C(12)	H(17)	111.2
H(16)	C(12)	H(17)	109.2	N(3)	C(13)	H(18)	111.3
N(3)	C(13)	H(19)	111.3	C(12)	C(13)	H(18)	111.3
C(12)	C(13)	H(19)	111.3	H(18)	C(13)	H(19)	109.2
N(2)	C(14)	H(20)	107.2	C(15)	C(14)	H(20)	107.2
C(19)	C(14)	H(20)	107.2	C(14)	C(15)	H(21)	109.6
C(14)	C(15)	H(22)	109.6	C(16)	C(15)	H(21)	109.6
C(16)	C(15)	H(22)	109.6	H(21)	C(15)	H(22)	108.1
C(15)	C(16)	H(23)	109.4	C(15)	C(16)	H(24)	109.4
C(17)	C(16)	H(23)	109.4	C(17)	C(16)	H(24)	109.4
H(23)	C(16)	H(24)	108.0	C(16)	C(17)	H(25)	109.4
C(16)	C(17)	H(26)	109.4	C(18)	C(17)	H(25)	109.4
C(18)	C(17)	H(26)	109.4	H(25)	C(17)	H(26)	108.0
C(17)	C(18)	H(27)	109.3	C(17)	C(18)	H(28)	109.3
C(19)	C(18)	H(27)	109.2	C(19)	C(18)	H(28)	109.3
H(27)	C(18)	H(28)	107.9	C(14)	C(19)	H(29)	109.7
C(14)	C(19)	H(30)	109.7	C(18)	C(19)	H(29)	109.7
C(18)	C(19)	H(30)	109.7	H(29)	C(19)	H(30)	108.2
N(3)	C(20)	H(31)	107.4	C(21)	C(20)	H(31)	107.4
C(25)	C(20)	H(31)	107.4	C(20)	C(21)	H(32)	109.5
C(20)	C(21)	H(33)	109.5	C(22)	C(21)	H(32)	109.5

Table 7. Bond angles involving hydrogens (°) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
C(22)	C(21)	H(33)	109.5	H(32)	C(21)	H(33)	108.1
C(21)	C(22)	H(34)	109.4	C(21)	C(22)	H(35)	109.4
C(23)	C(22)	H(34)	109.4	C(23)	C(22)	H(35)	109.4
H(34)	C(22)	H(35)	108.0	C(22)	C(23)	H(36)	109.4
C(22)	C(23)	H(37)	109.4	C(24)	C(23)	H(36)	109.4
C(24)	C(23)	H(37)	109.4	H(36)	C(23)	H(37)	108.0
C(23)	C(24)	H(38)	109.3	C(23)	C(24)	H(39)	109.3
C(25)	C(24)	H(38)	109.3	C(25)	C(24)	H(39)	109.3
H(38)	C(24)	H(39)	108.0	C(20)	C(25)	H(40)	109.7
C(20)	C(25)	H(41)	109.7	C(24)	C(25)	H(40)	109.7
C(24)	C(25)	H(41)	109.7	H(40)	C(25)	H(41)	108.2

Table 8. Torsion Angles(°)

atom1	atom2	atom3	atom4	angle	atom1	atom2	atom3	atom4	angle
Cl(1)	Ti(1)	N(1)	C(11)	94.4(6)	Cl(1)	Ti(1)	C(1)	C(2)	-87.02(9)
Cl(1)	Ti(1)	C(1)	C(5)	27.93(10)	Cl(1)	Ti(1)	C(1)	C(6)	150.93(9)
Cl(1)	Ti(1)	C(2)	C(1)	128.95(6)	Cl(1)	Ti(1)	C(2)	C(3)	13.06(10)
Cl(1)	Ti(1)	C(2)	C(7)	-108.38(10)	Cl(1)	Ti(1)	C(3)	C(2)	-169.92(7)
Cl(1)	Ti(1)	C(3)	C(4)	75.26(7)	Cl(1)	Ti(1)	C(3)	C(8)	-47.31(10)
Cl(1)	Ti(1)	C(4)	C(3)	-105.01(7)	Cl(1)	Ti(1)	C(4)	C(5)	137.60(7)
Cl(1)	Ti(1)	C(4)	C(9)	15.35(11)	Cl(1)	Ti(1)	C(5)	C(1)	-162.50(6)
Cl(1)	Ti(1)	C(5)	C(4)	-45.91(7)	Cl(1)	Ti(1)	C(5)	C(10)	76.29(10)
Cl(2)	Ti(1)	N(1)	C(11)	-158.9(6)	Cl(2)	Ti(1)	C(1)	C(2)	159.38(7)
Cl(2)	Ti(1)	C(1)	C(5)	-85.67(6)	Cl(2)	Ti(1)	C(1)	C(6)	37.33(11)
Cl(2)	Ti(1)	C(2)	C(1)	-25.07(8)	Cl(2)	Ti(1)	C(2)	C(3)	-140.96(7)
Cl(2)	Ti(1)	C(2)	C(7)	97.59(11)	Cl(2)	Ti(1)	C(3)	C(2)	68.29(10)
Cl(2)	Ti(1)	C(3)	C(4)	-46.53(10)	Cl(2)	Ti(1)	C(3)	C(8)	-169.10(7)
Cl(2)	Ti(1)	C(4)	C(3)	152.62(6)	Cl(2)	Ti(1)	C(4)	C(5)	35.23(8)
Cl(2)	Ti(1)	C(4)	C(9)	-87.02(11)	Cl(2)	Ti(1)	C(5)	C(1)	94.28(7)
Cl(2)	Ti(1)	C(5)	C(4)	-149.14(7)	Cl(2)	Ti(1)	C(5)	C(10)	-26.93(10)
N(1)	Ti(1)	C(1)	C(2)	53.93(8)	N(1)	Ti(1)	C(1)	C(5)	168.88(7)
N(1)	Ti(1)	C(1)	C(6)	-68.12(12)	C(1)	Ti(1)	N(1)	C(11)	-62.9(6)
N(1)	Ti(1)	C(2)	C(1)	-129.37(8)	N(1)	Ti(1)	C(2)	C(3)	114.74(8)
N(1)	Ti(1)	C(2)	C(7)	-6.70(11)	C(2)	Ti(1)	N(1)	C(11)	-35.1(6)
N(1)	Ti(1)	C(3)	C(2)	-66.94(9)	N(1)	Ti(1)	C(3)	C(4)	178.24(8)
N(1)	Ti(1)	C(3)	C(8)	55.66(11)	C(3)	Ti(1)	N(1)	C(11)	-3.0(6)
N(1)	Ti(1)	C(4)	C(3)	-2.45(11)	N(1)	Ti(1)	C(4)	C(5)	-119.84(9)
N(1)	Ti(1)	C(4)	C(9)	117.91(11)	C(4)	Ti(1)	N(1)	C(11)	-1.6(7)
N(1)	Ti(1)	C(5)	C(1)	-17.18(11)	N(1)	Ti(1)	C(5)	C(4)	99.41(9)
N(1)	Ti(1)	C(5)	C(10)	-138.39(10)	C(5)	Ti(1)	N(1)	C(11)	-52.7(7)
C(1)	Ti(1)	C(2)	C(3)	-115.89(11)	C(1)	Ti(1)	C(2)	C(7)	122.67(14)
C(2)	Ti(1)	C(1)	C(5)	114.95(10)	C(2)	Ti(1)	C(1)	C(6)	-122.05(15)
C(1)	Ti(1)	C(3)	C(2)	37.44(8)	C(1)	Ti(1)	C(3)	C(4)	-77.38(8)
C(1)	Ti(1)	C(3)	C(8)	160.05(12)	C(3)	Ti(1)	C(1)	C(2)	-37.41(7)
C(3)	Ti(1)	C(1)	C(5)	77.53(7)	C(3)	Ti(1)	C(1)	C(6)	-159.46(13)
C(1)	Ti(1)	C(4)	C(3)	80.01(8)	C(1)	Ti(1)	C(4)	C(5)	-37.37(7)
C(1)	Ti(1)	C(4)	C(9)	-159.63(13)	C(4)	Ti(1)	C(1)	C(2)	-78.66(8)
C(4)	Ti(1)	C(1)	C(5)	36.29(7)	C(4)	Ti(1)	C(1)	C(6)	159.29(13)
C(1)	Ti(1)	C(5)	C(4)	116.58(11)	C(1)	Ti(1)	C(5)	C(10)	-121.21(13)
C(5)	Ti(1)	C(1)	C(2)	-114.95(10)	C(5)	Ti(1)	C(1)	C(6)	123.00(14)
C(2)	Ti(1)	C(3)	C(4)	-114.82(12)	C(2)	Ti(1)	C(3)	C(8)	122.61(14)

Table 8. Torsion angles (°) (continued)

atom1	atom2	atom3	atom4	angle	atom1	atom2	atom3	atom4	angle
C(3)	Ti(1)	C(2)	C(1)	115.89(11)	C(3)	Ti(1)	C(2)	C(7)	-121.44(15)
C(2)	Ti(1)	C(4)	C(3)	38.14(7)	C(2)	Ti(1)	C(4)	C(5)	-79.25(8)
C(2)	Ti(1)	C(4)	C(9)	158.50(13)	C(4)	Ti(1)	C(2)	C(1)	78.15(8)
C(4)	Ti(1)	C(2)	C(3)	-37.74(8)	C(4)	Ti(1)	C(2)	C(7)	-159.18(13)
C(2)	Ti(1)	C(5)	C(1)	-38.02(7)	C(2)	Ti(1)	C(5)	C(4)	78.57(8)
C(2)	Ti(1)	C(5)	C(10)	-159.23(12)	C(5)	Ti(1)	C(2)	C(1)	37.80(7)
C(5)	Ti(1)	C(2)	C(3)	-78.10(8)	C(5)	Ti(1)	C(2)	C(7)	160.46(12)
C(3)	Ti(1)	C(4)	C(5)	-117.38(11)	C(3)	Ti(1)	C(4)	C(9)	120.36(15)
C(4)	Ti(1)	C(3)	C(2)	114.82(12)	C(4)	Ti(1)	C(3)	C(8)	-122.57(14)
C(3)	Ti(1)	C(5)	C(1)	-79.78(8)	C(3)	Ti(1)	C(5)	C(4)	36.81(7)
C(3)	Ti(1)	C(5)	C(10)	159.01(12)	C(5)	Ti(1)	C(3)	C(2)	78.88(8)
C(5)	Ti(1)	C(3)	C(4)	-35.94(7)	C(5)	Ti(1)	C(3)	C(8)	-158.51(12)
C(4)	Ti(1)	C(5)	C(1)	-116.58(11)	C(4)	Ti(1)	C(5)	C(10)	122.21(14)
C(5)	Ti(1)	C(4)	C(3)	117.38(11)	C(5)	Ti(1)	C(4)	C(9)	-122.26(14)
Ti(1)	N(1)	C(11)	N(2)	109.9(6)	Ti(1)	N(1)	C(11)	N(3)	-71.0(7)
C(11)	N(2)	C(12)	C(13)	18.54(14)	C(12)	N(2)	C(11)	N(1)	166.66(13)
C(12)	N(2)	C(11)	N(3)	-12.54(15)	C(11)	N(2)	C(14)	C(15)	75.03(16)
C(11)	N(2)	C(14)	C(19)	-159.39(13)	C(14)	N(2)	C(11)	N(1)	11.5(2)
C(14)	N(2)	C(11)	N(3)	-167.67(12)	C(12)	N(2)	C(14)	C(15)	-76.53(15)
C(12)	N(2)	C(14)	C(19)	49.05(17)	C(14)	N(2)	C(12)	C(13)	172.71(11)
C(11)	N(3)	C(13)	C(12)	11.01(15)	C(13)	N(3)	C(11)	N(1)	-178.89(13)
C(13)	N(3)	C(11)	N(2)	0.32(16)	C(11)	N(3)	C(20)	C(21)	-93.48(17)
C(11)	N(3)	C(20)	C(25)	141.13(14)	C(20)	N(3)	C(11)	N(1)	-3.3(2)
C(20)	N(3)	C(11)	N(2)	175.90(12)	C(13)	N(3)	C(20)	C(21)	81.45(16)
C(13)	N(3)	C(20)	C(25)	-43.94(19)	C(20)	N(3)	C(13)	C(12)	-164.42(13)
Ti(1)	C(1)	C(2)	C(3)	64.51(10)	Ti(1)	C(1)	C(2)	C(7)	-118.87(16)
Ti(1)	C(1)	C(5)	C(4)	-64.43(10)	Ti(1)	C(1)	C(5)	C(10)	118.65(15)
C(2)	C(1)	C(5)	Ti(1)	65.40(10)	C(2)	C(1)	C(5)	C(4)	0.96(17)
C(2)	C(1)	C(5)	C(10)	-175.95(14)	C(5)	C(1)	C(2)	Ti(1)	-66.86(10)
C(5)	C(1)	C(2)	C(3)	-2.34(17)	C(5)	C(1)	C(2)	C(7)	174.27(15)
C(6)	C(1)	C(2)	Ti(1)	116.23(15)	C(6)	C(1)	C(2)	C(3)	-179.25(14)
C(6)	C(1)	C(2)	C(7)	-2.6(2)	C(6)	C(1)	C(5)	Ti(1)	-117.68(15)
C(6)	C(1)	C(5)	C(4)	177.88(14)	C(6)	C(1)	C(5)	C(10)	1.0(2)
Ti(1)	C(2)	C(3)	C(4)	67.11(10)	Ti(1)	C(2)	C(3)	C(8)	-115.72(15)
C(1)	C(2)	C(3)	Ti(1)	-64.29(10)	C(1)	C(2)	C(3)	C(4)	2.82(17)
C(1)	C(2)	C(3)	C(8)	179.99(12)	C(7)	C(2)	C(3)	Ti(1)	119.05(16)
C(7)	C(2)	C(3)	C(4)	-173.84(14)	C(7)	C(2)	C(3)	C(8)	3.3(2)

Table 8. Torsion angles (°) (continued)

atom1	atom2	atom3	atom4	angle
Ti(1)	C(3)	C(4)	C(5)	63.00(10)
C(2)	C(3)	C(4)	Ti(1)	-65.24(10)
C(2)	C(3)	C(4)	C(9)	173.02(14)
C(8)	C(3)	C(4)	C(5)	-179.45(14)
Ti(1)	C(4)	C(5)	C(1)	62.35(10)
C(3)	C(4)	C(5)	Ti(1)	-61.57(10)
C(3)	C(4)	C(5)	C(10)	177.73(14)
C(9)	C(4)	C(5)	C(1)	-174.45(14)
N(2)	C(12)	C(13)	N(3)	-17.00(14)
N(2)	C(14)	C(19)	C(18)	175.88(12)
C(19)	C(14)	C(15)	C(16)	58.23(15)
C(15)	C(16)	C(17)	C(18)	54.92(17)
C(17)	C(18)	C(19)	C(14)	56.02(17)
N(3)	C(20)	C(25)	C(24)	-178.35(13)
C(25)	C(20)	C(21)	C(22)	-56.72(16)
C(21)	C(22)	C(23)	C(24)	-55.41(18)
C(23)	C(24)	C(25)	C(20)	-55.91(17)
Ti(1)	C(3)	C(4)	C(9)	-121.75(14)
C(2)	C(3)	C(4)	C(5)	-2.23(16)
C(8)	C(3)	C(4)	Ti(1)	117.55(15)
C(8)	C(3)	C(4)	C(9)	-4.2(2)
Ti(1)	C(4)	C(5)	C(10)	-120.70(15)
C(3)	C(4)	C(5)	C(1)	0.78(16)
C(9)	C(4)	C(5)	Ti(1)	123.20(14)
C(9)	C(4)	C(5)	C(10)	2.5(2)
N(2)	C(14)	C(15)	C(16)	-176.35(11)
C(15)	C(14)	C(19)	C(18)	-57.75(17)
C(14)	C(15)	C(16)	C(17)	-56.30(16)
C(16)	C(17)	C(18)	C(19)	-54.98(17)
N(3)	C(20)	C(21)	C(22)	177.84(12)
C(21)	C(20)	C(25)	C(24)	56.48(16)
C(20)	C(21)	C(22)	C(23)	55.60(18)
C(22)	C(23)	C(24)	C(25)	55.86(18)

The sign is positive if when looking from atom 2 to atom 3 a clock-wise motion of atom 1 would superimpose it on atom 4.

Table 9. Distances beyond the asymmetric unit out to 3.60 Å

atom	atom	distance	atom	atom	distance
Ti(1)	C(6)	3.3823(17)	Ti(1)	C(7)	3.4130(14)
Ti(1)	C(8)	3.3859(15)	Ti(1)	C(9)	3.5303(15)
Ti(1)	C(10)	3.4796(18)	Ti(1)	C(11)	3.0782(13)
Cl(1)	N(1)	3.1936(11)	Cl(1)	C(3)	3.4461(15)
Cl(1)	C(4)	3.2257(15)	Cl(1)	C(9)	3.3710(17)
Cl(2)	N(1)	3.2432(11)	Cl(2)	C(1)	3.3299(14)
Cl(2)	C(5)	3.2923(14)	Cl(2)	C(6)	3.5166(17)
Cl(2)	C(10)	3.4577(18)	Cl(2)	C(13)[1)]	3.3981(15)
N(1)	Cl(1)	3.1936(11)	N(1)	Cl(2)	3.2432(11)
N(1)	N(2)	2.3712(15)	N(1)	N(3)	2.3503(18)
N(1)	C(1)	3.347(2)	N(1)	C(2)	2.838(2)
N(1)	C(3)	3.1954(18)	N(1)	C(7)	3.089(2)
N(1)	C(12)	3.5703(18)	N(1)	C(13)	3.5804(19)
N(1)	C(14)	2.8815(16)	N(1)	C(15)	3.3829(17)
N(1)	C(20)	2.8864(18)	N(2)	N(1)	2.3712(15)
N(2)	N(3)	2.2156(15)	N(2)	C(7)	3.566(2)
N(2)	C(13)	2.3432(18)	N(2)	C(15)	2.4899(16)
N(2)	C(19)	2.4633(17)	N(3)	N(1)	2.3503(18)
N(3)	N(2)	2.2156(15)	N(3)	C(12)	2.3408(17)
N(3)	C(14)	3.5889(17)	N(3)	C(21)	2.465(2)
N(3)	C(25)	2.4721(16)	C(1)	Cl(2)	3.3299(14)
C(1)	N(1)	3.347(2)	C(1)	C(3)	2.2944(18)
C(1)	C(4)	2.2949(17)	C(1)	C(7)	2.605(2)
C(1)	C(10)	2.614(2)	C(1)	C(15)[2)]	3.527(2)
C(2)	N(1)	2.838(2)	C(2)	C(4)	2.3017(17)
C(2)	C(5)	2.3023(19)	C(2)	C(6)	2.6042(19)
C(2)	C(8)	2.6122(19)	C(3)	Cl(1)	3.4461(15)
C(3)	N(1)	3.1954(18)	C(3)	C(1)	2.2944(18)
C(3)	C(5)	2.2962(19)	C(3)	C(7)	2.5930(19)
C(3)	C(9)	2.606(2)	C(4)	Cl(1)	3.2257(15)
C(4)	C(1)	2.2949(17)	C(4)	C(2)	2.3017(17)
C(4)	C(8)	2.604(2)	C(4)	C(10)	2.587(2)
C(5)	Cl(2)	3.2923(14)	C(5)	C(2)	2.3023(19)
C(5)	C(3)	2.2962(19)	C(5)	C(6)	2.6107(19)
C(5)	C(9)	2.5921(18)	C(5)	C(15)[2)]	3.527(2)
C(6)	Ti(1)	3.3823(17)	C(6)	Cl(2)	3.5166(17)
C(6)	C(2)	2.6042(19)	C(6)	C(5)	2.6107(19)

Table 9. Distances beyond the asymmetric unit out to 3.60 Å (continued)

atom	atom	distance	atom	atom	distance
C(6)	C(7)	3.197(2)	C(6)	C(10)	3.198(2)
C(7)	Ti(1)	3.4130(14)	C(7)	N(1)	3.089(2)
C(7)	N(2)	3.566(2)	C(7)	C(1)	2.605(2)
C(7)	C(3)	2.5930(19)	C(7)	C(6)	3.197(2)
C(7)	C(8)	3.186(2)	C(7)	C(11)	3.320(2)
C(8)	Ti(1)	3.3859(15)	C(8)	C(2)	2.6122(19)
C(8)	C(4)	2.604(2)	C(8)	C(7)	3.186(2)
C(8)	C(9)	3.175(2)	C(9)	Ti(1)	3.5303(15)
C(9)	Cl(1)	3.3710(17)	C(9)	C(3)	2.606(2)
C(9)	C(5)	2.5921(18)	C(9)	C(8)	3.175(2)
C(9)	C(10)	3.164(2)	C(10)	Ti(1)	3.4796(18)
C(10)	Cl(2)	3.4577(18)	C(10)	C(1)	2.614(2)
C(10)	C(4)	2.587(2)	C(10)	C(6)	3.198(2)
C(10)	C(9)	3.164(2)	C(11)	Ti(1)	3.0782(13)
C(11)	C(7)	3.320(2)	C(11)	C(12)	2.3137(19)
C(11)	C(13)	2.319(2)	C(11)	C(14)	2.4538(17)
C(11)	C(15)	3.1698(17)	C(11)	C(20)	2.4663(18)
C(11)	C(21)	3.320(2)	C(12)	N(1)	3.5703(18)
C(12)	N(3)	2.3408(17)	C(12)	C(11)	2.3137(19)
C(12)	C(14)	2.584(2)	C(12)	C(15)	3.3019(19)
C(12)	C(19)	3.038(2)	C(13)	Cl(2)[3)]	3.3981(15)
C(13)	N(1)	3.5804(19)	C(13)	N(2)	2.3432(18)
C(13)	C(11)	2.319(2)	C(13)	C(20)	2.6020(19)
C(13)	C(21)	3.339(2)	C(13)	C(25)	3.0466(18)
C(14)	N(1)	2.8815(16)	C(14)	N(3)	3.5889(17)
C(14)	C(11)	2.4538(17)	C(14)	C(12)	2.584(2)
C(14)	C(16)	2.5050(18)	C(14)	C(17)	2.9355(17)
C(14)	C(18)	2.5002(18)	C(15)	N(1)	3.3829(17)
C(15)	N(2)	2.4899(16)	C(15)	C(1)[4)]	3.527(2)
C(15)	C(5)[4)]	3.527(2)	C(15)	C(11)	3.1698(17)
C(15)	C(12)	3.3019(19)	C(15)	C(17)	2.5227(19)
C(15)	C(18)	2.941(2)	C(15)	C(19)	2.520(2)
C(16)	C(14)	2.5050(18)	C(16)	C(18)	2.517(2)
C(16)	C(19)	2.9533(19)	C(17)	C(14)	2.9355(17)
C(17)	C(15)	2.5227(19)	C(17)	C(19)	2.5319(19)
C(18)	C(14)	2.5002(18)	C(18)	C(15)	2.941(2)
C(18)	C(16)	2.517(2)	C(19)	N(2)	2.4633(17)

Table 9. Distances beyond the asymmetric unit out to 3.60 Å (continued)

atom	atom	distance	atom	atom	distance
C(19)	C(12)	3.038(2)	C(19)	C(15)	2.520(2)
C(19)	C(16)	2.9533(19)	C(19)	C(17)	2.5319(19)
C(20)	N(1)	2.8864(18)	C(20)	C(11)	2.4663(18)
C(20)	C(13)	2.6020(19)	C(20)	C(22)	2.511(2)
C(20)	C(23)	2.932(2)	C(20)	C(24)	2.5030(19)
C(21)	N(3)	2.465(2)	C(21)	C(11)	3.320(2)
C(21)	C(13)	3.339(2)	C(21)	C(23)	2.516(2)
C(21)	C(24)	2.939(2)	C(21)	C(25)	2.523(2)
C(22)	C(20)	2.511(2)	C(22)	C(24)	2.515(2)
C(22)	C(25)	2.954(2)	C(23)	C(20)	2.932(2)
C(23)	C(21)	2.516(2)	C(23)	C(25)	2.523(2)
C(24)	C(20)	2.5030(19)	C(24)	C(21)	2.939(2)
C(24)	C(22)	2.515(2)	C(25)	N(3)	2.4721(16)
C(25)	C(13)	3.0466(18)	C(25)	C(21)	2.523(2)
C(25)	C(22)	2.954(2)	C(25)	C(23)	2.523(2)

Symmetry Operators:

(1)	-X+2,Y+1/2-1,-Z+1/2	(2)	X-1,Y,Z
(3)	-X+2,Y+1/2,-Z+1/2	(4)	X+1,Y,Z

Table 10. Distances beyond the asymmetric unit out to 3.60 Å involving hydrogens

atom	atom	distance	atom	atom	distance
Ti(1)	H(1)	3.548	Ti(1)	H(2)	3.473
Ti(1)	H(5)	3.533	Ti(1)	H(6)	3.573
Ti(1)	H(9)	3.412	Ti(1)	H(15)	3.560
Ti(1)	H(20)	3.541	Ti(1)	H(31)	3.287
Cl(1)	H(4)[1)]	2.756	Cl(1)	H(9)	3.149
Cl(1)	H(11)	3.356	Cl(1)	H(12)	3.003
Cl(1)	H(16)[2)]	3.437	Cl(1)	H(17)[2)]	3.081
Cl(1)	H(30)[2)]	3.129	Cl(1)	H(31)	2.954
Cl(1)	H(32)	3.504	Cl(1)	H(35)	3.064
Cl(1)	H(37)[3)]	2.945	Cl(1)	H(39)[3)]	3.378
Cl(2)	H(2)	2.968	Cl(2)	H(14)	3.117
Cl(2)	H(15)	3.413	Cl(2)	H(17)[2)]	3.208
Cl(2)	H(18)[2)]	3.110	Cl(2)	H(19)[2)]	3.125
Cl(2)	H(22)	3.364	Cl(2)	H(23)	3.532
Cl(2)	H(23)[4)]	3.486	Cl(2)	H(25)[4)]	3.045
N(1)	H(5)	2.861	N(1)	H(6)	3.043
N(1)	H(7)	3.505	N(1)	H(20)	2.587
N(1)	H(22)	2.875	N(1)	H(31)	2.491
N(1)	H(32)	3.232	N(2)	H(5)	3.211
N(2)	H(6)	3.076	N(2)	H(11)[5)]	3.427
N(2)	H(16)	2.044	N(2)	H(17)	2.044
N(2)	H(18)	2.890	N(2)	H(19)	3.115
N(2)	H(20)	2.002	N(2)	H(21)	2.725
N(2)	H(22)	2.674	N(2)	H(29)	2.640
N(2)	H(30)	2.699	N(3)	H(5)	3.359
N(3)	H(8)[6)]	3.394	N(3)	H(16)	2.888
N(3)	H(17)	3.112	N(3)	H(18)	2.042
N(3)	H(19)	2.042	N(3)	H(31)	2.002
N(3)	H(32)	2.651	N(3)	H(33)	2.682
N(3)	H(40)	2.691	N(3)	H(41)	2.667
C(1)	H(1)	2.050	C(1)	H(2)	2.050
C(1)	H(3)	2.050	C(1)	H(4)	3.049
C(1)	H(5)	3.331	C(1)	H(6)	2.729
C(1)	H(13)	3.103	C(1)	H(14)	2.711
C(1)	H(15)	3.316	C(1)	H(21)[7)]	2.772
C(1)	H(24)[7)]	3.339	C(2)	H(1)	2.713
C(2)	H(2)	3.319	C(2)	H(3)	3.071

Table 10. Distances beyond the asymmetric unit out to 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
C(2)	H(4)	2.045	C(2)	H(5)	2.045
C(2)	H(6)	2.045	C(2)	H(7)	2.703
C(2)	H(8)	3.130	C(2)	H(9)	3.295
C(2)	H(16)[7)]	3.393	C(2)	H(20)	3.536
C(2)	H(21)[7)]	2.794	C(3)	H(4)	3.006
C(3)	H(5)	2.727	C(3)	H(6)	3.336
C(3)	H(7)	2.050	C(3)	H(8)	2.050
C(3)	H(9)	2.050	C(3)	H(10)	3.029
C(3)	H(11)	3.343	C(3)	H(12)	2.733
C(3)	H(16)[7)]	3.282	C(3)	H(21)[7)]	3.135
C(4)	H(7)	3.370	C(4)	H(8)	2.943
C(4)	H(9)	2.789	C(4)	H(10)	2.048
C(4)	H(11)	2.048	C(4)	H(12)	2.048
C(4)	H(13)	2.956	C(4)	H(14)	3.344
C(4)	H(15)	2.756	C(4)	H(21)[7)]	3.257
C(4)	H(22)[7)]	3.264	C(5)	H(1)	3.360
C(5)	H(2)	2.760	C(5)	H(3)	3.001
C(5)	H(10)	3.016	C(5)	H(11)	2.726
C(5)	H(12)	3.328	C(5)	H(13)	2.048
C(5)	H(14)	2.048	C(5)	H(15)	2.048
C(5)	H(21)[7)]	3.059	C(5)	H(22)[7)]	3.242
C(5)	H(24)[7)]	3.323	C(6)	H(4)	3.544
C(6)	H(6)	2.869	C(6)	H(13)[8)]	3.457
C(6)	H(14)	2.825	C(6)	H(14)[8)]	3.567
C(6)	H(20)	3.264	C(6)	H(21)[7)]	3.409
C(6)	H(24)[7)]	3.261	C(6)	H(26)[7)]	3.424
C(6)	H(39)[9)]	3.454	C(6)	H(40)[9)]	3.305
C(7)	H(1)	2.858	C(7)	H(3)	3.560
C(7)	H(7)	2.803	C(7)	H(11)[5)]	2.965
C(7)	H(16)[7)]	3.339	C(7)	H(20)	3.150
C(7)	H(21)[7)]	3.405	C(7)	H(39)[9)]	3.391
C(8)	H(4)	3.477	C(8)	H(5)	2.883
C(8)	H(10)	3.491	C(8)	H(12)	2.854
C(8)	H(16)[7)]	3.160	C(8)	H(19)[7)]	3.332
C(8)	H(27)[10)]	3.573	C(8)	H(31)	3.219
C(8)	H(33)[7)]	3.416	C(8)	H(37)[3)]	3.466
C(9)	H(5)[1)]	3.387	C(9)	H(6)[1)]	3.597

Table 10. Distances beyond the asymmetric unit out to 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
C(9)	H(8)	3.278	C(9)	H(9)	3.011
C(9)	H(13)	3.333	C(9)	H(15)	2.950
C(9)	H(17)[1)]	3.425	C(9)	H(29)[1)]	3.301
C(9)	H(32)[7)]	3.291	C(9)	H(37)[3)]	3.513
C(10)	H(2)	2.945	C(10)	H(3)	3.423
C(10)	H(3)[8)]	3.305	C(10)	H(10)	3.470
C(10)	H(11)	2.855	C(10)	H(18)[1)]	3.365
C(10)	H(24)[7)]	3.213	C(10)	H(24)[4)]	3.468
C(10)	H(25)[4)]	3.231	C(10)	H(41)[1)]	3.284
C(11)	H(5)	2.830	C(11)	H(6)	3.162
C(11)	H(16)	2.854	C(11)	H(17)	3.075
C(11)	H(18)	2.911	C(11)	H(19)	3.041
C(11)	H(20)	2.580	C(11)	H(21)	3.536
C(11)	H(22)	2.908	C(11)	H(31)	2.533
C(11)	H(32)	3.124	C(12)	H(4)[6)]	3.571
C(12)	H(8)[6)]	3.225	C(12)	H(10)[5)]	3.543
C(12)	H(18)	2.108	C(12)	H(19)	2.108
C(12)	H(20)	3.358	C(12)	H(21)	3.078
C(12)	H(22)	3.578	C(12)	H(29)	3.181
C(12)	H(30)	2.782	C(13)	H(8)[6)]	3.077
C(13)	H(16)	2.108	C(13)	H(17)	2.108
C(13)	H(31)	3.362	C(13)	H(33)	3.109
C(13)	H(40)	2.783	C(13)	H(41)	3.187
C(14)	H(1)	3.434	C(14)	H(6)	3.030
C(14)	H(16)	2.823	C(14)	H(17)	2.910
C(14)	H(21)	2.081	C(14)	H(22)	2.081
C(14)	H(23)	2.731	C(14)	H(24)	3.358
C(14)	H(26)	3.312	C(14)	H(27)	3.354
C(14)	H(28)	2.727	C(14)	H(29)	2.080
C(14)	H(30)	2.080	C(15)	H(3)[6)]	3.555
C(15)	H(13)[6)]	3.561	C(15)	H(16)	3.076
C(15)	H(20)	2.058	C(15)	H(23)	2.079
C(15)	H(24)	2.079	C(15)	H(25)	3.372
C(15)	H(26)	2.762	C(15)	H(28)	3.304
C(15)	H(29)	3.372	C(15)	H(30)	2.740
C(16)	H(2)[4)]	3.399	C(16)	H(3)[6)]	3.137
C(16)	H(13)[6)]	3.402	C(16)	H(14)[4)]	3.151

Table 10. Distances beyond the asymmetric unit out to 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
C(16)	H(20)	2.657	C(16)	H(21)	2.083
C(16)	H(22)	2.083	C(16)	H(25)	2.077
C(16)	H(26)	2.077	C(16)	H(27)	3.365
C(16)	H(28)	2.755	C(16)	H(30)	3.304
C(17)	H(3)[6)]	3.177	C(17)	H(14)[4)]	3.088
C(17)	H(20)	3.197	C(17)	H(21)	2.754
C(17)	H(22)	3.373	C(17)	H(23)	2.077
C(17)	H(24)	2.077	C(17)	H(27)	2.073
C(17)	H(28)	2.073	C(17)	H(29)	3.380
C(17)	H(30)	2.768	C(17)	H(39)[11)]	3.470
C(17)	H(41)[11)]	3.393	C(18)	H(19)[9)]	3.537
C(18)	H(20)	2.653	C(18)	H(21)	3.287
C(18)	H(23)	2.757	C(18)	H(24)	3.365
C(18)	H(25)	2.075	C(18)	H(26)	2.075
C(18)	H(29)	2.087	C(18)	H(30)	2.088
C(18)	H(33)[9)]	3.233	C(18)	H(34)[12)]	3.294
C(18)	H(36)[9)]	3.305	C(18)	H(40)[9)]	3.476
C(19)	H(6)	3.497	C(19)	H(16)	3.274
C(19)	H(17)	2.858	C(19)	H(20)	2.056
C(19)	H(21)	2.736	C(19)	H(22)	3.371
C(19)	H(23)	3.315	C(19)	H(25)	3.379
C(19)	H(26)	2.772	C(19)	H(27)	2.082
C(19)	H(28)	2.082	C(19)	H(34)[12)]	3.408
C(19)	H(35)[12)]	3.542	C(19)	H(36)[9)]	3.306
C(20)	H(7)	3.536	C(20)	H(18)	2.984
C(20)	H(19)	2.806	C(20)	H(32)	2.077
C(20)	H(33)	2.077	C(20)	H(34)	3.363
C(20)	H(35)	2.745	C(20)	H(36)	3.295
C(20)	H(38)	2.731	C(20)	H(39)	3.356
C(20)	H(40)	2.079	C(20)	H(41)	2.079
C(21)	H(8)[6)]	3.261	C(21)	H(19)	3.126
C(21)	H(27)[13)]	3.598	C(21)	H(31)	2.058
C(21)	H(34)	2.078	C(21)	H(34)[14)]	3.448
C(21)	H(35)	2.078	C(21)	H(36)	2.751
C(21)	H(37)	3.366	C(21)	H(38)	3.295
C(21)	H(40)	2.754	C(21)	H(41)	3.373
C(22)	H(27)[2)]	3.189	C(22)	H(30)[2)]	3.586

Table 10. Distances beyond the asymmetric unit out to 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
C(22)	H(31)	2.684	C(22)	H(32)	2.079
C(22)	H(33)	2.079	C(22)	H(34)[14)]	3.205
C(22)	H(36)	2.075	C(22)	H(37)	2.075
C(22)	H(38)	2.747	C(22)	H(38)[3)]	3.351
C(22)	H(39)	3.363	C(22)	H(40)	3.310
C(23)	H(9)[3)]	3.401	C(23)	H(12)[3)]	3.107
C(23)	H(29)[13)]	3.524	C(23)	H(31)	3.220
C(23)	H(32)	3.367	C(23)	H(33)	2.751
C(23)	H(34)	2.076	C(23)	H(35)	2.076
C(23)	H(38)	2.071	C(23)	H(38)[3)]	3.573
C(23)	H(39)	2.071	C(23)	H(40)	2.759
C(23)	H(41)	3.372	C(24)	H(26)[10)]	3.034
C(24)	H(31)	2.674	C(24)	H(33)	3.295
C(24)	H(34)	3.363	C(24)	H(35)	2.752
C(24)	H(35)[3)]	3.358	C(24)	H(36)	2.072
C(24)	H(37)	2.072	C(24)	H(40)	2.084
C(24)	H(41)	2.084	C(25)	H(1)[13)]	3.444
C(25)	H(3)[13)]	3.363	C(25)	H(18)	2.973
C(25)	H(19)	3.155	C(25)	H(26)[10)]	3.259
C(25)	H(28)[13)]	3.448	C(25)	H(31)	2.058
C(25)	H(32)	3.372	C(25)	H(33)	2.751
C(25)	H(35)	3.315	C(25)	H(36)	2.755
C(25)	H(37)	3.371	C(25)	H(38)	2.080
C(25)	H(39)	2.080	H(1)	Ti(1)	3.548
H(1)	C(1)	2.050	H(1)	C(2)	2.713
H(1)	C(5)	3.360	H(1)	C(7)	2.858
H(1)	C(14)	3.434	H(1)	C(25)[9)]	3.444
H(1)	H(2)	1.600	H(1)	H(3)	1.600
H(1)	H(4)	3.277	H(1)	H(6)	2.265
H(1)	H(20)	2.452	H(1)	H(23)	3.342
H(1)	H(28)	3.017	H(1)	H(39)[9)]	3.061
H(1)	H(40)[9)]	2.760	H(1)	H(41)[9)]	3.544
H(2)	Ti(1)	3.473	H(2)	Cl(2)	2.968
H(2)	C(1)	2.050	H(2)	C(2)	3.319
H(2)	C(5)	2.760	H(2)	C(10)	2.945
H(2)	C(16)[4)]	3.399	H(2)	H(1)	1.600
H(2)	H(3)	1.600	H(2)	H(13)	3.487

Table 10. Distances beyond the asymmetric unit out to 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
H(2)	H(13)[8)]	3.084	H(2)	H(14)	2.318
H(2)	H(14)[8)]	3.450	H(2)	H(20)	3.525
H(2)	H(23)	3.509	H(2)	H(23)[4)]	3.215
H(2)	H(24)[7)]	3.581	H(2)	H(24)[4)]	2.711
H(3)	C(1)	2.050	H(3)	C(2)	3.071
H(3)	C(5)	3.001	H(3)	C(7)	3.560
H(3)	C(10)	3.423	H(3)	C(10)[8)]	3.305
H(3)	C(15)[7)]	3.555	H(3)	C(16)[7)]	3.137
H(3)	C(17)[7)]	3.177	H(3)	C(25)[9)]	3.363
H(3)	H(1)	1.600	H(3)	H(2)	1.600
H(3)	H(6)	3.301	H(3)	H(13)	3.590
H(3)	H(13)[8)]	2.978	H(3)	H(14)	3.075
H(3)	H(14)[8)]	2.813	H(3)	H(21)[7)]	3.008
H(3)	H(24)[7)]	2.544	H(3)	H(25)[7)]	3.498
H(3)	H(26)[7)]	2.515	H(3)	H(39)[9)]	3.011
H(3)	H(40)[9)]	3.030	H(3)	H(41)[9)]	3.018
H(4)	Cl(1)[5)]	2.756	H(4)	C(1)	3.049
H(4)	C(2)	2.045	H(4)	C(3)	3.006
H(4)	C(6)	3.544	H(4)	C(8)	3.477
H(4)	C(12)[7)]	3.571	H(4)	H(1)	3.277
H(4)	H(5)	1.600	H(4)	H(6)	1.600
H(4)	H(7)	3.125	H(4)	H(11)[5)]	3.039
H(4)	H(12)[5)]	3.529	H(4)	H(16)[7)]	2.688
H(4)	H(21)[7)]	2.985	H(4)	H(30)[7)]	3.426
H(4)	H(39)[9)]	2.919	H(5)	Ti(1)	3.533
H(5)	N(1)	2.861	H(5)	N(2)	3.211
H(5)	N(3)	3.359	H(5)	C(1)	3.331
H(5)	C(2)	2.045	H(5)	C(3)	2.727
H(5)	C(8)	2.883	H(5)	C(9)[5)]	3.387
H(5)	C(11)	2.830	H(5)	H(4)	1.600
H(5)	H(6)	1.600	H(5)	H(7)	2.244
H(5)	H(8)	3.435	H(5)	H(11)[5)]	2.462
H(5)	H(12)[5)]	3.583	H(5)	H(15)[5)]	3.050
H(5)	H(16)[7)]	3.552	H(5)	H(20)	3.380
H(6)	Ti(1)	3.573	H(6)	N(1)	3.043
H(6)	N(2)	3.076	H(6)	C(1)	2.729
H(6)	C(2)	2.045	H(6)	C(3)	3.336

Table 10. Distances beyond the asymmetric unit out to 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
H(6)	C(6)	2.869	H(6)	C(9)[5)]	3.597
H(6)	C(11)	3.162	H(6)	C(14)	3.030
H(6)	C(19)	3.497	H(6)	H(1)	2.265
H(6)	H(3)	3.301	H(6)	H(4)	1.600
H(6)	H(5)	1.600	H(6)	H(11)[5)]	2.917
H(6)	H(12)[5)]	3.395	H(6)	H(20)	2.344
H(6)	H(29)	3.037	H(6)	H(36)[9)]	3.277
H(6)	H(39)[9)]	3.016	H(7)	N(1)	3.505
H(7)	C(2)	2.703	H(7)	C(3)	2.050
H(7)	C(4)	3.370	H(7)	C(7)	2.803
H(7)	C(20)	3.536	H(7)	H(4)	3.125
H(7)	H(5)	2.244	H(7)	H(8)	1.600
H(7)	H(9)	1.600	H(7)	H(15)[5)]	3.327
H(7)	H(16)[7)]	3.236	H(7)	H(19)[7)]	3.432
H(7)	H(25)[10)]	3.273	H(7)	H(31)	2.878
H(7)	H(41)	2.977	H(8)	N(3)[7)]	3.394
H(8)	C(2)	3.130	H(8)	C(3)	2.050
H(8)	C(4)	2.943	H(8)	C(9)	3.278
H(8)	C(12)[7)]	3.225	H(8)	C(13)[7)]	3.077
H(8)	C(21)[7)]	3.261	H(8)	H(5)	3.435
H(8)	H(7)	1.600	H(8)	H(9)	1.600
H(8)	H(10)	3.316	H(8)	H(12)	2.999
H(8)	H(16)[7)]	2.591	H(8)	H(19)[7)]	2.450
H(8)	H(25)[10)]	3.592	H(8)	H(27)[10)]	3.254
H(8)	H(32)[7)]	3.071	H(8)	H(33)[7)]	2.632
H(9)	Ti(1)	3.412	H(9)	Cl(1)	3.149
H(9)	C(2)	3.295	H(9)	C(3)	2.050
H(9)	C(4)	2.789	H(9)	C(9)	3.011
H(9)	C(23)[3)]	3.401	H(9)	H(7)	1.600
H(9)	H(8)	1.600	H(9)	H(10)	3.472
H(9)	H(12)	2.424	H(9)	H(27)[10)]	3.288
H(9)	H(31)	2.836	H(9)	H(33)[7)]	3.350
H(9)	H(34)[3)]	3.553	H(9)	H(37)[3)]	2.505
H(9)	H(38)	3.134	H(10)	C(3)	3.029
H(10)	C(4)	2.048	H(10)	C(5)	3.016
H(10)	C(8)	3.491	H(10)	C(10)	3.470
H(10)	C(12)[1)]	3.543	H(10)	H(8)	3.316

Table 10. Distances beyond the asymmetric unit out to 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
H(10)	H(9)	3.472	H(10)	H(11)	1.600
H(10)	H(12)	1.600	H(10)	H(13)	3.357
H(10)	H(15)	3.382	H(10)	H(17)[1)]	2.766
H(10)	H(18)[1)]	3.365	H(10)	H(22)[7)]	3.097
H(10)	H(29)[1)]	3.117	H(10)	H(32)[7)]	2.655
H(11)	Cl(1)	3.356	H(11)	N(2)[1)]	3.427
H(11)	C(3)	3.343	H(11)	C(4)	2.048
H(11)	C(5)	2.726	H(11)	C(7)[1)]	2.965
H(11)	C(10)	2.855	H(11)	H(4)[1)]	3.039
H(11)	H(5)[1)]	2.462	H(11)	H(6)[1)]	2.917
H(11)	H(10)	1.600	H(11)	H(12)	1.600
H(11)	H(13)	3.084	H(11)	H(15)	2.367
H(11)	H(17)[1)]	3.233	H(11)	H(18)[1)]	3.205
H(11)	H(29)[1)]	3.254	H(12)	Cl(1)	3.003
H(12)	C(3)	2.733	H(12)	C(4)	2.048
H(12)	C(5)	3.328	H(12)	C(8)	2.854
H(12)	C(23)[3)]	3.107	H(12)	H(4)[1)]	3.529
H(12)	H(5)[1)]	3.583	H(12)	H(6)[1)]	3.395
H(12)	H(8)	2.999	H(12)	H(9)	2.424
H(12)	H(10)	1.600	H(12)	H(11)	1.600
H(12)	H(29)[1)]	2.979	H(12)	H(32)[7)]	3.068
H(12)	H(36)[3)]	2.751	H(12)	H(37)[3)]	2.552
H(13)	C(1)	3.103	H(13)	C(4)	2.956
H(13)	C(5)	2.048	H(13)	C(6)[8)]	3.457
H(13)	C(9)	3.333	H(13)	C(15)[7)]	3.561
H(13)	C(16)[7)]	3.402	H(13)	H(2)	3.487
H(13)	H(2)[8)]	3.084	H(13)	H(3)	3.590
H(13)	H(3)[8)]	2.978	H(13)	H(10)	3.357
H(13)	H(11)	3.084	H(13)	H(14)	1.600
H(13)	H(15)	1.600	H(13)	H(18)[1)]	2.754
H(13)	H(22)[7)]	3.091	H(13)	H(24)[7)]	2.644
H(13)	H(41)[1)]	3.176	H(14)	Cl(2)	3.117
H(14)	C(1)	2.711	H(14)	C(4)	3.344
H(14)	C(5)	2.048	H(14)	C(6)	2.825
H(14)	C(6)[8)]	3.567	H(14)	C(16)[4)]	3.151
H(14)	C(17)[4)]	3.088	H(14)	H(2)	2.318
H(14)	H(2)[8)]	3.450	H(14)	H(3)	3.075

Table 10. Distances beyond the asymmetric unit out to 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
H(14)	H(3)[8)]	2.813	H(14)	H(13)	1.600
H(14)	H(15)	1.600	H(14)	H(23)[4)]	3.478
H(14)	H(24)[7)]	3.289	H(14)	H(24)[4)]	2.502
H(14)	H(25)[4)]	2.586	H(14)	H(26)[4)]	3.107
H(14)	H(41)[1)]	3.365	H(15)	Ti(1)	3.560
H(15)	Cl(2)	3.413	H(15)	C(1)	3.316
H(15)	C(4)	2.756	H(15)	C(5)	2.048
H(15)	C(9)	2.950	H(15)	H(5)[1)]	3.050
H(15)	H(7)[1)]	3.327	H(15)	H(10)	3.382
H(15)	H(11)	2.367	H(15)	H(13)	1.600
H(15)	H(14)	1.600	H(15)	H(18)[1)]	3.090
H(15)	H(25)[4)]	2.998	H(15)	H(41)[1)]	2.790
H(16)	Cl(1)[12)]	3.437	H(16)	N(2)	2.044
H(16)	N(3)	2.888	H(16)	C(2)[6)]	3.393
H(16)	C(3)[6)]	3.282	H(16)	C(7)[6)]	3.339
H(16)	C(8)[6)]	3.160	H(16)	C(11)	2.854
H(16)	C(13)	2.108	H(16)	C(14)	2.823
H(16)	C(15)	3.076	H(16)	C(19)	3.274
H(16)	H(4)[6)]	2.688	H(16)	H(5)[6)]	3.552
H(16)	H(7)[6)]	3.236	H(16)	H(8)[6)]	2.591
H(16)	H(17)	1.614	H(16)	H(18)	2.840
H(16)	H(19)	2.271	H(16)	H(21)	2.581
H(16)	H(22)	3.361	H(16)	H(30)	2.818
H(17)	Cl(1)[12)]	3.081	H(17)	Cl(2)[12)]	3.208
H(17)	N(2)	2.044	H(17)	N(3)	3.112
H(17)	C(9)[5)]	3.425	H(17)	C(11)	3.075
H(17)	C(13)	2.108	H(17)	C(14)	2.910
H(17)	C(19)	2.858	H(17)	H(10)[5)]	2.766
H(17)	H(11)[5)]	3.233	H(17)	H(16)	1.614
H(17)	H(18)	2.271	H(17)	H(19)	2.688
H(17)	H(21)	3.576	H(17)	H(29)	2.803
H(17)	H(30)	2.481	H(18)	Cl(2)[12)]	3.110
H(18)	N(2)	2.890	H(18)	N(3)	2.042
H(18)	C(10)[5)]	3.365	H(18)	C(11)	2.911
H(18)	C(12)	2.108	H(18)	C(20)	2.984
H(18)	C(25)	2.973	H(18)	H(10)[5)]	3.365
H(18)	H(11)[5)]	3.205	H(18)	H(13)[5)]	2.754

Table 10. Distances beyond the asymmetric unit out to 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
H(18)	H(15)[5)]	3.090	H(18)	H(16)	2.840
H(18)	H(17)	2.271	H(18)	H(19)	1.614
H(18)	H(40)	2.642	H(18)	H(41)	2.866
H(19)	Cl(2)[12)]	3.125	H(19)	N(2)	3.115
H(19)	N(3)	2.042	H(19)	C(8)[6)]	3.332
H(19)	C(11)	3.041	H(19)	C(12)	2.108
H(19)	C(18)[13)]	3.537	H(19)	C(20)	2.806
H(19)	C(21)	3.126	H(19)	C(25)	3.155
H(19)	H(7)[6)]	3.432	H(19)	H(8)[6)]	2.450
H(19)	H(16)	2.271	H(19)	H(17)	2.688
H(19)	H(18)	1.614	H(19)	H(25)[13)]	3.157
H(19)	H(27)[13)]	3.407	H(19)	H(28)[13)]	2.980
H(19)	H(32)	3.486	H(19)	H(33)	2.617
H(19)	H(40)	2.655	H(19)	H(41)	3.535
H(20)	Ti(1)	3.541	H(20)	N(1)	2.587
H(20)	N(2)	2.002	H(20)	C(2)	3.536
H(20)	C(6)	3.264	H(20)	C(7)	3.150
H(20)	C(11)	2.580	H(20)	C(12)	3.358
H(20)	C(15)	2.058	H(20)	C(16)	2.657
H(20)	C(17)	3.197	H(20)	C(18)	2.653
H(20)	C(19)	2.056	H(20)	H(1)	2.452
H(20)	H(2)	3.525	H(20)	H(5)	3.380
H(20)	H(6)	2.344	H(20)	H(21)	2.865
H(20)	H(22)	2.365	H(20)	H(23)	2.503
H(20)	H(24)	3.568	H(20)	H(27)	3.565
H(20)	H(28)	2.500	H(20)	H(29)	2.361
H(20)	H(30)	2.865	H(21)	N(2)	2.725
H(21)	C(1)[6)]	2.772	H(21)	C(2)[6)]	2.794
H(21)	C(3)[6)]	3.135	H(21)	C(4)[6)]	3.257
H(21)	C(5)[6)]	3.059	H(21)	C(6)[6)]	3.409
H(21)	C(7)[6)]	3.405	H(21)	C(11)	3.536
H(21)	C(12)	3.078	H(21)	C(14)	2.081
H(21)	C(16)	2.083	H(21)	C(17)	2.754
H(21)	C(18)	3.287	H(21)	C(19)	2.736
H(21)	H(3)[6)]	3.008	H(21)	H(4)[6)]	2.985
H(21)	H(16)	2.581	H(21)	H(17)	3.576
H(21)	H(20)	2.865	H(21)	H(22)	1.603

Table 10. Distances beyond the asymmetric unit out to 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
H(21)	H(23)	2.877	H(21)	H(24)	2.362
H(21)	H(26)	2.628	H(21)	H(30)	2.587
H(22)	Cl(2)	3.364	H(22)	N(1)	2.875
H(22)	N(2)	2.674	H(22)	C(4)[6)]	3.264
H(22)	C(5)[6)]	3.242	H(22)	C(11)	2.908
H(22)	C(12)	3.578	H(22)	C(14)	2.081
H(22)	C(16)	2.083	H(22)	C(17)	3.373
H(22)	C(19)	3.371	H(22)	H(10)[6)]	3.097
H(22)	H(13)[6)]	3.091	H(22)	H(16)	3.361
H(22)	H(20)	2.365	H(22)	H(21)	1.603
H(22)	H(23)	2.360	H(22)	H(24)	2.392
H(23)	Cl(2)	3.532	H(23)	Cl(2)[4)]	3.486
H(23)	C(14)	2.731	H(23)	C(15)	2.079
H(23)	C(17)	2.077	H(23)	C(18)	2.757
H(23)	C(19)	3.315	H(23)	H(1)	3.342
H(23)	H(2)	3.509	H(23)	H(2)[4)]	3.215
H(23)	H(14)[4)]	3.478	H(23)	H(20)	2.503
H(23)	H(21)	2.877	H(23)	H(22)	2.360
H(23)	H(24)	1.602	H(23)	H(25)	2.347
H(23)	H(26)	2.871	H(23)	H(28)	2.628
H(24)	C(1)[6)]	3.339	H(24)	C(5)[6)]	3.323
H(24)	C(6)[6)]	3.261	H(24)	C(10)[6)]	3.213
H(24)	C(10)[4)]	3.468	H(24)	C(14)	3.358
H(24)	C(15)	2.079	H(24)	C(17)	2.077
H(24)	C(18)	3.365	H(24)	H(2)[6)]	3.581
H(24)	H(2)[4)]	2.711	H(24)	H(3)[6)]	2.544
H(24)	H(13)[6)]	2.644	H(24)	H(14)[6)]	3.289
H(24)	H(14)[4)]	2.502	H(24)	H(20)	3.568
H(24)	H(21)	2.362	H(24)	H(22)	2.392
H(24)	H(23)	1.602	H(24)	H(25)	2.393
H(24)	H(26)	2.347	H(25)	Cl(2)[4)]	3.045
H(25)	C(10)[4)]	3.231	H(25)	C(15)	3.372
H(25)	C(16)	2.077	H(25)	C(18)	2.075
H(25)	C(19)	3.379	H(25)	H(3)[6)]	3.498
H(25)	H(7)[11)]	3.273	H(25)	H(8)[11)]	3.592
H(25)	H(14)[4)]	2.586	H(25)	H(15)[4)]	2.998
H(25)	H(19)[9)]	3.157	H(25)	H(23)	2.347

Table 10. Distances beyond the asymmetric unit out to 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
H(25)	H(24)	2.393	H(25)	H(26)	1.602
H(25)	H(27)	2.388	H(25)	H(28)	2.343
H(25)	H(41)[11)]	3.229	H(26)	C(6)[6)]	3.424
H(26)	C(14)	3.312	H(26)	C(15)	2.762
H(26)	C(16)	2.077	H(26)	C(18)	2.075
H(26)	C(19)	2.772	H(26)	C(24)[11)]	3.034
H(26)	C(25)[11)]	3.259	H(26)	H(3)[6)]	2.515
H(26)	H(14)[4)]	3.107	H(26)	H(21)	2.628
H(26)	H(23)	2.871	H(26)	H(24)	2.347
H(26)	H(25)	1.602	H(26)	H(27)	2.345
H(26)	H(28)	2.868	H(26)	H(30)	2.644
H(26)	H(38)[11)]	2.969	H(26)	H(39)[11)]	2.516
H(26)	H(41)[11)]	2.660	H(27)	C(8)[11)]	3.573
H(27)	C(14)	3.354	H(27)	C(16)	3.365
H(27)	C(17)	2.073	H(27)	C(19)	2.082
H(27)	C(21)[9)]	3.598	H(27)	C(22)[12)]	3.189
H(27)	H(8)[11)]	3.254	H(27)	H(9)[11)]	3.288
H(27)	H(19)[9)]	3.407	H(27)	H(20)	3.565
H(27)	H(25)	2.388	H(27)	H(26)	2.345
H(27)	H(28)	1.601	H(27)	H(29)	2.397
H(27)	H(30)	2.365	H(27)	H(33)[9)]	2.644
H(27)	H(34)[12)]	2.496	H(27)	H(35)[12)]	2.996
H(27)	H(36)[9)]	3.215	H(27)	H(38)[11)]	3.233
H(28)	C(14)	2.727	H(28)	C(15)	3.304
H(28)	C(16)	2.755	H(28)	C(17)	2.073
H(28)	C(19)	2.082	H(28)	C(25)[9)]	3.448
H(28)	H(1)	3.017	H(28)	H(19)[9)]	2.980
H(28)	H(20)	2.500	H(28)	H(23)	2.628
H(28)	H(25)	2.343	H(28)	H(26)	2.868
H(28)	H(27)	1.601	H(28)	H(29)	2.361
H(28)	H(30)	2.880	H(28)	H(33)[9)]	2.905
H(28)	H(36)[9)]	2.896	H(28)	H(40)[9)]	2.546
H(29)	N(2)	2.640	H(29)	C(9)[5)]	3.301
H(29)	C(12)	3.181	H(29)	C(14)	2.080
H(29)	C(15)	3.372	H(29)	C(17)	3.380
H(29)	C(18)	2.087	H(29)	C(23)[9)]	3.524
H(29)	H(6)	3.037	H(29)	H(10)[5)]	3.117

Table 10. Distances beyond the asymmetric unit out to 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
H(29)	H(11)[5)]	3.254	H(29)	H(12)[5)]	2.979
H(29)	H(17)	2.803	H(29)	H(20)	2.361
H(29)	H(27)	2.397	H(29)	H(28)	2.361
H(29)	H(30)	1.604	H(29)	H(32)[12)]	3.298
H(29)	H(34)[12)]	3.060	H(29)	H(35)[12)]	3.472
H(29)	H(36)[9)]	2.546	H(30)	Cl(1)[12)]	3.129
H(30)	N(2)	2.699	H(30)	C(12)	2.782
H(30)	C(14)	2.080	H(30)	C(15)	2.740
H(30)	C(16)	3.304	H(30)	C(17)	2.768
H(30)	C(18)	2.088	H(30)	C(22)[12)]	3.586
H(30)	H(4)[6)]	3.426	H(30)	H(16)	2.818
H(30)	H(17)	2.481	H(30)	H(20)	2.865
H(30)	H(21)	2.587	H(30)	H(26)	2.644
H(30)	H(27)	2.365	H(30)	H(28)	2.880
H(30)	H(29)	1.604	H(30)	H(34)[12)]	3.332
H(30)	H(35)[12)]	3.015	H(30)	H(39)[11)]	3.296
H(31)	Ti(1)	3.287	H(31)	Cl(1)	2.954
H(31)	N(1)	2.491	H(31)	N(3)	2.002
H(31)	C(8)	3.219	H(31)	C(11)	2.533
H(31)	C(13)	3.362	H(31)	C(21)	2.058
H(31)	C(22)	2.684	H(31)	C(23)	3.220
H(31)	C(24)	2.674	H(31)	C(25)	2.058
H(31)	H(7)	2.878	H(31)	H(9)	2.836
H(31)	H(32)	2.353	H(31)	H(33)	2.864
H(31)	H(34)	3.592	H(31)	H(35)	2.540
H(31)	H(38)	2.524	H(31)	H(39)	3.583
H(31)	H(40)	2.865	H(31)	H(41)	2.353
H(32)	Cl(1)	3.504	H(32)	N(1)	3.232
H(32)	N(3)	2.651	H(32)	C(9)[6)]	3.291
H(32)	C(11)	3.124	H(32)	C(20)	2.077
H(32)	C(22)	2.079	H(32)	C(23)	3.367
H(32)	C(25)	3.372	H(32)	H(8)[6)]	3.071
H(32)	H(10)[6)]	2.655	H(32)	H(12)[6)]	3.068
H(32)	H(19)	3.486	H(32)	H(29)[2)]	3.298
H(32)	H(31)	2.353	H(32)	H(33)	1.603
H(32)	H(34)	2.393	H(32)	H(35)	2.354
H(33)	N(3)	2.682	H(33)	C(8)[6)]	3.416

Table 10. Distances beyond the asymmetric unit out to 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
H(33)	C(13)	3.109	H(33)	C(18)[13)]	3.233
H(33)	C(20)	2.077	H(33)	C(22)	2.079
H(33)	C(23)	2.751	H(33)	C(24)	3.295
H(33)	C(25)	2.751	H(33)	H(8)[6)]	2.632
H(33)	H(9)[6)]	3.350	H(33)	H(19)	2.617
H(33)	H(27)[13)]	2.644	H(33)	H(28)[13)]	2.905
H(33)	H(31)	2.864	H(33)	H(32)	1.603
H(33)	H(34)	2.355	H(33)	H(34)[14)]	2.897
H(33)	H(35)	2.874	H(33)	H(36)	2.619
H(33)	H(40)	2.615	H(34)	C(18)[2)]	3.294
H(34)	C(19)[2)]	3.408	H(34)	C(20)	3.363
H(34)	C(21)	2.078	H(34)	C(21)[14)]	3.448
H(34)	C(22)[14)]	3.205	H(34)	C(23)	2.076
H(34)	C(24)	3.363	H(34)	H(9)[3)]	3.553
H(34)	H(27)[2)]	2.496	H(34)	H(29)[2)]	3.060
H(34)	H(30)[2)]	3.332	H(34)	H(31)	3.592
H(34)	H(32)	2.393	H(34)	H(33)	2.355
H(34)	H(33)[14)]	2.897	H(34)	H(34)[14)]	2.487
H(34)	H(35)	1.602	H(34)	H(36)	2.349
H(34)	H(36)[14)]	3.115	H(34)	H(37)	2.390
H(34)	H(38)[3)]	3.580	H(35)	Cl(1)	3.064
H(35)	C(19)[2)]	3.542	H(35)	C(20)	2.745
H(35)	C(21)	2.078	H(35)	C(23)	2.076
H(35)	C(24)	2.752	H(35)	C(24)[3)]	3.358
H(35)	C(25)	3.315	H(35)	H(27)[2)]	2.996
H(35)	H(29)[2)]	3.472	H(35)	H(30)[2)]	3.015
H(35)	H(31)	2.540	H(35)	H(32)	2.354
H(35)	H(33)	2.874	H(35)	H(34)	1.602
H(35)	H(36)	2.871	H(35)	H(37)	2.349
H(35)	H(37)[3)]	3.267	H(35)	H(38)	2.617
H(35)	H(38)[3)]	2.587	H(35)	H(39)[3)]	3.454
H(36)	C(18)[13)]	3.305	H(36)	C(19)[13)]	3.306
H(36)	C(20)	3.295	H(36)	C(21)	2.751
H(36)	C(22)	2.075	H(36)	C(24)	2.072
H(36)	C(25)	2.755	H(36)	H(6)[13)]	3.277
H(36)	H(12)[3)]	2.751	H(36)	H(27)[13)]	3.215
H(36)	H(28)[13)]	2.896	H(36)	H(29)[13)]	2.546

Table 10. Distances beyond the asymmetric unit out to 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
H(36)	H(33)	2.619	H(36)	H(34)	2.349
H(36)	H(34)[14)]	3.115	H(36)	H(35)	2.871
H(36)	H(37)	1.602	H(36)	H(38)	2.867
H(36)	H(39)	2.346	H(36)	H(40)	2.625
H(37)	Cl(1)[3)]	2.945	H(37)	C(8)[3)]	3.466
H(37)	C(9)[3)]	3.513	H(37)	C(21)	3.366
H(37)	C(22)	2.075	H(37)	C(24)	2.072
H(37)	C(25)	3.371	H(37)	H(9)[3)]	2.505
H(37)	H(12)[3)]	2.552	H(37)	H(34)	2.390
H(37)	H(35)	2.349	H(37)	H(35)[3)]	3.267
H(37)	H(36)	1.602	H(37)	H(38)	2.346
H(37)	H(38)[3)]	3.041	H(37)	H(39)	2.381
H(38)	C(20)	2.731	H(38)	C(21)	3.295
H(38)	C(22)	2.747	H(38)	C(22)[3)]	3.351
H(38)	C(23)	2.071	H(38)	C(23)[3)]	3.573
H(38)	C(25)	2.080	H(38)	H(9)	3.134
H(38)	H(26)[10)]	2.969	H(38)	H(27)[10)]	3.233
H(38)	H(31)	2.524	H(38)	H(34)[3)]	3.580
H(38)	H(35)	2.617	H(38)	H(35)[3)]	2.587
H(38)	H(36)	2.867	H(38)	H(37)	2.346
H(38)	H(37)[3)]	3.041	H(38)	H(38)[3)]	3.478
H(38)	H(39)	1.602	H(38)	H(40)	2.877
H(38)	H(41)	2.358	H(39)	Cl(1)[3)]	3.378
H(39)	C(6)[13)]	3.454	H(39)	C(7)[13)]	3.391
H(39)	C(17)[10)]	3.470	H(39)	C(20)	3.356
H(39)	C(22)	3.363	H(39)	C(23)	2.071
H(39)	C(25)	2.080	H(39)	H(1)[13)]	3.061
H(39)	H(3)[13)]	3.011	H(39)	H(4)[13)]	2.919
H(39)	H(6)[13)]	3.016	H(39)	H(26)[10)]	2.516
H(39)	H(30)[10)]	3.296	H(39)	H(31)	3.583
H(39)	H(35)[3)]	3.454	H(39)	H(36)	2.346
H(39)	H(37)	2.381	H(39)	H(38)	1.602
H(39)	H(40)	2.361	H(39)	H(41)	2.395
H(40)	N(3)	2.691	H(40)	C(6)[13)]	3.305
H(40)	C(13)	2.783	H(40)	C(18)[13)]	3.476
H(40)	C(20)	2.079	H(40)	C(21)	2.754
H(40)	C(22)	3.310	H(40)	C(23)	2.759

Table 10. Distances beyond the asymmetric unit out to 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
H(40)	C(24)	2.084	H(40)	H(1)[13)]	2.760
H(40)	H(3)[13)]	3.030	H(40)	H(18)	2.642
H(40)	H(19)	2.655	H(40)	H(28)[13)]	2.546
H(40)	H(31)	2.865	H(40)	H(33)	2.615
H(40)	H(36)	2.625	H(40)	H(38)	2.877
H(40)	H(39)	2.361	H(40)	H(41)	1.604
H(41)	N(3)	2.667	H(41)	C(10)[5)]	3.284
H(41)	C(13)	3.187	H(41)	C(17)[10)]	3.393
H(41)	C(20)	2.079	H(41)	C(21)	3.373
H(41)	C(23)	3.372	H(41)	C(24)	2.084
H(41)	H(1)[13)]	3.544	H(41)	H(3)[13)]	3.018
H(41)	H(7)	2.977	H(41)	H(13)[5)]	3.176
H(41)	H(14)[5)]	3.365	H(41)	H(15)[5)]	2.790
H(41)	H(18)	2.866	H(41)	H(19)	3.535
H(41)	H(25)[10)]	3.229	H(41)	H(26)[10)]	2.660
H(41)	H(31)	2.353	H(41)	H(38)	2.358
H(41)	H(39)	2.395	H(41)	H(40)	1.604

Symmetry Operators:

(1) -X+1,Y+1/2-1,-Z+1/2
(2) -X+2,Y+1/2-1,-Z+1/2
(3) -X+1,-Y,-Z
(4) -X+2,-Y,-Z+1
(5) -X+1,Y+1/2,-Z+1/2
(6) X+1,Y,Z
(7) X-1,Y,Z
(8) -X+1,-Y,-Z+1
(9) X,-Y+1/2,Z+1/2
(10) X-1,-Y+1/2,Z+1/2-1
(11) X+1,-Y+1/2,Z+1/2
(12) -X+2,Y+1/2,-Z+1/2
(13) X,-Y+1/2,Z+1/2-1
(14) -X+2,-Y,-Z

X-ray Structure Report for $Cp^*TiCl_2[1,3\text{-}(C_6H_5)_2(CH_2N)_2C{=}N]$ (**1c**)

Experimental

Data Collection

A yellow block crystal of $C_{25}H_{29}Cl_2N_3Ti$ having approximate dimensions of 0.150 x 0.120 x 0.060 mm was mounted on a glass fiber. All measurements were made on a Rigaku R-AXIS RAPID diffractometer using filtered Mo-Kα radiation.

The crystal-to-detector distance was 127.40 mm.

Cell constants and an orientation matrix for data collection corresponded to a primitive monoclinic cell with dimensions:

a = 8.6563(3) Å
b = 7.4257(2) Å β = 94.0965(9)^o
c = 36.557(1) Å
V = 2343.9(1) Å^3

For Z = 4 and F.W. = 490.33, the calculated density is 1.389 g/cm^3. The reflection conditions of:

h0l: h+l = 2n
0k0: k = 2n

uniquely determine the space group to be:

$P2_1/n$ (#14)

The data were collected at a temperature of -150 $\pm$ 1^{o}C to a maximum 2θ value of 55.0^o. A total of 148 oscillation images were collected. A sweep of data was done using ω scans from 130.0 to 190.0^o in 1.5^o step, at χ=45.0^o and ϕ = 0.0^o. The exposure rate was 50.0 [sec./^{o}]. A second sweep was performed using ω scans from 0.0 to 162.0^o in 1.5^o step, at χ=45.0^o and ϕ = 180.0^o. The exposure rate was 50.0 [sec./^{o}]. The crystal-to-detector distance was 127.40 mm. Readout was performed in the 0.100 mm pixel mode.

Data Reduction

Of the 22274 reflections that were collected, 5362 were unique (R_{int} = 0.0264); equivalent reflections were merged.

The linear absorption coefficient, μ, for Mo-Kα radiation is 6.108 cm^{-1}. An empirical absorption correction was applied which resulted in transmission factors ranging from 0.883 to 0.964. The data were corrected for Lorentz and polarization effects.

Structure Solution and Refinement

The structure was solved by direct methods[1] and expanded using Fourier techniques. The non-hydrogen atoms were refined anisotropically. Hydrogen atoms were refined using the riding model. The final cycle of full-matrix least-squares refinement[2] on F^2 was based on 5362 observed reflections and 280 variable parameters and converged (largest parameter shift was 0.00 times its esd) with unweighted and weighted agreement factors of:

$$R1 = \Sigma \, ||Fo| - |Fc|| \, / \, \Sigma \, |Fo| = 0.0390$$

$$wR2 = [\Sigma \, (w \, (Fo^2 - Fc^2)^2) / \Sigma \, w(Fo^2)^2]^{1/2} = 0.0968$$

The standard deviation of an observation of unit weight[3] was 1.20. Unit weights were used. The maximum and minimum peaks on the final difference Fourier map corresponded to 0.50 and -0.31 $e^-/Å^3$, respectively.

Neutral atom scattering factors were taken from Cromer and Waber[4]. Anomalous dispersion effects were included in Fcalc[5]; the values for Δf' and Δf'' were those of Creagh and McAuley[6]. The values for the mass attenuation coefficients are those of Creagh and Hubbell[7]. All calculations were performed using the CrystalStructure[8] crystallographic software package except for refinement, which was performed using SHELXL-97[9].

References

(1) SIR2004: M.C. Burla, R. Caliandro, M. Camalli, B. Carrozzini, G.L. Cascarano, L. De Caro, C. Giacovazzo, G. Polidori, R. Spagna (2005)

(2) Least Squares function minimized: (SHELXL97)

$\Sigma w(F_o^2-F_c^2)^2$ where w = Least Squares weights.

(3) Standard deviation of an observation of unit weight:

$[\Sigma w(F_o^2-F_c^2)^2/(N_o-N_v)]^{1/2}$

where: N_o = number of observations
N_v = number of variables

(4) Cromer, D. T. & Waber, J. T.; "International Tables for X-ray Crystallography", Vol. IV, The Kynoch Press, Birmingham, England, Table 2.2 A (1974).

(5) Ibers, J. A. & Hamilton, W. C.; Acta Crystallogr., 17, 781 (1964).

(6) Creagh, D. C. & McAuley, W.J .; "International Tables for Crystallography", Vol C, (A.J.C. Wilson, ed.), Kluwer Academic Publishers, Boston, Table 4.2.6.8, pages 219-222 (1992).

(7) Creagh, D. C. & Hubbell, J.H..; "International Tables for Crystallography", Vol C, (A.J.C. Wilson, ed.), Kluwer Academic Publishers, Boston, Table 4.2.4.3, pages 200-206 (1992).

(8) CrystalStructure 4.0: Crystal Structure Analysis Package, Rigaku Corporation (2000-2010). Tokyo 196-8666, Japan.

(9) SHELX97: Sheldrick, G.M. (2008). Acta Cryst. A64, 112-122.

EXPERIMENTAL DETAILS

A. Crystal Data

Empirical Formula	$C_{25}H_{29}Cl_2N_3Ti$
Formula Weight	490.33
Crystal Color, Habit	yellow, block
Crystal Dimensions	0.150 X 0.120 X 0.060 mm
Crystal System	monoclinic
Lattice Type	Primitive
Lattice Parameters	a = 8.6563(3) Å b = 7.4257(2) Å c = 36.557(1) Å β = 94.0965(9) ^{o} V = 2343.9(1) Å^3
Space Group	$P2_1/n$ (#14)
Z value	4
D_{calc}	1.389 g/cm^3
F_{000}	1024.00
μ(MoKα)	6.108 cm^{-1}

B. Intensity Measurements

Diffractometer	R-AXIS RAPID
Radiation Voltage, Current	MoKα (λ = 0.71075 Å) 50kV, 24mA
Temperature	-150.0^{o}C
Detector Aperture	280 x 256 mm
Data Images	148 exposures
ω oscillation Range (χ=45.0, ϕ=0.0)	130.0 - 190.0^{o}
Exposure Rate	50.0 sec./^{o}
ω oscillation Range (χ=45.0, ϕ=180.0)	0.0 - 162.0^{o}
Exposure Rate	50.0 sec./^{o}
Detector Position	127.40 mm
Pixel Size	0.100 mm
$2\theta_{max}$	55.0^{o}
No. of Reflections Measured	Total: 22274 Unique: 5362 (R_{int} = 0.0264)
Corrections	Lorentz-polarization Absorption (trans. factors: 0.883 - 0.964)

C. Structure Solution and Refinement

Structure Solution	Direct Methods
Refinement	Full-matrix least-squares on F^2
Function Minimized	Σ w $(Fo^2 - Fc^2)^2$
Least Squares Weights	$w = 1/ [\sigma^2(Fo^2) + (0.0476 \cdot P)^2 + 0.8443 \cdot P]$ where $P = (Max(Fo^2,0) + 2Fc^2)/3$
$2\theta_{max}$ cutoff	55.0^o
Anomalous Dispersion	All non-hydrogen atoms
No. Observations (All reflections)	5362
No. Variables	280
Reflection/Parameter Ratio	19.15
Residuals: R1 ($I>2.00\sigma(I)$)	0.0390
Residuals: R (All reflections)	0.0501
Residuals: wR2 (All reflections)	0.0968
Goodness of Fit Indicator	1.203
Max Shift/Error in Final Cycle	0.002
Maximum peak in Final Diff. Map	0.50 $e^-/Å^3$
Minimum peak in Final Diff. Map	-0.31 $e^-/Å^3$

Table 1. Atomic coordinates and B_{iso}/B_{eq}

atom	x	y	z	B_{eq}
Ti1	0.29448(3)	0.36498(4)	0.862486(8)	1.033(7)
Cl1	0.52951(5)	0.36063(6)	0.89723(2)	1.630(9)
Cl2	0.35841(5)	0.21308(6)	0.81085(1)	1.682(9)
N1	0.1737(2)	0.2089(2)	0.88574(4)	1.23(3)
N2	-0.0740(2)	0.0701(2)	0.88360(4)	1.26(3)
N3	0.0381(2)	0.1358(2)	0.93840(4)	1.32(3)
C1	0.2846(2)	0.6352(3)	0.82697(5)	1.38(3)
C2	0.1341(2)	0.5560(3)	0.82532(5)	1.35(3)
C3	0.0804(2)	0.5617(3)	0.86113(5)	1.25(3)
C4	0.1994(2)	0.6371(3)	0.88504(5)	1.24(3)
C5	0.3246(2)	0.6855(3)	0.86373(5)	1.31(3)
C6	0.3818(3)	0.6707(3)	0.79531(5)	2.22(4)
C7	0.0421(3)	0.4867(3)	0.79188(5)	1.98(4)
C8	-0.0802(2)	0.5151(3)	0.87049(6)	1.82(3)
C9	0.1921(3)	0.6689(3)	0.92565(5)	1.72(3)
C10	0.4665(3)	0.7881(3)	0.87705(5)	1.85(3)
C11	0.0557(2)	0.1425(3)	0.90100(4)	1.15(3)
C12	-0.1832(2)	0.0073(3)	0.90975(5)	1.43(3)
C13	-0.1250(2)	0.1036(3)	0.94482(5)	1.43(3)
C14	-0.0988(2)	0.0401(3)	0.84504(4)	1.21(3)
C15	0.0205(2)	-0.0221(3)	0.82491(5)	1.37(3)
C16	-0.0081(3)	-0.0522(3)	0.78743(5)	1.59(3)
C17	-0.1543(3)	-0.0234(3)	0.77036(5)	1.86(3)
C18	-0.2726(3)	0.0382(3)	0.79070(5)	1.91(4)
C19	-0.2454(2)	0.0716(3)	0.82810(5)	1.56(3)
C20	0.1461(2)	0.2035(3)	0.96572(4)	1.33(3)
C21	0.3046(3)	0.1770(3)	0.96327(5)	1.74(3)
C22	0.4089(3)	0.2457(3)	0.99032(5)	2.24(4)
C23	0.3575(3)	0.3385(3)	1.02022(5)	2.32(4)
C24	0.2010(3)	0.3598(3)	1.02306(5)	2.03(4)
C25	0.0937(3)	0.2924(3)	0.99617(5)	1.65(3)

$B_{eq} = 8/3\ \pi^2(U_{11}(aa^*)^2 + U_{22}(bb^*)^2 + U_{33}(cc^*)^2 + 2U_{12}(aa^*bb^*)\cos\gamma + 2U_{13}(aa^*cc^*)\cos\beta + 2U_{23}(bb^*cc^*)\cos\alpha)$

Table 2. Atomic coordinates and B_{iso} involving hydrogen atoms

atom	x	y	z	B_{iso}
H1	0.4842	0.6161	0.8003	2.67
H2	0.3931	0.8009	0.7921	2.67
H3	0.3314	0.6182	0.7729	2.67
H4	0.0065	0.3640	0.7965	2.38
H5	0.1073	0.4858	0.7711	2.38
H6	-0.0477	0.5649	0.7863	2.38
H7	-0.0775	0.4710	0.8958	2.19
H8	-0.1224	0.4212	0.8538	2.19
H9	-0.1460	0.6225	0.8680	2.19
H10	0.1197	0.5832	0.9355	2.06
H11	0.1566	0.7920	0.9298	2.06
H12	0.2953	0.6520	0.9380	2.06
H13	0.4909	0.7627	0.9031	2.22
H14	0.4478	0.9174	0.8737	2.22
H15	0.5537	0.7514	0.8631	2.22
H16	-0.1783	-0.1251	0.9128	1.71
H17	-0.2907	0.0430	0.9020	1.71
H18	-0.1812	0.2180	0.9479	1.71
H19	-0.1352	0.0267	0.9666	1.71
H20	0.1203	-0.0439	0.8366	1.64
H21	0.0734	-0.0929	0.7734	1.91
H22	-0.1732	-0.0458	0.7449	2.23
H23	-0.3728	0.0577	0.7791	2.29
H24	-0.3263	0.1156	0.8419	1.88
H25	0.3409	0.1122	0.9432	2.09
H26	0.5169	0.2292	0.9884	2.69
H27	0.4296	0.3865	1.0385	2.78
H28	0.1654	0.4212	1.0436	2.43
H29	-0.0141	0.3070	0.9986	1.98

Table 3. Anisotropic displacement parameters

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Ti1	0.0109(2)	0.0142(2)	0.0141(2)	0.0007(2)	0.0004(1)	-0.0009(1)
Cl1	0.0138(2)	0.0237(3)	0.0237(2)	0.0015(2)	-0.0037(2)	-0.0017(2)
Cl2	0.0200(3)	0.0243(3)	0.0199(2)	0.0034(2)	0.0035(2)	-0.0057(2)
N1	0.0151(7)	0.0162(7)	0.0151(7)	0.0003(6)	-0.0017(6)	0.0002(6)
N2	0.0150(7)	0.0184(8)	0.0145(7)	-0.0030(6)	0.0009(6)	0.0008(6)
N3	0.0166(8)	0.0192(8)	0.0143(7)	-0.0011(6)	-0.0000(6)	-0.0001(6)
C1	0.0193(9)	0.0155(8)	0.0176(8)	0.0017(7)	0.0018(7)	0.0019(7)
C2	0.0181(9)	0.0155(8)	0.0172(8)	0.0033(7)	-0.0024(7)	-0.0003(7)
C3	0.0140(9)	0.0123(8)	0.0210(8)	0.0022(7)	0.0003(7)	-0.0008(7)
C4	0.0161(8)	0.0136(8)	0.0175(8)	0.0017(7)	0.0004(7)	-0.0006(7)
C5	0.0164(9)	0.0142(8)	0.0190(8)	-0.0002(7)	0.0002(7)	0.0016(7)
C6	0.033(1)	0.029(1)	0.024(1)	-0.0003(9)	0.0107(9)	0.0047(8)
C7	0.028(1)	0.024(1)	0.0215(9)	0.0031(9)	-0.0095(8)	-0.0031(8)
C8	0.0145(9)	0.0177(9)	0.037(1)	0.0016(8)	0.0051(8)	-0.0027(8)
C9	0.027(1)	0.0198(9)	0.0187(9)	0.0014(8)	0.0028(7)	-0.0027(7)
C10	0.0194(9)	0.0204(9)	0.030(1)	-0.0049(8)	-0.0029(8)	0.0014(8)
C11	0.0158(8)	0.0127(8)	0.0148(8)	0.0029(7)	-0.0006(6)	0.0002(6)
C12	0.0168(9)	0.0192(9)	0.0184(8)	-0.0039(7)	0.0023(7)	0.0021(7)
C13	0.0172(9)	0.0199(9)	0.0174(8)	-0.0025(8)	0.0033(7)	0.0007(7)
C14	0.0174(9)	0.0136(8)	0.0148(8)	-0.0033(7)	-0.0009(7)	0.0008(6)
C15	0.0164(9)	0.0142(8)	0.0209(8)	0.0006(7)	-0.0017(7)	-0.0005(7)
C16	0.0213(9)	0.0191(9)	0.0205(9)	0.0006(8)	0.0034(7)	-0.0018(7)
C17	0.025(1)	0.029(1)	0.0160(8)	-0.0030(9)	-0.0016(7)	-0.0015(8)
C18	0.0171(9)	0.034(1)	0.0202(9)	-0.0012(9)	-0.0040(7)	-0.0002(8)
C19	0.0147(9)	0.025(1)	0.0201(9)	-0.0008(8)	0.0011(7)	-0.0005(7)
C20	0.0216(9)	0.0144(8)	0.0141(8)	-0.0014(8)	-0.0025(7)	0.0024(7)
C21	0.023(1)	0.025(1)	0.0172(8)	0.0004(8)	-0.0029(7)	0.0004(7)
C22	0.024(1)	0.037(2)	0.0226(9)	-0.0028(9)	-0.0056(8)	0.0024(9)
C23	0.038(2)	0.030(1)	0.0182(9)	-0.008(1)	-0.0097(8)	0.0006(8)
C24	0.042(2)	0.020(1)	0.0148(8)	-0.0013(9)	-0.0006(8)	-0.0011(7)
C25	0.027(1)	0.0189(9)	0.0165(8)	0.0011(8)	0.0013(7)	0.0022(7)

The general temperature factor expression: $\exp(-2\pi^2(a^{*2}U_{11}h^2 + b^{*2}U_{22}k^2 + c^{*2}U_{33}l^2 + 2a^*b^*U_{12}hk + 2a^*c^*U_{13}hl + 2b^*c^*U_{23}kl))$

Table 4. Bond lengths (Å)

atom	atom	distance	atom	atom	distance
Ti1	Cl1	2.3204(5)	Ti1	Cl2	2.3002(6)
Ti1	N1	1.8124(16)	Ti1	C1	2.3881(18)
Ti1	C2	2.3484(18)	Ti1	C3	2.3578(18)
Ti1	C4	2.3533(18)	Ti1	C5	2.3946(18)
N1	C11	1.296(3)	N2	C11	1.360(3)
N2	C12	1.468(3)	N2	C14	1.428(2)
N3	C11	1.387(2)	N3	C13	1.467(3)
N3	C20	1.411(3)	C1	C2	1.426(3)
C1	C5	1.414(3)	C1	C6	1.502(3)
C2	C3	1.421(3)	C2	C7	1.502(3)
C3	C4	1.418(3)	C3	C8	1.496(3)
C4	C5	1.426(3)	C4	C9	1.509(3)
C5	C10	1.497(3)	C12	C13	1.522(3)
C14	C15	1.389(3)	C14	C19	1.392(3)
C15	C16	1.393(3)	C16	C17	1.387(3)
C17	C18	1.385(3)	C18	C19	1.393(3)
C20	C21	1.396(3)	C20	C25	1.397(3)
C21	C22	1.388(3)	C22	C23	1.392(3)
C23	C24	1.374(4)	C24	C25	1.396(3)

Table 5. Bond lengths involving hydrogens (Å)

atom	atom	distance	atom	atom	distance
C6	H1	0.980	C6	H2	0.980
C6	H3	0.980	C7	H4	0.980
C7	H5	0.980	C7	H6	0.980
C8	H7	0.980	C8	H8	0.980
C8	H9	0.980	C9	H10	0.980
C9	H11	0.980	C9	H12	0.980
C10	H13	0.980	C10	H14	0.980
C10	H15	0.980	C12	H16	0.990
C12	H17	0.990	C13	H18	0.990
C13	H19	0.990	C15	H20	0.950
C16	H21	0.950	C17	H22	0.950
C18	H23	0.950	C19	H24	0.950
C21	H25	0.950	C22	H26	0.950
C23	H27	0.950	C24	H28	0.950
C25	H29	0.950			

Table 6. Bond angles (°)

atom	atom	atom	angle	atom	atom	atom	angle
Cl1	Ti1	Cl2	100.921(19)	Cl1	Ti1	N1	104.29(5)
Cl1	Ti1	C1	107.78(5)	Cl1	Ti1	C2	141.63(5)
Cl1	Ti1	C3	132.64(5)	Cl1	Ti1	C4	97.77(5)
Cl1	Ti1	C5	85.03(5)	Cl2	Ti1	N1	104.60(5)
Cl2	Ti1	C1	88.12(5)	Cl2	Ti1	C2	89.33(5)
Cl2	Ti1	C3	121.43(5)	Cl2	Ti1	C4	145.02(5)
Cl2	Ti1	C5	118.08(5)	N1	Ti1	C1	142.44(7)
N1	Ti1	C2	108.70(7)	N1	Ti1	C3	85.82(7)
N1	Ti1	C4	99.01(7)	N1	Ti1	C5	133.82(7)
C1	Ti1	C2	35.04(7)	C1	Ti1	C3	58.02(7)
C1	Ti1	C4	57.94(7)	C1	Ti1	C5	34.39(6)
C2	Ti1	C3	35.15(7)	C2	Ti1	C4	58.46(7)
C2	Ti1	C5	57.98(6)	C3	Ti1	C4	35.03(6)
C3	Ti1	C5	57.93(6)	C4	Ti1	C5	34.94(7)
Ti1	N1	C11	160.73(14)	C11	N2	C12	111.66(14)
C11	N2	C14	125.74(15)	C12	N2	C14	122.33(14)
C11	N3	C13	109.75(14)	C11	N3	C20	124.84(15)
C13	N3	C20	122.76(15)	Ti1	C1	C2	70.96(10)
Ti1	C1	C5	73.06(10)	Ti1	C1	C6	124.48(13)
C2	C1	C5	108.08(16)	C2	C1	C6	126.86(17)
C5	C1	C6	124.96(17)	Ti1	C2	C1	74.00(10)
Ti1	C2	C3	72.79(10)	Ti1	C2	C7	121.42(13)
C1	C2	C3	107.87(16)	C1	C2	C7	127.27(17)
C3	C2	C7	124.79(17)	Ti1	C3	C2	72.06(10)
Ti1	C3	C4	72.31(10)	Ti1	C3	C8	126.43(13)
C2	C3	C4	107.97(16)	C2	C3	C8	125.08(17)
C4	C3	C8	126.62(17)	Ti1	C4	C3	72.66(10)
Ti1	C4	C5	74.11(10)	Ti1	C4	C9	121.27(12)
C3	C4	C5	108.07(16)	C3	C4	C9	126.08(17)
C5	C4	C9	125.78(16)	Ti1	C5	C1	72.55(10)
Ti1	C5	C4	70.95(10)	Ti1	C5	C10	126.72(12)
C1	C5	C4	107.95(15)	C1	C5	C10	125.70(17)
C4	C5	C10	126.09(17)	N1	C11	N2	126.76(15)
N1	C11	N3	125.66(15)	N2	C11	N3	107.57(15)
N2	C12	C13	102.10(15)	N3	C13	C12	101.89(15)
N2	C14	C15	120.64(15)	N2	C14	C19	118.75(16)
C15	C14	C19	120.59(15)	C14	C15	C16	119.22(16)

Table 6. Bond angles (°) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
C15	C16	C17	120.66(18)	C16	C17	C18	119.66(17)
C17	C18	C19	120.44(17)	C14	C19	C18	119.41(17)
N3	C20	C21	120.60(15)	N3	C20	C25	119.75(17)
C21	C20	C25	119.61(16)	C20	C21	C22	119.68(18)
C21	C22	C23	120.9(2)	C22	C23	C24	119.24(18)
C23	C24	C25	121.02(18)	C20	C25	C24	119.53(19)

Table 7. Bond angles involving hydrogens (°)

atom	atom	atom	angle	atom	atom	atom	angle
C1	C6	H1	109.5	C1	C6	H2	109.5
C1	C6	H3	109.5	H1	C6	H2	109.5
H1	C6	H3	109.5	H2	C6	H3	109.5
C2	C7	H4	109.5	C2	C7	H5	109.5
C2	C7	H6	109.5	H4	C7	H5	109.5
H4	C7	H6	109.5	H5	C7	H6	109.5
C3	C8	H7	109.5	C3	C8	H8	109.5
C3	C8	H9	109.5	H7	C8	H8	109.5
H7	C8	H9	109.5	H8	C8	H9	109.5
C4	C9	H10	109.5	C4	C9	H11	109.5
C4	C9	H12	109.5	H10	C9	H11	109.5
H10	C9	H12	109.5	H11	C9	H12	109.5
C5	C10	H13	109.5	C5	C10	H14	109.5
C5	C10	H15	109.5	H13	C10	H14	109.5
H13	C10	H15	109.5	H14	C10	H15	109.5
N2	C12	H16	111.4	N2	C12	H17	111.4
C13	C12	H16	111.3	C13	C12	H17	111.3
H16	C12	H17	109.2	N3	C13	H18	111.4
N3	C13	H19	111.4	C12	C13	H18	111.4
C12	C13	H19	111.4	H18	C13	H19	109.3
C14	C15	H20	120.4	C16	C15	H20	120.4
C15	C16	H21	119.7	C17	C16	H21	119.7
C16	C17	H22	120.2	C18	C17	H22	120.2
C17	C18	H23	119.8	C19	C18	H23	119.8
C14	C19	H24	120.3	C18	C19	H24	120.3
C20	C21	H25	120.2	C22	C21	H25	120.2
C21	C22	H26	119.6	C23	C22	H26	119.6
C22	C23	H27	120.4	C24	C23	H27	120.4
C23	C24	H28	119.5	C25	C24	H28	119.5
C20	C25	H29	120.2	C24	C25	H29	120.2

Table 8. Torsion Angles(°)
(Those having bond angles > 160 or < 20 degrees are excluded.)

atom1	atom2	atom3	atom4	angle	atom1	atom2	atom3	atom4	angle
Cl1	Ti1	C1	C2	-167.62(6)	Cl1	Ti1	C1	C5	-50.98(8)
Cl1	Ti1	C1	C6	70.18(12)	Cl1	Ti1	C2	C1	19.20(13)
Cl1	Ti1	C2	C3	-95.83(9)	Cl1	Ti1	C2	C7	143.46(8)
Cl1	Ti1	C3	C2	122.92(6)	Cl1	Ti1	C3	C4	6.59(11)
Cl1	Ti1	C3	C8	-116.29(11)	Cl1	Ti1	C4	C3	-175.11(6)
Cl1	Ti1	C4	C5	69.63(7)	Cl1	Ti1	C4	C9	-52.95(11)
Cl1	Ti1	C5	C1	132.04(7)	Cl1	Ti1	C5	C4	-111.20(7)
Cl1	Ti1	C5	C10	10.12(12)	Cl2	Ti1	C1	C2	91.51(7)
Cl2	Ti1	C1	C5	-151.85(7)	Cl2	Ti1	C1	C6	-30.68(11)
Cl2	Ti1	C2	C1	-87.69(7)	Cl2	Ti1	C2	C3	157.29(7)
Cl2	Ti1	C2	C7	36.58(12)	Cl2	Ti1	C3	C2	-26.90(9)
Cl2	Ti1	C3	C4	-143.23(5)	Cl2	Ti1	C3	C8	93.89(13)
Cl2	Ti1	C4	C3	62.98(11)	Cl2	Ti1	C4	C5	-52.28(11)
Cl2	Ti1	C4	C9	-174.86(5)	Cl2	Ti1	C5	C1	32.31(9)
Cl2	Ti1	C5	C4	149.07(5)	Cl2	Ti1	C5	C10	-89.61(13)
N1	Ti1	C1	C2	-20.26(14)	N1	Ti1	C1	C5	96.38(12)
N1	Ti1	C1	C6	-142.46(11)	N1	Ti1	C2	C1	167.12(7)
N1	Ti1	C2	C3	52.09(9)	N1	Ti1	C2	C7	-68.61(13)
N1	Ti1	C3	C2	-131.47(8)	N1	Ti1	C3	C4	112.20(8)
N1	Ti1	C3	C8	-10.68(13)	N1	Ti1	C4	C3	-69.22(8)
N1	Ti1	C4	C5	175.52(8)	N1	Ti1	C4	C9	52.94(12)
N1	Ti1	C5	C1	-122.89(9)	N1	Ti1	C5	C4	-6.14(12)
N1	Ti1	C5	C10	115.18(13)	C1	Ti1	C2	C1	0.00(8)
C1	Ti1	C2	C3	-115.03(13)	C1	Ti1	C2	C7	124.27(18)
C2	Ti1	C1	C2	0.00(8)	C2	Ti1	C1	C5	116.64(14)
C2	Ti1	C1	C6	-122.19(17)	C1	Ti1	C3	C2	37.83(7)
C1	Ti1	C3	C4	-78.50(8)	C1	Ti1	C3	C8	158.62(15)
C3	Ti1	C1	C2	-37.95(7)	C3	Ti1	C1	C5	78.69(9)
C3	Ti1	C1	C6	-160.15(15)	C1	Ti1	C4	C3	78.74(8)
C1	Ti1	C4	C5	-36.52(7)	C1	Ti1	C4	C9	-159.10(14)
C4	Ti1	C1	C2	-79.53(9)	C4	Ti1	C1	C5	37.11(7)
C4	Ti1	C1	C6	158.28(15)	C1	Ti1	C5	C1	0.00(8)
C1	Ti1	C5	C4	116.76(13)	C1	Ti1	C5	C10	-121.92(19)
C5	Ti1	C1	C2	-116.64(14)	C5	Ti1	C1	C5	0.00(8)
C5	Ti1	C1	C6	121.16(17)	C2	Ti1	C3	C2	0.00(8)
C2	Ti1	C3	C4	-116.33(13)	C2	Ti1	C3	C8	120.79(17)
C3	Ti1	C2	C1	115.03(13)	C3	Ti1	C2	C3	0.00(8)

Table 8. Torsion angles (°) (continued)

atom1	atom2	atom3	atom4	angle	atom1	atom2	atom3	atom4	angle
C3	Ti1	C2	C7	-120.71(17)	C2	Ti1	C4	C3	37.26(7)
C2	Ti1	C4	C5	-78.01(9)	C2	Ti1	C4	C9	159.42(14)
C4	Ti1	C2	C1	77.90(8)	C4	Ti1	C2	C3	-37.12(7)
C4	Ti1	C2	C7	-157.83(15)	C2	Ti1	C5	C1	-37.25(7)
C2	Ti1	C5	C4	79.51(8)	C2	Ti1	C5	C10	-159.17(16)
C5	Ti1	C2	C1	36.55(7)	C5	Ti1	C2	C3	-78.48(8)
C5	Ti1	C2	C7	160.81(15)	C3	Ti1	C4	C3	0.00(8)
C3	Ti1	C4	C5	-115.26(13)	C3	Ti1	C4	C9	122.16(17)
C4	Ti1	C3	C2	116.33(13)	C4	Ti1	C3	C4	0.00(8)
C4	Ti1	C3	C8	-122.88(18)	C3	Ti1	C5	C1	-78.99(8)
C3	Ti1	C5	C4	37.77(7)	C3	Ti1	C5	C10	159.09(16)
C5	Ti1	C3	C2	78.65(8)	C5	Ti1	C3	C4	-37.68(7)
C5	Ti1	C3	C8	-160.56(16)	C4	Ti1	C5	C1	-116.76(13)
C4	Ti1	C5	C4	0.00(8)	C4	Ti1	C5	C10	121.32(18)
C5	Ti1	C4	C3	115.26(13)	C5	Ti1	C4	C5	0.00(8)
C5	Ti1	C4	C9	-122.58(16)	C11	N2	C12	C13	16.97(17)
C12	N2	C11	N1	179.68(15)	C12	N2	C11	N3	-1.41(18)
C11	N2	C14	C15	39.6(3)	C11	N2	C14	C19	-141.39(16)
C14	N2	C11	N1	5.5(3)	C14	N2	C11	N3	-175.57(14)
C12	N2	C14	C15	-133.95(16)	C12	N2	C14	C19	45.0(3)
C14	N2	C12	C13	-168.65(14)	C11	N3	C13	C12	25.66(17)
C13	N3	C11	N1	162.94(15)	C13	N3	C11	N2	-15.98(18)
C11	N3	C20	C21	-41.8(3)	C11	N3	C20	C25	140.44(16)
C20	N3	C11	N1	1.0(3)	C20	N3	C11	N2	-177.89(14)
C13	N3	C20	C21	158.53(14)	C13	N3	C20	C25	-19.2(3)
C20	N3	C13	C12	-171.98(14)	Ti1	C1	C2	Ti1	0.0
Ti1	C1	C2	C3	65.42(10)	Ti1	C1	C2	C7	-117.60(16)
Ti1	C1	C5	Ti1	0.0	Ti1	C1	C5	C4	-62.52(10)
Ti1	C1	C5	C10	123.09(15)	C2	C1	C5	Ti1	62.73(12)
C2	C1	C5	C4	0.21(19)	C2	C1	C5	C10	-174.18(14)
C5	C1	C2	Ti1	-64.09(13)	C5	C1	C2	C3	1.34(19)
C5	C1	C2	C7	178.31(14)	C6	C1	C2	Ti1	119.33(19)
C6	C1	C2	C3	-175.25(16)	C6	C1	C2	C7	1.7(3)
C6	C1	C5	Ti1	-120.61(18)	C6	C1	C5	C4	176.88(16)
C6	C1	C5	C10	2.5(3)	Ti1	C2	C3	Ti1	0.0
Ti1	C2	C3	C4	63.85(10)	Ti1	C2	C3	C8	-122.37(15)
C1	C2	C3	Ti1	-66.23(12)	C1	C2	C3	C4	-2.38(18)

Table 8. Torsion angles (°) (continued)

atom1	atom2	atom3	atom4	angle	atom1	atom2	atom3	atom4	angle
C1	C2	C3	C8	171.40(14)	C7	C2	C3	Ti1	116.70(18)
C7	C2	C3	C4	-179.45(15)	C7	C2	C3	C8	-5.7(3)
Ti1	C3	C4	Ti1	0.0	Ti1	C3	C4	C5	66.20(10)
Ti1	C3	C4	C9	-116.45(15)	C2	C3	C4	Ti1	-63.69(12)
C2	C3	C4	C5	2.51(18)	C2	C3	C4	C9	179.86(14)
C8	C3	C4	Ti1	122.65(18)	C8	C3	C4	C5	-171.15(15)
C8	C3	C4	C9	6.2(3)	Ti1	C4	C5	Ti1	0.0
Ti1	C4	C5	C1	63.56(10)	Ti1	C4	C5	C10	-122.07(15)
C3	C4	C5	Ti1	-65.24(12)	C3	C4	C5	C1	-1.69(18)
C3	C4	C5	C10	172.68(14)	C9	C4	C5	Ti1	117.40(18)
C9	C4	C5	C1	-179.04(15)	C9	C4	C5	C10	-4.7(3)
N2	C12	C13	N3	-24.43(16)	N2	C14	C15	C16	179.18(14)
N2	C14	C19	C18	-178.22(14)	C15	C14	C19	C18	0.8(3)
C19	C14	C15	C16	0.2(3)	C14	C15	C16	C17	-1.0(3)
C15	C16	C17	C18	0.9(3)	C16	C17	C18	C19	0.1(3)
C17	C18	C19	C14	-1.0(3)	N3	C20	C21	C22	179.58(14)
N3	C20	C25	C24	-179.75(14)	C21	C20	C25	C24	2.5(3)
C25	C20	C21	C22	-2.7(3)	C20	C21	C22	C23	1.0(3)
C21	C22	C23	C24	0.9(3)	C22	C23	C24	C25	-1.1(3)
C23	C24	C25	C20	-0.6(3)					

Table 9. Intramolecular contacts less than 3.60 Å

atom	atom	distance	atom	atom	distance
Cl1	C10	3.296(2)	Cl1	C21	3.486(2)
Cl2	C6	3.454(3)	Cl2	C7	3.440(2)
Cl2	C15	3.4767(19)	N1	C8	3.184(3)
N1	C12	3.598(3)	N1	C13	3.572(3)
N1	C14	2.975(3)	N1	C15	3.038(3)
N1	C20	2.951(2)	N1	C21	2.986(3)
N2	C8	3.339(3)	N2	C20	3.578(2)
C3	C11	3.451(3)	C6	C7	3.237(3)
C6	C10	3.149(3)	C7	C8	3.140(3)
C8	C9	3.201(3)	C8	C11	3.177(3)
C9	C10	3.191(3)	C11	C15	3.034(3)
C11	C21	3.031(3)	C12	C19	3.033(3)
C13	C25	2.927(3)	C14	C17	2.778(3)
C15	C18	2.783(3)	C16	C19	2.777(3)
C20	C23	2.793(3)	C21	C24	2.775(3)
C22	C25	2.774(3)			

Table 10. Intramolecular contacts less than 3.60 Å involving hydrogens

atom	atom	distance	atom	atom	distance
Ti1	H1	3.446	Ti1	H4	3.343
Ti1	H10	3.552	Ti1	H12	3.488
Ti1	H20	3.491	Ti1	H25	3.496
Cl1	H12	3.383	Cl1	H13	3.014
Cl1	H15	3.172	Cl1	H25	3.047
Cl1	H26	3.482	Cl2	H1	3.218
Cl2	H3	3.314	Cl2	H4	3.253
Cl2	H5	3.239	Cl2	H20	3.008
Cl2	H21	3.555	N1	H7	2.961
N1	H8	3.161	N1	H10	3.373
N1	H20	2.617	N1	H25	2.567
N2	H7	3.011	N2	H8	2.845
N2	H18	2.813	N2	H19	3.135
N2	H20	2.629	N2	H24	2.595
N3	H7	3.066	N3	H10	3.399
N3	H16	2.809	N3	H17	3.132
N3	H25	2.620	N3	H29	2.607
C1	H4	3.272	C1	H5	2.705
C1	H6	3.185	C1	H13	3.336
C1	H14	2.993	C1	H15	2.734
C2	H1	3.258	C2	H2	3.194
C2	H3	2.696	C2	H7	3.327
C2	H8	2.711	C2	H9	3.016
C3	H4	2.816	C3	H5	3.365
C3	H6	2.878	C3	H10	2.721
C3	H11	3.070	C3	H12	3.326
C4	H7	2.749	C4	H8	3.344
C4	H9	3.011	C4	H13	2.727
C4	H14	3.043	C4	H15	3.336
C5	H1	2.830	C5	H2	2.859
C5	H3	3.361	C5	H10	3.358
C5	H11	3.012	C5	H12	2.757
C6	H5	2.831	C6	H14	3.414
C6	H15	2.861	C7	H3	2.821
C7	H8	2.801	C7	H9	3.473
C8	H4	3.071	C8	H6	3.133
C8	H10	2.884	C8	H11	3.535

Table 10. Intramolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
C9	H7	2.904	C9	H9	3.499
C9	H13	2.856	C9	H14	3.538
C10	H1	3.096	C10	H2	3.128
C10	H11	3.413	C10	H12	2.942
C11	H7	2.699	C11	H8	3.043
C11	H10	3.537	C11	H16	2.892
C11	H17	3.091	C11	H18	2.822
C11	H19	3.129	C11	H20	2.822
C11	H25	2.825	C12	H24	2.809
C13	H7	3.306	C13	H29	2.606
C14	H4	3.162	C14	H8	2.857
C14	H16	2.890	C14	H17	2.754
C14	H21	3.257	C14	H23	3.262
C15	H4	3.049	C15	H22	3.272
C15	H24	3.273	C16	H4	3.110
C16	H23	3.254	C17	H4	3.307
C17	H20	3.273	C17	H24	3.269
C18	H4	3.415	C18	H21	3.253
C19	H4	3.341	C19	H8	2.935
C19	H16	3.435	C19	H17	2.765
C19	H20	3.274	C19	H22	3.269
C20	H10	3.031	C20	H18	2.863
C20	H19	2.768	C20	H26	3.263
C20	H28	3.269	C21	H10	3.529
C21	H27	3.275	C21	H29	3.274
C22	H28	3.245	C23	H25	3.274
C23	H29	3.266	C24	H26	3.243
C25	H10	3.114	C25	H18	2.912
C25	H19	2.946	C25	H25	3.273
C25	H27	3.270	H1	H5	3.497
H1	H14	3.524	H1	H15	2.537
H2	H5	3.452	H2	H14	3.110
H2	H15	2.879	H3	H4	3.545
H3	H5	2.172	H3	H6	3.375
H4	H8	2.479	H4	H9	3.571
H4	H20	3.476	H4	H21	3.553
H6	H8	2.807	H6	H9	3.194

Table 10. Intramolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
H7	H10	2.316	H7	H11	3.313
H7	H18	2.865	H8	H24	2.889
H9	H10	3.264	H9	H11	3.563
H10	H29	3.353	H11	H13	3.126
H11	H14	3.488	H12	H13	2.340
H12	H14	3.406	H16	H18	2.855
H16	H19	2.277	H16	H24	3.327
H17	H18	2.277	H17	H19	2.639
H17	H24	2.260	H18	H29	2.360
H19	H29	2.572	H20	H21	2.344
H21	H22	2.335	H22	H23	2.335
H23	H24	2.344	H25	H26	2.334
H26	H27	2.341	H27	H28	2.323
H28	H29	2.342			

Table 11. Intermolecular contacts less than 3.60 Å

atom	atom	distance	atom	atom	distance
Cl2	C18[1]	3.574(2)	Cl2	C19[1]	3.5988(19)
C1	C15[2]	3.418(3)	C2	C15[2]	3.283(3)
C2	C16[2]	3.414(3)	C3	C15[2]	3.387(3)
C7	C16[2]	3.454(3)	C10	C12[3]	3.572(3)
C12	C10[4]	3.572(3)	C15	C1[5]	3.418(3)
C15	C2[5]	3.283(3)	C15	C3[5]	3.387(3)
C16	C2[5]	3.414(3)	C16	C7[5]	3.454(3)
C18	Cl2[6]	3.574(2)	C19	Cl2[6]	3.5988(19)
C25	C25[7]	3.504(3)			

Symmetry Operators:

(1) X+1,Y,Z
(2) X,Y+1,Z
(3) X+1,Y+1,Z
(4) X-1,Y-1,Z
(5) X,Y-1,Z
(6) X-1,Y,Z
(7) -X,-Y+1,-Z+2

Table 12. Intermolecular contacts less than 3.60 Å involving hydrogens

atom	atom	distance	atom	atom	distance
Ti1	H14[1]	3.591	Cl1	H7[2]	3.503
Cl1	H8[2]	3.533	Cl1	H14[1]	3.462
Cl1	H17[2]	2.824	Cl1	H18[2]	3.188
Cl1	H24[2]	3.052	Cl1	H27[3]	3.010
Cl2	H2[1]	3.156	Cl2	H3[4]	3.444
Cl2	H5[4]	3.468	Cl2	H14[1]	3.231
Cl2	H21[5]	3.489	Cl2	H23[2]	2.912
Cl2	H24[2]	2.970	N1	H11[1]	3.497
N1	H14[1]	3.265	N2	H9[1]	3.422
N2	H11[1]	3.258	N3	H11[1]	2.778
C1	H20[6]	2.810	C1	H21[6]	3.277
C2	H20[6]	3.003	C2	H21[6]	3.245
C3	H20[6]	3.090	C4	H20[6]	3.008
C5	H20[6]	2.811	C6	H5[5]	3.377
C6	H20[6]	3.518	C6	H21[6]	3.247
C6	H21[5]	3.230	C6	H22[5]	3.411
C7	H2[4]	3.447	C7	H21[6]	3.210
C7	H22[7]	3.383	C7	H23[7]	2.934
C8	H16[6]	3.230	C8	H28[8]	3.309
C9	H16[6]	3.554	C9	H25[6]	3.576
C9	H27[3]	3.464	C9	H28[8]	3.433
C9	H29[8]	3.270	C10	H16[9]	3.316
C10	H17[9]	2.925	C10	H20[6]	3.477
C10	H24[9]	3.333	C10	H27[3]	3.411
C11	H11[1]	2.918	C12	H9[1]	3.266
C12	H11[1]	3.382	C12	H13[10]	3.350
C12	H14[10]	3.433	C12	H15[10]	3.340
C13	H11[1]	3.434	C13	H28[8]	3.574
C14	H9[1]	3.246	C15	H6[1]	3.410
C15	H9[1]	3.442	C16	H1[4]	3.462
C16	H3[4]	3.048	C16	H6[1]	2.863
C17	H1[4]	3.234	C17	H3[4]	3.472
C17	H6[1]	3.234	C17	H6[11]	3.257
C18	H2[10]	3.391	C18	H5[11]	3.565
C18	H6[11]	3.123	C18	H22[7]	3.371
C19	H14[10]	3.431	C19	H15[10]	3.260
C20	H11[1]	3.330	C20	H19[12]	3.013

Table 12. Intermolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
C21	H11[1]	3.330	C21	H19[12]	3.397
C22	H19[12]	3.566	C22	H27[3]	3.276
C23	H12[3]	3.273	C23	H13[3]	3.101
C23	H16[12]	3.385	C23	H19[12]	3.379
C23	H26[3]	3.412	C23	H27[3]	3.568
C24	H7[8]	3.460	C24	H10[8]	3.284
C24	H16[12]	2.940	C24	H18[8]	3.318
C24	H19[12]	2.955	C24	H29[8]	3.031
C25	H10[8]	3.341	C25	H16[12]	3.580
C25	H19[12]	2.743	C25	H28[8]	3.347
C25	H29[8]	3.063	H1	C16[5]	3.462
H1	C17[5]	3.234	H1	H21[5]	3.119
H1	H22[5]	2.690	H2	Cl2[6]	3.156
H2	C7[5]	3.447	H2	C18[9]	3.391
H2	H4[5]	3.443	H2	H5[5]	2.685
H2	H20[6]	3.178	H2	H21[6]	2.912
H2	H23[9]	2.847	H3	Cl2[5]	3.444
H3	C16[5]	3.048	H3	C17[5]	3.472
H3	H4[5]	3.500	H3	H5[5]	3.231
H3	H21[6]	3.098	H3	H21[5]	2.491
H3	H22[5]	3.307	H4	H2[4]	3.443
H4	H3[4]	3.500	H4	H22[7]	3.230
H4	H23[7]	3.253	H5	Cl2[5]	3.468
H5	C6[4]	3.377	H5	C18[7]	3.565
H5	H2[4]	2.685	H5	H3[4]	3.231
H5	H21[6]	3.144	H5	H21[5]	3.357
H5	H23[7]	2.689	H6	C15[6]	3.410
H6	C16[6]	2.863	H6	C17[6]	3.234
H6	C17[7]	3.257	H6	C18[7]	3.123
H6	H21[6]	2.801	H6	H22[6]	3.405
H6	H22[7]	2.723	H6	H23[7]	2.439
H7	Cl1[13]	3.503	H7	C24[8]	3.460
H7	H16[6]	3.196	H7	H28[8]	2.522
H8	Cl1[13]	3.533	H9	N2[6]	3.422
H9	C12[6]	3.266	H9	C14[6]	3.246
H9	C15[6]	3.442	H9	H15[13]	2.764
H9	H16[6]	2.517	H9	H28[8]	3.262

Table 12. Intermolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
H10	C24[8]	3.284	H10	C25[8]	3.341
H10	H16[6]	3.425	H10	H28[8]	2.635
H10	H29[8]	2.761	H11	N1[6]	3.497
H11	N2[6]	3.258	H11	N3[6]	2.778
H11	C11[6]	2.918	H11	C12[6]	3.382
H11	C13[6]	3.434	H11	C20[6]	3.330
H11	C21[6]	3.330	H11	H16[6]	2.986
H11	H19[6]	3.423	H11	H25[6]	2.885
H11	H28[8]	3.407	H11	H29[8]	3.064
H12	C23[3]	3.273	H12	H25[6]	3.443
H12	H26[3]	3.168	H12	H27[3]	2.490
H12	H29[8]	3.493	H13	C12[9]	3.350
H13	C23[3]	3.101	H13	H16[9]	2.979
H13	H17[9]	2.814	H13	H25[6]	3.292
H13	H27[3]	2.460	H14	Ti1[6]	3.591
H14	Cl1[6]	3.462	H14	Cl2[6]	3.231
H14	N1[6]	3.265	H14	C12[9]	3.433
H14	C19[9]	3.431	H14	H16[9]	3.458
H14	H17[9]	2.594	H14	H20[6]	3.067
H14	H24[9]	2.768	H14	H25[6]	3.122
H15	C12[9]	3.340	H15	C19[9]	3.260
H15	H9[2]	2.764	H15	H16[9]	2.987
H15	H17[9]	2.873	H15	H24[9]	3.018
H16	C8[1]	3.230	H16	C9[1]	3.554
H16	C10[10]	3.316	H16	C23[12]	3.385
H16	C24[12]	2.940	H16	C25[12]	3.580
H16	H7[1]	3.196	H16	H9[1]	2.517
H16	H10[1]	3.425	H16	H11[1]	2.986
H16	H13[10]	2.979	H16	H14[10]	3.458
H16	H15[10]	2.987	H16	H27[12]	3.497
H16	H28[12]	2.713	H17	Cl1[13]	2.824
H17	C10[10]	2.925	H17	H13[10]	2.814
H17	H14[10]	2.594	H17	H15[10]	2.873
H18	Cl1[13]	3.188	H18	C24[8]	3.318
H18	H26[13]	3.095	H18	H28[8]	2.699
H19	C20[12]	3.013	H19	C21[12]	3.397
H19	C22[12]	3.566	H19	C23[12]	3.379

Table 12. Intermolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
H19	C24[12]	2.955	H19	C25[12]	2.743
H19	H11[1]	3.423	H19	H19[12]	3.281
H19	H26[13]	3.508	H19	H28[12]	3.356
H19	H29[12]	3.032	H20	C1[1]	2.810
H20	C2[1]	3.003	H20	C3[1]	3.090
H20	C4[1]	3.008	H20	C5[1]	2.811
H20	C6[1]	3.518	H20	C10[1]	3.477
H20	H2[1]	3.178	H20	H14[1]	3.067
H21	Cl2[4]	3.489	H21	C1[1]	3.277
H21	C2[1]	3.245	H21	C6[1]	3.247
H21	C6[4]	3.230	H21	C7[1]	3.210
H21	H1[4]	3.119	H21	H2[1]	2.912
H21	H3[1]	3.098	H21	H3[4]	2.491
H21	H5[1]	3.144	H21	H5[4]	3.357
H21	H6[1]	2.801	H21	H23[11]	3.599
H22	C6[4]	3.411	H22	C7[11]	3.383
H22	C18[11]	3.371	H22	H1[4]	2.690
H22	H3[4]	3.307	H22	H4[11]	3.230
H22	H6[1]	3.405	H22	H6[11]	2.723
H22	H23[11]	3.105	H23	Cl2[13]	2.912
H23	C7[11]	2.934	H23	H2[10]	2.847
H23	H4[11]	3.253	H23	H5[11]	2.689
H23	H6[11]	2.439	H23	H21[7]	3.599
H23	H22[7]	3.105	H24	Cl1[13]	3.052
H24	Cl2[13]	2.970	H24	C10[10]	3.333
H24	H14[10]	2.768	H24	H15[10]	3.018
H25	C9[1]	3.576	H25	H11[1]	2.885
H25	H12[1]	3.443	H25	H13[1]	3.292
H25	H14[1]	3.122	H26	C23[3]	3.412
H26	H12[3]	3.168	H26	H18[2]	3.095
H26	H19[2]	3.508	H26	H26[14]	3.525
H26	H27[3]	3.064	H27	Cl1[3]	3.010
H27	C9[3]	3.464	H27	C10[3]	3.411
H27	C22[3]	3.276	H27	C23[3]	3.568
H27	H12[3]	2.490	H27	H13[3]	2.460
H27	H16[12]	3.497	H27	H26[3]	3.064
H27	H27[3]	3.567	H28	C8[8]	3.309

Table 12. Intermolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
H28	$C9^{8}$	3.433	H28	$C13^{8}$	3.574
H28	$C25^{8}$	3.347	H28	$H7^{8}$	2.522
H28	$H9^{8}$	3.262	H28	$H10^{8}$	2.635
H28	$H11^{8}$	3.407	H28	$H16^{12}$	2.713
H28	$H18^{8}$	2.699	H28	$H19^{12}$	3.356
H28	$H29^{8}$	2.807	H29	$C9^{8}$	3.270
H29	$C24^{8}$	3.031	H29	$C25^{8}$	3.063
H29	$H10^{8}$	2.761	H29	$H11^{8}$	3.064
H29	$H12^{8}$	3.493	H29	$H19^{12}$	3.032
H29	$H28^{8}$	2.807	H29	$H29^{8}$	2.879

Symmetry Operators:

(1) X,Y-1,Z
(2) X+1,Y,Z
(3) -X+1,-Y+1,-Z+2
(4) -X+1/2,Y+1/2-1,-Z+1/2+1
(5) -X+1/2,Y+1/2,-Z+1/2+1
(6) X,Y+1,Z
(7) -X+1/2-1,Y+1/2,-Z+1/2+1
(8) -X,-Y+1,-Z+2
(9) X+1,Y+1,Z
(10) X-1,Y-1,Z
(11) -X+1/2-1,Y+1/2-1,-Z+1/2+1
(12) -X,-Y,-Z+2
(13) X-1,Y,Z
(14) -X+1,-Y,-Z+2

X-ray Structure Report for $Cp^*TiCl_2[1,3\text{-}(2,6\text{-}Me_2C_6H_3)_2(CH_2N)_2C{=}N]$ (**1d**)

Experimental

Data Collection

A yellow block crystal of $C_{117}H_{148}Cl_{10}N_{12}Ti_4$ having approximate dimensions of 0.620 x 0.200 x 0.180 mm was mounted on a glass fiber. All measurements were made on a Rigaku R-AXIS RAPID diffractometer using graphite monochromated Mo-Kα radiation.

The crystal-to-detector distance was 127.40 mm.

Cell constants and an orientation matrix for data collection corresponded to a primitive orthorhombic cell with dimensions:

a = 21.8842(5) Å
b = 28.7235(7) Å
c = 9.4156(2) Å
V = 5918.6(3) Å^3

For Z = 2 and F.W. = 2268.67, the calculated density is 1.273 g/cm^3. The reflection conditions of:

h00: h = 2n
0k0: k = 2n

uniquely determine the space group to be:

$P2_12_12$ (#18)

The data were collected at a temperature of -60 $\pm$ 1^{o}C to a maximum 2θ value of 54.9^o. A total of 148 oscillation images were collected. A sweep of data was done using ω scans from 130.0 to 190.0^o in 1.5^o step, at χ=45.0^o and ϕ = 30.0^o. The exposure rate was 100.0 [sec./^{o}]. A second sweep was performed using ω scans from 0.0 to 162.0^o in 1.5^o step, at χ=45.0^o and ϕ = 210.0^o. The exposure rate was 100.0 [sec./^{o}]. The crystal-to-detector distance was 127.40 mm. Readout was performed in the 0.100 mm pixel mode.

Data Reduction

Of the 58490 reflections that were collected, 13519 were unique (R_{int} = 0.0309); equivalent reflections were merged.

The linear absorption coefficient, μ, for Mo-Kα radiation is 5.368 cm^{-1}. An empirical absorption correction was applied which resulted in transmission factors ranging from 0.597 to 0.908. The data were corrected for Lorentz and polarization effects.

Structure Solution and Refinement

The structure was solved by direct methods[1] and expanded using Fourier techniques. Some non-hydrogen atoms were refined anisotropically, while the rest were refined isotropically. Hydrogen atoms were refined using the riding model. The final cycle of full-matrix least-squares refinement[2] on F^2 was based on 13519 observed reflections and 643 variable parameters and converged (largest parameter shift was 0.00 times its esd) with unweighted and weighted agreement factors of:

$$R1 = \Sigma \; ||Fo| - |Fc|| \; / \; \Sigma \; |Fo| = 0.0366$$

$$wR2 = [\; \Sigma \; (\; w \; (Fo^2 - Fc^2)^2 \;) / \; \Sigma \; w(Fo^2)^2]^{1/2} = 0.0971$$

The standard deviation of an observation of unit weight[3] was 1.05. Unit weights were used. The maximum and minimum peaks on the final difference Fourier map corresponded to 0.79 and -0.64 $e^-/Å^3$, respectively. The absolute structure was deduced based on Flack parameter, -0.024(16), using 6051 Friedel pairs.[4]

Neutral atom scattering factors were taken from Cromer and Waber[5]. Anomalous dispersion effects were included in Fcalc[6]; the values for Δf' and Δf'' were those of Creagh and McAuley[7]. The values for the mass attenuation coefficients are those of Creagh and Hubbell[8]. All calculations were performed using the CrystalStructure[9] crystallographic software package except for refinement, which was performed using SHELXL-97[10].

References

(1) SIR92: Altomare, A., Cascarano, G., Giacovazzo, C., Guagliardi, A., Burla, M., Polidori, G., and Camalli, M. (1994) J. Appl. Cryst., 27, 435.

(2) Least Squares function minimized: (SHELXL97)

$\Sigma w(F_o^2-F_c^2)^2$ where w = Least Squares weights.

(3) Standard deviation of an observation of unit weight:

$[\Sigma w(F_o^2-F_c^2)^2/(N_o-N_v)]^{1/2}$

where: N_o = number of observations
N_v = number of variables

(4) Flack, H. D. (1983), Acta Cryst. A39, 876-881.

(5) Cromer, D. T. & Waber, J. T.; "International Tables for X-ray Crystallography", Vol. IV, The Kynoch Press, Birmingham, England, Table 2.2 A (1974).

(6) Ibers, J. A. & Hamilton, W. C.; Acta Crystallogr., 17, 781 (1964).

(7) Creagh, D. C. & McAuley, W.J .; "International Tables for Crystallography", Vol C, (A.J.C. Wilson, ed.), Kluwer Academic Publishers, Boston, Table 4.2.6.8, pages 219-222 (1992).

(8) Creagh, D. C. & Hubbell, J.H..; "International Tables for Crystallography", Vol C, (A.J.C. Wilson, ed.), Kluwer Academic Publishers, Boston, Table 4.2.4.3, pages 200-206 (1992).

(9) CrystalStructure 4.0: Crystal Structure Analysis Package, Rigaku Corporation (2000-2010). Tokyo 196-8666, Japan.

(10) SHELX97: Sheldrick, G.M. (2008). Acta Cryst. A64, 112-122.

EXPERIMENTAL DETAILS

A. Crystal Data

Empirical Formula	$C_{117}H_{148}Cl_{10}N_{12}Ti_4$
Formula Weight	2268.67
Crystal Color, Habit	yellow, block
Crystal Dimensions	0.620 X 0.200 X 0.180 mm
Crystal System	orthorhombic
Lattice Type	Primitive
Lattice Parameters	a = 21.8842(5) Å b = 28.7235(7) Å c = 9.4156(2) Å V = 5918.6(3) Å^3
Space Group	$P2_12_12$ (#18)
Z value	2
D_{calc}	1.273 g/cm^3
F_{000}	2384.00
μ(MoKα)	5.368 cm^{-1}

B. Intensity Measurements

Diffractometer	R-AXIS RAPID
Radiation	MoKα (λ = 0.71075 Å) graphite monochromated
Voltage, Current	50kV, 30mA
Temperature	-60.0^{o}C
Detector Aperture	280 x 256 mm
Data Images	148 exposures
ω oscillation Range (χ=45.0, ϕ=30.0)	130.0 - 190.0^{o}
Exposure Rate	100.0 sec./^{o}
ω oscillation Range (χ=45.0, ϕ=210.0)	0.0 - 162.0^{o}
Exposure Rate	100.0 sec./^{o}
Detector Position	127.40 mm
Pixel Size	0.100 mm
$2\theta_{max}$	54.9^{o}
No. of Reflections Measured	Total: 58490 Unique: 13519 (R_{int} = 0.0309) Friedel pairs: 6051
Corrections	Lorentz-polarization Absorption (trans. factors: 0.597 - 0.908)

C. Structure Solution and Refinement

Structure Solution	Direct Methods (SIR92)
Refinement	Full-matrix least-squares on F^2
Function Minimized	Σ w $(Fo^2 - Fc^2)^2$
Least Squares Weights	$w = 1/ [\sigma^2(Fo^2) + (0.0537 \cdot P)^2 + 1.5844 \cdot P]$ where $P = (Max(Fo^2,0) + 2Fc^2)/3$
$2\theta_{max}$ cutoff	54.9^o
Anomalous Dispersion	All non-hydrogen atoms
No. Observations (All reflections)	13519
No. Variables	643
Reflection/Parameter Ratio	21.02
Residuals: R1 (I>2.00σ(I))	0.0366
Residuals: R (All reflections)	0.0405
Residuals: wR2 (All reflections)	0.0971
Goodness of Fit Indicator	1.047
Flack Parameter (Friedel pairs = 6051)	-0.024(16)
Max Shift/Error in Final Cycle	0.001
Maximum peak in Final Diff. Map	0.79 $e^-/Å^3$
Minimum peak in Final Diff. Map	-0.64 $e^-/Å^3$

Table 1. Atomic coordinates and B_{iso}/B_{eq} and occupancy

atom	x	y	z	B_{eq}	occ
Ti(1)	0.18498(2)	0.01418(2)	0.20568(4)	2.273(7)	1
Ti(2)	0.48109(2)	0.23197(1)	0.27901(4)	2.203(7)	1
Cl(1)	0.22043(3)	-0.05359(2)	0.30525(7)	3.93(2)	1
Cl(2)	0.23563(3)	0.06716(3)	0.34648(7)	4.37(2)	1
Cl(3)	0.49679(3)	0.16849(2)	0.13311(6)	3.92(2)	1
Cl(4)	0.38938(2)	0.25780(2)	0.19069(7)	3.57(1)	1
Cl(5)	0.5278(2)	0.0038(2)	0.7347(4)	12.7(1)	1/2
Cl(6)	0.4914(2)	0.0199(2)	1.0225(4)	11.56(9)	1/2
N(1)	0.22215(8)	0.01786(6)	0.0367(2)	2.44(3)	1
N(2)	0.26098(8)	0.05984(6)	-0.1614(2)	2.56(3)	1
N(3)	0.26171(9)	-0.01702(6)	-0.1712(2)	2.82(3)	1
N(4)	0.46230(8)	0.20696(6)	0.4473(2)	2.58(3)	1
N(5)	0.40328(9)	0.20705(7)	0.6569(2)	3.09(4)	1
N(6)	0.47599(9)	0.15423(7)	0.6382(2)	3.16(4)	1
C(1)	0.0979(1)	0.06223(9)	0.2047(3)	3.80(5)	1
C(2)	0.0938(1)	0.03231(9)	0.0858(3)	3.25(4)	1
C(3)	0.08779(9)	-0.01352(9)	0.1357(3)	3.15(4)	1
C(4)	0.08621(9)	-0.01229(9)	0.2860(3)	3.43(4)	1
C(5)	0.0926(1)	0.0338(1)	0.3283(3)	3.76(5)	1
C(6)	0.1040(2)	0.1141(1)	0.2009(5)	6.8(1)	1
C(7)	0.0933(2)	0.0473(2)	-0.0681(3)	4.77(7)	1
C(8)	0.0814(2)	-0.0569(1)	0.0482(4)	5.30(7)	1
C(9)	0.0739(2)	-0.0542(2)	0.3785(4)	5.77(8)	1
C(10)	0.0924(2)	0.0499(2)	0.4805(4)	6.13(9)	1
C(11)	0.24654(9)	0.02037(7)	-0.0892(2)	2.21(3)	1
C(12)	0.2961(2)	0.04969(8)	-0.2903(3)	3.52(4)	1
C(13)	0.2888(2)	-0.00286(8)	-0.3067(3)	3.62(5)	1
C(14)	0.2605(1)	0.10571(7)	-0.1014(3)	2.67(4)	1
C(15)	0.3008(1)	0.11616(8)	0.0095(3)	3.05(4)	1
C(16)	0.2990(2)	0.16101(9)	0.0664(3)	4.17(6)	1
C(17)	0.2608(2)	0.19394(9)	0.0124(4)	4.91(7)	1
C(18)	0.2233(2)	0.18372(9)	-0.1010(4)	4.42(6)	1
C(19)	0.2218(1)	0.13926(8)	-0.1606(3)	3.23(4)	1
C(20)	0.3464(2)	0.0817(1)	0.0649(3)	3.91(5)	1
C(21)	0.1810(2)	0.12931(9)	-0.2858(3)	4.14(5)	1
C(22)	0.2547(1)	-0.06442(7)	-0.1278(3)	2.86(4)	1
C(23)	0.2929(2)	-0.08209(8)	-0.0226(3)	3.61(5)	1

Table 1. Atomic coordinates and B_{iso}/B_{eq} and occupancy (continued)

atom	x	y	z	B_{eq}	occ
C(24)	0.2831(2)	-0.1276(1)	0.0220(4)	5.28(7)	1
C(25)	0.2391(2)	-0.1550(1)	-0.0401(5)	6.22(9)	1
C(26)	0.2035(2)	-0.1377(1)	-0.1485(4)	5.20(7)	1
C(27)	0.2098(2)	-0.09167(8)	-0.1935(3)	3.57(5)	1
C(28)	0.3429(2)	-0.0533(2)	0.0416(4)	4.79(6)	1
C(29)	0.1688(2)	-0.0731(1)	-0.3063(4)	4.92(6)	1
C(30)	0.5188(1)	0.30564(7)	0.3488(3)	2.95(4)	1
C(31)	0.5607(1)	0.27160(8)	0.3953(3)	2.98(4)	1
C(32)	0.5858(1)	0.24969(8)	0.2751(3)	3.08(4)	1
C(33)	0.5609(1)	0.27169(8)	0.1520(3)	2.96(4)	1
C(34)	0.5199(1)	0.30628(7)	0.1975(3)	2.91(4)	1
C(35)	0.4809(2)	0.3376(1)	0.4391(4)	4.94(7)	1
C(36)	0.5784(2)	0.2630(2)	0.5474(3)	4.55(6)	1
C(37)	0.6321(2)	0.2110(1)	0.2779(4)	4.89(6)	1
C(38)	0.5761(2)	0.2607(1)	0.0004(3)	4.59(6)	1
C(39)	0.4864(2)	0.34056(9)	0.1068(4)	4.48(6)	1
C(40)	0.44854(9)	0.19073(7)	0.5720(3)	2.49(4)	1
C(41)	0.3981(2)	0.1801(1)	0.7895(3)	4.15(5)	1
C(42)	0.4447(2)	0.14165(9)	0.7705(3)	3.90(5)	1
C(43)	0.3594(1)	0.24129(8)	0.6157(3)	3.09(4)	1
C(44)	0.3142(1)	0.2294(1)	0.5178(3)	3.94(5)	1
C(45)	0.2724(2)	0.2638(2)	0.4779(4)	5.20(7)	1
C(46)	0.2753(2)	0.3077(2)	0.5364(5)	6.08(9)	1
C(47)	0.3187(2)	0.3183(1)	0.6363(4)	5.21(7)	1
C(48)	0.3620(2)	0.28560(9)	0.6787(3)	3.84(5)	1
C(49)	0.3108(2)	0.1811(2)	0.4579(4)	4.99(7)	1
C(50)	0.4086(2)	0.2975(1)	0.7877(4)	5.10(6)	1
C(51)	0.5234(1)	0.12654(8)	0.5754(3)	3.13(4)	1
C(52)	0.5094(2)	0.09647(9)	0.4634(3)	3.78(5)	1
C(53)	0.5571(2)	0.0714(1)	0.4028(4)	4.78(6)	1
C(54)	0.6160(2)	0.0755(1)	0.4512(4)	5.18(7)	1
C(55)	0.6287(2)	0.1040(1)	0.5662(4)	4.56(6)	1
C(56)	0.5829(2)	0.12988(9)	0.6317(3)	3.63(5)	1
C(57)	0.4450(2)	0.0905(1)	0.4128(3)	4.42(6)	1
C(58)	0.5974(2)	0.1587(1)	0.7591(4)	4.77(6)	1
C(59)	0.5041(7)	-0.0250(4)	0.891(2)	10.8(4)	1/2

$B_{eq} = 8/3\ \pi^2(U_{11}(aa^*)^2 + U_{22}(bb^*)^2 + U_{33}(cc^*)^2 + 2U_{12}(aa^*bb^*)\cos\gamma + 2U_{13}(aa^*cc^*)\cos\beta + 2U_{23}(bb^*cc^*)\cos\alpha)$

Table 2. Atomic coordinates and B_{iso} involving hydrogen atoms

atom	x	y	z	B_{iso}	occ
H(1)	0.1370	0.1236	0.2632	8.14	1
H(2)	0.0661	0.1282	0.2323	8.14	1
H(3)	0.1128	0.1240	0.1046	8.14	1
H(4)	0.1158	0.0249	-0.1246	5.73	1
H(5)	0.1123	0.0777	-0.0766	5.73	1
H(6)	0.0515	0.0490	-0.1017	5.73	1
H(7)	0.1150	-0.0778	0.0688	6.37	1
H(8)	0.0819	-0.0488	-0.0518	6.37	1
H(9)	0.0430	-0.0721	0.0710	6.37	1
H(10)	0.0352	-0.0681	0.3517	6.92	1
H(11)	0.0723	-0.0446	0.4772	6.92	1
H(12)	0.1064	-0.0768	0.3660	6.92	1
H(13)	0.1184	0.0297	0.5366	7.36	1
H(14)	0.0510	0.0489	0.5174	7.36	1
H(15)	0.1077	0.0816	0.4855	7.36	1
H(16)	0.3391	0.0583	-0.2785	4.22	1
H(17)	0.2793	0.0663	-0.3725	4.22	1
H(18)	0.2617	-0.0104	-0.3864	4.34	1
H(19)	0.3284	-0.0180	-0.3217	4.34	1
H(20)	0.3246	0.1686	0.1431	5.00	1
H(21)	0.2600	0.2239	0.0527	5.89	1
H(22)	0.1981	0.2072	-0.1389	5.30	1
H(23)	0.3623	0.0633	-0.0132	4.69	1
H(24)	0.3267	0.0613	0.1332	4.69	1
H(25)	0.3797	0.0982	0.1107	4.69	1
H(26)	0.1401	0.1407	-0.2661	4.97	1
H(27)	0.1796	0.0960	-0.3025	4.97	1
H(28)	0.1970	0.1448	-0.3693	4.97	1
H(29)	0.3069	-0.1399	0.0961	6.34	1
H(30)	0.2333	-0.1857	-0.0085	7.47	1
H(31)	0.1746	-0.1571	-0.1927	6.23	1
H(32)	0.3663	-0.0385	-0.0335	5.75	1
H(33)	0.3695	-0.0731	0.0974	5.75	1
H(34)	0.3252	-0.0296	0.1022	5.75	1
H(35)	0.1883	-0.0765	-0.3981	5.90	1
H(36)	0.1606	-0.0404	-0.2884	5.90	1
H(37)	0.1306	-0.0902	-0.3058	5.90	1

Table 2. Atomic coordinates and B_{iso} involving hydrogens/B_{eq} and occupancy (continued)

atom	x	y	z	B_{eq}	occ
H(38)	0.4381	0.3340	0.4147	5.92	1
H(39)	0.4933	0.3696	0.4224	5.92	1
H(40)	0.4869	0.3299	0.5384	5.92	1
H(41)	0.6012	0.2342	0.5540	5.46	1
H(42)	0.5418	0.2608	0.6052	5.46	1
H(43)	0.6035	0.2885	0.5812	5.46	1
H(44)	0.6186	0.1869	0.3428	5.86	1
H(45)	0.6712	0.2232	0.3095	5.86	1
H(46)	0.6364	0.1980	0.1834	5.86	1
H(47)	0.5387	0.2588	-0.0547	5.51	1
H(48)	0.5975	0.2312	-0.0042	5.51	1
H(49)	0.6020	0.2851	-0.0381	5.51	1
H(50)	0.4984	0.3719	0.1329	5.37	1
H(51)	0.4428	0.3369	0.1208	5.37	1
H(52)	0.4963	0.3351	0.0077	5.37	1
H(53)	0.3569	0.1673	0.8007	4.98	1
H(54)	0.4078	0.1994	0.8723	4.98	1
H(55)	0.4734	0.1408	0.8504	4.68	1
H(56)	0.4248	0.1112	0.7622	4.68	1
H(57)	0.2420	0.2569	0.4106	6.24	1
H(58)	0.2472	0.3306	0.5075	7.29	1
H(59)	0.3193	0.3482	0.6768	6.25	1
H(60)	0.3462	0.1754	0.3986	5.99	1
H(61)	0.2739	0.1780	0.4014	5.99	1
H(62)	0.3099	0.1587	0.5350	5.99	1
H(63)	0.4471	0.2827	0.7635	6.13	1
H(64)	0.3951	0.2865	0.8800	6.13	1
H(65)	0.4141	0.3310	0.7908	6.13	1
H(66)	0.5488	0.0511	0.3269	5.74	1
H(67)	0.6477	0.0591	0.4063	6.22	1
H(68)	0.6689	0.1059	0.6005	5.48	1
H(69)	0.4330	0.1176	0.3580	5.30	1
H(70)	0.4181	0.0871	0.4939	5.30	1
H(71)	0.4424	0.0629	0.3537	5.30	1
H(72)	0.5712	0.1859	0.7608	5.73	1
H(73)	0.6398	0.1685	0.7551	5.73	1
H(74)	0.5908	0.1404	0.8444	5.73	1

Table 2. Atomic coordinates and B_{iso} involving hydrogens/B_{eq} and occupancy (continued)

atom	x	y	z	B_{eq}	occ

Table 3. Anisotropic displacement parameters

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Ti(1)	0.0288(2)	0.0323(2)	0.0253(2)	-0.0005(2)	-0.0018(2)	0.0006(2)
Ti(2)	0.0313(2)	0.0271(2)	0.0253(2)	-0.0019(2)	-0.0008(2)	0.0008(2)
Cl(1)	0.0418(3)	0.0519(3)	0.0555(4)	0.0098(3)	0.0076(3)	0.0238(3)
Cl(2)	0.0593(4)	0.0681(4)	0.0387(3)	-0.0218(3)	-0.0017(3)	-0.0158(3)
Cl(3)	0.0720(4)	0.0385(3)	0.0383(3)	-0.0051(3)	0.0073(3)	-0.0097(3)
Cl(4)	0.0365(3)	0.0420(3)	0.0570(4)	-0.0050(2)	-0.0121(3)	0.0128(3)
N(1)	0.0316(8)	0.0306(8)	0.0306(9)	-0.0002(7)	-0.0022(7)	0.0013(7)
N(2)	0.044(1)	0.0273(8)	0.0262(8)	-0.0030(7)	0.0025(7)	-0.0009(7)
N(3)	0.050(1)	0.0285(8)	0.0282(9)	-0.0001(8)	0.0050(8)	-0.0002(7)
N(4)	0.0349(9)	0.0325(9)	0.0306(9)	-0.0005(7)	0.0013(7)	0.0003(7)
N(5)	0.042(1)	0.046(1)	0.0291(9)	0.0051(9)	0.0080(8)	0.0031(8)
N(6)	0.050(1)	0.041(1)	0.0295(9)	0.0084(9)	0.0031(9)	0.0073(8)
C(1)	0.043(2)	0.046(2)	0.056(2)	0.016(1)	-0.007(2)	-0.009(2)
C(2)	0.032(1)	0.057(2)	0.035(2)	0.011(1)	-0.0051(9)	-0.000(1)
C(3)	0.026(1)	0.051(2)	0.043(2)	-0.001(1)	-0.0047(9)	-0.007(1)
C(4)	0.0269(9)	0.061(2)	0.042(2)	0.002(1)	0.001(1)	0.006(2)
C(5)	0.032(1)	0.074(2)	0.036(2)	0.014(1)	0.0012(9)	-0.011(2)
C(6)	0.098(3)	0.047(2)	0.113(3)	0.026(2)	-0.028(3)	-0.011(2)
C(7)	0.049(2)	0.091(3)	0.041(2)	0.014(2)	-0.007(2)	0.016(2)
C(8)	0.054(2)	0.063(2)	0.084(3)	-0.009(2)	-0.009(2)	-0.029(2)
C(9)	0.041(2)	0.106(3)	0.072(2)	-0.013(2)	0.009(2)	0.035(2)
C(10)	0.058(2)	0.127(4)	0.048(2)	0.019(2)	-0.002(2)	-0.031(2)
C(11)	0.0295(9)	0.0288(9)	0.0257(9)	-0.0012(8)	-0.0029(8)	-0.0011(8)
C(12)	0.063(2)	0.037(1)	0.033(1)	-0.003(1)	0.014(2)	-0.001(1)
C(13)	0.069(2)	0.035(1)	0.034(1)	-0.005(1)	0.015(2)	-0.001(1)
C(14)	0.043(2)	0.028(1)	0.031(1)	-0.0063(9)	0.0042(9)	-0.0002(8)
C(15)	0.046(2)	0.039(1)	0.030(1)	-0.015(1)	0.0014(9)	-0.0001(9)
C(16)	0.073(2)	0.050(2)	0.036(2)	-0.025(2)	0.005(2)	-0.009(1)
C(17)	0.091(3)	0.036(2)	0.059(2)	-0.013(2)	0.017(2)	-0.016(2)
C(18)	0.069(2)	0.032(2)	0.067(2)	0.007(2)	0.013(2)	0.000(2)
C(19)	0.048(2)	0.034(1)	0.042(2)	0.001(1)	0.003(1)	0.0018(9)
C(20)	0.045(2)	0.062(2)	0.042(2)	-0.013(2)	-0.009(1)	0.007(2)
C(21)	0.055(2)	0.050(2)	0.052(2)	0.004(2)	-0.010(2)	0.011(2)
C(22)	0.044(2)	0.028(1)	0.036(1)	0.0018(9)	0.007(1)	-0.0002(9)
C(23)	0.049(2)	0.041(2)	0.047(2)	0.013(1)	0.007(1)	0.007(1)
C(24)	0.085(3)	0.051(2)	0.065(2)	0.027(2)	0.018(2)	0.019(2)
C(25)	0.110(3)	0.028(2)	0.098(3)	0.010(2)	0.038(3)	0.011(2)

Table 3. Anisotropic displacement parameters (continued)

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
C(26)	0.081(2)	0.038(2)	0.079(3)	-0.015(2)	0.029(2)	-0.012(2)
C(27)	0.053(2)	0.037(1)	0.046(2)	-0.006(1)	0.012(2)	-0.009(1)
C(28)	0.049(2)	0.080(2)	0.053(2)	0.014(2)	-0.007(2)	0.008(2)
C(29)	0.060(2)	0.074(2)	0.053(2)	-0.016(2)	-0.005(2)	-0.015(2)
C(30)	0.037(1)	0.031(1)	0.045(2)	-0.0077(9)	0.002(1)	-0.0068(9)
C(31)	0.038(1)	0.042(2)	0.032(1)	-0.010(1)	-0.0044(9)	0.001(1)
C(32)	0.032(1)	0.042(1)	0.043(2)	-0.0012(9)	-0.000(1)	0.001(1)
C(33)	0.037(1)	0.044(2)	0.032(1)	-0.009(1)	0.0028(9)	0.0023(9)
C(34)	0.036(1)	0.033(1)	0.042(2)	-0.0089(9)	-0.004(1)	0.0081(9)
C(35)	0.066(2)	0.045(2)	0.077(2)	-0.005(2)	0.012(2)	-0.023(2)
C(36)	0.064(2)	0.072(2)	0.037(2)	-0.017(2)	-0.017(2)	0.003(2)
C(37)	0.043(2)	0.058(2)	0.084(2)	0.011(2)	-0.002(2)	-0.003(2)
C(38)	0.064(2)	0.072(2)	0.038(2)	-0.022(2)	0.015(2)	-0.005(2)
C(39)	0.050(2)	0.045(2)	0.075(2)	-0.009(2)	-0.011(2)	0.024(2)
C(40)	0.035(1)	0.032(1)	0.028(1)	-0.0017(8)	-0.0012(8)	-0.0010(8)
C(41)	0.064(2)	0.058(2)	0.035(2)	0.004(2)	0.011(2)	0.012(2)
C(42)	0.065(2)	0.049(2)	0.034(2)	0.001(2)	0.004(2)	0.011(1)
C(43)	0.039(1)	0.043(2)	0.035(1)	0.004(1)	0.0085(9)	0.003(1)
C(44)	0.037(2)	0.069(2)	0.044(2)	-0.004(2)	0.005(1)	0.003(2)
C(45)	0.038(2)	0.099(3)	0.060(2)	0.007(2)	0.002(2)	0.016(2)
C(46)	0.053(2)	0.091(3)	0.088(3)	0.029(2)	0.021(2)	0.028(2)
C(47)	0.068(2)	0.052(2)	0.077(2)	0.017(2)	0.026(2)	0.006(2)
C(48)	0.052(2)	0.045(2)	0.049(2)	-0.000(1)	0.014(2)	-0.000(1)
C(49)	0.058(2)	0.084(3)	0.048(2)	-0.022(2)	-0.002(2)	-0.007(2)
C(50)	0.087(2)	0.055(2)	0.052(2)	-0.006(2)	0.006(2)	-0.011(2)
C(51)	0.049(2)	0.036(1)	0.034(1)	0.006(1)	-0.003(1)	0.0066(9)
C(52)	0.066(2)	0.040(2)	0.038(2)	0.005(2)	-0.004(2)	0.004(1)
C(53)	0.084(2)	0.054(2)	0.044(2)	0.019(2)	0.002(2)	-0.001(2)
C(54)	0.069(2)	0.064(2)	0.063(2)	0.032(2)	0.006(2)	0.006(2)
C(55)	0.051(2)	0.058(2)	0.065(2)	0.016(2)	-0.005(2)	0.016(2)
C(56)	0.051(2)	0.041(2)	0.046(2)	0.006(1)	-0.009(2)	0.012(1)
C(57)	0.070(2)	0.051(2)	0.046(2)	-0.005(2)	-0.012(2)	-0.004(2)
C(58)	0.065(2)	0.059(2)	0.057(2)	0.005(2)	-0.025(2)	0.003(2)

The general temperature factor expression: $\exp(-2\pi^2(a^{*2}U_{11}h^2 + b^{*2}U_{22}k^2 + c^{*2}U_{33}l^2 + 2a^*b^*U_{12}hk + 2a^*c^*U_{13}hl + 2b^*c^*U_{23}kl))$

Table 4. Fragment Analysis

fragment: 1

Ti1	Cl1	Cl2	N1	N2
N3	C1	C2	C3	C4
C5	C6	C7	C8	C9
C10	C11	C12	C13	C14
C15	C16	C17	C18	C19
C20	C21	C22	C23	C24
C25	C26	C27	C28	C29

fragment: 2

Ti2	Cl3	Cl4	N4	N5
N6	C30	C31	C32	C33
C34	C35	C36	C37	C38
C39	C40	C41	C42	C43
C44	C45	C46	C47	C48
C49	C50	C51	C52	C53
C54	C55	C56	C57	C58

fragment: 3

Cl5	Cl6	C59

Table 5. Bond lengths (Å)

atom	atom	distance	atom	atom	distance
Ti(1)	Cl(1)	2.2955(7)	Ti(1)	Cl(2)	2.3026(9)
Ti(1)	N(1)	1.7898(18)	Ti(1)	C(1)	2.354(3)
Ti(1)	C(2)	2.352(3)	Ti(1)	C(3)	2.365(3)
Ti(1)	C(4)	2.413(3)	Ti(1)	C(5)	2.396(3)
Ti(2)	Cl(3)	2.3087(7)	Ti(2)	Cl(4)	2.2956(6)
Ti(2)	N(4)	1.7874(19)	Ti(2)	C(30)	2.364(2)
Ti(2)	C(31)	2.352(3)	Ti(2)	C(32)	2.348(3)
Ti(2)	C(33)	2.404(3)	Ti(2)	C(34)	2.422(2)
Cl(5)	C(59)	1.767(13)	Cl(5)	C(59)[1]	1.739(13)
Cl(6)	C(59)	1.808(12)	N(1)	C(11)	1.303(3)
N(2)	C(11)	1.359(3)	N(2)	C(12)	1.465(3)
N(2)	C(14)	1.433(3)	N(3)	C(11)	1.364(3)
N(3)	C(13)	1.464(3)	N(3)	C(22)	1.430(3)
N(4)	C(40)	1.299(3)	N(5)	C(40)	1.356(3)
N(5)	C(41)	1.474(4)	N(5)	C(43)	1.429(3)
N(6)	C(40)	1.360(3)	N(6)	C(42)	1.466(4)
N(6)	C(51)	1.436(3)	C(1)	C(2)	1.414(4)
C(1)	C(5)	1.426(4)	C(1)	C(6)	1.495(4)
C(2)	C(3)	1.404(4)	C(2)	C(7)	1.511(4)
C(3)	C(4)	1.416(4)	C(3)	C(8)	1.499(5)
C(4)	C(5)	1.391(4)	C(4)	C(9)	1.509(5)
C(5)	C(10)	1.505(5)	C(12)	C(13)	1.526(4)
C(14)	C(15)	1.399(4)	C(14)	C(19)	1.399(4)
C(15)	C(16)	1.396(4)	C(15)	C(20)	1.500(4)
C(16)	C(17)	1.361(5)	C(17)	C(18)	1.379(5)
C(18)	C(19)	1.395(4)	C(19)	C(21)	1.506(4)
C(22)	C(23)	1.391(4)	C(22)	C(27)	1.400(4)
C(23)	C(24)	1.391(4)	C(23)	C(28)	1.499(4)
C(24)	C(25)	1.373(6)	C(25)	C(26)	1.377(6)
C(26)	C(27)	1.395(4)	C(27)	C(29)	1.490(4)
C(30)	C(31)	1.411(3)	C(30)	C(34)	1.424(4)
C(30)	C(35)	1.501(4)	C(31)	C(32)	1.407(4)
C(31)	C(36)	1.503(4)	C(32)	C(33)	1.428(4)
C(32)	C(37)	1.505(4)	C(33)	C(34)	1.405(3)
C(33)	C(38)	1.500(4)	C(34)	C(39)	1.495(4)
C(41)	C(42)	1.515(4)	C(43)	C(44)	1.393(4)
C(43)	C(48)	1.405(4)	C(44)	C(45)	1.397(5)

Table 5. Bond lengths (Å) (continued)

atom	atom	distance	atom	atom	distance
C(44)	C(49)	1.501(5)	C(45)	C(46)	1.377(6)
C(46)	C(47)	1.372(5)	C(47)	C(48)	1.393(5)
C(48)	C(50)	1.488(5)	C(51)	C(52)	1.397(4)
C(51)	C(56)	1.409(4)	C(52)	C(53)	1.392(5)
C(52)	C(57)	1.497(5)	C(53)	C(54)	1.372(5)
C(54)	C(55)	1.386(5)	C(55)	C(56)	1.391(4)
C(56)	C(58)	1.492(4)	C(59)	C(59)[1]	1.446(16)

Symmetry Operators:

(1) -X+1,-Y,Z

Table 6. Bond lengths involving hydrogens (Å)

atom	atom	distance	atom	atom	distance
C(6)	H(1)	0.970	C(6)	H(2)	0.970
C(6)	H(3)	0.970	C(7)	H(4)	0.970
C(7)	H(5)	0.970	C(7)	H(6)	0.970
C(8)	H(7)	0.970	C(8)	H(8)	0.970
C(8)	H(9)	0.970	C(9)	H(10)	0.970
C(9)	H(11)	0.970	C(9)	H(12)	0.970
C(10)	H(13)	0.970	C(10)	H(14)	0.970
C(10)	H(15)	0.970	C(12)	H(16)	0.980
C(12)	H(17)	0.980	C(13)	H(18)	0.980
C(13)	H(19)	0.980	C(16)	H(20)	0.940
C(17)	H(21)	0.940	C(18)	H(22)	0.940
C(20)	H(23)	0.970	C(20)	H(24)	0.970
C(20)	H(25)	0.970	C(21)	H(26)	0.970
C(21)	H(27)	0.970	C(21)	H(28)	0.970
C(24)	H(29)	0.940	C(25)	H(30)	0.940
C(26)	H(31)	0.940	C(28)	H(32)	0.970
C(28)	H(33)	0.970	C(28)	H(34)	0.970
C(29)	H(35)	0.970	C(29)	H(36)	0.970
C(29)	H(37)	0.970	C(35)	H(38)	0.970
C(35)	H(39)	0.970	C(35)	H(40)	0.970
C(36)	H(41)	0.970	C(36)	H(42)	0.970
C(36)	H(43)	0.970	C(37)	H(44)	0.970
C(37)	H(45)	0.970	C(37)	H(46)	0.970
C(38)	H(47)	0.970	C(38)	H(48)	0.970
C(38)	H(49)	0.970	C(39)	H(50)	0.970
C(39)	H(51)	0.970	C(39)	H(52)	0.970
C(41)	H(53)	0.980	C(41)	H(54)	0.980
C(42)	H(55)	0.980	C(42)	H(56)	0.980
C(45)	H(57)	0.940	C(46)	H(58)	0.940
C(47)	H(59)	0.940	C(49)	H(60)	0.970
C(49)	H(61)	0.970	C(49)	H(62)	0.970
C(50)	H(63)	0.970	C(50)	H(64)	0.970
C(50)	H(65)	0.970	C(53)	H(66)	0.940
C(54)	H(67)	0.940	C(55)	H(68)	0.940
C(57)	H(69)	0.970	C(57)	H(70)	0.970
C(57)	H(71)	0.970	C(58)	H(72)	0.970
C(58)	H(73)	0.970	C(58)	H(74)	0.970

Table 6. Bond lengths involving hydrogens (Å) (continued)

atom	atom	distance	atom	atom	distance

Table 7. Bond angles (°)

atom	atom	atom	angle	atom	atom	atom	angle
Cl(1)	Ti(1)	Cl(2)	99.36(3)	Cl(1)	Ti(1)	N(1)	105.04(6)
Cl(1)	Ti(1)	C(1)	140.59(7)	Cl(1)	Ti(1)	C(2)	132.12(7)
Cl(1)	Ti(1)	C(3)	97.61(7)	Cl(1)	Ti(1)	C(4)	84.70(7)
Cl(1)	Ti(1)	C(5)	106.76(8)	Cl(2)	Ti(1)	N(1)	104.71(6)
Cl(2)	Ti(1)	C(1)	90.26(7)	Cl(2)	Ti(1)	C(2)	122.59(7)
Cl(2)	Ti(1)	C(3)	144.66(7)	Cl(2)	Ti(1)	C(4)	117.33(7)
Cl(2)	Ti(1)	C(5)	88.45(7)	N(1)	Ti(1)	C(1)	109.26(9)
N(1)	Ti(1)	C(2)	86.91(8)	N(1)	Ti(1)	C(3)	100.43(9)
N(1)	Ti(1)	C(4)	134.77(9)	N(1)	Ti(1)	C(5)	142.93(9)
C(1)	Ti(1)	C(2)	34.98(9)	C(1)	Ti(1)	C(3)	57.83(9)
C(1)	Ti(1)	C(4)	57.34(9)	C(1)	Ti(1)	C(5)	34.92(10)
C(2)	Ti(1)	C(3)	34.64(9)	C(2)	Ti(1)	C(4)	57.30(9)
C(2)	Ti(1)	C(5)	57.50(9)	C(3)	Ti(1)	C(4)	34.45(9)
C(3)	Ti(1)	C(5)	56.94(9)	C(4)	Ti(1)	C(5)	33.62(10)
Cl(3)	Ti(2)	Cl(4)	99.78(3)	Cl(3)	Ti(2)	N(4)	104.13(6)
Cl(3)	Ti(2)	C(30)	145.11(6)	Cl(3)	Ti(2)	C(31)	123.29(6)
Cl(3)	Ti(2)	C(32)	90.95(6)	Cl(3)	Ti(2)	C(33)	88.32(6)
Cl(3)	Ti(2)	C(34)	117.09(6)	Cl(4)	Ti(2)	N(4)	104.47(6)
Cl(4)	Ti(2)	C(30)	96.69(6)	Cl(4)	Ti(2)	C(31)	131.31(6)
Cl(4)	Ti(2)	C(32)	141.05(6)	Cl(4)	Ti(2)	C(33)	107.55(6)
Cl(4)	Ti(2)	C(34)	84.66(6)	N(4)	Ti(2)	C(30)	101.18(8)
N(4)	Ti(2)	C(31)	87.26(8)	N(4)	Ti(2)	C(32)	109.00(9)
N(4)	Ti(2)	C(33)	142.99(8)	N(4)	Ti(2)	C(34)	135.70(8)
C(30)	Ti(2)	C(31)	34.82(8)	C(30)	Ti(2)	C(32)	57.98(8)
C(30)	Ti(2)	C(33)	57.32(8)	C(30)	Ti(2)	C(34)	34.60(8)
C(31)	Ti(2)	C(32)	34.83(8)	C(31)	Ti(2)	C(33)	57.57(8)
C(31)	Ti(2)	C(34)	57.40(8)	C(32)	Ti(2)	C(33)	34.96(8)
C(32)	Ti(2)	C(34)	57.43(8)	C(33)	Ti(2)	C(34)	33.86(8)
C(59)	Cl(5)	C(59)[1]	48.7(6)	Ti(1)	N(1)	C(11)	177.15(16)
C(11)	N(2)	C(12)	111.71(17)	C(11)	N(2)	C(14)	124.62(17)
C(12)	N(2)	C(14)	120.85(18)	C(11)	N(3)	C(13)	111.90(17)
C(11)	N(3)	C(22)	124.19(18)	C(13)	N(3)	C(22)	123.84(18)
Ti(2)	N(4)	C(40)	177.32(16)	C(40)	N(5)	C(41)	112.0(2)
C(40)	N(5)	C(43)	124.73(19)	C(41)	N(5)	C(43)	122.6(2)
C(40)	N(6)	C(42)	111.93(19)	C(40)	N(6)	C(51)	123.90(19)
C(42)	N(6)	C(51)	123.4(2)	Ti(1)	C(1)	C(2)	72.43(14)
Ti(1)	C(1)	C(5)	74.18(15)	Ti(1)	C(1)	C(6)	120.8(2)

Table 7. Bond angles (°) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
C(2)	C(1)	C(5)	107.1(3)	C(2)	C(1)	C(6)	126.3(3)
C(5)	C(1)	C(6)	126.6(3)	Ti(1)	C(2)	C(1)	72.59(14)
Ti(1)	C(2)	C(3)	73.19(13)	Ti(1)	C(2)	C(7)	121.92(17)
C(1)	C(2)	C(3)	108.1(3)	C(1)	C(2)	C(7)	125.9(3)
C(3)	C(2)	C(7)	126.0(3)	Ti(1)	C(3)	C(2)	72.18(13)
Ti(1)	C(3)	C(4)	74.64(13)	Ti(1)	C(3)	C(8)	121.11(17)
C(2)	C(3)	C(4)	108.3(3)	C(2)	C(3)	C(8)	127.1(3)
C(4)	C(3)	C(8)	124.6(3)	Ti(1)	C(4)	C(3)	70.91(12)
Ti(1)	C(4)	C(5)	72.54(14)	Ti(1)	C(4)	C(9)	126.25(17)
C(3)	C(4)	C(5)	107.9(3)	C(3)	C(4)	C(9)	124.1(3)
C(5)	C(4)	C(9)	127.7(3)	Ti(1)	C(5)	C(1)	70.90(14)
Ti(1)	C(5)	C(4)	73.83(14)	Ti(1)	C(5)	C(10)	122.20(19)
C(1)	C(5)	C(4)	108.6(3)	C(1)	C(5)	C(10)	127.0(3)
C(4)	C(5)	C(10)	124.4(3)	N(1)	C(11)	N(2)	126.64(19)
N(1)	C(11)	N(3)	124.87(19)	N(2)	C(11)	N(3)	108.50(17)
N(2)	C(12)	C(13)	103.06(19)	N(3)	C(13)	C(12)	103.22(19)
N(2)	C(14)	C(15)	119.12(19)	N(2)	C(14)	C(19)	118.73(19)
C(15)	C(14)	C(19)	122.1(2)	C(14)	C(15)	C(16)	117.9(3)
C(14)	C(15)	C(20)	122.5(2)	C(16)	C(15)	C(20)	119.5(3)
C(15)	C(16)	C(17)	121.0(3)	C(16)	C(17)	C(18)	120.5(3)
C(17)	C(18)	C(19)	121.3(3)	C(14)	C(19)	C(18)	117.1(3)
C(14)	C(19)	C(21)	122.7(2)	C(18)	C(19)	C(21)	120.1(3)
N(3)	C(22)	C(23)	119.1(2)	N(3)	C(22)	C(27)	118.8(2)
C(23)	C(22)	C(27)	122.1(2)	C(22)	C(23)	C(24)	117.7(3)
C(22)	C(23)	C(28)	121.6(3)	C(24)	C(23)	C(28)	120.7(3)
C(23)	C(24)	C(25)	121.2(4)	C(24)	C(25)	C(26)	120.4(3)
C(25)	C(26)	C(27)	120.7(3)	C(22)	C(27)	C(26)	117.7(3)
C(22)	C(27)	C(29)	122.5(3)	C(26)	C(27)	C(29)	119.8(3)
Ti(2)	C(30)	C(31)	72.14(13)	Ti(2)	C(30)	C(34)	74.92(12)
Ti(2)	C(30)	C(35)	120.81(17)	C(31)	C(30)	C(34)	107.98(19)
C(31)	C(30)	C(35)	127.4(3)	C(34)	C(30)	C(35)	124.6(3)
Ti(2)	C(31)	C(30)	73.04(13)	Ti(2)	C(31)	C(32)	72.40(13)
Ti(2)	C(31)	C(36)	123.66(18)	C(30)	C(31)	C(32)	108.3(2)
C(30)	C(31)	C(36)	125.2(3)	C(32)	C(31)	C(36)	126.4(3)
Ti(2)	C(32)	C(31)	72.77(13)	Ti(2)	C(32)	C(33)	74.69(13)
Ti(2)	C(32)	C(37)	119.83(17)	C(31)	C(32)	C(33)	107.8(2)
C(31)	C(32)	C(37)	125.4(3)	C(33)	C(32)	C(37)	126.8(3)

Table 7. Bond angles (°) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
Ti(2)	C(33)	C(32)	70.36(13)	Ti(2)	C(33)	C(34)	73.76(13)
Ti(2)	C(33)	C(38)	122.36(18)	C(32)	C(33)	C(34)	108.0(2)
C(32)	C(33)	C(38)	126.5(3)	C(34)	C(33)	C(38)	125.5(3)
Ti(2)	C(34)	C(30)	70.48(12)	Ti(2)	C(34)	C(33)	72.38(13)
Ti(2)	C(34)	C(39)	126.12(16)	C(30)	C(34)	C(33)	107.85(19)
C(30)	C(34)	C(39)	124.8(2)	C(33)	C(34)	C(39)	127.2(3)
N(4)	C(40)	N(5)	125.30(19)	N(4)	C(40)	N(6)	126.07(19)
N(5)	C(40)	N(6)	108.62(19)	N(5)	C(41)	C(42)	103.4(2)
N(6)	C(42)	C(41)	103.6(2)	N(5)	C(43)	C(44)	119.2(3)
N(5)	C(43)	C(48)	118.8(2)	C(44)	C(43)	C(48)	122.0(3)
C(43)	C(44)	C(45)	118.1(3)	C(43)	C(44)	C(49)	120.7(3)
C(45)	C(44)	C(49)	121.3(3)	C(44)	C(45)	C(46)	120.6(3)
C(45)	C(46)	C(47)	120.7(4)	C(46)	C(47)	C(48)	121.2(3)
C(43)	C(48)	C(47)	117.5(3)	C(43)	C(48)	C(50)	121.8(3)
C(47)	C(48)	C(50)	120.7(3)	N(6)	C(51)	C(52)	119.6(3)
N(6)	C(51)	C(56)	118.4(2)	C(52)	C(51)	C(56)	122.0(3)
C(51)	C(52)	C(53)	117.7(3)	C(51)	C(52)	C(57)	121.3(3)
C(53)	C(52)	C(57)	121.0(3)	C(52)	C(53)	C(54)	121.5(3)
C(53)	C(54)	C(55)	120.0(3)	C(54)	C(55)	C(56)	121.2(3)
C(51)	C(56)	C(55)	117.5(3)	C(51)	C(56)	C(58)	122.5(3)
C(55)	C(56)	C(58)	120.0(3)	Cl(5)	C(59)	Cl(5)[1]	41.3(4)
Cl(5)	C(59)	Cl(6)	106.4(6)	Cl(5)	C(59)	C(59)[1]	64.6(7)
Cl(5)[1]	C(59)	Cl(6)	105.6(7)	Cl(5)[1]	C(59)	C(59)[1]	66.7(7)
Cl(6)	C(59)	C(59)[1]	43.5(6)				

Symmetry Operators:

(1) -X+1,-Y,Z

Table 8. Bond angles involving hydrogens (^{o})

atom	atom	atom	angle	atom	atom	atom	angle
C(1)	C(6)	H(1)	109	C(1)	C(6)	H(2)	109
C(1)	C(6)	H(3)	109	H(1)	C(6)	H(2)	109
H(1)	C(6)	H(3)	109	H(2)	C(6)	H(3)	109
C(2)	C(7)	H(4)	109	C(2)	C(7)	H(5)	109
C(2)	C(7)	H(6)	109	H(4)	C(7)	H(5)	109
H(4)	C(7)	H(6)	109	H(5)	C(7)	H(6)	109
C(3)	C(8)	H(7)	109	C(3)	C(8)	H(8)	109
C(3)	C(8)	H(9)	109	H(7)	C(8)	H(8)	109
H(7)	C(8)	H(9)	109	H(8)	C(8)	H(9)	109
C(4)	C(9)	H(10)	109	C(4)	C(9)	H(11)	109
C(4)	C(9)	H(12)	109	H(10)	C(9)	H(11)	109
H(10)	C(9)	H(12)	109	H(11)	C(9)	H(12)	109
C(5)	C(10)	H(13)	109	C(5)	C(10)	H(14)	109
C(5)	C(10)	H(15)	109	H(13)	C(10)	H(14)	109
H(13)	C(10)	H(15)	109	H(14)	C(10)	H(15)	109
N(2)	C(12)	H(16)	111	N(2)	C(12)	H(17)	111
C(13)	C(12)	H(16)	111	C(13)	C(12)	H(17)	111
H(16)	C(12)	H(17)	109	N(3)	C(13)	H(18)	111
N(3)	C(13)	H(19)	111	C(12)	C(13)	H(18)	111
C(12)	C(13)	H(19)	111	H(18)	C(13)	H(19)	109
C(15)	C(16)	H(20)	120	C(17)	C(16)	H(20)	120
C(16)	C(17)	H(21)	120	C(18)	C(17)	H(21)	120
C(17)	C(18)	H(22)	119	C(19)	C(18)	H(22)	119
C(15)	C(20)	H(23)	109	C(15)	C(20)	H(24)	109
C(15)	C(20)	H(25)	109	H(23)	C(20)	H(24)	109
H(23)	C(20)	H(25)	109	H(24)	C(20)	H(25)	109
C(19)	C(21)	H(26)	109	C(19)	C(21)	H(27)	109
C(19)	C(21)	H(28)	109	H(26)	C(21)	H(27)	109
H(26)	C(21)	H(28)	109	H(27)	C(21)	H(28)	109
C(23)	C(24)	H(29)	119	C(25)	C(24)	H(29)	119
C(24)	C(25)	H(30)	120	C(26)	C(25)	H(30)	120
C(25)	C(26)	H(31)	120	C(27)	C(26)	H(31)	120
C(23)	C(28)	H(32)	109	C(23)	C(28)	H(33)	109
C(23)	C(28)	H(34)	109	H(32)	C(28)	H(33)	109
H(32)	C(28)	H(34)	109	H(33)	C(28)	H(34)	109
C(27)	C(29)	H(35)	109	C(27)	C(29)	H(36)	109
C(27)	C(29)	H(37)	109	H(35)	C(29)	H(36)	109

Table 8. Bond angles involving hydrogens (^{o}) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
H(35)	C(29)	H(37)	109	H(36)	C(29)	H(37)	109
C(30)	C(35)	H(38)	109	C(30)	C(35)	H(39)	109
C(30)	C(35)	H(40)	109	H(38)	C(35)	H(39)	109
H(38)	C(35)	H(40)	109	H(39)	C(35)	H(40)	109
C(31)	C(36)	H(41)	109	C(31)	C(36)	H(42)	109
C(31)	C(36)	H(43)	109	H(41)	C(36)	H(42)	109
H(41)	C(36)	H(43)	109	H(42)	C(36)	H(43)	109
C(32)	C(37)	H(44)	109	C(32)	C(37)	H(45)	109
C(32)	C(37)	H(46)	109	H(44)	C(37)	H(45)	109
H(44)	C(37)	H(46)	109	H(45)	C(37)	H(46)	109
C(33)	C(38)	H(47)	109	C(33)	C(38)	H(48)	109
C(33)	C(38)	H(49)	109	H(47)	C(38)	H(48)	109
H(47)	C(38)	H(49)	109	H(48)	C(38)	H(49)	109
C(34)	C(39)	H(50)	109	C(34)	C(39)	H(51)	109
C(34)	C(39)	H(52)	109	H(50)	C(39)	H(51)	109
H(50)	C(39)	H(52)	109	H(51)	C(39)	H(52)	109
N(5)	C(41)	H(53)	111	N(5)	C(41)	H(54)	111
C(42)	C(41)	H(53)	111	C(42)	C(41)	H(54)	111
H(53)	C(41)	H(54)	109	N(6)	C(42)	H(55)	111
N(6)	C(42)	H(56)	111	C(41)	C(42)	H(55)	111
C(41)	C(42)	H(56)	111	H(55)	C(42)	H(56)	109
C(44)	C(45)	H(57)	120	C(46)	C(45)	H(57)	120
C(45)	C(46)	H(58)	120	C(47)	C(46)	H(58)	120
C(46)	C(47)	H(59)	119	C(48)	C(47)	H(59)	119
C(44)	C(49)	H(60)	109	C(44)	C(49)	H(61)	109
C(44)	C(49)	H(62)	109	H(60)	C(49)	H(61)	109
H(60)	C(49)	H(62)	109	H(61)	C(49)	H(62)	109
C(48)	C(50)	H(63)	109	C(48)	C(50)	H(64)	109
C(48)	C(50)	H(65)	109	H(63)	C(50)	H(64)	109
H(63)	C(50)	H(65)	109	H(64)	C(50)	H(65)	109
C(52)	C(53)	H(66)	119	C(54)	C(53)	H(66)	119
C(53)	C(54)	H(67)	120	C(55)	C(54)	H(67)	120
C(54)	C(55)	H(68)	119	C(56)	C(55)	H(68)	119
C(52)	C(57)	H(69)	109	C(52)	C(57)	H(70)	109
C(52)	C(57)	H(71)	109	H(69)	C(57)	H(70)	109
H(69)	C(57)	H(71)	109	H(70)	C(57)	H(71)	109
C(56)	C(58)	H(72)	109	C(56)	C(58)	H(73)	109

Table 8. Bond angles involving hydrogens (°) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
C(56)	C(58)	H(74)	109	H(72)	C(58)	H(73)	109
H(72)	C(58)	H(74)	109	H(73)	C(58)	H(74)	109

Table 9. Torsion Angles(°)

(Those having bond angles > 160 or < 20 degrees are excluded.)

atom1	atom2	atom3	atom4	angle	atom1	atom2	atom3	atom4	angle
Cl(1)	Ti(1)	C(1)	C(2)	-95.94(13)	Cl(1)	Ti(1)	C(1)	C(5)	18.26(18)
Cl(1)	Ti(1)	C(1)	C(6)	141.80(12)	Cl(1)	Ti(1)	C(2)	C(1)	121.64(9)
Cl(1)	Ti(1)	C(2)	C(3)	5.86(14)	Cl(1)	Ti(1)	C(2)	C(7)	-116.47(14)
Cl(1)	Ti(1)	C(3)	C(2)	-175.62(8)	Cl(1)	Ti(1)	C(3)	C(4)	68.93(10)
Cl(1)	Ti(1)	C(3)	C(8)	-52.52(16)	Cl(1)	Ti(1)	C(4)	C(3)	-111.74(10)
Cl(1)	Ti(1)	C(4)	C(5)	131.49(10)	Cl(1)	Ti(1)	C(4)	C(9)	7.12(16)
Cl(1)	Ti(1)	C(5)	C(1)	-168.01(8)	Cl(1)	Ti(1)	C(5)	C(4)	-51.17(11)
Cl(1)	Ti(1)	C(5)	C(10)	69.7(2)	Cl(2)	Ti(1)	C(1)	C(2)	158.89(10)
Cl(2)	Ti(1)	C(1)	C(5)	-86.91(10)	Cl(2)	Ti(1)	C(1)	C(6)	36.63(18)
Cl(2)	Ti(1)	C(2)	C(1)	-25.31(12)	Cl(2)	Ti(1)	C(2)	C(3)	-141.09(7)
Cl(2)	Ti(1)	C(2)	C(7)	96.58(16)	Cl(2)	Ti(1)	C(3)	C(2)	66.20(15)
Cl(2)	Ti(1)	C(3)	C(4)	-49.25(17)	Cl(2)	Ti(1)	C(3)	C(8)	-170.70(8)
Cl(2)	Ti(1)	C(4)	C(3)	150.45(7)	Cl(2)	Ti(1)	C(4)	C(5)	33.67(12)
Cl(2)	Ti(1)	C(4)	C(9)	-90.69(17)	Cl(2)	Ti(1)	C(5)	C(1)	92.68(10)
Cl(2)	Ti(1)	C(5)	C(4)	-150.48(10)	Cl(2)	Ti(1)	C(5)	C(10)	-29.65(19)
N(1)	Ti(1)	C(1)	C(2)	53.19(12)	N(1)	Ti(1)	C(1)	C(5)	167.39(10)
N(1)	Ti(1)	C(1)	C(6)	-69.1(2)	N(1)	Ti(1)	C(2)	C(1)	-130.81(11)
N(1)	Ti(1)	C(2)	C(3)	113.41(11)	N(1)	Ti(1)	C(2)	C(7)	-8.92(16)
N(1)	Ti(1)	C(3)	C(2)	-68.71(11)	N(1)	Ti(1)	C(3)	C(4)	175.84(10)
N(1)	Ti(1)	C(3)	C(8)	54.39(17)	N(1)	Ti(1)	C(4)	C(3)	-5.77(17)
N(1)	Ti(1)	C(4)	C(5)	-122.54(12)	N(1)	Ti(1)	C(4)	C(9)	113.09(17)
N(1)	Ti(1)	C(5)	C(1)	-20.0(3)	N(1)	Ti(1)	C(5)	C(4)	96.85(17)
N(1)	Ti(1)	C(5)	C(10)	-142.32(15)	C(1)	Ti(1)	C(2)	C(3)	-115.78(18)
C(1)	Ti(1)	C(2)	C(7)	121.9(3)	C(2)	Ti(1)	C(1)	C(5)	114.20(18)
C(2)	Ti(1)	C(1)	C(6)	-122.3(3)	C(1)	Ti(1)	C(3)	C(2)	37.58(11)
C(1)	Ti(1)	C(3)	C(4)	-77.87(12)	C(1)	Ti(1)	C(3)	C(8)	160.7(2)
C(3)	Ti(1)	C(1)	C(2)	-37.20(10)	C(3)	Ti(1)	C(1)	C(5)	77.00(12)
C(3)	Ti(1)	C(1)	C(6)	-159.5(3)	C(1)	Ti(1)	C(4)	C(3)	79.42(12)
C(1)	Ti(1)	C(4)	C(5)	-37.35(11)	C(1)	Ti(1)	C(4)	C(9)	-161.7(3)
C(4)	Ti(1)	C(1)	C(2)	-78.27(12)	C(4)	Ti(1)	C(1)	C(5)	35.93(10)
C(4)	Ti(1)	C(1)	C(6)	159.5(3)	C(1)	Ti(1)	C(5)	C(4)	116.84(19)
C(1)	Ti(1)	C(5)	C(10)	-122.3(3)	C(5)	Ti(1)	C(1)	C(2)	-114.20(19)
C(5)	Ti(1)	C(1)	C(6)	123.5(3)	C(2)	Ti(1)	C(3)	C(4)	-115.45(18)
C(2)	Ti(1)	C(3)	C(8)	123.1(3)	C(3)	Ti(1)	C(2)	C(1)	115.78(18)
C(3)	Ti(1)	C(2)	C(7)	-122.3(3)	C(2)	Ti(1)	C(4)	C(3)	37.58(10)
C(2)	Ti(1)	C(4)	C(5)	-79.19(12)	C(2)	Ti(1)	C(4)	C(9)	156.4(3)
C(4)	Ti(1)	C(2)	C(1)	78.41(11)	C(4)	Ti(1)	C(2)	C(3)	-37.38(10)

Table 9. Torsion angles (°) (continued)

atom1	atom2	atom3	atom4	angle
C(4)	Ti(1)	C(2)	C(7)	-159.7(2)
C(2)	Ti(1)	C(5)	C(4)	78.52(12)
C(5)	Ti(1)	C(2)	C(1)	38.25(11)
C(5)	Ti(1)	C(2)	C(7)	160.1(3)
C(3)	Ti(1)	C(4)	C(9)	118.9(3)
C(4)	Ti(1)	C(3)	C(8)	-121.4(3)
C(3)	Ti(1)	C(5)	C(4)	37.06(10)
C(5)	Ti(1)	C(3)	C(2)	79.31(12)
C(5)	Ti(1)	C(3)	C(8)	-157.6(2)
C(4)	Ti(1)	C(5)	C(4)	-0(609037)
C(5)	Ti(1)	C(4)	C(3)	116.77(19)
Cl(3)	Ti(2)	C(30)	C(31)	-67.60(14)
Cl(3)	Ti(2)	C(30)	C(35)	169.01(7)
Cl(3)	Ti(2)	C(31)	C(32)	24.61(12)
Cl(3)	Ti(2)	C(32)	C(31)	-159.62(9)
Cl(3)	Ti(2)	C(32)	C(37)	-38.23(15)
Cl(3)	Ti(2)	C(33)	C(34)	149.46(8)
Cl(3)	Ti(2)	C(34)	C(30)	-151.77(6)
Cl(3)	Ti(2)	C(34)	C(39)	88.77(15)
Cl(4)	Ti(2)	C(30)	C(34)	-70.44(8)
Cl(4)	Ti(2)	C(31)	C(30)	-7.20(13)
Cl(4)	Ti(2)	C(31)	C(36)	114.25(14)
Cl(4)	Ti(2)	C(32)	C(33)	-21.19(16)
Cl(4)	Ti(2)	C(33)	C(32)	166.21(7)
Cl(4)	Ti(2)	C(33)	C(38)	-72.37(15)
Cl(4)	Ti(2)	C(34)	C(33)	-133.05(9)
N(4)	Ti(2)	C(30)	C(31)	68.32(11)
N(4)	Ti(2)	C(30)	C(35)	-55.06(16)
N(4)	Ti(2)	C(31)	C(32)	129.75(10)
N(4)	Ti(2)	C(32)	C(31)	-54.31(12)
N(4)	Ti(2)	C(32)	C(37)	67.08(17)
N(4)	Ti(2)	C(33)	C(34)	-99.01(14)
N(4)	Ti(2)	C(34)	C(30)	4.68(16)
N(4)	Ti(2)	C(34)	C(39)	-114.78(16)
C(30)	Ti(2)	C(31)	C(36)	121.5(3)
C(31)	Ti(2)	C(30)	C(35)	-123.4(3)
C(30)	Ti(2)	C(32)	C(33)	-77.47(11)
C(2)	Ti(1)	C(5)	C(1)	-38.32(10)
C(2)	Ti(1)	C(5)	C(10)	-160.6(3)
C(5)	Ti(1)	C(2)	C(3)	-77.53(12)
C(3)	Ti(1)	C(4)	C(5)	-116.77(19)
C(4)	Ti(1)	C(3)	C(2)	115.45(18)
C(3)	Ti(1)	C(5)	C(1)	-79.78(12)
C(3)	Ti(1)	C(5)	C(10)	157.9(3)
C(5)	Ti(1)	C(3)	C(4)	-36.15(11)
C(4)	Ti(1)	C(5)	C(1)	-116.84(19)
C(4)	Ti(1)	C(5)	C(10)	120.8(3)
C(5)	Ti(1)	C(4)	C(9)	-124.4(3)
Cl(3)	Ti(2)	C(30)	C(34)	47.40(15)
Cl(3)	Ti(2)	C(31)	C(30)	140.75(6)
Cl(3)	Ti(2)	C(31)	C(36)	-97.80(14)
Cl(3)	Ti(2)	C(32)	C(33)	85.71(9)
Cl(3)	Ti(2)	C(33)	C(32)	-94.07(8)
Cl(3)	Ti(2)	C(33)	C(38)	27.36(14)
Cl(3)	Ti(2)	C(34)	C(33)	-34.79(11)
Cl(4)	Ti(2)	C(30)	C(31)	174.56(8)
Cl(4)	Ti(2)	C(30)	C(35)	51.18(14)
Cl(4)	Ti(2)	C(31)	C(32)	-123.34(8)
Cl(4)	Ti(2)	C(32)	C(31)	93.48(12)
Cl(4)	Ti(2)	C(32)	C(37)	-145.13(10)
Cl(4)	Ti(2)	C(33)	C(34)	49.73(9)
Cl(4)	Ti(2)	C(34)	C(30)	109.96(8)
Cl(4)	Ti(2)	C(34)	C(39)	-9.50(15)
N(4)	Ti(2)	C(30)	C(34)	-176.67(9)
N(4)	Ti(2)	C(31)	C(30)	-114.12(10)
N(4)	Ti(2)	C(31)	C(36)	7.34(15)
N(4)	Ti(2)	C(32)	C(33)	-168.98(9)
N(4)	Ti(2)	C(33)	C(32)	17.47(18)
N(4)	Ti(2)	C(33)	C(38)	138.89(14)
N(4)	Ti(2)	C(34)	C(33)	121.66(11)
C(30)	Ti(2)	C(31)	C(32)	-116.13(17)
C(31)	Ti(2)	C(30)	C(34)	115.01(16)
C(30)	Ti(2)	C(32)	C(31)	37.20(9)
C(30)	Ti(2)	C(32)	C(37)	158.59(19)

Table 9. Torsion angles (°) (continued)

atom1	atom2	atom3	atom4	angle
C(32)	Ti(2)	C(30)	C(31)	-37.21(9)
C(32)	Ti(2)	C(30)	C(35)	-160.59(19)
C(30)	Ti(2)	C(33)	C(34)	-36.95(9)
C(33)	Ti(2)	C(30)	C(31)	-78.86(10)
C(33)	Ti(2)	C(30)	C(35)	157.76(18)
C(30)	Ti(2)	C(34)	C(39)	-119.5(3)
C(34)	Ti(2)	C(30)	C(35)	121.6(2)
C(31)	Ti(2)	C(32)	C(33)	-114.67(17)
C(32)	Ti(2)	C(31)	C(30)	116.13(17)
C(31)	Ti(2)	C(33)	C(32)	37.94(9)
C(31)	Ti(2)	C(33)	C(38)	159.36(18)
C(33)	Ti(2)	C(31)	C(32)	-38.09(9)
C(31)	Ti(2)	C(34)	C(30)	-37.90(9)
C(31)	Ti(2)	C(34)	C(39)	-157.35(19)
C(34)	Ti(2)	C(31)	C(32)	-78.49(10)
C(32)	Ti(2)	C(33)	C(34)	-116.48(17)
C(33)	Ti(2)	C(32)	C(31)	114.67(17)
C(32)	Ti(2)	C(34)	C(30)	-79.50(11)
C(32)	Ti(2)	C(34)	C(39)	161.0(2)
C(34)	Ti(2)	C(32)	C(33)	-36.28(9)
C(33)	Ti(2)	C(34)	C(30)	-116.98(17)
C(33)	Ti(2)	C(34)	C(39)	123.6(3)
C(34)	Ti(2)	C(33)	C(34)	-0(899792)
C(59)	Cl(5)	C(59)[1]	Cl(5)[1]	-77.5(8)
C(59)[1]	Cl(5)	C(59)	Cl(5)[1]	82.9(8)
C(11)	N(2)	C(12)	C(13)	12.8(3)
C(12)	N(2)	C(11)	N(3)	-8.9(3)
C(11)	N(2)	C(14)	C(19)	-119.9(2)
C(14)	N(2)	C(11)	N(3)	-169.92(17)
C(12)	N(2)	C(14)	C(19)	80.7(3)
C(11)	N(3)	C(13)	C(12)	7.0(3)
C(13)	N(3)	C(11)	N(2)	0.7(3)
C(11)	N(3)	C(22)	C(27)	110.1(3)
C(22)	N(3)	C(11)	N(2)	178.00(18)
C(13)	N(3)	C(22)	C(27)	-73.0(3)
C(40)	N(5)	C(41)	C(42)	-3.8(3)
C(41)	N(5)	C(40)	N(6)	-0.8(3)
C(32)	Ti(2)	C(30)	C(34)	77.80(11)
C(30)	Ti(2)	C(33)	C(32)	79.52(10)
C(30)	Ti(2)	C(33)	C(38)	-159.06(18)
C(33)	Ti(2)	C(30)	C(34)	36.15(9)
C(30)	Ti(2)	C(34)	C(33)	116.98(17)
C(34)	Ti(2)	C(30)	C(31)	-115.01(16)
C(31)	Ti(2)	C(32)	C(31)	0(612250)
C(31)	Ti(2)	C(32)	C(37)	121.4(3)
C(32)	Ti(2)	C(31)	C(36)	-122.4(3)
C(31)	Ti(2)	C(33)	C(34)	-78.54(11)
C(33)	Ti(2)	C(31)	C(30)	78.05(10)
C(33)	Ti(2)	C(31)	C(36)	-160.50(19)
C(31)	Ti(2)	C(34)	C(33)	79.09(11)
C(34)	Ti(2)	C(31)	C(30)	37.65(9)
C(34)	Ti(2)	C(31)	C(36)	159.10(19)
C(32)	Ti(2)	C(33)	C(38)	121.4(3)
C(33)	Ti(2)	C(32)	C(37)	-123.9(3)
C(32)	Ti(2)	C(34)	C(33)	37.48(9)
C(34)	Ti(2)	C(32)	C(31)	78.39(11)
C(34)	Ti(2)	C(32)	C(37)	-160.22(19)
C(33)	Ti(2)	C(34)	C(33)	-0(904273)
C(34)	Ti(2)	C(33)	C(32)	116.48(17)
C(34)	Ti(2)	C(33)	C(38)	-122.1(2)
C(59)	Cl(5)	C(59)[1]	Cl(6)[1]	19.7(7)
C(59)[1]	Cl(5)	C(59)	Cl(6)	-12.3(7)
C(12)	N(2)	C(11)	N(1)	171.30(18)
C(11)	N(2)	C(14)	C(15)	63.2(3)
C(14)	N(2)	C(11)	N(1)	10.3(4)
C(12)	N(2)	C(14)	C(15)	-96.2(3)
C(14)	N(2)	C(12)	C(13)	174.65(16)
C(13)	N(3)	C(11)	N(1)	-179.46(19)
C(11)	N(3)	C(22)	C(23)	-70.3(3)
C(22)	N(3)	C(11)	N(1)	-2.2(4)
C(13)	N(3)	C(22)	C(23)	106.6(3)
C(22)	N(3)	C(13)	C(12)	-170.24(18)
C(41)	N(5)	C(40)	N(4)	178.04(19)
C(40)	N(5)	C(43)	C(44)	70.9(3)

Table 9. Torsion angles (°) (continued)

atom1	atom2	atom3	atom4	angle	atom1	atom2	atom3	atom4	angle
C(40)	N(5)	C(43)	C(48)	-111.0(3)	C(43)	N(5)	C(40)	N(4)	7.2(4)
C(43)	N(5)	C(40)	N(6)	-171.60(18)	C(41)	N(5)	C(43)	C(44)	-98.9(3)
C(41)	N(5)	C(43)	C(48)	79.2(3)	C(43)	N(5)	C(41)	C(42)	167.21(18)
C(40)	N(6)	C(42)	C(41)	-7.6(3)	C(42)	N(6)	C(40)	N(4)	-173.37(19)
C(42)	N(6)	C(40)	N(5)	5.5(3)	C(40)	N(6)	C(51)	C(52)	-70.4(3)
C(40)	N(6)	C(51)	C(56)	111.1(3)	C(51)	N(6)	C(40)	N(4)	-2.9(4)
C(51)	N(6)	C(40)	N(5)	175.94(18)	C(42)	N(6)	C(51)	C(52)	99.0(3)
C(42)	N(6)	C(51)	C(56)	-79.5(3)	C(51)	N(6)	C(42)	C(41)	-178.12(18)
Ti(1)	C(1)	C(2)	C(3)	65.07(13)	Ti(1)	C(1)	C(2)	C(7)	-117.2(2)
Ti(1)	C(1)	C(5)	C(4)	-64.70(15)	Ti(1)	C(1)	C(5)	C(10)	116.4(3)
C(2)	C(1)	C(5)	Ti(1)	65.46(17)	C(2)	C(1)	C(5)	C(4)	0.8(3)
C(2)	C(1)	C(5)	C(10)	-178.1(2)	C(5)	C(1)	C(2)	Ti(1)	-66.64(17)
C(5)	C(1)	C(2)	C(3)	-1.6(3)	C(5)	C(1)	C(2)	C(7)	176.16(19)
C(6)	C(1)	C(2)	Ti(1)	115.7(3)	C(6)	C(1)	C(2)	C(3)	-179.2(3)
C(6)	C(1)	C(2)	C(7)	-1.5(4)	C(6)	C(1)	C(5)	Ti(1)	-116.9(3)
C(6)	C(1)	C(5)	C(4)	178.4(3)	C(6)	C(1)	C(5)	C(10)	-0.4(5)
Ti(1)	C(2)	C(3)	C(4)	66.48(12)	Ti(1)	C(2)	C(3)	C(8)	-115.94(18)
C(1)	C(2)	C(3)	Ti(1)	-64.68(16)	C(1)	C(2)	C(3)	C(4)	1.8(3)
C(1)	C(2)	C(3)	C(8)	179.38(18)	C(7)	C(2)	C(3)	Ti(1)	117.6(3)
C(7)	C(2)	C(3)	C(4)	-175.9(2)	C(7)	C(2)	C(3)	C(8)	1.7(4)
Ti(1)	C(3)	C(4)	C(5)	63.53(12)	Ti(1)	C(3)	C(4)	C(9)	-121.42(17)
C(2)	C(3)	C(4)	Ti(1)	-64.86(15)	C(2)	C(3)	C(4)	C(5)	-1.3(3)
C(2)	C(3)	C(4)	C(9)	173.72(17)	C(8)	C(3)	C(4)	Ti(1)	117.5(3)
C(8)	C(3)	C(4)	C(5)	-179.0(2)	C(8)	C(3)	C(4)	C(9)	-3.9(4)
Ti(1)	C(4)	C(5)	Ti(1)	0(979275)	Ti(1)	C(4)	C(5)	C(1)	62.81(14)
Ti(1)	C(4)	C(5)	C(10)	-118.3(2)	C(3)	C(4)	C(5)	Ti(1)	-62.47(15)
C(3)	C(4)	C(5)	C(1)	0.3(3)	C(3)	C(4)	C(5)	C(10)	179.25(18)
C(9)	C(4)	C(5)	Ti(1)	122.7(3)	C(9)	C(4)	C(5)	C(1)	-174.5(2)
C(9)	C(4)	C(5)	C(10)	4.4(4)	N(2)	C(12)	C(13)	N(3)	-11.3(3)
N(2)	C(14)	C(15)	C(16)	-179.62(17)	N(2)	C(14)	C(15)	C(20)	2.4(3)
N(2)	C(14)	C(19)	C(18)	-178.98(17)	N(2)	C(14)	C(19)	C(21)	-0.6(4)
C(15)	C(14)	C(19)	C(18)	-2.2(4)	C(15)	C(14)	C(19)	C(21)	176.17(19)
C(19)	C(14)	C(15)	C(16)	3.6(4)	C(19)	C(14)	C(15)	C(20)	-174.36(19)
C(14)	C(15)	C(16)	C(17)	-2.2(4)	C(20)	C(15)	C(16)	C(17)	175.9(2)
C(15)	C(16)	C(17)	C(18)	-0.6(5)	C(16)	C(17)	C(18)	C(19)	2.1(5)
C(17)	C(18)	C(19)	C(14)	-0.7(4)	C(17)	C(18)	C(19)	C(21)	-179.1(3)
N(3)	C(22)	C(23)	C(24)	177.01(18)	N(3)	C(22)	C(23)	C(28)	-2.7(4)

Table 9. Torsion angles (°) (continued)

atom1	atom2	atom3	atom4	angle
N(3)	C(22)	C(27)	C(26)	-179.46(18)
C(23)	C(22)	C(27)	C(26)	1.0(4)
C(27)	C(22)	C(23)	C(24)	-3.4(4)
C(22)	C(23)	C(24)	C(25)	3.0(5)
C(23)	C(24)	C(25)	C(26)	-0.2(6)
C(25)	C(26)	C(27)	C(22)	2.0(5)
Ti(2)	C(30)	C(31)	C(32)	64.31(13)
Ti(2)	C(30)	C(34)	C(33)	-63.16(12)
C(31)	C(30)	C(34)	Ti(2)	65.08(15)
C(31)	C(30)	C(34)	C(39)	-173.91(18)
C(34)	C(30)	C(31)	C(32)	-2.6(3)
C(35)	C(30)	C(31)	Ti(2)	115.5(3)
C(35)	C(30)	C(31)	C(36)	-4.1(4)
C(35)	C(30)	C(34)	C(33)	179.5(2)
Ti(2)	C(31)	C(32)	Ti(2)	0(665142)
Ti(2)	C(31)	C(32)	C(37)	-114.7(2)
C(30)	C(31)	C(32)	C(33)	2.3(3)
C(36)	C(31)	C(32)	Ti(2)	119.2(3)
C(36)	C(31)	C(32)	C(37)	4.5(4)
Ti(2)	C(32)	C(33)	C(38)	-116.3(2)
C(31)	C(32)	C(33)	C(34)	-1.1(3)
C(37)	C(32)	C(33)	Ti(2)	116.0(3)
C(37)	C(32)	C(33)	C(38)	-0.2(4)
Ti(2)	C(33)	C(34)	C(39)	-122.4(2)
C(32)	C(33)	C(34)	C(30)	-0.5(3)
C(38)	C(33)	C(34)	Ti(2)	118.5(3)
C(38)	C(33)	C(34)	C(39)	-3.9(4)
N(5)	C(43)	C(44)	C(45)	-179.10(18)
N(5)	C(43)	C(48)	C(47)	179.81(19)
C(44)	C(43)	C(48)	C(47)	-2.1(4)
C(48)	C(43)	C(44)	C(45)	2.9(4)
C(43)	C(44)	C(45)	C(46)	-1.3(4)
C(44)	C(45)	C(46)	C(47)	-0.9(5)
C(46)	C(47)	C(48)	C(43)	-0.2(5)
N(6)	C(51)	C(52)	C(53)	178.06(18)
N(6)	C(51)	C(56)	C(55)	-177.78(19)
C(52)	C(51)	C(56)	C(55)	3.8(4)
N(3)	C(22)	C(27)	C(29)	-0.4(4)
C(23)	C(22)	C(27)	C(29)	-180.0(2)
C(27)	C(22)	C(23)	C(28)	176.8(2)
C(28)	C(23)	C(24)	C(25)	-177.2(3)
C(24)	C(25)	C(26)	C(27)	-2.4(6)
C(25)	C(26)	C(27)	C(29)	-177.1(3)
Ti(2)	C(30)	C(31)	C(36)	-119.6(2)
Ti(2)	C(30)	C(34)	C(39)	121.02(18)
C(31)	C(30)	C(34)	C(33)	1.9(3)
C(34)	C(30)	C(31)	Ti(2)	-66.92(15)
C(34)	C(30)	C(31)	C(36)	173.46(18)
C(35)	C(30)	C(31)	C(32)	179.8(3)
C(35)	C(30)	C(34)	Ti(2)	-117.3(3)
C(35)	C(30)	C(34)	C(39)	3.7(4)
Ti(2)	C(31)	C(32)	C(33)	67.03(13)
C(30)	C(31)	C(32)	Ti(2)	-64.73(16)
C(30)	C(31)	C(32)	C(37)	-179.47(18)
C(36)	C(31)	C(32)	C(33)	-173.7(3)
Ti(2)	C(32)	C(33)	C(34)	64.64(13)
C(31)	C(32)	C(33)	Ti(2)	-65.75(16)
C(31)	C(32)	C(33)	C(38)	177.96(19)
C(37)	C(32)	C(33)	C(34)	-179.3(2)
Ti(2)	C(33)	C(34)	C(30)	61.93(12)
C(32)	C(33)	C(34)	Ti(2)	-62.43(16)
C(32)	C(33)	C(34)	C(39)	175.20(18)
C(38)	C(33)	C(34)	C(30)	-179.6(2)
N(5)	C(41)	C(42)	N(6)	6.5(3)
N(5)	C(43)	C(44)	C(49)	1.1(4)
N(5)	C(43)	C(48)	C(50)	-0.7(4)
C(44)	C(43)	C(48)	C(50)	177.4(2)
C(48)	C(43)	C(44)	C(49)	-176.9(2)
C(49)	C(44)	C(45)	C(46)	178.4(3)
C(45)	C(46)	C(47)	C(48)	1.7(6)
C(46)	C(47)	C(48)	C(50)	-179.7(3)
N(6)	C(51)	C(52)	C(57)	-3.5(4)
N(6)	C(51)	C(56)	C(58)	3.9(4)
C(52)	C(51)	C(56)	C(58)	-174.5(2)

Table 9. Torsion angles (°) (continued)

atom1	atom2	atom3	atom4	angle
C(56)	C(51)	C(52)	C(53)	-3.5(4)
C(51)	C(52)	C(53)	C(54)	0.4(4)
C(52)	C(53)	C(54)	C(55)	2.3(5)
C(54)	C(55)	C(56)	C(51)	-1.0(4)
Cl(5)	C(59)	C(59)[1]	Cl(5)[1]	45.5(3)
Cl(5)[1]	C(59)	C(59)[1]	Cl(5)	-45.5(3)
Cl(6)	C(59)	C(59)[1]	Cl(5)[1]	-151.8(9)
Cl(6)	C(59)	C(59)[1]	Cl(6)[1]	10.9(8)
C(56)	C(51)	C(52)	C(57)	174.9(2)
C(57)	C(52)	C(53)	C(54)	-178.0(3)
C(53)	C(54)	C(55)	C(56)	-2.0(5)
C(54)	C(55)	C(56)	C(58)	177.4(3)
Cl(5)	C(59)	C(59)[1]	Cl(6)[1]	-151.8(9)
Cl(5)[1]	C(59)	C(59)[1]	Cl(6)[1]	162.7(10)
Cl(6)	C(59)	C(59)[1]	Cl(5)	162.7(10)

Symmetry Operators:

(1) -X+1,-Y,Z

Table 10. Intramolecular contacts less than 3.60 Å

atom	atom	distance	atom	atom	distance
Cl(1)	C(9)	3.279(4)	Cl(1)	C(23)	3.566(3)
Cl(2)	C(6)	3.464(5)	Cl(2)	C(10)	3.415(4)
Cl(3)	C(37)	3.482(3)	Cl(3)	C(38)	3.405(4)
Cl(4)	C(39)	3.284(3)	Cl(4)	C(44)	3.586(3)
N(1)	C(7)	3.104(4)	N(1)	C(12)	3.596(3)
N(1)	C(13)	3.597(3)	N(1)	C(14)	2.960(3)
N(1)	C(15)	3.316(3)	N(1)	C(20)	3.291(4)
N(1)	C(22)	2.914(3)	N(1)	C(23)	3.309(3)
N(1)	C(28)	3.340(4)	N(2)	C(20)	2.904(4)
N(2)	C(21)	2.901(4)	N(2)	C(22)	3.586(3)
N(3)	C(14)	3.586(3)	N(3)	C(28)	2.873(4)
N(3)	C(29)	2.889(4)	N(4)	C(36)	3.152(4)
N(4)	C(41)	3.599(4)	N(4)	C(42)	3.596(3)
N(4)	C(43)	2.926(3)	N(4)	C(44)	3.371(3)
N(4)	C(49)	3.400(4)	N(4)	C(51)	2.929(3)
N(4)	C(52)	3.340(4)	N(4)	C(57)	3.383(4)
N(5)	C(49)	2.857(4)	N(5)	C(50)	2.877(4)
N(5)	C(51)	3.585(3)	N(6)	C(43)	3.579(3)
N(6)	C(57)	2.884(4)	N(6)	C(58)	2.894(4)
C(6)	C(7)	3.185(6)	C(6)	C(10)	3.223(6)
C(7)	C(8)	3.197(5)	C(7)	C(11)	3.447(4)
C(8)	C(9)	3.115(6)	C(9)	C(10)	3.166(6)
C(11)	C(15)	3.137(3)	C(11)	C(19)	3.522(3)
C(11)	C(20)	3.160(4)	C(11)	C(23)	3.175(3)
C(11)	C(27)	3.459(3)	C(11)	C(28)	3.230(4)
C(12)	C(15)	3.409(4)	C(12)	C(19)	3.279(4)
C(12)	C(21)	3.402(4)	C(13)	C(23)	3.513(4)
C(13)	C(27)	3.260(4)	C(13)	C(29)	3.311(4)
C(14)	C(17)	2.752(4)	C(15)	C(18)	2.779(4)
C(16)	C(19)	2.796(4)	C(22)	C(25)	2.751(4)
C(23)	C(26)	2.789(5)	C(24)	C(27)	2.784(5)
C(35)	C(36)	3.191(5)	C(35)	C(39)	3.132(5)
C(36)	C(37)	3.170(5)	C(36)	C(40)	3.527(4)
C(37)	C(38)	3.221(5)	C(38)	C(39)	3.181(5)
C(40)	C(44)	3.184(4)	C(40)	C(48)	3.468(4)
C(40)	C(49)	3.213(4)	C(40)	C(52)	3.186(4)
C(40)	C(56)	3.467(4)	C(40)	C(57)	3.248(4)

Table 10. Intramolecular contacts less than 3.60 Å (continued)

atom	atom	distance	atom	atom	distance
C(41)	C(44)	3.452(4)	C(41)	C(48)	3.301(4)
C(41)	C(50)	3.380(4)	C(42)	C(52)	3.471(4)
C(42)	C(56)	3.312(4)	C(42)	C(58)	3.379(5)
C(43)	C(46)	2.753(5)	C(44)	C(47)	2.787(5)
C(45)	C(48)	2.795(4)	C(51)	C(54)	2.759(5)
C(52)	C(55)	2.792(4)	C(53)	C(56)	2.792(4)

Table 11. Intramolecular contacts less than 3.60 Å involving hydrogens

atom	atom	distance	atom	atom	distance
Ti(1)	H(1)	3.358	Ti(1)	H(4)	3.472
Ti(1)	H(5)	3.595	Ti(1)	H(7)	3.314
Ti(1)	H(12)	3.472	Ti(1)	H(13)	3.469
Ti(1)	H(24)	3.453	Ti(1)	H(34)	3.455
Ti(2)	H(38)	3.332	Ti(2)	H(42)	3.447
Ti(2)	H(44)	3.331	Ti(2)	H(47)	3.472
Ti(2)	H(51)	3.465	Ti(2)	H(60)	3.553
Ti(2)	H(69)	3.530	Cl(1)	H(7)	3.280
Cl(1)	H(12)	2.645	Cl(1)	H(34)	3.063
Cl(2)	H(1)	2.811	Cl(2)	H(13)	3.309
Cl(2)	H(15)	3.118	Cl(2)	H(24)	2.835
Cl(3)	H(44)	3.360	Cl(3)	H(46)	3.207
Cl(3)	H(47)	3.271	Cl(3)	H(48)	3.126
Cl(3)	H(69)	2.928	Cl(4)	H(38)	3.221
Cl(4)	H(51)	2.638	Cl(4)	H(60)	3.214
N(1)	H(4)	2.786	N(1)	H(5)	3.141
N(1)	H(23)	3.367	N(1)	H(24)	2.761
N(1)	H(34)	2.705	N(2)	H(4)	3.349
N(2)	H(5)	3.389	N(2)	H(18)	2.926
N(2)	H(19)	3.074	N(2)	H(23)	2.622
N(2)	H(24)	3.125	N(2)	H(27)	2.453
N(2)	H(28)	3.429	N(3)	H(4)	3.440
N(3)	H(16)	2.927	N(3)	H(17)	3.076
N(3)	H(23)	3.520	N(3)	H(32)	2.702
N(3)	H(34)	2.947	N(3)	H(35)	3.172
N(3)	H(36)	2.561	N(4)	H(41)	3.296
N(4)	H(42)	2.762	N(4)	H(60)	2.736
N(4)	H(69)	2.777	N(5)	H(42)	3.436
N(5)	H(55)	3.049	N(5)	H(56)	2.963
N(5)	H(60)	2.881	N(5)	H(62)	2.724
N(5)	H(63)	2.579	N(5)	H(64)	3.107
N(6)	H(42)	3.396	N(6)	H(53)	3.046
N(6)	H(54)	2.961	N(6)	H(69)	2.993
N(6)	H(70)	2.679	N(6)	H(72)	2.549
N(6)	H(74)	3.199	C(1)	H(4)	3.304
C(1)	H(5)	2.704	C(1)	H(6)	3.082
C(1)	H(13)	3.293	C(1)	H(14)	3.141

Table 11. Intramolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
C(1)	H(15)	2.711	C(2)	H(1)	3.249
C(2)	H(2)	3.139	C(2)	H(3)	2.672
C(2)	H(7)	3.200	C(2)	H(8)	2.678
C(2)	H(9)	3.200	C(3)	H(4)	2.757
C(3)	H(5)	3.339	C(3)	H(6)	2.975
C(3)	H(10)	2.813	C(3)	H(11)	3.354
C(3)	H(12)	2.858	C(4)	H(7)	2.849
C(4)	H(8)	3.350	C(4)	H(9)	2.817
C(4)	H(13)	2.742	C(4)	H(14)	2.903
C(4)	H(15)	3.320	C(5)	H(1)	2.822
C(5)	H(2)	2.915	C(5)	H(3)	3.367
C(5)	H(10)	3.192	C(5)	H(11)	2.690
C(5)	H(12)	3.211	C(6)	H(5)	2.820
C(6)	H(6)	3.596	C(6)	H(15)	2.839
C(7)	H(3)	2.770	C(7)	H(8)	2.775
C(7)	H(26)	3.423	C(7)	H(27)	3.224
C(7)	H(36)	3.580	C(8)	H(4)	2.955
C(8)	H(6)	3.415	C(8)	H(10)	3.048
C(8)	H(12)	3.095	C(9)	H(7)	3.125
C(9)	H(9)	3.017	C(9)	H(13)	2.994
C(9)	H(14)	3.274	C(10)	H(1)	3.101
C(10)	H(2)	3.293	C(10)	H(11)	2.750
C(11)	H(4)	2.882	C(11)	H(5)	3.369
C(11)	H(16)	2.910	C(11)	H(17)	3.060
C(11)	H(18)	2.953	C(11)	H(19)	3.035
C(11)	H(23)	2.908	C(11)	H(24)	2.975
C(11)	H(27)	3.302	C(11)	H(32)	3.163
C(11)	H(34)	2.875	C(11)	H(36)	3.177
C(12)	H(23)	3.010	C(12)	H(27)	2.878
C(12)	H(28)	3.567	C(13)	H(32)	3.248
C(13)	H(35)	3.169	C(13)	H(36)	3.009
C(14)	H(5)	3.349	C(14)	H(16)	2.757
C(14)	H(17)	2.822	C(14)	H(20)	3.246
C(14)	H(22)	3.238	C(14)	H(23)	2.671
C(14)	H(24)	2.934	C(14)	H(25)	3.293
C(14)	H(26)	3.218	C(14)	H(27)	2.608
C(14)	H(28)	3.092	C(15)	H(16)	3.290

Table 11. Intramolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
C(15)	H(21)	3.245	C(16)	H(22)	3.220
C(16)	H(23)	3.217	C(16)	H(24)	2.994
C(16)	H(25)	2.559	C(18)	H(3)	3.540
C(18)	H(20)	3.224	C(18)	H(26)	2.694
C(18)	H(27)	3.296	C(18)	H(28)	2.821
C(19)	H(3)	3.480	C(19)	H(5)	3.081
C(19)	H(17)	3.156	C(19)	H(21)	3.262
C(20)	H(16)	3.307	C(20)	H(20)	2.645
C(20)	H(34)	3.248	C(21)	H(5)	2.887
C(21)	H(17)	2.928	C(21)	H(22)	2.656
C(22)	H(7)	3.595	C(22)	H(18)	2.891
C(22)	H(19)	2.777	C(22)	H(29)	3.233
C(22)	H(31)	3.245	C(22)	H(32)	2.703
C(22)	H(33)	3.297	C(22)	H(34)	2.841
C(22)	H(35)	2.951	C(22)	H(36)	2.646
C(22)	H(37)	3.277	C(23)	H(19)	3.453
C(23)	H(30)	3.253	C(24)	H(31)	3.230
C(24)	H(32)	3.185	C(24)	H(33)	2.558
C(24)	H(34)	3.059	C(26)	H(7)	3.302
C(26)	H(29)	3.230	C(26)	H(35)	2.954
C(26)	H(36)	3.228	C(26)	H(37)	2.568
C(27)	H(7)	3.251	C(27)	H(8)	3.336
C(27)	H(18)	3.168	C(27)	H(19)	3.560
C(27)	H(30)	3.255	C(28)	H(19)	3.581
C(28)	H(23)	3.415	C(28)	H(24)	3.421
C(28)	H(29)	2.660	C(29)	H(4)	3.491
C(29)	H(8)	3.137	C(29)	H(18)	2.818
C(29)	H(31)	2.642	C(30)	H(41)	3.348
C(30)	H(42)	2.783	C(30)	H(43)	2.910
C(30)	H(50)	2.820	C(30)	H(51)	2.860
C(30)	H(52)	3.357	C(31)	H(38)	3.232
C(31)	H(39)	3.188	C(31)	H(40)	2.690
C(31)	H(44)	2.788	C(31)	H(45)	2.904
C(31)	H(46)	3.346	C(32)	H(41)	2.685
C(32)	H(42)	3.269	C(32)	H(43)	3.115
C(32)	H(47)	3.282	C(32)	H(48)	2.695
C(32)	H(49)	3.139	C(33)	H(44)	3.280

Table 11. Intramolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
C(33)	H(45)	3.157	C(33)	H(46)	2.702
C(33)	H(50)	3.192	C(33)	H(51)	3.206
C(33)	H(52)	2.676	C(34)	H(38)	2.831
C(34)	H(39)	2.851	C(34)	H(40)	3.359
C(34)	H(47)	2.769	C(34)	H(48)	3.338
C(34)	H(49)	2.918	C(35)	H(42)	3.016
C(35)	H(43)	3.312	C(35)	H(50)	3.070
C(35)	H(51)	3.111	C(35)	H(63)	3.516
C(36)	H(40)	2.777	C(36)	H(44)	3.044
C(36)	H(45)	3.233	C(36)	H(63)	3.566
C(36)	H(72)	2.994	C(37)	H(41)	2.766
C(37)	H(48)	2.823	C(38)	H(46)	2.821
C(38)	H(52)	2.760	C(39)	H(38)	3.092
C(39)	H(39)	3.090	C(39)	H(47)	3.023
C(39)	H(49)	3.285	C(40)	H(41)	3.571
C(40)	H(42)	2.883	C(40)	H(53)	3.019
C(40)	H(54)	2.975	C(40)	H(55)	3.036
C(40)	H(56)	2.948	C(40)	H(60)	2.807
C(40)	H(62)	3.189	C(40)	H(63)	3.199
C(40)	H(69)	2.932	C(40)	H(70)	3.139
C(40)	H(72)	3.222	C(41)	H(62)	3.137
C(41)	H(63)	3.147	C(41)	H(64)	3.174
C(42)	H(70)	3.096	C(42)	H(72)	3.046
C(42)	H(74)	3.271	C(43)	H(53)	2.749
C(43)	H(54)	2.900	C(43)	H(57)	3.244
C(43)	H(59)	3.246	C(43)	H(60)	2.802
C(43)	H(61)	3.298	C(43)	H(62)	2.716
C(43)	H(63)	2.653	C(43)	H(64)	2.914
C(43)	H(65)	3.285	C(44)	H(53)	3.340
C(44)	H(58)	3.255	C(45)	H(59)	3.231
C(45)	H(60)	3.101	C(45)	H(61)	2.568
C(45)	H(62)	3.174	C(47)	H(38)	3.374
C(47)	H(57)	3.232	C(47)	H(63)	3.222
C(47)	H(64)	2.983	C(47)	H(65)	2.571
C(48)	H(38)	3.300	C(48)	H(40)	3.292
C(48)	H(53)	3.589	C(48)	H(54)	3.234
C(48)	H(58)	3.252	C(49)	H(53)	3.405

Table 11. Intramolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
C(49)	H(57)	2.683	C(49)	H(69)	3.372
C(49)	H(70)	3.594	C(50)	H(40)	3.051
C(50)	H(42)	3.544	C(50)	H(54)	2.928
C(50)	H(59)	2.654	C(51)	H(41)	3.535
C(51)	H(44)	3.483	C(51)	H(55)	2.841
C(51)	H(56)	2.819	C(51)	H(66)	3.238
C(51)	H(68)	3.247	C(51)	H(69)	2.859
C(51)	H(70)	2.682	C(51)	H(71)	3.293
C(51)	H(72)	2.654	C(51)	H(73)	3.287
C(51)	H(74)	2.958	C(52)	H(56)	3.394
C(52)	H(67)	3.256	C(53)	H(68)	3.232
C(53)	H(69)	3.052	C(53)	H(70)	3.193
C(53)	H(71)	2.564	C(54)	H(44)	3.357
C(55)	H(44)	3.183	C(55)	H(66)	3.233
C(55)	H(72)	3.235	C(55)	H(73)	2.579
C(55)	H(74)	2.940	C(56)	H(41)	3.109
C(56)	H(44)	3.269	C(56)	H(55)	3.175
C(56)	H(67)	3.263	C(57)	H(56)	3.372
C(57)	H(60)	3.262	C(57)	H(66)	2.663
C(58)	H(41)	2.904	C(58)	H(42)	3.489
C(58)	H(55)	2.892	C(58)	H(68)	2.641
H(1)	H(5)	3.502	H(1)	H(15)	2.500
H(2)	H(5)	3.405	H(2)	H(14)	3.536
H(2)	H(15)	2.882	H(3)	H(4)	3.572
H(3)	H(5)	2.163	H(3)	H(6)	3.196
H(3)	H(26)	3.573	H(4)	H(7)	3.466
H(4)	H(8)	2.345	H(4)	H(27)	2.987
H(4)	H(36)	2.618	H(5)	H(26)	2.612
H(5)	H(27)	2.639	H(6)	H(8)	2.924
H(7)	H(10)	3.196	H(7)	H(12)	2.804
H(7)	H(31)	3.599	H(7)	H(37)	3.562
H(8)	H(36)	2.826	H(8)	H(37)	2.876
H(9)	H(10)	2.651	H(9)	H(12)	3.108
H(11)	H(13)	2.425	H(11)	H(14)	2.750
H(12)	H(13)	3.464	H(16)	H(18)	2.792
H(16)	H(19)	2.240	H(16)	H(23)	2.553
H(17)	H(18)	2.239	H(17)	H(19)	2.690

Table 11. Intramolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
H(17)	H(27)	2.435	H(17)	H(28)	2.888
H(18)	H(35)	2.488	H(18)	H(36)	2.546
H(19)	H(32)	2.898	H(19)	H(35)	3.569
H(20)	H(21)	2.291	H(20)	H(23)	3.462
H(20)	H(24)	3.082	H(20)	H(25)	2.373
H(21)	H(22)	2.306	H(22)	H(26)	2.588
H(22)	H(27)	3.569	H(22)	H(28)	2.813
H(23)	H(32)	2.933	H(23)	H(34)	2.994
H(24)	H(32)	3.382	H(24)	H(34)	2.627
H(29)	H(30)	2.302	H(29)	H(32)	3.415
H(29)	H(33)	2.359	H(29)	H(34)	3.196
H(30)	H(31)	2.309	H(31)	H(35)	3.032
H(31)	H(36)	3.484	H(31)	H(37)	2.397
H(38)	H(42)	3.576	H(38)	H(50)	3.157
H(38)	H(51)	2.770	H(38)	H(65)	3.581
H(39)	H(50)	2.729	H(39)	H(51)	3.189
H(40)	H(42)	2.406	H(40)	H(43)	2.844
H(40)	H(63)	2.662	H(40)	H(65)	2.861
H(41)	H(44)	2.437	H(41)	H(45)	2.783
H(41)	H(72)	2.479	H(41)	H(73)	2.802
H(42)	H(63)	2.629	H(42)	H(72)	2.680
H(43)	H(45)	3.503	H(43)	H(72)	3.472
H(44)	H(48)	3.537	H(44)	H(68)	3.536
H(45)	H(48)	3.373	H(46)	H(47)	3.556
H(46)	H(48)	2.180	H(46)	H(49)	3.342
H(47)	H(51)	3.489	H(47)	H(52)	2.452
H(49)	H(52)	2.756	H(53)	H(55)	2.703
H(53)	H(56)	2.221	H(53)	H(62)	2.716
H(54)	H(55)	2.221	H(54)	H(56)	2.761
H(54)	H(63)	2.742	H(54)	H(64)	2.519
H(55)	H(72)	2.638	H(55)	H(74)	2.569
H(56)	H(62)	3.571	H(56)	H(70)	2.624
H(57)	H(58)	2.308	H(57)	H(60)	3.270
H(57)	H(61)	2.372	H(57)	H(62)	3.395
H(58)	H(59)	2.299	H(59)	H(63)	3.469
H(59)	H(64)	3.091	H(59)	H(65)	2.389
H(60)	H(69)	2.551	H(60)	H(70)	3.116

Table 11. Intramolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
H(62)	H(69)	3.380	H(62)	H(70)	3.159
H(66)	H(67)	2.301	H(66)	H(69)	3.187
H(66)	H(70)	3.424	H(66)	H(71)	2.366
H(67)	H(68)	2.317	H(68)	H(72)	3.483
H(68)	H(73)	2.399	H(68)	H(74)	3.030

Table 12. Intermolecular contacts less than 3.60 Å

atom	atom	distance	atom	atom	distance
C(15)	C(41)[1]	3.492(4)	C(16)	C(41)[1]	3.434(4)
C(41)	C(15)[2]	3.492(4)	C(41)	C(16)[2]	3.434(4)

Symmetry Operators:

(1) X,Y,Z-1 (2) X,Y,Z+1

Table 13. Intermolecular contacts less than 3.60 Å involving hydrogens

atom	atom	distance	atom	atom	distance
Cl(1)	H(18)[1]	3.284	Cl(1)	H(35)[1]	2.954
Cl(1)	H(59)[2]	2.956	Cl(1)	H(67)[3]	3.043
Cl(2)	H(17)[1]	2.814	Cl(2)	H(18)[1]	3.409
Cl(2)	H(28)[1]	3.585	Cl(2)	H(61)	3.332
Cl(2)	H(62)	3.565	Cl(3)	H(25)	3.269
Cl(3)	H(54)[4]	3.258	Cl(3)	H(55)[4]	2.824
Cl(3)	H(74)[4]	3.503	Cl(4)	H(20)	2.962
Cl(4)	H(21)	3.264	Cl(4)	H(30)[5]	3.575
Cl(4)	H(31)[5]	2.818	Cl(4)	H(54)[4]	3.459
Cl(4)	H(64)[4]	3.042	Cl(5)	H(16)[6]	3.417
Cl(5)	H(19)[6]	3.217	Cl(5)	H(32)[6]	3.336
Cl(5)	H(56)[3]	3.474	Cl(6)	H(23)[1]	3.106
Cl(6)	H(25)[1]	3.424	Cl(6)	H(32)[1]	3.253
Cl(6)	H(32)[6]	3.204	Cl(6)	H(33)[6]	3.479
Cl(6)	H(66)[1]	3.255	Cl(6)	H(71)[1]	3.521
C(1)	H(9)[7]	3.342	C(1)	H(10)[7]	3.229
C(2)	H(9)[7]	3.207	C(4)	H(10)[7]	3.574
C(5)	H(10)[7]	2.972	C(6)	H(43)[8]	3.470
C(6)	H(49)[9]	3.278	C(6)	H(52)[9]	3.397
C(7)	H(9)[7]	3.335	C(7)	H(50)[9]	3.173
C(8)	H(6)[7]	3.240	C(8)	H(50)[10]	3.185
C(8)	H(51)[10]	3.482	C(8)	H(52)[10]	3.578
C(8)	H(65)[2]	3.562	C(9)	H(14)[7]	3.036
C(9)	H(35)[1]	3.332	C(9)	H(37)[1]	3.384
C(9)	H(39)[2]	3.237	C(10)	H(10)[7]	3.090
C(10)	H(27)[1]	3.092	C(10)	H(39)[8]	3.300
C(12)	H(56)[4]	3.362	C(12)	H(62)[4]	3.550
C(12)	H(70)[4]	3.523	C(13)	H(67)[11]	3.441
C(13)	H(68)[11]	3.222	C(14)	H(53)[4]	2.902
C(15)	H(53)[4]	2.743	C(15)	H(54)[4]	3.587
C(15)	H(56)[4]	3.579	C(16)	H(53)[4]	2.809
C(16)	H(54)[4]	3.197	C(16)	H(60)	3.319
C(16)	H(61)	3.239	C(17)	H(30)[5]	3.459
C(17)	H(49)[9]	3.536	C(17)	H(53)[4]	2.996
C(17)	H(54)[4]	3.480	C(18)	H(45)[9]	3.508
C(18)	H(49)[9]	3.092	C(18)	H(53)[4]	3.103
C(19)	H(53)[4]	3.085	C(19)	H(62)[4]	3.500

Table 13. Intermolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
C(20)	H(53)[4]	3.505	C(20)	H(56)[4]	3.434
C(20)	H(69)	3.502	C(20)	H(71)	3.478
C(21)	H(13)[4]	3.587	C(21)	H(15)[4]	3.015
C(21)	H(62)[4]	3.395	C(22)	H(68)[11]	3.280
C(23)	H(73)[11]	3.566	C(23)	H(74)[11]	3.295
C(24)	H(46)[3]	3.082	C(24)	H(73)[11]	3.247
C(24)	H(74)[11]	3.249	C(25)	H(21)[10]	3.481
C(25)	H(73)[11]	3.300	C(26)	H(51)[10]	3.294
C(27)	H(68)[11]	3.312	C(28)	H(66)[3]	3.583
C(28)	H(67)[3]	3.445	C(28)	H(74)[11]	3.438
C(29)	H(11)[4]	3.048	C(29)	H(12)[4]	3.376
C(29)	H(13)[4]	3.480	C(30)	H(26)[12]	3.168
C(31)	H(26)[12]	3.294	C(32)	H(22)[12]	3.037
C(32)	H(26)[12]	3.367	C(33)	H(22)[12]	3.067
C(33)	H(26)[12]	3.240	C(34)	H(26)[12]	3.108
C(35)	H(10)[13]	3.369	C(35)	H(37)[5]	3.439
C(37)	H(22)[12]	3.053	C(37)	H(29)[3]	2.980
C(37)	H(58)[14]	3.441	C(38)	H(3)[12]	3.548
C(38)	H(22)[12]	3.111	C(38)	H(72)[4]	3.118
C(39)	H(3)[12]	3.557	C(39)	H(6)[12]	3.478
C(39)	H(8)[5]	3.551	C(39)	H(9)[5]	3.085
C(39)	H(64)[4]	3.311	C(39)	H(65)[4]	3.380
C(42)	H(16)[1]	3.360	C(42)	H(23)[1]	3.530
C(45)	H(45)[8]	3.009	C(46)	H(31)[5]	3.563
C(46)	H(45)[8]	2.842	C(47)	H(12)[13]	3.430
C(47)	H(45)[8]	3.478	C(49)	H(20)	3.001
C(49)	H(28)[1]	3.151	C(50)	H(47)[1]	3.397
C(50)	H(51)[1]	3.416	C(50)	H(52)[1]	3.023
C(53)	H(33)[3]	3.294	C(54)	H(19)[6]	2.965
C(54)	H(33)[3]	3.347	C(55)	H(19)[6]	2.847
C(55)	H(58)[14]	3.277	C(57)	H(25)	3.191
C(58)	H(48)[1]	3.050	C(59)	H(23)[6]	3.253
C(59)	H(32)[1]	3.122	C(59)	H(32)[6]	3.447
C(59)	H(55)[3]	3.386	C(59)	H(56)[3]	3.168
H(1)	H(43)[8]	3.009	H(1)	H(49)[9]	3.458
H(2)	H(9)[7]	3.257	H(2)	H(10)[7]	3.026
H(2)	H(40)[8]	3.018	H(2)	H(42)[8]	3.577

Table 13. Intermolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
H(2)	H(43)[8]	3.078	H(2)	H(49)[9]	3.189
H(2)	H(52)[9]	2.924	H(2)	H(65)[8]	3.533
H(3)	C(38)[9]	3.548	H(3)	C(39)[9]	3.557
H(3)	H(49)[9]	2.696	H(3)	H(50)[9]	3.359
H(3)	H(52)[9]	3.000	H(4)	H(13)[4]	3.193
H(5)	H(50)[9]	2.931	H(6)	C(8)[7]	3.240
H(6)	C(39)[9]	3.478	H(6)	H(8)[7]	2.957
H(6)	H(9)[7]	2.713	H(6)	H(14)[4]	3.586
H(6)	H(50)[9]	2.569	H(7)	H(50)[10]	3.444
H(7)	H(51)[10]	3.285	H(7)	H(52)[10]	3.566
H(7)	H(59)[2]	3.510	H(7)	H(65)[2]	3.003
H(8)	C(39)[10]	3.551	H(8)	H(6)[7]	2.957
H(8)	H(50)[10]	2.978	H(8)	H(51)[10]	3.391
H(9)	C(1)[7]	3.342	H(9)	C(2)[7]	3.207
H(9)	C(7)[7]	3.335	H(9)	C(39)[10]	3.085
H(9)	H(2)[7]	3.257	H(9)	H(6)[7]	2.713
H(9)	H(50)[10]	2.664	H(9)	H(51)[10]	3.193
H(9)	H(52)[10]	2.899	H(9)	H(65)[2]	3.214
H(10)	C(1)[7]	3.229	H(10)	C(4)[7]	3.574
H(10)	C(5)[7]	2.972	H(10)	C(10)[7]	3.090
H(10)	C(35)[2]	3.369	H(10)	H(2)[7]	3.026
H(10)	H(14)[7]	2.510	H(10)	H(15)[7]	3.395
H(10)	H(39)[2]	2.850	H(10)	H(40)[2]	3.145
H(10)	H(65)[2]	3.382	H(11)	C(29)[1]	3.048
H(11)	H(14)[7]	2.728	H(11)	H(35)[1]	2.944
H(11)	H(36)[1]	2.937	H(11)	H(37)[1]	2.744
H(11)	H(39)[2]	3.006	H(12)	C(29)[1]	3.376
H(12)	C(47)[2]	3.430	H(12)	H(35)[1]	2.854
H(12)	H(37)[1]	3.159	H(12)	H(38)[2]	3.433
H(12)	H(39)[2]	3.333	H(12)	H(40)[2]	3.487
H(12)	H(59)[2]	2.729	H(12)	H(65)[2]	3.067
H(13)	C(21)[1]	3.587	H(13)	C(29)[1]	3.480
H(13)	H(4)[1]	3.193	H(13)	H(18)[1]	3.419
H(13)	H(27)[1]	2.778	H(13)	H(35)[1]	3.466
H(13)	H(36)[1]	2.761	H(14)	C(9)[7]	3.036
H(14)	H(6)[1]	3.586	H(14)	H(10)[7]	2.510
H(14)	H(11)[7]	2.728	H(14)	H(14)[7]	3.589

Table 13. Intermolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
H(14)	H(27)[1]	3.552	H(14)	H(39)[8]	2.722
H(15)	C(21)[1]	3.015	H(15)	H(10)[7]	3.395
H(15)	H(26)[1]	2.975	H(15)	H(27)[1]	2.574
H(15)	H(28)[1]	2.998	H(15)	H(39)[8]	2.998
H(16)	Cl(5)[11]	3.417	H(16)	C(42)[4]	3.360
H(16)	H(53)[4]	3.242	H(16)	H(56)[4]	2.445
H(16)	H(62)[4]	3.437	H(16)	H(70)[4]	2.874
H(17)	Cl(2)[4]	2.814	H(17)	H(62)[4]	2.874
H(17)	H(70)[4]	3.341	H(18)	Cl(1)[4]	3.284
H(18)	Cl(2)[4]	3.409	H(18)	H(13)[4]	3.419
H(18)	H(67)[11]	3.114	H(18)	H(68)[11]	3.138
H(19)	Cl(5)[11]	3.217	H(19)	C(54)[11]	2.965
H(19)	C(55)[11]	2.847	H(19)	H(67)[11]	2.868
H(19)	H(68)[11]	2.631	H(20)	Cl(4)	2.962
H(20)	C(49)	3.001	H(20)	H(53)[4]	3.300
H(20)	H(54)[4]	3.255	H(20)	H(60)	2.459
H(20)	H(61)	2.687	H(20)	H(69)	3.444
H(21)	Cl(4)	3.264	H(21)	C(25)[5]	3.481
H(21)	H(30)[5]	2.634	H(21)	H(49)[9]	3.471
H(21)	H(53)[4]	3.572	H(21)	H(57)	3.523
H(21)	H(61)	3.551	H(22)	C(32)[9]	3.037
H(22)	C(33)[9]	3.067	H(22)	C(37)[9]	3.053
H(22)	C(38)[9]	3.111	H(22)	H(45)[9]	2.632
H(22)	H(46)[9]	3.068	H(22)	H(48)[9]	3.130
H(22)	H(49)[9]	2.693	H(23)	Cl(6)[4]	3.106
H(23)	C(42)[4]	3.530	H(23)	C(59)[11]	3.253
H(23)	H(53)[4]	3.464	H(23)	H(55)[4]	3.538
H(23)	H(56)[4]	2.870	H(24)	H(69)	3.534
H(24)	H(71)	3.273	H(25)	Cl(3)	3.269
H(25)	Cl(6)[4]	3.424	H(25)	C(57)	3.191
H(25)	H(53)[4]	3.565	H(25)	H(55)[4]	3.423
H(25)	H(56)[4]	3.448	H(25)	H(60)	3.577
H(25)	H(69)	2.662	H(25)	H(71)	2.853
H(26)	C(30)[9]	3.168	H(26)	C(31)[9]	3.294
H(26)	C(32)[9]	3.367	H(26)	C(33)[9]	3.240
H(26)	C(34)[9]	3.108	H(26)	H(15)[4]	2.975
H(26)	H(39)[9]	3.546	H(26)	H(50)[9]	3.364

Table 13. Intermolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
H(27)	C(10)^{4}	3.092	H(27)	H(13)^{4}	2.778
H(27)	H(14)^{4}	3.552	H(27)	H(15)^{4}	2.574
H(28)	Cl(2)^{4}	3.585	H(28)	C(49)^{4}	3.151
H(28)	H(15)^{4}	2.998	H(28)	H(43)^{9}	3.439
H(28)	H(61)^{4}	2.898	H(28)	H(62)^{4}	2.660
H(29)	C(37)^{3}	2.980	H(29)	H(44)^{3}	3.142
H(29)	H(45)^{3}	3.160	H(29)	H(46)^{3}	2.235
H(29)	H(48)^{3}	3.484	H(29)	H(59)^{2}	3.509
H(29)	H(73)^{11}	3.513	H(29)	H(74)^{11}	3.260
H(30)	Cl(4)^{10}	3.575	H(30)	C(17)^{10}	3.459
H(30)	H(21)^{10}	2.634	H(30)	H(46)^{3}	3.394
H(30)	H(59)^{2}	3.468	H(30)	H(64)^{2}	3.161
H(30)	H(73)^{11}	3.593	H(31)	Cl(4)^{10}	2.818
H(31)	C(46)^{10}	3.563	H(31)	H(38)^{10}	3.243
H(31)	H(51)^{10}	2.662	H(31)	H(58)^{10}	3.441
H(32)	Cl(5)^{11}	3.336	H(32)	Cl(6)^{4}	3.253
H(32)	Cl(6)^{11}	3.204	H(32)	C(59)^{4}	3.122
H(32)	C(59)^{11}	3.447	H(32)	H(74)^{11}	3.283
H(33)	Cl(6)^{11}	3.479	H(33)	C(53)^{3}	3.294
H(33)	C(54)^{3}	3.347	H(33)	H(66)^{3}	2.875
H(33)	H(67)^{3}	2.961	H(33)	H(74)^{11}	3.189
H(34)	H(66)^{3}	3.531	H(34)	H(67)^{3}	3.045
H(35)	Cl(1)^{4}	2.954	H(35)	C(9)^{4}	3.332
H(35)	H(11)^{4}	2.944	H(35)	H(12)^{4}	2.854
H(35)	H(13)^{4}	3.466	H(35)	H(58)^{10}	3.191
H(35)	H(59)^{10}	3.405	H(35)	H(68)^{11}	3.236
H(36)	H(11)^{4}	2.937	H(36)	H(13)^{4}	2.761
H(37)	C(9)^{4}	3.384	H(37)	C(35)^{10}	3.439
H(37)	H(11)^{4}	2.744	H(37)	H(12)^{4}	3.159
H(37)	H(38)^{10}	2.838	H(37)	H(39)^{10}	3.145
H(37)	H(50)^{10}	3.436	H(37)	H(51)^{10}	3.161
H(38)	H(12)^{13}	3.433	H(38)	H(31)^{5}	3.243
H(38)	H(37)^{5}	2.838	H(39)	C(9)^{13}	3.237
H(39)	C(10)^{14}	3.300	H(39)	H(10)^{13}	2.850
H(39)	H(11)^{13}	3.006	H(39)	H(12)^{13}	3.333
H(39)	H(14)^{14}	2.722	H(39)	H(15)^{14}	2.998
H(39)	H(26)^{12}	3.546	H(39)	H(37)^{5}	3.145

Table 13. Intermolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
H(40)	H(2)^{14}	3.018	H(40)	H(10)^{13}	3.145
H(40)	H(12)^{13}	3.487	H(41)	H(57)^{14}	3.109
H(42)	H(2)^{14}	3.577	H(42)	H(47)^{1}	3.203
H(43)	C(6)^{14}	3.470	H(43)	H(1)^{14}	3.009
H(43)	H(2)^{14}	3.078	H(43)	H(28)^{12}	3.439
H(43)	H(49)^{1}	3.587	H(43)	H(57)^{14}	3.301
H(44)	H(29)^{3}	3.142	H(44)	H(58)^{14}	3.186
H(45)	C(18)^{12}	3.508	H(45)	C(45)^{14}	3.009
H(45)	C(46)^{14}	2.842	H(45)	C(47)^{14}	3.478
H(45)	H(22)^{12}	2.632	H(45)	H(29)^{3}	3.160
H(45)	H(57)^{14}	3.111	H(45)	H(58)^{14}	2.849
H(46)	C(24)^{3}	3.082	H(46)	H(22)^{12}	3.068
H(46)	H(29)^{3}	2.235	H(46)	H(30)^{3}	3.394
H(47)	C(50)^{4}	3.397	H(47)	H(42)^{4}	3.203
H(47)	H(54)^{4}	3.405	H(47)	H(63)^{4}	2.724
H(47)	H(64)^{4}	3.300	H(47)	H(72)^{4}	2.812
H(48)	C(58)^{4}	3.050	H(48)	H(22)^{12}	3.130
H(48)	H(29)^{3}	3.484	H(48)	H(72)^{4}	2.631
H(48)	H(73)^{4}	3.039	H(48)	H(74)^{4}	2.974
H(49)	C(6)^{12}	3.278	H(49)	C(17)^{12}	3.536
H(49)	C(18)^{12}	3.092	H(49)	H(1)^{12}	3.458
H(49)	H(2)^{12}	3.189	H(49)	H(3)^{12}	2.696
H(49)	H(21)^{12}	3.471	H(49)	H(22)^{12}	2.693
H(49)	H(43)^{4}	3.587	H(49)	H(72)^{4}	3.487
H(50)	C(7)^{12}	3.173	H(50)	C(8)^{5}	3.185
H(50)	H(3)^{12}	3.359	H(50)	H(5)^{12}	2.931
H(50)	H(6)^{12}	2.569	H(50)	H(7)^{5}	3.444
H(50)	H(8)^{5}	2.978	H(50)	H(9)^{5}	2.664
H(50)	H(26)^{12}	3.364	H(50)	H(37)^{5}	3.436
H(51)	C(8)^{5}	3.482	H(51)	C(26)^{5}	3.294
H(51)	C(50)^{4}	3.416	H(51)	H(7)^{5}	3.285
H(51)	H(8)^{5}	3.391	H(51)	H(9)^{5}	3.193
H(51)	H(31)^{5}	2.662	H(51)	H(37)^{5}	3.161
H(51)	H(64)^{4}	2.885	H(51)	H(65)^{4}	3.174
H(52)	C(6)^{12}	3.397	H(52)	C(8)^{5}	3.578
H(52)	C(50)^{4}	3.023	H(52)	H(2)^{12}	2.924
H(52)	H(3)^{12}	3.000	H(52)	H(7)^{5}	3.566

Table 13. Intermolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
H(52)	H(9)^{5}	2.899	H(52)	H(63)^{4}	2.952
H(52)	H(64)^{4}	2.881	H(52)	H(65)^{4}	2.724
H(53)	C(14)^{1}	2.902	H(53)	C(15)^{1}	2.743
H(53)	C(16)^{1}	2.809	H(53)	C(17)^{1}	2.996
H(53)	C(18)^{1}	3.103	H(53)	C(19)^{1}	3.085
H(53)	C(20)^{1}	3.505	H(53)	H(16)^{1}	3.242
H(53)	H(20)^{1}	3.300	H(53)	H(21)^{1}	3.572
H(53)	H(23)^{1}	3.464	H(53)	H(25)^{1}	3.565
H(54)	Cl(3)^{1}	3.258	H(54)	Cl(4)^{1}	3.459
H(54)	C(15)^{1}	3.587	H(54)	C(16)^{1}	3.197
H(54)	C(17)^{1}	3.480	H(54)	H(20)^{1}	3.255
H(54)	H(47)^{1}	3.405	H(55)	Cl(3)^{1}	2.824
H(55)	C(59)^{3}	3.386	H(55)	H(23)^{1}	3.538
H(55)	H(25)^{1}	3.423	H(56)	Cl(5)^{3}	3.474
H(56)	C(12)^{1}	3.362	H(56)	C(15)^{1}	3.579
H(56)	C(20)^{1}	3.434	H(56)	C(59)^{3}	3.168
H(56)	H(16)^{1}	2.445	H(56)	H(23)^{1}	2.870
H(56)	H(25)^{1}	3.448	H(57)	H(21)	3.523
H(57)	H(41)^{8}	3.109	H(57)	H(43)^{8}	3.301
H(57)	H(45)^{8}	3.111	H(57)	H(73)^{8}	3.468
H(58)	C(37)^{8}	3.441	H(58)	C(55)^{8}	3.277
H(58)	H(31)^{5}	3.441	H(58)	H(35)^{5}	3.191
H(58)	H(44)^{8}	3.186	H(58)	H(45)^{8}	2.849
H(58)	H(68)^{8}	2.701	H(58)	H(73)^{8}	3.411
H(59)	Cl(1)^{13}	2.956	H(59)	H(7)^{13}	3.510
H(59)	H(12)^{13}	2.729	H(59)	H(29)^{13}	3.509
H(59)	H(30)^{13}	3.468	H(59)	H(35)^{5}	3.405
H(60)	C(16)	3.319	H(60)	H(20)	2.459
H(60)	H(25)	3.577	H(61)	Cl(2)	3.332
H(61)	C(16)	3.239	H(61)	H(20)	2.687
H(61)	H(21)	3.551	H(61)	H(28)^{1}	2.898
H(62)	Cl(2)	3.565	H(62)	C(12)^{1}	3.550
H(62)	C(19)^{1}	3.500	H(62)	C(21)^{1}	3.395
H(62)	H(16)^{1}	3.437	H(62)	H(17)^{1}	2.874
H(62)	H(28)^{1}	2.660	H(63)	H(47)^{1}	2.724
H(63)	H(52)^{1}	2.952	H(64)	Cl(4)^{1}	3.042
H(64)	C(39)^{1}	3.311	H(64)	H(30)^{13}	3.161

Table 13. Intermolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
H(64)	H(47)[1]	3.300	H(64)	H(51)[1]	2.885
H(64)	H(52)[1]	2.881	H(65)	C(8)[13]	3.562
H(65)	C(39)[1]	3.380	H(65)	H(2)[14]	3.533
H(65)	H(7)[13]	3.003	H(65)	H(9)[13]	3.214
H(65)	H(10)[13]	3.382	H(65)	H(12)[13]	3.067
H(65)	H(51)[1]	3.174	H(65)	H(52)[1]	2.724
H(66)	Cl(6)[4]	3.255	H(66)	C(28)[3]	3.583
H(66)	H(33)[3]	2.875	H(66)	H(34)[3]	3.531
H(66)	H(71)[3]	3.288	H(67)	Cl(1)[3]	3.043
H(67)	C(13)[6]	3.441	H(67)	C(28)[3]	3.445
H(67)	H(18)[6]	3.114	H(67)	H(19)[6]	2.868
H(67)	H(33)[3]	2.961	H(67)	H(34)[3]	3.045
H(68)	C(13)[6]	3.222	H(68)	C(22)[6]	3.280
H(68)	C(27)[6]	3.312	H(68)	H(18)[6]	3.138
H(68)	H(19)[6]	2.631	H(68)	H(35)[6]	3.236
H(68)	H(58)[14]	2.701	H(69)	C(20)	3.502
H(69)	H(20)	3.444	H(69)	H(24)	3.534
H(69)	H(25)	2.662	H(70)	C(12)[1]	3.523
H(70)	H(16)[1]	2.874	H(70)	H(17)[1]	3.341
H(71)	Cl(6)[4]	3.521	H(71)	C(20)	3.478
H(71)	H(24)	3.273	H(71)	H(25)	2.853
H(71)	H(66)[3]	3.288	H(72)	C(38)[1]	3.118
H(72)	H(47)[1]	2.812	H(72)	H(48)[1]	2.631
H(72)	H(49)[1]	3.487	H(73)	C(23)[6]	3.566
H(73)	C(24)[6]	3.247	H(73)	C(25)[6]	3.300
H(73)	H(29)[6]	3.513	H(73)	H(30)[6]	3.593
H(73)	H(48)[1]	3.039	H(73)	H(57)[14]	3.468
H(73)	H(58)[14]	3.411	H(74)	Cl(3)[1]	3.503
H(74)	C(23)[6]	3.295	H(74)	C(24)[6]	3.249
H(74)	C(28)[6]	3.438	H(74)	H(29)[6]	3.260
H(74)	H(32)[6]	3.283	H(74)	H(33)[6]	3.189
H(74)	H(48)[1]	2.974			

Symmetry Operators:

(1)	X,Y,Z+1	(2)	-X+1/2,Y+1/2-1,-Z+1
(3)	-X+1,-Y,Z	(4)	X,Y,Z-1
(5)	-X+1/2,Y+1/2,-Z	(6)	-X+1,-Y,Z+1

(7) -X,-Y,Z
(8) X+1/2-1,-Y+1/2,-Z+1
(9) X+1/2-1,-Y+1/2,-Z
(10) -X+1/2,Y+1/2-1,-Z
(11) -X+1,-Y,Z-1
(12) X+1/2,-Y+1/2,-Z
(13) -X+1/2,Y+1/2,-Z+1
(14) X+1/2,-Y+1/2,-Z+1

X-ray Structure Report for $Cp^*TiCl_2[1,3\text{-}(2,6\text{-}^iPr_2C_6H_3)_2(CH_2N)_2C{=}N]$ (**1e**)

Experimental

Data Collection

A yellow block crystal of $C_{39}H_{53}Cl_6N_3Ti$ having approximate dimensions of 0.200 x 0.160 x 0.100 mm was mounted on a glass fiber. All measurements were made on a Rigaku R-AXIS RAPID diffractometer using filtered Mo-Kα radiation.

The crystal-to-detector distance was 127.40 mm.

Cell constants and an orientation matrix for data collection corresponded to a primitive triclinic cell with dimensions:

a	= 11.1642(2) Å	α	= 94.0438(7)°
b	= 11.2931(2) Å	β	= 100.1681(7)°
c	= 19.4433(4) Å	γ	= 115.2973(7)°
V	= 2151.93(7) Å^3		

For Z = 2 and F.W. = 824.49, the calculated density is 1.272 g/cm^3. Based on a statistical analysis of intensity distribution, and the successful solution and refinement of the structure, the space group was determined to be:

P-1 (#2)

The data were collected at a temperature of -150 $\pm$ 1°C to a maximum 2θ value of 55.0°. A total of 128 oscillation images were collected. A sweep of data was done using ω scans from 130.0 to 190.0° in 3.0° step, at χ=45.0° and ϕ = 0.0°. The exposure rate was 26.0 [sec./°]. A second sweep was performed using ω scans from 0.0 to 162.0° in 3.0° step, at χ=45.0° and ϕ = 180.0°. The exposure rate was 26.0 [sec./°]. Another sweep was performed using ω scans from 0.0 to 162.0° in 3.0° step, at χ=45.0° and ϕ = 90.0°. The exposure rate was 26.0 [sec./°]. The crystal-to-detector distance was 127.40 mm. Readout was performed in the 0.100 mm pixel mode.

Data Reduction

Of the 37405 reflections that were collected, 9868 were unique (R_{int} = 0.0220);

equivalent reflections were merged.

The linear absorption coefficient, μ, for Mo-Kα radiation is 6.007 cm^{-1}. An empirical absorption correction was applied which resulted in transmission factors ranging from 0.823 to 0.942. The data were corrected for Lorentz and polarization effects.

Structure Solution and Refinement

The structure was solved by direct methods[1] and expanded using Fourier techniques. The non-hydrogen atoms were refined anisotropically. Hydrogen atoms were refined using the riding model. The final cycle of full-matrix least-squares refinement[2] on F^2 was based on 9868 observed reflections and 511 variable parameters and converged (largest parameter shift was 0.00 times its esd) with unweighted and weighted agreement factors of:

$$R1 = \Sigma \; ||Fo| - |Fc|| \; / \; \Sigma \; |Fo| = 0.0453$$

$$wR2 = [\; \Sigma \; (\; w \; (Fo^2 - Fc^2)^2 \;) / \; \Sigma \; w(Fo^2)^2]^{1/2} = 0.1224$$

The standard deviation of an observation of unit weight[3] was 1.14. Unit weights were used. The maximum and minimum peaks on the final difference Fourier map corresponded to 1.08 and -0.49 $e^-/Å^3$, respectively.

Neutral atom scattering factors were taken from Cromer and Waber[4]. Anomalous dispersion effects were included in Fcalc[5]; the values for Δf' and Δf'' were those of Creagh and McAuley[6]. The values for the mass attenuation coefficients are those of Creagh and Hubbell[7]. All calculations were performed using the CrystalStructure[8] crystallographic software package except for refinement, which was performed using SHELXL-97[9].

References

(1) SIR2008: M.C. Burla, R. Caliandro, M. Camalli, B. Carrozzini, G.L. Cascarano, L. De Caro, C. Giacovazzo, G. Polidori, D. Siliqi, R. Spagna (2007)

(2) Least Squares function minimized: (SHELXL97)

$\Sigma w(F_o^2-F_c^2)^2$ where w = Least Squares weights.

(3) Standard deviation of an observation of unit weight:

$[\Sigma w(F_o^2-F_c^2)^2/(N_o-N_v)]^{1/2}$

where: N_o = number of observations
N_v = number of variables

(4) Cromer, D. T. & Waber, J. T.; "International Tables for X-ray Crystallography", Vol. IV, The Kynoch Press, Birmingham, England, Table 2.2 A (1974).

(5) Ibers, J. A. & Hamilton, W. C.; Acta Crystallogr., 17, 781 (1964).

(6) Creagh, D. C. & McAuley, W.J .; "International Tables for Crystallography", Vol C, (A.J.C. Wilson, ed.), Kluwer Academic Publishers, Boston, Table 4.2.6.8, pages 219-222 (1992).

(7) Creagh, D. C. & Hubbell, J.H..; "International Tables for Crystallography", Vol C, (A.J.C. Wilson, ed.), Kluwer Academic Publishers, Boston, Table 4.2.4.3, pages 200-206 (1992).

(8) CrystalStructure 4.0: Crystal Structure Analysis Package, Rigaku Corporation (2000-2010). Tokyo 196-8666, Japan.

(9) SHELX97: Sheldrick, G.M. (2008). Acta Cryst. A64, 112-122.

EXPERIMENTAL DETAILS

A. Crystal Data

Empirical Formula	$C_{39}H_{53}Cl_6N_3Ti$
Formula Weight	824.49
Crystal Color, Habit	yellow, block
Crystal Dimensions	0.200 X 0.160 X 0.100 mm
Crystal System	triclinic
Lattice Type	Primitive
Lattice Parameters	a = 11.1642(2) Å b = 11.2931(2) Å c = 19.4433(4) Å α = 94.0438(7) ^{o} β = 100.1681(7) ^{o} γ = 115.2973(7) ^{o} V = 2151.93(7) Å^3
Space Group	P-1 (#2)
Z value	2
D_{calc}	1.272 g/cm^3
F_{000}	864.00
μ(MoKα)	6.007 cm^{-1}

B. Intensity Measurements

Diffractometer	R-AXIS RAPID
Radiation	MoKα (λ = 0.71075 Å)
Voltage, Current	50kV, 24mA
Temperature	-150.0^{o}C
Detector Aperture	280 x 256 mm
Data Images	128 exposures
ω oscillation Range (χ=45.0, ϕ=0.0)	130.0 - 190.0^{o}
Exposure Rate	26.0 sec./^{o}
ω oscillation Range (χ=45.0, ϕ=180.0)	0.0 - 162.0^{o}
Exposure Rate	26.0 sec./^{o}
ω oscillation Range (χ=45.0, ϕ=90.0)	0.0 - 162.0^{o}
Exposure Rate	26.0 sec./^{o}
Detector Position	127.40 mm
Pixel Size	0.100 mm
$2\theta_{max}$	55.0^{o}
No. of Reflections Measured	Total: 37405 Unique: 9868 (R_{int} = 0.0220)
Corrections	Lorentz-polarization Absorption (trans. factors: 0.823 - 0.942)

C. Structure Solution and Refinement

Structure Solution	Direct Methods
Refinement	Full-matrix least-squares on F^2
Function Minimized	$\Sigma\ w\ (Fo^2 - Fc^2)^2$
Least Squares Weights	$w = 1/\ [\ \sigma^2(Fo^2) + (0.0683 \cdot P)^2 + 0.9296 \cdot P\ ]$ where $P = (Max(Fo^2,0) + 2Fc^2)/3$
$2\theta_{max}$ cutoff	55.0^o
Anomalous Dispersion	All non-hydrogen atoms
No. Observations (All reflections)	9868
No. Variables	511
Reflection/Parameter Ratio	19.31
Residuals: R1 (I>2.00σ(I))	0.0453
Residuals: R (All reflections)	0.0485
Residuals: wR2 (All reflections)	0.1224
Goodness of Fit Indicator	1.142
Max Shift/Error in Final Cycle	0.001
Maximum peak in Final Diff. Map	1.08 $e^-/Å^3$
Minimum peak in Final Diff. Map	-0.49 $e^-/Å^3$

Table 1. Atomic coordinates and B_{iso}/B_{eq} and occupancy

atom	x	y	z	B_{eq}	occ
Ti1	0.03096(3)	0.27300(2)	0.31885(2)	1.331(7)	1
Cl1	-0.12110(4)	0.11819(4)	0.22218(2)	2.258(8)	1
Cl2	0.17613(4)	0.18046(4)	0.34967(2)	2.382(9)	1
Cl3A	0.0926(3)	0.8390(3)	0.1629(2)	4.09(5)	0.679(8)
Cl3B	0.0688(9)	0.8371(6)	0.1454(5)	6.3(2)	0.321(8)
Cl4A	-0.1003(2)	0.7557(2)	0.24650(8)	5.39(5)	0.679(8)
Cl4B	-0.155(2)	0.7636(6)	0.218(1)	18.9(6)	0.321(8)
Cl5A	0.4399(4)	0.9907(4)	0.1194(2)	3.64(4)	0.488(8)
Cl5B	0.4633(5)	0.9671(5)	0.1091(3)	6.8(1)	0.512(8)
Cl6A	0.5301(3)	0.8098(3)	0.0587(3)	6.43(9)	0.488(8)
Cl6B	0.5847(5)	0.7895(3)	0.0986(3)	8.5(2)	0.512(8)
N1	0.1265(2)	0.4122(2)	0.27894(6)	1.38(2)	1
N2	0.1524(2)	0.4986(2)	0.17223(6)	1.56(2)	1
N3	0.2951(2)	0.6272(2)	0.27140(6)	1.43(2)	1
C1	-0.0624(2)	0.3896(2)	0.37590(8)	1.70(3)	1
C2	0.0425(2)	0.3851(2)	0.42737(8)	1.72(3)	1
C3	-0.0008(2)	0.2509(2)	0.43854(8)	1.85(3)	1
C4	-0.1300(2)	0.1726(2)	0.39301(9)	1.92(3)	1
C5	-0.1691(2)	0.2585(2)	0.35487(9)	1.84(3)	1
C6	-0.0626(2)	0.5130(2)	0.3512(1)	2.30(3)	1
C7	0.1716(2)	0.5021(2)	0.46697(9)	2.29(3)	1
C8	0.0745(2)	0.2026(2)	0.4924(1)	2.48(3)	1
C9	-0.2136(2)	0.0252(2)	0.3856(1)	2.77(4)	1
C10	-0.3063(2)	0.2167(2)	0.3071(1)	2.55(3)	1
C11	0.1871(2)	0.5064(2)	0.24400(7)	1.26(2)	1
C12	0.2492(2)	0.6132(2)	0.14768(8)	1.77(3)	1
C13	0.3309(2)	0.7109(2)	0.21648(8)	1.91(3)	1
C14	0.0650(2)	0.3780(2)	0.12326(8)	1.63(3)	1
C15	-0.0681(2)	0.3555(2)	0.09348(8)	1.82(3)	1
C16	-0.1496(2)	0.2416(2)	0.04283(9)	2.28(3)	1
C17	-0.1005(2)	0.1538(2)	0.0234(1)	2.70(4)	1
C18	0.0314(2)	0.1784(2)	0.0532(1)	2.62(3)	1
C19	0.1180(2)	0.2917(2)	0.10344(8)	2.00(3)	1
C20	-0.1247(2)	0.4496(2)	0.11435(8)	1.96(3)	1
C21	-0.2516(3)	0.3776(3)	0.1428(2)	3.53(4)	1
C22	-0.1558(3)	0.5159(3)	0.0526(1)	3.42(4)	1
C23	0.2640(2)	0.3178(2)	0.13307(9)	2.24(3)	1

Table 1. Atomic coordinates and B_{iso}/B_{eq} and occupancy (continued)

atom	x	y	z	B_{eq}	occ
C24	0.2709(3)	0.2056(2)	0.1706(1)	3.08(4)	1
C25	0.3447(2)	0.3407(3)	0.0751(1)	3.23(4)	1
C26	0.3715(2)	0.6707(2)	0.34342(8)	1.44(3)	1
C27	0.3659(2)	0.7741(2)	0.38508(8)	1.60(3)	1
C28	0.4464(2)	0.8178(2)	0.45429(8)	2.06(3)	1
C29	0.5282(2)	0.7608(2)	0.48104(9)	2.31(3)	1
C30	0.5319(2)	0.6583(2)	0.43914(9)	2.17(3)	1
C31	0.4556(2)	0.6118(2)	0.36974(8)	1.69(3)	1
C32	0.2792(2)	0.8420(2)	0.35777(8)	1.70(3)	1
C33	0.2036(2)	0.8657(2)	0.4118(1)	2.38(3)	1
C34	0.3689(2)	0.9758(2)	0.33756(9)	2.10(3)	1
C35	0.4680(2)	0.5054(2)	0.32328(9)	2.01(3)	1
C36	0.5164(2)	0.4187(2)	0.3654(1)	3.07(4)	1
C37	0.5642(3)	0.5687(3)	0.2750(2)	3.48(4)	1
C38A	-0.0098(7)	0.8831(6)	0.2040(3)	3.33(9)	0.679(8)
C38B	-0.014(3)	0.902(3)	0.196(2)	11(1)	0.321(8)
C39A	0.5757(9)	0.963(1)	0.1035(7)	5.7(3)	0.488(8)
C39B	0.595(1)	0.944(2)	0.0813(5)	7.8(4)	0.512(8)

$B_{eq} = 8/3\ \pi^2(U_{11}(aa^*)^2 + U_{22}(bb^*)^2 + U_{33}(cc^*)^2 + 2U_{12}(aa^*bb^*)\cos\gamma + 2U_{13}(aa^*cc^*)\cos\beta + 2U_{23}(bb^*cc^*)\cos\alpha)$

Table 2. Atomic coordinates and B_{iso} involving hydrogen atoms

atom	x	y	z	B_{iso}	occ
H1	0.0282	0.5713	0.3449	2.76	1
H2	-0.0869	0.5595	0.3866	2.76	1
H3	-0.1292	0.4883	0.3061	2.76	1
H4	0.1574	0.5353	0.5112	2.74	1
H5	0.1974	0.5724	0.4378	2.74	1
H6	0.2444	0.4748	0.4777	2.74	1
H7	0.0544	0.1110	0.4748	2.97	1
H8	0.0455	0.2056	0.5370	2.97	1
H9	0.1726	0.2595	0.5005	2.97	1
H10	-0.2925	0.0068	0.4063	3.32	1
H11	-0.1581	-0.0133	0.4104	3.32	1
H12	-0.2449	-0.0141	0.3353	3.32	1
H13	-0.3745	0.1981	0.3356	3.06	1
H14	-0.3300	0.1365	0.2738	3.06	1
H15	-0.3039	0.2881	0.2807	3.06	1
H16	0.2015	0.6507	0.1149	2.12	1
H17	0.3086	0.5889	0.1236	2.12	1
H18	0.4299	0.7499	0.2187	2.29	1
H19	0.3037	0.7833	0.2213	2.29	1
H20	-0.2401	0.2243	0.0215	2.73	1
H21	-0.1577	0.0763	-0.0106	3.24	1
H22	0.0639	0.1173	0.0394	3.15	1
H23	-0.0540	0.5208	0.1532	2.35	1
H24	-0.2786	0.4423	0.1624	4.23	1
H25	-0.2319	0.3300	0.1800	4.23	1
H26	-0.3258	0.3141	0.1042	4.23	1
H27	-0.1895	0.5780	0.0682	4.10	1
H28	-0.2252	0.4481	0.0139	4.10	1
H29	-0.0727	0.5644	0.0361	4.10	1
H30	0.3080	0.4008	0.1689	2.69	1
H31	0.2293	0.1229	0.1365	3.69	1
H32	0.2215	0.1941	0.2086	3.69	1
H33	0.3662	0.2278	0.1909	3.69	1
H34	0.4394	0.3618	0.0962	3.88	1
H35	0.3420	0.4148	0.0527	3.88	1
H36	0.3044	0.2602	0.0395	3.88	1
H37	0.4446	0.8880	0.4833	2.47	1

Table 2. Atomic coordinates and B_{iso} involving hydrogens/B_{eq} and occupancy (continued)

atom	x	y	z	B_{eq}	occ
H38	0.5819	0.7917	0.5281	2.77	1
H39	0.5878	0.6191	0.4583	2.60	1
H40	0.2102	0.7840	0.3142	2.04	1
H41	0.1540	0.7825	0.4288	2.85	1
H42	0.1391	0.8968	0.3893	2.85	1
H43	0.2693	0.9328	0.4519	2.85	1
H44	0.3115	1.0156	0.3166	2.52	1
H45	0.4177	0.9613	0.3032	2.52	1
H46	0.4346	1.0355	0.3800	2.52	1
H47	0.3759	0.4465	0.2925	2.41	1
H48	0.4636	0.3890	0.4014	3.68	1
H49	0.6131	0.4701	0.3885	3.68	1
H50	0.5037	0.3412	0.3332	3.68	1
H51	0.6544	0.6300	0.3039	4.17	1
H52	0.5285	0.6175	0.2447	4.17	1
H53	0.5712	0.4991	0.2453	4.17	1

Table 3. Anisotropic displacement parameters

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Ti1	0.0168(2)	0.0141(2)	0.0214(2)	0.0073(1)	0.0071(1)	0.0045(1)
Cl1	0.0257(2)	0.0218(2)	0.0315(2)	0.0066(2)	0.0033(2)	-0.0018(2)
Cl2	0.0359(3)	0.0365(3)	0.0336(2)	0.0275(2)	0.0132(2)	0.0126(2)
Cl3A	0.0612(7)	0.0432(7)	0.062(2)	0.0335(6)	0.0171(7)	0.0008(7)
Cl3B	0.121(5)	0.035(2)	0.080(4)	0.014(3)	0.074(4)	0.005(2)
Cl4A	0.0698(9)	0.0512(8)	0.074(2)	0.0080(6)	0.0422(8)	0.0138(5)
Cl4B	0.25(1)	0.052(2)	0.47(2)	0.033(5)	0.31(1)	0.035(6)
Cl5A	0.0389(8)	0.050(1)	0.0484(9)	0.0194(7)	0.0101(6)	0.0042(7)
Cl5B	0.071(3)	0.077(2)	0.061(2)	-0.004(2)	-0.010(2)	0.024(2)
Cl6A	0.062(1)	0.080(2)	0.097(3)	0.029(1)	0.025(2)	-0.020(2)
Cl6B	0.091(3)	0.097(2)	0.097(3)	-0.005(2)	0.067(2)	-0.008(2)
N1	0.0176(6)	0.0171(6)	0.0184(6)	0.0076(5)	0.0058(5)	0.0023(5)
N2	0.0224(6)	0.0172(6)	0.0162(6)	0.0057(5)	0.0050(5)	0.0022(5)
N3	0.0207(6)	0.0150(6)	0.0155(6)	0.0046(5)	0.0044(5)	0.0035(5)
C1	0.0236(8)	0.0199(7)	0.0266(8)	0.0111(6)	0.0139(6)	0.0067(6)
C2	0.0241(8)	0.0217(8)	0.0226(8)	0.0097(6)	0.0129(6)	0.0053(6)
C3	0.0252(8)	0.0248(8)	0.0255(8)	0.0122(7)	0.0134(6)	0.0100(6)
C4	0.0233(8)	0.0219(8)	0.0323(9)	0.0099(7)	0.0149(7)	0.0111(7)
C5	0.0201(7)	0.0234(8)	0.0302(8)	0.0103(7)	0.0126(6)	0.0082(6)
C6	0.0367(9)	0.0229(8)	0.039(1)	0.0187(8)	0.0184(8)	0.0107(7)
C7	0.0303(9)	0.0271(9)	0.0228(8)	0.0057(7)	0.0097(7)	0.0021(7)
C8	0.0331(9)	0.037(1)	0.0308(9)	0.0187(8)	0.0124(7)	0.0160(8)
C9	0.034(1)	0.0220(9)	0.046(1)	0.0061(8)	0.0161(8)	0.0134(8)
C10	0.0206(8)	0.036(1)	0.043(1)	0.0131(7)	0.0104(7)	0.0110(8)
C11	0.0167(7)	0.0161(7)	0.0174(7)	0.0094(6)	0.0048(5)	0.0016(5)
C12	0.0276(8)	0.0196(7)	0.0185(7)	0.0079(6)	0.0080(6)	0.0054(6)
C13	0.0308(8)	0.0184(7)	0.0179(7)	0.0049(7)	0.0078(6)	0.0056(6)
C14	0.0245(8)	0.0186(7)	0.0158(7)	0.0071(6)	0.0048(6)	0.0010(6)
C15	0.0253(8)	0.0232(8)	0.0176(7)	0.0078(7)	0.0056(6)	0.0019(6)
C16	0.0268(8)	0.0283(9)	0.0236(8)	0.0070(7)	0.0028(6)	-0.0016(7)
C17	0.037(1)	0.0260(9)	0.0281(9)	0.0068(8)	0.0036(7)	-0.0080(7)
C18	0.041(1)	0.0264(9)	0.0318(9)	0.0159(8)	0.0083(8)	-0.0051(7)
C19	0.0294(8)	0.0234(8)	0.0223(8)	0.0109(7)	0.0075(6)	0.0013(6)
C20	0.0254(8)	0.0276(8)	0.0204(7)	0.0121(7)	0.0028(6)	0.0015(6)
C21	0.044(2)	0.046(2)	0.057(2)	0.025(1)	0.029(1)	0.015(1)
C22	0.069(2)	0.044(2)	0.030(1)	0.036(1)	0.0124(9)	0.0118(9)
C23	0.0326(9)	0.0298(9)	0.0267(8)	0.0181(8)	0.0069(7)	0.0016(7)

Table 3. Anisotropic displacement parameters (continued)

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
C24	0.051(2)	0.038(1)	0.039(1)	0.029(1)	0.0118(9)	0.0084(8)
C25	0.039(1)	0.060(2)	0.035(1)	0.029(1)	0.0139(8)	0.0096(9)
C26	0.0169(7)	0.0164(7)	0.0174(7)	0.0035(6)	0.0045(5)	0.0030(6)
C27	0.0208(7)	0.0147(7)	0.0208(7)	0.0032(6)	0.0062(6)	0.0031(6)
C28	0.0301(8)	0.0167(7)	0.0221(8)	0.0034(7)	0.0034(6)	-0.0004(6)
C29	0.0295(9)	0.0238(8)	0.0216(8)	0.0035(7)	-0.0025(7)	0.0012(6)
C30	0.0227(8)	0.0273(8)	0.0272(8)	0.0083(7)	0.0003(6)	0.0056(7)
C31	0.0177(7)	0.0209(7)	0.0234(8)	0.0064(6)	0.0050(6)	0.0045(6)
C32	0.0244(8)	0.0147(7)	0.0233(7)	0.0063(6)	0.0074(6)	0.0018(6)
C33	0.0337(9)	0.0240(8)	0.0345(9)	0.0118(7)	0.0161(7)	0.0033(7)
C34	0.0325(9)	0.0160(7)	0.0308(9)	0.0086(7)	0.0116(7)	0.0044(6)
C35	0.0223(8)	0.0292(8)	0.0280(8)	0.0145(7)	0.0066(6)	0.0038(7)
C36	0.041(1)	0.042(1)	0.041(1)	0.029(1)	0.0011(8)	0.0032(9)
C37	0.040(1)	0.050(2)	0.050(2)	0.021(1)	0.027(1)	0.010(1)
C38A	0.057(3)	0.020(2)	0.060(3)	0.021(2)	0.031(2)	0.006(2)
C38B	0.15(2)	0.09(2)	0.26(3)	0.07(1)	0.17(2)	0.10(2)
C39A	0.022(3)	0.057(4)	0.112(9)	-0.005(3)	0.023(5)	-0.015(5)
C39B	0.042(5)	0.14(1)	0.045(4)	-0.023(5)	0.007(3)	0.037(6)

The general temperature factor expression: $\exp(-2\pi^2(a^{*2}U_{11}h^2 + b^{*2}U_{22}k^2 + c^{*2}U_{33}l^2 + 2a^*b^*U_{12}hk + 2a^*c^*U_{13}hl + 2b^*c^*U_{23}kl))$

Table 4. Fragment Analysis

fragment: 1

Ti(1)	Cl(1)	Cl(2)	N(1)	N(2)
N(3)	C(1)	C(2)	C(3)	C(4)
C(5)	C(6)	C(7)	C(8)	C(9)
C(10)	C(11)	C(12)	C(13)	C(14)
C(15)	C(16)	C(17)	C(18)	C(19)
C(20)	C(21)	C(22)	C(23)	C(24)
C(25)	C(26)	C(27)	C(28)	C(29)
C(30)	C(31)	C(32)	C(33)	C(34)
C(35)	C(36)	C(37)		

fragment: 2

Cl(3A)	Cl(4A)	C(38A)

fragment: 3

Cl(3B)	Cl(4B)	C(38B)

fragment: 4

Cl(5A)	Cl(6A)	C(39A)

fragment: 5

Cl(5B)	Cl(6B)	C(39B)

Table 5. Bond lengths (Å)

atom	atom	distance	atom	atom	distance
Ti1	Cl1	2.3119(4)	Ti1	Cl2	2.2958(7)
Ti1	N1	1.8007(13)	Ti1	C1	2.330(2)
Ti1	C2	2.3365(17)	Ti1	C3	2.4291(17)
Ti1	C4	2.4487(18)	Ti1	C5	2.401(2)
Cl3A	C38A	1.716(9)	Cl3B	C38B	1.77(4)
Cl4A	C38A	1.730(7)	Cl4B	C38B	1.82(3)
Cl5A	C39A	1.743(13)	Cl5B	C39B	1.760(16)
Cl6A	C39A	1.705(12)	Cl6B	C39B	1.760(17)
N1	C11	1.3038(19)	N2	C11	1.3667(18)
N2	C12	1.4648(19)	N2	C14	1.4372(17)
N3	C11	1.3650(16)	N3	C13	1.471(2)
N3	C26	1.4328(18)	C1	C2	1.421(3)
C1	C5	1.4194(19)	C1	C6	1.505(3)
C2	C3	1.427(3)	C2	C7	1.5008(19)
C3	C4	1.412(2)	C3	C8	1.504(3)
C4	C5	1.426(3)	C4	C9	1.501(3)
C5	C10	1.499(3)	C12	C13	1.5296(19)
C14	C15	1.400(3)	C14	C19	1.403(3)
C15	C16	1.399(2)	C15	C20	1.516(3)
C16	C17	1.382(4)	C17	C18	1.382(3)
C18	C19	1.400(2)	C19	C23	1.519(3)
C20	C21	1.526(3)	C20	C22	1.524(3)
C23	C24	1.529(4)	C23	C25	1.533(3)
C26	C27	1.404(3)	C26	C31	1.413(3)
C27	C28	1.401(2)	C27	C32	1.522(3)
C28	C29	1.378(3)	C29	C30	1.388(3)
C30	C31	1.391(2)	C31	C35	1.520(3)
C32	C33	1.535(3)	C32	C34	1.539(3)
C35	C36	1.527(4)	C35	C37	1.530(3)

Table 6. Bond lengths involving hydrogens (Å)

atom	atom	distance	atom	atom	distance
C6	H1	0.980	C6	H2	0.980
C6	H3	0.980	C7	H4	0.980
C7	H5	0.980	C7	H6	0.980
C8	H7	0.980	C8	H8	0.980
C8	H9	0.980	C9	H10	0.980
C9	H11	0.980	C9	H12	0.980
C10	H13	0.980	C10	H14	0.980
C10	H15	0.980	C12	H16	0.990
C12	H17	0.990	C13	H18	0.990
C13	H19	0.990	C16	H20	0.950
C17	H21	0.950	C18	H22	0.950
C20	H23	1.000	C21	H24	0.980
C21	H25	0.980	C21	H26	0.980
C22	H27	0.980	C22	H28	0.980
C22	H29	0.980	C23	H30	1.000
C24	H31	0.980	C24	H32	0.980
C24	H33	0.980	C25	H34	0.980
C25	H35	0.980	C25	H36	0.980
C28	H37	0.950	C29	H38	0.950
C30	H39	0.950	C32	H40	1.000
C33	H41	0.980	C33	H42	0.980
C33	H43	0.980	C34	H44	0.980
C34	H45	0.980	C34	H46	0.980
C35	H47	1.000	C36	H48	0.980
C36	H49	0.980	C36	H50	0.980
C37	H51	0.980	C37	H52	0.980
C37	H53	0.980			

Table 7. Bond angles (°)

atom	atom	atom	angle	atom	atom	atom	angle
Cl1	Ti1	Cl2	100.257(19)	Cl1	Ti1	N1	102.89(4)
Cl1	Ti1	C1	113.45(4)	Cl1	Ti1	C2	142.41(5)
Cl1	Ti1	C3	121.67(4)	Cl1	Ti1	C4	89.79(4)
Cl1	Ti1	C5	84.75(4)	Cl2	Ti1	N1	104.11(6)
Cl2	Ti1	C1	137.77(5)	Cl2	Ti1	C2	102.76(5)
Cl2	Ti1	C3	83.31(6)	Cl2	Ti1	C4	99.70(5)
Cl2	Ti1	C5	133.87(5)	N1	Ti1	C1	92.77(7)
N1	Ti1	C2	99.81(6)	N1	Ti1	C3	132.99(5)
N1	Ti1	C4	150.37(7)	N1	Ti1	C5	119.54(7)
C1	Ti1	C2	35.47(6)	C1	Ti1	C3	57.86(7)
C1	Ti1	C4	57.61(6)	C1	Ti1	C5	34.88(5)
C2	Ti1	C3	34.77(6)	C2	Ti1	C4	57.37(5)
C2	Ti1	C5	57.93(6)	C3	Ti1	C4	33.66(5)
C3	Ti1	C5	56.73(7)	C4	Ti1	C5	34.18(7)
Ti1	N1	C11	174.25(9)	C11	N2	C12	111.87(10)
C11	N2	C14	124.74(13)	C12	N2	C14	120.02(12)
C11	N3	C13	111.61(11)	C11	N3	C26	126.49(13)
C13	N3	C26	121.85(11)	Ti1	C1	C2	72.52(12)
Ti1	C1	C5	75.30(12)	Ti1	C1	C6	120.39(13)
C2	C1	C5	107.77(16)	C2	C1	C6	125.79(12)
C5	C1	C6	126.36(16)	Ti1	C2	C1	72.00(10)
Ti1	C2	C3	76.16(10)	Ti1	C2	C7	121.08(13)
C1	C2	C3	107.97(12)	C1	C2	C7	126.12(16)
C3	C2	C7	125.78(16)	Ti1	C3	C2	69.06(10)
Ti1	C3	C4	73.93(10)	Ti1	C3	C8	125.31(15)
C2	C3	C4	108.12(16)	C2	C3	C8	125.89(13)
C4	C3	C8	125.90(16)	Ti1	C4	C3	72.41(10)
Ti1	C4	C5	71.07(11)	Ti1	C4	C9	122.55(15)
C3	C4	C5	107.91(14)	C3	C4	C9	126.87(18)
C5	C4	C9	125.22(15)	Ti1	C5	C1	69.82(11)
Ti1	C5	C4	74.75(12)	Ti1	C5	C10	126.18(13)
C1	C5	C4	108.20(14)	C1	C5	C10	126.91(18)
C4	C5	C10	124.59(14)	N1	C11	N2	124.68(11)
N1	C11	N3	126.91(12)	N2	C11	N3	108.40(12)
N2	C12	C13	102.85(12)	N3	C13	C12	103.00(11)
N2	C14	C15	118.32(18)	N2	C14	C19	119.22(15)
C15	C14	C19	122.32(13)	C14	C15	C16	117.74(19)

Table 7. Bond angles (°) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
C14	C15	C20	122.26(13)	C16	C15	C20	120.00(16)
C15	C16	C17	121.00(18)	C16	C17	C18	120.28(16)
C17	C18	C19	121.1(3)	C14	C19	C18	117.51(18)
C14	C19	C23	122.91(13)	C18	C19	C23	119.6(2)
C15	C20	C21	110.84(17)	C15	C20	C22	111.51(17)
C21	C20	C22	110.46(19)	C19	C23	C24	111.86(15)
C19	C23	C25	111.35(15)	C24	C23	C25	110.4(2)
N3	C26	C27	119.55(16)	N3	C26	C31	118.75(15)
C27	C26	C31	121.63(14)	C26	C27	C28	117.90(17)
C26	C27	C32	122.96(13)	C28	C27	C32	119.12(16)
C27	C28	C29	121.27(18)	C28	C29	C30	119.96(15)
C29	C30	C31	121.4(2)	C26	C31	C30	117.78(17)
C26	C31	C35	121.61(14)	C30	C31	C35	120.56(18)
C27	C32	C33	112.77(15)	C27	C32	C34	109.95(14)
C33	C32	C34	109.12(15)	C31	C35	C36	113.38(16)
C31	C35	C37	110.34(16)	C36	C35	C37	109.4(2)
Cl3A	C38A	Cl4A	109.1(5)	Cl3B	C38B	Cl4B	108.5(14)
Cl5A	C39A	Cl6A	114.6(5)	Cl5B	C39B	Cl6B	109.5(7)

Table 8. Bond angles involving hydrogens (°)

atom	atom	atom	angle	atom	atom	atom	angle
C1	C6	H1	109.5	C1	C6	H2	109.5
C1	C6	H3	109.5	H1	C6	H2	109.5
H1	C6	H3	109.5	H2	C6	H3	109.5
C2	C7	H4	109.5	C2	C7	H5	109.5
C2	C7	H6	109.5	H4	C7	H5	109.5
H4	C7	H6	109.5	H5	C7	H6	109.5
C3	C8	H7	109.5	C3	C8	H8	109.5
C3	C8	H9	109.5	H7	C8	H8	109.5
H7	C8	H9	109.5	H8	C8	H9	109.5
C4	C9	H10	109.5	C4	C9	H11	109.5
C4	C9	H12	109.5	H10	C9	H11	109.5
H10	C9	H12	109.5	H11	C9	H12	109.5
C5	C10	H13	109.5	C5	C10	H14	109.5
C5	C10	H15	109.5	H13	C10	H14	109.5
H13	C10	H15	109.5	H14	C10	H15	109.5
N2	C12	H16	111.2	N2	C12	H17	111.2
C13	C12	H16	111.2	C13	C12	H17	111.2
H16	C12	H17	109.1	N3	C13	H18	111.2
N3	C13	H19	111.2	C12	C13	H18	111.2
C12	C13	H19	111.2	H18	C13	H19	109.1
C15	C16	H20	119.5	C17	C16	H20	119.5
C16	C17	H21	119.9	C18	C17	H21	119.9
C17	C18	H22	119.4	C19	C18	H22	119.4
C15	C20	H23	108.0	C21	C20	H23	108.0
C22	C20	H23	108.0	C20	C21	H24	109.5
C20	C21	H25	109.5	C20	C21	H26	109.5
H24	C21	H25	109.5	H24	C21	H26	109.5
H25	C21	H26	109.5	C20	C22	H27	109.5
C20	C22	H28	109.5	C20	C22	H29	109.5
H27	C22	H28	109.5	H27	C22	H29	109.5
H28	C22	H29	109.5	C19	C23	H30	107.7
C24	C23	H30	107.7	C25	C23	H30	107.7
C23	C24	H31	109.5	C23	C24	H32	109.5
C23	C24	H33	109.5	H31	C24	H32	109.5
H31	C24	H33	109.5	H32	C24	H33	109.5
C23	C25	H34	109.5	C23	C25	H35	109.5
C23	C25	H36	109.5	H34	C25	H35	109.5

Table 8. Bond angles involving hydrogens (°) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
H34	C25	H36	109.5	H35	C25	H36	109.5
C27	C28	H37	119.4	C29	C28	H37	119.4
C28	C29	H38	120.0	C30	C29	H38	120.0
C29	C30	H39	119.3	C31	C30	H39	119.3
C27	C32	H40	108.3	C33	C32	H40	108.3
C34	C32	H40	108.3	C32	C33	H41	109.5
C32	C33	H42	109.5	C32	C33	H43	109.5
H41	C33	H42	109.5	H41	C33	H43	109.5
H42	C33	H43	109.5	C32	C34	H44	109.5
C32	C34	H45	109.5	C32	C34	H46	109.5
H44	C34	H45	109.5	H44	C34	H46	109.5
H45	C34	H46	109.5	C31	C35	H47	107.9
C36	C35	H47	107.8	C37	C35	H47	107.9
C35	C36	H48	109.5	C35	C36	H49	109.5
C35	C36	H50	109.5	H48	C36	H49	109.5
H48	C36	H50	109.5	H49	C36	H50	109.5
C35	C37	H51	109.5	C35	C37	H52	109.5
C35	C37	H53	109.5	H51	C37	H52	109.5
H51	C37	H53	109.5	H52	C37	H53	109.5

Table 9. Torsion Angles(°)

(Those having bond angles > 160 or < 20 degrees are excluded.)

atom1	atom2	atom3	atom4	angle	atom1	atom2	atom3	atom4	angle
Cl1	Ti1	C1	C2	151.60(4)	Cl1	Ti1	C1	C5	37.18(8)
Cl1	Ti1	C1	C6	-86.65(8)	Cl1	Ti1	C2	C1	-45.66(11)
Cl1	Ti1	C2	C3	68.79(11)	Cl1	Ti1	C2	C7	-167.52(7)
Cl1	Ti1	C3	C2	-138.07(5)	Cl1	Ti1	C3	C4	-20.89(11)
Cl1	Ti1	C3	C8	102.05(9)	Cl1	Ti1	C4	C3	162.33(8)
Cl1	Ti1	C4	C5	-80.94(6)	Cl1	Ti1	C4	C9	39.35(11)
Cl1	Ti1	C5	C1	-146.17(7)	Cl1	Ti1	C5	C4	97.40(6)
Cl1	Ti1	C5	C10	-24.58(12)	Cl2	Ti1	C1	C2	11.55(9)
Cl2	Ti1	C1	C5	-102.87(6)	Cl2	Ti1	C1	C6	133.30(7)
Cl2	Ti1	C2	C1	-172.07(5)	Cl2	Ti1	C2	C3	-57.61(7)
Cl2	Ti1	C2	C7	66.07(12)	Cl2	Ti1	C3	C2	123.98(7)
Cl2	Ti1	C3	C4	-118.84(8)	Cl2	Ti1	C3	C8	4.10(9)
Cl2	Ti1	C4	C3	61.96(8)	Cl2	Ti1	C4	C5	178.69(5)
Cl2	Ti1	C4	C9	-61.02(11)	Cl2	Ti1	C5	C1	114.64(7)
Cl2	Ti1	C5	C4	-1.79(9)	Cl2	Ti1	C5	C10	-123.77(11)
N1	Ti1	C1	C2	-103.06(7)	N1	Ti1	C1	C5	142.52(7)
N1	Ti1	C1	C6	18.69(9)	N1	Ti1	C2	C1	80.91(7)
N1	Ti1	C2	C3	-164.63(8)	N1	Ti1	C2	C7	-40.95(13)
N1	Ti1	C3	C2	20.91(13)	N1	Ti1	C3	C4	138.09(8)
N1	Ti1	C3	C8	-98.97(13)	N1	Ti1	C4	C3	-81.25(14)
N1	Ti1	C4	C5	35.48(13)	N1	Ti1	C4	C9	155.77(10)
N1	Ti1	C5	C1	-44.31(9)	N1	Ti1	C5	C4	-160.75(6)
N1	Ti1	C5	C10	77.28(13)	C1	Ti1	C2	C1	-0.00(7)
C1	Ti1	C2	C3	114.46(11)	C1	Ti1	C2	C7	-121.86(16)
C2	Ti1	C1	C2	-0.00(7)	C2	Ti1	C1	C5	-114.42(12)
C2	Ti1	C1	C6	121.75(13)	C1	Ti1	C3	C2	-38.59(7)
C1	Ti1	C3	C4	78.59(9)	C1	Ti1	C3	C8	-158.48(11)
C3	Ti1	C1	C2	37.81(6)	C3	Ti1	C1	C5	-76.61(7)
C3	Ti1	C1	C6	159.56(11)	C1	Ti1	C4	C3	-79.40(8)
C1	Ti1	C4	C5	37.33(6)	C1	Ti1	C4	C9	157.62(14)
C4	Ti1	C1	C2	77.86(7)	C4	Ti1	C1	C5	-36.56(6)
C4	Ti1	C1	C6	-160.39(11)	C1	Ti1	C5	C1	0.00(7)
C1	Ti1	C5	C4	-116.44(12)	C1	Ti1	C5	C10	121.59(18)
C5	Ti1	C1	C2	114.42(13)	C5	Ti1	C1	C5	0.00(8)
C5	Ti1	C1	C6	-123.83(15)	C2	Ti1	C3	C2	0.00(8)
C2	Ti1	C3	C4	117.18(15)	C2	Ti1	C3	C8	-119.88(14)
C3	Ti1	C2	C1	-114.46(12)	C3	Ti1	C2	C3	-0.00(8)

Table 9. Torsion angles (°) (continued)

atom1	atom2	atom3	atom4	angle	atom1	atom2	atom3	atom4	angle
C3	Ti1	C2	C7	123.68(18)	C2	Ti1	C4	C3	-37.05(8)
C2	Ti1	C4	C5	79.68(9)	C2	Ti1	C4	C9	-160.02(15)
C4	Ti1	C2	C1	-78.62(8)	C4	Ti1	C2	C3	35.84(7)
C4	Ti1	C2	C7	159.52(16)	C2	Ti1	C5	C1	38.57(7)
C2	Ti1	C5	C4	-77.86(8)	C2	Ti1	C5	C10	160.16(16)
C5	Ti1	C2	C1	-37.91(7)	C5	Ti1	C2	C3	76.55(8)
C5	Ti1	C2	C7	-159.77(15)	C3	Ti1	C4	C3	-0.00(9)
C3	Ti1	C4	C5	116.73(14)	C3	Ti1	C4	C9	-123.0(2)
C4	Ti1	C3	C2	-117.18(16)	C4	Ti1	C3	C4	-0.00(9)
C4	Ti1	C3	C8	122.94(17)	C3	Ti1	C5	C1	80.13(8)
C3	Ti1	C5	C4	-36.30(6)	C3	Ti1	C5	C10	-158.28(15)
C5	Ti1	C3	C2	-80.30(9)	C5	Ti1	C3	C4	36.88(7)
C5	Ti1	C3	C8	159.82(12)	C4	Ti1	C5	C1	116.44(11)
C4	Ti1	C5	C4	-0.00(6)	C4	Ti1	C5	C10	-121.97(16)
C5	Ti1	C4	C3	-116.73(13)	C5	Ti1	C4	C5	-0.00(6)
C5	Ti1	C4	C9	120.30(15)	C11	N2	C12	C13	-13.3(2)
C12	N2	C11	N1	-173.11(16)	C12	N2	C11	N3	6.3(2)
C11	N2	C14	C15	105.0(2)	C11	N2	C14	C19	-79.2(2)
C14	N2	C11	N1	-14.0(3)	C14	N2	C11	N3	165.40(16)
C12	N2	C14	C15	-97.48(19)	C12	N2	C14	C19	78.4(2)
C14	N2	C12	C13	-173.56(15)	C11	N3	C13	C12	-12.1(2)
C13	N3	C11	N1	-176.46(17)	C13	N3	C11	N2	4.2(2)
C11	N3	C26	C27	-113.44(19)	C11	N3	C26	C31	69.3(3)
C26	N3	C11	N1	5.9(3)	C26	N3	C11	N2	-173.45(16)
C13	N3	C26	C27	69.2(2)	C13	N3	C26	C31	-108.12(18)
C26	N3	C13	C12	165.69(15)	Ti1	C1	C2	Ti1	0.0
Ti1	C1	C2	C3	-68.30(11)	Ti1	C1	C2	C7	115.78(16)
Ti1	C1	C5	Ti1	0.0	Ti1	C1	C5	C4	65.42(12)
Ti1	C1	C5	C10	-120.70(17)	C2	C1	C5	Ti1	-65.79(14)
C2	C1	C5	C4	-0.4(2)	C2	C1	C5	C10	173.52(16)
C5	C1	C2	Ti1	67.65(14)	C5	C1	C2	C3	-0.7(2)
C5	C1	C2	C7	-176.57(16)	C6	C1	C2	Ti1	-115.27(19)
C6	C1	C2	C3	176.43(17)	C6	C1	C2	C7	0.5(3)
C6	C1	C5	Ti1	117.15(19)	C6	C1	C5	C4	-177.43(17)
C6	C1	C5	C10	-3.5(3)	Ti1	C2	C3	Ti1	0.0
Ti1	C2	C3	C4	-64.09(11)	Ti1	C2	C3	C8	119.14(17)
C1	C2	C3	Ti1	65.52(13)	C1	C2	C3	C4	1.4(2)

Table 9. Torsion angles (°) (continued)

atom1	atom2	atom3	atom4	angle	atom1	atom2	atom3	atom4	angle
C1	C2	C3	C8	-175.34(16)	C7	C2	C3	Ti1	-118.5(2)
C7	C2	C3	C4	177.37(17)	C7	C2	C3	C8	0.6(3)
Ti1	C3	C4	Ti1	-0.0	Ti1	C3	C4	C5	-62.61(11)
Ti1	C3	C4	C9	117.88(18)	C2	C3	C4	Ti1	60.95(13)
C2	C3	C4	C5	-1.7(2)	C2	C3	C4	C9	178.84(16)
C8	C3	C4	Ti1	-122.3(2)	C8	C3	C4	C5	175.12(17)
C8	C3	C4	C9	-4.4(4)	Ti1	C4	C5	Ti1	0.0
Ti1	C4	C5	C1	-62.22(11)	Ti1	C4	C5	C10	123.72(17)
C3	C4	C5	Ti1	63.47(14)	C3	C4	C5	C1	1.3(2)
C3	C4	C5	C10	-172.80(16)	C9	C4	C5	Ti1	-117.0(2)
C9	C4	C5	C1	-179.23(18)	C9	C4	C5	C10	6.7(3)
N2	C12	C13	N3	14.44(19)	N2	C14	C15	C16	176.39(12)
N2	C14	C15	C20	-3.6(3)	N2	C14	C19	C18	-177.19(12)
N2	C14	C19	C23	1.8(3)	C15	C14	C19	C18	-1.5(3)
C15	C14	C19	C23	177.43(14)	C19	C14	C15	C16	0.7(3)
C19	C14	C15	C20	-179.30(14)	C14	C15	C16	C17	0.6(3)
C14	C15	C20	C21	-121.88(15)	C14	C15	C20	C22	114.61(16)
C16	C15	C20	C21	58.13(19)	C16	C15	C20	C22	-65.38(19)
C20	C15	C16	C17	-179.45(14)	C15	C16	C17	C18	-0.9(3)
C16	C17	C18	C19	0.0(3)	C17	C18	C19	C14	1.2(3)
C17	C18	C19	C23	-177.83(16)	C14	C19	C23	C24	121.06(17)
C14	C19	C23	C25	-114.92(17)	C18	C19	C23	C24	-60.0(2)
C18	C19	C23	C25	64.0(2)	N3	C26	C27	C28	-177.36(11)
N3	C26	C27	C32	1.2(2)	N3	C26	C31	C30	178.13(11)
N3	C26	C31	C35	0.9(2)	C27	C26	C31	C30	0.9(2)
C27	C26	C31	C35	-176.36(12)	C31	C26	C27	C28	-0.1(2)
C31	C26	C27	C32	178.42(12)	C26	C27	C28	C29	-0.4(3)
C26	C27	C32	C33	137.13(13)	C26	C27	C32	C34	-100.85(14)
C28	C27	C32	C33	-44.32(17)	C28	C27	C32	C34	77.70(17)
C32	C27	C28	C29	-178.98(12)	C27	C28	C29	C30	0.1(3)
C28	C29	C30	C31	0.7(3)	C29	C30	C31	C26	-1.2(3)
C29	C30	C31	C35	176.11(14)	C26	C31	C35	C36	-158.11(12)
C26	C31	C35	C37	78.82(16)	C30	C31	C35	C36	24.70(19)
C30	C31	C35	C37	-98.36(17)					

Table 10. Intramolecular contacts less than 3.60 Å

atom	atom	distance	atom	atom	distance
Cl1	C10	3.339(3)	Cl2	C8	3.210(3)
Cl2	C36	3.536(2)	N1	C6	3.255(3)
N1	C12	3.597(2)	N1	C14	2.9424(19)
N1	C19	3.553(2)	N1	C26	3.0042(15)
N1	C31	3.4305(17)	N1	C35	3.416(3)
N2	C20	2.892(3)	N2	C23	2.931(3)
N3	C14	3.5888(17)	N3	C32	2.939(3)
N3	C35	2.900(3)	N3	C37	3.331(4)
C6	C7	3.186(3)	C6	C10	3.213(3)
C7	C8	3.186(3)	C7	C27	3.591(3)
C8	C9	3.196(3)	C9	C10	3.146(4)
C11	C15	3.4337(18)	C11	C19	3.265(3)
C11	C23	3.390(3)	C11	C27	3.5200(18)
C11	C31	3.2138(19)	C11	C35	3.245(3)
C12	C15	3.4009(19)	C12	C19	3.261(3)
C12	C23	3.404(3)	C13	C27	3.223(3)
C13	C31	3.522(3)	C13	C32	3.285(3)
C13	C34	3.499(3)	C14	C17	2.763(2)
C14	C22	3.574(4)	C14	C25	3.593(4)
C15	C18	2.799(4)	C16	C19	2.802(3)
C16	C21	3.047(4)	C16	C22	3.122(4)
C18	C24	3.081(3)	C18	C25	3.108(3)
C26	C29	2.774(2)	C26	C34	3.467(3)
C26	C37	3.262(4)	C27	C30	2.798(3)
C28	C31	2.801(3)	C28	C33	2.975(4)
C28	C34	3.206(3)	C30	C36	2.894(4)
C30	C37	3.407(4)			

Table 11. Intramolecular contacts less than 3.60 Å involving hydrogens

atom	atom	distance	atom	atom	distance
Ti1	H1	3.385	Ti1	H3	3.580
Ti1	H5	3.499	Ti1	H6	3.490
Ti1	H12	3.473	Ti1	H14	3.555
Ti1	H32	3.589	Cl1	H12	2.959
Cl1	H14	2.775	Cl1	H25	3.220
Cl2	H7	2.984	Cl2	H9	3.017
Cl2	H32	2.880	Cl2	H47	3.295
Cl2	H48	2.987	Cl2	H50	3.404
N1	H1	2.817	N1	H3	3.425
N1	H5	3.250	N1	H23	3.512
N1	H30	3.228	N1	H32	3.367
N1	H47	2.604	N2	H18	3.099
N2	H19	2.908	N2	H23	2.390
N2	H30	2.432	N2	H47	3.381
N3	H1	3.369	N3	H16	3.107
N3	H17	2.915	N3	H30	3.197
N3	H40	2.497	N3	H45	3.384
N3	H47	2.589	N3	H52	2.790
C1	H4	3.051	C1	H5	2.724
C1	H6	3.331	C1	H13	3.129
C1	H14	3.293	C1	H15	2.703
C2	H1	2.773	C2	H2	2.973
C2	H3	3.361	C2	H7	3.340
C2	H8	3.048	C2	H9	2.731
C3	H4	3.011	C3	H5	3.351
C3	H6	2.746	C3	H10	3.156
C3	H11	2.690	C3	H12	3.265
C4	H7	2.733	C4	H8	3.017
C4	H9	3.335	C4	H13	2.903
C4	H14	2.790	C4	H15	3.363
C5	H1	3.311	C5	H2	3.101
C5	H3	2.710	C5	H10	2.918
C5	H11	3.369	C5	H12	2.799
C5	H25	3.568	C6	H4	3.526
C6	H5	2.856	C6	H15	2.819
C6	H25	3.521	C6	H40	3.504
C6	H41	3.027	C7	H1	2.966

Table 11. Intramolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
C7	H2	3.367	C7	H8	3.512
C7	H9	2.864	C7	H41	3.381
C8	H4	3.439	C8	H6	2.909
C8	H11	2.794	C9	H7	2.889
C9	H8	3.506	C9	H13	3.261
C9	H14	2.962	C10	H3	2.856
C10	H10	3.196	C10	H12	3.026
C10	H25	2.949	C11	H1	3.111
C11	H16	3.079	C11	H17	2.921
C11	H18	3.073	C11	H19	2.930
C11	H23	3.022	C11	H30	2.683
C11	H40	3.216	C11	H47	2.528
C11	H52	3.463	C12	H23	3.112
C12	H30	2.783	C12	H35	3.403
C12	H52	3.326	C13	H30	3.446
C13	H40	2.783	C13	H45	2.861
C13	H52	2.814	C14	H16	2.824
C14	H17	2.743	C14	H20	3.258
C14	H22	3.258	C14	H23	2.583
C14	H25	3.512	C14	H29	3.466
C14	H30	2.596	C14	H32	3.562
C14	H35	3.479	C15	H16	3.336
C15	H21	3.275	C15	H24	3.343
C15	H25	2.638	C15	H26	2.760
C15	H27	3.353	C15	H28	2.720
C15	H29	2.695	C16	H22	3.250
C16	H23	3.323	C16	H25	3.197
C16	H26	2.834	C16	H28	2.858
C16	H29	3.387	C18	H20	3.250
C18	H30	3.321	C18	H31	2.821
C18	H32	3.316	C18	H35	3.355
C18	H36	2.851	C19	H17	3.060
C19	H21	3.277	C19	H31	2.740
C19	H32	2.702	C19	H33	3.363
C19	H34	3.360	C19	H35	2.694
C19	H36	2.736	C20	H16	3.366
C20	H20	2.669	C21	H3	3.155

Table 11. Intramolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
C21	H15	2.996	C21	H20	2.881
C21	H27	2.681	C21	H28	2.710
C21	H29	3.351	C22	H16	3.541
C22	H20	2.995	C22	H24	2.728
C22	H25	3.349	C22	H26	2.665
C23	H17	2.910	C23	H22	2.663
C23	H47	3.119	C23	H53	3.384
C24	H22	2.903	C24	H34	2.688
C24	H35	3.358	C24	H36	2.717
C24	H47	3.127	C24	H50	3.480
C24	H53	3.528	C25	H17	3.104
C25	H22	2.983	C25	H31	2.717
C25	H32	3.359	C25	H33	2.688
C25	H53	3.591	C26	H1	3.510
C26	H5	2.843	C26	H18	2.733
C26	H19	2.905	C26	H37	3.264
C26	H39	3.262	C26	H40	2.629
C26	H45	3.272	C26	H47	2.676
C26	H51	3.581	C26	H52	3.008
C27	H1	3.376	C27	H5	2.670
C27	H18	3.451	C27	H19	3.156
C27	H38	3.277	C27	H41	2.685
C27	H42	3.375	C27	H43	2.807
C27	H44	3.350	C27	H45	2.663
C27	H46	2.728	C28	H5	2.913
C28	H39	3.247	C28	H40	3.312
C28	H41	3.057	C28	H43	2.787
C28	H45	3.485	C28	H46	2.977
C29	H5	3.288	C29	H6	3.410
C30	H5	3.429	C30	H6	3.248
C30	H37	3.249	C30	H47	3.257
C30	H48	2.806	C30	H49	2.824
C30	H51	3.227	C31	H5	3.255
C31	H6	3.384	C31	H18	3.445
C31	H38	3.277	C31	H48	2.666
C31	H49	2.837	C31	H50	3.370
C31	H51	2.694	C31	H52	2.694

Table 11. Intramolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
C31	H53	3.348	C32	H1	3.097
C32	H5	3.365	C32	H19	2.778
C32	H37	2.655	C33	H1	3.083
C33	H2	3.511	C33	H5	3.359
C33	H37	2.699	C33	H44	2.690
C33	H45	3.353	C33	H46	2.686
C34	H19	2.782	C34	H37	3.162
C34	H41	3.352	C34	H42	2.734
C34	H43	2.642	C35	H30	3.065
C35	H33	3.541	C35	H39	2.673
C36	H33	3.584	C36	H39	2.528
C36	H51	2.721	C36	H52	3.341
C36	H53	2.641	C37	H18	3.161
C37	H30	2.959	C37	H33	3.598
C37	H39	3.514	C37	H48	3.340
C37	H49	2.617	C37	H50	2.745
H1	H4	3.426	H1	H5	2.367
H1	H40	2.591	H1	H41	2.469
H1	H42	3.328	H2	H4	3.432
H2	H5	3.091	H2	H15	3.242
H2	H41	2.718	H2	H42	3.548
H3	H13	3.424	H3	H14	3.570
H3	H15	2.212	H3	H23	3.233
H3	H24	2.874	H3	H25	2.676
H4	H8	3.490	H4	H9	3.185
H4	H41	3.326	H5	H37	3.375
H5	H40	3.485	H5	H41	2.628
H6	H8	3.335	H6	H9	2.316
H6	H39	3.572	H6	H48	3.499
H7	H10	3.495	H7	H11	2.241
H7	H12	3.569	H8	H11	3.114
H10	H13	3.010	H10	H14	3.103
H12	H13	3.287	H12	H14	2.548
H14	H25	2.920	H15	H24	2.961
H15	H25	2.250	H15	H26	3.439
H16	H18	2.693	H16	H19	2.257
H16	H23	2.858	H16	H29	2.872

Table 11. Intramolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
H17	H18	2.257	H17	H19	2.824
H17	H30	2.355	H17	H34	3.505
H17	H35	2.517	H17	H52	2.974
H18	H30	3.570	H18	H40	3.453
H18	H45	2.866	H18	H51	3.552
H18	H52	2.241	H19	H40	2.242
H19	H44	3.064	H19	H45	2.201
H20	H21	2.323	H20	H25	3.197
H20	H26	2.383	H20	H28	2.477
H20	H29	3.442	H21	H22	2.322
H22	H31	2.372	H22	H32	3.303
H22	H35	3.417	H22	H36	2.471
H23	H24	2.321	H23	H25	2.393
H23	H26	2.860	H23	H27	2.353
H23	H28	2.860	H23	H29	2.355
H24	H27	2.536	H24	H28	3.050
H25	H27	3.590	H25	H28	3.581
H26	H27	2.912	H26	H28	2.500
H26	H29	3.571	H30	H31	2.861
H30	H32	2.359	H30	H33	2.351
H30	H34	2.354	H30	H35	2.362
H30	H36	2.864	H30	H47	2.337
H30	H52	2.698	H30	H53	2.741
H31	H34	2.988	H31	H36	2.554
H32	H34	3.577	H32	H47	2.813
H32	H50	3.290	H33	H34	2.492
H33	H35	3.576	H33	H36	2.987
H33	H47	3.005	H33	H50	2.825
H33	H53	2.906	H34	H53	2.981
H37	H38	2.319	H37	H40	3.582
H37	H41	2.893	H37	H43	2.220
H37	H46	2.716	H38	H39	2.328
H39	H47	3.502	H39	H48	2.423
H39	H49	2.229	H39	H50	3.498
H39	H51	3.215	H40	H41	2.417
H40	H42	2.323	H40	H43	2.868
H40	H44	2.358	H40	H45	2.386

Table 11. Intramolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
H40	H46	2.873	H41	H46	3.557
H42	H44	2.554	H42	H46	3.034
H43	H44	2.904	H43	H45	3.547
H43	H46	2.453	H47	H48	2.422
H47	H49	2.855	H47	H50	2.294
H47	H51	2.863	H47	H52	2.345
H47	H53	2.372	H48	H51	3.569
H48	H53	3.569	H49	H51	2.480
H49	H52	3.543	H49	H53	2.806
H50	H51	3.115	H50	H53	2.531

Table 12. Intermolecular contacts less than 3.60 Å

atom	atom	distance	atom	atom	distance
Cl1	C38A[1]	3.400(8)	Cl1	C38B[1]	3.19(4)
Cl1	C39A[2]	3.384(9)	Cl1	C39B[2]	3.505(9)
Cl3A	C13	3.576(5)	Cl3B	C17[3]	3.368(10)
Cl3B	C22	3.523(7)	Cl4A	C37[4]	3.596(3)
Cl4B	Cl6B[4]	3.514(19)	Cl4B	C37[4]	3.409(18)
Cl6B	Cl4B[5]	3.514(19)	C13	Cl3A	3.576(5)
C16	C39B[2]	3.595(12)	C17	Cl3B[3]	3.368(10)
C22	Cl3B	3.523(7)	C37	Cl4A[5]	3.596(3)
C37	Cl4B[5]	3.409(18)	C38A	Cl1[6]	3.400(8)
C38B	Cl1[6]	3.19(4)	C39A	Cl1[7]	3.384(9)
C39B	Cl1[7]	3.505(9)	C39B	C16[7]	3.595(12)

Symmetry Operators:

(1) X,Y-1,Z
(2) X-1,Y-1,Z
(3) -X,-Y+1,-Z
(4) X-1,Y,Z
(5) X+1,Y,Z
(6) X,Y+1,Z
(7) X+1,Y+1,Z

Table 13. Intermolecular contacts less than 3.60 Å involving hydrogens

atom	atom	distance	atom	atom	distance
Cl2	H38[1]	3.153	Cl2	H42[2]	3.218
Cl2	H44[2]	2.956	Cl3A	H16	3.034
Cl3A	H19	2.769	Cl3A	H21[3]	3.284
Cl3A	H23	3.224	Cl3A	H27	3.354
Cl3A	H29	3.396	Cl3A	H31[4]	3.033
Cl3A	H40	3.219	Cl3A	H44	3.360
Cl3B	H16	3.127	Cl3B	H19	3.090
Cl3B	H21[3]	3.045	Cl3B	H23	3.260
Cl3B	H27	3.127	Cl3B	H29	3.200
Cl3B	H31[4]	2.984	Cl3B	H40	3.589
Cl4A	H1	3.493	Cl4A	H3	3.218
Cl4A	H23	3.380	Cl4A	H24	3.343
Cl4A	H40	3.352	Cl4A	H42	3.242
Cl4A	H51[5]	2.957	Cl4A	H53[5]	3.567
Cl4B	H24	3.296	Cl4B	H27	3.320
Cl4B	H51[5]	2.918	Cl4B	H52[5]	3.363
Cl4B	H53[5]	3.403	Cl5A	H14[6]	3.360
Cl5A	H18	3.419	Cl5A	H19	3.225
Cl5A	H20[3]	3.264	Cl5A	H21[3]	3.219
Cl5A	H26[6]	3.540	Cl5A	H31[4]	3.328
Cl5A	H33[4]	3.397	Cl5B	H14[6]	3.464
Cl5B	H16	3.546	Cl5B	H18	3.307
Cl5B	H19	3.331	Cl5B	H20[3]	3.117
Cl5B	H21[3]	3.418	Cl6A	H17	3.194
Cl6A	H18	3.503	Cl6A	H20[3]	3.182
Cl6A	H26[3]	3.359	Cl6A	H28[3]	3.362
Cl6A	H36[7]	3.157	Cl6B	H17	3.096
Cl6B	H18	3.091	Cl6B	H36[7]	3.258
Cl6B	H52	3.549	C1	H4[8]	2.826
C2	H2[8]	3.535	C2	H4[8]	3.117
C3	H41[8]	3.297	C4	H41[8]	3.541
C5	H4[8]	3.314	C6	H4[8]	3.047
C7	H2[8]	3.185	C7	H49[1]	3.259
C8	H2[8]	3.383	C8	H7[9]	3.363
C8	H11[9]	3.265	C8	H39[1]	3.339
C8	H41[8]	3.256	C8	H42[8]	3.500
C9	H43[8]	3.365	C10	H45[10]	3.180

Table 13. Intermolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
C10	H46[10]	3.371	C10	H50[5]	3.094
C12	H28[3]	3.107	C14	H29[3]	3.218
C15	H29[3]	3.184	C16	H16[3]	3.424
C16	H29[3]	3.238	C17	H22[11]	3.428
C17	H29[3]	3.355	C18	H22[11]	3.311
C18	H29[3]	3.394	C19	H29[3]	3.331
C21	H34[5]	3.332	C22	H16[3]	3.484
C22	H17[3]	3.419	C22	H35[3]	3.039
C25	H27[3]	3.410	C25	H28[3]	3.599
C27	H10[6]	3.514	C28	H10[6]	3.139
C28	H37[12]	3.074	C28	H43[12]	3.305
C28	H46[12]	3.277	C29	H9[1]	3.404
C29	H10[6]	3.268	C29	H43[12]	3.228
C29	H46[12]	3.266	C29	H48[1]	2.950
C30	H9[1]	2.998	C30	H48[1]	3.179
C33	H8[8]	2.924	C33	H10[8]	3.519
C33	H38[12]	3.539	C34	H13[6]	2.901
C34	H14[6]	3.564	C34	H37[12]	3.574
C34	H38[12]	3.363	C36	H6[1]	3.427
C36	H13[13]	3.265	C36	H15[13]	3.503
C36	H38[1]	3.225	C38A	H31[4]	3.427
C38A	H32[4]	3.337	C38A	H40	3.566
C38A	H44	3.475	C38B	H31[4]	3.260
C38B	H32[4]	3.176	C38B	H44	3.597
C39A	H14[6]	3.463	C39A	H18	3.489
C39A	H20[6]	3.479	C39B	H20[6]	3.328
C39B	H21[6]	3.415	H1	Cl4A	3.493
H2	C2[8]	3.535	H2	C7[8]	3.185
H2	C8[8]	3.383	H2	H4[8]	2.417
H2	H6[8]	3.376	H2	H8[8]	2.759
H2	H9[8]	3.418	H2	H49[5]	3.066
H2	H51[5]	3.474	H3	Cl4A	3.218
H3	H49[5]	3.472	H3	H51[5]	3.416
H3	H53[5]	3.401	H4	C1[8]	2.826
H4	C2[8]	3.117	H4	C5[8]	3.314
H4	C6[8]	3.047	H4	H2[8]	2.417
H4	H4[8]	3.192	H4	H49[1]	2.960

Table 13. Intermolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
H6	C36[1]	3.427	H6	H2[8]	3.376
H6	H39[1]	2.691	H6	H48[1]	3.320
H6	H49[1]	2.674	H7	C8[9]	3.363
H7	H7[9]	2.625	H7	H8[9]	3.236
H7	H11[9]	2.840	H7	H42[2]	3.384
H8	C33[8]	2.924	H8	H2[8]	2.759
H8	H7[9]	3.236	H8	H11[9]	3.088
H8	H41[8]	2.489	H8	H42[8]	2.623
H8	H43[8]	3.235	H9	C29[1]	3.404
H9	C30[1]	2.998	H9	H2[8]	3.418
H9	H11[9]	3.339	H9	H38[1]	3.163
H9	H39[1]	2.373	H9	H49[1]	3.272
H10	C27[10]	3.514	H10	C28[10]	3.139
H10	C29[10]	3.268	H10	C33[8]	3.519
H10	H37[10]	3.337	H10	H37[8]	3.399
H10	H38[10]	3.543	H10	H41[8]	3.517
H10	H43[8]	2.732	H10	H45[10]	3.301
H10	H46[10]	3.157	H11	C8[9]	3.265
H11	H7[9]	2.840	H11	H8[9]	3.088
H11	H9[9]	3.339	H11	H43[8]	3.366
H12	H45[10]	3.592	H13	C34[10]	2.901
H13	C36[5]	3.265	H13	H44[10]	3.152
H13	H45[10]	2.622	H13	H46[10]	2.488
H13	H49[5]	3.237	H13	H50[5]	2.516
H14	Cl5A[10]	3.360	H14	Cl5B[10]	3.464
H14	C34[10]	3.564	H14	C39A[10]	3.463
H14	H45[10]	2.852	H14	H46[10]	3.486
H15	C36[5]	3.503	H15	H33[5]	3.535
H15	H49[5]	3.345	H15	H50[5]	2.796
H15	H53[5]	3.291	H16	Cl3A	3.034
H16	Cl3B	3.127	H16	Cl5B	3.546
H16	C16[3]	3.424	H16	C22[3]	3.484
H16	H20[3]	3.101	H16	H28[3]	2.770
H16	H29[3]	3.332	H17	Cl6A	3.194
H17	Cl6B	3.096	H17	C22[3]	3.419
H17	H28[3]	2.611	H17	H29[3]	3.469
H18	Cl5A	3.419	H18	Cl5B	3.307

Table 13. Intermolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
H18	Cl6A	3.503	H18	Cl6B	3.091
H18	C39A	3.489	H19	Cl3A	2.769
H19	Cl3B	3.090	H19	Cl5A	3.225
H19	Cl5B	3.331	H20	Cl5A[3]	3.264
H20	Cl5B[3]	3.117	H20	Cl6A[3]	3.182
H20	C39A[10]	3.479	H20	C39B[10]	3.328
H20	H16[3]	3.101	H21	Cl3A[3]	3.284
H21	Cl3B[3]	3.045	H21	Cl5A[3]	3.219
H21	Cl5B[3]	3.418	H21	C39B[10]	3.415
H21	H22[11]	2.860	H21	H31[11]	2.948
H21	H36[11]	3.391	H22	C17[11]	3.428
H22	C18[11]	3.311	H22	H21[11]	2.860
H22	H22[11]	2.613	H23	Cl3A	3.224
H23	Cl3B	3.260	H23	Cl4A	3.380
H24	Cl4A	3.343	H24	Cl4B	3.296
H24	H34[5]	2.891	H24	H53[5]	2.748
H26	Cl5A[10]	3.540	H26	Cl6A[3]	3.359
H26	H34[5]	2.873	H27	Cl3A	3.354
H27	Cl3B	3.127	H27	Cl4B	3.320
H27	C25[3]	3.410	H27	H35[3]	2.676
H27	H36[3]	3.310	H28	Cl6A[3]	3.362
H28	C12[3]	3.107	H28	C25[3]	3.599
H28	H16[3]	2.770	H28	H17[3]	2.611
H28	H35[3]	2.680	H29	Cl3A	3.396
H29	Cl3B	3.200	H29	C14[3]	3.218
H29	C15[3]	3.184	H29	C16[3]	3.238
H29	C17[3]	3.355	H29	C18[3]	3.394
H29	C19[3]	3.331	H29	H16[3]	3.332
H29	H17[3]	3.469	H29	H29[3]	3.041
H29	H35[3]	3.302	H31	Cl3A[2]	3.033
H31	Cl3B[2]	2.984	H31	Cl5A[2]	3.328
H31	C38A[2]	3.427	H31	C38B[2]	3.260
H31	H21[11]	2.948	H32	C38A[2]	3.337
H32	C38B[2]	3.176	H32	H44[2]	3.326
H33	Cl5A[2]	3.397	H33	H15[13]	3.535
H33	H44[2]	3.492	H34	C21[13]	3.332
H34	H24[13]	2.891	H34	H26[13]	2.873

Table 13. Intermolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
H35	C22^{3}	3.039	H35	H27^{3}	2.676
H35	H28^{3}	2.680	H35	H29^{3}	3.302
H36	Cl6A^{7}	3.157	H36	Cl6B^{7}	3.258
H36	H21^{11}	3.391	H36	H27^{3}	3.310
H37	C28^{12}	3.074	H37	C34^{12}	3.574
H37	H10^{6}	3.337	H37	H10^{8}	3.399
H37	H37^{12}	2.272	H37	H43^{12}	2.929
H37	H46^{12}	2.653	H38	Cl2^{1}	3.153
H38	C33^{12}	3.539	H38	C34^{12}	3.363
H38	C36^{1}	3.225	H38	H9^{1}	3.163
H38	H10^{6}	3.543	H38	H42^{12}	3.568
H38	H43^{12}	2.789	H38	H44^{12}	3.295
H38	H46^{12}	2.639	H38	H48^{1}	2.460
H38	H49^{1}	3.540	H38	H50^{1}	3.269
H39	C8^{1}	3.339	H39	H6^{1}	2.691
H39	H9^{1}	2.373	H39	H39^{1}	3.308
H39	H48^{1}	2.886	H40	Cl3A	3.219
H40	Cl3B	3.589	H40	Cl4A	3.352
H40	C38A	3.566	H41	C3^{8}	3.297
H41	C4^{8}	3.541	H41	C8^{8}	3.256
H41	H8^{8}	2.489	H41	H10^{8}	3.517
H42	Cl2^{4}	3.218	H42	Cl4A	3.242
H42	C8^{8}	3.500	H42	H7^{4}	3.384
H42	H8^{8}	2.623	H42	H38^{12}	3.568
H43	C9^{8}	3.365	H43	C28^{12}	3.305
H43	C29^{12}	3.228	H43	H8^{8}	3.235
H43	H10^{8}	2.732	H43	H11^{8}	3.366
H43	H37^{12}	2.929	H43	H38^{12}	2.789
H44	Cl2^{4}	2.956	H44	Cl3A	3.360
H44	C38A	3.475	H44	C38B	3.597
H44	H13^{6}	3.152	H44	H32^{4}	3.326
H44	H33^{4}	3.492	H44	H38^{12}	3.295
H44	H50^{4}	3.328	H45	C10^{6}	3.180
H45	H10^{6}	3.301	H45	H12^{6}	3.592
H45	H13^{6}	2.622	H45	H14^{6}	2.852
H46	C10^{6}	3.371	H46	C28^{12}	3.277
H46	C29^{12}	3.266	H46	H10^{6}	3.157

Table 13. Intermolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
H46	$H13^{6}$	2.488	H46	$H14^{6}$	3.486
H46	$H37^{12}$	2.653	H46	$H38^{12}$	2.639
H46	$H50^{4}$	3.429	H48	$C29^{1}$	2.950
H48	$C30^{1}$	3.179	H48	$H6^{1}$	3.320
H48	$H38^{1}$	2.460	H48	$H39^{1}$	2.886
H49	$C7^{1}$	3.259	H49	$H2^{13}$	3.066
H49	$H3^{13}$	3.472	H49	$H4^{1}$	2.960
H49	$H6^{1}$	2.674	H49	$H9^{1}$	3.272
H49	$H13^{13}$	3.237	H49	$H15^{13}$	3.345
H49	$H38^{1}$	3.540	H50	$C10^{13}$	3.094
H50	$H13^{13}$	2.516	H50	$H15^{13}$	2.796
H50	$H38^{1}$	3.269	H50	$H44^{2}$	3.328
H50	$H46^{2}$	3.429	H51	$Cl4A^{13}$	2.957
H51	$Cl4B^{13}$	2.918	H51	$H2^{13}$	3.474
H51	$H3^{13}$	3.416	H52	$Cl4B^{13}$	3.363
H52	Cl6B	3.549	H53	$Cl4A^{13}$	3.567
H53	$Cl4B^{13}$	3.403	H53	$H3^{13}$	3.401
H53	$H15^{13}$	3.291	H53	$H24^{13}$	2.748

Symmetry Operators:

(1) -X+1,-Y+1,-Z+1
(2) X,Y-1,Z
(3) -X,-Y+1,-Z
(4) X,Y+1,Z
(5) X-1,Y,Z
(6) X+1,Y+1,Z
(7) -X+1,-Y+1,-Z
(8) -X,-Y+1,-Z+1
(9) -X,-Y,-Z+1
(10) X-1,Y-1,Z
(11) -X,-Y,-Z
(12) -X+1,-Y+2,-Z+1
(13) X+1,Y,Z

or $Cp^{*}TiCl_{2}[1,3\text{-}(2,6\text{-}^{i}Pr_{2}C_{6}H_{3})_{2}(CH_{2}N)_{2}C{=}N]$ (**1e**)