Supporting Information

for

Synthesis of Titanium Complexes Containing Amine Triphenolate Ligand of the Type, [TiX{(O-2,4-$R_2C_6H_2$)-6-CH_2}$_3$N], and the Ti-Al Hetero-bimetallic Complexes with $AlMe_3$: Effect of Terminal Donor Ligand in Ethylene Polymerization

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Contents

1. Additional polymerization results (for demonstration of reproducibility in the experiments).

Table S1. Ethylene polymerization by TiX[(O-2,4-$R_2C_6H_2$-6-$CH_2)_3N$] [R = Me (**1**), ^{t}Bu (**2**); X = O^{i}Pr (**a**), O^{t}Bu (**b**), $OCH(CF_3)_2$ (**c**), $OC(CF_3)_3$ (**d**), Cl (**e**), Et (**f**), Me (**g**)], [TiMe{(O-2,4-$Me_2C_6H_2$-6-$CH_2)_2(\mu_2$-O-2,4-Me_2-C_6H_2-6-$CH_2)$}N][$Me_2Al(\mu_2$-OR')] [R' = ^{t}Bu (**3b**), $CH(CF_3)_2$ (**3c**), $C(CF_3)_3$ (**3d**)] – MAO catalyst systems.[a]

run	catalyst	$AlMe_3$ / µmol (Al/Ti)[b]	yield/ mg	activity[c]
1	**1a**	---	149.7	1500
2	**1a**	1.0 (10)	163.3	1630
S1	**1a**	1.0 (10)	162.3	1620
3	**1a**	0.5 (5.0)	180.9	1810
S2	**1a**	0.3 (3.0)	181.4	1810
4	**1a**	0.3 (3.0)	181.5	1810
S3	**2a**	---	128.1	1280
5	**2a**	---	129.2	1290
6	**2a**	1.0 (10)	142.1	1420
7	**2a**	0.5 (5.0)	132.5	1330
S4	**2a**	0.5 (5.0)	130.1	1300
8	**2a**	0.3 (3.0)	132.7	1330
9	**1b**	---	236.6	2370
10	**1b**	1.0 (10)	212.7	2130
S5	**1b**	1.0 (10)	205.0	2050
11	**1b**	0.35 (3.5)	200.6	2010
S6	**1b**	0.3 (3.0)	200.9	2010
S7	**1b**	0.3 (3.0)	207.3	2070
12	**3b**	---	213.6	2140
S8	**3b**	---	208.5	2090
13	**2b**	---	191.1	1910
S9	**2b**	---	185.9	1860
S10	**2b**	1.0 (10)	201.2	2010
14	**2b**	1.0 (10)	208.8	2090
15	**1c**	---	243.3	2430
16	**1c**	1.0 (10)	243.2	2430
S11	**1c**	1.0 (10)	232.7	2330
17	**1c**	0.5 (5.0)	252.9	2530
18	**1c**	0.3 (3.0)	270.7	2710
19	**3c**	---	251.3	2510
S12	**3c**	---	244.8	2450
20	**2c**	---	178.5	1790
S13	**2c**	---	169.6	1700
21	**2c**	1.0 (10.0)	177.2	1770
S14	**2c**	1.0 (10.0)	166.7	1670

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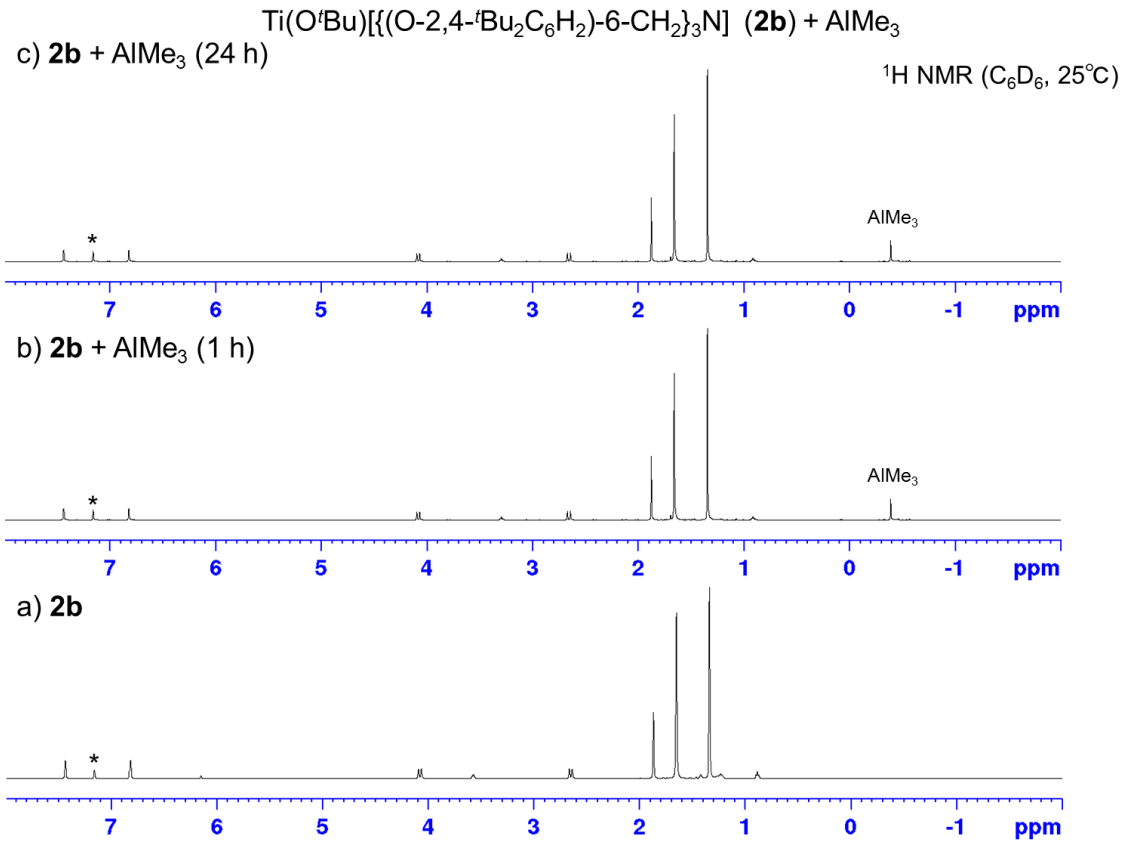
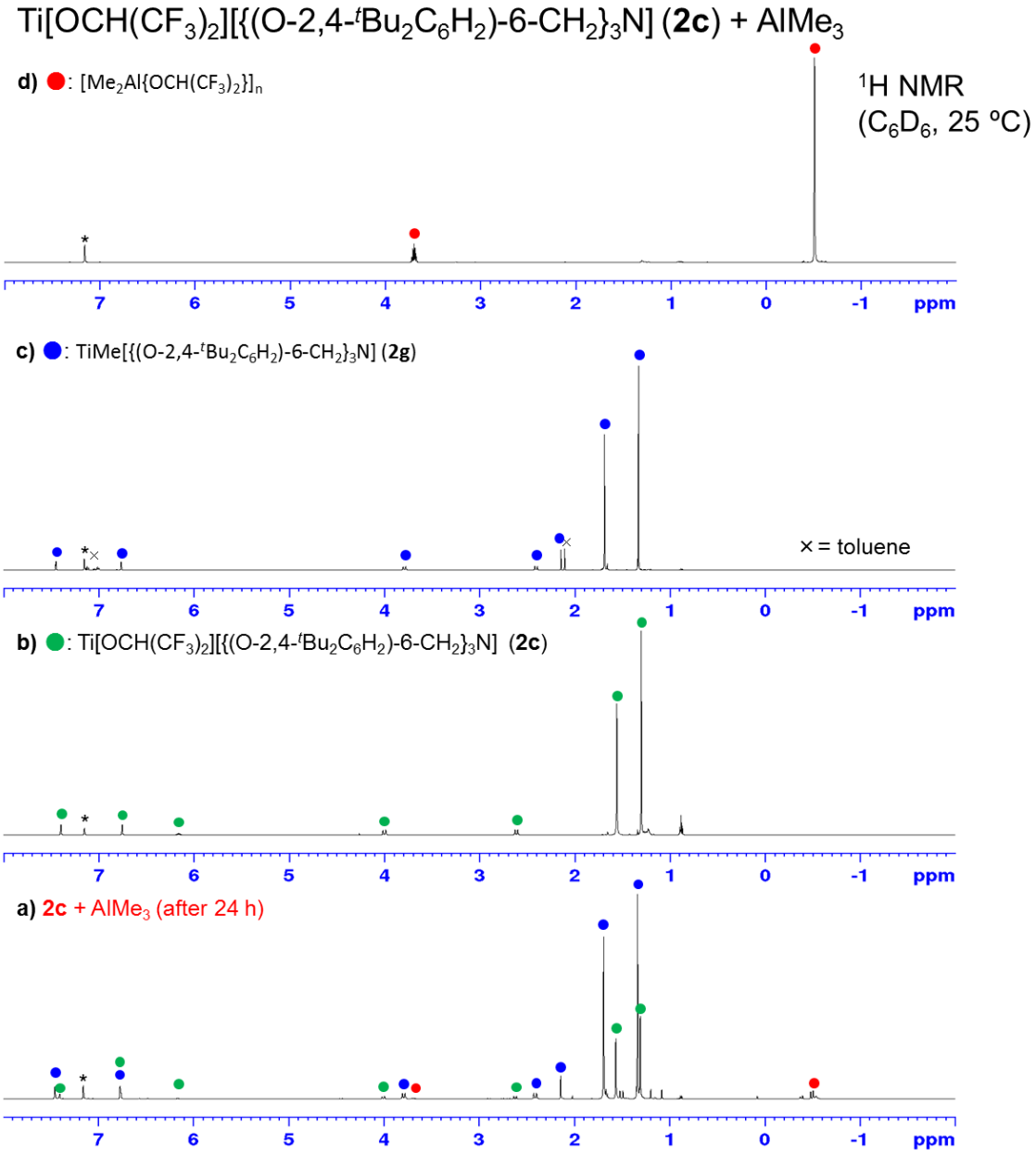
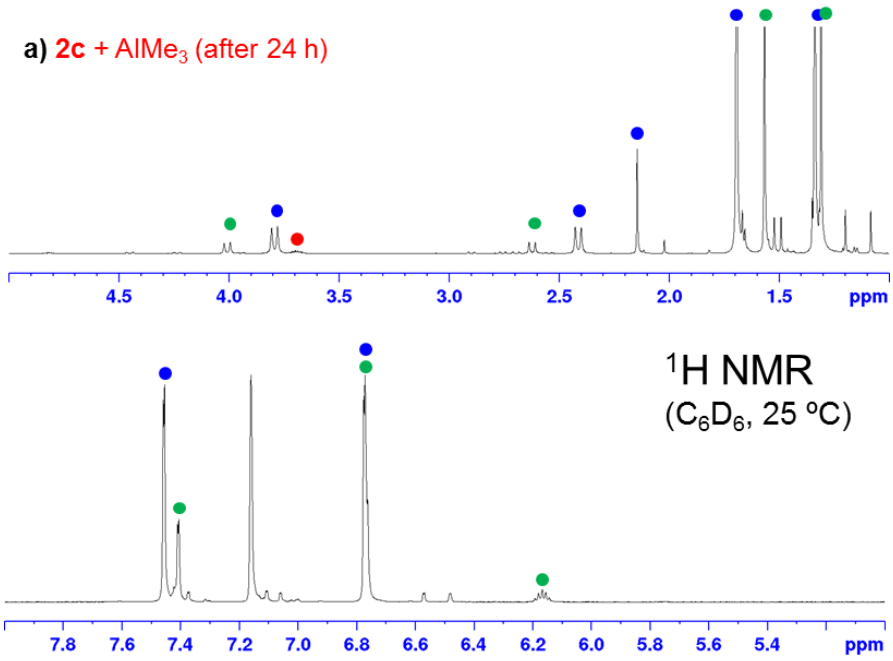
22	**1d**	---	201.2	2010
S15	**1d**	---	195.9	1960
23	**1d**	1.0 (10)	177.6	1780
S16	**1d**	1.0 (10)	176.5	1770
24	**1d**	0.5 (5.0)	206.9	2070
S17	**1d**	0.5 (5.0)	185.0	1850
25	**1d**	0.3 (3.0)	229.9	2300
S18	**1d**	0.3 (3.0)	228.5	2290
26	**3d**	---	285.8	2860
S19	**3d**	---	264.4	2640
27	**1e**	---	200.2	2000
28	**1e**	1.0 (10)	178.5	1790
S20	**1e**	1.0 (10)	168.7	1690
29	**1e**	0.35 (3.5)	167.7	1670
S21	**1e**	0.35 (3.5)	163.9	1640
30	**2e**	---	168.5	1690
S22	**2e**	---	165.5	1660
31	**2e**	1.0 (10)	226.7	2270
S23	**2e**	1.0 (10)	207.4	2070
32	**2f**	---	180.2	1800
S24	**2f**	---	170.2	1700
33	**2f**	1.0 (10)	208.8	2100
34	**2g**	---	158.8	1590
S25	**2g**	---	152.4	1520
35	**2g**	1.0 (10)	193.9	1940

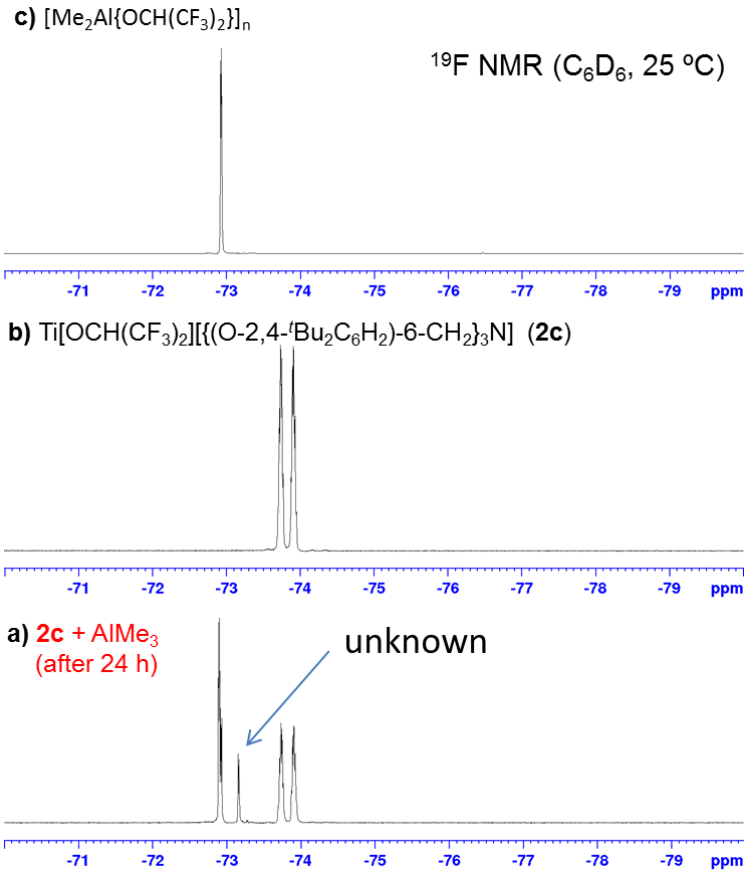
[a]Conditions: Ti complex 0.1 μmol, *n*-octane 30.0 mL, MAO 3.0 mmol, ethylene 8 atm, 100 °C, 60 min. [b]Al/Ti molar ratio. [c]Activity in kg-PE/mol-Ti·h.

2. Reactions of Ti(OR')[{(O-2,4-^{t}Bu$_2$C$_6$H$_2$)-6-CH$_2$}$_3$N] [R' = ^{t}Bu (**2b**), CH(CF$_3$)$_2$ (**2c**)] with AlMe$_3$ monitored by NMR spectra.




Ti[OCH(CF3)2][{(O-2,4-tBu2C6H2)-6-CH2}3N] (2c) + AlMe3
d) ●: [Me2Al{OCH(CF3)2}]n
1H NMR
(C6D6, 25 °C)
c) ●: TiMe[{(O-2,4-tBu2C6H2)-6-CH2}3N] (2g)
× = toluene
b) ●: Ti[OCH(CF3)2][{(O-2,4-tBu2C6H2)-6-CH2}3N] (2c)
a) 2c + AlMe3 (after 24 h)
7
6
5
4
3
2
1
0
-1
ppm


a) 2c + AlMe3 (after 24 h)
4.5
4.0
3.5
3.0
2.5
2.0
1.5
ppm
1H NMR
(C6D6, 25 ºC)
7.8
7.6
7.4
7.2
7.0
6.8
6.6
6.4
6.2
6.0
5.8
5.6
5.4
ppm


c) [Me2Al{OCH(CF3)2}]n
19F NMR (C6D6, 25 ºC)
-71
-72
-73
-74
-75
-76
-77
-78
-79
ppm
b) Ti[OCH(CF3)2][{(O-2,4-tBu2C6H2)-6-CH2}3N] (2c)
-71
-72
-73
-74
-75
-76
-77
-78
-79
ppm
a) 2c + AlMe3
(after 24 h)
unknown
-71
-72
-73
-74
-75
-76
-77
-78
-79
ppm

X-ray Structure Report

for

[TiMe{(O-2,4-$Me_2C_6H_2$-6-CH_2)$_2$(μ_2-O-2,4-Me_2-C_6H_2-6-CH_2)}N][Me_2Al(μ_2-O^{t}Bu)] (**3b**)

October 25, 2013

Experimental

Data Collection

An orange prism crystal of $C_{35}H_{50}AlCl_2NO_4Ti$ having approximate dimensions of 0.200 x 0.180 x 0.150 mm was mounted on a glass fiber. All measurements were made on a Rigaku XtaLAB mini diffractometer Mo-Kα radiation.

The crystal-to-detector distance was 0.00 mm.

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

a	= 9.537(4) Å	α	= 77.075(11)^o
b	= 11.805(5) Å	β	= 81.444(8)^o
c	= 16.938(7) Å	γ	= 83.505(10)^o
V	= 1831.6(13) Å^3		

For Z = 2 and F.W. = 694.57, the calculated density is 1.259 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 0 $\pm$ 1^{o}C to a maximum 2θ value of 55.0^o. The crystal-to-detector distance was 0.00 mm. Readout was performed in the 0.000 mm pixel mode.

Data Reduction

Of the 17857 reflections that were collected, 8324 were unique (R_{int} = 0.0243); equivalent reflections were merged. Data were collected and processed using CrystalClear (Rigaku).

The linear absorption coefficient, μ, for Mo-Kα radiation is 4.397 cm^{-1}. An empirical

absorption correction was applied which resulted in transmission factors ranging from 0.830 to 0.936. The data were corrected for Lorentz and polarization effects.

Structure Solution and Refinement

The structure was solved by direct methods[2] 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[3] on F^2 was based on 8324 observed reflections and 397 variable parameters and converged (largest parameter shift was 0.00 times its esd) with unweighted and weighted agreement factors of:

$$R1 = \Sigma \, ||Fo| - |Fc|| \, / \, \Sigma \, |Fo| = 0.0539$$

$$wR2 = [\Sigma \, (w \, (Fo^2 - Fc^2)^2) / \Sigma \, w(Fo^2)^2]^{1/2} = 0.1532$$

The standard deviation of an observation of unit weight[4] was 1.04. Unit weights were used. The maximum and minimum peaks on the final difference Fourier map corresponded to 1.64 and -1.10 $e^-/Å^3$, respectively.

Neutral atom scattering factors were taken from Cromer and Waber[5]. Anomalous dispersion effects were included in Fcalc[6]; the values for $\Delta f'$ and $\Delta f''$ 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) CrystalClear: Rigaku Corporation, 1999. CrystalClear Software User's Guide, Molecular Structure Corporation, (c) 2000.J.W.Pflugrath (1999) Acta Cryst. D55, 1718-1725.

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

(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 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	$C_{35}H_{50}AlCl_2NO_4Ti$
Formula Weight	694.57
Crystal Color, Habit	orange, prism
Crystal Dimensions	0.200 X 0.180 X 0.150 mm
Crystal System	triclinic
Lattice Type	Primitive
Lattice Parameters	a = 9.537(4) Å b = 11.805(5) Å c = 16.938(7) Å α = 77.075(11) ^{o} β = 81.444(8) ^{o} γ = 83.505(10) ^{o} V = 1831.6(13) Å^3
Space Group	P-1 (#2)
Z value	2
D_{calc}	1.259 g/cm^3
F_{000}	736.00
μ(MoKα)	4.397 cm^{-1}

B. Intensity Measurements

Diffractometer	XtaLAB mini
Radiation	MoKα (λ = 0.71075 Å)
Voltage, Current	50kV, 12mA
Temperature	0.0^{o}C
Detector Aperture	75 mm (diameter)
Detector Position	0.00 mm
Pixel Size	0.073 mm
$2\theta_{max}$	55.0^{o}
No. of Reflections Measured	Total: 17857 Unique: 8324 (R_{int} = 0.0243)
Corrections	Lorentz-polarization Absorption (trans. factors: 0.830 - 0.936)

C. Structure Solution and Refinement

Structure Solution	Direct Methods (SIR92)
Refinement	Full-matrix least-squares on F^2
Function Minimized	$\Sigma\, w\,(Fo^2 - Fc^2)^2$
Least Squares Weights	$w = 1/\,[\,\sigma^2(Fo^2) + (0.0824 \cdot P)^2 + 2.2478 \cdot P\,]$ 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)	8324
No. Variables	397
Reflection/Parameter Ratio	20.97
Residuals: R1 ($I>2.00\sigma(I)$)	0.0539
Residuals: R (All reflections)	0.0621
Residuals: wR2 (All reflections)	0.1532
Goodness of Fit Indicator	1.041
Max Shift/Error in Final Cycle	0.001
Maximum peak in Final Diff. Map	1.64 $e^-/Å^3$
Minimum peak in Final Diff. Map	-1.10 $e^-/Å^3$

Table S2-1. Atomic coordinates and B_{iso}/B_{eq}

atom	x	y	z	B_{eq}
Ti1	0.69565(4)	0.29166(3)	0.20502(2)	0.995(9)
Cl1	1.10908(11)	0.84662(7)	0.17711(7)	4.44(2)
Cl3	1.36443(10)	0.72609(8)	0.24317(7)	4.35(2)
Al1	0.57055(7)	0.05999(6)	0.28941(4)	1.361(13)
O1	0.6088(2)	0.1461(2)	0.18493(9)	1.42(3)
O2	0.6615(2)	0.17513(13)	0.31376(9)	1.18(3)
O3	0.7645(2)	0.39408(13)	0.25451(9)	1.22(3)
O4	0.7739(2)	0.33304(13)	0.09869(9)	1.25(3)
N1	0.9418(2)	0.2020(2)	0.21515(10)	1.00(3)
C10	0.8699(3)	0.4168(2)	0.29222(12)	1.09(3)
C11	0.9620(3)	0.1410(2)	0.43134(13)	1.36(4)
C12	1.0080(3)	0.3656(2)	0.27526(12)	1.07(3)
C13	0.4963(3)	0.3912(2)	0.2050(2)	1.67(4)
C14	1.1269(3)	0.3015(2)	-0.07443(13)	1.41(4)
C15	0.8408(3)	0.4921(2)	0.34758(13)	1.32(4)
C16	0.8840(3)	0.1411(2)	0.36813(12)	1.14(4)
C17	0.8950(3)	0.3987(2)	-0.03415(13)	1.25(4)
C18	1.0924(3)	0.4658(2)	0.36796(13)	1.40(4)
C19	1.0147(3)	0.3867(2)	-0.09125(13)	1.40(4)
C20	0.9892(3)	0.1477(2)	0.14258(12)	1.11(3)
C21	1.1175(3)	0.3904(2)	0.31344(13)	1.23(4)
C22	0.8971(3)	0.1738(2)	0.50329(13)	1.58(4)
C23	0.7750(3)	0.4913(2)	-0.0520(2)	1.54(4)
C24	1.1164(3)	0.2255(2)	0.00202(13)	1.32(4)
C25	0.9981(3)	0.2336(2)	0.06113(12)	1.13(4)
C26	0.7377(3)	0.1728(2)	0.37846(12)	1.14(4)
C27	0.5669(3)	0.1169(2)	0.1121(2)	1.75(4)
C28	0.6903(3)	0.5433(2)	0.3677(2)	1.75(4)
C29	0.9533(3)	0.1069(2)	0.28944(12)	1.13(3)
C30	1.0411(3)	0.2931(2)	0.21089(12)	1.14(4)
C31	1.2129(3)	0.4903(3)	0.4094(2)	1.93(4)
C32	0.6754(3)	-0.0949(2)	0.3109(2)	1.98(4)
C33	0.3698(3)	0.0665(3)	0.3385(2)	2.19(5)
C34	0.8883(3)	0.3212(2)	0.04240(12)	1.12(3)
C35	0.9534(3)	0.5158(2)	0.38356(13)	1.46(4)
C36	0.4994(3)	0.2259(3)	0.0596(2)	2.44(5)
C37	0.6683(3)	0.2061(2)	0.44953(13)	1.46(4)

Table S2-1. Atomic coordinates and B_{iso}/B_{eq} (continued)

atom	x	y	z	B_{eq}
C38	0.9839(3)	0.1769(3)	0.5701(2)	2.21(5)
C39	1.2557(3)	0.2939(3)	-0.1379(2)	2.02(4)
C40	0.6985(3)	0.0667(3)	0.0643(2)	2.37(5)
C41	0.5106(3)	0.2433(3)	0.4588(2)	2.28(5)
C42	0.7511(3)	0.2061(2)	0.51096(13)	1.69(4)
C43	0.4581(3)	0.0256(3)	0.1404(2)	2.59(5)
C44	1.2074(4)	0.7124(3)	0.2036(3)	3.64(7)

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

Table S2-2. Atomic coordinates and B_{iso} involving hydrogen atoms

atom	x	y	z	B_{iso}
H11	1.0591	0.1187	0.4256	1.63
H13A	0.4427	0.3700	0.1676	2.00
H13B	0.5112	0.4726	0.1884	2.00
H13C	0.4448	0.3760	0.2589	2.00
H19	1.0199	0.4372	-0.1422	1.68
H20A	0.9236	0.0908	0.1422	1.33
H20B	1.0821	0.1063	0.1486	1.33
H21	1.2090	0.3562	0.3024	1.47
H23A	0.7765	0.5172	-0.1100	1.85
H23B	0.7861	0.5561	-0.0285	1.85
H23C	0.6859	0.4598	-0.0289	1.85
H24	1.1898	0.1681	0.0140	1.59
H28A	0.6875	0.6269	0.3536	2.11
H28B	0.6600	0.5186	0.4250	2.11
H28C	0.6281	0.5169	0.3372	2.11
H29A	1.0531	0.0834	0.2938	1.36
H29B	0.9095	0.0400	0.2827	1.36
H30A	1.0423	0.3453	0.1577	1.37
H30B	1.1362	0.2549	0.2144	1.37
H31A	1.2375	0.4227	0.4498	2.31
H31B	1.1832	0.5552	0.4351	2.31
H31C	1.2942	0.5083	0.3694	2.31
H32A	0.7758	-0.0863	0.3018	2.38
H32B	0.6524	-0.1405	0.2749	2.38
H32C	0.6492	-0.1335	0.3665	2.38
H33A	0.3134	0.0381	0.3058	2.63
H33B	0.3367	0.1457	0.3410	2.63
H33C	0.3617	0.0189	0.3927	2.63
H35	0.9357	0.5667	0.4193	1.75
H36A	0.5654	0.2850	0.0445	2.92
H36B	0.4146	0.2541	0.0899	2.92
H36C	0.4757	0.2069	0.0112	2.92
H38A	0.9477	0.1257	0.6196	2.65
H38B	0.9779	0.2550	0.5789	2.65
H38C	1.0814	0.1519	0.5545	2.65
H39A	1.2664	0.2182	-0.1513	2.42
H39B	1.3393	0.3058	-0.1164	2.42

Table S2-2. Atomic coordinates and B_{iso} involving hydrogens/B_{eq} (continued)

atom	x	y	z	B_{eq}
H39C	1.2432	0.3527	-0.1861	2.42
H40A	0.7653	0.1249	0.0453	2.85
H40B	0.6715	0.0429	0.0185	2.85
H40C	0.7417	0.0004	0.0992	2.85
H41A	0.4578	0.1764	0.4655	2.74
H41B	0.4880	0.2993	0.4109	2.74
H41C	0.4860	0.2777	0.5058	2.74
H42	0.7074	0.2283	0.5587	2.03
H43A	0.5008	-0.0434	0.1727	3.11
H43B	0.4280	0.0067	0.0936	3.11
H43C	0.3773	0.0563	0.1725	3.11
H44A	1.2324	0.6786	0.1556	4.37
H44B	1.1490	0.6597	0.2440	4.37

Table S2-3. Anisotropic displacement parameters

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Ti1	0.0109(2)	0.0139(2)	0.0120(2)	-0.00050(13)	-0.00195(13)	-0.00068(13)
Cl1	0.0606(6)	0.0329(4)	0.0779(7)	0.0065(4)	-0.0243(5)	-0.0121(4)
Cl3	0.0428(5)	0.0404(5)	0.0783(7)	-0.0112(4)	-0.0137(5)	0.0033(4)
Al1	0.0144(3)	0.0164(4)	0.0199(4)	-0.0032(3)	-0.0043(3)	0.0008(3)
O1	0.0193(8)	0.0189(8)	0.0174(8)	-0.0043(6)	-0.0078(6)	-0.0023(6)
O2	0.0129(7)	0.0177(8)	0.0135(7)	-0.0016(6)	-0.0037(6)	-0.0006(6)
O3	0.0139(7)	0.0160(7)	0.0167(7)	0.0001(6)	-0.0040(6)	-0.0033(6)
O4	0.0140(7)	0.0187(8)	0.0133(7)	0.0012(6)	-0.0022(6)	-0.0012(6)
N1	0.0148(9)	0.0119(8)	0.0113(8)	-0.0012(7)	-0.0023(7)	-0.0021(7)
C10	0.0150(10)	0.0142(10)	0.0115(9)	-0.0021(8)	-0.0026(8)	0.0000(8)
C11	0.0184(11)	0.0142(10)	0.0182(10)	-0.0021(8)	-0.0058(9)	0.0007(8)
C12	0.0153(10)	0.0107(9)	0.0131(9)	-0.0019(8)	-0.0005(8)	0.0001(8)
C13	0.0133(10)	0.0247(12)	0.0238(11)	0.0044(9)	-0.0033(9)	-0.0041(9)
C14	0.0186(11)	0.0204(11)	0.0149(10)	-0.0024(9)	0.0004(8)	-0.0060(9)
C15	0.0187(11)	0.0155(10)	0.0149(10)	-0.0012(8)	-0.0005(8)	-0.0021(8)
C16	0.0175(10)	0.0120(9)	0.0129(9)	-0.0029(8)	-0.0022(8)	0.0002(8)
C17	0.0190(11)	0.0142(10)	0.0150(10)	-0.0020(8)	-0.0047(8)	-0.0024(8)
C18	0.0193(11)	0.0185(11)	0.0160(10)	-0.0056(9)	-0.0021(8)	-0.0028(8)
C19	0.0214(11)	0.0180(11)	0.0132(10)	-0.0042(9)	-0.0023(8)	-0.0008(8)
C20	0.0154(10)	0.0131(10)	0.0134(9)	0.0010(8)	-0.0024(8)	-0.0028(8)
C21	0.0141(10)	0.0157(10)	0.0160(10)	-0.0021(8)	-0.0010(8)	-0.0019(8)
C22	0.0295(12)	0.0147(10)	0.0153(10)	-0.0015(9)	-0.0082(9)	0.0010(8)
C23	0.0210(11)	0.0190(11)	0.0166(10)	0.0002(9)	-0.0046(9)	0.0008(8)
C24	0.0181(11)	0.0168(10)	0.0158(10)	0.0002(8)	-0.0029(8)	-0.0046(8)
C25	0.0160(10)	0.0148(10)	0.0131(9)	-0.0005(8)	-0.0034(8)	-0.0038(8)
C26	0.0166(10)	0.0137(10)	0.0121(9)	-0.0021(8)	-0.0041(8)	0.0012(8)
C27	0.0254(12)	0.0247(12)	0.0194(11)	-0.0061(10)	-0.0102(9)	-0.0045(9)
C28	0.0199(11)	0.0240(12)	0.0223(11)	0.0042(9)	-0.0004(9)	-0.0086(9)
C29	0.0143(10)	0.0141(10)	0.0136(10)	0.0006(8)	-0.0038(8)	-0.0001(8)
C30	0.0131(10)	0.0161(10)	0.0141(10)	-0.0027(8)	-0.0007(8)	-0.0028(8)
C31	0.0215(12)	0.0319(13)	0.0238(12)	-0.0055(10)	-0.0049(10)	-0.0111(10)
C32	0.0250(12)	0.0194(11)	0.0316(13)	-0.0026(10)	-0.0102(10)	-0.0019(10)
C33	0.0171(11)	0.0260(13)	0.037(2)	-0.0058(10)	-0.0021(10)	0.0019(11)
C34	0.0154(10)	0.0149(10)	0.0125(9)	-0.0026(8)	-0.0021(8)	-0.0027(8)
C35	0.0227(11)	0.0179(11)	0.0162(10)	-0.0034(9)	-0.0006(9)	-0.0069(8)
C36	0.038(2)	0.030(2)	0.0277(13)	-0.0043(12)	-0.0199(12)	-0.0016(11)
C37	0.0204(11)	0.0186(11)	0.0142(10)	-0.0011(9)	0.0008(8)	-0.0010(8)

Table S2-3. Anisotropic displacement parameters (continued)

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
C38	0.042(2)	0.0244(13)	0.0211(12)	0.0012(11)	-0.0150(11)	-0.0060(10)
C39	0.0255(12)	0.0283(13)	0.0187(11)	0.0013(10)	0.0048(10)	-0.0030(10)
C40	0.031(2)	0.037(2)	0.0276(13)	-0.0050(12)	-0.0088(11)	-0.0149(11)
C41	0.0214(12)	0.039(2)	0.0226(12)	0.0049(11)	0.0035(10)	-0.0066(11)
C42	0.0308(13)	0.0185(11)	0.0127(10)	0.0003(9)	-0.0000(9)	-0.0020(8)
C43	0.034(2)	0.037(2)	0.033(2)	-0.0168(12)	-0.0135(12)	-0.0063(12)
C44	0.056(2)	0.023(2)	0.063(3)	-0.007(2)	-0.022(2)	-0.006(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 S2-4. Fragment Analysis

fragment: 1

Ti(1)	Al(1)	O(1)	O(2)	O(3)
O(4)	N(1)	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)
C(38)	C(39)	C(40)	C(41)	C(42)
C(43)				

fragment: 2

Cl(1)	Cl(3)	C(44)

Table S2-5. Bond lengths (Å)

atom	atom	distance	atom	atom	distance
Ti1	Al1	3.0705(12)	Ti1	O1	2.103(2)
Ti1	O2	2.0446(15)	Ti1	O3	1.8419(19)
Ti1	O4	1.8242(16)	Ti1	N1	2.477(2)
Ti1	C13	2.119(3)	Cl1	C44	1.750(4)
Cl3	C44	1.767(5)	Al1	O1	1.8398(17)
Al1	O2	1.842(2)	Al1	C32	1.968(3)
Al1	C33	1.971(3)	O1	C27	1.472(4)
O2	C26	1.396(3)	O3	C10	1.349(3)
O4	C34	1.355(3)	N1	C20	1.499(3)
N1	C29	1.496(3)	N1	C30	1.495(3)
C10	C12	1.403(3)	C10	C15	1.409(4)
C11	C16	1.391(4)	C11	C22	1.397(4)
C12	C21	1.397(4)	C12	C30	1.508(4)
C14	C19	1.399(3)	C14	C24	1.397(3)
C14	C39	1.516(4)	C15	C28	1.513(4)
C15	C35	1.394(4)	C16	C26	1.399(3)
C16	C29	1.514(3)	C17	C19	1.398(3)
C17	C23	1.507(3)	C17	C34	1.407(3)
C18	C21	1.398(4)	C18	C31	1.517(4)
C18	C35	1.401(4)	C20	C25	1.516(3)
C22	C38	1.507(4)	C22	C42	1.396(4)
C24	C25	1.402(3)	C25	C34	1.404(3)
C26	C37	1.399(3)	C27	C36	1.527(4)
C27	C40	1.526(4)	C27	C43	1.530(4)
C37	C41	1.513(4)	C37	C42	1.397(4)

Table S2-6. Bond lengths involving hydrogens (Å)

atom	atom	distance	atom	atom	distance
C11	H11	0.930	C13	H13A	0.960
C13	H13B	0.960	C13	H13C	0.960
C19	H19	0.930	C20	H20A	0.970
C20	H20B	0.970	C21	H21	0.930
C23	H23A	0.960	C23	H23B	0.960
C23	H23C	0.960	C24	H24	0.930
C28	H28A	0.960	C28	H28B	0.960
C28	H28C	0.960	C29	H29A	0.970
C29	H29B	0.970	C30	H30A	0.970
C30	H30B	0.970	C31	H31A	0.960
C31	H31B	0.960	C31	H31C	0.960
C32	H32A	0.960	C32	H32B	0.960
C32	H32C	0.960	C33	H33A	0.960
C33	H33B	0.960	C33	H33C	0.960
C35	H35	0.930	C36	H36A	0.960
C36	H36B	0.960	C36	H36C	0.960
C38	H38A	0.960	C38	H38B	0.960
C38	H38C	0.960	C39	H39A	0.960
C39	H39B	0.960	C39	H39C	0.960
C40	H40A	0.960	C40	H40B	0.960
C40	H40C	0.960	C41	H41A	0.960
C41	H41B	0.960	C41	H41C	0.960
C42	H42	0.930	C43	H43A	0.960
C43	H43B	0.960	C43	H43C	0.960
C44	H44A	0.970	C44	H44B	0.970

Table S2-7. Bond angles (°)

atom	atom	atom	angle	atom	atom	atom	angle
Al1	Ti1	O1	35.87(5)	Al1	Ti1	O2	35.55(6)
Al1	Ti1	O3	126.87(6)	Al1	Ti1	O4	126.87(6)
Al1	Ti1	N1	91.65(5)	Al1	Ti1	C13	94.80(7)
O1	Ti1	O2	71.20(7)	O1	Ti1	O3	162.72(6)
O1	Ti1	O4	92.93(7)	O1	Ti1	N1	97.35(7)
O1	Ti1	C13	92.27(9)	O2	Ti1	O3	91.53(8)
O2	Ti1	O4	152.87(7)	O2	Ti1	N1	80.61(6)
O2	Ti1	C13	100.40(8)	O3	Ti1	O4	103.24(8)
O3	Ti1	N1	79.83(7)	O3	Ti1	C13	90.28(10)
O4	Ti1	N1	79.80(7)	O4	Ti1	C13	102.13(8)
N1	Ti1	C13	170.09(9)	Ti1	Al1	O1	42.05(6)
Ti1	Al1	O2	40.19(5)	Ti1	Al1	C32	126.64(9)
Ti1	Al1	C33	117.61(9)	O1	Al1	O2	81.97(8)
O1	Al1	C32	115.09(10)	O1	Al1	C33	116.20(10)
O2	Al1	C32	113.46(11)	O2	Al1	C33	110.12(11)
C32	Al1	C33	115.37(11)	Ti1	O1	Al1	102.08(9)
Ti1	O1	C27	133.34(13)	Al1	O1	C27	124.17(15)
Ti1	O2	Al1	104.25(9)	Ti1	O2	C26	121.82(13)
Al1	O2	C26	130.50(13)	Ti1	O3	C10	147.22(14)
Ti1	O4	C34	146.69(14)	Ti1	N1	C20	108.11(13)
Ti1	N1	C29	113.07(12)	Ti1	N1	C30	110.60(12)
C20	N1	C29	106.84(16)	C20	N1	C30	106.84(15)
C29	N1	C30	111.07(17)	O3	C10	C12	119.4(2)
O3	C10	C15	119.93(19)	C12	C10	C15	120.7(3)
C16	C11	C22	121.2(2)	C10	C12	C21	119.4(2)
C10	C12	C30	120.5(2)	C21	C12	C30	119.95(19)
C19	C14	C24	118.1(2)	C19	C14	C39	120.17(19)
C24	C14	C39	121.8(2)	C10	C15	C28	120.2(3)
C10	C15	C35	118.1(2)	C28	C15	C35	121.7(3)
C11	C16	C26	118.6(2)	C11	C16	C29	121.73(19)
C26	C16	C29	119.6(2)	C19	C17	C23	122.22(18)
C19	C17	C34	118.18(19)	C23	C17	C34	119.60(19)
C21	C18	C31	120.3(2)	C21	C18	C35	118.0(3)
C31	C18	C35	121.7(3)	C14	C19	C17	122.25(19)
N1	C20	C25	114.42(17)	C12	C21	C18	121.3(2)
C11	C22	C38	120.5(3)	C11	C22	C42	118.5(3)
C38	C22	C42	121.0(2)	C14	C24	C25	121.8(2)

Table S2-7. Bond angles (°) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
C20	C25	C24	120.11(18)	C20	C25	C34	121.34(17)
C24	C25	C34	118.54(18)	O2	C26	C16	117.97(18)
O2	C26	C37	119.86(19)	C16	C26	C37	122.1(3)
O1	C27	C36	109.9(2)	O1	C27	C40	108.8(2)
O1	C27	C43	108.28(19)	C36	C27	C40	110.8(2)
C36	C27	C43	109.3(3)	C40	C27	C43	109.7(3)
N1	C29	C16	113.91(17)	N1	C30	C12	116.37(16)
O4	C34	C17	118.71(18)	O4	C34	C25	120.11(17)
C17	C34	C25	121.18(18)	C15	C35	C18	122.5(3)
C26	C37	C41	121.4(3)	C26	C37	C42	117.3(2)
C41	C37	C42	121.3(3)	C22	C42	C37	122.3(3)
Cl1	C44	Cl3	112.2(2)				

Table S2-8. Bond angles involving hydrogens (^{o})

atom	atom	atom	angle	atom	atom	atom	angle
C16	C11	H11	119.4	C22	C11	H11	119.4
Ti1	C13	H13A	109.5	Ti1	C13	H13B	109.5
Ti1	C13	H13C	109.5	H13A	C13	H13B	109.5
H13A	C13	H13C	109.5	H13B	C13	H13C	109.5
C14	C19	H19	118.9	C17	C19	H19	118.9
N1	C20	H20A	108.7	N1	C20	H20B	108.7
C25	C20	H20A	108.6	C25	C20	H20B	108.7
H20A	C20	H20B	107.6	C12	C21	H21	119.3
C18	C21	H21	119.3	C17	C23	H23A	109.5
C17	C23	H23B	109.5	C17	C23	H23C	109.5
H23A	C23	H23B	109.5	H23A	C23	H23C	109.5
H23B	C23	H23C	109.5	C14	C24	H24	119.1
C25	C24	H24	119.1	C15	C28	H28A	109.5
C15	C28	H28B	109.5	C15	C28	H28C	109.5
H28A	C28	H28B	109.5	H28A	C28	H28C	109.5
H28B	C28	H28C	109.5	N1	C29	H29A	108.8
N1	C29	H29B	108.8	C16	C29	H29A	108.8
C16	C29	H29B	108.8	H29A	C29	H29B	107.7
N1	C30	H30A	108.2	N1	C30	H30B	108.2
C12	C30	H30A	108.2	C12	C30	H30B	108.2
H30A	C30	H30B	107.4	C18	C31	H31A	109.5
C18	C31	H31B	109.5	C18	C31	H31C	109.5
H31A	C31	H31B	109.5	H31A	C31	H31C	109.5
H31B	C31	H31C	109.5	Al1	C32	H32A	109.5
Al1	C32	H32B	109.5	Al1	C32	H32C	109.5
H32A	C32	H32B	109.5	H32A	C32	H32C	109.5
H32B	C32	H32C	109.5	Al1	C33	H33A	109.5
Al1	C33	H33B	109.5	Al1	C33	H33C	109.5
H33A	C33	H33B	109.5	H33A	C33	H33C	109.5
H33B	C33	H33C	109.5	C15	C35	H35	118.7
C18	C35	H35	118.7	C27	C36	H36A	109.5
C27	C36	H36B	109.5	C27	C36	H36C	109.5
H36A	C36	H36B	109.5	H36A	C36	H36C	109.5
H36B	C36	H36C	109.5	C22	C38	H38A	109.5
C22	C38	H38B	109.5	C22	C38	H38C	109.5
H38A	C38	H38B	109.5	H38A	C38	H38C	109.5
H38B	C38	H38C	109.5	C14	C39	H39A	109.5

Table S2-8. Bond angles involving hydrogens (°) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
C14	C39	H39B	109.5	C14	C39	H39C	109.5
H39A	C39	H39B	109.5	H39A	C39	H39C	109.5
H39B	C39	H39C	109.5	C27	C40	H40A	109.5
C27	C40	H40B	109.5	C27	C40	H40C	109.5
H40A	C40	H40B	109.5	H40A	C40	H40C	109.5
H40B	C40	H40C	109.5	C37	C41	H41A	109.5
C37	C41	H41B	109.5	C37	C41	H41C	109.5
H41A	C41	H41B	109.5	H41A	C41	H41C	109.5
H41B	C41	H41C	109.5	C22	C42	H42	118.8
C37	C42	H42	118.8	C27	C43	H43A	109.5
C27	C43	H43B	109.5	C27	C43	H43C	109.5
H43A	C43	H43B	109.5	H43A	C43	H43C	109.5
H43B	C43	H43C	109.5	Cl1	C44	H44A	109.2
Cl1	C44	H44B	109.2	Cl3	C44	H44A	109.2
Cl3	C44	H44B	109.2	H44A	C44	H44B	107.9

Table S2-9. Torsion Angles(O)

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

atom1	atom2	atom3	atom4	angle	atom1	atom2	atom3	atom4	angle
Al1	Ti1	O1	Al1	0.00(2)	Al1	Ti1	O1	C27	172.63(19)
O1	Ti1	Al1	O1	0.00(8)	O1	Ti1	Al1	O2	171.57(8)
O1	Ti1	Al1	C32	87.97(9)	O1	Ti1	Al1	C33	-99.43(9)
Al1	Ti1	O2	Al1	-0.00(3)	Al1	Ti1	O2	C26	161.12(16)
O2	Ti1	Al1	O1	-171.57(8)	O2	Ti1	Al1	O2	-0.00(8)
O2	Ti1	Al1	C32	-83.60(9)	O2	Ti1	Al1	C33	88.99(9)
Al1	Ti1	O3	C10	73.26(19)	O3	Ti1	Al1	O1	-178.80(7)
O3	Ti1	Al1	O2	-7.23(7)	O3	Ti1	Al1	C32	-90.83(8)
O3	Ti1	Al1	C33	81.76(7)	Al1	Ti1	O4	C34	-76.5(3)
O4	Ti1	Al1	O1	-21.83(7)	O4	Ti1	Al1	O2	149.74(7)
O4	Ti1	Al1	C32	66.14(8)	O4	Ti1	Al1	C33	-121.26(7)
Al1	Ti1	N1	C20	85.99(9)	Al1	Ti1	N1	C29	-32.08(11)
Al1	Ti1	N1	C30	-157.37(9)	N1	Ti1	Al1	O1	-100.30(5)
N1	Ti1	Al1	O2	71.28(5)	N1	Ti1	Al1	C32	-12.33(6)
N1	Ti1	Al1	C33	160.27(6)	C13	Ti1	Al1	O1	87.24(8)
C13	Ti1	Al1	O2	-101.19(8)	C13	Ti1	Al1	C32	175.21(9)
C13	Ti1	Al1	C33	-12.20(9)	O1	Ti1	O2	Al1	-5.21(7)
O1	Ti1	O2	C26	155.91(12)	O2	Ti1	O1	Al1	5.17(7)
O2	Ti1	O1	C27	177.80(15)	O1	Ti1	O4	C34	-89.1(3)
O4	Ti1	O1	Al1	162.67(8)	O4	Ti1	O1	C27	-24.70(14)
O1	Ti1	N1	C20	50.45(10)	O1	Ti1	N1	C29	-67.62(12)
O1	Ti1	N1	C30	167.10(9)	N1	Ti1	O1	Al1	82.59(8)
N1	Ti1	O1	C27	-104.78(13)	C13	Ti1	O1	Al1	-95.05(9)
C13	Ti1	O1	C27	77.58(14)	O2	Ti1	O3	C10	69.06(18)
O3	Ti1	O2	Al1	174.22(8)	O3	Ti1	O2	C26	-24.66(11)
O2	Ti1	O4	C34	-36.6(4)	O4	Ti1	O2	Al1	-62.11(19)
O4	Ti1	O2	C26	99.01(19)	O2	Ti1	N1	C20	119.92(10)
O2	Ti1	N1	C29	1.84(11)	O2	Ti1	N1	C30	-123.44(11)
N1	Ti1	O2	Al1	-106.35(8)	N1	Ti1	O2	C26	54.77(11)
C13	Ti1	O2	Al1	83.66(11)	C13	Ti1	O2	C26	-115.23(13)
O3	Ti1	O4	C34	84.7(3)	O4	Ti1	O3	C10	-87.99(18)
O3	Ti1	N1	C20	-146.80(10)	O3	Ti1	N1	C29	95.12(12)
O3	Ti1	N1	C30	-30.16(9)	N1	Ti1	O3	C10	-11.12(17)
C13	Ti1	O3	C10	169.47(19)	O4	Ti1	N1	C20	-41.22(10)
O4	Ti1	N1	C29	-159.29(13)	O4	Ti1	N1	C30	75.43(10)
N1	Ti1	O4	C34	7.8(2)	C13	Ti1	O4	C34	177.9(3)
Ti1	Al1	O1	Ti1	-0.0	Ti1	Al1	O1	C27	-173.52(16)

Table S2-9. Torsion angles (°) (continued)

atom1	atom2	atom3	atom4	angle	atom1	atom2	atom3	atom4	angle
Ti1	Al1	O2	Ti1	-0.000(11)	Ti1	Al1	O2	C26	-158.80(17)
O1	Al1	O2	Ti1	5.69(8)	O1	Al1	O2	C26	-153.11(14)
O2	Al1	O1	Ti1	-5.48(7)	O2	Al1	O1	C27	-179.01(12)
C32	Al1	O1	Ti1	-117.69(12)	C32	Al1	O1	C27	68.79(16)
C33	Al1	O1	Ti1	103.05(13)	C33	Al1	O1	C27	-70.48(16)
C32	Al1	O2	Ti1	119.62(10)	C32	Al1	O2	C26	-39.18(16)
C33	Al1	O2	Ti1	-109.34(10)	C33	Al1	O2	C26	91.86(15)
Ti1	O1	C27	C36	-38.0(3)	Ti1	O1	C27	C40	83.5(2)
Ti1	O1	C27	C43	-157.29(11)	Al1	O1	C27	C36	133.33(13)
Al1	O1	C27	C40	-105.19(16)	Al1	O1	C27	C43	14.0(3)
Ti1	O2	C26	C16	-65.7(2)	Ti1	O2	C26	C37	111.73(16)
Al1	O2	C26	C16	89.9(2)	Al1	O2	C26	C37	-92.6(2)
Ti1	O3	C10	C12	26.5(4)	Ti1	O3	C10	C15	-153.98(16)
Ti1	O4	C34	C17	-167.86(18)	Ti1	O4	C34	C25	11.5(4)
Ti1	N1	C20	C25	63.51(17)	Ti1	N1	C29	C16	-50.4(2)
Ti1	N1	C30	C12	58.64(17)	C20	N1	C29	C16	-169.25(16)
C29	N1	C20	C25	-174.50(15)	C20	N1	C30	C12	176.07(14)
C30	N1	C20	C25	-55.5(2)	C29	N1	C30	C12	-67.8(2)
C30	N1	C29	C16	74.6(2)	O3	C10	C12	C21	179.11(14)
O3	C10	C12	C30	4.6(3)	O3	C10	C15	C28	2.7(3)
O3	C10	C15	C35	-178.30(15)	C12	C10	C15	C28	-177.76(15)
C12	C10	C15	C35	1.3(3)	C15	C10	C12	C21	-0.5(3)
C15	C10	C12	C30	-174.94(15)	C16	C11	C22	C38	-178.10(17)
C16	C11	C22	C42	0.5(3)	C22	C11	C16	C26	-1.2(3)
C22	C11	C16	C29	179.35(17)	C10	C12	C21	C18	-0.3(3)
C10	C12	C30	N1	-48.6(3)	C21	C12	C30	N1	136.97(18)
C30	C12	C21	C18	174.22(15)	C19	C14	C24	C25	-0.4(4)
C24	C14	C19	C17	0.8(4)	C39	C14	C19	C17	-178.7(3)
C39	C14	C24	C25	179.1(3)	C10	C15	C35	C18	-1.4(3)
C28	C15	C35	C18	177.63(17)	C11	C16	C26	O2	178.49(17)
C11	C16	C26	C37	1.1(3)	C11	C16	C29	N1	-118.8(2)
C26	C16	C29	N1	61.7(3)	C29	C16	C26	O2	-2.0(3)
C29	C16	C26	C37	-179.40(16)	C23	C17	C19	C14	179.3(2)
C19	C17	C34	O4	179.0(2)	C19	C17	C34	C25	-0.4(4)
C34	C17	C19	C14	-0.4(4)	C23	C17	C34	O4	-0.8(4)
C23	C17	C34	C25	179.9(2)	C31	C18	C21	C12	179.28(17)
C21	C18	C35	C15	0.7(3)	C35	C18	C21	C12	0.2(3)

Table S2-9. Torsion angles (°) (continued)

atom1	atom2	atom3	atom4	angle	atom1	atom2	atom3	atom4	angle
C31	C18	C35	C15	-178.41(17)	N1	C20	C25	C24	135.22(19)
N1	C20	C25	C34	-45.9(3)	C11	C22	C42	C37	0.2(4)
C38	C22	C42	C37	178.85(19)	C14	C24	C25	C20	178.6(2)
C14	C24	C25	C34	-0.3(4)	C20	C25	C34	O4	2.5(4)
C20	C25	C34	C17	-178.16(19)	C24	C25	C34	O4	-178.6(2)
C24	C25	C34	C17	0.7(4)	O2	C26	C37	C41	1.0(3)
O2	C26	C37	C42	-177.72(16)	C16	C26	C37	C41	178.33(17)
C16	C26	C37	C42	-0.4(3)	C26	C37	C42	C22	-0.3(4)
C41	C37	C42	C22	-179.0(2)					

Table S2-10. Intramolecular contacts less than 3.60 Å

atom	atom	distance	atom	atom	distance
Ti1	C16	3.547(3)	Ti1	C25	3.597(3)
Ti1	C36	3.568(4)	Al1	C43	3.008(4)
O1	C20	3.594(3)	O2	C10	3.582(3)
O2	C29	2.804(3)	O2	C41	2.885(4)
O3	C16	3.352(3)	O3	C26	2.972(3)
O3	C28	2.846(4)	O3	C30	2.833(3)
O3	C37	3.599(3)	O4	C20	2.876(3)
O4	C23	2.805(3)	O4	C27	3.347(4)
O4	C30	3.331(3)	O4	C36	3.245(4)
O4	C40	3.493(4)	N1	C10	3.070(3)
N1	C26	3.112(3)	N1	C34	3.040(3)
C10	C16	3.217(3)	C10	C18	2.811(4)
C10	C26	3.227(3)	C11	C12	3.315(3)
C11	C21	3.512(3)	C11	C37	2.810(4)
C12	C16	3.031(3)	C12	C29	3.106(4)
C12	C35	2.782(4)	C13	C36	3.463(5)
C14	C34	2.810(3)	C15	C21	2.808(4)
C16	C30	3.137(3)	C16	C42	2.783(4)
C17	C24	2.803(3)	C19	C25	2.795(3)
C20	C40	3.552(4)	C22	C26	2.785(4)
C25	C30	2.875(4)	C30	C34	3.329(4)
C33	C43	3.463(5)			

Table S2-11. Intramolecular contacts less than 3.60 Å involving hydrogens

atom	atom	distance	atom	atom	distance
Ti1	H20A	3.279	Ti1	H29B	3.521
Ti1	H30A	3.381	Ti1	H36A	3.172
Al1	H29B	3.202	Al1	H40C	3.568
Al1	H41A	3.534	Al1	H43A	2.737
Al1	H43C	2.908	O1	H13A	2.903
O1	H13C	3.371	O1	H20A	3.014
O1	H29B	3.494	O1	H32A	3.391
O1	H32B	3.392	O1	H33A	3.417
O1	H33B	3.417	O1	H36A	2.629
O1	H36B	2.660	O1	H36C	3.279
O1	H40A	2.648	O1	H40B	3.265
O1	H40C	2.598	O1	H43A	2.626
O1	H43B	3.263	O1	H43C	2.609
O2	H13C	3.039	O2	H29B	2.751
O2	H32A	3.196	O2	H32C	3.563
O2	H33B	3.110	O2	H33C	3.509
O2	H41A	2.984	O2	H41B	2.705
O3	H13B	2.790	O3	H13C	3.069
O3	H28A	3.485	O3	H28B	3.494
O3	H28C	2.386	O3	H30A	2.970
O3	H41B	3.534	O4	H13A	3.217
O4	H13B	3.217	O4	H20A	3.034
O4	H23B	3.007	O4	H23C	2.533
O4	H30A	2.914	O4	H36A	2.479
O4	H40A	2.815	C10	H21	3.254
C10	H28A	3.145	C10	H28B	3.136
C10	H28C	2.561	C10	H30A	2.835
C10	H30B	3.297	C10	H35	3.242
C11	H29A	2.572	C11	H29B	3.141
C11	H38A	3.137	C11	H38B	3.121
C11	H38C	2.554	C11	H42	3.237
C12	H11	3.456	C12	H29A	3.259
C13	H28C	3.397	C13	H36A	3.193
C13	H36B	3.028	C13	H41B	3.405
C16	H30B	3.416	C16	H32A	3.444
C17	H36A	3.516	C17	H40A	3.499
C19	H23A	2.615	C19	H23B	3.026

Table S2-11. Intramolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
C19	H23C	3.241	C19	H24	3.238
C19	H39A	3.139	C19	H39B	3.130
C19	H39C	2.558	C20	H24	2.662
C20	H29A	2.645	C20	H29B	2.482
C20	H30A	2.518	C20	H30B	2.578
C20	H40A	2.954	C20	H40C	3.340
C21	H11	3.402	C21	H30A	3.005
C21	H30B	2.540	C21	H31A	2.841
C21	H31B	3.298	C21	H31C	2.696
C21	H35	3.237	C23	H19	2.690
C23	H36A	3.308	C24	H19	3.236
C24	H20A	3.037	C24	H20B	2.559
C24	H30A	3.216	C24	H39A	2.786
C24	H39B	2.789	C24	H39C	3.316
C24	H40A	3.597	C25	H30A	2.427
C25	H30B	3.150	C25	H40A	2.761
C26	H11	3.240	C26	H29A	3.301
C26	H29B	2.746	C26	H32A	3.545
C26	H41A	2.852	C26	H41B	2.716
C26	H41C	3.306	C26	H42	3.228
C27	H13A	3.366	C27	H20A	3.484
C28	H35	2.679	C28	H41B	3.528
C29	H11	2.688	C29	H20A	2.601
C29	H20B	2.517	C29	H30A	3.284
C29	H30B	2.598	C29	H32A	2.944
C30	H20A	3.248	C30	H20B	2.618
C30	H21	2.654	C30	H29A	2.557
C30	H29B	3.279	C31	H21	2.666
C31	H35	2.688	C32	H29B	2.810
C32	H33C	3.372	C32	H40C	3.494
C32	H43A	2.986	C33	H32C	3.369
C33	H41A	3.008	C33	H41B	3.598
C33	H43A	3.368	C33	H43C	2.831
C34	H19	3.245	C34	H20A	2.877
C34	H20B	3.313	C34	H23A	3.278
C34	H23B	2.886	C34	H23C	2.637
C34	H24	3.251	C34	H30A	2.694

Table S2-11. Intramolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
C34	H36A	3.150	C34	H40A	2.700
C35	H21	3.241	C35	H28A	2.783
C35	H28B	2.781	C35	H28C	3.310
C35	H31A	3.080	C35	H31B	2.601
C35	H31C	3.215	C36	H13A	2.725
C36	H23C	3.391	C36	H40A	2.678
C36	H40B	2.715	C36	H40C	3.338
C36	H43A	3.324	C36	H43B	2.665
C36	H43C	2.678	C38	H11	2.664
C38	H42	2.664	C39	H19	2.657
C39	H24	2.691	C40	H20A	2.753
C40	H36A	2.714	C40	H36B	3.338
C40	H36C	2.679	C40	H43A	2.660
C40	H43B	2.698	C40	H43C	3.328
C41	H13C	3.514	C41	H28B	3.591
C41	H33B	3.241	C41	H33C	3.597
C41	H42	2.674	C42	H11	3.240
C42	H38A	2.765	C42	H38B	2.767
C42	H38C	3.302	C42	H41A	3.085
C42	H41B	3.192	C42	H41C	2.582
C43	H32B	3.303	C43	H33A	2.960
C43	H36A	3.324	C43	H36B	2.646
C43	H36C	2.697	C43	H40A	3.329
C43	H40B	2.665	C43	H40C	2.691
H11	H21	3.415	H11	H29A	2.371
H11	H29B	3.330	H11	H30B	3.582
H11	H38A	3.316	H11	H38B	3.304
H11	H38C	2.346	H13A	H33B	3.592
H13A	H36A	2.582	H13A	H36B	2.159
H13A	H36C	3.566	H13B	H28C	3.070
H13B	H36A	3.590	H13C	H28C	3.148
H13C	H33B	2.984	H13C	H36B	3.539
H13C	H41B	2.609	H19	H23A	2.437
H19	H23B	3.143	H19	H23C	3.481
H19	H39A	3.306	H19	H39B	3.301
H19	H39C	2.337	H20A	H24	3.161
H20A	H29A	2.990	H20A	H29B	2.307

Table S2-11. Intramolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
H20A	H30A	3.405	H20A	H30B	3.471
H20A	H32A	3.266	H20A	H40A	2.333
H20A	H40B	3.582	H20A	H40C	2.413
H20B	H24	2.347	H20B	H29A	2.391
H20B	H29B	2.620	H20B	H30A	2.840
H20B	H30B	2.417	H21	H30A	3.145
H21	H30B	2.329	H21	H31A	2.838
H21	H31B	3.564	H21	H31C	2.587
H23C	H36A	2.466	H24	H30A	3.588
H24	H39A	2.733	H24	H39B	2.745
H24	H39C	3.596	H28A	H35	2.719
H28B	H35	2.735	H28B	H41B	3.287
H28B	H41C	3.371	H28C	H35	3.585
H28C	H41B	2.965	H29A	H30A	3.419
H29A	H30B	2.315	H29A	H32A	3.465
H29B	H30B	3.411	H29B	H32A	2.012
H29B	H32B	3.460	H29B	H32C	3.343
H31A	H35	3.223	H31A	H38B	3.521
H31B	H35	2.401	H31C	H35	3.427
H32A	H40C	3.408	H32A	H43A	3.581
H32B	H40C	3.115	H32B	H43A	2.426
H32C	H33C	3.136	H33A	H43A	2.929
H33A	H43C	2.217	H33B	H41A	2.661
H33B	H41B	2.973	H33B	H43C	3.213
H33C	H41A	2.751	H36A	H40A	2.527
H36A	H40B	3.027	H36A	H40C	3.572
H36A	H43B	3.554	H36A	H43C	3.540
H36B	H40A	3.563	H36B	H40B	3.573
H36B	H43A	3.531	H36B	H43B	2.896
H36B	H43C	2.473	H36C	H40A	2.919
H36C	H40B	2.529	H36C	H40C	3.564
H36C	H43A	3.563	H36C	H43B	2.514
H36C	H43C	2.992	H38A	H42	2.702
H38B	H42	2.714	H38C	H42	3.573
H40A	H43A	3.545	H40A	H43B	3.562
H40B	H43A	2.904	H40B	H43B	2.509
H40B	H43C	3.551	H40C	H43A	2.496

Table S2-11. Intramolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
H40C	H43B	2.999	H40C	H43C	3.552
H41A	H42	3.226	H41B	H42	3.401
H41C	H42	2.378			

Table S2-12. Intermolecular contacts less than 3.60 Å

atom	atom	distance	atom	atom	distance
Cl1	C20[1]	3.554(3)	C19	C44[2]	3.497(5)
C20	Cl1[3]	3.554(3)	C44	C19[2]	3.497(5)

Symmetry Operators:

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

Table S2-13. Intermolecular contacts less than 3.60 Å involving hydrogens

atom	atom	distance	atom	atom	distance
Cl1	H20A[1]	3.191	Cl1	H20B[1]	2.982
Cl1	H29B[1]	3.444	Cl1	H38A[2]	3.488
Cl3	H13B[3]	3.418	Cl3	H31C	3.022
Cl3	H32B[4]	3.480	Cl3	H39B[5]	3.324
Cl3	H42[2]	3.474	Cl3	H43A[4]	3.067
O3	H19[6]	3.144	O3	H39C[6]	2.951
C10	H19[6]	2.862	C10	H39C[6]	3.085
C11	H11[7]	3.462	C11	H38A[7]	3.432
C11	H38C[7]	3.480	C12	H19[6]	2.875
C12	H23A[6]	3.343	C13	H21[8]	3.001
C13	H23A[9]	3.218	C13	H31C[8]	3.593
C14	H23B[6]	2.934	C15	H19[6]	3.485
C15	H31B[2]	3.574	C15	H39C[6]	3.091
C16	H38A[7]	3.346	C16	H38C[7]	3.411
C17	H23B[6]	3.499	C17	H30A[6]	3.328
C17	H44A[6]	2.894	C18	H35[2]	3.510
C18	H38B[2]	3.574	C18	H44B	2.780
C19	H23B[6]	3.198	C19	H30A[6]	3.125
C19	H44A[6]	2.981	C19	H44B[6]	3.386
C21	H13C[3]	3.117	C21	H19[6]	3.487
C21	H23A[6]	3.408	C21	H33B[3]	3.355
C21	H44B	3.164	C22	H11[7]	3.393
C22	H31B[2]	3.551	C22	H33C[10]	3.543
C23	H13A[9]	3.135	C23	H30A[6]	2.872
C23	H36B[9]	3.311	C23	H44A[6]	2.959
C24	H23B[6]	2.982	C24	H36B[3]	3.482
C24	H36C[3]	3.433	C24	H40C[11]	3.525
C25	H23B[6]	3.303	C28	H31A[2]	3.382
C28	H39C[6]	3.045	C28	H41C[12]	3.469
C29	H33A[3]	3.476	C29	H38A[7]	2.959
C29	H38C[7]	3.576	C30	H19[6]	3.155
C30	H23A[6]	3.041	C30	H23B[6]	3.482
C31	H13C[3]	3.520	C31	H28B[2]	3.194
C31	H35[2]	3.000	C31	H38B[2]	3.364
C31	H41B[3]	3.259	C31	H44B	3.153
C32	H28A[13]	3.193	C32	H38C[7]	3.401
C32	H39A[11]	3.297	C33	H11[8]	3.167

Table S2-13. Intermolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
C33	H21[8]	3.546	C33	H29A[8]	3.196
C33	H30B[8]	3.537	C34	H23B[6]	3.528
C35	H31A[2]	3.301	C35	H31B[2]	3.121
C35	H35[2]	3.547	C35	H38B[2]	3.075
C35	H44B	3.092	C36	H23B[9]	3.542
C36	H24[8]	3.339	C36	H39B[8]	3.446
C37	H33C[10]	3.324	C38	H11[7]	3.543
C38	H29A[7]	3.423	C38	H29B[7]	3.333
C38	H31B[2]	3.365	C38	H32A[7]	3.315
C38	H35[2]	3.255	C39	H28A[6]	3.537
C39	H32B[11]	3.217	C39	H36C[3]	3.428
C39	H40C[11]	3.386	C40	H24[11]	3.336
C40	H39A[11]	3.356	C40	H43B[14]	3.405
C41	H31A[8]	3.165	C41	H32C[10]	3.185
C42	H31B[2]	3.300	C42	H33C[10]	3.010
C43	H20B[8]	3.595	C43	H40B[14]	3.408
C44	H19[6]	3.355	C44	H23A[6]	3.411
C44	H31C	3.404	H11	C11[7]	3.462
H11	C22[7]	3.393	H11	C33[3]	3.167
H11	C38[7]	3.543	H11	H11[7]	3.491
H11	H33A[3]	3.128	H11	H33B[3]	2.832
H11	H33C[3]	3.012	H11	H38A[7]	3.156
H11	H38C[7]	3.531	H13A	C23[9]	3.135
H13A	H21[8]	2.934	H13A	H23A[9]	2.547
H13A	H23B[9]	3.354	H13A	H23C[9]	3.042
H13A	H30B[8]	3.278	H13B	Cl3[8]	3.418
H13B	H21[8]	3.461	H13B	H23A[9]	3.200
H13B	H23C[9]	3.417	H13B	H31C[8]	3.515
H13B	H39B[6]	3.044	H13B	H39C[6]	3.283
H13B	H44A[8]	3.415	H13C	C21[8]	3.117
H13C	C31[8]	3.520	H13C	H21[8]	2.281
H13C	H23A[9]	3.459	H13C	H31C[8]	2.830
H19	O3[6]	3.144	H19	C10[6]	2.862
H19	C12[6]	2.875	H19	C15[6]	3.485
H19	C21[6]	3.487	H19	C30[6]	3.155
H19	C44[6]	3.355	H19	H30A[6]	2.532
H19	H44A[6]	2.959	H19	H44B[6]	3.001

Table S2-13. Intermolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
H20A	Cl1[13]	3.191	H20B	Cl1[13]	2.982
H20B	C43[3]	3.595	H20B	H43B[3]	3.439
H20B	H43C[3]	2.880	H21	C13[3]	3.001
H21	C33[3]	3.546	H21	H13A[3]	2.934
H21	H13B[3]	3.461	H21	H13C[3]	2.281
H21	H23A[6]	3.257	H21	H33B[3]	2.629
H21	H41B[3]	3.377	H21	H44B	3.501
H23A	C12[6]	3.343	H23A	C13[9]	3.218
H23A	C21[6]	3.408	H23A	C30[6]	3.041
H23A	C44[6]	3.411	H23A	H13A[9]	2.547
H23A	H13B[9]	3.200	H23A	H13C[9]	3.459
H23A	H21[6]	3.257	H23A	H30A[6]	2.430
H23A	H30B[6]	3.000	H23A	H36B[9]	3.136
H23A	H44A[6]	2.609	H23A	H44B[6]	3.365
H23B	C14[6]	2.934	H23B	C17[6]	3.499
H23B	C19[6]	3.198	H23B	C24[6]	2.982
H23B	C25[6]	3.303	H23B	C30[6]	3.482
H23B	C34[6]	3.528	H23B	C36[9]	3.542
H23B	H13A[9]	3.354	H23B	H24[6]	3.355
H23B	H30A[6]	2.656	H23B	H30B[6]	3.462
H23B	H36B[9]	2.889	H23B	H36C[9]	3.565
H23B	H39B[6]	3.253	H23C	H13A[9]	3.042
H23C	H13B[9]	3.417	H23C	H36B[9]	3.376
H23C	H44A[6]	2.944	H24	C36[3]	3.339
H24	C40[11]	3.336	H24	H23B[6]	3.355
H24	H36B[3]	3.030	H24	H36C[3]	2.807
H24	H40B[11]	2.812	H24	H40C[11]	3.016
H24	H43B[3]	3.065	H24	H43C[3]	3.385
H28A	C32[1]	3.193	H28A	C39[6]	3.537
H28A	H31A[2]	3.418	H28A	H32A[1]	3.469
H28A	H32B[1]	2.778	H28A	H32C[1]	2.864
H28A	H39A[6]	3.494	H28A	H39C[6]	2.777
H28A	H41C[12]	3.047	H28B	C31[2]	3.194
H28B	H31A[2]	2.712	H28B	H31B[2]	2.906
H28B	H31C[2]	3.513	H28B	H41C[12]	3.019
H28C	H31C[8]	3.159	H28C	H39C[6]	2.855
H29A	C33[3]	3.196	H29A	C38[7]	3.423

Table S2-13. Intermolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
H29A	H33A[3]	2.508	H29A	H33B[3]	3.138
H29A	H33C[3]	3.526	H29A	H38A[7]	2.574
H29A	H38C[7]	3.550	H29A	H43C[3]	3.473
H29B	Cl1[13]	3.444	H29B	C38[7]	3.333
H29B	H38A[7]	2.653	H29B	H38C[7]	3.159
H30A	C17[6]	3.328	H30A	C19[6]	3.125
H30A	C23[6]	2.872	H30A	H19[6]	2.532
H30A	H23A[6]	2.430	H30A	H23B[6]	2.656
H30B	C33[3]	3.537	H30B	H13A[3]	3.278
H30B	H23A[6]	3.000	H30B	H23B[6]	3.462
H30B	H33A[3]	3.135	H30B	H33B[3]	3.056
H30B	H36B[3]	3.136	H30B	H43C[3]	3.214
H31A	C28[2]	3.382	H31A	C35[2]	3.301
H31A	C41[3]	3.165	H31A	H28A[2]	3.418
H31A	H28B[2]	2.712	H31A	H35[2]	2.578
H31A	H41A[3]	3.373	H31A	H41B[3]	2.727
H31A	H41C[3]	2.910	H31B	C15[2]	3.574
H31B	C22[2]	3.551	H31B	C35[2]	3.121
H31B	C38[2]	3.365	H31B	C42[2]	3.300
H31B	H28B[2]	2.906	H31B	H35[2]	2.718
H31B	H38B[2]	2.555	H31B	H42[2]	2.896
H31B	H44B	3.247	H31C	Cl3	3.022
H31C	C13[3]	3.593	H31C	C44	3.404
H31C	H13B[3]	3.515	H31C	H13C[3]	2.830
H31C	H28B[2]	3.513	H31C	H28C[3]	3.159
H31C	H41B[3]	2.929	H31C	H42[2]	3.582
H31C	H44B	2.870	H32A	C38[7]	3.315
H32A	H28A[13]	3.469	H32A	H38A[7]	3.072
H32A	H38B[7]	3.482	H32A	H38C[7]	2.879
H32A	H39A[11]	3.362	H32B	Cl3[15]	3.480
H32B	C39[11]	3.217	H32B	H28A[13]	2.778
H32B	H39A[11]	2.459	H32B	H39C[11]	3.194
H32C	C41[10]	3.185	H32C	H28A[13]	2.864
H32C	H38C[7]	3.034	H32C	H41A[10]	2.828
H32C	H41C[10]	2.693	H33A	C29[8]	3.476
H33A	H11[8]	3.128	H33A	H29A[8]	2.508
H33A	H30B[8]	3.135	H33A	H38A[10]	3.255

Table S2-13. Intermolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
H33A	H42[10]	3.461	H33B	C21[8]	3.355
H33B	H11[8]	2.832	H33B	H21[8]	2.629
H33B	H29A[8]	3.138	H33B	H30B[8]	3.056
H33C	C22[10]	3.543	H33C	C37[10]	3.324
H33C	C42[10]	3.010	H33C	H11[8]	3.012
H33C	H29A[8]	3.526	H33C	H41A[10]	3.451
H33C	H42[10]	2.971	H35	C18[2]	3.510
H35	C31[2]	3.000	H35	C35[2]	3.547
H35	C38[2]	3.255	H35	H31A[2]	2.578
H35	H31B[2]	2.718	H35	H35[2]	3.177
H35	H38B[2]	2.355	H35	H38C[2]	3.432
H35	H44B	3.378	H36B	C23[9]	3.311
H36B	C24[8]	3.482	H36B	H23A[9]	3.136
H36B	H23B[9]	2.889	H36B	H23C[9]	3.376
H36B	H24[8]	3.030	H36B	H30B[8]	3.136
H36B	H39B[8]	3.577	H36C	C24[8]	3.433
H36C	C39[8]	3.428	H36C	H23B[9]	3.565
H36C	H24[8]	2.807	H36C	H39B[8]	2.662
H36C	H40B[14]	3.568	H36C	H43B[14]	3.368
H38A	Cl1[2]	3.488	H38A	C11[7]	3.432
H38A	C16[7]	3.346	H38A	C29[7]	2.959
H38A	H11[7]	3.156	H38A	H29A[7]	2.574
H38A	H29B[7]	2.653	H38A	H32A[7]	3.072
H38A	H33A[10]	3.255	H38B	C18[2]	3.574
H38B	C31[2]	3.364	H38B	C35[2]	3.075
H38B	H31B[2]	2.555	H38B	H32A[7]	3.482
H38B	H35[2]	2.355	H38B	H44B[2]	3.387
H38C	C11[7]	3.480	H38C	C16[7]	3.411
H38C	C29[7]	3.576	H38C	C32[7]	3.401
H38C	H11[7]	3.531	H38C	H29A[7]	3.550
H38C	H29B[7]	3.159	H38C	H32A[7]	2.879
H38C	H32C[7]	3.034	H38C	H35[2]	3.432
H39A	C32[11]	3.297	H39A	C40[11]	3.356
H39A	H28A[6]	3.494	H39A	H32A[11]	3.362
H39A	H32B[11]	2.459	H39A	H40B[11]	3.434
H39A	H40C[11]	2.540	H39A	H43A[11]	2.895
H39B	Cl3[5]	3.324	H39B	C36[3]	3.446

Table S2-13. Intermolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
H39B	H13B[6]	3.044	H39B	H23B[6]	3.253
H39B	H36B[3]	3.577	H39B	H36C[3]	2.662
H39B	H43A[11]	3.557	H39C	O3[6]	2.951
H39C	C10[6]	3.085	H39C	C15[6]	3.091
H39C	C28[6]	3.045	H39C	H13B[6]	3.283
H39C	H28A[6]	2.777	H39C	H28C[6]	2.855
H39C	H32B[11]	3.194	H40B	C43[14]	3.408
H40B	H24[11]	2.812	H40B	H36C[14]	3.568
H40B	H39A[11]	3.434	H40B	H43B[14]	2.451
H40C	C24[11]	3.525	H40C	C39[11]	3.386
H40C	H24[11]	3.016	H40C	H39A[11]	2.540
H41A	H31A[8]	3.373	H41A	H32C[10]	2.828
H41A	H33C[10]	3.451	H41B	C31[8]	3.259
H41B	H21[8]	3.377	H41B	H31A[8]	2.727
H41B	H31C[8]	2.929	H41C	C28[12]	3.469
H41C	H28A[12]	3.047	H41C	H28B[12]	3.019
H41C	H31A[8]	2.910	H41C	H32C[10]	2.693
H42	Cl3[2]	3.474	H42	H31B[2]	2.896
H42	H31C[2]	3.582	H42	H33A[10]	3.461
H42	H33C[10]	2.971	H43A	Cl3[15]	3.067
H43A	H39A[11]	2.895	H43A	H39B[11]	3.557
H43B	C40[14]	3.405	H43B	H20B[8]	3.439
H43B	H24[8]	3.065	H43B	H36C[14]	3.368
H43B	H40B[14]	2.451	H43B	H43B[14]	3.293
H43C	H20B[8]	2.880	H43C	H24[8]	3.385
H43C	H29A[8]	3.473	H43C	H30B[8]	3.214
H44A	C17[6]	2.894	H44A	C19[6]	2.981
H44A	C23[6]	2.959	H44A	H13B[3]	3.415
H44A	H19[6]	2.959	H44A	H23A[6]	2.609
H44A	H23C[6]	2.944	H44B	C18	2.780
H44B	C19[6]	3.386	H44B	C21	3.164
H44B	C31	3.153	H44B	C35	3.092
H44B	H19[6]	3.001	H44B	H21	3.501
H44B	H23A[6]	3.365	H44B	H31B	3.247
H44B	H31C	2.870	H44B	H35	3.378
H44B	H38B[2]	3.387			

Symmetry Operators:

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

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

X-ray Structure Report

for

[TiMe{(O-2,4-$Me_2C_6H_2$-6-CH_2)$_2$(μ_2-O-2,4-Me_2-C_6H_2-6-CH_2)}N][Me_2Al{μ_2-OCH(CF_3)$_2$}] (**3c**)

October 25, 2013

Experimental

Data Collection

A colorless prism crystal of $C_{33}H_{40}AlF_6NO_4Ti$ having approximate dimensions of 0.180 x 0.160 x 0.070 mm was mounted on a glass fiber. All measurements were made on a Rigaku XtaLAB mini diffractometer Mo-Kα radiation.

The crystal-to-detector distance was 0.00 mm.

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

a	= 9.9894(5) Å	α	= 70.26(2)^o
b	= 11.8733(2) Å	β	= 81.40(2)^o
c	= 15.8248(6) Å	γ	= 70.67(2)^o
V	= 1665.6(3) Å^3		

For Z = 2 and F.W. = 703.56, the calculated density is 1.403 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 0 $\pm$ 1^{o}C to a maximum 2θ value of 55.1^o. The crystal-to-detector distance was 0.00 mm. Readout was performed in the 0.000 mm pixel mode.

Data Reduction

Of the 17304 reflections that were collected, 7613 were unique (R_{int} = 0.0347); equivalent reflections were merged. Data were collected and processed using CrystalClear (Rigaku).

The linear absorption coefficient, μ, for Mo-Kα radiation is 3.545 cm^{-1}. An empirical

absorption correction was applied which resulted in transmission factors ranging from 0.878 to 0.975. The data were corrected for Lorentz and polarization effects.

Structure Solution and Refinement

The structure was solved by direct methods[2] 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[3] on F^2 was based on 7613 observed reflections and 415 variable parameters and converged (largest parameter shift was 0.00 times its esd) with unweighted and weighted agreement factors of:

$$R1 = \Sigma \, ||Fo| - |Fc|| \, / \, \Sigma \, |Fo| = 0.0530$$

$$wR2 = [\, \Sigma \, (\, w \, (Fo^2 - Fc^2)^2 \,) / \, \Sigma \, w(Fo^2)^2]^{1/2} = 0.1415$$

The standard deviation of an observation of unit weight[4] was 1.06. Unit weights were used. The maximum and minimum peaks on the final difference Fourier map corresponded to 0.50 and -0.57 $e^-/Å^3$, respectively.

Neutral atom scattering factors were taken from Cromer and Waber[5]. Anomalous dispersion effects were included in Fcalc[6]; the values for $\Delta f'$ and $\Delta f''$ 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) CrystalClear: Rigaku Corporation, 1999. CrystalClear Software User's Guide, Molecular Structure Corporation, (c) 2000.J.W.Pflugrath (1999) Acta Cryst. D55, 1718-1725.

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

(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 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	$C_{33}H_{40}AlF_6NO_4Ti$
Formula Weight	703.56
Crystal Color, Habit	colorless, prism
Crystal Dimensions	0.180 X 0.160 X 0.070 mm
Crystal System	triclinic
Lattice Type	Primitive
Lattice Parameters	a = 9.9894(5) Å b = 11.8733(2) Å c = 15.8248(6) Å α = 70.26(2) ^{o} β = 81.40(2) ^{o} γ = 70.67(2) ^{o} V = 1665.6(3) Å^3
Space Group	P-1 (#2)
Z value	2
D_{calc}	1.403 g/cm^3
F_{000}	732.00
μ(MoKα)	3.545 cm^{-1}

B. Intensity Measurements

Diffractometer	XtaLAB mini
Radiation	MoKα (λ = 0.71075 Å)
Voltage, Current	50kV, 12mA
Temperature	0.0^{o}C
Detector Aperture	75 mm (diameter)
Detector Position	0.00 mm
Pixel Size	0.073 mm
$2\theta_{max}$	55.1^{o}
No. of Reflections Measured	Total: 17304 Unique: 7613 (R_{int} = 0.0347)
Corrections	Lorentz-polarization Absorption (trans. factors: 0.878 - 0.975)

C. Structure Solution and Refinement

Structure Solution	Direct Methods (SIR92)
Refinement	Full-matrix least-squares on F^2
Function Minimized	$\Sigma\, w\,(Fo^2 - Fc^2)^2$
Least Squares Weights	$w = 1/\,[\,\sigma^2(Fo^2) + (0.0600 \cdot P)^2 + 1.4228 \cdot P\,]$ where $P = (Max(Fo^2,0) + 2Fc^2)/3$
$2\theta_{max}$ cutoff	55.1^o
Anomalous Dispersion	All non-hydrogen atoms
No. Observations (All reflections)	7613
No. Variables	415
Reflection/Parameter Ratio	18.34
Residuals: R1 ($I>2.00\sigma(I)$)	0.0530
Residuals: R (All reflections)	0.0766
Residuals: wR2 (All reflections)	0.1415
Goodness of Fit Indicator	1.056
Max Shift/Error in Final Cycle	0.001
Maximum peak in Final Diff. Map	0.50 $e^-/Å^3$
Minimum peak in Final Diff. Map	-0.57 $e^-/Å^3$

Table S3-1. Atomic coordinates and B_{iso}/B_{eq}

atom	x	y	z	B_{eq}
Ti1	0.22889(5)	0.09751(4)	0.77482(3)	1.599(10)
Al1	0.15765(8)	-0.02221(7)	0.64634(5)	1.64(2)
F1	-0.0870(2)	0.3473(2)	0.66907(13)	3.68(4)
F2	-0.1314(2)	0.2328(2)	0.6034(2)	4.02(5)
F3	-0.1160(2)	0.4166(2)	0.5263(2)	3.79(4)
F4	0.2724(2)	0.1937(2)	0.47073(11)	2.54(3)
F5	0.1096(2)	0.3683(2)	0.42204(12)	3.41(4)
F6	0.0604(2)	0.1938(2)	0.45913(12)	2.99(4)
O1	0.2616(2)	-0.0642(2)	0.74479(11)	1.60(3)
O2	0.1515(2)	0.1385(2)	0.64010(12)	1.73(3)
O3	0.3196(2)	0.0182(2)	0.87943(12)	1.81(3)
O4	0.2207(2)	0.2628(2)	0.73992(12)	1.79(3)
N1	0.4705(2)	0.0731(2)	0.71464(13)	1.50(4)
C1	0.3776(3)	-0.1704(3)	0.7759(2)	1.62(4)
C2	0.3548(3)	-0.2801(3)	0.8343(2)	1.86(5)
C3	0.4737(3)	-0.3831(3)	0.8638(2)	2.12(5)
C4	0.6115(3)	-0.3786(3)	0.8370(2)	2.18(5)
C5	0.6290(3)	-0.2651(3)	0.7789(2)	2.00(5)
C6	0.5136(3)	-0.1603(3)	0.7479(2)	1.64(4)
C7	0.5341(3)	-0.0396(3)	0.6832(2)	1.79(4)
C8	0.4467(3)	-0.0550(3)	0.9163(2)	1.68(4)
C9	0.4521(3)	-0.1518(3)	0.9980(2)	2.05(5)
C10	0.5849(3)	-0.2248(3)	1.0307(2)	2.26(5)
C11	0.7108(3)	-0.2061(3)	0.9859(2)	2.33(5)
C12	0.7011(3)	-0.1106(3)	0.9050(2)	2.03(5)
C13	0.5710(3)	-0.0345(3)	0.8691(2)	1.68(4)
C14	0.5602(3)	0.0713(3)	0.7828(2)	1.70(4)
C15	0.2963(3)	0.3453(3)	0.7026(2)	1.61(4)
C16	0.2453(3)	0.4657(3)	0.7119(2)	1.78(4)
C17	0.3325(3)	0.5434(3)	0.6799(2)	1.99(5)
C18	0.4654(3)	0.5063(3)	0.6379(2)	1.97(5)
C19	0.5080(3)	0.3896(3)	0.6241(2)	1.90(5)
C20	0.4256(3)	0.3084(3)	0.6553(2)	1.62(4)
C21	0.4731(3)	0.1851(3)	0.6346(2)	1.60(4)
C22	0.0260(3)	0.1024(3)	0.8367(2)	2.41(5)
C23	0.1349(3)	0.2536(3)	0.4816(2)	2.35(5)
C24	0.0999(3)	0.2574(3)	0.5785(2)	2.03(5)

Table S3-1. Atomic coordinates and B_{iso}/B_{eq} (continued)

atom	x	y	z	B_{eq}
C25	-0.0605(4)	0.3139(3)	0.5943(3)	2.86(6)
C26	-0.0245(3)	-0.0557(3)	0.6804(2)	2.39(5)
C27	0.2729(3)	-0.0878(3)	0.5519(2)	2.07(5)
C28	0.2056(3)	-0.2864(3)	0.8649(2)	2.20(5)
C29	0.7383(4)	-0.4910(3)	0.8701(3)	3.12(6)
C30	0.3171(4)	-0.1728(3)	1.0467(2)	2.66(6)
C31	0.8544(4)	-0.2882(4)	1.0235(2)	3.39(7)
C32	0.0996(3)	0.5115(3)	0.7531(2)	2.14(5)
C33	0.5605(3)	0.5894(3)	0.6093(3)	2.63(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 S3-2. Atomic coordinates and B_{iso} involving hydrogen atoms

atom	x	y	z	B_{iso}
H3	0.4605	-0.4575	0.9029	2.54
H5	0.7203	-0.2599	0.7606	2.41
H7A	0.6351	-0.0513	0.6713	2.15
H7B	0.4930	-0.0230	0.6268	2.15
H10	0.5904	-0.2890	1.0850	2.71
H12	0.7840	-0.0972	0.8740	2.44
H14A	0.5219	0.1499	0.7966	2.04
H14B	0.6551	0.0671	0.7564	2.04
H17	0.3007	0.6229	0.6868	2.39
H19	0.5938	0.3652	0.5931	2.28
H21A	0.4122	0.1908	0.5901	1.92
H21B	0.5690	0.1724	0.6083	1.92
H22A	0.0272	0.0197	0.8748	2.89
H22B	-0.0423	0.1311	0.7915	2.89
H22C	0.0006	0.1586	0.8722	2.89
H24	0.1475	0.3122	0.5876	2.44
H26A	-0.0686	-0.0245	0.7296	2.86
H26B	-0.0097	-0.1445	0.6983	2.86
H26C	-0.0849	-0.0146	0.6301	2.86
H27A	0.3654	-0.0777	0.5473	2.48
H27B	0.2279	-0.0426	0.4956	2.48
H27C	0.2818	-0.1753	0.5667	2.48
H28A	0.1545	-0.2737	0.8140	2.64
H28B	0.1578	-0.2223	0.8926	2.64
H28C	0.2099	-0.3672	0.9075	2.64
H29A	0.7335	-0.5593	0.8523	3.74
H29B	0.7385	-0.5153	0.9344	3.74
H29C	0.8237	-0.4702	0.8446	3.74
H30A	0.2790	-0.2131	1.0170	3.19
H30B	0.2495	-0.0935	1.0468	3.19
H30C	0.3366	-0.2251	1.1075	3.19
H31A	0.9039	-0.2369	1.0331	4.07
H31B	0.9089	-0.3304	0.9817	4.07
H31C	0.8413	-0.3491	1.0796	4.07
H32A	0.1081	0.5093	0.8134	2.57
H32B	0.0445	0.4583	0.7543	2.57
H32C	0.0535	0.5959	0.7180	2.57

Table S3-2. Atomic coordinates and B_{iso} involving hydrogens/B_{eq} (continued)

atom	x	y	z	B_{eq}
H33A	0.5802	0.6090	0.5457	3.16
H33B	0.6478	0.5465	0.6400	3.16
H33C	0.5140	0.6655	0.6242	3.16

Table S3-3. Anisotropic displacement parameters

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Ti1	0.0180(3)	0.0235(3)	0.0227(3)	-0.0088(2)	0.0037(2)	-0.0108(2)
Al1	0.0213(4)	0.0204(4)	0.0223(4)	-0.0073(3)	0.0002(3)	-0.0082(3)
F1	0.0343(10)	0.0433(11)	0.0572(12)	0.0049(9)	0.0004(9)	-0.0265(10)
F2	0.0233(9)	0.0386(11)	0.094(2)	-0.0041(8)	-0.0078(10)	-0.0270(11)
F3	0.0402(11)	0.0307(10)	0.0650(13)	0.0088(8)	-0.0228(10)	-0.0148(9)
F4	0.0365(9)	0.0325(9)	0.0270(9)	-0.0117(8)	-0.0013(7)	-0.0073(7)
F5	0.0639(13)	0.0240(9)	0.0353(10)	-0.0098(9)	-0.0178(9)	0.0021(8)
F6	0.0450(10)	0.0352(10)	0.0414(10)	-0.0129(8)	-0.0148(8)	-0.0155(8)
O1	0.0185(9)	0.0218(9)	0.0213(9)	-0.0067(7)	0.0003(7)	-0.0074(7)
O2	0.0213(9)	0.0194(9)	0.0250(9)	-0.0054(8)	-0.0017(7)	-0.0075(7)
O3	0.0203(9)	0.0298(10)	0.0228(9)	-0.0115(8)	0.0048(7)	-0.0119(8)
O4	0.0187(9)	0.0247(10)	0.0285(10)	-0.0098(8)	0.0047(7)	-0.0124(8)
N1	0.0206(10)	0.0205(11)	0.0174(10)	-0.0083(9)	0.0019(8)	-0.0066(8)
C1	0.0221(12)	0.0191(12)	0.0210(12)	-0.0060(10)	0.0019(10)	-0.0085(10)
C2	0.0263(13)	0.026(2)	0.0208(13)	-0.0117(11)	0.0012(10)	-0.0078(11)
C3	0.035(2)	0.022(2)	0.0240(13)	-0.0125(12)	0.0001(11)	-0.0043(11)
C4	0.029(2)	0.023(2)	0.029(2)	-0.0055(12)	0.0002(12)	-0.0081(11)
C5	0.0233(13)	0.026(2)	0.027(2)	-0.0078(11)	0.0035(11)	-0.0106(11)
C6	0.0233(13)	0.0208(13)	0.0197(12)	-0.0067(10)	0.0020(10)	-0.0094(10)
C7	0.0229(13)	0.0238(13)	0.0215(13)	-0.0076(11)	0.0046(10)	-0.0088(10)
C8	0.0232(13)	0.0232(13)	0.0195(12)	-0.0080(11)	0.0018(10)	-0.0091(10)
C9	0.033(2)	0.027(2)	0.0224(13)	-0.0134(12)	0.0057(11)	-0.0116(11)
C10	0.041(2)	0.024(2)	0.0195(13)	-0.0108(13)	0.0019(12)	-0.0054(11)
C11	0.031(2)	0.029(2)	0.0219(13)	-0.0042(12)	-0.0013(12)	-0.0045(11)
C12	0.0239(13)	0.034(2)	0.0201(13)	-0.0100(12)	0.0034(10)	-0.0092(11)
C13	0.0251(13)	0.0224(13)	0.0192(12)	-0.0092(11)	0.0032(10)	-0.0095(10)
C14	0.0201(12)	0.0258(13)	0.0202(12)	-0.0089(11)	0.0010(10)	-0.0077(10)
C15	0.0213(12)	0.0222(13)	0.0196(12)	-0.0092(10)	-0.0014(10)	-0.0060(10)
C16	0.0215(13)	0.0227(13)	0.0233(13)	-0.0039(11)	-0.0019(10)	-0.0091(11)
C17	0.031(2)	0.0155(12)	0.028(2)	-0.0056(11)	-0.0042(11)	-0.0056(11)
C18	0.027(2)	0.0218(13)	0.0250(13)	-0.0084(11)	-0.0037(11)	-0.0037(11)
C19	0.0211(13)	0.024(2)	0.0246(13)	-0.0071(11)	-0.0014(10)	-0.0038(11)
C20	0.0191(12)	0.0200(13)	0.0202(12)	-0.0038(10)	-0.0033(10)	-0.0045(10)
C21	0.0195(12)	0.0221(13)	0.0192(12)	-0.0082(10)	0.0020(10)	-0.0059(10)
C22	0.026(2)	0.041(2)	0.031(2)	-0.0165(13)	0.0106(12)	-0.0175(13)
C23	0.037(2)	0.0191(13)	0.032(2)	-0.0066(12)	-0.0126(12)	-0.0034(11)
C24	0.0252(13)	0.0168(13)	0.035(2)	-0.0026(11)	-0.0095(12)	-0.0076(11)

Table S3-3. Anisotropic displacement parameters (continued)

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
C25	0.029(2)	0.025(2)	0.053(2)	0.0000(12)	-0.011(2)	-0.013(2)
C26	0.029(2)	0.036(2)	0.031(2)	-0.0164(13)	-0.0032(12)	-0.0113(13)
C27	0.033(2)	0.0212(13)	0.0234(13)	-0.0052(11)	-0.0004(11)	-0.0083(11)
C28	0.030(2)	0.026(2)	0.028(2)	-0.0139(12)	0.0009(12)	-0.0048(11)
C29	0.037(2)	0.028(2)	0.043(2)	-0.006(2)	0.000(2)	-0.003(2)
C30	0.042(2)	0.036(2)	0.026(2)	-0.022(2)	0.0053(13)	-0.0064(12)
C31	0.038(2)	0.050(2)	0.027(2)	-0.004(2)	-0.0023(13)	-0.003(2)
C32	0.027(2)	0.024(2)	0.030(2)	-0.0046(11)	0.0010(11)	-0.0123(12)
C33	0.032(2)	0.023(2)	0.046(2)	-0.0119(12)	0.0002(13)	-0.0091(13)

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 S3-4. Bond lengths (Å)

atom	atom	distance	atom	atom	distance
Ti1	Al1	3.1169(12)	Ti1	O1	2.043(3)
Ti1	O2	2.218(2)	Ti1	O3	1.8110(19)
Ti1	O4	1.827(2)	Ti1	N1	2.419(2)
Ti1	C22	2.107(3)	Al1	O1	1.835(2)
Al1	O2	1.858(3)	Al1	C26	1.950(4)
Al1	C27	1.960(3)	F1	C25	1.335(5)
F2	C25	1.333(5)	F3	C25	1.341(4)
F4	C23	1.337(3)	F5	C23	1.335(3)
F6	C23	1.336(5)	O1	C1	1.399(3)
O2	C24	1.396(3)	O3	C8	1.363(3)
O4	C15	1.359(4)	N1	C7	1.494(4)
N1	C14	1.493(4)	N1	C21	1.500(3)
C1	C2	1.388(4)	C1	C6	1.395(4)
C2	C3	1.394(4)	C2	C28	1.515(4)
C3	C4	1.392(5)	C4	C5	1.401(4)
C4	C29	1.506(4)	C5	C6	1.387(4)
C6	C7	1.513(4)	C8	C9	1.404(4)
C8	C13	1.400(4)	C9	C10	1.386(4)
C9	C30	1.502(5)	C10	C11	1.394(5)
C11	C12	1.385(4)	C11	C31	1.516(4)
C12	C13	1.387(4)	C13	C14	1.500(3)
C15	C16	1.401(4)	C15	C20	1.406(4)
C16	C17	1.396(5)	C16	C32	1.507(4)
C17	C18	1.395(4)	C18	C19	1.392(5)
C18	C33	1.507(5)	C19	C20	1.390(5)
C20	C21	1.514(4)	C23	C24	1.533(5)
C24	C25	1.536(4)			

Table S3-5. Bond lengths involving hydrogens (Å)

atom	atom	distance	atom	atom	distance
C3	H3	0.930	C5	H5	0.930
C7	H7A	0.970	C7	H7B	0.970
C10	H10	0.930	C12	H12	0.930
C14	H14A	0.970	C14	H14B	0.970
C17	H17	0.930	C19	H19	0.930
C21	H21A	0.970	C21	H21B	0.970
C22	H22A	0.960	C22	H22B	0.960
C22	H22C	0.960	C24	H24	0.980
C26	H26A	0.960	C26	H26B	0.960
C26	H26C	0.960	C27	H27A	0.960
C27	H27B	0.960	C27	H27C	0.960
C28	H28A	0.960	C28	H28B	0.960
C28	H28C	0.960	C29	H29A	0.960
C29	H29B	0.960	C29	H29C	0.960
C30	H30A	0.960	C30	H30B	0.960
C30	H30C	0.960	C31	H31A	0.960
C31	H31B	0.960	C31	H31C	0.960
C32	H32A	0.960	C32	H32B	0.960
C32	H32C	0.960	C33	H33A	0.960
C33	H33B	0.960	C33	H33C	0.960

Table S3-6. Bond angles (°)

atom	atom	atom	angle	atom	atom	atom	angle
Al1	Ti1	O1	34.31(5)	Al1	Ti1	O2	36.03(6)
Al1	Ti1	O3	128.03(8)	Al1	Ti1	O4	122.16(7)
Al1	Ti1	N1	93.13(7)	Al1	Ti1	C22	87.30(11)
O1	Ti1	O2	68.99(7)	O1	Ti1	O3	94.14(9)
O1	Ti1	O4	150.43(8)	O1	Ti1	N1	82.11(8)
O1	Ti1	C22	95.29(12)	O2	Ti1	O3	162.49(9)
O2	Ti1	O4	86.22(9)	O2	Ti1	N1	91.27(8)
O2	Ti1	C22	92.26(10)	O3	Ti1	O4	108.39(11)
O3	Ti1	N1	81.41(8)	O3	Ti1	C22	94.04(10)
O4	Ti1	N1	82.60(8)	O4	Ti1	C22	101.78(11)
N1	Ti1	C22	174.54(8)	Ti1	Al1	O1	38.87(7)
Ti1	Al1	O2	44.61(7)	Ti1	Al1	C26	111.47(11)
Ti1	Al1	C27	131.25(11)	O1	Al1	O2	81.78(10)
O1	Al1	C26	111.76(11)	O1	Al1	C27	111.58(11)
O2	Al1	C26	113.76(12)	O2	Al1	C27	116.17(11)
C26	Al1	C27	116.67(16)	Ti1	O1	Al1	106.82(8)
Ti1	O1	C1	122.00(19)	Al1	O1	C1	127.82(19)
Ti1	O2	Al1	99.36(8)	Ti1	O2	C24	126.0(2)
Al1	O2	C24	134.2(2)	Ti1	O3	C8	144.17(17)
Ti1	O4	C15	144.55(15)	Ti1	N1	C7	114.10(18)
Ti1	N1	C14	109.41(14)	Ti1	N1	C21	108.95(13)
C7	N1	C14	110.75(18)	C7	N1	C21	106.53(19)
C14	N1	C21	106.8(3)	O1	C1	C2	119.7(3)
O1	C1	C6	118.0(2)	C2	C1	C6	122.3(2)
C1	C2	C3	117.6(3)	C1	C2	C28	120.8(2)
C3	C2	C28	121.7(3)	C2	C3	C4	122.4(3)
C3	C4	C5	117.9(3)	C3	C4	C29	121.4(3)
C5	C4	C29	120.7(3)	C4	C5	C6	121.6(3)
C1	C6	C5	118.3(3)	C1	C6	C7	120.7(2)
C5	C6	C7	121.0(3)	N1	C7	C6	115.0(2)
O3	C8	C9	120.4(3)	O3	C8	C13	118.41(19)
C9	C8	C13	121.2(3)	C8	C9	C10	117.5(3)
C8	C9	C30	120.1(3)	C10	C9	C30	122.5(3)
C9	C10	C11	122.8(3)	C10	C11	C12	118.0(3)
C10	C11	C31	121.4(3)	C12	C11	C31	120.6(3)
C11	C12	C13	121.7(3)	C8	C13	C12	118.9(2)
C8	C13	C14	119.3(2)	C12	C13	C14	121.8(3)

Table S3-6. Bond angles (°) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
N1	C14	C13	115.3(3)	O4	C15	C16	119.8(3)
O4	C15	C20	119.4(3)	C16	C15	C20	120.8(3)
C15	C16	C17	117.9(3)	C15	C16	C32	121.2(3)
C17	C16	C32	120.9(3)	C16	C17	C18	122.5(3)
C17	C18	C19	117.8(3)	C17	C18	C33	121.1(3)
C19	C18	C33	121.1(3)	C18	C19	C20	121.8(3)
C15	C20	C19	118.9(3)	C15	C20	C21	121.3(3)
C19	C20	C21	119.7(3)	N1	C21	C20	114.4(2)
F4	C23	F5	106.8(3)	F4	C23	F6	107.2(3)
F4	C23	C24	110.6(3)	F5	C23	F6	107.6(3)
F5	C23	C24	112.2(3)	F6	C23	C24	112.1(3)
O2	C24	C23	111.2(3)	O2	C24	C25	111.3(3)
C23	C24	C25	111.0(3)	F1	C25	F2	107.3(3)
F1	C25	F3	107.4(3)	F1	C25	C24	110.7(3)
F2	C25	F3	107.4(3)	F2	C25	C24	112.1(3)
F3	C25	C24	111.7(3)				

Table S3-7. Bond angles involving hydrogens (°)

atom	atom	atom	angle	atom	atom	atom	angle
C2	C3	H3	118.8	C4	C3	H3	118.8
C4	C5	H5	119.2	C6	C5	H5	119.2
N1	C7	H7A	108.5	N1	C7	H7B	108.5
C6	C7	H7A	108.5	C6	C7	H7B	108.5
H7A	C7	H7B	107.5	C9	C10	H10	118.6
C11	C10	H10	118.6	C11	C12	H12	119.2
C13	C12	H12	119.2	N1	C14	H14A	108.5
N1	C14	H14B	108.5	C13	C14	H14A	108.5
C13	C14	H14B	108.5	H14A	C14	H14B	107.5
C16	C17	H17	118.7	C18	C17	H17	118.7
C18	C19	H19	119.1	C20	C19	H19	119.1
N1	C21	H21A	108.7	N1	C21	H21B	108.7
C20	C21	H21A	108.7	C20	C21	H21B	108.7
H21A	C21	H21B	107.6	Ti1	C22	H22A	109.5
Ti1	C22	H22B	109.5	Ti1	C22	H22C	109.5
H22A	C22	H22B	109.5	H22A	C22	H22C	109.5
H22B	C22	H22C	109.5	O2	C24	H24	107.7
C23	C24	H24	107.7	C25	C24	H24	107.7
Al1	C26	H26A	109.5	Al1	C26	H26B	109.5
Al1	C26	H26C	109.5	H26A	C26	H26B	109.5
H26A	C26	H26C	109.5	H26B	C26	H26C	109.5
Al1	C27	H27A	109.5	Al1	C27	H27B	109.5
Al1	C27	H27C	109.5	H27A	C27	H27B	109.5
H27A	C27	H27C	109.5	H27B	C27	H27C	109.5
C2	C28	H28A	109.5	C2	C28	H28B	109.5
C2	C28	H28C	109.5	H28A	C28	H28B	109.5
H28A	C28	H28C	109.5	H28B	C28	H28C	109.5
C4	C29	H29A	109.5	C4	C29	H29B	109.5
C4	C29	H29C	109.5	H29A	C29	H29B	109.5
H29A	C29	H29C	109.5	H29B	C29	H29C	109.5
C9	C30	H30A	109.5	C9	C30	H30B	109.5
C9	C30	H30C	109.5	H30A	C30	H30B	109.5
H30A	C30	H30C	109.5	H30B	C30	H30C	109.5
C11	C31	H31A	109.5	C11	C31	H31B	109.5
C11	C31	H31C	109.5	H31A	C31	H31B	109.5
H31A	C31	H31C	109.5	H31B	C31	H31C	109.5
C16	C32	H32A	109.5	C16	C32	H32B	109.5

Table S3-7. Bond angles involving hydrogens (°) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
C16	C32	H32C	109.5	H32A	C32	H32B	109.5
H32A	C32	H32C	109.5	H32B	C32	H32C	109.5
C18	C33	H33A	109.5	C18	C33	H33B	109.5
C18	C33	H33C	109.5	H33A	C33	H33B	109.5
H33A	C33	H33C	109.5	H33B	C33	H33C	109.5

Table S3-8. Torsion Angles(O)

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

atom1	atom2	atom3	atom4	angle	atom1	atom2	atom3	atom4	angle
Al1	Ti1	O1	Al1	-0.00(3)	Al1	Ti1	O1	C1	160.77(18)
O1	Ti1	Al1	O1	-0.00(9)	O1	Ti1	Al1	O2	-158.96(10)
O1	Ti1	Al1	C26	98.45(9)	O1	Ti1	Al1	C27	-72.03(9)
Al1	Ti1	O2	Al1	0.00(3)	Al1	Ti1	O2	C24	173.45(19)
O2	Ti1	Al1	O1	158.96(9)	O2	Ti1	Al1	O2	0.00(8)
O2	Ti1	Al1	C26	-102.59(9)	O2	Ti1	Al1	C27	86.93(9)
Al1	Ti1	O3	C8	67.6(3)	O3	Ti1	Al1	O1	-10.44(8)
O3	Ti1	Al1	O2	-169.40(8)	O3	Ti1	Al1	C26	88.01(8)
O3	Ti1	Al1	C27	-82.47(9)	Al1	Ti1	O4	C15	-91.0(3)
O4	Ti1	Al1	O1	154.32(8)	O4	Ti1	Al1	O2	-4.64(7)
O4	Ti1	Al1	C26	-107.23(8)	O4	Ti1	Al1	C27	82.29(8)
Al1	Ti1	N1	C7	-32.04(10)	Al1	Ti1	N1	C14	-156.72(10)
Al1	Ti1	N1	C21	86.85(13)	N1	Ti1	Al1	O1	71.10(5)
N1	Ti1	Al1	O2	-87.86(5)	N1	Ti1	Al1	C26	169.55(5)
N1	Ti1	Al1	C27	-0.94(6)	C22	Ti1	Al1	O1	-103.46(8)
C22	Ti1	Al1	O2	97.58(8)	C22	Ti1	Al1	C26	-5.01(8)
C22	Ti1	Al1	C27	-175.49(8)	O1	Ti1	O2	Al1	12.52(7)
O1	Ti1	O2	C24	-174.03(15)	O2	Ti1	O1	Al1	-13.07(7)
O2	Ti1	O1	C1	147.70(13)	O1	Ti1	O3	C8	61.8(3)
O3	Ti1	O1	Al1	171.77(9)	O3	Ti1	O1	C1	-27.45(13)
O1	Ti1	O4	C15	-61.4(4)	O4	Ti1	O1	Al1	-48.01(19)
O4	Ti1	O1	C1	112.77(17)	O1	Ti1	N1	C7	0.54(11)
O1	Ti1	N1	C14	-124.15(12)	O1	Ti1	N1	C21	119.42(14)
N1	Ti1	O1	Al1	-107.50(9)	N1	Ti1	O1	C1	53.27(12)
C22	Ti1	O1	Al1	77.32(11)	C22	Ti1	O1	C1	-121.90(13)
O2	Ti1	O4	C15	-93.8(3)	O4	Ti1	O2	Al1	176.07(9)
O4	Ti1	O2	C24	-10.48(13)	O2	Ti1	N1	C7	-68.05(11)
O2	Ti1	N1	C14	167.27(11)	O2	Ti1	N1	C21	50.84(14)
N1	Ti1	O2	Al1	93.57(9)	N1	Ti1	O2	C24	-92.98(14)
C22	Ti1	O2	Al1	-82.28(11)	C22	Ti1	O2	C24	91.18(16)
O3	Ti1	O4	C15	76.4(3)	O4	Ti1	O3	C8	-98.8(3)
O3	Ti1	N1	C7	95.97(12)	O3	Ti1	N1	C14	-28.71(12)
O3	Ti1	N1	C21	-145.14(16)	N1	Ti1	O3	C8	-19.6(3)
C22	Ti1	O3	C8	157.4(3)	O4	Ti1	N1	C7	-154.07(13)
O4	Ti1	N1	C14	81.25(13)	O4	Ti1	N1	C21	-35.19(14)
N1	Ti1	O4	C15	-2.0(3)	C22	Ti1	O4	C15	174.7(3)
Ti1	Al1	O1	Ti1	-0.000(14)	Ti1	Al1	O1	C1	-159.3(2)

Table S3-8. Torsion angles (°) (continued)

atom1	atom2	atom3	atom4	angle	atom1	atom2	atom3	atom4	angle
Ti1	Al1	O2	Ti1	-0.000(18)	Ti1	Al1	O2	C24	-172.6(2)
O1	Al1	O2	Ti1	-13.16(8)	O1	Al1	O2	C24	174.23(17)
O2	Al1	O1	Ti1	14.76(9)	O2	Al1	O1	C1	-144.54(15)
C26	Al1	O1	Ti1	-97.62(13)	C26	Al1	O1	C1	103.08(17)
C27	Al1	O1	Ti1	129.72(12)	C27	Al1	O1	C1	-29.57(19)
C26	Al1	O2	Ti1	97.07(12)	C26	Al1	O2	C24	-75.55(19)
C27	Al1	O2	Ti1	-123.22(11)	C27	Al1	O2	C24	64.2(2)
Ti1	O1	C1	C2	116.2(3)	Ti1	O1	C1	C6	-62.5(3)
Al1	O1	C1	C2	-87.3(3)	Al1	O1	C1	C6	94.0(3)
Ti1	O2	C24	C23	147.65(15)	Ti1	O2	C24	C25	-88.1(3)
Al1	O2	C24	C23	-41.4(3)	Al1	O2	C24	C25	82.9(3)
Ti1	O3	C8	C9	-141.2(3)	Ti1	O3	C8	C13	36.3(5)
Ti1	O4	C15	C16	-162.8(2)	Ti1	O4	C15	C20	16.9(5)
Ti1	N1	C7	C6	-47.3(3)	Ti1	N1	C14	C13	62.0(2)
Ti1	N1	C21	C20	62.1(3)	C7	N1	C14	C13	-64.6(3)
C14	N1	C7	C6	76.7(3)	C7	N1	C21	C20	-174.4(2)
C21	N1	C7	C6	-167.5(2)	C14	N1	C21	C20	-56.0(3)
C21	N1	C14	C13	179.74(17)	O1	C1	C2	C3	-179.6(3)
O1	C1	C2	C28	-0.1(5)	O1	C1	C6	C5	179.7(3)
O1	C1	C6	C7	-2.2(4)	C2	C1	C6	C5	1.1(5)
C2	C1	C6	C7	179.1(3)	C6	C1	C2	C3	-1.0(5)
C6	C1	C2	C28	178.5(3)	C1	C2	C3	C4	0.1(5)
C28	C2	C3	C4	-179.4(3)	C2	C3	C4	C5	0.7(5)
C2	C3	C4	C29	179.8(3)	C3	C4	C5	C6	-0.6(5)
C29	C4	C5	C6	-179.7(3)	C4	C5	C6	C1	-0.3(5)
C4	C5	C6	C7	-178.3(3)	C1	C6	C7	N1	59.0(4)
C5	C6	C7	N1	-123.0(3)	O3	C8	C9	C10	178.5(3)
O3	C8	C9	C30	-1.8(5)	O3	C8	C13	C12	-178.4(3)
O3	C8	C13	C14	3.5(5)	C9	C8	C13	C12	-0.9(5)
C9	C8	C13	C14	-179.0(3)	C13	C8	C9	C10	1.1(5)
C13	C8	C9	C30	-179.3(3)	C8	C9	C10	C11	-0.4(5)
C30	C9	C10	C11	179.9(3)	C9	C10	C11	C12	-0.3(5)
C9	C10	C11	C31	-179.7(3)	C10	C11	C12	C13	0.4(5)
C31	C11	C12	C13	179.9(3)	C11	C12	C13	C8	0.2(5)
C11	C12	C13	C14	178.2(3)	C8	C13	C14	N1	-52.8(4)
C12	C13	C14	N1	129.2(3)	O4	C15	C16	C17	174.2(2)
O4	C15	C16	C32	-7.3(4)	O4	C15	C20	C19	-174.5(2)

Table S3-8. Torsion angles (°) (continued)

atom1	atom2	atom3	atom4	angle	atom1	atom2	atom3	atom4	angle
O4	C15	C20	C21	8.0(4)	C16	C15	C20	C19	5.2(4)
C16	C15	C20	C21	-172.2(2)	C20	C15	C16	C17	-5.6(4)
C20	C15	C16	C32	172.9(2)	C15	C16	C17	C18	1.4(4)
C32	C16	C17	C18	-177.2(3)	C16	C17	C18	C19	3.2(4)
C16	C17	C18	C33	-176.1(3)	C17	C18	C19	C20	-3.6(4)
C33	C18	C19	C20	175.7(3)	C18	C19	C20	C15	-0.5(4)
C18	C19	C20	C21	177.0(3)	C15	C20	C21	N1	-51.6(3)
C19	C20	C21	N1	131.0(3)	F4	C23	C24	O2	-49.7(4)
F4	C23	C24	C25	-174.1(2)	F5	C23	C24	O2	-168.8(3)
F5	C23	C24	C25	66.8(4)	F6	C23	C24	O2	70.0(3)
F6	C23	C24	C25	-54.5(3)	O2	C24	C25	F1	71.8(4)
O2	C24	C25	F2	-47.9(4)	O2	C24	C25	F3	-168.6(3)
C23	C24	C25	F1	-163.8(3)	C23	C24	C25	F2	76.5(3)
C23	C24	C25	F3	-44.2(4)					

Table S3-9. Intramolecular contacts less than 3.60 Å

atom	atom	distance	atom	atom	distance
Ti1	C6	3.521(3)	Ti1	C13	3.572(3)
Ti1	C20	3.558(3)	Al1	F2	3.3730(19)
Al1	F4	3.4333(19)	Al1	F6	3.2211(19)
Al1	C23	3.390(3)	F1	O2	2.926(3)
F1	O4	3.152(3)	F1	C22	3.206(3)
F2	F6	2.814(3)	F2	O2	2.745(3)
F2	C23	3.071(4)	F2	C26	3.083(4)
F3	F5	2.607(3)	F3	F6	3.080(3)
F3	O2	3.587(3)	F3	C23	2.776(4)
F4	O2	2.728(3)	F4	C21	3.464(4)
F4	C27	3.148(4)	F5	O2	3.584(3)
F5	C25	2.981(4)	F6	O2	2.928(3)
F6	C25	2.866(5)	F6	C27	3.280(3)
O1	C7	2.827(4)	O1	C8	3.555(4)
O1	C28	2.856(4)	O2	C21	3.419(4)
O3	C1	3.061(4)	O3	C6	3.411(4)
O3	C14	2.786(4)	O3	C30	2.848(3)
O4	C14	3.417(3)	O4	C21	2.868(3)
O4	C24	3.012(4)	O4	C32	2.864(4)
N1	C1	3.125(4)	N1	C8	3.048(3)
N1	C15	3.078(4)	C1	C4	2.782(4)
C1	C8	3.229(5)	C1	C27	3.563(4)
C2	C5	2.794(4)	C3	C6	2.779(4)
C5	C12	3.413(5)	C5	C13	3.349(5)
C6	C8	3.205(4)	C6	C13	3.012(5)
C6	C14	3.168(5)	C7	C13	3.042(4)
C8	C11	2.791(4)	C9	C12	2.796(4)
C10	C13	2.768(4)	C14	C15	3.417(3)
C14	C20	2.876(3)	C15	C18	2.802(5)
C15	C24	3.563(5)	C16	C19	2.797(4)
C17	C20	2.776(4)			

Table S3-10. Intramolecular contacts less than 3.60 Å involving hydrogens

atom	atom	distance	atom	atom	distance
Ti1	H7B	3.524	Ti1	H14A	3.275
Ti1	H21A	3.268	Ti1	H24	3.191
Al1	H7B	3.315	Al1	H22B	3.409
Al1	H28A	3.263	F1	H22B	2.585
F1	H22C	3.285	F1	H24	2.477
F1	H32B	2.856	F2	H22B	2.961
F2	H24	3.176	F2	H26A	2.950
F2	H26C	2.709	F3	H24	2.683
F4	H7B	3.340	F4	H21A	2.496
F4	H24	2.620	F4	H27A	2.904
F4	H27B	2.873	F5	H24	2.531
F6	H24	3.184	F6	H26C	3.498
F6	H27B	2.664	O1	H7B	2.813
O1	H22A	3.018	O1	H22B	3.311
O1	H26A	3.207	O1	H26B	3.402
O1	H27A	3.182	O1	H27C	3.448
O1	H28A	2.846	O1	H28B	2.768
O2	H7B	3.329	O2	H21A	2.813
O2	H22B	2.842	O2	H26A	3.259
O2	H26C	3.472	O2	H27A	3.360
O2	H27B	3.486	O3	H14A	2.856
O3	H22A	2.927	O3	H22C	3.068
O3	H30A	2.980	O3	H30B	2.636
O4	H14A	2.996	O4	H21A	2.991
O4	H22B	3.351	O4	H22C	3.069
O4	H24	2.444	O4	H32A	3.303
O4	H32B	2.463	C1	H3	3.218
C1	H5	3.228	C1	H7A	3.303
C1	H7B	2.773	C1	H27A	3.415
C1	H28A	2.783	C1	H28B	2.744
C1	H28C	3.297	C2	H30A	3.173
C3	H5	3.232	C3	H28A	3.129
C3	H28B	3.159	C3	H28C	2.583
C3	H29A	2.769	C3	H29B	2.768
C3	H29C	3.300	C5	H3	3.231
C5	H7A	2.549	C5	H7B	3.102
C5	H29A	3.138	C5	H29B	3.130

Table S3-10. Intramolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
C5	H29C	2.560	C6	H14B	3.484
C6	H27A	3.402	C7	H5	2.665
C7	H14A	3.283	C7	H14B	2.614
C7	H21A	2.597	C7	H21B	2.510
C7	H27A	3.148	C8	H10	3.224
C8	H12	3.238	C8	H14A	2.783
C8	H14B	3.284	C8	H30A	2.852
C8	H30B	2.664	C8	H30C	3.285
C10	H12	3.223	C10	H30A	3.050
C10	H30B	3.206	C10	H30C	2.594
C10	H31A	3.146	C10	H31B	3.141
C10	H31C	2.579	C12	H5	3.284
C12	H10	3.218	C12	H14A	3.064
C12	H14B	2.554	C12	H31A	2.761
C12	H31B	2.760	C12	H31C	3.295
C13	H5	3.469	C13	H7A	3.160
C14	H7A	2.533	C14	H7B	3.266
C14	H12	2.671	C14	H21A	3.247
C14	H21B	2.614	C15	H14A	2.807
C15	H17	3.234	C15	H19	3.246
C15	H21A	2.840	C15	H21B	3.319
C15	H24	2.712	C15	H32A	3.048
C15	H32B	2.586	C15	H32C	3.214
C16	H24	3.510	C17	H19	3.227
C17	H32A	2.874	C17	H32B	3.285
C17	H32C	2.668	C17	H33A	3.136
C17	H33B	3.129	C17	H33C	2.563
C19	H14A	3.190	C19	H17	3.224
C19	H21A	3.046	C19	H21B	2.535
C19	H33A	2.765	C19	H33B	2.764
C19	H33C	3.298	C20	H14A	2.464
C20	H14B	3.111	C20	H24	3.104
C21	H7A	2.647	C21	H7B	2.457
C21	H14A	2.549	C21	H14B	2.553
C21	H19	2.641	C21	H24	3.182
C22	H26A	3.030	C22	H28B	3.473
C23	H21A	3.219	C23	H27B	3.265

Table S3-10. Intramolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
C24	H21A	2.972	C24	H22B	3.492
C25	H22B	3.133	C26	H22B	3.212
C26	H27B	3.561	C26	H27C	3.438
C26	H28A	2.956	C27	H7B	3.056
C27	H26B	3.470	C27	H26C	3.523
C28	H3	2.680	C28	H22A	3.525
C28	H26B	3.273	C28	H30A	3.074
C29	H3	2.666	C29	H5	2.668
C30	H10	2.675	C30	H28B	3.402
C31	H10	2.673	C31	H12	2.656
C32	H17	2.660	C33	H17	2.663
C33	H19	2.667	H3	H28A	3.299
H3	H28B	3.349	H3	H28C	2.375
H3	H29A	2.713	H3	H29B	2.712
H3	H29C	3.574	H5	H7A	2.336
H5	H7B	3.276	H5	H12	3.295
H5	H29A	3.320	H5	H29B	3.308
H5	H29C	2.352	H7A	H12	3.536
H7A	H14A	3.415	H7A	H14B	2.318
H7A	H21A	2.999	H7A	H21B	2.394
H7B	H14B	3.405	H7B	H21A	2.285
H7B	H21B	2.586	H7B	H27A	2.281
H7B	H27C	3.593	H10	H30A	3.184
H10	H30B	3.433	H10	H30C	2.401
H10	H31A	3.322	H10	H31B	3.315
H10	H31C	2.365	H12	H14A	3.226
H12	H14B	2.351	H12	H31A	2.700
H12	H31B	2.700	H12	H31C	3.565
H14A	H19	3.519	H14A	H21A	3.430
H14A	H21B	2.880	H14B	H19	3.527
H14B	H21A	3.451	H14B	H21B	2.388
H17	H32A	2.876	H17	H32B	3.549
H17	H32C	2.549	H17	H33A	3.301
H17	H33B	3.317	H17	H33C	2.350
H19	H21A	3.188	H19	H21B	2.312
H19	H33A	2.696	H19	H33B	2.729
H19	H33C	3.575	H21A	H24	2.557

Table S3-10. Intramolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
H22A	H26A	2.877	H22A	H28B	2.668
H22A	H30A	3.452	H22A	H30B	3.391
H22B	H26A	2.462	H22C	H32B	3.555
H24	H32B	3.481	H26A	H28A	3.060
H26A	H28B	3.379	H26B	H27C	3.309
H26B	H28A	2.394	H26B	H28B	3.421
H26C	H27B	3.494	H28B	H30A	2.509
H28C	H30A	3.187	H29B	H31B	3.498
H29C	H31B	3.478			

Table S3-11. Intermolecular contacts less than 3.60 Å

atom	atom	distance	atom	atom	distance
F1	F5[1]	3.136(3)	F2	C19[2]	3.488(3)
F3	F3[1]	3.365(4)	F3	F5[1]	2.954(4)
F3	C33[2]	3.542(4)	F4	C7[3]	3.504(4)
F4	C33[4]	3.322(4)	F5	F1[1]	3.136(3)
F5	F3[1]	2.954(4)	F5	C25[1]	3.563(4)
F5	C32[1]	3.343(4)	F5	C33[4]	3.435(4)
F6	C26[5]	3.281(5)	O3	C11[6]	3.490(5)
C7	F4[3]	3.504(4)	C8	C10[6]	3.598(5)
C9	C13[6]	3.469(5)	C10	C8[6]	3.598(5)
C11	O3[6]	3.490(5)	C13	C9[6]	3.469(5)
C19	F2[7]	3.488(3)	C25	F5[1]	3.563(4)
C26	F6[5]	3.281(5)	C32	F5[1]	3.343(4)
C33	F3[7]	3.542(4)	C33	F4[4]	3.322(4)
C33	F5[4]	3.435(4)			

Symmetry Operators:

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

Table S3-12. Intermolecular contacts less than 3.60 Å involving hydrogens

atom	atom	distance	atom	atom	distance
F1	H19[1]	3.491	F1	H29A[2]	3.487
F1	H33B[1]	2.882	F2	H14B[1]	3.507
F2	H19[1]	2.671	F2	H21B[1]	3.285
F2	H27B[3]	3.572	F3	H19[1]	3.117
F3	H24[4]	3.048	F3	H33A[1]	3.182
F3	H33B[1]	3.063	F4	H5[5]	3.469
F4	H7A[5]	3.110	F4	H7B[5]	3.141
F4	H27A[5]	3.424	F4	H33A[6]	3.079
F4	H33B[6]	3.283	F4	H33C[6]	3.052
F5	H5[5]	3.534	F5	H32B[4]	3.115
F5	H32C[4]	2.781	F5	H33A[6]	3.324
F5	H33B[6]	2.845	F6	H26B[3]	2.891
F6	H26C[3]	2.857	F6	H27C[3]	3.589
F6	H32C[4]	3.120	O3	H31A[7]	3.363
O4	H31A[7]	3.566	O4	H31C[7]	3.259
C1	H17[8]	3.538	C1	H33C[8]	3.441
C2	H17[8]	3.109	C3	H3[9]	3.581
C3	H17[8]	3.474	C4	H33B[8]	3.458
C4	H33C[8]	3.466	C5	H33B[8]	3.575
C5	H33C[8]	3.289	C6	H33C[8]	3.291
C7	H27A[5]	3.556	C7	H27B[5]	3.503
C9	H14A[7]	3.308	C10	H14A[7]	3.088
C11	H30B[7]	3.566	C12	H26A[10]	3.431
C12	H30B[7]	2.976	C13	H30B[7]	3.344
C14	H26A[10]	3.560	C14	H30C[7]	3.366
C15	H10[7]	3.485	C15	H31C[7]	3.524
C16	H10[7]	3.488	C16	H31C[7]	3.226
C17	H27C[11]	3.120	C17	H28A[11]	3.437
C18	H19[6]	3.510	C18	H27C[11]	3.475
C19	H33A[6]	2.942	C20	H33A[6]	2.998
C21	H27A[5]	3.500	C21	H33A[6]	3.046
C22	H30B[12]	3.086	C22	H30C[12]	3.527
C22	H31A[7]	3.268	C23	H32C[4]	3.529
C25	H19[1]	3.304	C25	H33B[1]	3.469
C26	H7A[1]	3.407	C26	H12[1]	3.337
C26	H14B[1]	3.280	C26	H27B[3]	3.343
C27	H7A[5]	3.485	C27	H7B[5]	3.570

Table S3-12. Intermolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
C27	H17[8]	3.321	C27	H21B[5]	3.067
C27	H26C[3]	3.323	C27	H33C[8]	3.094
C28	H17[8]	3.252	C28	H29B[9]	3.248
C28	H31B[1]	3.348	C28	H32A[8]	3.261
C29	H28C[9]	3.384	C29	H30A[9]	3.411
C29	H30C[9]	3.582	C29	H32B[13]	3.305
C30	H14A[7]	3.278	C30	H22A[12]	3.576
C30	H22B[12]	3.492	C30	H22C[12]	3.213
C30	H29A[9]	3.213	C31	H22C[7]	3.331
C31	H28B[10]	3.562	C31	H32A[7]	2.960
C31	H32B[7]	3.518	C32	H28A[11]	3.237
C32	H29C[2]	2.891	C32	H31C[7]	2.709
C33	H19[6]	3.562	C33	H21A[6]	3.391
C33	H27C[11]	3.186	H3	C3[9]	3.581
H3	H3[9]	3.031	H3	H10[9]	3.154
H3	H29B[9]	3.002	H5	F4[5]	3.469
H5	F5[5]	3.534	H5	H26B[10]	3.296
H5	H32C[13]	3.286	H7A	F4[5]	3.110
H7A	C26[10]	3.407	H7A	C27[5]	3.485
H7A	H26A[10]	3.369	H7A	H26B[10]	3.395
H7A	H26C[10]	2.916	H7A	H27A[5]	3.276
H7A	H27B[5]	2.834	H7B	F4[5]	3.141
H7B	C27[5]	3.570	H7B	H27A[5]	2.958
H7B	H27B[5]	3.307	H10	C15[7]	3.485
H10	C16[7]	3.488	H10	H3[9]	3.154
H10	H14A[7]	2.780	H10	H32A[7]	3.449
H12	C26[10]	3.337	H12	H22A[10]	3.175
H12	H22B[10]	3.480	H12	H26A[10]	2.576
H12	H26B[10]	3.296	H12	H28B[10]	3.549
H12	H30B[7]	2.847	H14A	C9[7]	3.308
H14A	C10[7]	3.088	H14A	C30[7]	3.278
H14A	H10[7]	2.780	H14A	H30B[7]	3.372
H14A	H30C[7]	2.737	H14B	F2[10]	3.507
H14B	C26[10]	3.280	H14B	H22B[10]	3.512
H14B	H26A[10]	2.637	H14B	H26C[10]	3.125
H14B	H30B[7]	3.530	H14B	H30C[7]	3.325
H17	C1[11]	3.538	H17	C2[11]	3.109

Table S3-12. Intermolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
H17	C3[11]	3.474	H17	C27[11]	3.321
H17	C28[11]	3.252	H17	H26B[11]	3.432
H17	H27C[11]	2.475	H17	H28A[11]	2.701
H17	H28C[11]	3.506	H19	F1[10]	3.491
H19	F2[10]	2.671	H19	F3[10]	3.117
H19	C18[6]	3.510	H19	C25[10]	3.304
H19	C33[6]	3.562	H19	H33A[6]	2.876
H21A	C33[6]	3.391	H21A	H27A[5]	3.165
H21A	H33A[6]	2.625	H21A	H33C[6]	3.336
H21B	F2[10]	3.285	H21B	C27[5]	3.067
H21B	H26C[10]	3.429	H21B	H27A[5]	2.943
H21B	H27B[5]	2.800	H21B	H27C[5]	2.937
H21B	H33A[6]	3.025	H22A	C30[12]	3.576
H22A	H12[1]	3.175	H22A	H30B[12]	2.838
H22B	C30[12]	3.492	H22B	H12[1]	3.480
H22B	H14B[1]	3.512	H22B	H30B[12]	3.048
H22B	H30C[12]	3.174	H22C	C30[12]	3.213
H22C	C31[7]	3.331	H22C	H29A[2]	3.473
H22C	H30A[12]	3.067	H22C	H30B[12]	2.852
H22C	H30C[12]	3.188	H22C	H31A[7]	2.446
H22C	H31C[7]	3.477	H24	F3[4]	3.048
H24	H33A[6]	3.370	H26A	C12[1]	3.431
H26A	C14[1]	3.560	H26A	H7A[1]	3.369
H26A	H12[1]	2.576	H26A	H14B[1]	2.637
H26B	F6[3]	2.891	H26B	H5[1]	3.296
H26B	H7A[1]	3.395	H26B	H12[1]	3.296
H26B	H17[8]	3.432	H26B	H32C[8]	2.848
H26C	F6[3]	2.857	H26C	C27[3]	3.323
H26C	H7A[1]	2.916	H26C	H14B[1]	3.125
H26C	H21B[1]	3.429	H26C	H27B[3]	2.399
H26C	H27C[3]	3.578	H27A	F4[5]	3.424
H27A	C7[5]	3.556	H27A	C21[5]	3.500
H27A	H7A[5]	3.276	H27A	H7B[5]	2.958
H27A	H21A[5]	3.165	H27A	H21B[5]	2.943
H27A	H33C[8]	2.831	H27B	F2[3]	3.572
H27B	C7[5]	3.503	H27B	C26[3]	3.343
H27B	H7A[5]	2.834	H27B	H7B[5]	3.307

Table S3-12. Intermolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
H27B	H21B^{5}	2.800	H27B	H26C^{3}	2.399
H27C	F6^{3}	3.589	H27C	C17^{8}	3.120
H27C	C18^{8}	3.475	H27C	C33^{8}	3.186
H27C	H17^{8}	2.475	H27C	H21B^{5}	2.937
H27C	H26C^{3}	3.578	H27C	H33A^{8}	3.283
H27C	H33C^{8}	2.519	H28A	C17^{8}	3.437
H28A	C32^{8}	3.237	H28A	H17^{8}	2.701
H28A	H31B^{1}	3.384	H28A	H32A^{8}	2.768
H28A	H32C^{8}	2.967	H28B	C31^{1}	3.562
H28B	H12^{1}	3.549	H28B	H29B^{9}	3.351
H28B	H31A^{1}	3.123	H28B	H31B^{1}	3.109
H28C	C29^{9}	3.384	H28C	H17^{8}	3.506
H28C	H29B^{9}	2.454	H28C	H31A^{1}	3.580
H28C	H31B^{1}	3.006	H28C	H31C^{9}	3.506
H28C	H32A^{8}	2.885	H29A	F1^{13}	3.487
H29A	C30^{9}	3.213	H29A	H22C^{13}	3.473
H29A	H30A^{9}	2.823	H29A	H30C^{9}	2.721
H29A	H32B^{13}	3.297	H29A	H33B^{8}	3.301
H29B	C28^{9}	3.248	H29B	H3^{9}	3.002
H29B	H28B^{9}	3.351	H29B	H28C^{9}	2.454
H29B	H30A^{9}	3.112	H29C	C32^{13}	2.891
H29C	H31C^{14}	3.457	H29C	H32A^{13}	2.752
H29C	H32B^{13}	2.503	H29C	H32C^{13}	2.942
H30A	C29^{9}	3.411	H30A	H22C^{12}	3.067
H30A	H29A^{9}	2.823	H30A	H29B^{9}	3.112
H30B	C11^{7}	3.566	H30B	C12^{7}	2.976
H30B	C13^{7}	3.344	H30B	C22^{12}	3.086
H30B	H12^{7}	2.847	H30B	H14A^{7}	3.372
H30B	H14B^{7}	3.530	H30B	H22A^{12}	2.838
H30B	H22B^{12}	3.048	H30B	H22C^{12}	2.852
H30B	H31A^{7}	3.548	H30C	C14^{7}	3.366
H30C	C22^{12}	3.527	H30C	C29^{9}	3.582
H30C	H14A^{7}	2.737	H30C	H14B^{7}	3.325
H30C	H22B^{12}	3.174	H30C	H22C^{12}	3.188
H30C	H29A^{9}	2.721	H31A	O3^{7}	3.363
H31A	O4^{7}	3.566	H31A	C22^{7}	3.268
H31A	H22C^{7}	2.446	H31A	H28B^{10}	3.123

Table S3-12. Intermolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
H31A	H28C[10]	3.580	H31A	H30B[7]	3.548
H31A	H32A[7]	3.353	H31A	H32B[7]	3.485
H31B	C28[10]	3.348	H31B	H28A[10]	3.384
H31B	H28B[10]	3.109	H31B	H28C[10]	3.006
H31B	H32A[7]	3.237	H31C	O4[7]	3.259
H31C	C15[7]	3.524	H31C	C16[7]	3.226
H31C	C32[7]	2.709	H31C	H22C[7]	3.477
H31C	H28C[9]	3.506	H31C	H29C[14]	3.457
H31C	H32A[7]	2.047	H31C	H32B[7]	2.740
H31C	H32C[7]	3.547	H32A	C28[11]	3.261
H32A	C31[7]	2.960	H32A	H10[7]	3.449
H32A	H28A[11]	2.768	H32A	H28C[11]	2.885
H32A	H29C[2]	2.752	H32A	H31A[7]	3.353
H32A	H31B[7]	3.237	H32A	H31C[7]	2.047
H32B	F5[4]	3.115	H32B	C29[2]	3.305
H32B	C31[7]	3.518	H32B	H29A[2]	3.297
H32B	H29C[2]	2.503	H32B	H31A[7]	3.485
H32B	H31C[7]	2.740	H32C	F5[4]	2.781
H32C	F6[4]	3.120	H32C	C23[4]	3.529
H32C	H5[2]	3.286	H32C	H26B[11]	2.848
H32C	H28A[11]	2.967	H32C	H29C[2]	2.942
H32C	H31C[7]	3.547	H33A	F3[10]	3.182
H33A	F4[6]	3.079	H33A	F5[6]	3.324
H33A	C19[6]	2.942	H33A	C20[6]	2.998
H33A	C21[6]	3.046	H33A	H19[6]	2.876
H33A	H21A[6]	2.625	H33A	H21B[6]	3.025
H33A	H24[6]	3.370	H33A	H27C[11]	3.283
H33B	F1[10]	2.882	H33B	F3[10]	3.063
H33B	F4[6]	3.283	H33B	F5[6]	2.845
H33B	C4[11]	3.458	H33B	C5[11]	3.575
H33B	C25[10]	3.469	H33B	H29A[11]	3.301
H33C	F4[6]	3.052	H33C	C1[11]	3.441
H33C	C4[11]	3.466	H33C	C5[11]	3.289
H33C	C6[11]	3.291	H33C	C27[11]	3.094
H33C	H21A[6]	3.336	H33C	H27A[11]	2.831
H33C	H27C[11]	2.519			

Symmetry Operators:

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

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