Electronic Supplementary Information for Dalton Transactions

Electronic Supplementary Information (ESI)

Effect of Aryloxo Substituents in Ethylene Polymerization by Tris(pyrazolyl)borate Titanium(IV) Complexes Containing Aryloxo Ligands of Type, $TpTiCl_2(OAr)$

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Contents

Electronic Supplementary Information for Dalton Transactions

X-ray Structure Report for $TpTiCl_2(OC_6F_5)$ (**3**)

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Experimental

Data Collection

A red block crystal of $C_{16}H_{10}BCl_4F_5N_6OTi$ having approximate dimensions of 0.40 x 0.20 x 0.12 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 200 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 = 11.5340(4) Å
b = 12.9265(4) Å β = 98.7577(12)^o
c = 15.6367(7) Å
V = 2304.15(15) Å^3

For Z = 4 and F.W. = 597.81, the calculated density is 1.723 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 -80 ± 1^{o}C to a maximum 2θ value of 50.6^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 280.0 [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 280.0 [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 18147 reflections that were collected, 4185 were unique (R_{int} = 0.021); equivalent reflections were merged.

The linear absorption coefficient, μ, for Mo-Kα radiation is 8.980 cm^{-1}. An empirical absorption correction was applied which resulted in transmission factors ranging from 0.718 to 0.898. 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 4185 observed reflections and 326 variable parameters and converged (largest parameter shift was 0.00 times its esd) with unweighted and weighted agreement factors of:

$$R1 = \Sigma \; ||Fo| - |Fc|| \; / \; \Sigma \; |Fo| = 0.0624$$

$$wR2 = [\Sigma \; (\; w \; (Fo^2 - Fc^2)^2 \;) / \; \Sigma \; w(Fo^2)^2]^{1/2} = 0.1842$$

The standard deviation of an observation of unit weight[4] was 1.07. A Sheldrick weighting scheme was used. The maximum and minimum peaks on the final difference Fourier map corresponded to 1.04 and -1.70 $e^-/Å^3$, 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).

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(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).

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(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	$C_{16}H_{10}BCl_4F_5N_6OTi$
Formula Weight	597.81
Crystal Color, Habit	red, block
Crystal Dimensions	0.40 X 0.20 X 0.12 mm
Crystal System	monoclinic
Lattice Type	Primitive
Indexing Images	3 oscillations @ 200.0 seconds
Detector Position	127.40 mm
Pixel Size	0.100 mm
Lattice Parameters	a = 11.5340(4) Å b = 12.9265(4) Å c = 15.6367(7) Å β = 98.7577(12) ^{o} V = 2304.15(15) Å^3
Space Group	$P2_1/c$ (#14)
Z value	4
D_{calc}	1.723 g/cm^3
F_{000}	1184.00
μ(MoKα)	8.980 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	280.0 sec./^{o}
ω oscillation Range (χ=45.0, ϕ=180.0)	0.0 - 162.0^{o}
Exposure Rate	280.0 sec./^{o}
Detector Position	127.40 mm
Pixel Size	0.100 mm
$2\theta_{max}$	50.6^{o}
No. of Reflections Measured	Total: 18147 Unique: 4185 (R_{int} = 0.021)
Corrections	Lorentz-polarization Absorption (trans. factors: 0.718 - 0.898)

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	$w = 1/ [\sigma^2(Fo^2) + (0.1048 \cdot P)^2 + 6.5259 \cdot P]$ where $P = (Max(Fo^2,0) + 2Fc^2)/3$
$2\theta_{max}$ cutoff	50.6^o
Anomalous Dispersion	All non-hydrogen atoms
No. Observations (All reflections)	4185
No. Variables	326
Reflection/Parameter Ratio	12.84
Residuals: R1 (I>2.00σ(I))	0.0624
Residuals: R (All reflections)	0.0660
Residuals: wR2 (All reflections)	0.1842
Goodness of Fit Indicator	1.067
Max Shift/Error in Final Cycle	0.000
Maximum peak in Final Diff. Map	1.04 $e^-/Å^3$
Minimum peak in Final Diff. Map	-1.70 $e^-/Å^3$

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

atom	x	y	z	B_{eq}	occ
Ti(1)	0.26783(6)	0.20009(5)	0.68940(4)	1.941(18)	
Cl(1)	0.22698(9)	0.04087(8)	0.73886(7)	2.75(2)	
Cl(2)	0.18584(9)	0.18311(9)	0.54876(7)	3.04(2)	
Cl(3)	-0.0333(4)	0.4724(3)	0.6099(2)	7.19(9)	1/2
Cl(4)	-0.2024(5)	0.3265(3)	0.5849(2)	16.42(17)	
Cl(5)	-0.0308(8)	0.4466(6)	0.5000(5)	13.7(2)	1/2
F(1)	0.1764(2)	0.4513(2)	0.81124(19)	3.50(5)	
F(2)	0.0224(2)	0.5160(2)	0.91350(19)	4.02(5)	
F(3)	-0.1641(2)	0.3921(2)	0.93774(18)	4.17(5)	
F(4)	-0.1931(2)	0.2073(2)	0.85613(19)	3.74(5)	
F(5)	-0.0419(2)	0.1439(2)	0.7512(2)	3.79(5)	
O(1)	0.1478(2)	0.2650(2)	0.7282(2)	2.78(5)	
N(1)	0.5386(2)	0.1811(2)	0.6850(2)	1.96(5)	
N(2)	0.4310(2)	0.1361(2)	0.6601(2)	1.96(5)	
N(3)	0.4917(2)	0.2640(2)	0.8186(2)	2.07(5)	
N(4)	0.3790(2)	0.2294(2)	0.8118(2)	2.25(5)	
N(5)	0.4655(2)	0.3627(2)	0.6805(2)	2.08(5)	
N(6)	0.3486(2)	0.3409(2)	0.6577(2)	2.26(5)	
C(1)	0.6219(3)	0.1205(3)	0.6606(2)	2.56(6)	
C(2)	0.5692(3)	0.0349(3)	0.6182(2)	2.85(7)	
C(3)	0.4509(3)	0.0482(3)	0.6193(2)	2.50(6)	
C(4)	0.5364(3)	0.2737(3)	0.9029(2)	2.41(6)	
C(5)	0.4529(4)	0.2450(3)	0.9522(2)	2.87(7)	
C(6)	0.3557(4)	0.2181(3)	0.8930(2)	2.74(7)	
C(7)	0.4886(4)	0.4564(3)	0.6503(2)	2.85(7)	
C(8)	0.3847(4)	0.4969(3)	0.6058(3)	3.69(9)	
C(9)	0.3011(4)	0.4230(3)	0.6122(3)	3.20(8)	
C(10)	0.0728(3)	0.2957(3)	0.7802(2)	2.34(6)	
C(11)	0.0855(3)	0.3904(3)	0.8225(2)	2.49(6)	
C(12)	0.0071(3)	0.4235(3)	0.8756(2)	2.75(7)	
C(13)	-0.0855(3)	0.3617(3)	0.8872(2)	2.88(7)	
C(14)	-0.1010(3)	0.2673(3)	0.8457(2)	2.75(7)	
C(15)	-0.0234(3)	0.2344(3)	0.7928(2)	2.51(6)	
C(16)	-0.0723(16)	0.3573(14)	0.5548(10)	9.1(6)	1/2
C(17)	-0.1002(8)	0.4339(8)	0.5818(6)	3.7(2)	1/2
B(1)	0.5453(3)	0.2841(3)	0.7355(2)	1.99(6)	

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

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

atom	x	y	z	B_{eq}	occ
H(1)	0.7038	0.1341	0.6707	3.07	
H(2)	0.6064	-0.0209	0.5936	3.42	
H(3)	0.3916	0.0015	0.5946	2.99	
H(4)	0.6134	0.2968	0.9248	2.89	
H(5)	0.4602	0.2439	1.0135	3.45	
H(6)	0.2830	0.1950	0.9076	3.28	
H(7)	0.5631	0.4895	0.6580	3.41	
H(8)	0.3740	0.5617	0.5771	4.43	
H(9)	0.2207	0.4290	0.5879	3.84	
H(10)	0.6278	0.3098	0.7491	2.39	

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

Table 3. Anisotropic displacement parameters

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Ti(1)	0.0207(3)	0.0239(3)	0.0295(4)	-0.0011(2)	0.0049(2)	0.0008(2)
Cl(1)	0.0317(5)	0.0300(5)	0.0427(5)	-0.0066(3)	0.0052(4)	0.0059(3)
Cl(2)	0.0340(5)	0.0464(6)	0.0329(5)	-0.0100(4)	-0.0020(4)	0.0029(4)
Cl(3)	0.111(3)	0.092(2)	0.077(2)	-0.006(2)	0.038(2)	-0.004(2)
Cl(4)	0.337(7)	0.153(3)	0.135(2)	-0.005(4)	0.042(3)	0.010(2)
Cl(5)	0.203(8)	0.152(6)	0.168(6)	-0.022(5)	0.039(5)	-0.006(5)
F(1)	0.0341(13)	0.0347(13)	0.0643(17)	-0.0077(10)	0.0074(12)	-0.0023(11)
F(2)	0.0613(17)	0.0409(14)	0.0507(16)	0.0033(13)	0.0086(13)	-0.0139(12)
F(3)	0.0488(15)	0.0674(19)	0.0467(15)	0.0105(14)	0.0217(12)	-0.0022(13)
F(4)	0.0301(12)	0.0545(16)	0.0594(17)	-0.0043(11)	0.0125(11)	0.0125(13)
F(5)	0.0395(14)	0.0350(13)	0.0706(18)	-0.0065(11)	0.0122(12)	-0.0107(12)
O(1)	0.0267(13)	0.0342(15)	0.0465(16)	0.0019(11)	0.0115(12)	-0.0016(12)
N(1)	0.0220(15)	0.0257(15)	0.0266(15)	-0.0001(12)	0.0035(12)	-0.0005(12)
N(2)	0.0256(15)	0.0223(15)	0.0266(15)	-0.0019(12)	0.0041(12)	-0.0011(12)
N(3)	0.0268(15)	0.0229(15)	0.0285(16)	0.0002(12)	0.0030(12)	-0.0027(12)
N(4)	0.0287(16)	0.0293(17)	0.0288(16)	-0.0016(13)	0.0086(13)	-0.0027(13)
N(5)	0.0254(15)	0.0228(15)	0.0303(16)	-0.0027(12)	0.0029(12)	-0.0001(12)
N(6)	0.0235(15)	0.0240(16)	0.0376(17)	0.0012(12)	0.0022(13)	0.0014(13)
C(1)	0.0254(19)	0.035(2)	0.037(2)	0.0066(16)	0.0065(15)	-0.0006(16)
C(2)	0.038(2)	0.030(2)	0.042(2)	0.0075(17)	0.0109(18)	-0.0066(17)
C(3)	0.036(2)	0.0251(19)	0.033(2)	-0.0017(16)	0.0032(16)	-0.0043(15)
C(4)	0.037(2)	0.0237(18)	0.0289(19)	0.0028(16)	-0.0012(16)	-0.0050(15)
C(5)	0.050(2)	0.036(2)	0.0248(19)	0.0040(19)	0.0081(17)	-0.0029(16)
C(6)	0.041(2)	0.035(2)	0.031(2)	-0.0003(18)	0.0138(17)	-0.0006(16)
C(7)	0.040(2)	0.026(2)	0.041(2)	-0.0075(17)	0.0033(18)	0.0045(16)
C(8)	0.049(2)	0.026(2)	0.061(3)	-0.0045(19)	-0.005(2)	0.013(2)
C(9)	0.034(2)	0.029(2)	0.055(2)	0.0051(17)	-0.0038(19)	0.0097(19)
C(10)	0.0216(18)	0.032(2)	0.035(2)	0.0056(15)	0.0034(15)	0.0045(15)
C(11)	0.0242(18)	0.030(2)	0.039(2)	0.0009(15)	0.0010(16)	0.0037(16)
C(12)	0.037(2)	0.033(2)	0.033(2)	0.0063(17)	-0.0009(17)	-0.0009(16)
C(13)	0.032(2)	0.047(2)	0.031(2)	0.0114(18)	0.0074(16)	0.0036(18)
C(14)	0.0245(19)	0.040(2)	0.039(2)	0.0025(17)	0.0044(16)	0.0118(18)
C(15)	0.0237(18)	0.029(2)	0.041(2)	0.0008(15)	0.0012(16)	0.0007(16)
C(16)	0.149(17)	0.133(16)	0.074(9)	-0.090(14)	0.046(10)	-0.034(10)
C(17)	0.045(5)	0.052(5)	0.041(5)	-0.040(5)	-0.006(4)	-0.020(4)
B(1)	0.0228(19)	0.0228(19)	0.030(2)	-0.0018(16)	0.0038(16)	-0.0008(16)

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)	2.2731(12)	Ti(1)	Cl(2)	2.2683(11)
Ti(1)	O(1)	1.801(3)	Ti(1)	N(2)	2.168(3)
Ti(1)	N(4)	2.168(3)	Ti(1)	N(6)	2.138(3)
Cl(3)	Cl(5)	1.755(10)	Cl(3)	Cl(5)[1)]	2.231(10)
Cl(3)	C(16)	1.743(18)	Cl(3)	C(17)	0.966(10)
Cl(4)	C(16)	1.69(2)	Cl(4)	C(17)	1.826(12)
Cl(5)	Cl(5)[1)]	1.554(12)	Cl(5)	C(16)	1.56(2)
Cl(5)	C(17)	1.618(14)	F(1)	C(11)	1.343(4)
F(2)	C(12)	1.333(5)	F(3)	C(13)	1.348(5)
F(4)	C(14)	1.345(5)	F(5)	C(15)	1.338(5)
O(1)	C(10)	1.335(5)	N(1)	N(2)	1.373(4)
N(1)	C(1)	1.340(5)	N(1)	B(1)	1.544(5)
N(2)	C(3)	1.339(5)	N(3)	N(4)	1.364(4)
N(3)	C(4)	1.345(4)	N(3)	B(1)	1.544(5)
N(4)	C(6)	1.345(5)	N(5)	N(6)	1.370(4)
N(5)	C(7)	1.341(5)	N(5)	B(1)	1.542(5)
N(6)	C(9)	1.347(5)	C(1)	C(2)	1.382(5)
C(2)	C(3)	1.378(6)	C(4)	C(5)	1.374(6)
C(5)	C(6)	1.385(5)	C(7)	C(8)	1.394(6)
C(8)	C(9)	1.371(6)	C(10)	C(11)	1.389(5)
C(10)	C(15)	1.402(5)	C(11)	C(12)	1.385(6)
C(12)	C(13)	1.369(6)	C(13)	C(14)	1.381(6)
C(14)	C(15)	1.376(6)	C(16)	C(17)	1.14(2)

Symmetry Operators:

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

Table 5. Bond lengths involving hydrogens (Å)

atom	atom	distance	atom	atom	distance
C(1)	H(1)	0.950	C(2)	H(2)	0.950
C(3)	H(3)	0.950	C(4)	H(4)	0.950
C(5)	H(5)	0.950	C(6)	H(6)	0.950
C(7)	H(7)	0.950	C(8)	H(8)	0.950
C(9)	H(9)	0.950	B(1)	H(10)	1.000

Table 6. Bond angles (°)

atom	atom	atom	angle	atom	atom	atom	angle
Cl(1)	Ti(1)	Cl(2)	99.49(4)	Cl(1)	Ti(1)	O(1)	95.59(10)
Cl(1)	Ti(1)	N(2)	87.61(9)	Cl(1)	Ti(1)	N(4)	89.03(9)
Cl(1)	Ti(1)	N(6)	166.00(9)	Cl(2)	Ti(1)	O(1)	98.24(9)
Cl(2)	Ti(1)	N(2)	90.29(8)	Cl(2)	Ti(1)	N(4)	167.35(10)
Cl(2)	Ti(1)	N(6)	89.41(9)	O(1)	Ti(1)	N(2)	170.25(12)
O(1)	Ti(1)	N(4)	90.16(13)	O(1)	Ti(1)	N(6)	93.78(13)
N(2)	Ti(1)	N(4)	80.67(12)	N(2)	Ti(1)	N(6)	81.52(12)
N(4)	Ti(1)	N(6)	80.56(12)	Cl(5)	Cl(3)	Cl(5)[1)]	43.9(3)
Cl(5)	Cl(3)	C(16)	52.8(6)	Cl(5)	Cl(3)	C(17)	65.7(7)
Cl(5)[1)]	Cl(3)	C(16)	96.4(6)	Cl(5)[1)]	Cl(3)	C(17)	103.2(7)
C(16)	Cl(3)	C(17)	37.6(8)	C(16)	Cl(4)	C(17)	37.7(7)
Cl(3)	Cl(5)	Cl(3)[1)]	136.1(4)	Cl(3)	Cl(5)	Cl(5)[1)]	84.6(5)
Cl(3)	Cl(5)	C(16)	63.2(7)	Cl(3)	Cl(5)	C(17)	33.0(4)
Cl(3)[1)]	Cl(5)	Cl(5)[1)]	51.5(4)	Cl(3)[1)]	Cl(5)	C(16)	159.7(8)
Cl(3)[1)]	Cl(5)	C(17)	156.7(6)	Cl(5)[1)]	Cl(5)	C(16)	146.9(9)
Cl(5)[1)]	Cl(5)	C(17)	111.8(7)	C(16)	Cl(5)	C(17)	42.1(8)
Ti(1)	O(1)	C(10)	161.2(2)	N(2)	N(1)	C(1)	109.1(3)
N(2)	N(1)	B(1)	118.9(3)	C(1)	N(1)	B(1)	131.9(3)
Ti(1)	N(2)	N(1)	123.7(2)	Ti(1)	N(2)	C(3)	129.9(2)
N(1)	N(2)	C(3)	106.4(3)	N(4)	N(3)	C(4)	109.0(3)
N(4)	N(3)	B(1)	119.2(2)	C(4)	N(3)	B(1)	131.7(3)
Ti(1)	N(4)	N(3)	123.7(2)	Ti(1)	N(4)	C(6)	129.7(2)
N(3)	N(4)	C(6)	106.6(3)	N(6)	N(5)	C(7)	109.5(3)
N(6)	N(5)	B(1)	119.3(3)	C(7)	N(5)	B(1)	131.1(3)
Ti(1)	N(6)	N(5)	124.1(2)	Ti(1)	N(6)	C(9)	129.5(2)
N(5)	N(6)	C(9)	106.3(3)	N(1)	C(1)	C(2)	108.8(3)
C(1)	C(2)	C(3)	104.9(3)	N(2)	C(3)	C(2)	110.7(3)
N(3)	C(4)	C(5)	109.1(3)	C(4)	C(5)	C(6)	105.0(3)
N(4)	C(6)	C(5)	110.3(3)	N(5)	C(7)	C(8)	108.2(3)
C(7)	C(8)	C(9)	105.3(4)	N(6)	C(9)	C(8)	110.7(3)
O(1)	C(10)	C(11)	121.4(3)	O(1)	C(10)	C(15)	121.2(3)
C(11)	C(10)	C(15)	117.4(3)	F(1)	C(11)	C(10)	118.8(3)
F(1)	C(11)	C(12)	119.4(3)	C(10)	C(11)	C(12)	121.8(3)
F(2)	C(12)	C(11)	119.3(3)	F(2)	C(12)	C(13)	121.2(4)
C(11)	C(12)	C(13)	119.5(3)	F(3)	C(13)	C(12)	121.0(4)
F(3)	C(13)	C(14)	118.9(3)	C(12)	C(13)	C(14)	120.1(4)
F(4)	C(14)	C(13)	120.1(3)	F(4)	C(14)	C(15)	119.5(3)

Table 6. Bond angles (°) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
C(13)	C(14)	C(15)	120.4(3)	F(5)	C(15)	C(10)	119.8(3)
F(5)	C(15)	C(14)	119.5(3)	C(10)	C(15)	C(14)	120.7(3)
Cl(3)	C(16)	Cl(4)	103.7(10)	Cl(3)	C(16)	Cl(5)	64.0(7)
Cl(3)	C(16)	C(17)	31.1(7)	Cl(4)	C(16)	Cl(5)	133.6(12)
Cl(4)	C(16)	C(17)	77.8(11)	Cl(5)	C(16)	C(17)	71.8(11)
Cl(3)	C(17)	Cl(4)	148.6(9)	Cl(3)	C(17)	Cl(5)	81.3(7)
Cl(3)	C(17)	C(16)	111.3(13)	Cl(4)	C(17)	Cl(5)	119.8(6)
Cl(4)	C(17)	C(16)	64.6(10)	Cl(5)	C(17)	C(16)	66.1(11)
N(1)	B(1)	N(3)	106.9(3)	N(1)	B(1)	N(5)	107.7(2)
N(3)	B(1)	N(5)	107.4(3)				

Symmetry Operators:

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

Table 7. Bond angles involving hydrogens (°)

atom	atom	atom	angle	atom	atom	atom	angle
N(1)	C(1)	H(1)	125.6	C(2)	C(1)	H(1)	125.6
C(1)	C(2)	H(2)	127.5	C(3)	C(2)	H(2)	127.5
N(2)	C(3)	H(3)	124.6	C(2)	C(3)	H(3)	124.6
N(3)	C(4)	H(4)	125.5	C(5)	C(4)	H(4)	125.4
C(4)	C(5)	H(5)	127.5	C(6)	C(5)	H(5)	127.5
N(4)	C(6)	H(6)	124.9	C(5)	C(6)	H(6)	124.9
N(5)	C(7)	H(7)	125.9	C(8)	C(7)	H(7)	125.9
C(7)	C(8)	H(8)	127.4	C(9)	C(8)	H(8)	127.4
N(6)	C(9)	H(9)	124.7	C(8)	C(9)	H(9)	124.7
N(1)	B(1)	H(10)	111.5	N(3)	B(1)	H(10)	111.5
N(5)	B(1)	H(10)	111.5				

Table 8. Torsion Angles(°)

atom1	atom2	atom3	atom4	angle
Cl(1)	Ti(1)	O(1)	C(10)	47.4(8)
Cl(1)	Ti(1)	N(2)	C(3)	47.3(3)
Cl(1)	Ti(1)	N(4)	C(6)	-50.5(3)
Cl(1)	Ti(1)	N(6)	C(9)	178.9(3)
Cl(2)	Ti(1)	N(2)	N(1)	130.4(2)
Cl(2)	Ti(1)	N(4)	N(3)	-3.5(6)
Cl(2)	Ti(1)	N(6)	N(5)	-129.5(2)
O(1)	Ti(1)	N(2)	N(1)	-20.7(9)
N(2)	Ti(1)	O(1)	C(10)	-61.4(12)
O(1)	Ti(1)	N(4)	C(6)	45.1(3)
O(1)	Ti(1)	N(6)	N(5)	132.3(3)
N(6)	Ti(1)	O(1)	C(10)	-122.2(8)
N(2)	Ti(1)	N(4)	C(6)	-138.2(3)
N(4)	Ti(1)	N(2)	C(3)	136.7(3)
N(2)	Ti(1)	N(6)	C(9)	139.4(4)
N(6)	Ti(1)	N(2)	C(3)	-141.6(3)
N(4)	Ti(1)	N(6)	C(9)	-138.7(4)
N(6)	Ti(1)	N(4)	C(6)	138.9(3)
Cl(5)	Cl(3)	Cl(5)[1)]	C(17)[1)]	-49.8(15)
Cl(5)[1)]	Cl(3)	Cl(5)	C(17)	-146.2(9)
Cl(5)	Cl(3)	C(16)	C(17)	-97.9(13)
C(16)	Cl(3)	Cl(5)	C(17)	41.5(10)
Cl(5)	Cl(3)	C(17)	Cl(4)	136(2)
C(17)	Cl(3)	Cl(5)	Cl(3)[1)]	146.2(10)
C(17)	Cl(3)	Cl(5)	Cl(5)[1)]	146.2(9)
Cl(5)[1)]	Cl(3)	C(16)	Cl(5)	-5.4(6)
C(16)	Cl(3)	Cl(5)[1)]	Cl(3)[1)]	6.2(9)
C(16)	Cl(3)	Cl(5)[1)]	C(17)[1)]	-43.7(17)
Cl(5)[1)]	Cl(3)	C(17)	Cl(4)	159.1(16)
Cl(5)[1)]	Cl(3)	C(17)	C(16)	83.3(12)
C(17)	Cl(3)	Cl(5)[1)]	C(16)[1)]	128(2)
C(17)	Cl(3)	Cl(5)[1)]	Cl(5)	-31.4(8)
C(16)	Cl(3)	C(17)	Cl(5)	-60.0(12)
C(17)	Cl(3)	C(16)	Cl(5)	97.9(13)
C(16)	Cl(4)	C(17)	Cl(5)	37.8(10)
C(17)	Cl(4)	C(16)	Cl(5)	-49.7(13)
Cl(3)	Cl(5)	Cl(5)[1)]	C(17)[1)]	161.0(6)

atom1	atom2	atom3	atom4	angle
Cl(1)	Ti(1)	N(2)	N(1)	-130.1(2)
Cl(1)	Ti(1)	N(4)	N(3)	129.1(2)
Cl(1)	Ti(1)	N(6)	N(5)	0.3(6)
Cl(2)	Ti(1)	O(1)	C(10)	147.8(8)
Cl(2)	Ti(1)	N(2)	C(3)	-52.2(3)
Cl(2)	Ti(1)	N(4)	C(6)	176.9(3)
Cl(2)	Ti(1)	N(6)	C(9)	49.1(3)
O(1)	Ti(1)	N(2)	C(3)	156.7(7)
O(1)	Ti(1)	N(4)	N(3)	-135.3(2)
N(4)	Ti(1)	O(1)	C(10)	-41.7(8)
O(1)	Ti(1)	N(6)	C(9)	-49.2(4)
N(2)	Ti(1)	N(4)	N(3)	41.4(2)
N(4)	Ti(1)	N(2)	N(1)	-40.7(2)
N(2)	Ti(1)	N(6)	N(5)	-39.1(2)
N(6)	Ti(1)	N(2)	N(1)	41.1(2)
N(4)	Ti(1)	N(6)	N(5)	42.7(2)
N(6)	Ti(1)	N(4)	N(3)	-41.5(2)
Cl(5)	Cl(3)	Cl(5)[1)]	C(16)[1)]	160(2)
Cl(5)[1)]	Cl(3)	Cl(5)	C(16)	172.3(9)
Cl(5)	Cl(3)	C(16)	Cl(4)	-132.1(11)
C(16)	Cl(3)	Cl(5)	Cl(3)[1)]	-172.3(11)
C(16)	Cl(3)	Cl(5)	Cl(5)[1)]	-172.3(9)
Cl(5)	Cl(3)	C(17)	C(16)	60.0(12)
C(17)	Cl(3)	Cl(5)	C(16)	-41.5(10)
Cl(5)[1)]	Cl(3)	C(16)	Cl(4)	-137.5(7)
Cl(5)[1)]	Cl(3)	C(16)	C(17)	-103.3(12)
C(16)	Cl(3)	Cl(5)[1)]	C(16)[1)]	166(2)
C(16)	Cl(3)	Cl(5)[1)]	Cl(5)	6.2(7)
Cl(5)[1)]	Cl(3)	C(17)	Cl(5)	23.3(5)
C(17)	Cl(3)	Cl(5)[1)]	Cl(3)[1)]	-31.4(10)
C(17)	Cl(3)	Cl(5)[1)]	C(17)[1)]	-81.2(17)
C(16)	Cl(3)	C(17)	Cl(4)	76(2)
C(17)	Cl(3)	C(16)	Cl(4)	-34.2(11)
C(16)	Cl(4)	C(17)	Cl(3)	-90(2)
C(17)	Cl(4)	C(16)	Cl(3)	17.3(5)
Cl(3)	Cl(5)	Cl(5)[1)]	C(16)[1)]	-167.3(17)
Cl(3)	Cl(5)	C(16)	Cl(4)	84.2(15)

Table 8. Torsion angles (°) (continued)

atom1	atom2	atom3	atom4	angle
Cl(3)	Cl(5)	C(16)	C(17)	32.6(6)
Cl(3)	Cl(5)	C(17)	C(16)	-118.0(12)
Cl(3)[1)]	Cl(5)	Cl(5)[1)]	C(17)[1)]	-19.0(4)
Cl(3)[1)]	Cl(5)	C(16)	Cl(4)	-111(2)
Cl(3)[1)]	Cl(5)	C(17)	Cl(3)	-76.7(16)
Cl(3)[1)]	Cl(5)	C(17)	C(16)	165.2(17)
Cl(5)[1)]	Cl(5)	C(16)	Cl(4)	98(2)
C(16)	Cl(5)	Cl(5)[1)]	Cl(3)	-12.7(16)
C(16)	Cl(5)	Cl(5)[1)]	C(17)[1)]	148.3(17)
Cl(5)[1)]	Cl(5)	C(17)	Cl(4)	168.1(6)
C(17)	Cl(5)	Cl(5)[1)]	Cl(3)	19.0(4)
C(17)	Cl(5)	Cl(5)[1)]	C(16)[1)]	-148.3(17)
C(16)	Cl(5)	C(17)	Cl(4)	-37.2(10)
C(17)	Cl(5)	C(16)	Cl(4)	51.7(13)
Ti(1)	O(1)	C(10)	C(15)	-81.5(8)
C(1)	N(1)	N(2)	Ti(1)	177.1(2)
N(2)	N(1)	B(1)	N(3)	58.9(3)
B(1)	N(1)	N(2)	Ti(1)	-1.1(4)
C(1)	N(1)	B(1)	N(3)	-118.9(4)
B(1)	N(1)	C(1)	C(2)	178.5(3)
N(1)	N(2)	C(3)	C(2)	0.6(4)
C(4)	N(3)	N(4)	Ti(1)	-179.7(2)
N(4)	N(3)	B(1)	N(1)	-58.4(3)
B(1)	N(3)	N(4)	Ti(1)	-0.0(3)
C(4)	N(3)	B(1)	N(1)	121.2(4)
B(1)	N(3)	C(4)	C(5)	-179.4(3)
N(3)	N(4)	C(6)	C(5)	-0.2(3)
C(7)	N(5)	N(6)	Ti(1)	179.4(2)
N(6)	N(5)	B(1)	N(1)	58.8(4)
B(1)	N(5)	N(6)	Ti(1)	-2.4(4)
C(7)	N(5)	B(1)	N(1)	-123.4(4)
B(1)	N(5)	C(7)	C(8)	-178.5(4)
N(5)	N(6)	C(9)	C(8)	-0.2(4)
C(1)	C(2)	C(3)	N(2)	-0.2(4)
C(4)	C(5)	C(6)	N(4)	0.3(4)
C(7)	C(8)	C(9)	N(6)	-0.1(4)
O(1)	C(10)	C(11)	C(12)	179.1(3)

atom1	atom2	atom3	atom4	angle
Cl(3)	Cl(5)	C(17)	Cl(4)	-155.3(11)
Cl(3)[1)]	Cl(5)	Cl(5)[1)]	C(16)[1)]	12.7(16)
Cl(3)[1)]	Cl(5)	C(16)	Cl(3)	164(2)
Cl(3)[1)]	Cl(5)	C(16)	C(17)	-163(2)
Cl(3)[1)]	Cl(5)	C(17)	Cl(4)	128.0(13)
Cl(5)[1)]	Cl(5)	C(16)	Cl(3)	14.2(18)
Cl(5)[1)]	Cl(5)	C(16)	C(17)	47(2)
C(16)	Cl(5)	Cl(5)[1)]	Cl(3)[1)]	167.3(17)
Cl(5)[1)]	Cl(5)	C(17)	Cl(3)	-36.6(9)
Cl(5)[1)]	Cl(5)	C(17)	C(16)	-154.7(11)
C(17)	Cl(5)	Cl(5)[1)]	Cl(3)[1)]	-161.0(6)
C(16)	Cl(5)	C(17)	Cl(3)	118.0(12)
C(17)	Cl(5)	C(16)	Cl(3)	-32.6(6)
Ti(1)	O(1)	C(10)	C(11)	99.9(8)
N(2)	N(1)	C(1)	C(2)	0.6(4)
C(1)	N(1)	N(2)	C(3)	-0.8(4)
N(2)	N(1)	B(1)	N(5)	-56.3(4)
B(1)	N(1)	N(2)	C(3)	-179.0(3)
C(1)	N(1)	B(1)	N(5)	126.0(4)
Ti(1)	N(2)	C(3)	C(2)	-177.1(2)
N(4)	N(3)	C(4)	C(5)	0.2(4)
C(4)	N(3)	N(4)	C(6)	-0.0(3)
N(4)	N(3)	B(1)	N(5)	57.0(4)
B(1)	N(3)	N(4)	C(6)	179.6(3)
C(4)	N(3)	B(1)	N(5)	-123.5(4)
Ti(1)	N(4)	C(6)	C(5)	179.5(2)
N(6)	N(5)	C(7)	C(8)	-0.6(5)
C(7)	N(5)	N(6)	C(9)	0.5(4)
N(6)	N(5)	B(1)	N(3)	-56.0(4)
B(1)	N(5)	N(6)	C(9)	178.7(3)
C(7)	N(5)	B(1)	N(3)	121.7(4)
Ti(1)	N(6)	C(9)	C(8)	-179.0(3)
N(1)	C(1)	C(2)	C(3)	-0.3(4)
N(3)	C(4)	C(5)	C(6)	-0.3(4)
N(5)	C(7)	C(8)	C(9)	0.4(5)
O(1)	C(10)	C(11)	F(1)	-0.8(5)
O(1)	C(10)	C(15)	F(5)	-0.9(5)

Table 8. Torsion angles (°) (continued)

atom1	atom2	atom3	atom4	angle
O(1)	C(10)	C(15)	C(14)	-179.2(3)
C(11)	C(10)	C(15)	C(14)	-0.5(5)
C(15)	C(10)	C(11)	C(12)	0.4(5)
F(1)	C(11)	C(12)	C(13)	-180.0(2)
C(10)	C(11)	C(12)	C(13)	0.1(4)
F(2)	C(12)	C(13)	C(14)	178.5(3)
C(11)	C(12)	C(13)	C(14)	-0.5(6)
F(3)	C(13)	C(14)	C(15)	179.1(3)
C(12)	C(13)	C(14)	C(15)	0.3(6)
F(4)	C(14)	C(15)	C(10)	179.5(3)
C(13)	C(14)	C(15)	C(10)	0.2(5)
Cl(3)	C(16)	C(17)	Cl(5)	69.5(10)
Cl(4)	C(16)	C(17)	Cl(5)	-144.5(8)
Cl(5)	C(16)	C(17)	Cl(4)	144.5(8)
C(11)	C(10)	C(15)	F(5)	177.8(3)
C(15)	C(10)	C(11)	F(1)	-179.5(3)
F(1)	C(11)	C(12)	F(2)	1.0(5)
C(10)	C(11)	C(12)	F(2)	-178.9(3)
F(2)	C(12)	C(13)	F(3)	-0.3(5)
C(11)	C(12)	C(13)	F(3)	-179.3(3)
F(3)	C(13)	C(14)	F(4)	-0.1(4)
C(12)	C(13)	C(14)	F(4)	-179.0(3)
F(4)	C(14)	C(15)	F(5)	1.1(5)
C(13)	C(14)	C(15)	F(5)	-178.1(3)
Cl(3)	C(16)	C(17)	Cl(4)	-146.0(9)
Cl(4)	C(16)	C(17)	Cl(3)	146.0(9)
Cl(5)	C(16)	C(17)	Cl(3)	-69.5(10)

Symmetry Operators:

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

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
Cl(1)	F(2)[1)]	3.459(2)	Cl(1)	F(3)[1)]	3.352(3)
Cl(1)	C(12)[1)]	3.365(4)	Cl(1)	C(13)[1)]	3.307(4)
Cl(2)	F(2)[1)]	3.349(3)	Cl(2)	C(6)[2)]	3.585(4)
Cl(2)	C(12)[2)]	3.432(4)	Cl(3)	F(5)[3)]	3.133(5)
Cl(3)	C(10)	3.580(5)	Cl(3)	C(11)	3.560(5)
Cl(5)	F(4)[2)]	3.352(8)	F(1)	F(5)[3)]	3.017(3)
F(1)	C(1)[4)]	3.175(4)	F(1)	C(2)[4)]	3.164(4)
F(2)	Cl(1)[3)]	3.459(2)	F(2)	Cl(2)[3)]	3.349(3)
F(2)	F(2)[5)]	2.860(4)	F(2)	F(3)[5)]	2.887(3)
F(2)	F(5)[3)]	3.098(4)	F(2)	C(12)[5)]	3.456(5)
F(2)	C(13)[5)]	3.471(5)	F(3)	Cl(1)[3)]	3.352(3)
F(3)	F(2)[5)]	2.887(3)	F(4)	Cl(5)[6)]	3.352(8)
F(4)	C(4)[7)]	3.420(5)	F(4)	C(16)[6)]	3.313(16)
F(4)	B(1)[7)]	3.451(4)	F(5)	Cl(3)[1)]	3.133(5)
F(5)	F(1)[1)]	3.017(3)	F(5)	F(2)[1)]	3.098(4)
F(5)	C(11)[1)]	3.485(4)	F(5)	C(12)[1)]	3.529(5)
C(1)	F(1)[8)]	3.175(4)	C(2)	F(1)[8)]	3.164(4)
C(2)	C(4)[8)]	3.587(5)	C(3)	C(4)[8)]	3.570(5)
C(4)	F(4)[9)]	3.420(5)	C(4)	C(2)[4)]	3.587(5)
C(4)	C(3)[4)]	3.570(5)	C(6)	Cl(2)[6)]	3.585(4)
C(10)	Cl(3)	3.580(5)	C(11)	Cl(3)	3.560(5)
C(11)	F(5)[3)]	3.485(4)	C(12)	Cl(1)[3)]	3.365(4)
C(12)	Cl(2)[6)]	3.432(4)	C(12)	F(2)[5)]	3.456(5)
C(12)	F(5)[3)]	3.529(5)	C(13)	Cl(1)[3)]	3.307(4)
C(13)	F(2)[5)]	3.471(5)	C(16)	F(4)[2)]	3.313(16)
B(1)	F(4)[9)]	3.451(4)			

Symmetry Operators:

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

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

atom	atom	distance	atom	atom	distance
Cl(1)	H(7)[1)]	2.778	Cl(1)	H(10)[1)]	3.416
Cl(2)	H(5)[2)]	3.426	Cl(2)	H(6)[2)]	3.060
Cl(3)	H(9)	3.053	Cl(4)	H(1)[3)]	3.099
Cl(4)	H(4)[4)]	3.421	Cl(4)	H(8)[5)]	3.301
Cl(4)	H(10)[3)]	3.465	Cl(5)	H(9)	3.024
Cl(5)	H(9)[5)]	2.891	F(1)	H(1)[6)]	2.730
F(1)	H(2)[6)]	2.736	F(3)	H(3)[7)]	2.955
F(3)	H(4)[3)]	2.826	F(4)	H(1)[3)]	3.108
F(4)	H(4)[3)]	2.863	F(4)	H(8)[8)]	3.106
F(4)	H(10)[3)]	2.787	F(5)	H(1)[3)]	3.013
N(1)	H(5)[2)]	2.866	N(2)	H(5)[2)]	2.829
N(2)	H(7)[1)]	3.410	N(3)	H(2)[6)]	3.371
N(3)	H(3)[6)]	3.538	N(3)	H(8)[1)]	3.336
N(4)	H(2)[6)]	3.544	N(4)	H(7)[1)]	3.192
N(5)	H(5)[2)]	2.945	N(6)	H(5)[2)]	2.970
C(1)	H(5)[2)]	3.247	C(2)	H(3)[9)]	3.458
C(2)	H(5)[2)]	3.437	C(3)	H(2)[9)]	3.314
C(3)	H(4)[1)]	3.382	C(3)	H(5)[2)]	3.166
C(3)	H(7)[1)]	3.591	C(4)	H(2)[6)]	3.129
C(4)	H(3)[6)]	3.057	C(4)	H(8)[1)]	2.929
C(5)	H(2)[6)]	3.160	C(5)	H(8)[1)]	3.176
C(6)	H(2)[6)]	3.404	C(6)	H(7)[1)]	3.237
C(7)	H(5)[2)]	3.343	C(8)	H(5)[2)]	3.592
C(9)	H(5)[2)]	3.356	C(9)	H(6)[2)]	3.522
C(14)	H(10)[3)]	3.306	C(16)	H(9)	3.466
C(17)	H(9)[5)]	3.316	B(1)	H(5)[2)]	3.480
H(1)	Cl(4)[10)]	3.099	H(1)	F(1)[1)]	2.730
H(1)	F(4)[10)]	3.108	H(1)	F(5)[10)]	3.013
H(2)	F(1)[1)]	2.736	H(2)	N(3)[1)]	3.371
H(2)	N(4)[1)]	3.544	H(2)	C(3)[9)]	3.314
H(2)	C(4)[1)]	3.129	H(2)	C(5)[1)]	3.160
H(2)	C(6)[1)]	3.404	H(2)	H(2)[9)]	3.564
H(2)	H(3)[9)]	2.958	H(2)	H(4)[1)]	3.442
H(2)	H(5)[1)]	3.500	H(3)	F(3)[8)]	2.955
H(3)	N(3)[1)]	3.538	H(3)	C(2)[9)]	3.458
H(3)	C(4)[1)]	3.057	H(3)	H(2)[9)]	2.958
H(3)	H(4)[1)]	2.663	H(3)	H(10)[1)]	3.511

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

atom	atom	distance	atom	atom	distance
H(4)	Cl(4)[11)]	3.421	H(4)	F(3)[10)]	2.826
H(4)	F(4)[10)]	2.863	H(4)	C(3)[6)]	3.382
H(4)	H(2)[6)]	3.442	H(4)	H(3)[6)]	2.663
H(4)	H(8)[1)]	3.043	H(5)	Cl(2)[12)]	3.426
H(5)	N(1)[12)]	2.866	H(5)	N(2)[12)]	2.829
H(5)	N(5)[12)]	2.945	H(5)	N(6)[12)]	2.970
H(5)	C(1)[12)]	3.247	H(5)	C(2)[12)]	3.437
H(5)	C(3)[12)]	3.166	H(5)	C(7)[12)]	3.343
H(5)	C(8)[12)]	3.592	H(5)	C(9)[12)]	3.356
H(5)	B(1)[12)]	3.480	H(5)	H(2)[6)]	3.500
H(5)	H(8)[1)]	3.469	H(6)	Cl(2)[12)]	3.060
H(6)	C(9)[12)]	3.522	H(6)	H(7)[1)]	3.438
H(6)	H(9)[12)]	3.413	H(7)	Cl(1)[6)]	2.778
H(7)	N(2)[6)]	3.410	H(7)	N(4)[6)]	3.192
H(7)	C(3)[6)]	3.591	H(7)	C(6)[6)]	3.237
H(7)	H(6)[6)]	3.438	H(8)	Cl(4)[5)]	3.301
H(8)	F(4)[7)]	3.106	H(8)	N(3)[6)]	3.336
H(8)	C(4)[6)]	2.929	H(8)	C(5)[6)]	3.176
H(8)	H(4)[6)]	3.043	H(8)	H(5)[6)]	3.469
H(9)	Cl(3)	3.053	H(9)	Cl(5)	3.024
H(9)	Cl(5)[5)]	2.891	H(9)	C(16)	3.466
H(9)	C(17)[5)]	3.316	H(9)	H(6)[2)]	3.413
H(10)	Cl(1)[6)]	3.416	H(10)	Cl(4)[10)]	3.465
H(10)	F(4)[10)]	2.787	H(10)	C(14)[10)]	3.306
H(10)	H(3)[6)]	3.511			

Symmetry Operators:

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

Electronic Supplementary Information for Dalton Transactions

X-ray Structure Report for $TpTiCl_2(O\text{-}2,6\text{-}Ph_2C_6H_3)$ (**4**)

July 15, 2009

Experimental

Data Collection

A red block crystal of $C_{27}H_{23}BCl_2N_6OTi$ having approximate dimensions of 0.35 x 0.32 x 0.25 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 240 seconds. 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 = 11.6472(3) Å
b = 13.6516(3) Å
c = 17.3088(5) Å
V = 2752.14(12) Å^3

For Z = 4 and F.W. = 577.13, the calculated density is 1.393 g/cm^3. The systematic absences of:

h00: h ± 2n
0k0: k ± 2n
00l: l ± 2n

uniquely determine the space group to be:

$P2_12_12_1$ (#19)

The data were collected at a temperature of -80 ± 1°C to a maximum 2θ value of 54.9°. A total of 74 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 200.0 [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 200.0 [sec./°]. The crystal-to-detector distance was 127.40 mm. Readout was performed in the 0.100 mm pixel mode.

Data Reduction

Of the 27327 reflections that were collected, 6279 were unique (R_{int} = 0.014); equivalent reflections were merged.

The linear absorption coefficient, μ, for Mo-Kα radiation is 5.372 cm^{-1}. An empirical absorption correction was applied which resulted in transmission factors ranging from 0.746 to 0.874. 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 6172 observed reflections and 367 variable parameters and converged (largest parameter shift was 0.00 times its esd) with unweighted and weighted agreement factors of:

$$R1 = \Sigma \; ||Fo| - |Fc|| \; / \; \Sigma \; |Fo| = 0.0195$$

$$wR2 = [\; \Sigma \; (\; w \; (Fo^2 - Fc^2)^2 \;) / \; \Sigma \; w(Fo^2)^2]^{1/2} = 0.0609$$

The standard deviation of an observation of unit weight[4] was 1.00. A Sheldrick weighting scheme was used. Plots of Σ w $(|Fo| - |Fc|)^2$ versus |Fo|, reflection order in data collection, sin θ/λ and various classes of indices showed no unusual trends. The maximum and minimum peaks on the final difference Fourier map corresponded to 0.35 and -0.36 $e^-/Å^3$, respectively. The absolute structure was deduced based on Flack parameter, -0.001(11), refined using 2761 Friedel pairs.[5]

Neutral atom scattering factors were taken from Cromer and Waber[6]. Anomalous dispersion effects were included in Fcalc[7]; the values for Δf' and Δf'' were those of Creagh and McAuley[8]. The values for the mass attenuation coefficients are those of Creagh and Hubbell[9]. All calculations were performed using the CrystalStructure[10,11] crystallographic software package.

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:

$\Sigma w(F_o^2-F_c^2)^2$ 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) Flack, H. D. (1983), Acta Cryst. A39, 876-881.

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EXPERIMENTAL DETAILS

A. Crystal Data

Empirical Formula	$C_{27}H_{23}BCl_2N_6OTi$
Formula Weight	577.13
Crystal Color, Habit	red, block
Crystal Dimensions	0.35 X 0.32 X 0.25 mm
Crystal System	orthorhombic
Lattice Type	Primitive
Indexing Images	3 oscillations @ 240.0 seconds
Detector Position	127.40 mm
Pixel Size	0.100 mm
Lattice Parameters	a = 11.6472(3) Å b = 13.6516(3) Å c = 17.3088(5) Å V = 2752.14(12) Å^3
Space Group	$P2_12_12_1$ (#19)
Z value	4
D_{calc}	1.393 g/cm^3
F_{000}	1184.00
μ(MoKα)	5.372 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	200.0 sec./^{o}
ω oscillation Range (χ=45.0, ϕ=180.0)	0.0 - 162.0^{o}
Exposure Rate	200.0 sec./^{o}
Detector Position	127.40 mm
Pixel Size	0.100 mm
$2\theta_{max}$	54.9^{o}
No. of Reflections Measured	Total: 27327 Unique: 6279 (R_{int} = 0.014) Friedel pairs: 2761
Corrections	Lorentz-polarization Absorption (trans. factors: 0.746 - 0.874)

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	$1/[0.0006Fo^2+1.0000\sigma(Fo^2)]/(4Fo^2)$
$2\theta_{max}$ cutoff	54.9^o
Anomalous Dispersion	All non-hydrogen atoms
No. Observations (I>1.00σ(I))	6172
No. Variables	367
Reflection/Parameter Ratio	16.82
Residuals: R1 (I>2.00σ(I))	0.0195
Residuals: R (I>1.00σ(I))	0.0198
Residuals: wR2 (I>1.00σ(I))	0.0609
Goodness of Fit Indicator	1.003
Flack Parameter (Friedel pairs = 2761)	-0.001(11)
Max Shift/Error in Final Cycle	0.000
Maximum peak in Final Diff. Map	0.35 $e^-/Å^3$
Minimum peak in Final Diff. Map	-0.36 $e^-/Å^3$

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

atom	x	y	z	B_{eq}
Ti(1)	0.69446(2)	0.182220(10)	0.279510(10)	1.148(3)
Cl(1)	0.74621(3)	0.06013(2)	0.36176(2)	2.163(6)
Cl(2)	0.74821(2)	0.31026(2)	0.35783(2)	1.843(5)
O(1)	0.81799(6)	0.17423(6)	0.21787(4)	1.429(13)
N(1)	0.42510(8)	0.17553(8)	0.29786(6)	1.709(18)
N(2)	0.52654(8)	0.17699(8)	0.33717(5)	1.452(17)
N(3)	0.49820(10)	0.08633(8)	0.18313(6)	1.88(2)
N(4)	0.60826(9)	0.07646(7)	0.20830(6)	1.668(19)
N(5)	0.49151(9)	0.26906(8)	0.18380(6)	1.757(19)
N(6)	0.60048(9)	0.28481(7)	0.21018(6)	1.582(18)
C(1)	0.33743(10)	0.17596(10)	0.34796(8)	2.22(2)
C(2)	0.38115(11)	0.17821(10)	0.42225(7)	2.16(2)
C(3)	0.49998(11)	0.17801(9)	0.41254(6)	1.68(2)
C(4)	0.46750(14)	0.00567(10)	0.14354(8)	2.56(2)
C(5)	0.55915(15)	-0.05794(10)	0.14230(9)	2.81(2)
C(6)	0.64520(14)	-0.01168(9)	0.18382(8)	2.20(2)
C(7)	0.45400(13)	0.34898(10)	0.14622(8)	2.34(2)
C(8)	0.53887(14)	0.41868(10)	0.14762(8)	2.47(2)
C(9)	0.62930(12)	0.37629(9)	0.18770(8)	2.08(2)
C(10)	0.89275(10)	0.11890(8)	0.17559(7)	1.39(2)
C(11)	0.86968(10)	0.10238(8)	0.09675(7)	1.54(2)
C(12)	0.93719(12)	0.03397(9)	0.05769(7)	2.04(2)
C(13)	1.02837(13)	-0.01245(10)	0.09378(8)	2.30(2)
C(14)	1.05496(12)	0.00984(9)	0.16966(8)	2.09(2)
C(15)	0.98803(10)	0.07560(8)	0.21245(7)	1.61(2)
C(16)	0.78177(10)	0.15835(9)	0.05289(7)	1.65(2)
C(17)	0.70226(13)	0.10985(10)	0.00605(8)	2.25(2)
C(18)	0.63045(13)	0.16343(11)	-0.04270(9)	2.92(2)
C(19)	0.63678(13)	0.26451(12)	-0.04498(9)	2.90(3)
C(20)	0.71349(14)	0.31251(11)	0.00214(8)	2.81(2)
C(21)	0.78574(12)	0.26024(10)	0.05084(8)	2.29(2)
C(22)	1.01961(10)	0.09769(9)	0.29375(7)	1.59(2)
C(23)	1.05424(11)	0.02227(10)	0.34328(8)	2.08(2)
C(24)	1.08417(13)	0.04120(11)	0.41934(8)	2.43(2)
C(25)	1.08024(12)	0.13631(11)	0.44766(8)	2.38(2)
C(26)	1.04740(12)	0.21160(10)	0.39890(8)	2.24(2)
C(27)	1.01715(10)	0.19320(10)	0.32264(7)	1.83(2)

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

atom	x	y	z	B_{eq}
B(1)	0.42693(11)	0.17570(11)	0.20839(8)	1.89(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)	0.3444	0.1764	0.1866	2.26
H(2)	0.2558	0.1749	0.3342	2.69
H(3)	0.3382	0.1795	0.4709	2.64
H(4)	0.5561	0.1787	0.4547	2.03
H(5)	0.3919	-0.0060	0.1191	3.16
H(6)	0.5628	-0.1231	0.1173	3.38
H(7)	0.7224	-0.0392	0.1939	2.58
H(8)	0.3778	0.3563	0.1216	2.82
H(9)	0.5361	0.4851	0.1247	3.02
H(10)	0.7038	0.4085	0.1984	2.51
H(11)	0.9199	0.0186	0.0042	2.54
H(12)	1.0737	-0.0604	0.0658	2.90
H(13)	1.1210	-0.0208	0.1938	2.53
H(14)	0.6970	0.0397	0.0075	2.65
H(15)	0.5761	0.1298	-0.0749	3.54
H(16)	0.5881	0.3009	-0.0793	3.48
H(17)	0.7169	0.3828	0.0015	3.41
H(18)	0.8391	0.2947	0.0832	2.75
H(19)	1.0575	-0.0431	0.3245	2.54
H(20)	1.1074	-0.0109	0.4522	2.94
H(21)	1.0998	0.1494	0.4999	2.86
H(22)	1.0456	0.2769	0.4179	2.75
H(23)	0.9947	0.2457	0.2900	2.19

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

Table 3. Anisotropic displacement parameters

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Ti(1)	0.01426(9)	0.01473(9)	0.01464(9)	0.00018(8)	0.00031(7)	-0.00061(7)
Cl(1)	0.02499(15)	0.02713(15)	0.03005(16)	0.00267(12)	-0.00173(13)	0.01141(12)
Cl(2)	0.02267(14)	0.02271(13)	0.02463(14)	-0.00314(12)	-0.00063(11)	-0.00745(11)
O(1)	0.0165(3)	0.0202(3)	0.0176(3)	0.0029(3)	0.0013(3)	-0.0013(3)
N(1)	0.0160(4)	0.0267(4)	0.0222(4)	-0.0017(4)	-0.0013(3)	0.0024(4)
N(2)	0.0173(4)	0.0197(4)	0.0181(4)	-0.0003(4)	-0.0005(3)	0.0013(3)
N(3)	0.0248(5)	0.0255(5)	0.0210(5)	-0.0063(4)	-0.0041(4)	-0.0024(4)
N(4)	0.0227(4)	0.0205(4)	0.0202(5)	-0.0027(4)	0.0013(4)	-0.0025(3)
N(5)	0.0196(4)	0.0270(5)	0.0202(5)	0.0034(4)	-0.0028(4)	0.0024(4)
N(6)	0.0193(4)	0.0201(4)	0.0206(4)	0.0017(3)	-0.0003(4)	0.0022(3)
C(1)	0.0185(5)	0.0341(6)	0.0317(6)	0.0007(5)	0.0050(4)	0.0047(5)
C(2)	0.0256(5)	0.0299(6)	0.0265(6)	0.0016(5)	0.0086(4)	0.0030(5)
C(3)	0.0258(5)	0.0193(4)	0.0188(5)	-0.0003(5)	0.0021(4)	-0.0003(4)
C(4)	0.0417(8)	0.0317(6)	0.0239(6)	-0.0161(6)	-0.0048(6)	-0.0047(5)
C(5)	0.0542(9)	0.0232(6)	0.0294(7)	-0.0115(6)	0.0031(6)	-0.0075(5)
C(6)	0.0405(7)	0.0188(5)	0.0242(6)	-0.0017(5)	0.0053(5)	-0.0038(4)
C(7)	0.0327(6)	0.0313(6)	0.0249(6)	0.0120(5)	-0.0026(5)	0.0035(5)
C(8)	0.0433(8)	0.0228(6)	0.0276(6)	0.0080(5)	-0.0030(6)	0.0052(5)
C(9)	0.0326(6)	0.0209(5)	0.0256(6)	-0.0003(5)	0.0009(5)	0.0024(4)
C(10)	0.0172(5)	0.0173(5)	0.0184(5)	-0.0004(4)	0.0030(4)	-0.0022(4)
C(11)	0.0212(5)	0.0192(5)	0.0180(5)	-0.0005(4)	0.0009(4)	-0.0005(4)
C(12)	0.0345(6)	0.0240(5)	0.0192(5)	0.0030(5)	0.0023(5)	-0.0050(4)
C(13)	0.0358(7)	0.0245(6)	0.0272(6)	0.0104(5)	0.0062(5)	-0.0054(4)
C(14)	0.0255(6)	0.0253(5)	0.0288(6)	0.0088(5)	0.0014(5)	-0.0005(5)
C(15)	0.0215(5)	0.0192(5)	0.0206(6)	0.0017(4)	0.0013(4)	-0.0001(4)
C(16)	0.0219(5)	0.0256(5)	0.0151(4)	0.0027(4)	0.0008(4)	-0.0013(4)
C(17)	0.0317(6)	0.0279(6)	0.0260(6)	-0.0016(5)	-0.0028(5)	-0.0034(4)
C(18)	0.0333(6)	0.0433(8)	0.0344(7)	-0.0020(6)	-0.0138(6)	-0.0051(6)
C(19)	0.0340(7)	0.0438(8)	0.0324(7)	0.0114(6)	-0.0093(6)	0.0028(6)
C(20)	0.0438(7)	0.0281(6)	0.0347(7)	0.0067(6)	-0.0086(6)	0.0028(5)
C(21)	0.0316(7)	0.0269(6)	0.0285(6)	-0.0005(5)	-0.0078(5)	-0.0013(5)
C(22)	0.0155(5)	0.0255(5)	0.0195(5)	0.0027(4)	0.0019(4)	-0.0012(4)
C(23)	0.0247(6)	0.0257(6)	0.0285(6)	0.0017(5)	-0.0015(5)	0.0012(4)
C(24)	0.0302(6)	0.0363(6)	0.0260(6)	0.0024(5)	-0.0027(5)	0.0070(5)
C(25)	0.0251(6)	0.0449(7)	0.0205(6)	0.0030(5)	-0.0030(5)	-0.0046(5)
C(26)	0.0255(6)	0.0321(6)	0.0276(6)	0.0034(5)	-0.0009(5)	-0.0084(5)
C(27)	0.0197(5)	0.0258(5)	0.0240(5)	0.0043(5)	-0.0012(4)	-0.0015(5)

Table 3. Anisotropic displacement parameters (continued)

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
B(1)	0.0193(5)	0.0309(6)	0.0217(6)	-0.0030(5)	-0.0039(4)	0.0004(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)	2.2733(3)	Ti(1)	Cl(2)	2.2989(3)
Ti(1)	O(1)	1.7945(7)	Ti(1)	N(2)	2.1969(9)
Ti(1)	N(4)	2.1475(10)	Ti(1)	N(6)	2.1447(10)
O(1)	C(10)	1.3654(13)	N(1)	N(2)	1.3635(13)
N(1)	C(1)	1.3397(15)	N(1)	B(1)	1.5488(17)
N(2)	C(3)	1.3408(13)	N(3)	N(4)	1.3606(15)
N(3)	C(4)	1.3453(17)	N(3)	B(1)	1.5391(18)
N(4)	C(6)	1.3463(16)	N(5)	N(6)	1.3659(14)
N(5)	C(7)	1.3433(17)	N(5)	B(1)	1.5399(18)
N(6)	C(9)	1.3504(15)	C(1)	C(2)	1.3834(18)
C(2)	C(3)	1.3942(18)	C(4)	C(5)	1.376(2)
C(5)	C(6)	1.386(2)	C(7)	C(8)	1.372(2)
C(8)	C(9)	1.388(2)	C(10)	C(11)	1.4090(17)
C(10)	C(15)	1.4100(16)	C(11)	C(12)	1.3955(17)
C(11)	C(16)	1.4861(16)	C(12)	C(13)	1.3855(19)
C(13)	C(14)	1.3833(19)	C(14)	C(15)	1.4008(17)
C(15)	C(22)	1.4854(17)	C(16)	C(17)	1.3976(18)
C(16)	C(21)	1.3922(18)	C(17)	C(18)	1.395(2)
C(18)	C(19)	1.382(2)	C(19)	C(20)	1.376(2)
C(20)	C(21)	1.388(2)	C(22)	C(23)	1.3992(18)
C(22)	C(27)	1.3968(18)	C(23)	C(24)	1.3862(19)
C(24)	C(25)	1.389(2)	C(25)	C(26)	1.3838(19)
C(26)	C(27)	1.3891(18)			

Table 5. Bond lengths involving hydrogens (Å)

atom	atom	distance	atom	atom	distance
C(1)	H(2)	0.980	C(2)	H(3)	0.980
C(3)	H(4)	0.980	C(4)	H(5)	0.990
C(5)	H(6)	0.990	C(6)	H(7)	0.990
C(7)	H(8)	0.990	C(8)	H(9)	0.990
C(9)	H(10)	0.990	C(12)	H(11)	0.970
C(13)	H(12)	0.970	C(14)	H(13)	0.970
C(17)	H(14)	0.960	C(18)	H(15)	0.960
C(19)	H(16)	0.960	C(20)	H(17)	0.960
C(21)	H(18)	0.960	C(23)	H(19)	0.950
C(24)	H(20)	0.950	C(25)	H(21)	0.950
C(26)	H(22)	0.950	C(27)	H(23)	0.950
B(1)	H(1)	1.033			

Table 6. Bond angles (°)

atom	atom	atom	angle	atom	atom	atom	angle
Cl(1)	Ti(1)	Cl(2)	96.660(13)	Cl(1)	Ti(1)	O(1)	96.61(2)
Cl(1)	Ti(1)	N(2)	85.85(2)	Cl(1)	Ti(1)	N(4)	89.45(2)
Cl(1)	Ti(1)	N(6)	164.69(3)	Cl(2)	Ti(1)	O(1)	100.28(2)
Cl(2)	Ti(1)	N(2)	89.96(2)	Cl(2)	Ti(1)	N(4)	167.67(3)
Cl(2)	Ti(1)	N(6)	88.42(2)	O(1)	Ti(1)	N(2)	169.08(3)
O(1)	Ti(1)	N(4)	89.58(3)	O(1)	Ti(1)	N(6)	96.67(3)
N(2)	Ti(1)	N(4)	79.79(3)	N(2)	Ti(1)	N(6)	79.69(3)
N(4)	Ti(1)	N(6)	83.07(3)	Ti(1)	O(1)	C(10)	149.72(7)
N(2)	N(1)	C(1)	109.72(9)	N(2)	N(1)	B(1)	119.14(8)
C(1)	N(1)	B(1)	131.13(10)	Ti(1)	N(2)	N(1)	123.04(6)
Ti(1)	N(2)	C(3)	130.32(7)	N(1)	N(2)	C(3)	106.60(9)
N(4)	N(3)	C(4)	109.42(11)	N(4)	N(3)	B(1)	119.72(9)
C(4)	N(3)	B(1)	130.55(11)	Ti(1)	N(4)	N(3)	123.89(7)
Ti(1)	N(4)	C(6)	129.21(9)	N(3)	N(4)	C(6)	106.79(10)
N(6)	N(5)	C(7)	109.65(10)	N(6)	N(5)	B(1)	119.46(9)
C(7)	N(5)	B(1)	130.33(11)	Ti(1)	N(6)	N(5)	123.95(7)
Ti(1)	N(6)	C(9)	129.66(8)	N(5)	N(6)	C(9)	106.27(10)
N(1)	C(1)	C(2)	108.74(10)	C(1)	C(2)	C(3)	104.67(10)
N(2)	C(3)	C(2)	110.26(10)	N(3)	C(4)	C(5)	108.56(13)
C(4)	C(5)	C(6)	105.39(12)	N(4)	C(6)	C(5)	109.84(13)
N(5)	C(7)	C(8)	108.68(12)	C(7)	C(8)	C(9)	105.45(12)
N(6)	C(9)	C(8)	109.94(11)	O(1)	C(10)	C(11)	119.08(9)
O(1)	C(10)	C(15)	119.43(10)	C(11)	C(10)	C(15)	121.42(10)
C(10)	C(11)	C(12)	117.96(10)	C(10)	C(11)	C(16)	122.95(10)
C(12)	C(11)	C(16)	119.00(10)	C(11)	C(12)	C(13)	121.30(11)
C(12)	C(13)	C(14)	119.94(12)	C(13)	C(14)	C(15)	121.23(12)
C(10)	C(15)	C(14)	117.87(11)	C(10)	C(15)	C(22)	122.58(10)
C(14)	C(15)	C(22)	119.55(10)	C(11)	C(16)	C(17)	120.62(11)
C(11)	C(16)	C(21)	120.25(10)	C(17)	C(16)	C(21)	118.72(11)
C(16)	C(17)	C(18)	119.98(12)	C(17)	C(18)	C(19)	120.57(13)
C(18)	C(19)	C(20)	119.55(14)	C(19)	C(20)	C(21)	120.58(13)
C(16)	C(21)	C(20)	120.59(12)	C(15)	C(22)	C(23)	120.16(11)
C(15)	C(22)	C(27)	121.57(10)	C(23)	C(22)	C(27)	118.26(11)
C(22)	C(23)	C(24)	121.15(12)	C(23)	C(24)	C(25)	120.09(13)
C(24)	C(25)	C(26)	119.23(12)	C(25)	C(26)	C(27)	121.02(12)
C(22)	C(27)	C(26)	120.25(11)	N(1)	B(1)	N(3)	106.88(10)
N(1)	B(1)	N(5)	106.52(10)	N(3)	B(1)	N(5)	108.31(9)

Table 7. Bond angles involving hydrogens (°)

atom	atom	atom	angle	atom	atom	atom	angle
N(1)	C(1)	H(2)	125.6	C(2)	C(1)	H(2)	125.6
C(1)	C(2)	H(3)	127.7	C(3)	C(2)	H(3)	127.7
N(2)	C(3)	H(4)	124.8	C(2)	C(3)	H(4)	124.9
N(3)	C(4)	H(5)	125.8	C(5)	C(4)	H(5)	125.6
C(4)	C(5)	H(6)	127.4	C(6)	C(5)	H(6)	127.2
N(4)	C(6)	H(7)	125.0	C(5)	C(6)	H(7)	125.1
N(5)	C(7)	H(8)	125.6	C(8)	C(7)	H(8)	125.7
C(7)	C(8)	H(9)	127.2	C(9)	C(8)	H(9)	127.4
N(6)	C(9)	H(10)	125.1	C(8)	C(9)	H(10)	124.9
C(11)	C(12)	H(11)	119.3	C(13)	C(12)	H(11)	119.4
C(12)	C(13)	H(12)	120.0	C(14)	C(13)	H(12)	120.0
C(13)	C(14)	H(13)	119.4	C(15)	C(14)	H(13)	119.3
C(16)	C(17)	H(14)	120.0	C(18)	C(17)	H(14)	120.0
C(17)	C(18)	H(15)	119.7	C(19)	C(18)	H(15)	119.8
C(18)	C(19)	H(16)	120.2	C(20)	C(19)	H(16)	120.3
C(19)	C(20)	H(17)	119.7	C(21)	C(20)	H(17)	119.7
C(16)	C(21)	H(18)	119.7	C(20)	C(21)	H(18)	119.7
C(22)	C(23)	H(19)	119.5	C(24)	C(23)	H(19)	119.3
C(23)	C(24)	H(20)	120.0	C(25)	C(24)	H(20)	119.9
C(24)	C(25)	H(21)	120.3	C(26)	C(25)	H(21)	120.5
C(25)	C(26)	H(22)	119.5	C(27)	C(26)	H(22)	119.5
C(22)	C(27)	H(23)	119.8	C(26)	C(27)	H(23)	119.9
N(1)	B(1)	H(1)	110.7	N(3)	B(1)	H(1)	113.9
N(5)	B(1)	H(1)	110.2				

Table 8. Torsion Angles(°)

atom1	atom2	atom3	atom4	angle	atom1	atom2	atom3	atom4	angle
Cl(1)	Ti(1)	O(1)	C(10)	47.48(14)	Cl(1)	Ti(1)	N(2)	N(1)	-133.06(9)
Cl(1)	Ti(1)	N(2)	C(3)	49.51(10)	Cl(1)	Ti(1)	N(4)	N(3)	129.53(8)
Cl(1)	Ti(1)	N(4)	C(6)	-46.14(11)	Cl(1)	Ti(1)	N(6)	N(5)	-25.11(17)
Cl(1)	Ti(1)	N(6)	C(9)	150.50(9)	Cl(2)	Ti(1)	O(1)	C(10)	145.51(13)
Cl(2)	Ti(1)	N(2)	N(1)	130.26(9)	Cl(2)	Ti(1)	N(2)	C(3)	-47.17(11)
Cl(2)	Ti(1)	N(4)	N(3)	9.5(2)	Cl(2)	Ti(1)	N(4)	C(6)	-166.12(10)
Cl(2)	Ti(1)	N(6)	N(5)	-134.90(8)	Cl(2)	Ti(1)	N(6)	C(9)	40.71(10)
O(1)	Ti(1)	N(2)	N(1)	-29.5(2)	O(1)	Ti(1)	N(2)	C(3)	153.05(17)
N(2)	Ti(1)	O(1)	C(10)	-55.1(2)	O(1)	Ti(1)	N(4)	N(3)	-133.86(9)
O(1)	Ti(1)	N(4)	C(6)	50.48(11)	N(4)	Ti(1)	O(1)	C(10)	-41.92(14)
O(1)	Ti(1)	N(6)	N(5)	124.93(9)	O(1)	Ti(1)	N(6)	C(9)	-59.46(11)
N(6)	Ti(1)	O(1)	C(10)	-124.89(14)	N(2)	Ti(1)	N(4)	N(3)	43.64(9)
N(2)	Ti(1)	N(4)	C(6)	-132.03(11)	N(4)	Ti(1)	N(2)	N(1)	-42.87(9)
N(4)	Ti(1)	N(2)	C(3)	139.70(11)	N(2)	Ti(1)	N(6)	N(5)	-44.65(8)
N(2)	Ti(1)	N(6)	C(9)	130.96(11)	N(6)	Ti(1)	N(2)	N(1)	41.86(9)
N(6)	Ti(1)	N(2)	C(3)	-135.57(11)	N(4)	Ti(1)	N(6)	N(5)	36.17(9)
N(4)	Ti(1)	N(6)	C(9)	-148.22(11)	N(6)	Ti(1)	N(4)	N(3)	-37.08(9)
N(6)	Ti(1)	N(4)	C(6)	147.25(11)	Ti(1)	O(1)	C(10)	C(11)	91.68(15)
Ti(1)	O(1)	C(10)	C(15)	-85.19(16)	N(2)	N(1)	C(1)	C(2)	0.28(15)
C(1)	N(1)	N(2)	Ti(1)	-177.76(8)	C(1)	N(1)	N(2)	C(3)	0.20(13)
N(2)	N(1)	B(1)	N(3)	56.99(14)	N(2)	N(1)	B(1)	N(5)	-58.63(13)
B(1)	N(1)	N(2)	Ti(1)	1.11(14)	B(1)	N(1)	N(2)	C(3)	179.06(10)
C(1)	N(1)	B(1)	N(3)	-124.43(13)	C(1)	N(1)	B(1)	N(5)	119.95(13)
B(1)	N(1)	C(1)	C(2)	-178.41(12)	Ti(1)	N(2)	C(3)	C(2)	177.15(8)
N(1)	N(2)	C(3)	C(2)	-0.60(14)	N(4)	N(3)	C(4)	C(5)	-0.37(15)
C(4)	N(3)	N(4)	Ti(1)	-176.62(8)	C(4)	N(3)	N(4)	C(6)	-0.13(13)
N(4)	N(3)	B(1)	N(1)	-57.12(13)	N(4)	N(3)	B(1)	N(5)	57.30(13)
B(1)	N(3)	N(4)	Ti(1)	-2.37(14)	B(1)	N(3)	N(4)	C(6)	174.12(10)
C(4)	N(3)	B(1)	N(1)	115.73(13)	C(4)	N(3)	B(1)	N(5)	-129.85(13)
B(1)	N(3)	C(4)	C(5)	-173.78(12)	Ti(1)	N(4)	C(6)	C(5)	176.81(9)
N(3)	N(4)	C(6)	C(5)	0.57(14)	N(6)	N(5)	C(7)	C(8)	-0.02(11)
C(7)	N(5)	N(6)	Ti(1)	176.28(8)	C(7)	N(5)	N(6)	C(9)	-0.20(13)
N(6)	N(5)	B(1)	N(1)	56.47(13)	N(6)	N(5)	B(1)	N(3)	-58.18(13)
B(1)	N(5)	N(6)	Ti(1)	4.01(14)	B(1)	N(5)	N(6)	C(9)	-172.47(10)
C(7)	N(5)	B(1)	N(1)	-113.97(13)	C(7)	N(5)	B(1)	N(3)	131.38(13)
B(1)	N(5)	C(7)	C(8)	171.15(12)	Ti(1)	N(6)	C(9)	C(8)	-175.87(9)
N(5)	N(6)	C(9)	C(8)	0.34(14)	N(1)	C(1)	C(2)	C(3)	-0.62(15)

Table 8. Torsion angles (°) (continued)

atom1	atom2	atom3	atom4	angle	atom1	atom2	atom3	atom4	angle
C(1)	C(2)	C(3)	N(2)	0.75(14)	N(3)	C(4)	C(5)	C(6)	0.69(16)
C(4)	C(5)	C(6)	N(4)	-0.78(16)	N(5)	C(7)	C(8)	C(9)	0.22(15)
C(7)	C(8)	C(9)	N(6)	-0.35(15)	O(1)	C(10)	C(11)	C(12)	-170.48(10)
O(1)	C(10)	C(11)	C(16)	13.09(16)	O(1)	C(10)	C(15)	C(14)	172.38(10)
O(1)	C(10)	C(15)	C(22)	-8.04(16)	C(11)	C(10)	C(15)	C(14)	-4.42(16)
C(11)	C(10)	C(15)	C(22)	175.16(10)	C(15)	C(10)	C(11)	C(12)	6.32(16)
C(15)	C(10)	C(11)	C(16)	-170.10(10)	C(10)	C(11)	C(12)	C(13)	-3.59(18)
C(10)	C(11)	C(16)	C(17)	-132.41(13)	C(10)	C(11)	C(16)	C(21)	55.02(16)
C(12)	C(11)	C(16)	C(17)	51.20(16)	C(12)	C(11)	C(16)	C(21)	-121.37(13)
C(16)	C(11)	C(12)	C(13)	172.98(11)	C(11)	C(12)	C(13)	C(14)	-1.0(2)
C(12)	C(13)	C(14)	C(15)	3.0(2)	C(13)	C(14)	C(15)	C(10)	-0.31(18)
C(13)	C(14)	C(15)	C(22)	-179.90(11)	C(10)	C(15)	C(22)	C(23)	138.08(12)
C(10)	C(15)	C(22)	C(27)	-42.72(16)	C(14)	C(15)	C(22)	C(23)	-42.35(16)
C(14)	C(15)	C(22)	C(27)	136.85(12)	C(11)	C(16)	C(17)	C(18)	-171.39(12)
C(11)	C(16)	C(21)	C(20)	171.56(12)	C(17)	C(16)	C(21)	C(20)	-1.15(19)
C(21)	C(16)	C(17)	C(18)	1.3(2)	C(16)	C(17)	C(18)	C(19)	-0.3(2)
C(17)	C(18)	C(19)	C(20)	-1.0(2)	C(18)	C(19)	C(20)	C(21)	1.1(2)
C(19)	C(20)	C(21)	C(16)	-0.05(16)	C(15)	C(22)	C(23)	C(24)	179.95(10)
C(15)	C(22)	C(27)	C(26)	-179.86(11)	C(23)	C(22)	C(27)	C(26)	-0.64(17)
C(27)	C(22)	C(23)	C(24)	0.73(18)	C(22)	C(23)	C(24)	C(25)	-0.06(15)
C(23)	C(24)	C(25)	C(26)	-0.7(2)	C(24)	C(25)	C(26)	C(27)	0.8(2)
C(25)	C(26)	C(27)	C(22)	-0.10(19)					

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
Cl(1)	C(17)[1)]	3.4616(14)	Cl(2)	C(14)[2)]	3.5924(13)
C(1)	C(25)[3)]	3.4992(18)	C(1)	C(26)[3)]	3.5249(18)
C(2)	C(25)[3)]	3.5783(18)	C(4)	C(9)[4)]	3.5949(19)
C(9)	C(4)[5)]	3.5949(19)	C(14)	Cl(2)[6)]	3.5924(13)
C(17)	Cl(1)[7)]	3.4616(14)	C(25)	C(1)[8)]	3.4992(18)
C(25)	C(2)[8)]	3.5783(18)	C(26)	C(1)[8)]	3.5249(18)

Symmetry Operators:

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

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

atom	atom	distance	atom	atom	distance
Cl(1)	H(8)[1)]	3.149	Cl(1)	H(9)[1)]	3.452
Cl(1)	H(11)[2)]	3.313	Cl(1)	H(14)[2)]	2.942
Cl(1)	H(15)[2)]	3.494	Cl(2)	H(3)[3)]	3.147
Cl(2)	H(5)[4)]	3.020	Cl(2)	H(12)[5)]	3.028
Cl(2)	H(13)[5)]	2.905	Cl(2)	H(21)[6)]	3.058
N(1)	H(6)[4)]	3.119	N(1)	H(9)[1)]	2.960
N(2)	H(6)[4)]	3.025	N(2)	H(9)[1)]	2.798
N(4)	H(9)[1)]	3.569	C(1)	H(6)[4)]	3.039
C(1)	H(9)[1)]	3.031	C(2)	H(6)[4)]	2.873
C(2)	H(9)[1)]	2.923	C(2)	H(12)[2)]	3.007
C(2)	H(21)[7)]	3.564	C(2)	H(22)[6)]	3.420
C(3)	H(6)[4)]	2.859	C(3)	H(9)[1)]	2.744
C(3)	H(11)[2)]	3.255	C(3)	H(12)[2)]	3.218
C(3)	H(21)[6)]	3.033	C(3)	H(22)[6)]	3.045
C(4)	H(20)[8)]	3.426	C(4)	H(21)[8)]	3.358
C(5)	H(21)[8)]	3.325	C(7)	H(11)[9)]	3.195
C(8)	H(11)[9)]	3.092	C(10)	H(16)[10)]	3.025
C(11)	H(16)[10)]	2.882	C(12)	H(4)[8)]	3.407
C(12)	H(8)[10)]	3.514	C(12)	H(9)[10)]	3.371
C(12)	H(16)[10)]	2.883	C(12)	H(17)[10)]	3.599
C(12)	H(22)[11)]	3.541	C(13)	H(3)[8)]	3.485
C(13)	H(4)[8)]	3.451	C(13)	H(16)[10)]	2.981
C(13)	H(17)[10)]	3.267	C(13)	H(22)[11)]	3.009
C(14)	H(16)[10)]	3.044	C(15)	H(16)[10)]	3.084
C(16)	H(8)[10)]	3.226	C(17)	H(8)[10)]	3.045
C(18)	H(8)[10)]	3.199	C(18)	H(18)[9)]	3.512
C(18)	H(19)[8)]	3.574	C(18)	H(20)[8)]	3.466
C(19)	H(1)[10)]	3.536	C(19)	H(8)[10)]	3.515
C(20)	H(20)[5)]	3.284	C(21)	H(8)[10)]	3.547
C(21)	H(20)[5)]	3.363	C(22)	H(2)[12)]	3.029
C(23)	H(2)[12)]	3.143	C(23)	H(10)[11)]	3.298
C(23)	H(15)[2)]	2.936	C(23)	H(18)[11)]	3.580
C(24)	H(2)[12)]	3.082	C(24)	H(5)[2)]	3.502
C(24)	H(15)[2)]	2.990	C(24)	H(17)[11)]	3.453
C(24)	H(18)[11)]	3.482	C(25)	H(2)[12)]	2.883
C(25)	H(3)[12)]	3.088	C(25)	H(4)[3)]	3.052
C(25)	H(5)[2)]	3.475	C(25)	H(6)[2)]	3.381

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

atom	atom	distance	atom	atom	distance
C(26)	H(2)[12)]	2.719	C(26)	H(4)[3)]	2.945
C(26)	H(12)[5)]	3.472	C(27)	H(2)[12)]	2.798
H(1)	C(19)[9)]	3.536	H(1)	H(16)[9)]	3.529
H(2)	C(22)[7)]	3.029	H(2)	C(23)[7)]	3.143
H(2)	C(24)[7)]	3.082	H(2)	C(25)[7)]	2.883
H(2)	C(26)[7)]	2.719	H(2)	C(27)[7)]	2.798
H(2)	H(6)[4)]	3.573	H(2)	H(21)[7)]	3.413
H(2)	H(22)[7)]	3.167	H(2)	H(23)[7)]	3.282
H(3)	Cl(2)[6)]	3.147	H(3)	C(13)[2)]	3.485
H(3)	C(25)[7)]	3.088	H(3)	H(6)[4)]	3.305
H(3)	H(9)[1)]	3.454	H(3)	H(12)[2)]	2.530
H(3)	H(21)[7)]	2.851	H(3)	H(22)[6)]	3.146
H(4)	C(12)[2)]	3.407	H(4)	C(13)[2)]	3.451
H(4)	C(25)[6)]	3.052	H(4)	C(26)[6)]	2.945
H(4)	H(6)[4)]	3.286	H(4)	H(9)[1)]	3.166
H(4)	H(11)[2)]	2.840	H(4)	H(12)[2)]	2.931
H(4)	H(21)[6)]	2.527	H(4)	H(22)[6)]	2.290
H(5)	Cl(2)[1)]	3.020	H(5)	C(24)[8)]	3.502
H(5)	C(25)[8)]	3.475	H(5)	H(10)[1)]	3.548
H(5)	H(13)[7)]	3.416	H(5)	H(17)[9)]	3.367
H(5)	H(20)[8)]	2.898	H(5)	H(21)[8)]	2.846
H(6)	N(1)[1)]	3.119	H(6)	N(2)[1)]	3.025
H(6)	C(1)[1)]	3.039	H(6)	C(2)[1)]	2.873
H(6)	C(3)[1)]	2.859	H(6)	C(25)[8)]	3.381
H(6)	H(2)[1)]	3.573	H(6)	H(3)[1)]	3.305
H(6)	H(4)[1)]	3.286	H(6)	H(21)[8)]	2.801
H(8)	Cl(1)[4)]	3.149	H(8)	C(12)[9)]	3.514
H(8)	C(16)[9)]	3.226	H(8)	C(17)[9)]	3.045
H(8)	C(18)[9)]	3.199	H(8)	C(19)[9)]	3.515
H(8)	C(21)[9)]	3.547	H(8)	H(11)[9)]	2.810
H(8)	H(14)[9)]	3.382	H(9)	Cl(1)[4)]	3.452
H(9)	N(1)[4)]	2.960	H(9)	N(2)[4)]	2.798
H(9)	N(4)[4)]	3.569	H(9)	C(1)[4)]	3.031
H(9)	C(2)[4)]	2.923	H(9)	C(3)[4)]	2.744
H(9)	C(12)[9)]	3.371	H(9)	H(3)[4)]	3.454
H(9)	H(4)[4)]	3.166	H(9)	H(11)[9)]	2.610
H(9)	H(12)[9)]	3.482	H(10)	C(23)[5)]	3.298

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

atom	atom	distance	atom	atom	distance
H(10)	H(5)[4)]	3.548	H(10)	H(13)[5)]	2.929
H(10)	H(19)[5)]	2.886	H(10)	H(20)[5)]	3.583
H(11)	Cl(1)[8)]	3.313	H(11)	C(3)[8)]	3.255
H(11)	C(7)[10)]	3.195	H(11)	C(8)[10)]	3.092
H(11)	H(4)[8)]	2.840	H(11)	H(8)[10)]	2.810
H(11)	H(9)[10)]	2.610	H(11)	H(16)[10)]	3.406
H(11)	H(22)[11)]	3.587	H(12)	Cl(2)[11)]	3.028
H(12)	C(2)[8)]	3.007	H(12)	C(3)[8)]	3.218
H(12)	C(26)[11)]	3.472	H(12)	H(3)[8)]	2.530
H(12)	H(4)[8)]	2.931	H(12)	H(9)[10)]	3.482
H(12)	H(16)[10)]	3.554	H(12)	H(17)[10)]	3.165
H(12)	H(22)[11)]	2.636	H(13)	Cl(2)[11)]	2.905
H(13)	H(5)[12)]	3.416	H(13)	H(10)[11)]	2.929
H(13)	H(23)[11)]	3.472	H(14)	Cl(1)[8)]	2.942
H(14)	H(8)[10)]	3.382	H(15)	Cl(1)[8)]	3.494
H(15)	C(23)[8)]	2.936	H(15)	C(24)[8)]	2.990
H(15)	H(18)[9)]	2.950	H(15)	H(19)[8)]	2.618
H(15)	H(20)[8)]	2.724	H(16)	C(10)[9)]	3.025
H(16)	C(11)[9)]	2.882	H(16)	C(12)[9)]	2.883
H(16)	C(13)[9)]	2.981	H(16)	C(14)[9)]	3.044
H(16)	C(15)[9)]	3.084	H(16)	H(1)[10)]	3.529
H(16)	H(11)[9)]	3.406	H(16)	H(12)[9)]	3.554
H(16)	H(18)[9)]	3.181	H(17)	C(12)[9)]	3.599
H(17)	C(13)[9)]	3.267	H(17)	C(24)[5)]	3.453
H(17)	H(5)[10)]	3.367	H(17)	H(12)[9)]	3.165
H(17)	H(20)[5)]	2.634	H(18)	C(18)[10)]	3.512
H(18)	C(23)[5)]	3.580	H(18)	C(24)[5)]	3.482
H(18)	H(15)[10)]	2.950	H(18)	H(16)[10)]	3.181
H(18)	H(19)[5)]	2.985	H(18)	H(20)[5)]	2.794
H(19)	C(18)[2)]	3.574	H(19)	H(10)[11)]	2.886
H(19)	H(15)[2)]	2.618	H(19)	H(18)[11)]	2.985
H(19)	H(23)[11)]	3.551	H(20)	C(4)[2)]	3.426
H(20)	C(18)[2)]	3.466	H(20)	C(20)[11)]	3.284
H(20)	C(21)[11)]	3.363	H(20)	H(5)[2)]	2.898
H(20)	H(10)[11)]	3.583	H(20)	H(15)[2)]	2.724
H(20)	H(17)[11)]	2.634	H(20)	H(18)[11)]	2.794
H(21)	Cl(2)[3)]	3.058	H(21)	C(2)[12)]	3.564

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

atom	atom	distance	atom	atom	distance
H(21)	C(3)[3)]	3.033	H(21)	C(4)[2)]	3.358
H(21)	C(5)[2)]	3.325	H(21)	H(2)[12)]	3.413
H(21)	H(3)[12)]	2.851	H(21)	H(4)[3)]	2.527
H(21)	H(5)[2)]	2.846	H(21)	H(6)[2)]	2.801
H(22)	C(2)[3)]	3.420	H(22)	C(3)[3)]	3.045
H(22)	C(12)[5)]	3.541	H(22)	C(13)[5)]	3.009
H(22)	H(2)[12)]	3.167	H(22)	H(3)[3)]	3.146
H(22)	H(4)[3)]	2.290	H(22)	H(11)[5)]	3.587
H(22)	H(12)[5)]	2.636	H(23)	H(2)[12)]	3.282
H(23)	H(13)[5)]	3.472	H(23)	H(19)[5)]	3.551

Symmetry Operators:

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