Electronic Supplementary Information (ESI)

for

Synthesis and Structural Analysis of Aryloxo-Modified Trinuclear Half-Titanocenes, and their Use as Catalyst Precursors for Ethylene Polymerization

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Contents

1. Additional experiments for the reactions of Cp'TiX_3 with [(LiO-2,4-$R_2C_6H_2$)-6-CH_2]$_3$N or [(HO-2,4-$R_2C_6H_2$)-6-CH_2]$_3$N.

1.1. Reaction of Cp*$TiCl_3$ with [(LiO-2,4-$Me_2C_6H_2$)-6-CH_2]$_3$N.

To a Et_2O (or toluene) solution (5 mL) containing Cp*$TiCl_3$ (87 mg, 0.3 mmol, or 145 mg, 0.5 mmol) was added Et_2O (or toluene) solution (2.5 mL) containing 44 mg (0.1 mmol) [(LiO-2,4-$Me_2C_6H_2$)-6-CH_2]$_3$N dropwise at -30 ºC. The reaction mixture was warmed slowly to room temperature and then was stirred overnight. After the removal of solvents, the reaction mixture was analyzed by ^{1}H NMR. As shown in Figures S1-1 and S1-2, bimetallic complex **2** and remained Cp*$TiCl_3$ were observed as major species in ^{1}H NMR spectra irrespective of equivalence (either 3 or 5 equiv) of Cp*$TiCl_3$ and solvent employed.

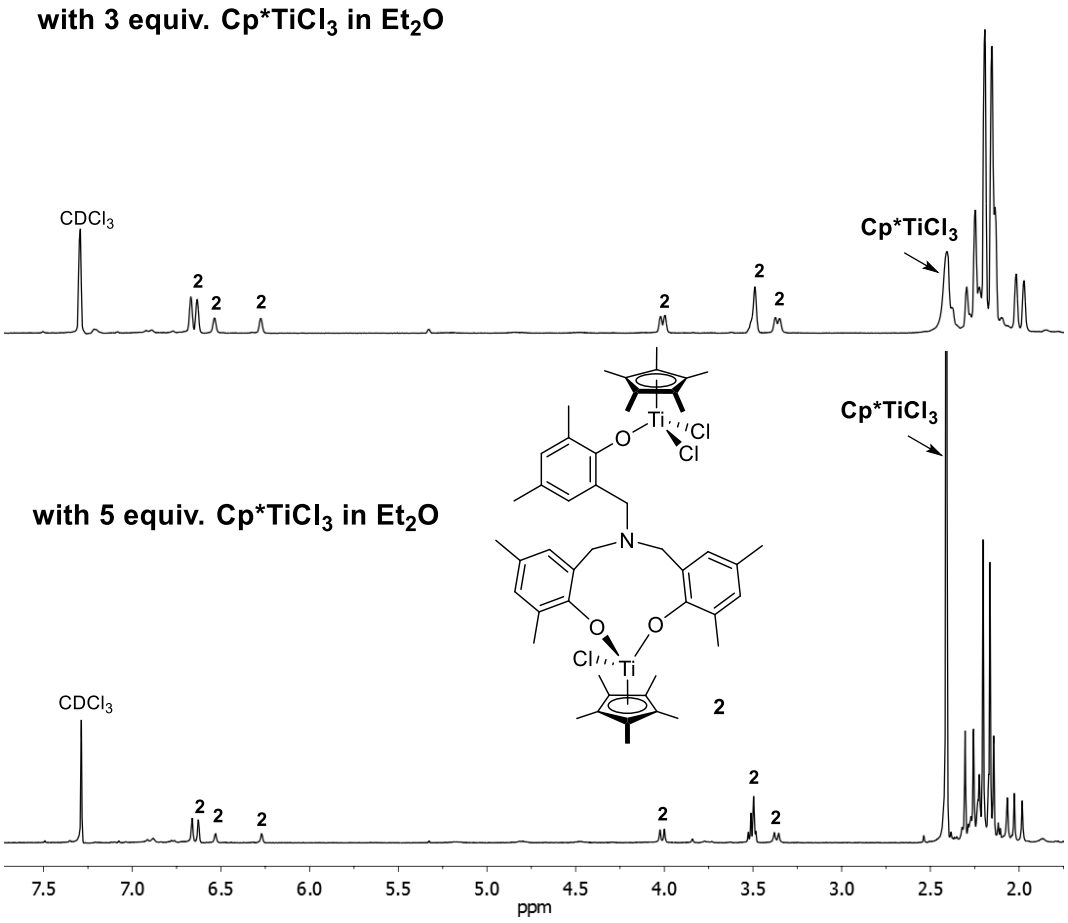

Figure S1-1. ^{1}H NMR spectra (in $CDCl_3$) for the reaction mixture of Cp*$TiCl_3$ with (LiO-2,4-$Me_2C_6H_2$-6-CH_2)$_3$N (conducted in Et_2O).

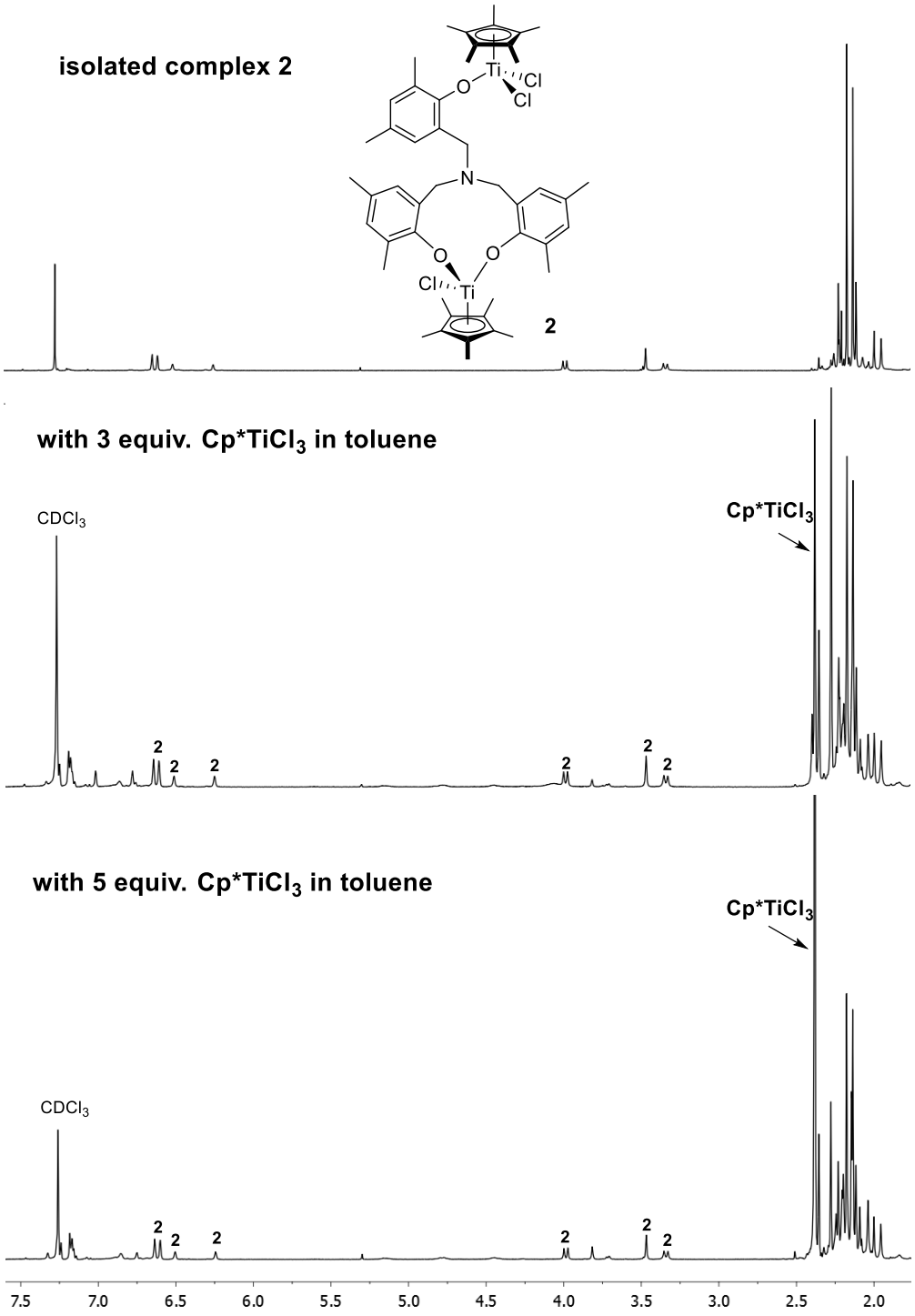

Figure S1-2. ^{1}H NMR spectra (in $CDCl_3$) for the reaction mixture of Cp^*TiCl_3 with $[(LiO\text{-}2,4\text{-}Me_2C_6H_2)\text{-}6\text{-}CH_2]_3N$ (conducted in toluene).

1.2. Reaction of (1,2,4-$Me_3C_5H_2$)$TiCl_3$ with [(LiO-2,4-$Me_2C_6H_2$)-6-CH_2]$_3$N.

The reactions were conducted similarly to those of Cp*$TiCl_3$ with [(LiO-2,4-$Me_2C_6H_2$)-6-CH_2]$_3$N (described in 1.1), except that (1,2,4-$Me_3C_5H_2$)$TiCl_3$ (78 mg, 0.3 mmol, or 131 mg, 0.5 mmol) was used in place of Cp*$TiCl_3$. As shown in Figure S1-3, bimetallic complex **3** and remained (1,2,4-$Me_3C_5H_2$)$TiCl_3$ were observed as major species in ^{1}H NMR spectra irrespective of equivalence (either 3 or 5 equiv) of (1,2,4-$Me_3C_5H_2$)$TiCl_3$ employed.

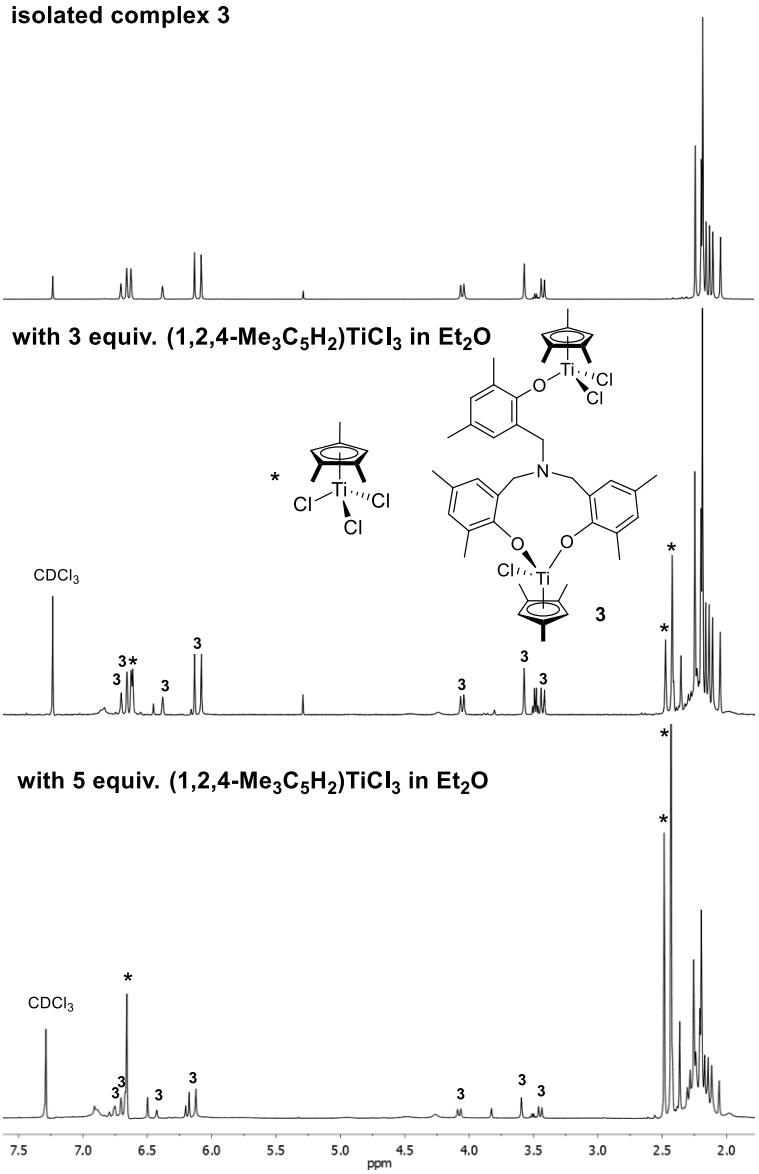

Figure S1-3. ^{1}H NMR spectra (in $CDCl_3$) for the reaction mixture of (1,2,4-$Me_3C_5H_2$)$TiCl_3$ with (LiO-2,4-$Me_2C_6H_2$-6-CH_2)$_3$N (conducted in Et_2O).

1.3. Reaction of Cp^*TiMe_3 (generated *in situ*) with $[(HO\text{-}2,4\text{-}^tBu_2C_6H_2)\text{-}6\text{-}CH_2]_3N$ for attempted synthesis of $[Cp^*TiMe_2\{(O\text{-}2,4\text{-}^tBu_2C_6H_2)\text{-}6\text{-}CH_2\}]_3N$ (9).

Into a toluene solution (18 mL) containing Cp^*TiCl_3 (87 mg, 0.30 mmol) was added MeLi (0.94 mmol, in 0.85 mL Et_2O solution) slowly at -30 ºC. The stirred reaction mixture was warmed slowly to room temperature, and the mixture covered by Al foil was then stirred for 3 h. Into the solution, toluene solution (6.0 mL) containing $[(HO\text{-}2,4\text{-}^tBu_2C_6H_2)\text{-}6\text{-}CH_2]_3N$ (67 mg, 0.10 mmol) was then added by several portions at -30 ºC. The reaction mixture was warmed slowly to room temperature, and then stirred overnight. After the removal of solvents, the reaction mixture was analyzed by ^1H NMR. As shown in Figure S1-4, Cp^*TiMe_3 and $[(HO\text{-}2,4\text{-}^tBu_2C_6H_2)\text{-}6\text{-}CH_2]_3N$ remained were observed in ^1H NMR spectra, whereas no other complexes, such as $[Cp^*TiMe_2\{(O\text{-}2,4\text{-}^tBu_2C_6H_2)\text{-}6\text{-}CH_2\}]_3N$ (**9**), were observed.

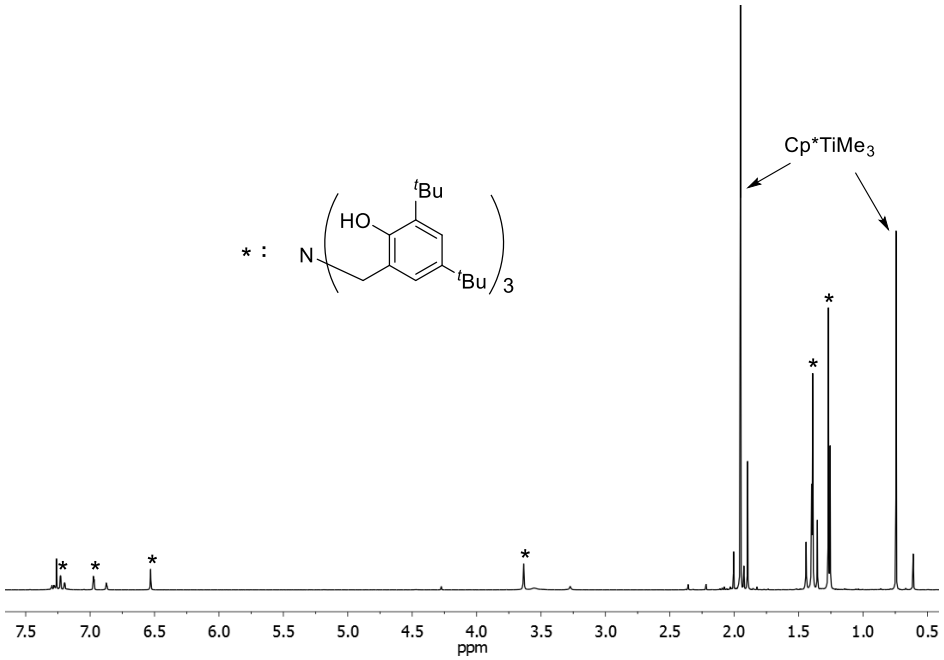

Figure S1-4. ^1H NMR spectra (in $CDCl_3$) for the reaction mixture of Cp^*TiMe_3 (generated *in situ*) with $[(HO\text{-}2,4\text{-}^tBu_2C_6H_2)\text{-}6\text{-}CH_2]_3N$.

2. Additional VT ^{1}H NMR spectra for [CpTiCl$_2${(O-2,4-Me$_2$C$_6$H$_2$)-6-CH$_2$}]$_3$N (1).

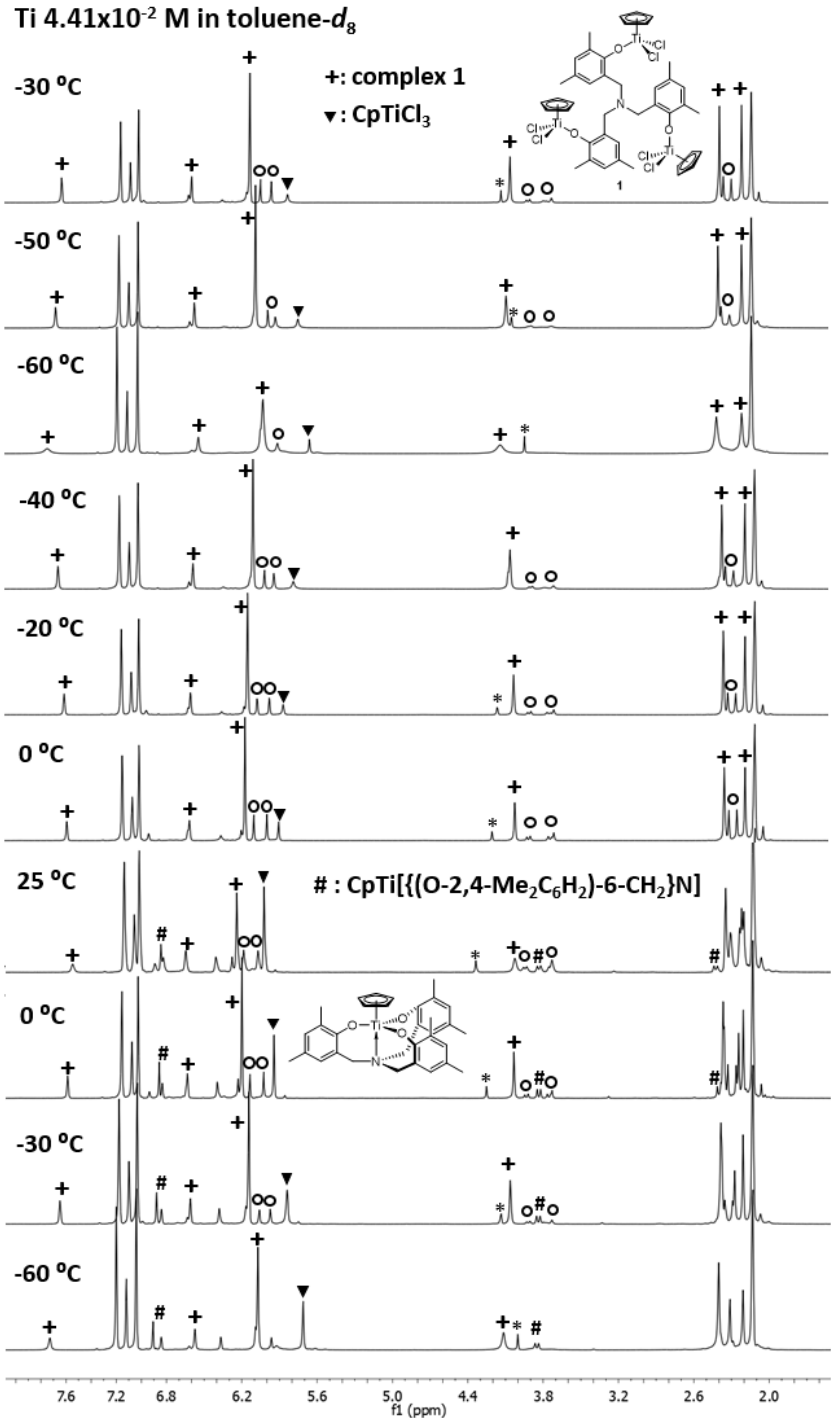

Figure S2-1. VT ^{1}H NMR spectra (prepared at -30 °C) of toluene-d_8 solution containing [CpTiCl$_2${(O-2,4-Me$_2$C$_6$H$_2$)-6-CH$_2$}]$_3$N (**1**) with rather high Ti concentration (Ti 4.41×10^{-2} M). Complex **1** (+), CpTiCl$_3$ (▼), CpTi[(O-2,4-Me$_2$C$_6$H$_2$)-6-CH$_2$]$_3$N (#), assumed bimetallic species (○). *Impurity.

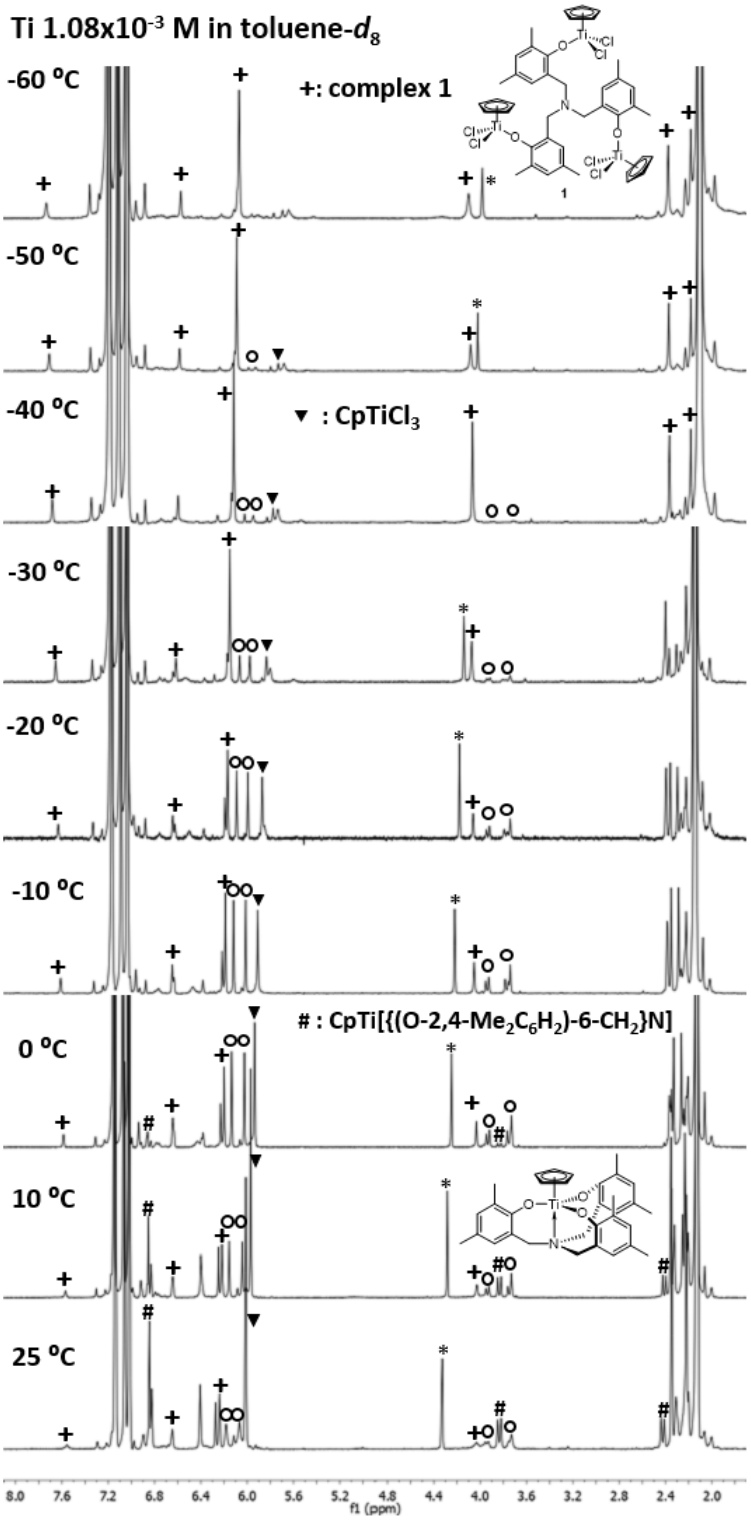

Figure S2-2. VT ^{1}H NMR spectra (prepared at -60 °C) of toluene-d_8 solution containing [$CpTiCl_2${(O-2,4-$Me_2C_6H_2$)-6-CH_2}]$_3$N (**1**) with rather low Ti concentration (Ti 1.08×10^{-3} M). Complex **1** (+), $CpTiCl_3$ (▼), CpTi[(O-2,4-$Me_2C_6H_2$)-6-CH_2]$_3$N (#), assumed bimetallic species (○). *Impurity.

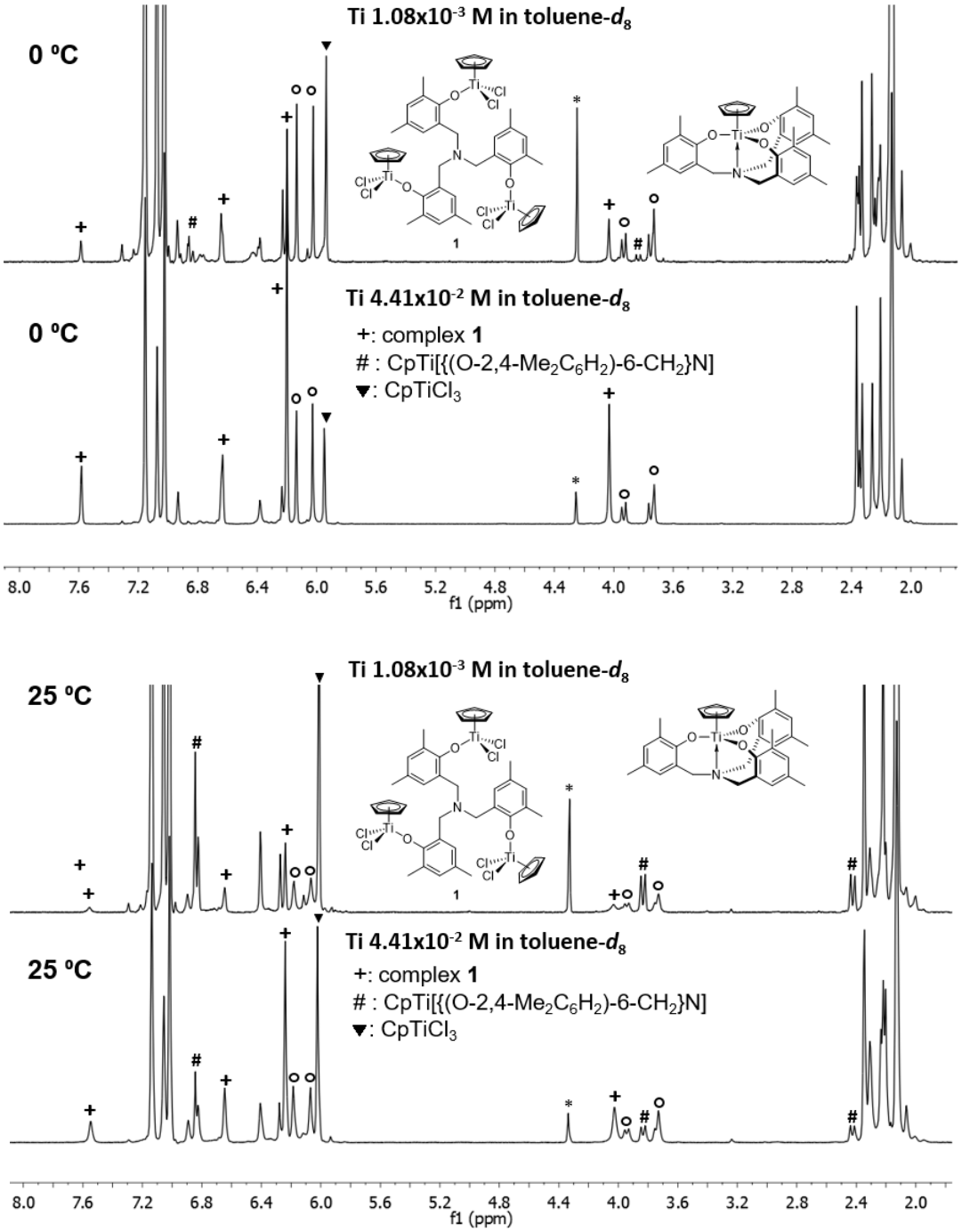

Figure S2-3. ^{1}H NMR spectra of toluene-d_8 solution (at 0 ºC or 25 ºC) containing $[CpTiCl_2\{(O\text{-}2,4\text{-}Me_2C_6H_2)\text{-}6\text{-}CH_2\}]_3N$ (**1**) under rather high Ti concentration (Ti 4.41×10^{-2} M) and low (Ti 1.08×10^{-3} M) concentration conditions. Complex **1** (+), $CpTiCl_3$ (▼), $CpTi[(O\text{-}2,4\text{-}Me_2C_6H_2)\text{-}6\text{-}CH_2]_3N$ (#), assumed bimetallic species (〇). *Impurity.

3. ^{1}H NMR spectra for [Cp'TiCl$_2${(O-2,4-Me$_2$C$_6$H$_2$)-6-CH$_2$}][Cp'TiCl{(O-2,4-Me$_2$C$_6$H$_2$)-6-CH$_2$}$_2$]N [Cp' = Cp* (2), 1,2,4-Me$_3$C$_5$H$_2$ (3)], and [Cp'TiCl$_2${(O-2,4-R$_2$C$_6$H$_2$)-6-CH$_2$}]$_3$N [R = Me, Cp' = Cp (1); R = ^{t}Bu, Cp' = Cp (4), Cp* (5), ^{t}BuC$_5$H$_4$ (6), 1,2,4-Me$_3$C$_5$H$_2$ (7)] upon heating in toluene-d_8 at 80 °C (for 30 min).

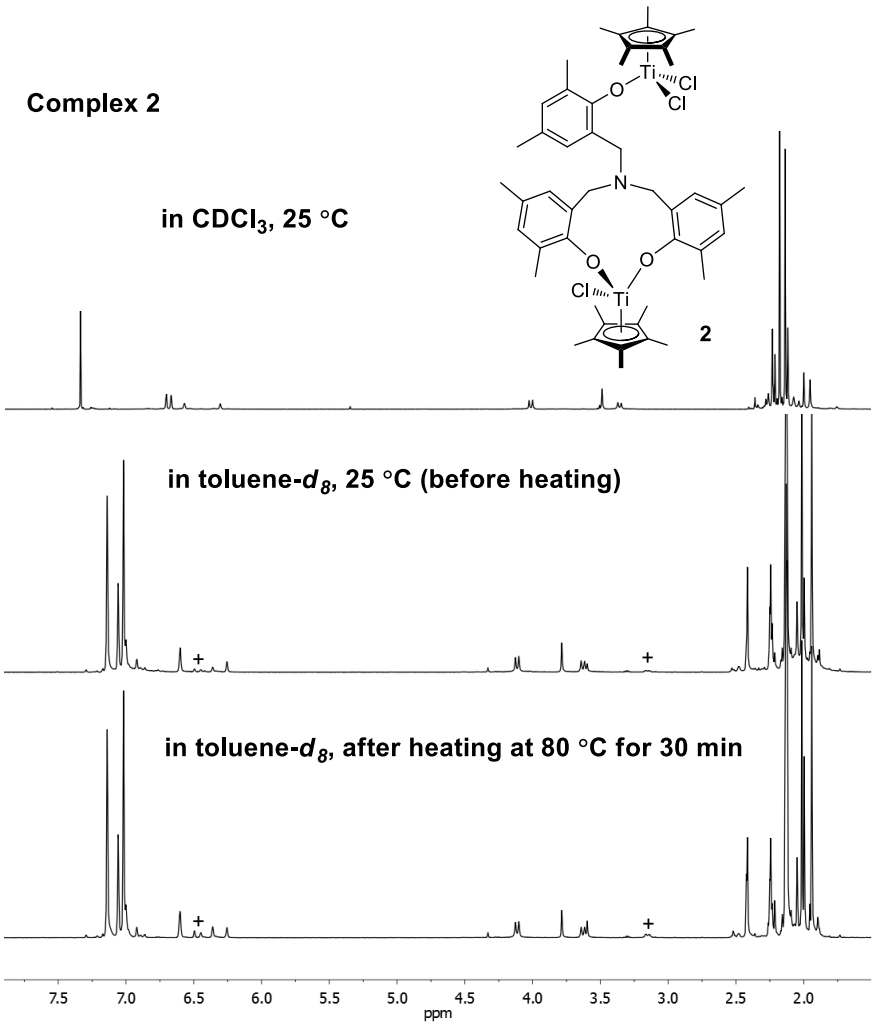

Figure S2-4. ^{1}H NMR spectra (at 25 °C) of toluene-d_8 solution containing [Cp*TiCl$_2${(O-2,4-Me$_2$C$_6$H$_2$)-6-CH$_2$}][Cp*TiCl{(O-2,4-Me$_2$C$_6$H$_2$)-6-CH$_2$}$_2$]N (**2**) after heating at 80 °C for 30 min. Resonances marked with + are resonances which would be different from **2**.

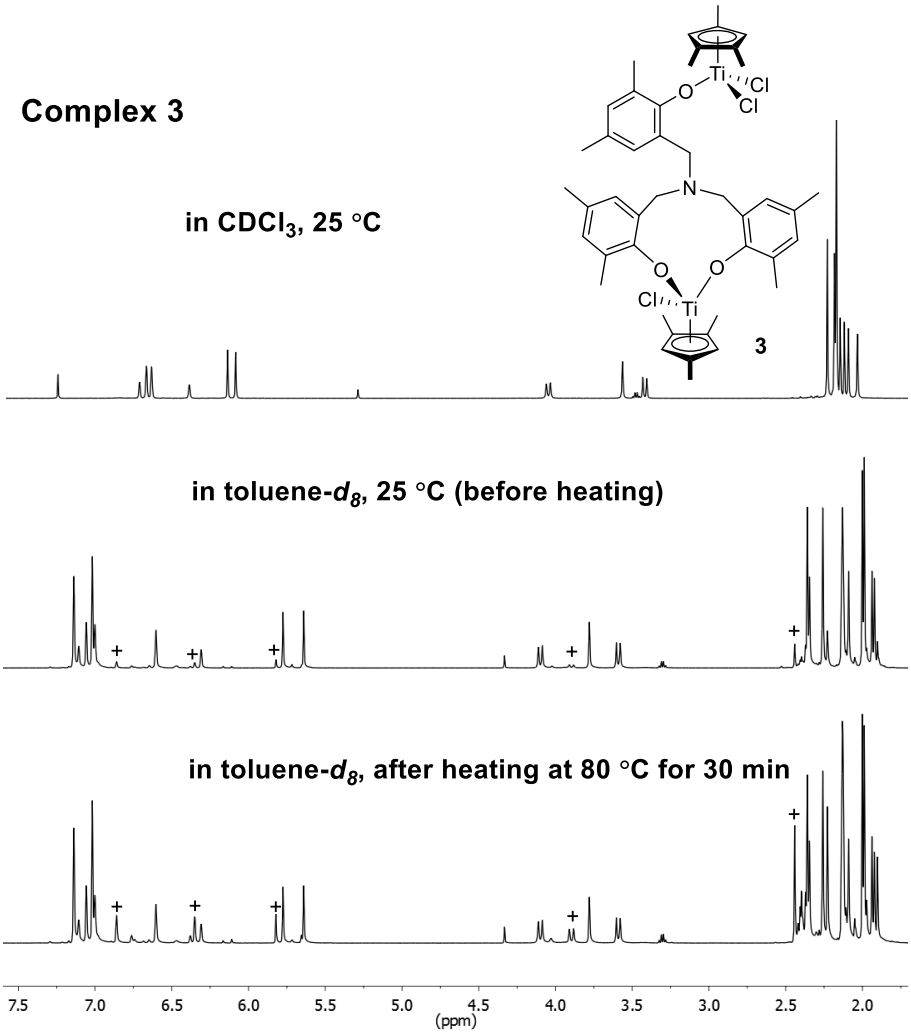

Figure S2-5. ^{1}H NMR spectra (at 25 ºC) of toluene-d_8 solution containing [(1,2,4-$Me_3C_5H_2$)$TiCl_2${(O-2,4-$Me_2C_6H_2$)-6-CH_2}][(1,2,4-$Me_3C_5H_2$)TiCl{(O-2,4-$Me_2C_6H_2$)-6-CH_2}$_2$]N (**3**) after heating at 80 ºC for 30 min. Resonances marked with + are resonances which would be different from **3**.

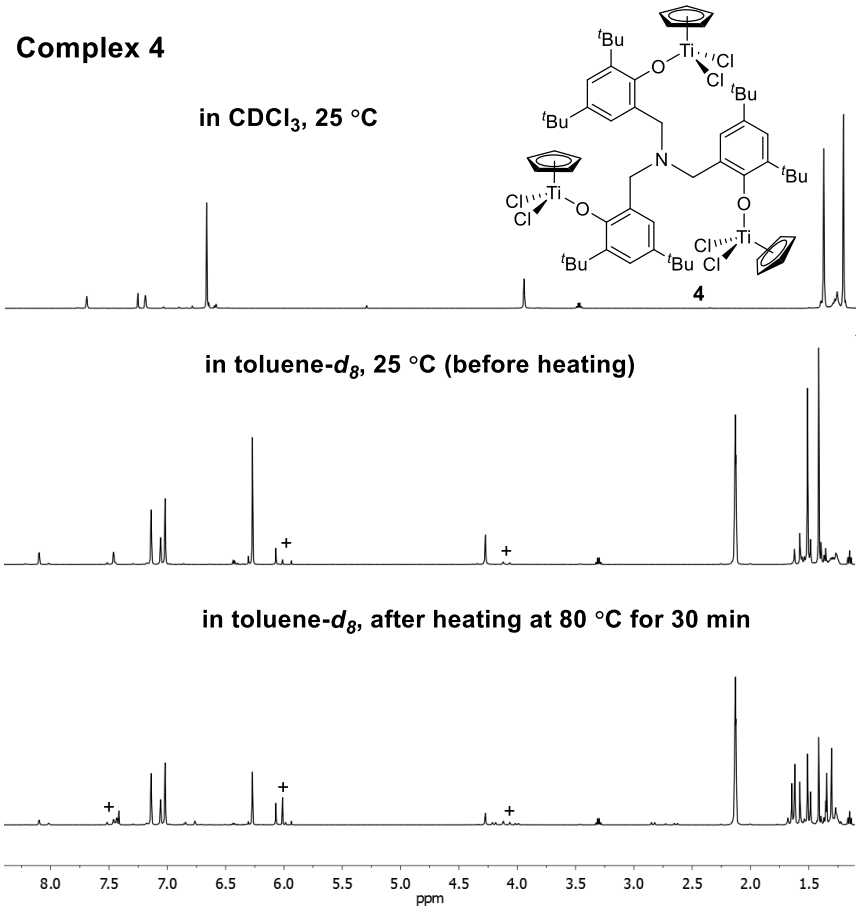

Figure S2-6. ^{1}H NMR spectra of toluene-d_8 solution (at 25 ºC) containing $[CpTiCl_2\{(O\text{-}2,4\text{-}^{t}Bu_2C_6H_2)\text{-}6\text{-}CH_2\}]_3N$ (**4**) after heating at 80 ºC for 30 min. Resonances marked with + are resonances which would be different from **4**.

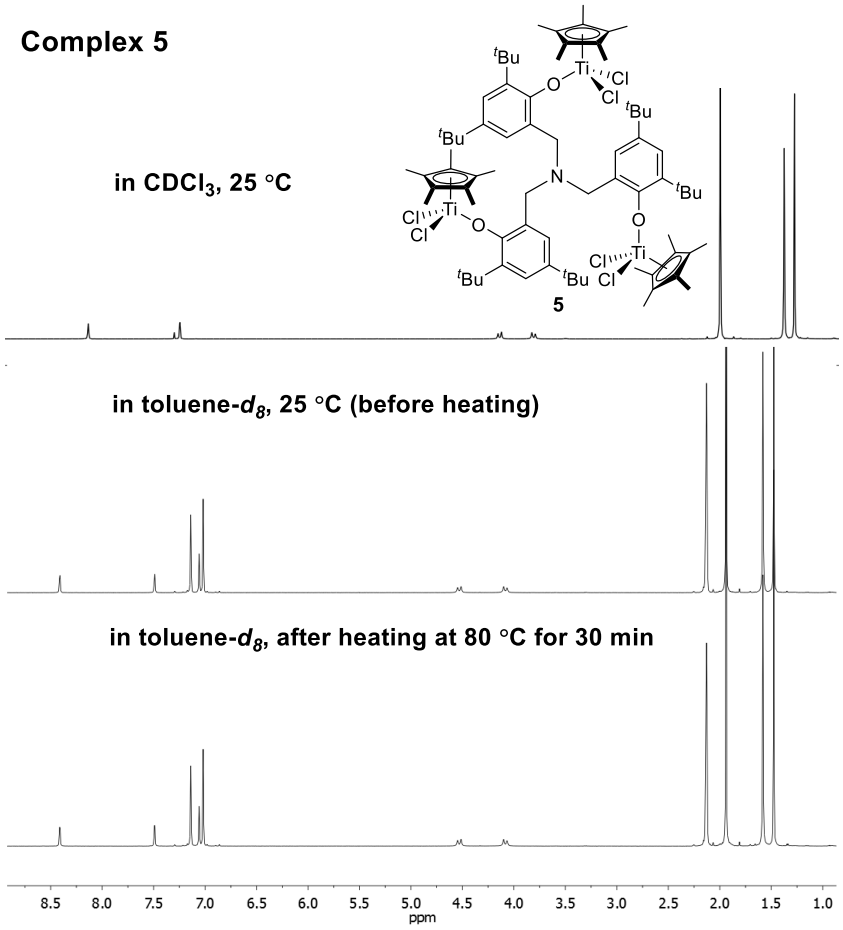

Figure S2-7. ^{1}H NMR spectra of toluene-d_8 solution (at 25 ºC) containing $[Cp^*TiCl_2\{(O\text{-}2,4\text{-}^tBu_2C_6H_2)\text{-}6\text{-}CH_2\}]_3N$ (**5**) after heating at 80 ºC for 30 min.

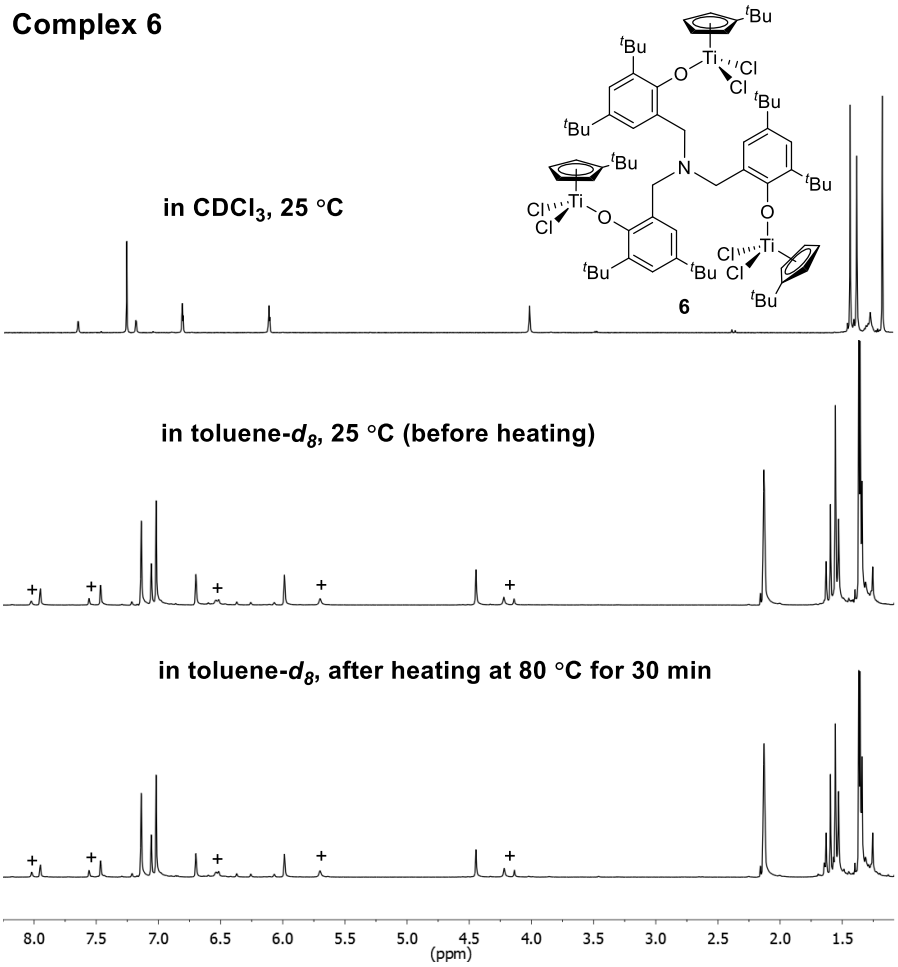

Figure S2-8. ^{1}H NMR spectra of toluene-d_8 solution (at 25 ºC) containing [(^{t}BuC$_5$H$_4$)TiCl$_2${(O-2,4-^{t}Bu$_2$C$_6$H$_2$)-6-CH$_2$}]$_3$N (**6**) after heating at 80 ºC for 30 min. Resonances marked with + are resonances which would be different from **6**.

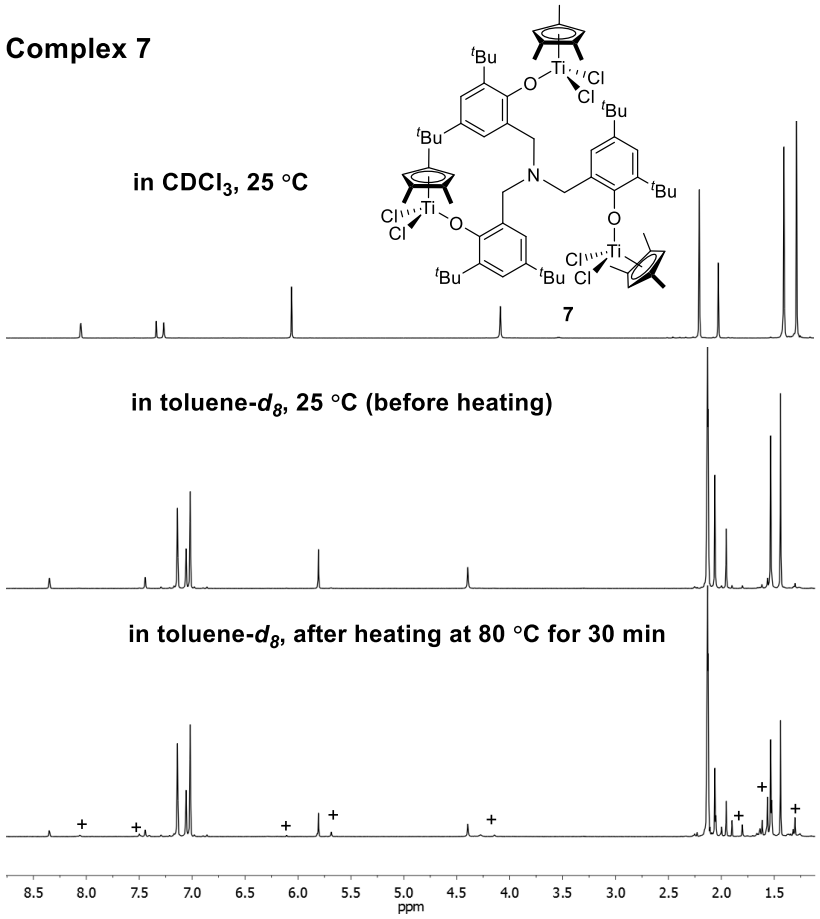

Figure S2-9. ^{1}H NMR spectra of toluene-d_8 solution (at 25 ºC) containing [(1,2,4-$Me_3C_5H_2$)$TiCl_2${(O-2,4-$^t Bu_2C_6H_2$)-6-CH_2}]$_3$N (**7**) after heating at 80 ºC for 30 min. Resonances marked with + are resonances which would be different from **7**.

4. Additional ethylene polymerization results.

Table S1. Ethylene polymerization by [Cp'$TiCl_2${(O-2,4-$R_2C_6H_2$)-6-CH_2}]$_3$N [R = Me, Cp' = Cp (**1**); R = ^{t}Bu, Cp' = Cp (**4**), Cp* (**5**), ^{t}BuC_5H_4 (**6**), 1,2,4-$Me_3C_5H_2$ (**7**)], [Cp'$TiCl_2${(O-2,4-$Me_2C_6H_2$)-6-CH_2}][Cp'TiCl{(O-2,4-$Me_2C_6H_2$)-6-CH_2}$_2$]N [Cp' = Cp* (**2**), 1,2,4-$Me_3C_5H_2$ (**3**)], and [Cp*$TiMe_2${(O-2,4-$R_2C_6H_2$)-6-CH_2}]$_3$N [R = Me (**8**), ^{t}Bu (**9**)] in the presence of MAO cocatalyst (ethylene 4 atm, 25 ºC).[a]

run	catalyst (μmol)	MAO / mmol	time / min	polymer / mg	activity [b]	M_n[c]×10^{-4}	M_w/M_n[c]
1	**1** (0.50)	3.0	10	80	320	341	2.13
S1	**1** (0.50)	3.0	10	70	280	358	2.06
2	**2** (0.03)	3.0	10	107	10700	309, 3.91	2.11, 1.95
S2	**2** (0.03)	3.0	10	93	9300	354, 3.97	1.62, 2.24
3	**2** (0.03)	3.0	5	78	15600	368, 3.09	2.67, 2.19
4	**2** (0.03)	3.0	5	75	15000	300, 1.93	2.29, 2.58
5	**3** (0.30)	3.0	10	116	1160	368, 0.96	1.72, 1.82
S3	**3** (0.30)	3.0	10	101	1010	375, 1.02	1.82, 2.02
6	**4** (0.50)	2.0	10	120	480	220	2.13
7	**4** (0.50)	2.0	10	124	496	239	2.21
8	**4** (0.50)	3.0	10	186	744	204	2.44
9	**4** (0.50)	3.0	10	180	720	202	2.48
10	**4** (0.50)	4.0	10	140	560	238	2.64
11	**4** (0.50)	4.0	10	136	544	232	2.66
12	**5** (0.50)	3.0	10	107	428	172	2.90
S4	**5** (0.50)	3.0	10	96	384	164	2.76
13	**6** (0.50)	3.0	10	44	176	277	2.26
S5	**6** (0.50)	3.0	10	38	157	268	2.06
14	**7** (0.25)	3.0	10	75	600	93.1, 1.12	3.95, 2.11
S6	**7** (0.25)	3.0	10	62	496	74.8, 0.82	4.00, 2.05
15	**7** (0.25)	3.0	5	26	416	238, 0.97	2.75, 2.05
S7	**7** (0.25)	3.0	5	23	368	238, 1.37	2.70, 1.68
16	**8** (0.01)	3.0	10	84	16800	214	2.20
S9	**8** (0.01)	3.0	10	75	15000	190	2.38
17	**9** (0.10)	3.0	10	453	9060	354	2.24
S10	**9** (0.10)	3.0	10	436	8720	368	2.16
18	**9** (0.01)	3.0	10	58	11600	128	3.04
S11	**9** (0.01)	3.0	10	55	11000	121	3.16

[a]Conditions: toluene total 30 mL, d-MAO (prepared by removing toluene and $AlMe_3$ from the ordinary MAO). [b]Activity in kg-PE/mol-Ti·h. [c]GPC data in *o*-dichlorobenzene *vs* polystyrene standards.

Table S2. Effect of polymerization temperature in ethylene polymerization by [Cp*$TiCl_2${(O-2,4-$Me_2C_6H_2$)-6-CH_2}][Cp*$TiCl${(O-2,4-$Me_2C_6H_2$)-6-CH_2}$_2$]N (**2**), [Cp'$TiCl_2${(O-2,4-$^tBu_2C_6H_2$)-6-CH_2}]$_3$N [Cp' = Cp (**4**), Cp* (**5**), $^tBuC_5H_4$ (**6**), 1,2,4-$Me_3C_5H_2$ (**7**)], and [Cp*$TiMe_2${(O-2,4-$R_2C_6H_2$)-6-CH_2}]$_3$N [R = Me (**8**), ^{t}Bu (**9**)] in the presence of MAO cocatalyst.[a]

run	catalyst (μmol)	temp. / ºC	time / min	polymer / mg	activity [b]	M_n[c]×10^{-4}	M_w/M_n[c]
8	**4** (0.50)	25	10	186	744	204	2.44
19	**4** (0.10)	50	10	74	1480	215	2.04
S12	**4** (0.10)	50	10	62	1240	208	2.24
13	**6** (0.50)	25	10	44	176	277	2.26
20	**6** (0. 30)	50	10	58	387	226	2.48
S13	**6** (0.30)	50	10	50	333	228	2.46
14	**7** (0.25)	25	10	75	600	93.1, 112	3.95, 2.11
21	**7** (0.10)	50	10	43	860	220, 0.67	2.15, 1.62
S14	**7** (0.10)	50	10	41	820	232, 0.58	2.27, 1.76
2	**2** (0.03)	25	10	107	10700	309, 3.91	2.11, 1.95
22	**2** (0.05)	50	10	140	8400	220, 1.44	1.67, 2.13
S15	**2** (0.05)	50	10	132	7920	228, 1.61	1.73, 1.81
23	**2** (0.05)	80	10	65	3900	173, 0.95	1.47, 1.81
S16	**2** (0.05)	80	10	61	3660	169, 0.85	1.59, 1.86
12	**5** (0.50)	25	10	107	428	172	2.90
24	**5** (0.10)	50	10	158	3160	113	2.85
S17	**5** (0.10)	50	10	145	2900	101	3.19
25	**5** (0.10)	80	10	150	3000	26, 0.83	3.08, 1.63
S18	**5** (0.10)	80	10	128	2560	30, 0.84	3.76, 1.33
26	**5** (0.10)	80	5	121	4840	38, 0.88	4.85, 1.64
S19	**5** (0.10)	80	5	117	4680	36, 0.97	4.81, 1.53
27	**5** (0.10)	100	10	68	1360	112, 0.61	1.92, 1.68
S20	**5** (0.10)	100	10	51	1020	100, 0.63	1.68, 1.98
16	**8** (0.01)	25	10	84	16800	214	2.2
28	**8** (0.02)	50	10	128	12800	215, 1.44	1.49, 2.06
S21	**8** (0.02)	50	10	112	11200	198, 1.37	1.66, 2.00
29	**8** (0.02)	50	5	110	22000	277, 2.09	2.33, 1.79
S22	**8** (0.02)	50	5	101	20200	273, 1.99	2.37, 1.87
30	**8** (0.04)	80	10	84	4200	180, 0.96	1.53, 1.69
S23	**8** (0.04)	80	10	80	4000	184, 0.99	1.50, 1.73
17	**9** (0.10)	25	10	453	9060	354	2.24
31	**9** (0.05)	50	10	107	4280	126, 2.44	3.94, 1.53
S24	**9** (0.05)	50	10	89	3560	120, 2.09	4.10, 1.32

[a] Conditions: toluene total 30 mL, d-MAO 3.0 mmol, ethylene 4 atm. [b] Activity in kg-PE/mol-Ti·h.
[c] GPC data in *o*-dichlorobenzene *vs* polystyrene standards.

Table S3. Ethylene polymerization by Cp'$TiCl_2$(O-2-R-4,6-$Me_2C_6H_2$) [Cp' = Cp, R = Me (**10**), ^{t}Bu (**11**); Cp' = Cp*, R = Me (**12**), ^{t}Bu (**13**)] in the presence of MAO cocatalyst.[a]

run	catalyst (μmol)	temp. / ºC	polymer / mg	activity [b]	M_n[c]×10^{-4}	M_w/M_n[c]
32	**10** (0.50)	25	110	1320	305	2.15
S25	**10** (0.50)	25	96	1150	301	2.10
33	**11** (0. 50)	25	128	1540	30.3	7.69
34	**11** (0.50)	50	144	1730	78.4	4.35
S26	**11** (0.50)	50	141	1690	75.8	4.06
35	**12** (0.50)	25	430	5160	208	2.09
36	**12** (0.10)	25	173	10400	139	2.71
S27	**12** (0.10)	25	158	9480	131	2.80
37	**13** (0.50)	25	189	2270	26.0	9.33
38	**13** (0.50)	50	199	2390	121	2.92
S28	**13** (0.50)	50	208	2500	121	3.37

[a] Conditions: toluene total 30 mL, d-MAO 3.0 mmol, ethylene 4 atm, 10 min. [b] Activity in kg-PE/mol-Ti·h. [c]GPC data in *o*-dichlorobenzene *vs* polystyrene standards.

Table S4. Ethylene polymerization by [Cp*TiX$_2$\{(O-2,4-^{t}Bu$_2$C$_6$H$_2$)-6-CH$_2$\}]$_3$N [X = Cl (**5**), Me (**9**)], [Cp*TiMe$_2$\{(O-2,4-Me$_2$C$_6$H$_2$)-6-CH$_2$\}]$_3$N (**8**), Cp*TiCl$_2$(2-R-4,6 Me$_2$C$_6$H$_2$)) [R = Me (**12**), ^{t}Bu (**13**)] in the presence of Al^{i}Bu$_3$/[Ph$_3$C][B(C$_6$F$_5$)$_4$] cocatalysts.[a]

run	catalyst (μmol)	Al/Ti[b]	temp. / ºC	polymer / mg	activity [c]	M_n[d]×10^{-4}	M_w/M_n[d]
39	**5** (0.02)	700	25	71	7100	71.6	3.37
S29	**5** (0.02)	700	25	63	6300	71.6	3.45
40	**8** (0.02)	100	25	trace			
41	**8** (0.01)	300	25	60	12000	71.6	3.78
42	**8** (0.01)	500	25	84	16800	88.1	3.79
43	**8** (0.01)	700	25	138	27600	115	3.15
S30	**8** (0.01)	700	25	112	22400	124	3.24
44	**8** (0.01)	900	25	36	7200	70.8	3.33
S31	**8** (0.01)	900	25	29	5800	71.6	3.23
45	**8** (0.01)	700	0	61	12200	77.7	2.70
46	**8** (0.01)	700	0	70	14000	78.4	2.70
47	**9** (0.02)	700	25	20	2000	78.5	4.21
S32	**9** (0.02)	700	25	15	1500	76.5	4.26
48	**12** (0.03)	700	25	109	21800	63.7	4.17
S33	**12** (0.03)	700	25	107	21400	65.1	4.98
49	**13** (0.06)	700	25	85	8500	54.9	2.82
S34	**13** (0.06)	700	25	72	7200	52.4	2.84

[a] Conditions: toluene total 30 mL, Al^{i}Bu$_3$, [Ph$_3$C][B(C$_6$F$_5$)$_4$] B/Ti = 1.5 (molar ratio), 4 atm, 10 min. [b]Molar ratio. [c]Activity in kg-PE/mol-Ti·h. [d]GPC data in *o*-dichlorobenzene *vs* polystyrene standards.

5. Tables summarized in the crystal collection parameter for [Cp'TiCl$_2${(O-2,4-R$_2$C$_6$H$_2$)-6-CH$_2$}]$_3$N [R = Me, Cp' = Cp (1); R = ^{t}Bu, Cp' = Cp (4), Cp* (5), 1,2,4-Me$_3$C$_5$H$_2$ (7)], [Cp'TiCl$_2${(O-2,4-Me$_2$C$_6$H$_2$)-6-CH$_2$}][Cp'TiCl{(O-2,4-Me$_2$C$_6$H$_2$)-6-CH$_2$}$_2$]N [Cp' = Cp* (2), 1,2,4-Me$_3$C$_5$H$_2$ (3)], and [Cp*TiMe$_2${(O-2,4-R$_2$C$_6$H$_2$)-6-CH$_2$}]$_3$N [R = Me (8), ^{t}Bu (9)].

Table S5. Crystal data and collection parameters of [Cp'TiCl$_2${(O-2,4-R$_2$C$_6$H$_2$)-6-CH$_2$}]$_3$N [R = Me, Cp' = Cp (**1**); R = ^{t}Bu, Cp' = Cp (**4**)], [Cp'TiCl$_2${(O-2,4-Me$_2$C$_6$H$_2$)-6-CH$_2$}] [Cp'TiCl{(O-2,4-Me$_2$C$_6$H$_2$)-6-CH$_2$}$_2$]N [Cp' = Cp* (**2**), 1,2,4-Me$_3$C$_5$H$_2$ (**3**)].

	1	**2**	**3**	**4**
Formula	$C_{42}H_{45}Cl_6NO_3Ti_3$	$C_{47}H_{60}Cl_3NO_3Ti_2$	$C_{43}H_{52}Cl_3NO_3Ti_2$	$C_{60}H_{81}Cl_6NO_3Ti_3$
Formula weight	968.24	889.15	833.05	1220.72
Crystal color, Habit	orange, block	red, platelet	red, block	orange, block
Crystal size (mm)	0.250×0.250×0.160	0.210×0.200×0.060	0.200×0.180×0.130	0.120×0.080×0.070
Crystal system	trigonal	monoclinic	monoclinic	trigonal
Space group	R-3c (#167)	P21/c (#14)	P21/c (#14)	R-3 (#148)
a (Å)	16.059(2)	14.275(7)	16.6846(7)	24.4075(13)
b (Å)		22.520(10)	18.4587(6)	
c (Å)	63.922(6)	14.984(7)	14.6183 (7)	23.4369(16)
α (deg)				
β (deg)		100.408(6)	114.144(5)	
γ (deg)				
V (Å^3)	14276(3)	4738(4)	4108.2(3)	12091.4(12)
Z value	12	4	4	6
D_{calcd} (g/cm^3)	1.351	1.246	1.347	1.006
F_{000}	5952	1872	1744	3840
Temp (K)	93	93	93	93
μ (MoKα) (cm^{-1})	8.635	5.443	6.228	5.211
No. of reflections measured (R_{int})	47281	49820	43125	43023
$2\theta_{max}$ (deg)	55.0	55.0	55.0	55.0
No. of observations [$I > 2.00\sigma(I)$]	3657	10837	9423	6172
No. of variables	166	505	469	220
*R*1 [$I > 2.00\sigma(I)$]	0.0982	0.0721	0.0553	0.075
*wR*2 [$I > 2.00\sigma(I)$]	0.222	0.2152	0.1477	0.2317
Goodness of Fit	1.096	1.063	1.037	0.984

Table S6. Crystal data and collection parameters of [Cp'TiCl$_2${(O-2,4-R$_2$C$_6$H$_2$)-6-CH$_2$}]$_3$N [R = ^{t}Bu, Cp' = Cp* (**5**), 1,2,4-Me$_3$C$_5$H$_2$ (**7**)] and [Cp*TiMe$_2${(O-2,4-R$_2$C$_6$H$_2$)-6-CH$_2$}]$_3$N [R = ^{t}Bu (**9**)].

	5	**7**	**9**
Formula	$C_{75}H_{111}Cl_6NO_3Ti_3$	$C_{69}H_{99}Cl_6NO_3Ti_3$	$C_{81}H_{129}NO_3Ti_3$
Formula weight	1431.12	1346.96	1308.62
Crystal color, Habit	red, block	red, plate	orange, block
Crystal size (mm)	0.230×0.190×0.100	0.330×0.130×0.050	0.108×0.090×0.046
Crystal system	monoclinic	monoclinic	monoclinic
Space group	P21/n (#14)	P21/n (#14)	P21/n (#14)
a (Å)	17.5836(9)	13.2258(6)	19.9129(4)
b (Å)	22.4075(10)	22.4804(11)	19.9654(3)
c (Å)	21.6663(10)	24.4338(12)	20.1690(4)
α (deg)			
β (deg)	94.814(4)	99.642(4)	98.7979(19)
γ (deg)			
V (Å^3)	8506.5(7)	7162.1(6)	7924.2(3)
Z value	4	4	4
D_{calcd} (g/cm^3)	1.175	1.249	1.097
F_{000}	3208	2848	2848
Temp (K)	93	93	93
μ (MoKα) (cm^{-1})	5.068	5.929	3.388
No. of reflections measured (R_{int})	89388	75160	65232
$2\theta_{max}$ (deg)	55	55	55
No. of observations [$I > 2.00\sigma(I)$]	19531	16446	17594
No. of variables	838	739	805
*R*1 [$I > 2.00\sigma(I)$]	0.0757	0.0571	0.0579
*wR*2 [$I > 2.00\sigma(I)$]	0.2209	0.133	0.1774
Goodness of Fit	0.945	1.012	1.008

X-ray Structure Report

for

$[CpTiCl_2\{(O\text{-}2,4\text{-}Me_2C_6H_2)\text{-}6\text{-}CH_2\}]_3N$ (**1**)

January 19, 2017

Experimental

Data Collection

An orange block crystal of $C_{42}H_{45}Cl_6NO_3Ti_3$ having approximate dimensions of 0.250 x 0.250 x 0.160 mm was mounted on a glass fiber. All measurements were made on a Rigaku XtaLAB mini diffractometer using multi-layer mirror monochromated Mo-Kα radiation.

The crystal-to-detector distance was 50.00 mm.

Cell constants and an orientation matrix for data collection corresponded to a R-centered trigonal cell (laue class: -3m1) with dimensions:

a = 16.059(2) Å
c = 63.922(6) Å
V = 14276(3) Å^3

For Z = 12 and F.W. = 968.24, the calculated density is 1.351 g/cm^3. Based on the reflection conditions of:

hkil: -h+k+l = 3n
h-h0l: l = 2n

packing considerations, a statistical analysis of intensity distribution, and the successful solution and refinement of the structure, the space group was determined to be:

R-3c(h) (#167)

The data were collected at a temperature of -180 $\pm$ 1^{o}C to a maximum 2θ value of 65.2^o. A total of 540 oscillation images were collected. A sweep of data was done using ω scans from -60.0 to 120.0^o in 1.00^o step, at χ=54.0^o and ϕ = 0.0^o. The exposure rate was 32.0 [sec./^{o}]. The detector swing angle was 30.00^o. A second sweep was performed using ω scans from -60.0 to 120.0^o in 1.00^o step, at χ=54.0^o and ϕ = 120.0^o. The exposure rate was 32.0 [sec./^{o}]. The detector swing angle was 30.00^o. Another sweep was performed using ω scans from -60.0 to 120.0^o in 1.00^o step, at χ=54.0^o and ϕ = 240.0^o. The exposure rate was 32.0 [sec./^{o}]. The detector swing angle

was 30.00°. The crystal-to-detector distance was 50.00 mm. Readout was performed in the 0.073 mm pixel mode.

Data Reduction

Of the 0 reflections were collected, where 0 were unique (R_{int} = 0.1014); equivalent reflections were merged. Data were collected and processed using CrysAlisPro (Rigaku Oxford Diffraction). [1]

The linear absorption coefficient, μ, for Mo-Kα radiation is 8.635 cm^{-1}. An empirical absorption correction was applied which resulted in transmission factors ranging from 0.471 to 0.871. 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 3657 observed reflections and 166 variable parameters and converged (largest parameter shift was 0.00 times its esd) with unweighted and weighted agreement factors of:

$$R1 = \Sigma \, ||Fo| - |Fc|| \, / \, \Sigma \, |Fo| = 0.0982$$

$$wR2 = [\Sigma \, (w \, (Fo^2 - Fc^2)^2) / \Sigma \, w(Fo^2)^2]^{1/2} = 0.2220$$

The goodness of fit[4] was 1.10. Unit weights were used. The maximum and minimum peaks on the final difference Fourier map corresponded to 0.61 and -1.14 $e^-/Å^3$, respectively.

Neutral atom scattering factors were taken from International Tables for Crystallography (IT), Vol. C, Table 6.1.1.4 [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 Version 2014/7[10].

References

(1) CrysAlisPro: Data Collection and Processing Software, Rigaku Corporation (2015). Tokyo 196-8666, Japan.

(2) SHELXT Version 2014/5: Sheldrick, G. M. (2014). Acta Cryst. A70, C1437.

(3) Least Squares function minimized: (SHELXL Version 2014/7)

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

(4) Goodness of fit is defined as:

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

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

(5) International Tables for Crystallography, Vol.C (1992). Ed. A.J.C. Wilson, Kluwer Academic Publishers, Dordrecht, Netherlands, Table 6.1.1.4, pp. 572.

(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 4.2: Crystal Structure Analysis Package, Rigaku Corporation (2000-2015). Tokyo 196-8666, Japan.

(10) SHELXL Version 2014/7: Sheldrick, G. M. (2008). Acta Cryst. A64, 112-122.

EXPERIMENTAL DETAILS

A. Crystal Data

Empirical Formula	$C_{42}H_{45}Cl_6NO_3Ti_3$
Formula Weight	968.24
Crystal Color, Habit	orange, block
Crystal Dimensions	0.250 X 0.250 X 0.160 mm
Crystal System	trigonal
Lattice Type	R-centered
Lattice Parameters	a = 16.059(2) Å c = 63.922(6) Å V = 14276(3) Å^3
Space Group	R-3c (#167)
Z value	12
D_{calc}	1.351 g/cm^3
F_{000}	5952.00
μ(MoKα)	8.635 cm^{-1}

B. Intensity Measurements

Diffractometer	XtaLAB mini
Radiation	MoKα (λ = 0.71073 Å) multi-layer mirror monochromated
Voltage, Current	50kV, 24mA
Temperature	-180.0^{o}C
Detector Aperture	75.0 mm (diameter)
Data Images	540 exposures
ω oscillation Range (χ=54.0, ϕ=0.0)	-60.0 - 120.0^{o}
Exposure Rate	32.0 sec./^{o}
Detector Swing Angle	30.00^{o}
ω oscillation Range (χ=54.0, ϕ=120.0)	-60.0 - 120.0^{o}
Exposure Rate	32.0 sec./^{o}
Detector Swing Angle	30.00^{o}
ω oscillation Range (χ=54.0, ϕ=240.0)	-60.0 - 120.0^{o}
Exposure Rate	32.0 sec./^{o}
Detector Swing Angle	30.00^{o}
Detector Position	50.00 mm
Pixel Size	0.073 mm
$2\theta_{max}$	55.0^{o}
No. of Reflections Measured	Total: 47281

	Unique: 3657 (R_{int} = 0.1014)
Corrections	Lorentz-polarization Absorption (trans. factors: 0.471 - 0.871)

C. Structure Solution and Refinement

Structure Solution	Direct Methods (SHELXT Version 2014/5)
Refinement	Full-matrix least-squares on F^2
Function Minimized	$\Sigma\ w\ (Fo^2 - Fc^2)^2$
Least Squares Weights	$w = 1/ [\ \sigma^2(Fo^2) + (0.0449 \cdot P)^2 + 338.0268 \cdot P\ ]$ 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)	3657
No. Variables	166
Reflection/Parameter Ratio	22.03
Residuals: R1 ($I>2.00\sigma(I)$)	0.0982
Residuals: R (All reflections)	0.1259
Residuals: wR2 (All reflections)	0.2220
Goodness of Fit Indicator	1.096
Max Shift/Error in Final Cycle	0.000
Maximum peak in Final Diff. Map	0.61 $e^-/Å^3$
Minimum peak in Final Diff. Map	-1.14 $e^-/Å^3$

Table S7-1. Atomic coordinates and B_{iso}/B_{eq} and occupancy

atom	x	y	z	B_{eq}	occ
Ti1	0.10567(9)	0.39766(9)	0.46057(2)	3.16(3)	1
Cl1	0.05200(17)	0.24779(17)	0.44836(3)	5.19(5)	1
Cl2	0.24579(14)	0.48561(18)	0.44358(2)	5.01(5)	1
O1	0.1440(3)	0.3950(3)	0.48670(5)	3.06(8)	1
N1	0.33333	0.66667	0.51144(11)	2.39(14)	1/3
C1	0.2969(5)	0.5680(4)	0.50426(8)	2.80(11)	1
C2	0.2109(5)	0.4955(5)	0.51663(8)	2.72(11)	1
C3	0.1397(5)	0.4092(5)	0.50783(8)	2.89(11)	1
C4	0.0659(5)	0.3379(5)	0.51960(9)	3.25(12)	1
C5	0.0618(5)	0.3545(5)	0.54089(9)	3.23(12)	1
C6	0.1293(5)	0.4399(4)	0.55009(8)	2.80(11)	1
C7	0.2032(5)	0.5098(4)	0.53813(8)	2.68(10)	1
C8	0.1255(6)	0.4572(5)	0.57326(8)	3.76(14)	1
C9	-0.0074(6)	0.2437(6)	0.50973(11)	4.50(15)	1
C10	-0.0035(5)	0.4343(5)	0.47604(9)	3.45(13)	1
C11	-0.0537(5)	0.3632(6)	0.46098(10)	4.05(15)	1
C12	-0.0150(5)	0.4056(6)	0.44122(9)	4.23(16)	1
C13	0.0583(5)	0.4992(6)	0.44436(10)	3.79(13)	1
C14	0.0674(5)	0.5182(5)	0.46590(9)	3.47(12)	1

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

Table S7-2. Atomic coordinates and B_{iso} involving hydrogen atoms

atom	x	y	z	B_{iso}	occ
H1A	0.34887	0.55200	0.50538	3.365	1
H1B	0.27880	0.56343	0.48932	3.365	1
H5	0.01183	0.30645	0.54920	3.871	1
H7	0.24939	0.56825	0.54453	3.217	1
H8A	0.17858	0.52105	0.57695	4.515	1
H8B	0.06415	0.45346	0.57660	4.515	1
H8C	0.13122	0.40816	0.58124	4.515	1
H9A	-0.05363	0.20250	0.52037	5.405	1
H9B	-0.04135	0.25617	0.49853	5.405	1
H9C	0.02544	0.21129	0.50391	5.405	1
H10	-0.01936	0.42865	0.49129	4.134	1
H11	-0.11189	0.29885	0.46345	4.857	1
H12	-0.04028	0.37479	0.42731	5.071	1
H13	0.09454	0.54702	0.43310	4.549	1
H14	0.10955	0.58199	0.47264	4.160	1

Table S7-3. Anisotropic displacement parameters

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Ti1	0.0452(7)	0.0625(8)	0.0161(4)	0.0297(6)	-0.0013(4)	-0.0059(5)
Cl1	0.0917(16)	0.0859(15)	0.0356(9)	0.0565(13)	-0.0161(9)	-0.0197(9)
Cl2	0.0530(11)	0.1152(18)	0.0243(7)	0.0437(12)	0.0036(7)	0.0033(9)
O1	0.046(3)	0.059(3)	0.0145(17)	0.029(2)	-0.0029(16)	-0.0026(17)
N1	0.036(3)	0.036(3)	0.019(3)	0.0179(14)	0.00000	0.00000
C1	0.043(3)	0.044(3)	0.017(2)	0.020(3)	0.002(2)	-0.002(2)
C2	0.046(4)	0.042(3)	0.017(2)	0.023(3)	0.001(2)	-0.002(2)
C3	0.047(4)	0.052(4)	0.014(2)	0.026(3)	-0.004(2)	-0.001(2)
C4	0.048(4)	0.051(4)	0.025(3)	0.025(3)	-0.001(3)	0.001(3)
C5	0.046(4)	0.048(4)	0.023(3)	0.019(3)	0.008(2)	0.011(3)
C6	0.050(4)	0.037(3)	0.022(3)	0.024(3)	0.004(2)	0.004(2)
C7	0.044(3)	0.038(3)	0.018(2)	0.019(3)	0.004(2)	0.001(2)
C8	0.072(5)	0.047(4)	0.021(3)	0.028(4)	0.010(3)	0.008(3)
C9	0.061(5)	0.062(5)	0.038(3)	0.023(4)	0.004(3)	0.003(3)
C10	0.057(4)	0.064(5)	0.022(3)	0.040(4)	0.002(3)	-0.005(3)
C11	0.038(4)	0.080(5)	0.038(3)	0.031(4)	-0.002(3)	-0.011(3)
C12	0.053(4)	0.102(6)	0.021(3)	0.051(5)	-0.009(3)	-0.013(3)
C13	0.054(4)	0.066(5)	0.031(3)	0.035(4)	-0.001(3)	0.007(3)
C14	0.054(4)	0.058(4)	0.029(3)	0.035(4)	-0.006(3)	-0.009(3)

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 S7-4. Bond lengths (Å)

atom	atom	distance	atom	atom	distance
Ti1	Cl1	2.252(3)	Ti1	Cl2	2.249(2)
Ti1	O1	1.788(4)	Ti1	C10	2.330(9)
Ti1	C11	2.333(9)	Ti1	C12	2.356(9)
Ti1	C13	2.357(10)	Ti1	C14	2.330(10)
O1	C3	1.377(6)	N1	C1	1.462(7)
N1	$C1^{1}$	1.462(7)	N1	$C1^{2}$	1.462(7)
C1	C2	1.510(7)	C2	C3	1.400(8)
C2	C7	1.409(8)	C3	C4	1.387(8)
C4	C5	1.395(8)	C4	C9	1.514(9)
C5	C6	1.384(8)	C6	C7	1.386(7)
C6	C8	1.514(8)	C10	C11	1.400(9)
C10	C14	1.414(9)	C11	C12	1.422(9)
C12	C13	1.384(10)	C13	C14	1.402(9)

Symmetry Operators:

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

Table S7-5. Bond lengths involving hydrogens (Å)

atom	atom	distance	atom	atom	distance
C1	H1A	0.990	C1	H1B	0.990
C5	H5	0.950	C7	H7	0.950
C8	H8A	0.980	C8	H8B	0.980
C8	H8C	0.980	C9	H9A	0.980
C9	H9B	0.980	C9	H9C	0.980
C10	H10	1.000	C11	H11	1.000
C12	H12	1.000	C13	H13	1.000
C14	H14	1.000			

Table S7-6. Bond angles (°)

atom	atom	atom	angle	atom	atom	atom	angle
Cl1	Ti1	Cl2	103.41(11)	Cl1	Ti1	O1	104.50(19)
Cl1	Ti1	C10	118.85(17)	Cl1	Ti1	C11	87.8(2)
Cl1	Ti1	C12	89.5(2)	Cl1	Ti1	C13	120.25(18)
Cl1	Ti1	C14	145.03(19)	Cl2	Ti1	O1	102.58(15)
Cl2	Ti1	C10	133.6(2)	Cl2	Ti1	C11	142.1(2)
Cl2	Ti1	C12	107.72(17)	Cl2	Ti1	C13	85.47(19)
Cl2	Ti1	C14	98.37(18)	O1	Ti1	C10	85.5(3)
O1	Ti1	C11	109.5(2)	O1	Ti1	C12	142.6(3)
O1	Ti1	C13	131.4(3)	O1	Ti1	C14	96.9(3)
C10	Ti1	C11	34.9(2)	C10	Ti1	C12	57.7(3)
C10	Ti1	C13	57.8(3)	C10	Ti1	C14	35.3(2)
C11	Ti1	C12	35.3(2)	C11	Ti1	C13	58.2(3)
C11	Ti1	C14	58.8(3)	C12	Ti1	C13	34.1(3)
C12	Ti1	C14	57.7(3)	C13	Ti1	C14	34.8(2)
Ti1	O1	C3	149.9(6)	C1	N1	C1[1]	110.6(5)
C1	N1	C1[2]	110.6(5)	C1[1]	N1	C1[2]	110.6(5)
N1	C1	C2	112.8(6)	C1	C2	C3	122.2(5)
C1	C2	C7	120.4(5)	C3	C2	C7	117.3(5)
O1	C3	C2	118.3(5)	O1	C3	C4	119.2(5)
C2	C3	C4	122.5(5)	C3	C4	C5	118.3(5)
C3	C4	C9	121.0(5)	C5	C4	C9	120.7(5)
C4	C5	C6	121.0(5)	C5	C6	C7	119.8(5)
C5	C6	C8	120.9(5)	C7	C6	C8	119.2(5)
C2	C7	C6	121.0(5)	Ti1	C10	C11	72.7(5)
Ti1	C10	C14	72.3(5)	C11	C10	C14	108.8(5)
Ti1	C11	C10	72.4(5)	Ti1	C11	C12	73.2(5)
C10	C11	C12	106.5(6)	Ti1	C12	C11	71.5(5)
Ti1	C12	C13	72.9(5)	C11	C12	C13	108.8(6)
Ti1	C13	C12	72.9(6)	Ti1	C13	C14	71.6(6)
C12	C13	C14	108.6(6)	Ti1	C14	C10	72.3(6)
Ti1	C14	C13	73.6(6)	C10	C14	C13	107.2(5)

Symmetry Operators:

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

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

Table S7-7. Bond angles involving hydrogens (°)

atom	atom	atom	angle	atom	atom	atom	angle
N1	C1	H1A	109.0	N1	C1	H1B	109.0
C2	C1	H1A	109.0	C2	C1	H1B	109.0
H1A	C1	H1B	107.8	C4	C5	H5	119.5
C6	C5	H5	119.5	C2	C7	H7	119.5
C6	C7	H7	119.5	C6	C8	H8A	109.5
C6	C8	H8B	109.5	C6	C8	H8C	109.5
H8A	C8	H8B	109.5	H8A	C8	H8C	109.5
H8B	C8	H8C	109.5	C4	C9	H9A	109.5
C4	C9	H9B	109.5	C4	C9	H9C	109.5
H9A	C9	H9B	109.5	H9A	C9	H9C	109.5
H9B	C9	H9C	109.5	Ti1	C10	H10	125.5
C11	C10	H10	125.5	C14	C10	H10	125.5
Ti1	C11	H11	126.4	C10	C11	H11	126.4
C12	C11	H11	126.4	Ti1	C12	H12	125.5
C11	C12	H12	125.5	C13	C12	H12	125.5
Ti1	C13	H13	125.6	C12	C13	H13	125.6
C14	C13	H13	125.6	Ti1	C14	H14	126.1
C10	C14	H14	126.1	C13	C14	H14	126.1

Table S7-8. Torsion Angles(°)

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

atom1	atom2	atom3	atom4	angle	atom1	atom2	atom3	atom4	angle
Cl1	Ti1	O1	C3	-124.7(5)	Cl1	Ti1	C10	C11	-30.2(4)
Cl1	Ti1	C10	C14	-147.23(17)	Cl1	Ti1	C11	C10	153.8(3)
Cl1	Ti1	C11	C12	-92.1(3)	Cl1	Ti1	C12	C11	87.0(3)
Cl1	Ti1	C12	C13	-155.7(3)	Cl1	Ti1	C13	C12	28.4(4)
Cl1	Ti1	C13	C14	145.40(18)	Cl1	Ti1	C14	C10	55.8(4)
Cl1	Ti1	C14	C13	-58.9(4)	Cl2	Ti1	O1	C3	127.6(5)
Cl2	Ti1	C10	C11	122.6(2)	Cl2	Ti1	C10	C14	5.6(4)
Cl2	Ti1	C11	C10	-96.9(3)	Cl2	Ti1	C11	C12	17.1(6)
Cl2	Ti1	C12	C11	-169.1(3)	Cl2	Ti1	C12	C13	-51.8(3)
Cl2	Ti1	C13	C12	131.3(3)	Cl2	Ti1	C13	C14	-111.7(2)
Cl2	Ti1	C14	C10	-175.9(2)	Cl2	Ti1	C14	C13	69.4(2)
O1	Ti1	C10	C11	-134.3(3)	O1	Ti1	C10	C14	108.7(3)
C10	Ti1	O1	C3	-6.0(6)	O1	Ti1	C11	C10	49.2(4)
O1	Ti1	C11	C12	163.3(3)	C11	Ti1	O1	C3	-31.8(6)
O1	Ti1	C12	C11	-26.5(6)	O1	Ti1	C12	C13	90.7(4)
C12	Ti1	O1	C3	-15.9(8)	O1	Ti1	C13	C12	-125.9(3)
O1	Ti1	C13	C14	-8.9(4)	C13	Ti1	O1	C3	32.5(7)
O1	Ti1	C14	C10	-72.0(3)	O1	Ti1	C14	C13	173.3(2)
C14	Ti1	O1	C3	27.4(6)	C10	Ti1	C11	C10	-0.0(3)
C10	Ti1	C11	C12	114.0(6)	C11	Ti1	C10	C11	0.0(4)
C11	Ti1	C10	C14	-117.0(5)	C10	Ti1	C12	C11	-38.2(3)
C10	Ti1	C12	C13	79.1(4)	C12	Ti1	C10	C11	38.6(3)
C12	Ti1	C10	C14	-78.4(3)	C10	Ti1	C13	C12	-78.6(3)
C10	Ti1	C13	C14	38.3(2)	C13	Ti1	C10	C11	79.3(3)
C13	Ti1	C10	C14	-37.8(2)	C10	Ti1	C14	C10	-0.0(3)
C10	Ti1	C14	C13	-114.7(5)	C14	Ti1	C10	C11	117.0(5)
C14	Ti1	C10	C14	-0.0(3)	C11	Ti1	C12	C11	-0.0(4)
C11	Ti1	C12	C13	117.3(7)	C12	Ti1	C11	C10	-114.0(7)
C12	Ti1	C11	C12	0.0(4)	C11	Ti1	C13	C12	-37.2(3)
C11	Ti1	C13	C14	79.8(3)	C13	Ti1	C11	C10	-78.1(4)
C13	Ti1	C11	C12	35.9(3)	C11	Ti1	C14	C10	36.6(2)
C11	Ti1	C14	C13	-78.1(3)	C14	Ti1	C11	C10	-37.0(3)
C14	Ti1	C11	C12	77.0(4)	C12	Ti1	C13	C12	-0.0(3)
C12	Ti1	C13	C14	117.0(5)	C13	Ti1	C12	C11	-117.3(6)
C13	Ti1	C12	C13	-0.0(3)	C12	Ti1	C14	C10	78.4(3)
C12	Ti1	C14	C13	-36.3(2)	C14	Ti1	C12	C11	-80.3(4)
C14	Ti1	C12	C13	37.0(3)	C13	Ti1	C14	C10	114.7(5)

Table S7-8. Torsion angles (°) (continued)

atom1	atom2	atom3	atom4	angle
C13	Ti1	C14	C13	0.0(3)
C14	Ti1	C13	C14	0.0(3)
Ti1	O1	C3	C4	82.3(10)
C1[1]	N1	C1	C2	161.0(5)
C1[2]	N1	C1	C2	-76.0(6)
C1[2]	N1	C1[1]	C2[1]	161.0(5)
N1	C1	C2	C7	-34.0(10)
C1	C2	C3	C4	173.2(7)
C3	C2	C7	C6	1.7(12)
C7	C2	C3	C4	-2.6(13)
O1	C3	C4	C9	2.3(13)
C2	C3	C4	C9	-177.2(7)
C9	C4	C5	C6	179.0(8)
C4	C5	C6	C8	-179.1(7)
C8	C6	C7	C2	178.2(7)
Ti1	C10	C11	C12	-65.8(5)
Ti1	C10	C14	C13	65.9(6)
C11	C10	C14	C13	1.9(11)
C14	C10	C11	C12	-2.1(11)
Ti1	C11	C12	C13	-63.8(6)
C10	C11	C12	C13	1.4(11)
Ti1	C12	C13	C14	-63.1(6)
C11	C12	C13	C14	-0.2(12)
Ti1	C13	C14	C10	-65.0(6)
C12	C13	C14	C10	-1.0(11)
C14	Ti1	C13	C12	-117.0(5)
Ti1	O1	C3	C2	-98.2(8)
C1	N1	C1[1]	C2[1]	-76.0(6)
C1	N1	C1[2]	C2[2]	161.0(5)
C1[1]	N1	C1[2]	C2[2]	-76.0(6)
N1	C1	C2	C3	150.4(6)
C1	C2	C3	O1	-6.3(12)
C1	C2	C7	C6	-174.1(7)
C7	C2	C3	O1	177.9(7)
O1	C3	C4	C5	-178.8(7)
C2	C3	C4	C5	1.7(13)
C3	C4	C5	C6	0.1(13)
C4	C5	C6	C7	-1.0(13)
C5	C6	C7	C2	0.0(13)
Ti1	C10	C11	Ti1	0.00(3)
Ti1	C10	C14	Ti1	-0.00(3)
C11	C10	C14	Ti1	-63.9(7)
C14	C10	C11	Ti1	63.7(7)
Ti1	C11	C12	Ti1	-0.00(4)
C10	C11	C12	Ti1	65.3(7)
Ti1	C12	C13	Ti1	-0.00(4)
C11	C12	C13	Ti1	62.9(8)
Ti1	C13	C14	Ti1	-0.00(3)
C12	C13	C14	Ti1	64.0(8)

Symmetry Operators:

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

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

Table S7-9. Intramolecular contacts less than 3.60 Å

atom	atom	distance	atom	atom	distance
O1	C1	2.861(6)	O1	C9	2.842(8)
N1	C2[1]	2.476(6)	N1	C2[2]	2.476(6)
N1	C7	2.891(7)	N1	C7[1]	2.891(7)
N1	C7[2]	2.891(7)	C1	C2[1]	3.075(9)
C1	C7[1]	3.482(8)	C2	C5	2.801(8)
C3	C6	2.766(8)	C3	C10	3.241(11)
C4	C7	2.792(8)			

Symmetry Operators:

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

Table S7-10. Intramolecular contacts less than 3.60 Å involving hydrogens

atom	atom	distance	atom	atom	distance
Ti1	H1B	3.285	Ti1	H9B	3.356
Cl1	H9B	3.571	Cl1	H9C	3.589
Cl1	H11	3.269	Cl1	H12	3.345
Cl2	H1B	3.119	Cl2	H13	3.117
Cl2	H13[1]	3.033	Cl2	H14[1]	3.113
O1	H1A	3.211	O1	H1B	2.485
O1	H9B	2.787	O1	H9C	2.814
O1	H10	2.946	O1	H14	3.434
N1	H1A[1]	2.016	N1	H1A[2]	2.016
N1	H1B[1]	2.016	N1	H1B[2]	2.016
N1	H7	2.580	N1	H7[1]	2.580
N1	H7[2]	2.580	C1	H1A[1]	3.238
C1	H1A[2]	2.464	C1	H1B[1]	2.497
C1	H1B[2]	2.737	C1	H7	2.686
C1	H7[1]	3.268	C1	H14[1]	3.090
C2	H1A[2]	2.664	C3	H1A	2.978
C3	H1A[2]	3.493	C3	H1B	2.645
C3	H5	3.247	C3	H7	3.261
C3	H9A	3.315	C3	H9B	2.775
C3	H9C	2.775	C3	H10	2.921
C4	H10	3.044	C5	H7	3.251
C5	H8A	3.312	C5	H8B	2.770
C5	H8C	2.771	C5	H9A	2.567
C5	H9B	3.155	C5	H9C	3.143
C7	H1A	2.954	C7	H1A[2]	3.088
C7	H1B	3.302	C7	H5	3.252
C7	H7[1]	3.333	C7	H7[2]	3.375
C7	H8A	2.533	C7	H8B	3.136
C7	H8C	3.116	C8	H5	2.672
C8	H7	2.639	C9	H5	2.677
C9	H10	3.290	C10	H9B	2.980
C10	H12	3.225	C10	H13	3.231
C11	H9B	3.016	C11	H13	3.245
C11	H14	3.250	C12	H10	3.227
C12	H14	3.224	C13	H10	3.229
C13	H11	3.243	C14	H1A[2]	3.320
C14	H1B	3.439	C14	H11	3.252

Table S7-10. Intramolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
C14	H12	3.224	H1A	H1A[1]	3.426
H1A	H1A[2]	3.426	H1A	H1B[1]	2.495
H1A	H1B[2]	3.508	H1A	H7	3.050
H1A	H7[1]	3.094	H1A	H14[1]	2.490
H1B	H1B[1]	2.488	H1B	H1B[2]	2.488
H1B	H7	3.567	H1B	H14	3.070
H1B	H14[1]	2.785	H5	H8B	2.714
H5	H8C	2.722	H5	H9A	2.352
H5	H9B	3.344	H5	H9C	3.331
H7	H7[1]	2.560	H7	H7[2]	2.560
H7	H8A	2.302	H7	H8B	3.312
H7	H8C	3.292	H9B	H10	2.652
H9B	H11	2.749	H10	H11	2.573
H10	H14	2.583	H11	H12	2.597
H12	H13	2.547	H13	H14	2.574

Symmetry Operators:

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

Table S7-11. Intermolecular contacts less than 3.60 Å

atom	atom	distance	atom	atom	distance
O1	C9[1]	3.414(11)	C2	C11[1]	3.564(11)
C5	C14[2]	3.593(14)	C7	C11[1]	3.558(11)
C8	C12[2]	3.573(15)	C8	C13[2]	3.540(14)
C9	O1[3]	3.414(11)	C11	C2[3]	3.564(11)
C11	C7[3]	3.558(11)	C12	C8[2]	3.573(15)
C13	C8[2]	3.540(14)	C14	C5[2]	3.593(14)

Symmetry Operators:

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

Table S7-12. Intermolecular contacts less than 3.60 Å involving hydrogens

atom	atom	distance	atom	atom	distance
Ti1	H9A[1]	3.550	Cl1	H8A[2]	3.558
Cl1	H8B[2]	3.459	Cl1	H9A[1]	3.087
Cl1	H12[3]	2.829	Cl2	H13[3]	2.885
O1	H9A[1]	2.855	O1	H9B[1]	3.067
C1	H10[1]	3.513	C1	H11[1]	3.273
C2	H11[1]	2.718	C3	H9A[1]	3.576
C3	H9B[1]	3.200	C3	H11[1]	3.137
C4	H11[1]	3.487	C5	H8C[4]	3.218
C5	H11[1]	3.457	C5	H14[5]	3.487
C6	H8C[4]	3.399	C6	H11[1]	3.108
C7	H11[1]	2.710	C8	H5[4]	3.191
C8	H8C[4]	2.911	C8	H12[5]	3.584
C8	H13[5]	3.524	C9	H9C[6]	3.348
C10	H1A[6]	3.028	C10	H10[5]	2.921
C11	H1A[6]	3.143	C12	H8A[5]	3.567
C12	H8B[5]	2.971	C12	H12[3]	3.285
C13	H8B[5]	2.781	C14	H10[5]	3.077
H1A	C10[1]	3.028	H1A	C11[1]	3.143
H1A	H9B[1]	3.591	H1A	H10[1]	2.572
H1A	H11[1]	2.818	H5	C8[4]	3.191
H5	H8A[4]	3.553	H5	H8B[4]	2.936
H5	H8C[4]	2.649	H5	H14[5]	3.528
H7	H11[1]	3.049	H8A	Cl1[7]	3.558
H8A	C12[5]	3.567	H8A	H5[4]	3.553
H8A	H12[5]	3.394	H8B	Cl1[7]	3.459
H8B	C12[5]	2.971	H8B	C13[5]	2.781
H8B	H5[4]	2.936	H8B	H8B[4]	3.450
H8B	H8C[4]	3.122	H8B	H12[5]	2.979
H8B	H13[5]	2.619	H8C	C5[4]	3.218
H8C	C6[4]	3.399	H8C	C8[4]	2.911
H8C	H5[4]	2.649	H8C	H8B[4]	3.122
H8C	H8C[4]	2.098	H9A	Ti1[6]	3.550
H9A	Cl1[6]	3.087	H9A	O1[6]	2.855
H9A	C3[6]	3.576	H9A	H9C[6]	2.994
H9B	O1[6]	3.067	H9B	C3[6]	3.200
H9B	H1A[6]	3.591	H9B	H9C[6]	3.247
H9C	C9[1]	3.348	H9C	H9A[1]	2.994

Table S7-12. Intermolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
H9C	H9B[1]	3.247	H9C	H9C[1]	3.247
H9C	H9C[6]	3.247	H10	C1[6]	3.513
H10	C10[5]	2.921	H10	C14[5]	3.077
H10	H1A[6]	2.572	H10	H10[5]	2.335
H10	H14[5]	2.682	H11	C1[6]	3.273
H11	C2[6]	2.718	H11	C3[6]	3.137
H11	C4[6]	3.487	H11	C5[6]	3.457
H11	C6[6]	3.108	H11	C7[6]	2.710
H11	H1A[6]	2.818	H11	H7[6]	3.049
H12	Cl1[3]	2.829	H12	C8[5]	3.584
H12	C12[3]	3.285	H12	H8A[5]	3.394
H12	H8B[5]	2.979	H12	H12[3]	2.650
H13	Cl2[3]	2.885	H13	C8[5]	3.524
H13	H8B[5]	2.619	H14	C5[5]	3.487
H14	H5[5]	3.528	H14	H10[5]	2.682

Symmetry Operators:

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

X-ray Structure Report

for

$[Cp^*TiCl_2\{(O\text{-}2,4\text{-}Me_2C_6H_2)\text{-}6\text{-}CH_2\}][Cp^*TiCl\{(O\text{-}2,4\text{-}Me_2C_6H_2)\text{-}6\text{-}CH_2\}_2]N$ (**2**)

January 19, 2017

Experimental

Data Collection

A red platelet crystal of $C_{47}H_{60}Cl_3NO_3Ti_2$ having approximate dimensions of 0.210 x 0.200 x 0.060 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 monoclinic cell with dimensions:

a = 14.275(7) Å
b = 22.520(10) Å β = 100.408(6)^o
c = 14.984(7) Å
V = 4738(4) Å^3

For Z = 4 and F.W. = 889.15, the calculated density is 1.246 g/cm^3. The reflection conditions 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 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 0.073 mm pixel mode.

Data Reduction

Of the 49820 reflections were collected, where 10837 were unique (R_{int} = 0.0801); equivalent reflections were merged. Data were collected and processed using CrystalClear (Rigaku). [1]

The linear absorption coefficient, μ, for Mo-Kα radiation is 5.443 cm^{-1}. An empirical absorption correction was applied which resulted in transmission factors ranging from 0.855 to 0.968. 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 10837 observed reflections and 505 variable parameters and converged (largest parameter shift was 0.00 times its esd) with unweighted and weighted agreement factors of:

$$R1 = \Sigma \, ||Fo| - |Fc|| \, / \, \Sigma \, |Fo| = 0.0721$$

$$wR2 = [\Sigma \, (w \, (Fo^2 - Fc^2)^2) / \Sigma \, w(Fo^2)^2]^{1/2} = 0.2152$$

The goodness of fit[4] was 1.06. Unit weights were used. The maximum and minimum peaks on the final difference Fourier map corresponded to 0.59 and -0.75 $e^-/Å^3$, respectively.

Neutral atom scattering factors were taken from International Tables for Crystallography (IT), Vol. C, Table 6.1.1.4 [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 Version 2014/7[10].

References

(1) CrystalClear: Data Collection and Processing Software, Rigaku Corporation (1998-2015). Tokyo 196-8666, Japan.

(2) SHELXT: Sheldrick, G. M. (2014). Acta Cryst. A70, C1437.

(3) Least Squares function minimized: (SHELXL Version 2014/7)

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

(4) Goodness of fit is defined as:

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

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

(5) International Tables for Crystallography, Vol.C (1992). Ed. A.J.C. Wilson, Kluwer Academic Publishers, Dordrecht, Netherlands, Table 6.1.1.4, pp. 572.

(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 4.2: Crystal Structure Analysis Package, Rigaku Corporation (2000-2015). Tokyo 196-8666, Japan.

(10) SHELXL Version 2014/7: Sheldrick, G. M. (2008). Acta Cryst. A64, 112-122.

EXPERIMENTAL DETAILS

A. Crystal Data

Empirical Formula	$C_{47}H_{60}Cl_3NO_3Ti_2$
Formula Weight	889.15
Crystal Color, Habit	red, platelet
Crystal Dimensions	0.210 X 0.200 X 0.060 mm
Crystal System	monoclinic
Lattice Type	Primitive
Lattice Parameters	a = 14.275(7) Å b = 22.520(10) Å c = 14.984(7) Å β = 100.408(6) ^{o} V = 4738(4) Å^3
Space Group	$P2_1/c$ (#14)
Z value	4
D_{calc}	1.246 g/cm^3
F_{000}	1872.00
μ(MoKα)	5.443 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	75.0 mm (diameter)
Detector Position	0.00 mm
Pixel Size	0.073 mm
$2\theta_{max}$	55.0^{o}
No. of Reflections Measured	Total: 49820 Unique: 10837 (R_{int} = 0.0801)
Corrections	Lorentz-polarization Absorption (trans. factors: 0.855 - 0.968)

C. Structure Solution and Refinement

Structure Solution	Direct Methods (SHELXT)
Refinement	Full-matrix least-squares on F^2
Function Minimized	Σ w (Fo^2 - Fc^2)^2
Least Squares Weights	w = 1/ [$\sigma^2(Fo^2)$ + (0.1005 · P)^2 + 9.5208 · 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)	10837
No. Variables	505
Reflection/Parameter Ratio	21.46
Residuals: R1 (I>2.00σ(I))	0.0721
Residuals: R (All reflections)	0.0999
Residuals: wR2 (All reflections)	0.2152
Goodness of Fit Indicator	1.063
Max Shift/Error in Final Cycle	0.000
Maximum peak in Final Diff. Map	0.59 e^-/Å^3
Minimum peak in Final Diff. Map	-0.75 e^-/Å^3

Table S8-1. Atomic coordinates and B_{iso}/B_{eq}

atom	x	y	z	B_{eq}
Ti1	0.19676(5)	0.41835(3)	0.27932(5)	1.536(13)
Ti2	0.67383(5)	0.19234(3)	0.47634(5)	1.369(13)
Cl1	0.24355(8)	0.42275(5)	0.43314(7)	2.52(2)
Cl2	0.03828(7)	0.39755(5)	0.26192(8)	2.52(2)
Cl3	0.71146(8)	0.13254(4)	0.36228(7)	2.099(18)
O1	0.24535(19)	0.34962(12)	0.25154(19)	1.71(5)
O2	0.54687(19)	0.18091(12)	0.46136(19)	1.64(5)
O3	0.69464(19)	0.26492(12)	0.43244(19)	1.66(5)
N1	0.4955(2)	0.30782(14)	0.4182(2)	1.33(5)
C1	0.4414(3)	0.33554(17)	0.3368(3)	1.53(6)
C2	0.3885(3)	0.29182(17)	0.2705(3)	1.52(6)
C3	0.2934(3)	0.30091(17)	0.2295(3)	1.64(6)
C4	0.2436(3)	0.25963(18)	0.1680(3)	1.92(7)
C5	0.2905(3)	0.20765(18)	0.1514(3)	1.89(7)
C6	0.3837(3)	0.19640(18)	0.1919(3)	1.83(7)
C7	0.4321(3)	0.23899(17)	0.2498(3)	1.56(6)
C8	0.4320(3)	0.13797(18)	0.1778(3)	2.06(7)
C9	0.1421(3)	0.2722(2)	0.1226(4)	3.02(9)
C10	0.2818(3)	0.46502(19)	0.1793(3)	2.09(7)
C11	0.3036(3)	0.49610(19)	0.2617(3)	2.19(7)
C12	0.2186(4)	0.52408(19)	0.2779(3)	2.42(8)
C13	0.1448(3)	0.5100(2)	0.2052(3)	2.36(8)
C14	0.1834(3)	0.47247(19)	0.1446(3)	2.12(7)
C15	0.3514(3)	0.4313(2)	0.1342(4)	2.78(9)
C16	0.4004(4)	0.5036(2)	0.3202(4)	3.33(10)
C17	0.2111(5)	0.5650(2)	0.3546(4)	3.83(11)
C18	0.0456(4)	0.5336(3)	0.1902(4)	3.92(12)
C19	0.1307(4)	0.4476(2)	0.0567(3)	3.02(9)
C20	0.4332(3)	0.28297(17)	0.4770(3)	1.66(6)
C21	0.3910(3)	0.22278(18)	0.4458(3)	1.58(6)
C22	0.4502(3)	0.17394(18)	0.4406(3)	1.55(6)
C23	0.4126(3)	0.11809(18)	0.4124(3)	1.79(6)
C24	0.3141(3)	0.1134(2)	0.3862(3)	2.07(7)
C25	0.2537(3)	0.1613(2)	0.3893(3)	2.08(7)
C26	0.2929(3)	0.2152(2)	0.4204(3)	2.03(7)
C27	0.1467(3)	0.1555(2)	0.3552(4)	2.73(8)
C28	0.4776(3)	0.06593(19)	0.4077(3)	2.39(8)

Table S8-1. Atomic coordinates and B_{iso}/B_{eq} (continued)

atom	x	y	z	B_{eq}
C29	0.5621(3)	0.35097(18)	0.4693(3)	1.61(6)
C30	0.6449(3)	0.36604(17)	0.4223(3)	1.42(6)
C31	0.7089(3)	0.32158(17)	0.4080(3)	1.43(6)
C32	0.7876(3)	0.33477(18)	0.3669(3)	1.71(6)
C33	0.7987(3)	0.39379(19)	0.3406(3)	1.96(7)
C34	0.7374(3)	0.43878(18)	0.3551(3)	1.71(6)
C35	0.6605(3)	0.42415(17)	0.3969(3)	1.56(6)
C36	0.7527(3)	0.5018(2)	0.3262(3)	2.44(8)
C37	0.8590(3)	0.28784(19)	0.3531(3)	2.16(7)
C38	0.7991(3)	0.21574(19)	0.6006(3)	1.68(6)
C39	0.8202(3)	0.15916(18)	0.5670(3)	1.70(6)
C40	0.7457(3)	0.11879(19)	0.5816(3)	1.90(7)
C41	0.6803(3)	0.15070(18)	0.6227(3)	1.67(6)
C42	0.7108(3)	0.21030(18)	0.6320(3)	1.81(6)
C43	0.6627(3)	0.2585(2)	0.6775(3)	2.19(7)
C44	0.8584(3)	0.2708(2)	0.6039(3)	2.45(8)
C45	0.9061(3)	0.1434(2)	0.5283(3)	2.74(8)
C46	0.7442(4)	0.05342(19)	0.5614(3)	2.71(8)
C47	0.5929(3)	0.1268(2)	0.6521(3)	2.33(8)

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

Table S8-2. Atomic coordinates and B_{iso} involving hydrogen atoms

atom	x	y	z	B_{iso}
H1A	0.48476	0.35803	0.30687	1.841
H1B	0.39608	0.36325	0.35457	1.841
H5	0.25802	0.17961	0.11191	2.267
H7	0.49550	0.23225	0.27560	1.867
H8A	0.49616	0.13842	0.21107	2.475
H8B	0.39758	0.10590	0.19908	2.475
H8C	0.43291	0.13263	0.11441	2.475
H9A	0.12262	0.31003	0.14261	3.619
H9B	0.13814	0.27296	0.05793	3.619
H9C	0.10098	0.24173	0.13832	3.619
H15A	0.31848	0.41410	0.07872	3.335
H15B	0.39972	0.45792	0.12122	3.335
H15C	0.38041	0.40040	0.17396	3.335
H16A	0.39474	0.52686	0.37262	3.994
H16B	0.42613	0.46528	0.33910	3.994
H16C	0.44200	0.52336	0.28611	3.994
H17A	0.27139	0.56693	0.39503	4.595
H17B	0.19358	0.60391	0.33123	4.595
H17C	0.16347	0.55048	0.38688	4.595
H18A	0.00981	0.51687	0.13562	4.708
H18B	0.01614	0.52316	0.24074	4.708
H18C	0.04714	0.57606	0.18457	4.708
H19A	0.06487	0.45893	0.04880	3.623
H19B	0.15796	0.46284	0.00735	3.623
H19C	0.13550	0.40506	0.05791	3.623
H20A	0.38167	0.31064	0.47937	1.994
H20B	0.46952	0.27903	0.53802	1.994
H24	0.28806	0.07690	0.36598	2.490
H26	0.25282	0.24720	0.42455	2.437
H27A	0.13184	0.11538	0.33632	3.279
H27B	0.11322	0.16577	0.40316	3.279
H27C	0.12780	0.18185	0.30479	3.279
H28A	0.54242	0.07781	0.42842	2.864
H28B	0.46154	0.03448	0.44548	2.864
H28C	0.47012	0.05224	0.34612	2.864
H29A	0.58691	0.33484	0.52893	1.937
H29B	0.52771	0.38711	0.47760	1.937

Table S8-2. Atomic coordinates and B_{iso} involving hydrogens/B_{eq} (continued)

atom	x	y	z	B_{eq}
H33	0.84957	0.40302	0.31214	2.357
H35	0.61892	0.45389	0.40802	1.870
H36A	0.70364	0.52687	0.34155	2.929
H36B	0.81376	0.51563	0.35677	2.929
H36C	0.75057	0.50293	0.26178	2.929
H37A	0.84024	0.25036	0.37486	2.588
H37B	0.86143	0.28471	0.28970	2.588
H37C	0.92070	0.29859	0.38608	2.588
H43A	0.69653	0.29524	0.67542	2.632
H43B	0.59824	0.26322	0.64632	2.632
H43C	0.66297	0.24783	0.73951	2.632
H44A	0.82746	0.30260	0.62986	2.940
H44B	0.91984	0.26367	0.64042	2.940
H44C	0.86583	0.28139	0.54352	2.940
H45A	0.90281	0.10238	0.51069	3.293
H45B	0.90845	0.16777	0.47617	3.293
H45C	0.96225	0.14999	0.57313	3.293
H46A	0.79737	0.04351	0.53312	3.253
H46B	0.74828	0.03147	0.61689	3.253
H46C	0.68599	0.04350	0.52124	3.253
H47A	0.56122	0.15827	0.67813	2.797
H47B	0.55078	0.11068	0.60061	2.797
H47C	0.61061	0.09619	0.69651	2.797

Table S8-3. Anisotropic displacement parameters

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Ti1	0.0179(4)	0.0200(4)	0.0212(4)	0.0006(3)	0.0056(3)	0.0003(3)
Ti2	0.0180(3)	0.0162(3)	0.0182(3)	0.0005(3)	0.0044(3)	0.0006(3)
Cl1	0.0386(6)	0.0360(6)	0.0216(5)	0.0048(5)	0.0061(4)	-0.0010(4)
Cl2	0.0190(5)	0.0389(6)	0.0396(6)	-0.0020(4)	0.0098(4)	0.0006(5)
Cl3	0.0353(6)	0.0228(5)	0.0233(5)	0.0029(4)	0.0099(4)	-0.0025(4)
O1	0.0186(14)	0.0216(14)	0.0248(14)	0.0011(11)	0.0043(11)	0.0016(11)
O2	0.0175(13)	0.0197(14)	0.0242(14)	-0.0006(11)	0.0012(11)	0.0030(11)
O3	0.0186(14)	0.0198(14)	0.0260(14)	0.0019(11)	0.0067(11)	0.0037(11)
N1	0.0172(15)	0.0185(16)	0.0151(15)	-0.0024(12)	0.0035(12)	0.0016(12)
C1	0.0168(18)	0.0196(19)	0.0214(19)	-0.0020(14)	0.0020(15)	0.0014(15)
C2	0.0197(19)	0.0186(18)	0.0208(19)	0.0004(14)	0.0073(15)	0.0046(15)
C3	0.024(2)	0.0171(18)	0.0212(19)	0.0020(15)	0.0051(16)	0.0025(15)
C4	0.025(2)	0.024(2)	0.023(2)	-0.0022(16)	0.0016(16)	0.0005(16)
C5	0.026(2)	0.020(2)	0.026(2)	-0.0029(16)	0.0066(17)	-0.0028(16)
C6	0.030(2)	0.0182(19)	0.023(2)	0.0002(16)	0.0104(17)	0.0014(15)
C7	0.0193(19)	0.023(2)	0.0183(18)	0.0010(15)	0.0067(14)	0.0032(15)
C8	0.038(2)	0.018(2)	0.024(2)	0.0024(17)	0.0097(18)	0.0002(16)
C9	0.025(2)	0.039(3)	0.044(3)	0.002(2)	-0.010(2)	-0.008(2)
C10	0.026(2)	0.024(2)	0.032(2)	-0.0009(17)	0.0116(18)	0.0056(17)
C11	0.023(2)	0.023(2)	0.036(2)	-0.0011(17)	0.0018(18)	0.0047(18)
C12	0.039(3)	0.021(2)	0.033(2)	-0.0012(18)	0.008(2)	-0.0004(18)
C13	0.027(2)	0.027(2)	0.038(3)	0.0074(17)	0.0109(19)	0.0092(19)
C14	0.027(2)	0.026(2)	0.028(2)	-0.0001(17)	0.0068(17)	0.0061(17)
C15	0.034(3)	0.036(3)	0.042(3)	0.006(2)	0.025(2)	0.011(2)
C16	0.033(3)	0.040(3)	0.046(3)	-0.016(2)	-0.010(2)	0.013(2)
C17	0.080(4)	0.029(3)	0.037(3)	0.005(3)	0.013(3)	-0.008(2)
C18	0.040(3)	0.051(3)	0.062(4)	0.028(3)	0.018(3)	0.026(3)
C19	0.043(3)	0.047(3)	0.022(2)	-0.018(2)	0.001(2)	0.006(2)
C20	0.0171(18)	0.0205(19)	0.027(2)	0.0001(15)	0.0090(15)	-0.0013(16)
C21	0.0209(19)	0.024(2)	0.0171(18)	-0.0013(15)	0.0080(15)	0.0057(15)
C22	0.0170(18)	0.027(2)	0.0151(18)	-0.0018(15)	0.0025(14)	0.0014(15)
C23	0.027(2)	0.022(2)	0.0196(19)	-0.0035(16)	0.0051(16)	0.0049(15)
C24	0.030(2)	0.027(2)	0.022(2)	-0.0094(17)	0.0040(17)	0.0010(16)
C25	0.022(2)	0.031(2)	0.026(2)	-0.0085(17)	0.0040(17)	0.0053(17)
C26	0.023(2)	0.029(2)	0.028(2)	-0.0044(17)	0.0097(17)	0.0017(17)
C27	0.023(2)	0.036(3)	0.043(3)	-0.0087(19)	0.0018(19)	0.004(2)
C28	0.037(3)	0.020(2)	0.032(2)	-0.0035(18)	0.0036(19)	0.0020(17)

Table S8-3. Anisotropic displacement parameters (continued)

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
C29	0.0183(18)	0.0211(19)	0.0220(19)	-0.0024(15)	0.0040(15)	-0.0033(15)
C30	0.0150(17)	0.0216(19)	0.0164(17)	-0.0034(14)	0.0001(14)	-0.0051(14)
C31	0.0195(19)	0.0180(18)	0.0168(18)	-0.0022(14)	0.0034(14)	-0.0014(14)
C32	0.0168(18)	0.026(2)	0.0217(19)	-0.0013(15)	0.0036(15)	0.0022(16)
C33	0.020(2)	0.031(2)	0.024(2)	-0.0031(16)	0.0079(16)	0.0051(17)
C34	0.0202(19)	0.0199(19)	0.024(2)	-0.0027(15)	0.0028(16)	0.0012(15)
C35	0.0182(19)	0.0205(19)	0.0188(18)	0.0000(15)	-0.0014(14)	-0.0029(15)
C36	0.033(2)	0.025(2)	0.035(2)	-0.0043(18)	0.0067(19)	0.0075(18)
C37	0.020(2)	0.026(2)	0.037(2)	-0.0006(17)	0.0097(18)	0.0019(18)
C38	0.0174(18)	0.028(2)	0.0176(18)	-0.0010(15)	-0.0005(14)	0.0004(16)
C39	0.0198(19)	0.023(2)	0.0220(19)	0.0043(15)	0.0034(15)	0.0013(15)
C40	0.023(2)	0.025(2)	0.022(2)	0.0027(16)	-0.0008(16)	0.0026(16)
C41	0.023(2)	0.026(2)	0.0138(17)	0.0005(16)	0.0004(14)	0.0031(15)
C42	0.024(2)	0.024(2)	0.021(2)	0.0030(16)	0.0060(16)	0.0012(16)
C43	0.028(2)	0.032(2)	0.023(2)	0.0082(18)	0.0033(17)	-0.0046(17)
C44	0.028(2)	0.031(2)	0.033(2)	-0.0050(18)	0.0015(18)	-0.0030(19)
C45	0.021(2)	0.044(3)	0.039(3)	0.0126(19)	0.0038(19)	-0.000(2)
C46	0.048(3)	0.021(2)	0.035(2)	0.003(2)	0.009(2)	0.0028(18)
C47	0.033(2)	0.030(2)	0.027(2)	-0.0053(18)	0.0094(18)	0.0023(18)

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 S8-4. Bond lengths (Å)

atom	atom	distance	atom	atom	distance
Ti1	Cl1	2.2830(16)	Ti1	Cl2	2.2787(16)
Ti1	O1	1.776(3)	Ti1	C10	2.341(5)
Ti1	C11	2.368(5)	Ti1	C12	2.402(4)
Ti1	C13	2.396(5)	Ti1	C14	2.336(5)
Ti2	Cl3	2.3140(15)	Ti2	O2	1.804(3)
Ti2	O3	1.806(3)	Ti2	C38	2.396(4)
Ti2	C39	2.396(4)	Ti2	C40	2.387(4)
Ti2	C41	2.371(4)	Ti2	C42	2.332(4)
O1	C3	1.365(5)	O2	C22	1.368(5)
O3	C31	1.353(5)	N1	C1	1.461(5)
N1	C20	1.471(5)	N1	C29	1.474(5)
C1	C2	1.502(5)	C2	C3	1.401(5)
C2	C7	1.403(6)	C3	C4	1.408(5)
C4	C5	1.393(6)	C4	C9	1.513(6)
C5	C6	1.383(6)	C6	C7	1.390(5)
C6	C8	1.518(6)	C10	C11	1.404(6)
C10	C14	1.417(6)	C10	C15	1.504(7)
C11	C12	1.427(7)	C11	C16	1.506(6)
C12	C13	1.408(6)	C12	C17	1.491(7)
C13	C14	1.422(7)	C13	C18	1.491(7)
C14	C19	1.502(6)	C20	C21	1.522(6)
C21	C22	1.398(6)	C21	C26	1.394(6)
C22	C23	1.402(6)	C23	C24	1.393(6)
C23	C28	1.506(6)	C24	C25	1.387(6)
C25	C26	1.382(6)	C25	C27	1.525(6)
C29	C30	1.519(6)	C30	C31	1.399(6)
C30	C35	1.392(5)	C31	C32	1.406(6)
C32	C33	1.403(6)	C32	C37	1.508(6)
C33	C34	1.381(6)	C34	C35	1.398(6)
C34	C36	1.511(6)	C38	C39	1.422(6)
C38	C42	1.429(6)	C38	C44	1.496(6)
C39	C40	1.445(6)	C39	C45	1.491(7)
C40	C41	1.405(6)	C40	C46	1.502(6)
C41	C42	1.410(6)	C41	C47	1.496(6)
C42	C43	1.511(6)			

Table S8-5. Bond lengths involving hydrogens (Å)

atom	atom	distance	atom	atom	distance
C1	H1A	0.970	C1	H1B	0.970
C5	H5	0.930	C7	H7	0.930
C8	H8A	0.960	C8	H8B	0.960
C8	H8C	0.960	C9	H9A	0.960
C9	H9B	0.960	C9	H9C	0.960
C15	H15A	0.960	C15	H15B	0.960
C15	H15C	0.960	C16	H16A	0.960
C16	H16B	0.960	C16	H16C	0.960
C17	H17A	0.960	C17	H17B	0.960
C17	H17C	0.960	C18	H18A	0.960
C18	H18B	0.960	C18	H18C	0.960
C19	H19A	0.960	C19	H19B	0.960
C19	H19C	0.960	C20	H20A	0.970
C20	H20B	0.970	C24	H24	0.930
C26	H26	0.930	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	0.970
C29	H29B	0.970	C33	H33	0.930
C35	H35	0.930	C36	H36A	0.960
C36	H36B	0.960	C36	H36C	0.960
C37	H37A	0.960	C37	H37B	0.960
C37	H37C	0.960	C43	H43A	0.960
C43	H43B	0.960	C43	H43C	0.960
C44	H44A	0.960	C44	H44B	0.960
C44	H44C	0.960	C45	H45A	0.960
C45	H45B	0.960	C45	H45C	0.960
C46	H46A	0.960	C46	H46B	0.960
C46	H46C	0.960	C47	H47A	0.960
C47	H47B	0.960	C47	H47C	0.960

Table S8-6. Bond angles (°)

atom	atom	atom	angle	atom	atom	atom	angle
Cl1	Ti1	Cl2	103.17(5)	Cl1	Ti1	O1	102.65(10)
Cl1	Ti1	C10	122.39(11)	Cl1	Ti1	C11	90.20(12)
Cl1	Ti1	C12	87.19(12)	Cl1	Ti1	C13	116.11(12)
Cl1	Ti1	C14	144.39(11)	Cl2	Ti1	O1	102.46(10)
Cl2	Ti1	C10	129.64(11)	Cl2	Ti1	C11	141.76(11)
Cl2	Ti1	C12	109.29(12)	Cl2	Ti1	C13	84.62(12)
Cl2	Ti1	C14	94.81(11)	O1	Ti1	C10	88.37(15)
O1	Ti1	C11	109.36(15)	O1	Ti1	C12	143.63(16)
O1	Ti1	C13	137.98(16)	O1	Ti1	C14	103.10(15)
C10	Ti1	C11	34.70(16)	C10	Ti1	C12	57.75(17)
C10	Ti1	C13	57.97(16)	C10	Ti1	C14	35.28(15)
C11	Ti1	C12	34.81(16)	C11	Ti1	C13	57.55(15)
C11	Ti1	C14	58.11(15)	C12	Ti1	C13	34.13(15)
C12	Ti1	C14	57.71(16)	C13	Ti1	C14	34.94(16)
Cl3	Ti2	O2	100.78(10)	Cl3	Ti2	O3	100.50(11)
Cl3	Ti2	C38	117.49(11)	Cl3	Ti2	C39	86.69(11)
Cl3	Ti2	C40	87.41(11)	Cl3	Ti2	C41	118.52(11)
Cl3	Ti2	C42	143.03(11)	O2	Ti2	O3	108.14(12)
O2	Ti2	C38	136.08(14)	O2	Ti2	C39	141.20(14)
O2	Ti2	C40	106.57(14)	O2	Ti2	C41	85.92(13)
O2	Ti2	C42	100.94(14)	O3	Ti2	C38	86.28(13)
O3	Ti2	C39	107.74(13)	O3	Ti2	C40	142.11(13)
O3	Ti2	C41	135.49(13)	O3	Ti2	C42	100.66(14)
C38	Ti2	C39	34.52(14)	C38	Ti2	C40	57.85(14)
C38	Ti2	C41	57.97(14)	C38	Ti2	C42	35.16(15)
C39	Ti2	C40	35.18(14)	C39	Ti2	C41	57.88(14)
C39	Ti2	C42	58.03(15)	C40	Ti2	C41	34.35(15)
C40	Ti2	C42	57.78(15)	C41	Ti2	C42	34.88(14)
Ti1	O1	C3	172.4(3)	Ti2	O2	C22	173.9(3)
Ti2	O3	C31	174.0(3)	C1	N1	C20	112.2(3)
C1	N1	C29	110.3(3)	C20	N1	C29	110.0(3)
N1	C1	C2	113.5(3)	C1	C2	C3	121.7(3)
C1	C2	C7	120.8(3)	C3	C2	C7	117.4(3)
O1	C3	C2	120.1(3)	O1	C3	C4	118.2(3)
C2	C3	C4	121.7(4)	C3	C4	C5	118.0(4)
C3	C4	C9	120.0(4)	C5	C4	C9	122.0(4)
C4	C5	C6	122.1(4)	C5	C6	C7	118.5(4)

Table S8-6. Bond angles (°) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
C5	C6	C8	121.6(4)	C7	C6	C8	119.8(4)
C2	C7	C6	122.2(4)	Ti1	C10	C11	73.7(3)
Ti1	C10	C14	72.2(3)	Ti1	C10	C15	121.5(3)
C11	C10	C14	108.1(4)	C11	C10	C15	125.9(4)
C14	C10	C15	125.9(4)	Ti1	C11	C10	71.6(3)
Ti1	C11	C12	73.9(3)	Ti1	C11	C16	124.0(3)
C10	C11	C12	108.0(4)	C10	C11	C16	127.0(4)
C12	C11	C16	124.8(4)	Ti1	C12	C11	71.3(2)
Ti1	C12	C13	72.7(3)	Ti1	C12	C17	125.3(4)
C11	C12	C13	108.0(4)	C11	C12	C17	125.8(4)
C13	C12	C17	126.0(5)	Ti1	C13	C12	73.1(3)
Ti1	C13	C14	70.2(2)	Ti1	C13	C18	125.7(4)
C12	C13	C14	107.9(4)	C12	C13	C18	126.4(5)
C14	C13	C18	125.6(4)	Ti1	C14	C10	72.6(3)
Ti1	C14	C13	74.9(3)	Ti1	C14	C19	120.8(3)
C10	C14	C13	108.0(4)	C10	C14	C19	125.7(4)
C13	C14	C19	126.2(4)	N1	C20	C21	113.8(3)
C20	C21	C22	120.5(3)	C20	C21	C26	121.1(4)
C22	C21	C26	118.4(4)	O2	C22	C21	119.5(3)
O2	C22	C23	119.2(4)	C21	C22	C23	121.4(4)
C22	C23	C24	117.7(4)	C22	C23	C28	120.5(4)
C24	C23	C28	121.7(4)	C23	C24	C25	122.3(4)
C24	C25	C26	118.5(4)	C24	C25	C27	120.9(4)
C26	C25	C27	120.5(4)	C21	C26	C25	121.8(4)
N1	C29	C30	112.9(3)	C29	C30	C31	119.7(3)
C29	C30	C35	120.9(3)	C31	C30	C35	119.3(4)
O3	C31	C30	119.9(4)	O3	C31	C32	119.3(3)
C30	C31	C32	120.8(4)	C31	C32	C33	117.5(4)
C31	C32	C37	121.6(4)	C33	C32	C37	120.8(4)
C32	C33	C34	122.9(4)	C33	C34	C35	117.9(4)
C33	C34	C36	121.0(4)	C35	C34	C36	121.1(4)
C30	C35	C34	121.5(4)	Ti2	C38	C39	72.7(2)
Ti2	C38	C42	70.0(2)	Ti2	C38	C44	123.1(3)
C39	C38	C42	107.2(4)	C39	C38	C44	126.9(4)
C42	C38	C44	126.0(4)	Ti2	C39	C38	72.7(2)
Ti2	C39	C40	72.1(2)	Ti2	C39	C45	123.2(3)
C38	C39	C40	107.6(4)	C38	C39	C45	126.3(4)

Table S8-6. Bond angles (°) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
C40	C39	C45	126.1(4)	Ti2	C40	C39	72.7(2)
Ti2	C40	C41	72.2(2)	Ti2	C40	C46	123.9(3)
C39	C40	C41	108.1(4)	C39	C40	C46	124.7(4)
C41	C40	C46	127.1(4)	Ti2	C41	C40	73.4(2)
Ti2	C41	C42	71.1(2)	Ti2	C41	C47	121.3(3)
C40	C41	C42	108.2(4)	C40	C41	C47	126.9(4)
C42	C41	C47	124.9(4)	Ti2	C42	C38	74.9(2)
Ti2	C42	C41	74.1(2)	Ti2	C42	C43	122.4(3)
C38	C42	C41	108.9(4)	C38	C42	C43	125.9(4)
C41	C42	C43	124.9(4)				

Table S8-7. Bond angles involving hydrogens (°)

atom	atom	atom	angle	atom	atom	atom	angle
N1	C1	H1A	108.9	N1	C1	H1B	108.9
C2	C1	H1A	108.9	C2	C1	H1B	108.9
H1A	C1	H1B	107.7	C4	C5	H5	118.9
C6	C5	H5	119.0	C2	C7	H7	118.9
C6	C7	H7	118.9	C6	C8	H8A	109.5
C6	C8	H8B	109.5	C6	C8	H8C	109.5
H8A	C8	H8B	109.5	H8A	C8	H8C	109.5
H8B	C8	H8C	109.5	C4	C9	H9A	109.5
C4	C9	H9B	109.5	C4	C9	H9C	109.5
H9A	C9	H9B	109.5	H9A	C9	H9C	109.5
H9B	C9	H9C	109.5	C10	C15	H15A	109.5
C10	C15	H15B	109.5	C10	C15	H15C	109.5
H15A	C15	H15B	109.5	H15A	C15	H15C	109.5
H15B	C15	H15C	109.5	C11	C16	H16A	109.5
C11	C16	H16B	109.5	C11	C16	H16C	109.5
H16A	C16	H16B	109.5	H16A	C16	H16C	109.5
H16B	C16	H16C	109.5	C12	C17	H17A	109.5
C12	C17	H17B	109.5	C12	C17	H17C	109.5
H17A	C17	H17B	109.5	H17A	C17	H17C	109.5
H17B	C17	H17C	109.5	C13	C18	H18A	109.5
C13	C18	H18B	109.5	C13	C18	H18C	109.5
H18A	C18	H18B	109.5	H18A	C18	H18C	109.5
H18B	C18	H18C	109.5	C14	C19	H19A	109.5
C14	C19	H19B	109.5	C14	C19	H19C	109.5
H19A	C19	H19B	109.5	H19A	C19	H19C	109.5
H19B	C19	H19C	109.5	N1	C20	H20A	108.8
N1	C20	H20B	108.8	C21	C20	H20A	108.8
C21	C20	H20B	108.8	H20A	C20	H20B	107.7
C23	C24	H24	118.9	C25	C24	H24	118.9
C21	C26	H26	119.1	C25	C26	H26	119.1
C25	C27	H27A	109.5	C25	C27	H27B	109.5
C25	C27	H27C	109.5	H27A	C27	H27B	109.5
H27A	C27	H27C	109.5	H27B	C27	H27C	109.5
C23	C28	H28A	109.5	C23	C28	H28B	109.5
C23	C28	H28C	109.5	H28A	C28	H28B	109.5
H28A	C28	H28C	109.5	H28B	C28	H28C	109.5
N1	C29	H29A	109.0	N1	C29	H29B	109.0

Table S8-7. Bond angles involving hydrogens (°) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
C30	C29	H29A	109.0	C30	C29	H29B	109.0
H29A	C29	H29B	107.8	C32	C33	H33	118.5
C34	C33	H33	118.5	C30	C35	H35	119.3
C34	C35	H35	119.3	C34	C36	H36A	109.5
C34	C36	H36B	109.5	C34	C36	H36C	109.5
H36A	C36	H36B	109.5	H36A	C36	H36C	109.5
H36B	C36	H36C	109.5	C32	C37	H37A	109.5
C32	C37	H37B	109.5	C32	C37	H37C	109.5
H37A	C37	H37B	109.5	H37A	C37	H37C	109.5
H37B	C37	H37C	109.5	C42	C43	H43A	109.5
C42	C43	H43B	109.5	C42	C43	H43C	109.5
H43A	C43	H43B	109.5	H43A	C43	H43C	109.5
H43B	C43	H43C	109.5	C38	C44	H44A	109.5
C38	C44	H44B	109.5	C38	C44	H44C	109.5
H44A	C44	H44B	109.5	H44A	C44	H44C	109.5
H44B	C44	H44C	109.5	C39	C45	H45A	109.5
C39	C45	H45B	109.5	C39	C45	H45C	109.5
H45A	C45	H45B	109.5	H45A	C45	H45C	109.5
H45B	C45	H45C	109.5	C40	C46	H46A	109.5
C40	C46	H46B	109.5	C40	C46	H46C	109.5
H46A	C46	H46B	109.5	H46A	C46	H46C	109.5
H46B	C46	H46C	109.5	C41	C47	H47A	109.5
C41	C47	H47B	109.5	C41	C47	H47C	109.5
H47A	C47	H47B	109.5	H47A	C47	H47C	109.5
H47B	C47	H47C	109.5				

Table S8-8. Torsion Angles(°)

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

atom1	atom2	atom3	atom4	angle	atom1	atom2	atom3	atom4	angle
Cl1	Ti1	C10	C11	-24.6(2)	Cl1	Ti1	C10	C14	-140.39(12)
Cl1	Ti1	C10	C15	97.9(3)	Cl1	Ti1	C11	C10	159.41(15)
Cl1	Ti1	C11	C12	-84.79(16)	Cl1	Ti1	C11	C16	36.7(3)
Cl1	Ti1	C12	C11	94.39(16)	Cl1	Ti1	C12	C13	-149.1(2)
Cl1	Ti1	C12	C17	-26.8(3)	Cl1	Ti1	C13	C12	34.9(2)
Cl1	Ti1	C13	C14	151.58(12)	Cl1	Ti1	C13	C18	-88.2(3)
Cl1	Ti1	C14	C10	67.6(3)	Cl1	Ti1	C14	C13	-47.2(3)
Cl1	Ti1	C14	C19	-170.69(14)	Cl2	Ti1	C10	C11	126.53(13)
Cl2	Ti1	C10	C14	10.8(2)	Cl2	Ti1	C10	C15	-110.9(2)
Cl2	Ti1	C11	C10	-88.7(2)	Cl2	Ti1	C11	C12	27.1(3)
Cl2	Ti1	C11	C16	148.55(19)	Cl2	Ti1	C12	C11	-162.64(13)
Cl2	Ti1	C12	C13	-46.1(2)	Cl2	Ti1	C12	C17	76.2(3)
Cl2	Ti1	C13	C12	136.90(19)	Cl2	Ti1	C13	C14	-106.38(16)
Cl2	Ti1	C13	C18	13.9(3)	Cl2	Ti1	C14	C10	-171.71(15)
Cl2	Ti1	C14	C13	73.45(16)	Cl2	Ti1	C14	C19	-50.0(3)
O1	Ti1	C10	C11	-128.59(17)	O1	Ti1	C10	C14	115.63(18)
O1	Ti1	C10	C15	-6.0(3)	O1	Ti1	C11	C10	55.91(19)
O1	Ti1	C11	C12	171.72(16)	O1	Ti1	C11	C16	-66.8(3)
O1	Ti1	C12	C11	-13.2(3)	O1	Ti1	C12	C13	103.3(3)
O1	Ti1	C12	C17	-134.4(3)	O1	Ti1	C13	C12	-120.4(2)
O1	Ti1	C13	C14	-3.7(3)	O1	Ti1	C13	C18	116.5(3)
O1	Ti1	C14	C10	-67.71(18)	O1	Ti1	C14	C13	177.45(15)
O1	Ti1	C14	C19	54.0(3)	C10	Ti1	C11	C10	-0.00(18)
C10	Ti1	C11	C12	115.8(3)	C10	Ti1	C11	C16	-122.7(4)
C11	Ti1	C10	C11	-0.00(18)	C11	Ti1	C10	C14	-115.8(3)
C11	Ti1	C10	C15	122.5(4)	C10	Ti1	C12	C11	-37.30(17)
C10	Ti1	C12	C13	79.2(2)	C10	Ti1	C12	C17	-158.5(4)
C12	Ti1	C10	C11	37.42(17)	C12	Ti1	C10	C14	-78.4(2)
C12	Ti1	C10	C15	160.0(3)	C10	Ti1	C13	C12	-78.5(2)
C10	Ti1	C13	C14	38.18(17)	C10	Ti1	C13	C18	158.4(4)
C13	Ti1	C10	C11	78.0(2)	C13	Ti1	C10	C14	-37.81(16)
C13	Ti1	C10	C15	-159.5(3)	C10	Ti1	C14	C10	0.00(19)
C10	Ti1	C14	C13	-114.8(3)	C10	Ti1	C14	C19	121.7(4)
C14	Ti1	C10	C11	115.8(3)	C14	Ti1	C10	C14	-0.00(19)
C14	Ti1	C10	C15	-121.7(4)	C11	Ti1	C12	C11	0.00(19)
C11	Ti1	C12	C13	116.5(4)	C11	Ti1	C12	C17	-121.2(4)
C12	Ti1	C11	C10	-115.8(3)	C12	Ti1	C11	C12	-0.00(19)

Table S8-8. Torsion angles (°) (continued)

atom1	atom2	atom3	atom4	angle	atom1	atom2	atom3	atom4	angle
C12	Ti1	C11	C16	121.5(5)	C11	Ti1	C13	C12	-37.25(19)
C11	Ti1	C13	C14	79.5(2)	C11	Ti1	C13	C18	-160.3(4)
C13	Ti1	C11	C10	-79.3(2)	C13	Ti1	C11	C12	36.50(17)
C13	Ti1	C11	C16	158.0(4)	C11	Ti1	C14	C10	37.14(17)
C11	Ti1	C14	C13	-77.7(2)	C11	Ti1	C14	C19	158.8(4)
C14	Ti1	C11	C10	-37.77(17)	C14	Ti1	C11	C12	78.0(2)
C14	Ti1	C11	C16	-160.5(4)	C12	Ti1	C13	C12	0.0(2)
C12	Ti1	C13	C14	116.7(4)	C12	Ti1	C13	C18	-123.0(5)
C13	Ti1	C12	C11	-116.5(4)	C13	Ti1	C12	C13	0.0(2)
C13	Ti1	C12	C17	122.3(5)	C12	Ti1	C14	C10	78.5(2)
C12	Ti1	C14	C13	-36.35(18)	C12	Ti1	C14	C19	-159.8(4)
C14	Ti1	C12	C11	-79.3(2)	C14	Ti1	C12	C13	37.23(18)
C14	Ti1	C12	C17	159.5(4)	C13	Ti1	C14	C10	114.8(3)
C13	Ti1	C14	C13	0.00(18)	C13	Ti1	C14	C19	-123.5(4)
C14	Ti1	C13	C12	-116.7(3)	C14	Ti1	C13	C14	0.00(18)
C14	Ti1	C13	C18	120.3(4)	Cl3	Ti2	C38	C39	-29.4(2)
Cl3	Ti2	C38	C42	-145.62(11)	Cl3	Ti2	C38	C44	93.8(3)
Cl3	Ti2	C39	C38	154.15(16)	Cl3	Ti2	C39	C40	-90.20(15)
Cl3	Ti2	C39	C45	31.7(2)	Cl3	Ti2	C40	C39	87.93(15)
Cl3	Ti2	C40	C41	-155.94(15)	Cl3	Ti2	C40	C46	-32.7(3)
Cl3	Ti2	C41	C40	27.61(19)	Cl3	Ti2	C41	C42	144.15(12)
Cl3	Ti2	C41	C47	-95.9(2)	Cl3	Ti2	C42	C38	56.4(3)
Cl3	Ti2	C42	C41	-58.8(3)	Cl3	Ti2	C42	C43	179.60(13)
O2	Ti2	C38	C39	118.22(19)	O2	Ti2	C38	C42	2.0(3)
O2	Ti2	C38	C44	-118.6(3)	O2	Ti2	C39	C38	-102.7(2)
O2	Ti2	C39	C40	12.9(3)	O2	Ti2	C39	C45	134.8(2)
O2	Ti2	C40	C39	-171.59(16)	O2	Ti2	C40	C41	-55.46(19)
O2	Ti2	C40	C46	67.8(3)	O2	Ti2	C41	C40	127.67(17)
O2	Ti2	C41	C42	-115.78(17)	O2	Ti2	C41	C47	4.1(3)
O2	Ti2	C42	C38	-178.60(15)	O2	Ti2	C42	C41	66.17(18)
O2	Ti2	C42	C43	-55.4(3)	O3	Ti2	C38	C39	-129.30(18)
O3	Ti2	C38	C42	114.47(18)	O3	Ti2	C38	C44	-6.1(3)
O3	Ti2	C39	C38	54.2(2)	O3	Ti2	C39	C40	169.82(15)
O3	Ti2	C39	C45	-68.3(3)	O3	Ti2	C40	C39	-15.9(3)
O3	Ti2	C40	C41	100.2(3)	O3	Ti2	C40	C46	-136.6(3)
O3	Ti2	C41	C40	-120.44(19)	O3	Ti2	C41	C42	-3.9(3)
O3	Ti2	C41	C47	116.0(2)	O3	Ti2	C42	C38	-67.55(18)

Table S8-8. Torsion angles (°) (continued)

atom1	atom2	atom3	atom4	angle	atom1	atom2	atom3	atom4	angle
O3	Ti2	C42	C41	177.22(16)	O3	Ti2	C42	C43	55.6(3)
C38	Ti2	C39	C38	-0.00(18)	C38	Ti2	C39	C40	115.6(3)
C38	Ti2	C39	C45	-122.5(4)	C39	Ti2	C38	C39	0.00(18)
C39	Ti2	C38	C42	-116.2(3)	C39	Ti2	C38	C44	123.2(4)
C38	Ti2	C40	C39	-37.11(16)	C38	Ti2	C40	C41	79.02(19)
C38	Ti2	C40	C46	-157.8(4)	C40	Ti2	C38	C39	37.84(17)
C40	Ti2	C38	C42	-78.40(19)	C40	Ti2	C38	C44	161.0(3)
C38	Ti2	C41	C40	-78.64(19)	C38	Ti2	C41	C42	37.91(15)
C38	Ti2	C41	C47	157.8(3)	C41	Ti2	C38	C39	78.63(19)
C41	Ti2	C38	C42	-37.61(16)	C41	Ti2	C38	C44	-158.2(3)
C38	Ti2	C42	C38	0.00(18)	C38	Ti2	C42	C41	-115.2(3)
C38	Ti2	C42	C43	123.2(4)	C42	Ti2	C38	C39	116.2(3)
C42	Ti2	C38	C42	-0.00(17)	C42	Ti2	C38	C44	-120.6(4)
C39	Ti2	C40	C39	-0.00(17)	C39	Ti2	C40	C41	116.1(3)
C39	Ti2	C40	C46	-120.7(4)	C40	Ti2	C39	C38	-115.6(3)
C40	Ti2	C39	C40	-0.00(18)	C40	Ti2	C39	C45	121.9(4)
C39	Ti2	C41	C40	-37.64(15)	C39	Ti2	C41	C42	78.90(18)
C39	Ti2	C41	C47	-161.2(3)	C41	Ti2	C39	C38	-78.92(19)
C41	Ti2	C39	C40	36.73(15)	C41	Ti2	C39	C45	158.6(3)
C39	Ti2	C42	C38	36.81(15)	C39	Ti2	C42	C41	-78.42(19)
C39	Ti2	C42	C43	160.0(3)	C42	Ti2	C39	C38	-37.50(16)
C42	Ti2	C39	C40	78.15(19)	C42	Ti2	C39	C45	-160.0(3)
C40	Ti2	C41	C40	-0.00(17)	C40	Ti2	C41	C42	116.5(3)
C40	Ti2	C41	C47	-123.5(4)	C41	Ti2	C40	C39	-116.1(3)
C41	Ti2	C40	C41	0.00(16)	C41	Ti2	C40	C46	123.2(4)
C40	Ti2	C42	C38	78.60(19)	C40	Ti2	C42	C41	-36.63(16)
C40	Ti2	C42	C43	-158.2(3)	C42	Ti2	C40	C39	-78.92(19)
C42	Ti2	C40	C41	37.21(16)	C42	Ti2	C40	C46	160.4(4)
C41	Ti2	C42	C38	115.2(3)	C41	Ti2	C42	C41	0.00(17)
C41	Ti2	C42	C43	-121.6(4)	C42	Ti2	C41	C40	-116.5(3)
C42	Ti2	C41	C42	0.00(18)	C42	Ti2	C41	C47	119.9(4)
C1	N1	C20	C21	79.9(4)	C20	N1	C1	C2	-70.1(4)
C1	N1	C29	C30	-71.1(4)	C29	N1	C1	C2	166.9(3)
C20	N1	C29	C30	164.6(3)	C29	N1	C20	C21	-156.9(3)
N1	C1	C2	C3	134.1(3)	N1	C1	C2	C7	-43.6(5)
C1	C2	C3	O1	-2.0(6)	C1	C2	C3	C4	-179.4(3)
C1	C2	C7	C6	177.0(3)	C3	C2	C7	C6	-0.8(6)

Table S8-8. Torsion angles (°) (continued)

atom1	atom2	atom3	atom4	angle	atom1	atom2	atom3	atom4	angle
C7	C2	C3	O1	175.8(3)	C7	C2	C3	C4	-1.6(6)
O1	C3	C4	C5	-174.8(3)	O1	C3	C4	C9	4.8(6)
C2	C3	C4	C5	2.7(6)	C2	C3	C4	C9	-177.7(3)
C3	C4	C5	C6	-1.3(6)	C9	C4	C5	C6	179.1(4)
C4	C5	C6	C7	-1.0(6)	C4	C5	C6	C8	176.2(4)
C5	C6	C7	C2	2.1(6)	C8	C6	C7	C2	-175.1(3)
Ti1	C10	C11	Ti1	0.000(17)	Ti1	C10	C11	C12	-65.4(3)
Ti1	C10	C11	C16	119.2(4)	Ti1	C10	C14	Ti1	0.000(18)
Ti1	C10	C14	C13	67.1(3)	Ti1	C10	C14	C19	-115.8(4)
C11	C10	C14	Ti1	-65.4(3)	C11	C10	C14	C13	1.6(5)
C11	C10	C14	C19	178.7(4)	C14	C10	C11	Ti1	64.4(3)
C14	C10	C11	C12	-1.0(5)	C14	C10	C11	C16	-176.4(4)
C15	C10	C11	Ti1	-117.4(5)	C15	C10	C11	C12	177.2(4)
C15	C10	C11	C16	1.8(7)	C15	C10	C14	Ti1	116.4(5)
C15	C10	C14	C13	-176.6(4)	C15	C10	C14	C19	0.5(7)
Ti1	C11	C12	Ti1	0.000(18)	Ti1	C11	C12	C13	-63.9(3)
Ti1	C11	C12	C17	120.6(4)	C10	C11	C12	Ti1	63.9(3)
C10	C11	C12	C13	0.0(5)	C10	C11	C12	C17	-175.5(4)
C16	C11	C12	Ti1	-120.6(5)	C16	C11	C12	C13	175.5(4)
C16	C11	C12	C17	-0.0(7)	Ti1	C12	C13	Ti1	0.00(2)
Ti1	C12	C13	C14	-62.0(3)	Ti1	C12	C13	C18	122.3(4)
C11	C12	C13	Ti1	63.0(3)	C11	C12	C13	C14	1.0(5)
C11	C12	C13	C18	-174.7(4)	C17	C12	C13	Ti1	-121.5(5)
C17	C12	C13	C14	176.5(4)	C17	C12	C13	C18	0.7(8)
Ti1	C13	C14	Ti1	0.000(17)	Ti1	C13	C14	C10	-65.5(2)
Ti1	C13	C14	C19	117.4(4)	C12	C13	C14	Ti1	63.9(3)
C12	C13	C14	C10	-1.6(5)	C12	C13	C14	C19	-178.7(4)
C18	C13	C14	Ti1	-120.3(5)	C18	C13	C14	C10	174.2(4)
C18	C13	C14	C19	-2.9(7)	N1	C20	C21	C22	61.5(4)
N1	C20	C21	C26	-117.4(4)	C20	C21	C22	O2	-1.7(5)
C20	C21	C22	C23	179.7(3)	C20	C21	C26	C25	177.9(3)
C22	C21	C26	C25	-1.0(6)	C26	C21	C22	O2	177.2(3)
C26	C21	C22	C23	-1.3(6)	O2	C22	C23	C24	-176.0(3)
O2	C22	C23	C28	1.8(5)	C21	C22	C23	C24	2.5(6)
C21	C22	C23	C28	-179.7(3)	C22	C23	C24	C25	-1.5(6)
C28	C23	C24	C25	-179.3(4)	C23	C24	C25	C26	-0.7(6)
C23	C24	C25	C27	176.6(4)	C24	C25	C26	C21	2.0(6)

Table S8-8. Torsion angles (°) (continued)

atom1	atom2	atom3	atom4	angle	atom1	atom2	atom3	atom4	angle
C27	C25	C26	C21	-175.3(4)	N1	C29	C30	C31	-62.8(4)
N1	C29	C30	C35	120.3(3)	C29	C30	C31	O3	2.9(5)
C29	C30	C31	C32	-178.2(3)	C29	C30	C35	C34	178.8(3)
C31	C30	C35	C34	1.9(5)	C35	C30	C31	O3	179.9(3)
C35	C30	C31	C32	-1.2(5)	O3	C31	C32	C33	178.5(3)
O3	C31	C32	C37	-2.8(5)	C30	C31	C32	C33	-0.3(5)
C30	C31	C32	C37	178.3(3)	C31	C32	C33	C34	1.4(5)
C37	C32	C33	C34	-177.3(3)	C32	C33	C34	C35	-0.8(5)
C32	C33	C34	C36	179.6(3)	C33	C34	C35	C30	-0.9(5)
C36	C34	C35	C30	178.8(3)	Ti2	C38	C39	Ti2	-0.000(19)
Ti2	C38	C39	C40	-64.1(2)	Ti2	C38	C39	C45	118.9(3)
Ti2	C38	C42	Ti2	0.000(18)	Ti2	C38	C42	C41	66.8(2)
Ti2	C38	C42	C43	-119.3(3)	C39	C38	C42	Ti2	-63.7(3)
C39	C38	C42	C41	3.1(4)	C39	C38	C42	C43	176.9(3)
C42	C38	C39	Ti2	61.9(3)	C42	C38	C39	C40	-2.2(4)
C42	C38	C39	C45	-179.2(3)	C44	C38	C39	Ti2	-118.8(4)
C44	C38	C39	C40	177.1(3)	C44	C38	C39	C45	0.1(6)
C44	C38	C42	Ti2	117.0(4)	C44	C38	C42	C41	-176.2(3)
C44	C38	C42	C43	-2.4(6)	Ti2	C39	C40	Ti2	-0.000(19)
Ti2	C39	C40	C41	-64.0(2)	Ti2	C39	C40	C46	119.7(3)
C38	C39	C40	Ti2	64.6(3)	C38	C39	C40	C41	0.5(4)
C38	C39	C40	C46	-175.7(3)	C45	C39	C40	Ti2	-118.5(4)
C45	C39	C40	C41	177.5(3)	C45	C39	C40	C46	1.3(6)
Ti2	C40	C41	Ti2	0.00(2)	Ti2	C40	C41	C42	-63.0(2)
Ti2	C40	C41	C47	117.1(3)	C39	C40	C41	Ti2	64.4(3)
C39	C40	C41	C42	1.4(4)	C39	C40	C41	C47	-178.5(3)
C46	C40	C41	Ti2	-119.5(4)	C46	C40	C41	C42	177.6(3)
C46	C40	C41	C47	-2.4(6)	Ti2	C41	C42	Ti2	-0.000(18)
Ti2	C41	C42	C38	-67.4(2)	Ti2	C41	C42	C43	118.7(3)
C40	C41	C42	Ti2	64.5(3)	C40	C41	C42	C38	-2.8(4)
C40	C41	C42	C43	-176.7(3)	C47	C41	C42	Ti2	-115.5(4)
C47	C41	C42	C38	177.1(3)	C47	C41	C42	C43	3.2(6)

Table S8-9. Intramolecular contacts less than 3.60 Å

atom	atom	distance	atom	atom	distance
Cl1	C16	3.544(6)	Cl1	C17	3.415(6)
Cl2	C18	3.255(6)	Cl3	C45	3.387(5)
Cl3	C46	3.434(5)	O1	C1	2.876(5)
O1	C9	2.814(6)	O1	C15	3.119(6)
O2	N1	2.992(4)	O2	C7	3.546(5)
O2	C20	2.847(5)	O2	C28	2.836(5)
O2	C47	3.067(5)	O3	N1	2.974(4)
O3	C29	2.832(5)	O3	C37	2.862(6)
O3	C44	3.148(5)	N1	C7	2.960(5)
N1	C22	3.114(5)	N1	C26	3.571(6)
N1	C31	3.094(5)	N1	C35	3.576(5)
C1	C21	3.172(6)	C1	C30	3.034(5)
C2	C5	2.798(5)	C2	C20	3.051(6)
C2	C21	3.048(6)	C2	C26	3.317(6)
C3	C6	2.790(6)	C3	C15	3.431(7)
C3	C26	3.453(6)	C4	C7	2.787(6)
C7	C20	3.543(6)	C7	C21	3.120(6)
C7	C22	3.181(6)	C7	C26	3.551(6)
C15	C16	3.193(7)	C15	C19	3.176(7)
C16	C17	3.160(9)	C17	C18	3.169(8)
C18	C19	3.179(8)	C21	C24	2.778(6)
C22	C25	2.786(6)	C23	C26	2.790(6)
C30	C33	2.771(6)	C31	C34	2.806(6)
C31	C44	3.495(6)	C32	C35	2.800(6)
C43	C44	3.194(7)	C43	C47	3.131(6)
C44	C45	3.202(7)	C45	C46	3.179(7)
C46	C47	3.210(7)			

Table S8-10. Intramolecular contacts less than 3.60 Å involving hydrogens

atom	atom	distance	atom	atom	distance
Ti1	H1B	3.122	Ti1	H9A	3.238
Ti1	H15C	3.320	Ti1	H16B	3.403
Ti1	H17C	3.457	Ti1	H18B	3.466
Ti1	H19C	3.288	Ti2	H28A	3.194
Ti2	H29A	3.579	Ti2	H37A	3.312
Ti2	H43B	3.345	Ti2	H44C	3.399
Ti2	H45B	3.395	Ti2	H46C	3.417
Ti2	H47B	3.334	Cl1	H1B	2.975
Cl1	H16A	3.418	Cl1	H16B	3.320
Cl1	H17A	3.333	Cl1	H17C	3.127
Cl1	H20A	3.201	Cl2	H9A	3.051
Cl2	H18A	3.269	Cl2	H18B	2.858
Cl2	H19A	3.562	Cl2	H19C	3.582
Cl3	H8A	3.476	Cl3	H28A	3.031
Cl3	H37A	3.214	Cl3	H45A	3.267
Cl3	H45B	3.117	Cl3	H46A	3.308
Cl3	H46C	3.184	O1	H1A	3.373
O1	H1B	2.430	O1	H9A	2.344
O1	H9B	3.483	O1	H9C	3.430
O1	H15A	3.299	O1	H15C	2.681
O1	H19C	3.285	O1	H26	3.457
O2	H7	2.981	O2	H20B	2.807
O2	H28A	2.372	O2	H28B	3.509
O2	H28C	3.449	O2	H43B	3.305
O2	H47A	3.257	O2	H47B	2.611
O3	H7	3.425	O3	H29A	2.782
O3	H37A	2.412	O3	H37B	3.505
O3	H37C	3.504	O3	H44A	3.322
O3	H44C	2.722	N1	H7	2.731
C1	H7	2.665	C1	H15C	2.842
C1	H16B	2.931	C1	H20A	2.503
C1	H20B	3.231	C1	H29A	3.232
C1	H29B	2.526	C2	H15C	2.832
C2	H20A	3.178	C2	H26	3.422
C3	H1A	3.053	C3	H1B	2.577
C3	H5	3.240	C3	H7	3.236
C3	H9A	2.556	C3	H9B	3.140

Table S8-10. Intramolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
C3	H9C	3.135	C3	H15A	3.467
C3	H15C	2.762	C3	H26	3.309
C4	H27C	3.351	C5	H7	3.220
C5	H8A	3.302	C5	H8B	2.775
C5	H8C	2.775	C5	H9A	3.311
C5	H9B	2.785	C5	H9C	2.785
C5	H27C	3.597	C7	H1A	2.873
C7	H1B	3.295	C7	H5	3.221
C7	H8A	2.548	C7	H8B	3.109
C7	H8C	3.140	C8	H5	2.672
C8	H7	2.645	C8	H28C	3.144
C9	H5	2.686	C9	H19C	3.140
C9	H27C	3.441	C10	H16A	3.353
C10	H16B	2.863	C10	H16C	2.862
C10	H19A	3.353	C10	H19B	2.850
C10	H19C	2.850	C11	H1B	3.459
C11	H15A	3.344	C11	H15B	2.846
C11	H15C	2.845	C11	H17A	2.660
C11	H17B	3.168	C11	H17C	3.221
C12	H16A	2.656	C12	H16B	3.224
C12	H16C	3.170	C12	H18A	3.340
C12	H18B	2.842	C12	H18C	2.842
C13	H17A	3.338	C13	H17B	2.837
C13	H17C	2.838	C13	H19A	2.674
C13	H19B	3.186	C13	H19C	3.219
C14	H15A	2.666	C14	H15B	3.187
C14	H15C	3.208	C14	H18A	2.653
C14	H18B	3.213	C14	H18C	3.163
C15	H1A	3.356	C15	H1B	3.591
C15	H16B	3.156	C15	H16C	3.176
C15	H19B	3.138	C15	H19C	3.144
C16	H1A	3.510	C16	H1B	3.204
C16	H15B	3.152	C16	H15C	3.171
C16	H17A	2.726	C16	H35	3.352
C17	H16A	2.726	C17	H18B	3.135
C17	H18C	3.143	C18	H17B	3.133
C18	H17C	3.141	C18	H19A	2.757

Table S8-10. Intramolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
C19	H9A	3.364	C19	H15A	2.747
C19	H18A	2.747	C20	H1A	3.252
C20	H1B	2.562	C20	H7	3.489
C20	H26	2.677	C20	H29A	2.483
C20	H29B	2.705	C20	H43B	3.166
C21	H1B	3.452	C21	H7	3.186
C22	H7	2.971	C22	H20A	3.313
C22	H20B	2.768	C22	H24	3.232
C22	H26	3.236	C22	H28A	2.557
C22	H28B	3.145	C22	H28C	3.121
C22	H47B	2.932	C23	H8A	3.469
C23	H8B	3.176	C23	H47B	3.141
C24	H8B	3.243	C24	H26	3.218
C24	H27A	2.575	C24	H27B	3.154
C24	H27C	3.125	C24	H28A	3.304
C24	H28B	2.775	C24	H28C	2.775
C26	H20A	2.570	C26	H20B	3.150
C26	H24	3.216	C26	H27A	3.298
C26	H27B	2.765	C26	H27C	2.765
C27	H24	2.667	C27	H26	2.658
C28	H8A	3.420	C28	H8B	3.255
C28	H24	2.676	C28	H46C	3.190
C28	H47B	3.062	C29	H1A	2.490
C29	H1B	2.679	C29	H16B	3.582
C29	H20A	2.761	C29	H20B	2.434
C29	H35	2.673	C29	H43A	3.557
C29	H43B	3.273	C30	H1A	2.611
C30	H1B	3.513	C31	H1A	3.385
C31	H29A	2.748	C31	H29B	3.307
C31	H33	3.240	C31	H35	3.245
C31	H37A	2.582	C31	H37B	3.156
C31	H37C	3.142	C31	H44A	3.473
C31	H44C	2.884	C32	H44C	2.938
C33	H35	3.221	C33	H36A	3.291
C33	H36B	2.759	C33	H36C	2.759
C33	H37A	3.307	C33	H37B	2.769
C33	H37C	2.769	C35	H1A	3.018

Table S8-10. Intramolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
C35	H16B	3.429	C35	H29A	3.133
C35	H29B	2.565	C35	H33	3.219
C35	H36A	2.570	C35	H36B	3.141
C35	H36C	3.137	C36	H33	2.647
C36	H35	2.677	C37	H33	2.663
C37	H44C	2.840	C37	H45B	3.277
C38	H43A	2.683	C38	H43B	3.248
C38	H43C	3.177	C38	H45A	3.353
C38	H45B	2.851	C38	H45C	2.851
C39	H37A	3.590	C39	H44A	3.361
C39	H44B	2.865	C39	H44C	2.865
C39	H46A	2.662	C39	H46B	3.187
C39	H46C	3.232	C40	H28A	3.483
C40	H45A	2.676	C40	H45B	3.231
C40	H45C	3.196	C40	H47A	3.345
C40	H47B	2.853	C40	H47C	2.853
C41	H43A	3.348	C41	H43B	2.840
C41	H43C	2.840	C41	H46A	3.352
C41	H46B	2.862	C41	H46C	2.862
C42	H29A	3.520	C42	H44A	2.668
C42	H44B	3.199	C42	H44C	3.207
C42	H47A	2.634	C42	H47B	3.175
C42	H47C	3.175	C43	H20B	3.179
C43	H29A	2.865	C43	H44A	2.762
C43	H47A	2.684	C44	H37A	3.426
C44	H37C	3.590	C44	H43A	2.772
C44	H45B	3.170	C44	H45C	3.171
C45	H37A	3.345	C45	H44B	3.174
C45	H44C	3.175	C45	H46A	2.741
C46	H28A	3.239	C46	H45A	2.746
C46	H47B	3.196	C46	H47C	3.171
C47	H28A	3.478	C47	H43B	3.074
C47	H43C	3.109	C47	H46B	3.199
C47	H46C	3.174	H1A	H7	2.880
H1A	H15C	2.454	H1A	H16B	2.629
H1A	H20A	3.370	H1A	H29A	3.423
H1A	H29B	2.604	H1A	H35	3.095

Table S8-10. Intramolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
H1B	H7	3.567	H1B	H15C	2.803
H1B	H16B	2.357	H1B	H20A	2.254
H1B	H20B	3.348	H1B	H26	3.590
H1B	H29A	3.476	H1B	H29B	2.443
H5	H8A	3.578	H5	H8B	2.737
H5	H8C	2.706	H5	H9A	3.591
H5	H9B	2.739	H5	H9C	2.731
H7	H8A	2.324	H7	H8B	3.284
H7	H8C	3.299	H8A	H28A	3.483
H8A	H28C	2.876	H8B	H24	3.246
H8B	H28C	2.562	H9A	H19C	2.512
H9B	H19C	2.975	H9C	H27C	2.800
H15A	H19B	2.591	H15A	H19C	2.582
H15B	H16B	3.222	H15B	H16C	2.846
H15B	H19B	3.565	H15C	H16B	2.846
H15C	H16C	3.276	H16A	H17A	2.059
H16A	H17B	3.316	H16A	H17C	3.389
H16A	H35	3.551	H16B	H17A	3.390
H16B	H29B	2.902	H16B	H35	2.771
H16C	H17A	3.316	H16C	H35	3.240
H17B	H18B	3.213	H17B	H18C	2.817
H17C	H18B	2.817	H17C	H18C	3.234
H18A	H19A	2.093	H18A	H19B	3.334
H18A	H19C	3.416	H18B	H19A	3.402
H18C	H19A	3.368	H20A	H26	2.357
H20A	H29A	2.940	H20A	H29B	2.708
H20B	H26	3.328	H20B	H29A	2.119
H20B	H29B	2.776	H20B	H43A	3.530
H20B	H43B	2.249	H20B	H47A	3.539
H24	H27A	2.359	H24	H27B	3.324
H24	H27C	3.302	H24	H28A	3.582
H24	H28B	2.720	H24	H28C	2.726
H26	H27A	3.566	H26	H27B	2.684
H26	H27C	2.723	H28A	H46C	2.388
H28A	H47B	2.666	H28B	H46C	3.207
H28B	H47B	2.983	H29A	H35	3.313
H29A	H43A	2.612	H29A	H43B	2.370

Table S8-10. Intramolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
H29A	H44A	3.568	H29B	H35	2.353
H33	H36A	3.556	H33	H36B	2.695
H33	H36C	2.691	H33	H37A	3.573
H33	H37B	2.695	H33	H37C	2.717
H35	H36A	2.365	H35	H36B	3.321
H35	H36C	3.323	H37A	H44C	2.584
H37A	H45B	2.485	H37C	H44C	2.645
H37C	H45B	3.258	H43A	H44A	2.109
H43A	H44B	3.398	H43A	H44C	3.401
H43B	H44A	3.442	H43B	H47A	2.487
H43B	H47B	3.544	H43C	H44A	3.336
H43C	H47A	2.557	H43C	H47C	3.530
H44B	H45B	3.256	H44B	H45C	2.856
H44C	H45B	2.856	H44C	H45C	3.260
H45A	H46A	2.078	H45A	H46B	3.349
H45A	H46C	3.397	H45B	H46A	3.400
H45C	H46A	3.338	H46B	H47B	3.308
H46B	H47C	2.873	H46C	H47B	2.874
H46C	H47C	3.238			

Table S8-11. Intermolecular contacts less than 3.60 Å

atom	atom	distance	atom	atom	distance
Cl3	C11[1]	3.577(5)	Cl3	C12[1]	3.484(5)
C5	C20[2]	3.599(6)	C6	C20[2]	3.450(6)
C8	C20[2]	3.499(6)	C11	Cl3[3]	3.577(5)
C12	Cl3[3]	3.484(5)	C20	C5[4]	3.599(6)
C20	C6[4]	3.450(6)	C20	C8[4]	3.499(6)
C33	C41[2]	3.540(5)	C37	C42[2]	3.594(6)
C41	C33[4]	3.540(5)	C42	C37[4]	3.594(6)

Symmetry Operators:

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

Table S8-12. Intermolecular contacts less than 3.60 Å involving hydrogens

atom	atom	distance	atom	atom	distance
Cl1	H5[1]	3.512	Cl1	H36A[2]	3.512
Cl2	H33[3]	2.928	Cl2	H37C[3]	3.518
Cl2	H45C[4]	3.036	Cl3	H17B[5]	3.476
Cl3	H43A[6]	3.212	Cl3	H43C[6]	3.265
O3	H43C[6]	2.859	N1	H8C[1]	3.492
C1	H47A[6]	3.173	C2	H47A[6]	3.239
C5	H20A[6]	3.118	C5	H20B[6]	3.329
C5	H26[6]	3.496	C6	H20A[6]	3.183
C6	H20B[6]	2.853	C6	H43B[6]	3.380
C7	H20B[6]	3.336	C7	H43B[6]	3.059
C7	H43C[6]	3.340	C7	H47A[6]	3.258
C8	H16C[5]	3.136	C8	H20A[6]	3.151
C8	H20B[6]	2.928	C8	H29A[6]	3.467
C8	H29B[6]	3.559	C8	H36A[5]	3.145
C8	H43B[6]	3.348	C9	H27B[6]	3.527
C9	H44B[4]	3.331	C9	H45C[4]	3.085
C10	H46C[7]	3.587	C14	H46A[7]	3.161
C15	H28B[6]	3.560	C15	H46C[7]	3.413
C15	H47A[6]	3.572	C15	H47B[6]	3.125
C16	H8A[7]	3.445	C16	H28C[7]	3.534
C17	H43A[2]	3.473	C17	H44A[2]	3.048
C18	H27A[8]	3.099	C18	H45A[7]	3.578
C19	H18A[9]	3.299	C19	H27A[6]	3.597
C19	H27B[6]	3.416	C19	H45A[4]	3.393
C19	H45C[4]	3.299	C19	H46A[7]	2.835
C20	H5[1]	3.589	C20	H8C[1]	2.803
C23	H15A[1]	3.123	C24	H15A[1]	2.940
C24	H19B[1]	3.560	C24	H36C[5]	3.349
C24	H46B[10]	3.380	C25	H9B[1]	3.578
C25	H15A[1]	3.293	C26	H9B[1]	3.293
C27	H9B[1]	3.459	C27	H18C[11]	3.259
C27	H19B[1]	3.492	C27	H19C[1]	3.360
C28	H15B[5]	3.074	C28	H16C[5]	3.446
C28	H28B[10]	3.165	C29	H8C[1]	3.116
C29	H17A[2]	3.384	C30	H17A[2]	3.165
C30	H47C[6]	3.436	C31	H43C[6]	2.941
C32	H43C[6]	3.007	C33	H47C[6]	3.135

Table S8-12. Intermolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
C34	H47C^{6}	2.827	C35	H17A^{2}	3.100
C35	H47C^{6}	2.994	C36	H8B^{7}	3.154
C36	H24^{7}	3.299	C36	H46B^{6}	3.213
C36	H47C^{6}	3.367	C37	H43C^{6}	3.107
C38	H37B^{1}	2.812	C39	H37B^{1}	3.517
C40	H33^{1}	3.539	C41	H33^{1}	3.590
C41	H37B^{1}	3.568	C42	H37B^{1}	2.895
C43	H7^{1}	3.029	C43	H8A^{1}	3.424
C43	H37A^{1}	3.536	C43	H37B^{1}	3.178
C44	H9C^{12}	3.420	C44	H17B^{2}	3.118
C44	H37B^{1}	3.045	C45	H9A^{12}	3.417
C45	H19A^{12}	3.209	C45	H19C^{12}	3.405
C46	H19B^{5}	2.774	C46	H24^{10}	3.192
C46	H28B^{10}	3.528	C46	H36C^{1}	3.246
C47	H1A^{1}	3.028	C47	H15B^{1}	3.316
C47	H15C^{1}	3.169	H1A	C47^{6}	3.028
H1A	H47A^{6}	2.410	H1A	H47B^{6}	3.462
H1A	H47C^{6}	2.846	H5	Cl1^{6}	3.512
H5	C20^{6}	3.589	H5	H20A^{6}	2.894
H5	H20B^{6}	3.524	H5	H26^{6}	3.245
H5	H36A^{5}	3.533	H7	C43^{6}	3.029
H7	H20B^{6}	3.521	H7	H43A^{6}	3.525
H7	H43B^{6}	2.634	H7	H43C^{6}	2.584
H7	H47A^{6}	3.096	H8A	C16^{5}	3.445
H8A	C43^{6}	3.424	H8A	H16A^{5}	3.319
H8A	H16C^{5}	2.735	H8A	H20B^{6}	3.157
H8A	H29A^{6}	3.281	H8A	H43A^{6}	3.354
H8A	H43B^{6}	2.912	H8A	H43C^{6}	3.471
H8B	C36^{5}	3.154	H8B	H16C^{5}	2.927
H8B	H36A^{5}	2.304	H8B	H36C^{5}	3.262
H8C	N1^{6}	3.492	H8C	C20^{6}	2.803
H8C	C29^{6}	3.116	H8C	H16A^{5}	3.405
H8C	H16C^{5}	3.241	H8C	H20A^{6}	2.393
H8C	H20B^{6}	2.399	H8C	H29A^{6}	2.833
H8C	H29B^{6}	2.690	H8C	H36A^{5}	3.221
H8C	H43B^{6}	3.300	H9A	C45^{4}	3.417
H9A	H44B^{4}	3.332	H9A	H45C^{4}	2.505

Table S8-12. Intermolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
H9B	C25[6]	3.578	H9B	C26[6]	3.293
H9B	C27[6]	3.459	H9B	H26[6]	2.839
H9B	H27B[6]	2.667	H9B	H45B[4]	3.547
H9B	H45C[4]	3.094	H9C	C44[4]	3.420
H9C	H44B[4]	2.595	H9C	H44C[4]	3.440
H9C	H45C[4]	3.182	H15A	C23[6]	3.123
H15A	C24[6]	2.940	H15A	C25[6]	3.293
H15A	H24[6]	3.145	H15A	H28B[6]	3.312
H15A	H46C[7]	3.272	H15A	H47B[6]	3.320
H15B	C28[7]	3.074	H15B	C47[6]	3.316
H15B	H28A[7]	2.958	H15B	H28B[7]	2.934
H15B	H28B[6]	2.929	H15B	H28C[7]	2.806
H15B	H46C[7]	2.971	H15B	H47A[6]	3.490
H15B	H47B[6]	2.715	H15B	H47C[6]	3.255
H15C	C47[6]	3.169	H15C	H47A[6]	2.890
H15C	H47B[6]	2.855	H15C	H47C[6]	3.243
H16A	H8A[7]	3.319	H16A	H8C[7]	3.405
H16A	H29A[2]	3.436	H16A	H29B[2]	3.020
H16A	H35[2]	3.356	H16C	C8[7]	3.136
H16C	C28[7]	3.446	H16C	H8A[7]	2.735
H16C	H8B[7]	2.927	H16C	H8C[7]	3.241
H16C	H28A[7]	3.485	H16C	H28C[7]	2.612
H17A	C29[2]	3.384	H17A	C30[2]	3.165
H17A	C35[2]	3.100	H17A	H29A[2]	3.074
H17A	H29B[2]	3.311	H17A	H35[2]	3.116
H17A	H43A[2]	3.337	H17A	H44A[2]	3.252
H17B	Cl3[7]	3.476	H17B	C44[2]	3.118
H17B	H43A[2]	2.772	H17B	H44A[2]	2.219
H17B	H44B[2]	3.456	H17B	H44C[2]	3.389
H17C	H44A[2]	3.322	H18A	C19[9]	3.299
H18A	H19A[9]	2.829	H18A	H19B[9]	2.946
H18A	H27A[8]	3.081	H18A	H45A[7]	3.325
H18A	H45A[4]	3.466	H18A	H46A[4]	3.424
H18B	H27A[8]	3.038	H18C	C27[8]	3.259
H18C	H27A[8]	2.669	H18C	H27B[8]	3.156
H18C	H27C[8]	3.476	H18C	H45A[7]	3.190
H18C	H45B[7]	3.320	H19A	C45[4]	3.209

Table S8-12. Intermolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
H19A	H18A^{9}	2.829	H19A	H19A^{9}	2.831
H19A	H45A^{7}	3.405	H19A	H45A^{4}	2.666
H19A	H45C^{4}	2.913	H19A	H46A^{7}	3.142
H19B	C24^{6}	3.560	H19B	C27^{6}	3.492
H19B	C46^{7}	2.774	H19B	H18A^{9}	2.946
H19B	H24^{6}	3.187	H19B	H27A^{6}	3.076
H19B	H27B^{6}	3.297	H19B	H45A^{7}	3.258
H19B	H46A^{7}	2.053	H19B	H46B^{7}	2.923
H19B	H46C^{7}	2.965	H19C	C27^{6}	3.360
H19C	C45^{4}	3.405	H19C	H27A^{6}	3.343
H19C	H27B^{6}	2.785	H19C	H45A^{4}	3.273
H19C	H45C^{4}	2.812	H20A	C5^{1}	3.118
H20A	C6^{1}	3.183	H20A	C8^{1}	3.151
H20A	H5^{1}	2.894	H20A	H8C^{1}	2.393
H20B	C5^{1}	3.329	H20B	C6^{1}	2.853
H20B	C7^{1}	3.336	H20B	C8^{1}	2.928
H20B	H5^{1}	3.524	H20B	H7^{1}	3.521
H20B	H8A^{1}	3.157	H20B	H8C^{1}	2.399
H24	C36^{5}	3.299	H24	C46^{10}	3.192
H24	H15A^{1}	3.145	H24	H19B^{1}	3.187
H24	H36A^{5}	3.330	H24	H36C^{5}	2.522
H24	H46A^{10}	3.434	H24	H46B^{10}	2.518
H24	H46C^{10}	3.181	H26	C5^{1}	3.496
H26	H5^{1}	3.245	H26	H9B^{1}	2.839
H27A	C18^{11}	3.099	H27A	C19^{1}	3.597
H27A	H18A^{11}	3.081	H27A	H18B^{11}	3.038
H27A	H18C^{11}	2.669	H27A	H19B^{1}	3.076
H27A	H19C^{1}	3.343	H27A	H36C^{5}	3.505
H27B	C9^{1}	3.527	H27B	C19^{1}	3.416
H27B	H9B^{1}	2.667	H27B	H18C^{11}	3.156
H27B	H19B^{1}	3.297	H27B	H19C^{1}	2.785
H27B	H45B^{3}	3.301	H27C	H18C^{11}	3.476
H28A	H15B^{5}	2.958	H28A	H16C^{5}	3.485
H28A	H28B^{10}	3.163	H28B	C15^{1}	3.560
H28B	C28^{10}	3.165	H28B	C46^{10}	3.528
H28B	H15A^{1}	3.312	H28B	H15B^{5}	2.934
H28B	H15B^{1}	2.929	H28B	H28A^{10}	3.163

Table S8-12. Intermolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
H28B	H28B[10]	2.375	H28B	H46B[10]	3.323
H28B	H46C[10]	2.854	H28B	H47B[10]	3.339
H28C	C16[5]	3.534	H28C	H15B[5]	2.806
H28C	H16C[5]	2.612	H28C	H36A[5]	3.445
H28C	H36C[5]	3.454	H28C	H47C[10]	3.556
H29A	C8[1]	3.467	H29A	H8A[1]	3.281
H29A	H8C[1]	2.833	H29A	H16A[2]	3.436
H29A	H17A[2]	3.074	H29B	C8[1]	3.559
H29B	H8C[1]	2.690	H29B	H16A[2]	3.020
H29B	H17A[2]	3.311	H33	Cl2[13]	2.928
H33	C40[6]	3.539	H33	C41[6]	3.590
H33	H46B[6]	3.361	H33	H47C[6]	3.536
H35	H16A[2]	3.356	H35	H17A[2]	3.116
H35	H47C[6]	3.346	H36A	Cl1[2]	3.512
H36A	C8[7]	3.145	H36A	H5[7]	3.533
H36A	H8B[7]	2.304	H36A	H8C[7]	3.221
H36A	H24[7]	3.330	H36A	H28C[7]	3.445
H36C	C24[7]	3.349	H36C	C46[6]	3.246
H36C	H8B[7]	3.262	H36C	H24[7]	2.522
H36C	H27A[7]	3.505	H36C	H28C[7]	3.454
H36C	H46B[6]	2.300	H36C	H47C[6]	3.037
H37A	C43[6]	3.536	H37A	H43A[6]	3.461
H37A	H43C[6]	2.943	H37B	C38[6]	2.812
H37B	C39[6]	3.517	H37B	C41[6]	3.568
H37B	C42[6]	2.895	H37B	C43[6]	3.178
H37B	C44[6]	3.045	H37B	H43A[6]	3.203
H37B	H43C[6]	2.891	H37B	H44A[6]	3.069
H37B	H44B[6]	2.749	H37C	Cl2[13]	3.518
H43A	Cl3[1]	3.212	H43A	C17[2]	3.473
H43A	H7[1]	3.525	H43A	H8A[1]	3.354
H43A	H17A[2]	3.337	H43A	H17B[2]	2.772
H43A	H37A[1]	3.461	H43A	H37B[1]	3.203
H43B	C6[1]	3.380	H43B	C7[1]	3.059
H43B	C8[1]	3.348	H43B	H7[1]	2.634
H43B	H8A[1]	2.912	H43B	H8C[1]	3.300
H43C	Cl3[1]	3.265	H43C	O3[1]	2.859
H43C	C7[1]	3.340	H43C	C31[1]	2.941

Table S8-12. Intermolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
H43C	C32[1]	3.007	H43C	C37[1]	3.107
H43C	H7[1]	2.584	H43C	H8A[1]	3.471
H43C	H37A[1]	2.943	H43C	H37B[1]	2.891
H44A	C17[2]	3.048	H44A	H17A[2]	3.252
H44A	H17B[2]	2.219	H44A	H17C[2]	3.322
H44A	H37B[1]	3.069	H44B	C9[12]	3.331
H44B	H9A[12]	3.332	H44B	H9C[12]	2.595
H44B	H17B[2]	3.456	H44B	H37B[1]	2.749
H44C	H9C[12]	3.440	H44C	H17B[2]	3.389
H45A	C18[5]	3.578	H45A	C19[12]	3.393
H45A	H18A[5]	3.325	H45A	H18A[12]	3.466
H45A	H18C[5]	3.190	H45A	H19A[5]	3.405
H45A	H19A[12]	2.666	H45A	H19B[5]	3.258
H45A	H19C[12]	3.273	H45B	H9B[12]	3.547
H45B	H18C[5]	3.320	H45B	H27B[13]	3.301
H45C	Cl2[12]	3.036	H45C	C9[12]	3.085
H45C	C19[12]	3.299	H45C	H9A[12]	2.505
H45C	H9B[12]	3.094	H45C	H9C[12]	3.182
H45C	H19A[12]	2.913	H45C	H19C[12]	2.812
H46A	C14[5]	3.161	H46A	C19[5]	2.835
H46A	H18A[12]	3.424	H46A	H19A[5]	3.142
H46A	H19B[5]	2.053	H46A	H24[10]	3.434
H46B	C24[10]	3.380	H46B	C36[1]	3.213
H46B	H19B[5]	2.923	H46B	H24[10]	2.518
H46B	H28B[10]	3.323	H46B	H33[1]	3.361
H46B	H36C[1]	2.300	H46C	C10[5]	3.587
H46C	C15[5]	3.413	H46C	H15A[5]	3.272
H46C	H15B[5]	2.971	H46C	H19B[5]	2.965
H46C	H24[10]	3.181	H46C	H28B[10]	2.854
H47A	C1[1]	3.173	H47A	C2[1]	3.239
H47A	C7[1]	3.258	H47A	C15[1]	3.572
H47A	H1A[1]	2.410	H47A	H7[1]	3.096
H47A	H15B[1]	3.490	H47A	H15C[1]	2.890
H47B	C15[1]	3.125	H47B	H1A[1]	3.462
H47B	H15A[1]	3.320	H47B	H15B[1]	2.715
H47B	H15C[1]	2.855	H47B	H28B[10]	3.339
H47C	C30[1]	3.436	H47C	C33[1]	3.135

Table S8-12. Intermolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
H47C	C34[1]	2.827	H47C	C35[1]	2.994
H47C	C36[1]	3.367	H47C	H1A[1]	2.846
H47C	H15B[1]	3.255	H47C	H15C[1]	3.243
H47C	H28C[10]	3.556	H47C	H33[1]	3.536
H47C	H35[1]	3.346	H47C	H36C[1]	3.037

Symmetry Operators:

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

X-ray Structure Report

for

[(1,2,4-$Me_3C_5H_2$)$TiCl_2${(O-2,4-$Me_2C_6H_2$)-6-CH_2}][(1,2,4-$Me_3C_5H_2$)TiCl{(O-2,4-$Me_2C_6H_2$)-6-CH_2}$_2$]N (**3**)

March 15, 2016

Experimental

Data Collection

A red block crystal of $C_{43}H_{52}Cl_3NO_3Ti_2$ having approximate dimensions of 0.200 x 0.180 x 0.130 mm was mounted on a glass fiber. All measurements were made on a Rigaku XtaLAB mini diffractometer using multi-layer mirror monochromated Mo-Kα radiation.

The crystal-to-detector distance was 50.00 mm.

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

a = 16.6846(7) Å
b = 18.4587(6) Å β = 114.144(5)^o
c = 14.6183(7) Å
V = 4108.2(3) Å^3

For Z = 4 and F.W. = 833.05, the calculated density is 1.347 g/cm^3. The reflection conditions 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 -180 $\pm$ 1^{o}C to a maximum 2θ value of 65.2^o. A total of 540 oscillation images were collected. A sweep of data was done using ω scans from -60.0 to 120.0^o in 1.00^o step, at χ=54.0^o and ϕ = 0.0^o. The exposure rate was 16.0 [sec./^{o}]. The detector swing angle was 30.00^o. A second sweep was performed using ω scans from -60.0 to 120.0^o in 1.00^o step, at χ=54.0^o and ϕ = 120.0^o. The exposure rate was 16.0 [sec./^{o}]. The detector swing angle was 30.00^o. Another sweep was performed using ω scans from -60.0 to 120.0^o in 1.00^o step, at χ=54.0^o and ϕ = 240.0^o. The exposure rate was 16.0 [sec./^{o}]. The detector swing angle

was 30.00°. The crystal-to-detector distance was 50.00 mm. Readout was performed in the 0.073 mm pixel mode.

Data Reduction

Of the 0 reflections were collected, where 0 were unique (R_{int} = 0.0777); equivalent reflections were merged. Data were collected and processed using CrysAlisPro (Rigaku Oxford Diffraction). [1]

The linear absorption coefficient, μ, for Mo-Kα radiation is 6.228 cm^{-1}. An empirical absorption correction was applied which resulted in transmission factors ranging from 0.890 to 0.922. 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 9423 observed reflections and 469 variable parameters and converged (largest parameter shift was 0.00 times its esd) with unweighted and weighted agreement factors of:

$$R1 = \Sigma \, ||Fo| - |Fc|| \, / \, \Sigma \, |Fo| = 0.0553$$

$$wR2 = [\Sigma \, (w \, (Fo^2 - Fc^2)^2) / \Sigma \, w(Fo^2)^2]^{1/2} = 0.1477$$

The goodness of fit[4] was 1.04. Unit weights were used. The maximum and minimum peaks on the final difference Fourier map corresponded to 0.69 and -0.69 $e^-/Å^3$, respectively.

Neutral atom scattering factors were taken from International Tables for Crystallography (IT), Vol. C, Table 6.1.1.4 [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 Version 2014/7[10].

References

(1) CrysAlisPro: Data Collection and Processing Software, Rigaku Corporation (2015). Tokyo 196-8666, Japan.

(2) SIR92: Altomare, A., Cascarano, G., Giacovazzo, C. and Guagliardi, A. (1993). J. Appl. Cryst. 26, 343-350.

(3) Least Squares function minimized: (SHELXL Version 2014/7)

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

(4) Goodness of fit is defined as:

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

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

(5) International Tables for Crystallography, Vol.C (1992). Ed. A.J.C. Wilson, Kluwer Academic Publishers, Dordrecht, Netherlands, Table 6.1.1.4, pp. 572.

(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 4.2: Crystal Structure Analysis Package, Rigaku Corporation (2000-2015). Tokyo 196-8666, Japan.

(10) SHELXL Version 2014/7: Sheldrick, G. M. (2008). Acta Cryst. A64, 112-122.

EXPERIMENTAL DETAILS

A. Crystal Data

Empirical Formula	$C_{43}H_{52}Cl_3NO_3Ti_2$
Formula Weight	833.05
Crystal Color, Habit	red, block
Crystal Dimensions	0.200 X 0.180 X 0.130 mm
Crystal System	monoclinic
Lattice Type	Primitive
Lattice Parameters	a = 16.6846(7) Å b = 18.4587(6) Å c = 14.6183(7) Å β = 114.144(5) ^{o} V = 4108.2(3) Å^3
Space Group	$P2_1/c$ (#14)
Z value	4
D_{calc}	1.347 g/cm^3
F_{000}	1744.00
μ(MoKα)	6.228 cm^{-1}

B. Intensity Measurements

Diffractometer	XtaLAB mini
Radiation	MoKα (λ = 0.71073 Å) multi-layer mirror monochromated
Voltage, Current	50kV, 24mA
Temperature	-180.0^{o}C
Detector Aperture	75.0 mm (diameter)
Data Images	540 exposures
ω oscillation Range (χ=54.0, ϕ=0.0)	-60.0 - 120.0^{o}
Exposure Rate	16.0 sec./^{o}
Detector Swing Angle	30.00^{o}
ω oscillation Range (χ=54.0, ϕ=120.0)	-60.0 - 120.0^{o}
Exposure Rate	16.0 sec./^{o}
Detector Swing Angle	30.00^{o}
ω oscillation Range (χ=54.0, ϕ=240.0)	-60.0 - 120.0^{o}
Exposure Rate	16.0 sec./^{o}
Detector Swing Angle	30.00^{o}
Detector Position	50.00 mm
Pixel Size	0.073 mm
$2\theta_{max}$	55.0^{o}
No. of Reflections Measured	Total: 43125

	Unique: 9423 (R_{int} = 0.0777)
Corrections	Lorentz-polarization Absorption (trans. factors: 0.890 - 0.922)

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	$w = 1/ [\sigma^2(Fo^2) + (0.0622 \cdot P)^2 + 5.1378 \cdot P]$ 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)	9423
No. Variables	469
Reflection/Parameter Ratio	20.09
Residuals: R1 ($I>2.00\sigma(I)$)	0.0553
Residuals: R (All reflections)	0.0898
Residuals: wR2 (All reflections)	0.1477
Goodness of Fit Indicator	1.037
Max Shift/Error in Final Cycle	0.000
Maximum peak in Final Diff. Map	0.69 $e^-/Å^3$
Minimum peak in Final Diff. Map	-0.69 $e^-/Å^3$

Table S9-1. Atomic coordinates and B_{iso}/B_{eq}

atom	x	y	z	B_{eq}
Ti1	-0.11264(4)	0.23007(3)	0.05337(4)	1.479(11)
Ti2	0.37407(4)	0.34402(3)	0.46534(4)	1.353(11)
Cl1	-0.09709(6)	0.18626(5)	0.20484(6)	2.413(17)
Cl2	-0.21522(6)	0.31738(5)	0.02666(8)	3.17(2)
Cl3	0.46139(5)	0.40871(5)	0.40655(7)	2.051(16)
O1	-0.01259(14)	0.27779(12)	0.08654(16)	1.44(4)
O2	0.38229(14)	0.25485(11)	0.41971(17)	1.59(4)
O3	0.26650(14)	0.37709(12)	0.38763(16)	1.49(4)
N1	0.19448(16)	0.23359(14)	0.33259(19)	1.26(4)
C1	0.1521(2)	0.21622(17)	0.2250(2)	1.50(5)
C2	0.1444(2)	0.28167(17)	0.1598(2)	1.42(5)
C3	0.0635(2)	0.30902(17)	0.0928(2)	1.31(5)
C4	0.0573(2)	0.37177(17)	0.0367(2)	1.48(5)
C5	0.1345(2)	0.40685(18)	0.0494(2)	1.73(6)
C6	0.2167(2)	0.38191(19)	0.1153(2)	1.73(6)
C7	0.2197(2)	0.31894(18)	0.1687(2)	1.58(5)
C8	0.2992(2)	0.4224(2)	0.1280(3)	2.41(7)
C9	-0.0313(2)	0.40098(19)	-0.0318(3)	2.04(6)
C10	-0.1428(2)	0.10913(18)	-0.0008(2)	1.68(5)
C11	-0.0715(2)	0.13391(18)	-0.0204(2)	1.53(5)
C12	-0.1041(2)	0.19026(19)	-0.0920(2)	1.78(6)
C13	-0.1954(2)	0.19839(19)	-0.1183(3)	1.94(6)
C14	-0.2192(2)	0.14900(19)	-0.0596(3)	1.80(6)
C15	-0.3094(2)	0.1399(2)	-0.0611(3)	2.30(6)
C16	-0.2558(2)	0.2487(2)	-0.1962(3)	2.80(7)
C17	0.0206(2)	0.10509(18)	0.0239(3)	1.80(6)
C18	0.2321(2)	0.16934(16)	0.3932(2)	1.41(5)
C19	0.3114(2)	0.13973(17)	0.3820(2)	1.47(5)
C20	0.3842(2)	0.18359(17)	0.3980(2)	1.50(5)
C21	0.4599(2)	0.15557(19)	0.3924(3)	1.90(6)
C22	0.4618(2)	0.0816(2)	0.3724(3)	2.28(6)
C23	0.3917(2)	0.03623(19)	0.3576(3)	2.21(6)
C24	0.3170(2)	0.06654(18)	0.3622(2)	1.81(6)
C25	0.3960(3)	-0.0439(2)	0.3384(3)	3.28(8)
C26	0.5379(2)	0.2033(2)	0.4101(3)	2.75(7)
C27	0.1358(2)	0.27123(17)	0.3685(2)	1.45(5)
C28	0.1140(2)	0.34778(17)	0.3314(2)	1.30(5)

Table S9-1. Atomic coordinates and B_{iso}/B_{eq} (continued)

atom	x	y	z	B_{eq}
C29	0.1806(2)	0.39804(17)	0.3443(2)	1.35(5)
C30	0.1613(2)	0.46905(17)	0.3109(2)	1.53(5)
C31	0.0737(2)	0.49055(18)	0.2695(2)	1.67(5)
C32	0.0059(2)	0.44287(18)	0.2578(2)	1.58(5)
C33	0.0276(2)	0.37157(18)	0.2869(2)	1.46(5)
C34	-0.0885(2)	0.4680(2)	0.2155(3)	2.22(6)
C35	0.2346(2)	0.51986(18)	0.3191(3)	2.17(6)
C36	0.3576(2)	0.31157(19)	0.6098(3)	2.01(6)
C37	0.3450(2)	0.38742(19)	0.6017(2)	1.83(6)
C38	0.4247(2)	0.41784(18)	0.6099(3)	1.79(6)
C39	0.4879(2)	0.36202(19)	0.6292(3)	1.99(6)
C40	0.4465(2)	0.29579(19)	0.6296(3)	2.11(6)
C41	0.4875(3)	0.22155(19)	0.6487(3)	2.97(8)
C42	0.5821(2)	0.3740(2)	0.6485(3)	2.68(7)
C43	0.2626(2)	0.4278(2)	0.5865(3)	2.48(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 S9-2. Atomic coordinates and B_{iso} involving hydrogen atoms

atom	x	y	z	B_{iso}
H1A	0.09266	0.19653	0.20917	1.799
H1B	0.18657	0.17827	0.20954	1.799
H5	0.13128	0.44954	0.01179	2.077
H7	0.27525	0.30066	0.21297	1.890
H8A	0.28365	0.46505	0.08428	2.892
H8B	0.32994	0.43773	0.19793	2.892
H8C	0.33747	0.39058	0.10990	2.892
H9A	-0.07733	0.36860	-0.03056	2.453
H9B	-0.03921	0.44934	-0.00916	2.453
H9C	-0.03486	0.40401	-0.10033	2.453
H10	-0.14097	0.06700	0.04304	2.013
H12	-0.07049	0.21470	-0.12626	2.139
H15A	-0.30783	0.10212	-0.01334	2.761
H15B	-0.32823	0.18577	-0.04228	2.761
H15C	-0.35089	0.12605	-0.12863	2.761
H16A	-0.22219	0.27686	-0.22534	3.357
H16B	-0.30115	0.22059	-0.24900	3.357
H16C	-0.28356	0.28170	-0.16532	3.357
H17A	0.05664	0.13236	-0.00294	2.156
H17B	0.04522	0.11032	0.09693	2.156
H17C	0.02019	0.05378	0.00645	2.156
H18A	0.18653	0.13109	0.37449	1.697
H18B	0.24849	0.18146	0.46459	1.697
H22	0.51306	0.06188	0.36881	2.740
H24	0.26802	0.03612	0.35145	2.169
H25A	0.34045	-0.06687	0.32984	3.934
H25B	0.40611	-0.05071	0.27749	3.934
H25C	0.44425	-0.06594	0.39548	3.934
H26A	0.58451	0.17461	0.40315	3.299
H26B	0.52051	0.24268	0.36084	3.299
H26C	0.55945	0.22369	0.47783	3.299
H27A	0.16338	0.27188	0.44273	1.735
H27B	0.08041	0.24337	0.34760	1.735
H31	0.05989	0.53940	0.24845	2.008
H33	-0.01830	0.33771	0.27598	1.753
H34A	-0.09105	0.51971	0.19931	2.667
H34B	-0.12258	0.44049	0.15461	2.667

Table S9-2. Atomic coordinates and B_{iso} involving hydrogens/B_{eq} (continued)

atom	x	y	z	B_{eq}
H34C	-0.11306	0.46015	0.26521	2.667
H35A	0.21014	0.56746	0.29250	2.602
H35B	0.27546	0.52471	0.38965	2.602
H35C	0.26598	0.50045	0.28059	2.602
H36	0.31393	0.27566	0.61301	2.411
H38	0.43714	0.47091	0.61106	2.151
H41A	0.44306	0.18538	0.64431	3.561
H41B	0.51071	0.21086	0.59852	3.561
H41C	0.53543	0.22012	0.71582	3.561
H42A	0.59236	0.42579	0.64327	3.218
H42B	0.61971	0.35686	0.71603	3.218
H42C	0.59596	0.34715	0.59900	3.218
H43A	0.21689	0.39330	0.58337	2.975
H43B	0.27427	0.46126	0.64254	2.975
H43C	0.24275	0.45519	0.52367	2.975

Table S9-3. Anisotropic displacement parameters

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Ti1	0.0140(3)	0.0208(3)	0.0207(3)	-0.0003(2)	0.0063(2)	-0.0012(2)
Ti2	0.0127(3)	0.0154(3)	0.0196(3)	-0.0015(2)	0.0028(2)	0.0023(2)
Cl1	0.0434(5)	0.0300(5)	0.0243(4)	-0.0137(4)	0.0199(4)	-0.0068(4)
Cl2	0.0187(4)	0.0331(5)	0.0605(7)	0.0061(4)	0.0080(4)	-0.0115(5)
Cl3	0.0201(4)	0.0257(4)	0.0309(5)	-0.0054(3)	0.0091(4)	0.0047(3)
O1	0.0146(11)	0.0202(11)	0.0173(11)	0.0003(9)	0.0037(9)	0.0025(9)
O2	0.0150(11)	0.0157(11)	0.0255(12)	0.0003(9)	0.0038(10)	0.0005(9)
O3	0.0145(11)	0.0181(11)	0.0209(12)	0.0003(9)	0.0040(9)	0.0001(9)
N1	0.0155(13)	0.0152(13)	0.0152(13)	0.0028(10)	0.0044(11)	0.0036(10)
C1	0.0188(16)	0.0166(16)	0.0180(16)	0.0003(13)	0.0039(13)	-0.0030(13)
C2	0.0196(16)	0.0207(16)	0.0127(15)	-0.0003(13)	0.0057(13)	-0.0036(12)
C3	0.0152(15)	0.0188(16)	0.0165(15)	-0.0011(12)	0.0071(13)	-0.0028(12)
C4	0.0227(17)	0.0176(16)	0.0149(15)	0.0030(13)	0.0068(13)	-0.0006(12)
C5	0.0312(19)	0.0200(17)	0.0172(16)	-0.0027(14)	0.0126(14)	0.0020(13)
C6	0.0243(17)	0.0266(18)	0.0193(16)	-0.0067(14)	0.0132(14)	-0.0083(14)
C7	0.0149(15)	0.0285(18)	0.0163(16)	0.0014(13)	0.0063(13)	-0.0034(13)
C8	0.0262(19)	0.041(2)	0.0287(19)	-0.0094(16)	0.0159(16)	-0.0067(17)
C9	0.0291(19)	0.0238(18)	0.0206(17)	0.0028(15)	0.0059(15)	0.0056(14)
C10	0.0210(16)	0.0236(17)	0.0168(16)	-0.0025(13)	0.0053(14)	-0.0040(13)
C11	0.0191(16)	0.0212(16)	0.0154(15)	0.0001(13)	0.0046(13)	-0.0014(13)
C12	0.0209(17)	0.0293(19)	0.0183(16)	0.0018(14)	0.0088(14)	0.0022(14)
C13	0.0190(17)	0.0307(19)	0.0211(17)	0.0008(14)	0.0052(14)	-0.0010(14)
C14	0.0151(16)	0.0281(18)	0.0216(17)	-0.0033(14)	0.0037(14)	-0.0059(14)
C15	0.0175(17)	0.038(2)	0.031(2)	-0.0041(15)	0.0088(15)	-0.0052(16)
C16	0.0196(18)	0.053(3)	0.029(2)	0.0096(17)	0.0045(16)	0.0091(18)
C17	0.0193(16)	0.0250(18)	0.0205(17)	0.0043(14)	0.0046(14)	-0.0003(14)
C18	0.0151(15)	0.0157(16)	0.0190(16)	-0.0008(12)	0.0029(13)	0.0013(12)
C19	0.0182(16)	0.0187(16)	0.0139(15)	0.0021(13)	0.0016(13)	0.0031(12)
C20	0.0191(16)	0.0168(16)	0.0178(16)	0.0028(13)	0.0043(13)	0.0008(12)
C21	0.0176(16)	0.0272(18)	0.0254(18)	0.0020(14)	0.0070(14)	0.0035(14)
C22	0.0256(19)	0.030(2)	0.0268(19)	0.0133(15)	0.0067(16)	0.0039(15)
C23	0.032(2)	0.0230(18)	0.0227(18)	0.0077(15)	0.0042(16)	-0.0014(14)
C24	0.0228(17)	0.0181(16)	0.0201(17)	0.0004(13)	0.0009(14)	0.0019(13)
C25	0.045(3)	0.025(2)	0.046(2)	0.0116(18)	0.010(2)	-0.0064(18)
C26	0.0217(18)	0.038(2)	0.047(2)	0.0042(16)	0.0155(18)	0.0063(18)
C27	0.0149(15)	0.0212(16)	0.0180(16)	-0.0016(13)	0.0059(13)	0.0001(13)
C28	0.0175(15)	0.0188(16)	0.0124(14)	0.0004(12)	0.0053(12)	-0.0018(12)

Table S9-3. Anisotropic displacement parameters (continued)

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
C29	0.0136(14)	0.0201(16)	0.0148(15)	0.0039(12)	0.0030(12)	-0.0006(12)
C30	0.0221(16)	0.0169(16)	0.0191(16)	0.0015(13)	0.0085(14)	-0.0017(13)
C31	0.0245(17)	0.0171(16)	0.0205(17)	0.0074(13)	0.0077(14)	0.0024(13)
C32	0.0175(16)	0.0257(18)	0.0158(16)	0.0038(13)	0.0059(13)	-0.0014(13)
C33	0.0152(15)	0.0231(17)	0.0172(16)	0.0001(13)	0.0065(13)	-0.0035(13)
C34	0.0207(17)	0.030(2)	0.0298(19)	0.0067(15)	0.0065(15)	0.0004(16)
C35	0.0275(19)	0.0192(17)	0.036(2)	0.0007(14)	0.0130(16)	0.0007(15)
C36	0.0258(18)	0.0273(19)	0.0197(17)	-0.0110(15)	0.0057(14)	0.0046(14)
C37	0.0225(17)	0.0291(19)	0.0134(15)	-0.0040(14)	0.0027(13)	0.0003(13)
C38	0.0203(17)	0.0200(17)	0.0224(17)	-0.0047(13)	0.0033(14)	0.0004(13)
C39	0.0196(17)	0.0254(18)	0.0200(17)	-0.0048(14)	-0.0027(14)	0.0028(14)
C40	0.0262(18)	0.0231(18)	0.0185(17)	-0.0042(14)	-0.0034(14)	0.0045(14)
C41	0.043(2)	0.0222(19)	0.030(2)	-0.0014(17)	-0.0030(18)	0.0073(16)
C42	0.0171(17)	0.037(2)	0.036(2)	-0.0013(16)	-0.0008(16)	0.0027(17)
C43	0.0229(18)	0.046(2)	0.0255(19)	-0.0011(17)	0.0097(16)	-0.0064(17)

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 S9-4. Bond lengths (Å)

atom	atom	distance	atom	atom	distance
Ti1	Cl1	2.2703(11)	Ti1	Cl2	2.2655(11)
Ti1	O1	1.771(2)	Ti1	C10	2.353(3)
Ti1	C11	2.322(4)	Ti1	C12	2.307(4)
Ti1	C13	2.390(3)	Ti1	C14	2.393(3)
Ti2	Cl3	2.3046(13)	Ti2	O2	1.802(2)
Ti2	O3	1.793(2)	Ti2	C36	2.317(4)
Ti2	C37	2.375(4)	Ti2	C38	2.361(3)
Ti2	C39	2.395(3)	Ti2	C40	2.376(3)
O1	C3	1.363(4)	O2	C20	1.357(4)
O3	C29	1.365(4)	N1	C1	1.472(4)
N1	C18	1.460(4)	N1	C27	1.463(5)
C1	C2	1.512(5)	C2	C3	1.398(4)
C2	C7	1.390(5)	C3	C4	1.399(5)
C4	C5	1.384(5)	C4	C9	1.506(4)
C5	C6	1.393(4)	C6	C7	1.389(5)
C6	C8	1.509(5)	C10	C11	1.408(6)
C10	C14	1.418(4)	C11	C12	1.417(5)
C11	C17	1.500(5)	C12	C13	1.418(5)
C13	C14	1.415(6)	C13	C16	1.495(5)
C14	C15	1.506(6)	C18	C19	1.501(5)
C19	C20	1.399(5)	C19	C24	1.393(5)
C20	C21	1.398(5)	C21	C22	1.400(5)
C21	C26	1.503(5)	C22	C23	1.381(5)
C23	C24	1.393(6)	C23	C25	1.512(5)
C27	C28	1.504(4)	C28	C29	1.400(5)
C28	C33	1.388(4)	C29	C30	1.390(4)
C30	C31	1.391(5)	C30	C35	1.507(5)
C31	C32	1.388(5)	C32	C33	1.385(5)
C32	C34	1.510(5)	C36	C37	1.414(5)
C36	C40	1.420(5)	C37	C38	1.403(5)
C37	C43	1.498(5)	C38	C39	1.418(5)
C39	C40	1.406(5)	C39	C42	1.495(5)
C40	C41	1.506(5)			

Table S9-5. Bond lengths involving hydrogens (Å)

atom	atom	distance	atom	atom	distance
C1	H1A	0.990	C1	H1B	0.990
C5	H5	0.950	C7	H7	0.950
C8	H8A	0.980	C8	H8B	0.980
C8	H8C	0.980	C9	H9A	0.980
C9	H9B	0.980	C9	H9C	0.980
C10	H10	1.000	C12	H12	1.000
C15	H15A	0.980	C15	H15B	0.980
C15	H15C	0.980	C16	H16A	0.980
C16	H16B	0.980	C16	H16C	0.980
C17	H17A	0.980	C17	H17B	0.980
C17	H17C	0.980	C18	H18A	0.990
C18	H18B	0.990	C22	H22	0.950
C24	H24	0.950	C25	H25A	0.980
C25	H25B	0.980	C25	H25C	0.980
C26	H26A	0.980	C26	H26B	0.980
C26	H26C	0.980	C27	H27A	0.990
C27	H27B	0.990	C31	H31	0.950
C33	H33	0.950	C34	H34A	0.980
C34	H34B	0.980	C34	H34C	0.980
C35	H35A	0.980	C35	H35B	0.980
C35	H35C	0.980	C36	H36	1.000
C38	H38	1.000	C41	H41A	0.980
C41	H41B	0.980	C41	H41C	0.980
C42	H42A	0.980	C42	H42B	0.980
C42	H42C	0.980	C43	H43A	0.980
C43	H43B	0.980	C43	H43C	0.980

Table S9-6. Bond angles (°)

atom	atom	atom	angle	atom	atom	atom	angle
Cl1	Ti1	Cl2	101.44(5)	Cl1	Ti1	O1	101.03(8)
Cl1	Ti1	C10	85.04(9)	Cl1	Ti1	C11	104.07(9)
Cl1	Ti1	C12	139.40(9)	Cl1	Ti1	C13	136.34(10)
Cl1	Ti1	C14	101.93(10)	Cl2	Ti1	O1	104.74(8)
Cl2	Ti1	C10	125.07(8)	Cl2	Ti1	C11	144.08(7)
Cl2	Ti1	C12	113.25(9)	Cl2	Ti1	C13	85.51(9)
Cl2	Ti1	C14	91.74(9)	O1	Ti1	C10	127.72(12)
O1	Ti1	C11	94.75(12)	O1	Ti1	C12	90.25(12)
O1	Ti1	C13	118.97(13)	O1	Ti1	C14	148.33(14)
C10	Ti1	C11	35.06(13)	C10	Ti1	C12	58.21(13)
C10	Ti1	C13	57.49(11)	C10	Ti1	C14	34.75(11)
C11	Ti1	C12	35.65(12)	C11	Ti1	C13	58.59(11)
C11	Ti1	C14	58.57(12)	C12	Ti1	C13	35.09(13)
C12	Ti1	C14	58.21(14)	C13	Ti1	C14	34.42(13)
Cl3	Ti2	O2	100.36(10)	Cl3	Ti2	O3	102.06(9)
Cl3	Ti2	C36	143.38(9)	Cl3	Ti2	C37	121.03(9)
Cl3	Ti2	C38	89.16(10)	Cl3	Ti2	C39	86.41(10)
Cl3	Ti2	C40	115.69(10)	O2	Ti2	O3	106.52(10)
O2	Ti2	C36	99.01(12)	O2	Ti2	C37	133.73(13)
O2	Ti2	C38	143.58(10)	O2	Ti2	C39	110.34(11)
O2	Ti2	C40	87.00(11)	O3	Ti2	C36	101.78(13)
O3	Ti2	C37	85.51(11)	O3	Ti2	C38	105.64(11)
O3	Ti2	C39	139.93(13)	O3	Ti2	C40	136.97(14)
C36	Ti2	C37	35.04(12)	C36	Ti2	C38	57.72(13)
C36	Ti2	C39	57.69(13)	C36	Ti2	C40	35.19(13)
C37	Ti2	C38	34.46(13)	C37	Ti2	C39	57.62(13)
C37	Ti2	C40	58.13(12)	C38	Ti2	C39	34.68(12)
C38	Ti2	C40	57.57(12)	C39	Ti2	C40	34.28(12)
Ti1	O1	C3	167.6(2)	Ti2	O2	C20	170.0(3)
Ti2	O3	C29	168.4(3)	C1	N1	C18	111.8(2)
C1	N1	C27	112.8(2)	C18	N1	C27	110.6(3)
N1	C1	C2	112.3(2)	C1	C2	C3	122.5(3)
C1	C2	C7	119.8(3)	C3	C2	C7	117.6(3)
O1	C3	C2	120.1(3)	O1	C3	C4	117.9(3)
C2	C3	C4	121.9(3)	C3	C4	C5	117.9(3)
C3	C4	C9	120.2(3)	C5	C4	C9	121.9(3)
C4	C5	C6	122.5(3)	C5	C6	C7	117.6(3)

Table S9-6. Bond angles (°) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
C5	C6	C8	120.8(3)	C7	C6	C8	121.6(3)
C2	C7	C6	122.5(3)	Ti1	C10	C11	71.24(19)
Ti1	C10	C14	74.16(19)	C11	C10	C14	109.4(3)
Ti1	C11	C10	73.7(2)	Ti1	C11	C12	71.6(2)
Ti1	C11	C17	121.1(2)	C10	C11	C12	106.7(3)
C10	C11	C17	126.8(3)	C12	C11	C17	126.5(4)
Ti1	C12	C11	72.7(2)	Ti1	C12	C13	75.7(2)
C11	C12	C13	108.9(3)	Ti1	C13	C12	69.25(18)
Ti1	C13	C14	72.91(18)	Ti1	C13	C16	124.6(3)
C12	C13	C14	107.7(3)	C12	C13	C16	125.9(4)
C14	C13	C16	126.4(3)	Ti1	C14	C10	71.09(17)
Ti1	C14	C13	72.67(18)	Ti1	C14	C15	122.4(3)
C10	C14	C13	107.3(3)	C10	C14	C15	126.6(3)
C13	C14	C15	126.1(3)	N1	C18	C19	114.1(3)
C18	C19	C20	121.0(3)	C18	C19	C24	120.9(3)
C20	C19	C24	117.9(3)	O2	C20	C19	119.9(3)
O2	C20	C21	118.8(3)	C19	C20	C21	121.4(3)
C20	C21	C22	118.1(3)	C20	C21	C26	120.8(3)
C22	C21	C26	121.1(4)	C21	C22	C23	122.3(4)
C22	C23	C24	117.8(3)	C22	C23	C25	121.4(4)
C24	C23	C25	120.8(4)	C19	C24	C23	122.5(3)
N1	C27	C28	114.5(3)	C27	C28	C29	120.9(3)
C27	C28	C33	121.2(3)	C29	C28	C33	117.9(3)
O3	C29	C28	120.0(3)	O3	C29	C30	118.6(3)
C28	C29	C30	121.4(3)	C29	C30	C31	118.2(3)
C29	C30	C35	119.7(3)	C31	C30	C35	122.1(3)
C30	C31	C32	122.1(3)	C31	C32	C33	117.8(3)
C31	C32	C34	121.1(3)	C33	C32	C34	121.1(3)
C28	C33	C32	122.4(3)	Ti2	C36	C37	74.7(2)
Ti2	C36	C40	74.7(2)	C37	C36	C40	109.1(3)
Ti2	C37	C36	70.2(2)	Ti2	C37	C38	72.2(2)
Ti2	C37	C43	122.2(2)	C36	C37	C38	106.6(3)
C36	C37	C43	126.9(3)	C38	C37	C43	126.4(3)
Ti2	C38	C37	73.3(2)	Ti2	C38	C39	73.96(19)
C37	C38	C39	109.2(3)	Ti2	C39	C38	71.36(17)
Ti2	C39	C40	72.12(17)	Ti2	C39	C42	123.5(3)
C38	C39	C40	107.8(3)	C38	C39	C42	124.7(3)

Table S9-6. Bond angles (°) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
C40	C39	C42	127.5(3)	Ti2	C40	C36	70.14(19)
Ti2	C40	C39	73.60(19)	Ti2	C40	C41	122.2(3)
C36	C40	C39	107.2(3)	C36	C40	C41	125.6(3)
C39	C40	C41	127.2(4)				

Table S9-7. Bond angles involving hydrogens (°)

atom	atom	atom	angle	atom	atom	atom	angle
N1	C1	H1A	109.1	N1	C1	H1B	109.1
C2	C1	H1A	109.1	C2	C1	H1B	109.1
H1A	C1	H1B	107.9	C4	C5	H5	118.8
C6	C5	H5	118.8	C2	C7	H7	118.7
C6	C7	H7	118.7	C6	C8	H8A	109.5
C6	C8	H8B	109.5	C6	C8	H8C	109.5
H8A	C8	H8B	109.5	H8A	C8	H8C	109.5
H8B	C8	H8C	109.5	C4	C9	H9A	109.5
C4	C9	H9B	109.5	C4	C9	H9C	109.5
H9A	C9	H9B	109.5	H9A	C9	H9C	109.5
H9B	C9	H9C	109.5	Ti1	C10	H10	125.2
C11	C10	H10	125.2	C14	C10	H10	125.2
Ti1	C12	H12	125.2	C11	C12	H12	125.2
C13	C12	H12	125.2	C14	C15	H15A	109.5
C14	C15	H15B	109.5	C14	C15	H15C	109.5
H15A	C15	H15B	109.5	H15A	C15	H15C	109.5
H15B	C15	H15C	109.5	C13	C16	H16A	109.5
C13	C16	H16B	109.5	C13	C16	H16C	109.5
H16A	C16	H16B	109.5	H16A	C16	H16C	109.5
H16B	C16	H16C	109.5	C11	C17	H17A	109.5
C11	C17	H17B	109.5	C11	C17	H17C	109.5
H17A	C17	H17B	109.5	H17A	C17	H17C	109.5
H17B	C17	H17C	109.5	N1	C18	H18A	108.7
N1	C18	H18B	108.7	C19	C18	H18A	108.7
C19	C18	H18B	108.7	H18A	C18	H18B	107.6
C21	C22	H22	118.9	C23	C22	H22	118.9
C19	C24	H24	118.8	C23	C24	H24	118.7
C23	C25	H25A	109.5	C23	C25	H25B	109.5
C23	C25	H25C	109.5	H25A	C25	H25B	109.5
H25A	C25	H25C	109.5	H25B	C25	H25C	109.5
C21	C26	H26A	109.5	C21	C26	H26B	109.5
C21	C26	H26C	109.5	H26A	C26	H26B	109.5
H26A	C26	H26C	109.5	H26B	C26	H26C	109.5
N1	C27	H27A	108.6	N1	C27	H27B	108.6
C28	C27	H27A	108.6	C28	C27	H27B	108.6
H27A	C27	H27B	107.6	C30	C31	H31	119.0
C32	C31	H31	119.0	C28	C33	H33	118.8

Table S9-7. Bond angles involving hydrogens (°) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
C32	C33	H33	118.8	C32	C34	H34A	109.5
C32	C34	H34B	109.5	C32	C34	H34C	109.5
H34A	C34	H34B	109.5	H34A	C34	H34C	109.5
H34B	C34	H34C	109.5	C30	C35	H35A	109.5
C30	C35	H35B	109.5	C30	C35	H35C	109.5
H35A	C35	H35B	109.5	H35A	C35	H35C	109.5
H35B	C35	H35C	109.5	Ti2	C36	H36	125.1
C37	C36	H36	125.1	C40	C36	H36	125.1
Ti2	C38	H38	125.2	C37	C38	H38	125.2
C39	C38	H38	125.2	C40	C41	H41A	109.5
C40	C41	H41B	109.5	C40	C41	H41C	109.5
H41A	C41	H41B	109.5	H41A	C41	H41C	109.5
H41B	C41	H41C	109.5	C39	C42	H42A	109.5
C39	C42	H42B	109.5	C39	C42	H42C	109.5
H42A	C42	H42B	109.5	H42A	C42	H42C	109.5
H42B	C42	H42C	109.5	C37	C43	H43A	109.5
C37	C43	H43B	109.5	C37	C43	H43C	109.5
H43A	C43	H43B	109.5	H43A	C43	H43C	109.5
H43B	C43	H43C	109.5				

Table S9-8. Torsion Angles(O)

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

atom1	atom2	atom3	atom4	angle	atom1	atom2	atom3	atom4	angle
Cl1	Ti1	C10	C11	-123.26(11)	Cl1	Ti1	C10	C14	119.29(15)
Cl1	Ti1	C11	C10	59.19(11)	Cl1	Ti1	C11	C12	173.60(10)
Cl1	Ti1	C11	C17	-64.3(2)	Cl1	Ti1	C12	C11	-9.6(2)
Cl1	Ti1	C12	C13	105.84(14)	Cl1	Ti1	C13	C12	-114.94(14)
Cl1	Ti1	C13	C14	2.2(2)	Cl1	Ti1	C13	C16	125.0(2)
Cl1	Ti1	C14	C10	-62.64(16)	Cl1	Ti1	C14	C13	-178.45(12)
Cl1	Ti1	C14	C15	59.3(2)	Cl2	Ti1	C10	C11	136.24(9)
Cl2	Ti1	C10	C14	18.8(2)	Cl2	Ti1	C11	C10	-74.8(2)
Cl2	Ti1	C11	C12	39.6(2)	Cl2	Ti1	C11	C17	161.72(12)
Cl2	Ti1	C12	C11	-155.99(9)	Cl2	Ti1	C12	C13	-40.57(16)
Cl2	Ti1	C13	C12	143.17(13)	Cl2	Ti1	C13	C14	-99.69(14)
Cl2	Ti1	C13	C16	23.1(3)	Cl2	Ti1	C14	C10	-164.72(15)
Cl2	Ti1	C14	C13	79.47(13)	Cl2	Ti1	C14	C15	-42.7(2)
O1	Ti1	C10	C11	-23.14(19)	O1	Ti1	C10	C14	-140.60(14)
O1	Ti1	C11	C10	161.82(12)	O1	Ti1	C11	C12	-83.77(13)
O1	Ti1	C11	C17	38.3(2)	O1	Ti1	C12	C11	97.83(14)
O1	Ti1	C12	C13	-146.76(14)	O1	Ti1	C13	C12	38.79(18)
O1	Ti1	C13	C14	155.93(13)	O1	Ti1	C13	C16	-81.3(3)
O1	Ti1	C14	C10	73.0(3)	O1	Ti1	C14	C13	-42.8(3)
O1	Ti1	C14	C15	-165.03(16)	C10	Ti1	C11	C10	-0.00(12)
C10	Ti1	C11	C12	114.4(2)	C10	Ti1	C11	C17	-123.5(3)
C11	Ti1	C10	C11	0.00(12)	C11	Ti1	C10	C14	-117.5(2)
C10	Ti1	C12	C11	-37.99(12)	C10	Ti1	C12	C13	77.42(16)
C12	Ti1	C10	C11	38.64(12)	C12	Ti1	C10	C14	-78.82(16)
C10	Ti1	C13	C12	-79.66(17)	C10	Ti1	C13	C14	37.48(14)
C10	Ti1	C13	C16	160.3(3)	C13	Ti1	C10	C11	80.34(17)
C13	Ti1	C10	C14	-37.12(15)	C10	Ti1	C14	C10	0.00(18)
C10	Ti1	C14	C13	-115.8(3)	C10	Ti1	C14	C15	122.0(4)
C14	Ti1	C10	C11	117.5(3)	C14	Ti1	C10	C14	0.00(18)
C11	Ti1	C12	C11	-0.00(14)	C11	Ti1	C12	C13	115.4(3)
C12	Ti1	C11	C10	-114.4(2)	C12	Ti1	C11	C12	-0.00(15)
C12	Ti1	C11	C17	122.1(3)	C11	Ti1	C13	C12	-38.08(14)
C11	Ti1	C13	C14	79.06(17)	C11	Ti1	C13	C16	-158.1(3)
C13	Ti1	C11	C10	-76.93(15)	C13	Ti1	C11	C12	37.47(13)
C13	Ti1	C11	C17	159.6(3)	C11	Ti1	C14	C10	36.69(14)
C11	Ti1	C14	C13	-79.13(17)	C11	Ti1	C14	C15	158.7(3)
C14	Ti1	C11	C10	-36.36(12)	C14	Ti1	C11	C12	78.05(14)

Table S9-8. Torsion angles (°) (continued)

atom1	atom2	atom3	atom4	angle	atom1	atom2	atom3	atom4	angle
C14	Ti1	C11	C17	-159.8(3)	C12	Ti1	C13	C12	0.00(15)
C12	Ti1	C13	C14	117.1(3)	C12	Ti1	C13	C16	-120.1(4)
C13	Ti1	C12	C11	-115.4(3)	C13	Ti1	C12	C13	0.00(15)
C12	Ti1	C14	C10	78.81(17)	C12	Ti1	C14	C13	-37.00(14)
C12	Ti1	C14	C15	-159.2(3)	C14	Ti1	C12	C11	-79.13(16)
C14	Ti1	C12	C13	36.29(13)	C13	Ti1	C14	C10	115.8(3)
C13	Ti1	C14	C13	0.00(16)	C13	Ti1	C14	C15	-122.2(3)
C14	Ti1	C13	C12	-117.1(3)	C14	Ti1	C13	C14	0.00(16)
C14	Ti1	C13	C16	122.8(4)	Cl3	Ti2	C36	C37	65.6(2)
Cl3	Ti2	C36	C40	-49.7(2)	Cl3	Ti2	C37	C36	-140.67(9)
Cl3	Ti2	C37	C38	-24.93(16)	Cl3	Ti2	C37	C43	97.4(2)
Cl3	Ti2	C38	C37	158.82(11)	Cl3	Ti2	C38	C39	-84.90(14)
Cl3	Ti2	C39	C38	93.72(14)	Cl3	Ti2	C39	C40	-149.71(15)
Cl3	Ti2	C39	C42	-26.1(2)	Cl3	Ti2	C40	C36	149.68(9)
Cl3	Ti2	C40	C39	33.96(19)	Cl3	Ti2	C40	C41	-90.1(2)
O2	Ti2	C36	C37	-173.21(12)	O2	Ti2	C36	C40	71.54(14)
O2	Ti2	C37	C36	9.3(2)	O2	Ti2	C37	C38	125.04(14)
O2	Ti2	C37	C43	-112.6(2)	O2	Ti2	C38	C37	-94.7(2)
O2	Ti2	C38	C39	21.5(3)	O2	Ti2	C39	C38	-166.56(15)
O2	Ti2	C39	C40	-50.0(2)	O2	Ti2	C39	C42	73.6(2)
O2	Ti2	C40	C36	-110.27(14)	O2	Ti2	C40	C39	134.02(17)
O2	Ti2	C40	C41	10.0(2)	O3	Ti2	C36	C37	-64.11(14)
O3	Ti2	C36	C40	-179.37(13)	O3	Ti2	C37	C36	117.95(14)
O3	Ti2	C37	C38	-126.31(14)	O3	Ti2	C37	C43	-3.9(2)
O3	Ti2	C38	C37	56.53(15)	O3	Ti2	C38	C39	172.81(14)
O3	Ti2	C39	C38	-10.8(3)	O3	Ti2	C39	C40	105.78(19)
O3	Ti2	C39	C42	-130.6(2)	O3	Ti2	C40	C36	0.9(2)
O3	Ti2	C40	C39	-114.81(18)	O3	Ti2	C40	C41	121.2(2)
C36	Ti2	C37	C36	0.00(14)	C36	Ti2	C37	C38	115.7(2)
C36	Ti2	C37	C43	-121.9(3)	C37	Ti2	C36	C37	-0.00(13)
C37	Ti2	C36	C40	-115.3(2)	C36	Ti2	C38	C37	-37.71(13)
C36	Ti2	C38	C39	78.57(17)	C38	Ti2	C36	C37	37.07(12)
C38	Ti2	C36	C40	-78.18(15)	C36	Ti2	C39	C38	-78.67(18)
C36	Ti2	C39	C40	37.90(15)	C36	Ti2	C39	C42	161.5(3)
C39	Ti2	C36	C37	78.36(15)	C39	Ti2	C36	C40	-36.90(13)
C36	Ti2	C40	C36	0.00(15)	C36	Ti2	C40	C39	-115.7(3)
C36	Ti2	C40	C41	120.3(3)	C40	Ti2	C36	C37	115.3(2)

Table S9-8. Torsion angles (°) (continued)

atom1	atom2	atom3	atom4	angle	atom1	atom2	atom3	atom4	angle
C40	Ti2	C36	C40	0.00(14)	C37	Ti2	C38	C37	-0.00(14)
C37	Ti2	C38	C39	116.3(3)	C38	Ti2	C37	C36	-115.7(2)
C38	Ti2	C37	C38	-0.00(13)	C38	Ti2	C37	C43	122.4(3)
C37	Ti2	C39	C38	-36.92(15)	C37	Ti2	C39	C40	79.65(18)
C37	Ti2	C39	C42	-156.7(3)	C39	Ti2	C37	C36	-78.58(15)
C39	Ti2	C37	C38	37.16(13)	C39	Ti2	C37	C43	159.5(3)
C37	Ti2	C40	C36	37.69(13)	C37	Ti2	C40	C39	-78.02(17)
C37	Ti2	C40	C41	158.0(3)	C40	Ti2	C37	C36	-37.86(13)
C40	Ti2	C37	C38	77.88(15)	C40	Ti2	C37	C43	-159.7(3)
C38	Ti2	C39	C38	0.00(17)	C38	Ti2	C39	C40	116.6(3)
C38	Ti2	C39	C42	-119.8(3)	C39	Ti2	C38	C37	-116.3(3)
C39	Ti2	C38	C39	-0.00(17)	C38	Ti2	C40	C36	78.64(17)
C38	Ti2	C40	C39	-37.07(15)	C38	Ti2	C40	C41	-161.1(3)
C40	Ti2	C38	C37	-79.64(17)	C40	Ti2	C38	C39	36.64(15)
C39	Ti2	C40	C36	115.7(3)	C39	Ti2	C40	C39	-0.00(17)
C39	Ti2	C40	C41	-124.0(4)	C40	Ti2	C39	C38	-116.6(3)
C40	Ti2	C39	C40	-0.00(18)	C40	Ti2	C39	C42	123.6(4)
C1	N1	C18	C19	70.2(3)	C18	N1	C1	C2	-157.9(3)
C1	N1	C27	C28	-70.4(3)	C27	N1	C1	C2	76.7(3)
C18	N1	C27	C28	163.55(19)	C27	N1	C18	C19	-163.2(2)
N1	C1	C2	C3	-118.3(3)	N1	C1	C2	C7	58.7(4)
C1	C2	C3	O1	1.8(5)	C1	C2	C3	C4	176.7(3)
C1	C2	C7	C6	-176.0(3)	C3	C2	C7	C6	1.0(5)
C7	C2	C3	O1	-175.1(3)	C7	C2	C3	C4	-0.3(5)
O1	C3	C4	C5	174.7(3)	O1	C3	C4	C9	-2.8(5)
C2	C3	C4	C5	-0.2(5)	C2	C3	C4	C9	-177.8(3)
C3	C4	C5	C6	0.0(5)	C9	C4	C5	C6	177.6(3)
C4	C5	C6	C7	0.6(5)	C4	C5	C6	C8	-179.2(3)
C5	C6	C7	C2	-1.2(5)	C8	C6	C7	C2	178.6(3)
Ti1	C10	C11	Ti1	-0.000(13)	Ti1	C10	C11	C12	-64.46(18)
Ti1	C10	C11	C17	116.9(3)	Ti1	C10	C14	Ti1	0.000(18)
Ti1	C10	C14	C13	64.14(19)	Ti1	C10	C14	C15	-116.8(3)
C11	C10	C14	Ti1	-63.0(2)	C11	C10	C14	C13	1.2(4)
C11	C10	C14	C15	-179.8(3)	C14	C10	C11	Ti1	64.8(2)
C14	C10	C11	C12	0.4(4)	C14	C10	C11	C17	-178.2(3)
Ti1	C11	C12	Ti1	0.000(16)	Ti1	C11	C12	C13	-67.6(2)
C10	C11	C12	Ti1	65.9(2)	C10	C11	C12	C13	-1.8(4)

Table S9-8. Torsion angles (°) (continued)

atom1	atom2	atom3	atom4	angle	atom1	atom2	atom3	atom4	angle
C17	C11	C12	Ti1	-115.5(3)	C17	C11	C12	C13	176.8(3)
Ti1	C12	C13	Ti1	-0.000(15)	Ti1	C12	C13	C14	-63.2(2)
Ti1	C12	C13	C16	118.4(3)	C11	C12	C13	Ti1	65.7(2)
C11	C12	C13	C14	2.5(4)	C11	C12	C13	C16	-175.9(3)
Ti1	C13	C14	Ti1	-0.000(16)	Ti1	C13	C14	C10	-63.10(19)
Ti1	C13	C14	C15	117.8(3)	C12	C13	C14	Ti1	60.9(2)
C12	C13	C14	C10	-2.2(4)	C12	C13	C14	C15	178.7(3)
C16	C13	C14	Ti1	-120.7(4)	C16	C13	C14	C10	176.2(3)
C16	C13	C14	C15	-2.9(6)	N1	C18	C19	C20	54.8(3)
N1	C18	C19	C24	-129.8(3)	C18	C19	C20	O2	-3.0(4)
C18	C19	C20	C21	176.9(3)	C18	C19	C24	C23	-175.8(3)
C20	C19	C24	C23	-0.2(5)	C24	C19	C20	O2	-178.5(3)
C24	C19	C20	C21	1.3(5)	O2	C20	C21	C22	178.5(3)
O2	C20	C21	C26	0.0(5)	C19	C20	C21	C22	-1.4(5)
C19	C20	C21	C26	-179.8(3)	C20	C21	C22	C23	0.4(5)
C26	C21	C22	C23	178.8(3)	C21	C22	C23	C24	0.6(5)
C21	C22	C23	C25	-178.6(3)	C22	C23	C24	C19	-0.7(5)
C25	C23	C24	C19	178.5(3)	N1	C27	C28	C29	-53.8(4)
N1	C27	C28	C33	128.7(3)	C27	C28	C29	O3	2.4(5)
C27	C28	C29	C30	-179.6(3)	C27	C28	C33	C32	175.8(3)
C29	C28	C33	C32	-1.8(5)	C33	C28	C29	O3	-180.0(3)
C33	C28	C29	C30	-1.9(5)	O3	C29	C30	C31	-178.1(3)
O3	C29	C30	C35	2.6(5)	C28	C29	C30	C31	3.8(5)
C28	C29	C30	C35	-175.4(3)	C29	C30	C31	C32	-2.1(5)
C35	C30	C31	C32	177.1(3)	C30	C31	C32	C33	-1.4(5)
C30	C31	C32	C34	178.1(3)	C31	C32	C33	C28	3.4(5)
C34	C32	C33	C28	-176.1(3)	Ti2	C36	C37	Ti2	-0.000(15)
Ti2	C36	C37	C38	-63.5(2)	Ti2	C36	C37	C43	116.0(3)
Ti2	C36	C40	Ti2	0.000(14)	Ti2	C36	C40	C39	64.8(2)
Ti2	C36	C40	C41	-116.0(3)	C37	C36	C40	Ti2	-67.4(3)
C37	C36	C40	C39	-2.6(4)	C37	C36	C40	C41	176.6(3)
C40	C36	C37	Ti2	67.4(3)	C40	C36	C37	C38	3.8(4)
C40	C36	C37	C43	-176.6(3)	Ti2	C37	C38	Ti2	0.000(13)
Ti2	C37	C38	C39	-65.8(2)	C36	C37	C38	Ti2	62.2(2)
C36	C37	C38	C39	-3.6(4)	C43	C37	C38	Ti2	-117.4(3)
C43	C37	C38	C39	176.8(3)	Ti2	C38	C39	Ti2	-0.000(17)
Ti2	C38	C39	C40	-63.4(2)	Ti2	C38	C39	C42	118.4(3)

Table S9-8. Torsion angles (°) (continued)

atom1	atom2	atom3	atom4	angle	atom1	atom2	atom3	atom4	angle
C37	C38	C39	Ti2	65.4(2)	C37	C38	C39	C40	2.0(4)
C37	C38	C39	C42	-176.3(3)	Ti2	C39	C40	Ti2	0.000(18)
Ti2	C39	C40	C36	-62.50(19)	Ti2	C39	C40	C41	118.3(3)
C38	C39	C40	Ti2	62.9(2)	C38	C39	C40	C36	0.4(4)
C38	C39	C40	C41	-178.8(3)	C42	C39	C40	Ti2	-118.9(4)
C42	C39	C40	C36	178.6(3)	C42	C39	C40	C41	-0.6(6)

Table S9-9. Intramolecular contacts less than 3.60 Å

atom	atom	distance	atom	atom	distance
Ti2	N1	3.485(2)	Cl2	C16	3.298(4)
Cl3	C42	3.340(4)	O1	C1	2.896(3)
O1	C9	2.797(4)	O1	C17	3.424(4)
O1	C28	3.572(3)	O1	C33	3.228(4)
O2	N1	2.886(3)	O2	C18	2.851(4)
O2	C26	2.822(5)	O2	C41	3.140(4)
O3	N1	2.884(3)	O3	C2	3.577(3)
O3	C7	3.156(4)	O3	C27	2.856(4)
O3	C35	2.792(4)	O3	C43	3.080(5)
N1	C3	3.568(4)	N1	C7	3.037(5)
N1	C20	3.052(4)	N1	C29	3.054(4)
C1	C17	3.520(4)	C1	C19	3.055(4)
C1	C28	3.087(5)	C2	C5	2.784(5)
C2	C27	3.120(5)	C2	C28	3.015(5)
C2	C29	3.305(5)	C3	C6	2.786(5)
C3	C28	3.314(5)	C3	C33	3.336(5)
C4	C7	2.781(4)	C7	C28	3.533(6)
C7	C29	3.243(5)	C15	C16	3.190(6)
C19	C22	2.786(5)	C20	C23	2.797(5)
C20	C41	3.425(5)	C21	C24	2.779(5)
C28	C31	2.778(4)	C29	C32	2.786(4)
C29	C43	3.279(5)	C30	C33	2.774(5)
C41	C42	3.227(6)			

Table S9-10. Intramolecular contacts less than 3.60 Å involving hydrogens

atom	atom	distance	atom	atom	distance
Ti1	H1A	3.305	Ti1	H9A	2.997
Ti1	H15B	3.383	Ti1	H16C	3.436
Ti1	H17B	3.295	Ti1	H33	3.581
Ti2	H7	3.463	Ti2	H41B	3.376
Ti2	H42C	3.407	Ti2	H43C	3.357
Cl1	H1A	3.146	Cl1	H10	3.092
Cl1	H27B	3.030	Cl1	H33	3.083
Cl2	H9A	2.909	Cl2	H15B	2.986
Cl2	H16C	2.644	Cl2	H34B	2.947
Cl3	H8B	2.988	Cl3	H26B	3.369
Cl3	H35C	3.461	Cl3	H38	3.378
Cl3	H42A	3.265	Cl3	H42C	3.013
O1	H1A	2.444	O1	H1B	3.572
O1	H9A	2.323	O1	H9B	3.417
O1	H9C	3.493	O1	H12	3.083
O1	H17A	3.389	O1	H17B	3.223
O1	H27B	3.540	O1	H33	3.019
O2	H7	2.936	O2	H18B	2.906
O2	H26B	2.781	O2	H26C	2.781
O2	H36	3.474	O2	H41A	3.276
O2	H41B	2.739	O3	H7	2.972
O3	H8B	3.531	O3	H27A	2.918
O3	H35B	2.728	O3	H35C	2.761
O3	H36	3.585	O3	H43A	3.301
O3	H43C	2.614	N1	H7	2.887
C1	H7	2.642	C1	H17A	3.420
C1	H17B	2.788	C1	H18A	2.559
C1	H18B	3.264	C1	H27A	3.275
C1	H27B	2.578	C2	H17A	3.542
C2	H17B	3.513	C2	H27B	3.403
C3	H1A	2.601	C3	H1B	3.176
C3	H5	3.241	C3	H7	3.242
C3	H9A	2.553	C3	H9B	3.127
C3	H9C	3.154	C3	H12	3.526
C3	H17A	3.532	C3	H33	3.507
C5	H7	3.237	C5	H8A	2.563
C5	H8B	3.143	C5	H8C	3.145

Table S9-10. Intramolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
C5	H9A	3.313	C5	H9B	2.778
C5	H9C	2.778	C6	H35C	3.111
C7	H1A	3.312	C7	H1B	2.770
C7	H5	3.237	C7	H8A	3.319
C7	H8B	2.781	C7	H8C	2.781
C8	H5	2.663	C8	H7	2.675
C8	H35C	2.893	C9	H5	2.674
C10	H12	3.229	C10	H15A	2.687
C10	H15B	3.226	C10	H15C	3.216
C10	H17A	3.367	C10	H17B	2.866
C10	H17C	2.866	C11	H1A	3.547
C12	H9A	3.393	C12	H10	3.231
C12	H16A	2.664	C12	H16B	3.196
C12	H16C	3.215	C12	H17A	2.679
C12	H17B	3.222	C12	H17C	3.206
C13	H10	3.243	C13	H15A	3.374
C13	H15B	2.866	C13	H15C	2.866
C14	H12	3.248	C14	H16A	3.368
C14	H16B	2.861	C14	H16C	2.861
C15	H10	2.920	C15	H16B	3.176
C15	H16C	3.145	C16	H12	2.900
C16	H15B	3.178	C16	H15C	3.147
C17	H1A	2.995	C17	H1B	3.273
C17	H10	2.909	C17	H12	2.914
C18	H1A	2.789	C18	H1B	2.479
C18	H24	2.661	C18	H27A	2.470
C18	H27B	2.708	C18	H36	3.529
C19	H1B	2.627	C20	H1B	3.323
C20	H7	3.357	C20	H18A	3.318
C20	H18B	2.808	C20	H22	3.256
C20	H24	3.249	C20	H26A	3.315
C20	H26B	2.768	C20	H26C	2.768
C20	H41A	3.322	C20	H41B	2.870
C21	H41B	2.958	C22	H24	3.232
C22	H25A	3.311	C22	H25B	2.774
C22	H25C	2.774	C22	H26A	2.567
C22	H26B	3.157	C22	H26C	3.140

Table S9-10. Intramolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
C24	H1B	3.162	C24	H18A	2.551
C24	H18B	3.073	C24	H22	3.234
C24	H25A	2.568	C24	H25B	3.152
C24	H25C	3.143	C25	H22	2.667
C25	H24	2.666	C26	H22	2.673
C26	H41B	2.972	C27	H1A	2.545
C27	H1B	3.267	C27	H18A	2.712
C27	H18B	2.469	C27	H33	2.664
C27	H36	3.595	C28	H1A	3.255
C28	H43A	3.470	C28	H43C	3.392
C29	H7	3.448	C29	H27A	2.813
C29	H27B	3.319	C29	H31	3.243
C29	H33	3.246	C29	H35A	3.302
C29	H35B	2.749	C29	H35C	2.749
C29	H43A	3.296	C29	H43C	2.616
C30	H43C	2.851	C31	H33	3.232
C31	H34A	2.567	C31	H34B	3.146
C31	H34C	3.142	C31	H35A	2.585
C31	H35B	3.159	C31	H35C	3.150
C33	H27A	3.080	C33	H27B	2.554
C33	H31	3.233	C33	H34A	3.311
C33	H34B	2.770	C33	H34C	2.770
C34	H31	2.669	C34	H33	2.663
C35	H8B	3.205	C35	H31	2.689
C35	H43C	3.171	C36	H18B	3.229
C36	H27A	3.245	C36	H38	3.224
C36	H41A	2.669	C36	H41B	3.218
C36	H41C	3.208	C36	H43A	2.682
C36	H43B	3.216	C36	H43C	3.211
C38	H36	3.221	C38	H42A	2.639
C38	H42B	3.183	C38	H42C	3.204
C38	H43A	3.358	C38	H43B	2.855
C38	H43C	2.855	C39	H36	3.235
C39	H41A	3.373	C39	H41B	2.876
C39	H41C	2.876	C40	H38	3.242
C40	H42A	3.366	C40	H42B	2.870
C40	H42C	2.870	C41	H26C	3.184

Table S9-10. Intramolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
C41	H36	2.902	C41	H42B	3.209
C41	H42C	3.202	C42	H38	2.875
C42	H41B	3.210	C42	H41C	3.204
C43	H27A	3.549	C43	H35B	3.469
C43	H36	2.915	C43	H38	2.896
H1A	H7	3.583	H1A	H17A	3.139
H1A	H17B	2.188	H1A	H18A	2.580
H1A	H18B	3.583	H1A	H27A	3.419
H1A	H27B	2.285	H1A	H33	3.557
H1B	H7	2.690	H1B	H17A	3.091
H1B	H17B	2.582	H1B	H18A	2.564
H1B	H18B	3.438	H1B	H24	3.275
H1B	H27B	3.403	H5	H8A	2.338
H5	H8B	3.326	H5	H8C	3.323
H5	H9B	2.734	H5	H9C	2.713
H7	H8B	2.729	H7	H8C	2.717
H8A	H35C	3.073	H8B	H35C	2.235
H9A	H12	3.189	H9A	H16A	3.345
H9A	H16C	3.570	H9A	H34B	3.366
H9B	H34B	3.228	H9C	H12	3.539
H10	H15A	2.641	H10	H15B	3.597
H10	H15C	3.544	H10	H17B	2.985
H10	H17C	2.958	H12	H16A	2.612
H12	H16B	3.520	H12	H16C	3.582
H12	H17A	2.633	H12	H17B	3.596
H12	H17C	3.532	H15B	H16B	3.296
H15B	H16C	2.832	H15C	H16B	2.833
H15C	H16C	3.209	H18A	H24	2.326
H18A	H27A	2.866	H18A	H27B	2.649
H18B	H24	3.237	H18B	H27A	2.129
H18B	H27B	2.859	H18B	H36	2.643
H18B	H41A	3.236	H22	H25A	3.595
H22	H25B	2.709	H22	H25C	2.721
H22	H26A	2.348	H22	H26B	3.343
H22	H26C	3.324	H24	H25A	2.342
H24	H25B	3.329	H24	H25C	3.326
H26B	H41B	3.593	H26C	H41B	2.237

Table S9-10. Intramolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
H26C	H42C	2.796	H27A	H33	3.250
H27A	H36	2.719	H27A	H43A	2.923
H27B	H33	2.330	H31	H34A	2.347
H31	H34B	3.327	H31	H34C	3.332
H31	H35A	2.376	H31	H35B	3.346
H31	H35C	3.353	H33	H34A	3.592
H33	H34B	2.692	H33	H34C	2.726
H35B	H38	3.405	H35B	H43C	2.580
H36	H41A	2.612	H36	H41B	3.581
H36	H41C	3.525	H36	H43A	2.636
H36	H43B	3.549	H36	H43C	3.582
H38	H42A	2.574	H38	H42B	3.499
H38	H42C	3.557	H38	H43B	2.941
H38	H43C	2.974	H41B	H42B	3.311
H41B	H42C	2.889	H41C	H42B	2.889
H41C	H42C	3.293			

Table S9-11. Intermolecular contacts less than 3.60 Å

atom	atom	distance	atom	atom	distance
C5	C18[1]	3.589(6)	C6	C18[1]	3.491(5)
C8	C18[1]	3.571(5)	C12	C33[1]	3.529(6)
C16	C42[2]	3.577(5)	C17	C33[1]	3.539(5)
C18	C5[3]	3.589(6)	C18	C6[3]	3.491(5)
C18	C8[3]	3.571(5)	C33	C12[3]	3.529(6)
C33	C17[3]	3.539(5)	C35	C42[4]	3.497(5)
C42	C16[5]	3.577(5)	C42	C35[4]	3.497(5)

Symmetry Operators:

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

Table S9-12. Intermolecular contacts less than 3.60 Å involving hydrogens

atom	atom	distance	atom	atom	distance
Cl1	H9C[1]	3.090	Cl1	H12[1]	2.956
Cl1	H16A[1]	2.758	Cl1	H31[2]	2.802
Cl1	H35A[2]	2.903	Cl2	H26A[3]	3.084
Cl3	H15A[4]	3.542	Cl3	H15C[4]	3.436
Cl3	H38[5]	2.868	Cl3	H42A[5]	3.183
C1	H43A[6]	3.373	C2	H27A[6]	3.459
C2	H36[6]	3.341	C3	H27A[6]	3.579
C4	H9B[7]	3.325	C5	H9B[7]	3.026
C5	H18A[6]	3.098	C5	H18B[6]	3.121
C6	H18A[6]	3.355	C6	H18B[6]	2.731
C6	H36[6]	3.337	C7	H18B[6]	3.210
C7	H27A[6]	3.473	C7	H36[6]	2.689
C8	H18A[6]	3.541	C8	H18B[6]	2.905
C8	H41A[6]	3.051	C9	H5[7]	3.299
C9	H9B[7]	2.966	C9	H31[7]	3.198
C10	H35B[2]	3.593	C10	H43B[2]	3.583
C10	H43C[2]	3.242	C11	H17C[8]	3.555
C11	H33[6]	3.476	C11	H34C[6]	3.397
C12	H33[6]	2.882	C12	H34C[6]	3.440
C15	H25B[8]	3.339	C15	H26B[3]	3.376
C15	H26C[3]	3.531	C15	H35B[2]	3.157
C15	H41C[9]	3.553	C15	H42C[3]	3.324
C15	H43C[2]	3.559	C16	H41C[9]	3.225
C16	H42B[9]	2.787	C16	H42C[9]	3.511
C17	H17C[8]	3.002	C17	H33[6]	3.569
C17	H43A[6]	3.025	C18	H8A[1]	3.568
C18	H8C[1]	3.129	C18	H34A[2]	3.520
C19	H8C[1]	3.228	C21	H25C[10]	3.294
C22	H25C[10]	3.115	C23	H25C[10]	3.569
C23	H43B[6]	2.947	C24	H8A[1]	3.559
C24	H8C[1]	3.584	C24	H43B[6]	3.035
C25	H15C[8]	3.222	C25	H41B[10]	3.406
C25	H43B[6]	3.145	C26	H15B[4]	2.898
C26	H16C[4]	3.585	C26	H41C[6]	3.158
C27	H12[1]	3.483	C27	H17A[1]	3.236
C28	H12[1]	3.570	C28	H17A[1]	2.968
C30	H10[11]	2.922	C31	H9C[7]	3.002

Table S9-12. Intermolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
C31	H10[11]	2.872	C32	H17A[1]	3.529
C32	H17C[1]	3.544	C33	H12[1]	2.920
C33	H17A[1]	2.909	C33	H17C[1]	3.541
C34	H5[7]	3.454	C34	H18A[11]	3.422
C34	H24[11]	3.019	C35	H10[11]	3.136
C35	H15A[11]	3.004	C35	H42A[5]	2.888
C35	H42B[5]	3.517	C35	H42C[5]	3.561
C36	H7[1]	3.186	C38	H22[1]	3.475
C38	H25B[1]	3.569	C40	H26B[1]	3.168
C41	H8C[1]	3.116	C41	H16B[12]	3.218
C41	H25B[10]	3.563	C41	H25C[10]	3.251
C41	H26B[1]	2.993	C42	H15A[4]	3.567
C42	H16A[12]	3.514	C42	H16B[12]	3.416
C42	H16C[12]	3.216	C42	H35A[5]	3.389
C42	H35B[5]	3.247	C42	H35C[5]	3.275
C43	H1B[1]	3.247	C43	H10[11]	3.341
C43	H15A[11]	3.568	C43	H17A[1]	3.328
H1A	H34A[2]	3.532	H1B	C43[6]	3.247
H1B	H36[6]	3.112	H1B	H43A[6]	2.483
H1B	H43B[6]	3.302	H5	C9[7]	3.299
H5	C34[7]	3.454	H5	H9A[7]	3.515
H5	H9B[7]	2.408	H5	H18A[6]	2.934
H5	H18B[6]	3.354	H5	H34A[7]	2.933
H5	H34B[7]	3.126	H7	C36[6]	3.186
H7	H18B[6]	3.488	H7	H36[6]	2.304
H7	H41A[6]	3.348	H8A	C18[6]	3.568
H8A	C24[6]	3.559	H8A	H18A[6]	3.334
H8A	H18B[6]	3.143	H8A	H24[6]	3.306
H8B	H41A[6]	3.248	H8B	H42A[5]	3.310
H8C	C18[6]	3.129	H8C	C19[6]	3.228
H8C	C24[6]	3.584	H8C	C41[6]	3.116
H8C	H18A[6]	3.355	H8C	H18B[6]	2.430
H8C	H36[6]	3.096	H8C	H41A[6]	2.144
H8C	H41B[6]	3.505	H9A	H5[7]	3.515
H9B	C4[7]	3.325	H9B	C5[7]	3.026
H9B	C9[7]	2.966	H9B	H5[7]	2.408
H9B	H9B[7]	2.235	H9B	H9C[7]	3.130

Table S9-12. Intermolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
H9B	H31^{7}	3.378	H9C	Cl1^{6}	3.090
H9C	C31^{7}	3.002	H9C	H9B^{7}	3.130
H9C	H27B^{6}	3.588	H9C	H31^{7}	2.283
H9C	H34A^{7}	3.313	H9C	H35A^{7}	3.162
H10	C30^{2}	2.922	H10	C31^{2}	2.872
H10	C35^{2}	3.136	H10	C43^{2}	3.341
H10	H17C^{8}	3.278	H10	H31^{2}	2.830
H10	H35A^{2}	3.063	H10	H35B^{2}	2.902
H10	H43B^{2}	3.344	H10	H43C^{2}	2.596
H12	Cl1^{6}	2.956	H12	C27^{6}	3.483
H12	C28^{6}	3.570	H12	C33^{6}	2.920
H12	H27B^{6}	2.806	H12	H33^{6}	2.180
H12	H34C^{6}	3.538	H15A	Cl3^{3}	3.542
H15A	C35^{2}	3.004	H15A	C42^{3}	3.567
H15A	C43^{2}	3.568	H15A	H35A^{2}	3.030
H15A	H35B^{2}	2.192	H15A	H38^{2}	3.169
H15A	H42A^{3}	3.376	H15A	H42C^{3}	2.882
H15A	H43B^{2}	3.392	H15A	H43C^{2}	2.948
H15B	C26^{3}	2.898	H15B	H26A^{3}	2.907
H15B	H26B^{3}	2.682	H15B	H26C^{3}	2.616
H15B	H41C^{9}	3.391	H15B	H42C^{3}	2.893
H15C	Cl3^{3}	3.436	H15C	C25^{8}	3.222
H15C	H25A^{8}	3.208	H15C	H25B^{8}	2.424
H15C	H26B^{3}	3.198	H15C	H38^{2}	3.262
H15C	H41C^{9}	2.873	H15C	H43B^{2}	3.338
H16A	Cl1^{6}	2.758	H16A	C42^{9}	3.514
H16A	H35A^{7}	3.070	H16A	H42B^{9}	2.833
H16A	H42C^{9}	3.333	H16B	C41^{9}	3.218
H16B	C42^{9}	3.416	H16B	H25A^{8}	3.040
H16B	H25B^{8}	3.532	H16B	H41B^{9}	3.022
H16B	H41C^{9}	2.560	H16B	H42B^{9}	2.789
H16B	H42C^{9}	3.197	H16C	C26^{3}	3.585
H16C	C42^{9}	3.216	H16C	H26A^{3}	2.881
H16C	H26B^{3}	3.472	H16C	H41C^{9}	3.023
H16C	H42B^{9}	2.291	H16C	H42C^{9}	3.421
H17A	C27^{6}	3.236	H17A	C28^{6}	2.968
H17A	C32^{6}	3.529	H17A	C33^{6}	2.909

Table S9-12. Intermolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
H17A	C43[6]	3.328	H17A	H27A[6]	2.843
H17A	H27B[6]	3.302	H17A	H33[6]	3.001
H17A	H43A[6]	2.491	H17A	H43C[6]	3.379
H17B	H17C[8]	3.362	H17B	H34A[2]	3.224
H17B	H34C[2]	3.341	H17B	H43A[6]	2.952
H17C	C11[8]	3.555	H17C	C17[8]	3.002
H17C	C32[6]	3.544	H17C	C33[6]	3.541
H17C	H10[8]	3.278	H17C	H17B[8]	3.362
H17C	H17C[8]	2.080	H17C	H34C[2]	3.507
H17C	H34C[6]	3.321	H17C	H43A[6]	3.158
H18A	C5[1]	3.098	H18A	C6[1]	3.355
H18A	C8[1]	3.541	H18A	C34[2]	3.422
H18A	H5[1]	2.934	H18A	H8A[1]	3.334
H18A	H8C[1]	3.355	H18A	H34A[2]	2.554
H18B	C5[1]	3.121	H18B	C6[1]	2.731
H18B	C7[1]	3.210	H18B	C8[1]	2.905
H18B	H5[1]	3.354	H18B	H7[1]	3.488
H18B	H8A[1]	3.143	H18B	H8C[1]	2.430
H22	C38[6]	3.475	H22	H25C[10]	3.221
H22	H38[6]	3.502	H24	C34[2]	3.019
H24	H8A[1]	3.306	H24	H34A[2]	2.751
H24	H34B[2]	2.973	H24	H34C[2]	2.820
H24	H43B[6]	3.098	H25A	H15C[8]	3.208
H25A	H16B[8]	3.040	H25A	H34C[2]	3.502
H25A	H41B[10]	3.493	H25A	H43B[6]	3.169
H25B	C15[8]	3.339	H25B	C38[6]	3.569
H25B	C41[10]	3.563	H25B	H15C[8]	2.424
H25B	H16B[8]	3.532	H25B	H38[6]	3.064
H25B	H41A[10]	3.386	H25B	H41B[10]	3.449
H25B	H41C[10]	3.265	H25B	H43B[6]	2.812
H25C	C21[10]	3.294	H25C	C22[10]	3.115
H25C	C23[10]	3.569	H25C	C41[10]	3.251
H25C	H22[10]	3.221	H25C	H26C[10]	3.465
H25C	H41A[10]	3.103	H25C	H41B[10]	2.770
H25C	H41C[10]	3.363	H26A	Cl2[4]	3.084
H26A	H15B[4]	2.907	H26A	H16C[4]	2.881
H26A	H41C[6]	3.180	H26A	H42B[6]	3.079

Table S9-12. Intermolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
H26B	C15[4]	3.376	H26B	C40[6]	3.168
H26B	C41[6]	2.993	H26B	H15B[4]	2.682
H26B	H15C[4]	3.198	H26B	H16C[4]	3.472
H26B	H41A[6]	3.179	H26B	H41C[6]	2.337
H26C	C15[4]	3.531	H26C	H15B[4]	2.616
H26C	H25C[10]	3.465	H27A	C2[1]	3.459
H27A	C3[1]	3.579	H27A	C7[1]	3.473
H27A	H17A[1]	2.843	H27B	H9C[1]	3.588
H27B	H12[1]	2.806	H27B	H17A[1]	3.302
H31	Cl1[11]	2.802	H31	C9[7]	3.198
H31	H9B[7]	3.378	H31	H9C[7]	2.283
H31	H10[11]	2.830	H33	C11[1]	3.476
H33	C12[1]	2.882	H33	C17[1]	3.569
H33	H12[1]	2.180	H33	H17A[1]	3.001
H34A	C18[11]	3.520	H34A	H1A[11]	3.532
H34A	H5[7]	2.933	H34A	H9C[7]	3.313
H34A	H17B[11]	3.224	H34A	H18A[11]	2.554
H34A	H24[11]	2.751	H34B	H5[7]	3.126
H34B	H24[11]	2.973	H34C	C11[1]	3.397
H34C	C12[1]	3.440	H34C	H12[1]	3.538
H34C	H17B[11]	3.341	H34C	H17C[11]	3.507
H34C	H17C[1]	3.321	H34C	H24[11]	2.820
H34C	H25A[11]	3.502	H35A	Cl1[11]	2.903
H35A	C42[5]	3.389	H35A	H9C[7]	3.162
H35A	H10[11]	3.063	H35A	H15A[11]	3.030
H35A	H16A[7]	3.070	H35A	H42A[5]	3.037
H35A	H42B[5]	3.212	H35A	H42C[5]	3.357
H35B	C10[11]	3.593	H35B	C15[11]	3.157
H35B	C42[5]	3.247	H35B	H10[11]	2.902
H35B	H15A[11]	2.192	H35B	H42A[5]	2.607
H35B	H42B[5]	3.526	H35B	H42C[5]	3.152
H35C	C42[5]	3.275	H35C	H42A[5]	2.555
H35C	H42B[5]	3.240	H36	C2[1]	3.341
H36	C6[1]	3.337	H36	C7[1]	2.689
H36	H1B[1]	3.112	H36	H7[1]	2.304
H36	H8C[1]	3.096	H38	Cl3[5]	2.868
H38	H15A[11]	3.169	H38	H15C[11]	3.262

Table S9-12. Intermolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
H38	$H22^{1}$	3.502	H38	$H25B^{1}$	3.064
H41A	$C8^{1}$	3.051	H41A	$H7^{1}$	3.348
H41A	$H8B^{1}$	3.248	H41A	$H8C^{1}$	2.144
H41A	$H25B^{10}$	3.386	H41A	$H25C^{10}$	3.103
H41A	$H26B^{1}$	3.179	H41B	$C25^{10}$	3.406
H41B	$H8C^{1}$	3.505	H41B	$H16B^{12}$	3.022
H41B	$H25A^{10}$	3.493	H41B	$H25B^{10}$	3.449
H41B	$H25C^{10}$	2.770	H41C	$C15^{12}$	3.553
H41C	$C16^{12}$	3.225	H41C	$C26^{1}$	3.158
H41C	$H15B^{12}$	3.391	H41C	$H15C^{12}$	2.873
H41C	$H16B^{12}$	2.560	H41C	$H16C^{12}$	3.023
H41C	$H25B^{10}$	3.265	H41C	$H25C^{10}$	3.363
H41C	$H26A^{1}$	3.180	H41C	$H26B^{1}$	2.337
H42A	$Cl3^{5}$	3.183	H42A	$C35^{5}$	2.888
H42A	$H8B^{5}$	3.310	H42A	$H15A^{4}$	3.376
H42A	$H35A^{5}$	3.037	H42A	$H35B^{5}$	2.607
H42A	$H35C^{5}$	2.555	H42B	$C16^{12}$	2.787
H42B	$C35^{5}$	3.517	H42B	$H16A^{12}$	2.833
H42B	$H16B^{12}$	2.789	H42B	$H16C^{12}$	2.291
H42B	$H26A^{1}$	3.079	H42B	$H35A^{5}$	3.212
H42B	$H35B^{5}$	3.526	H42B	$H35C^{5}$	3.240
H42C	$C15^{4}$	3.324	H42C	$C16^{12}$	3.511
H42C	$C35^{5}$	3.561	H42C	$H15A^{4}$	2.882
H42C	$H15B^{4}$	2.893	H42C	$H16A^{12}$	3.333
H42C	$H16B^{12}$	3.197	H42C	$H16C^{12}$	3.421
H42C	$H35A^{5}$	3.357	H42C	$H35B^{5}$	3.152
H43A	$C1^{1}$	3.373	H43A	$C17^{1}$	3.025
H43A	$H1B^{1}$	2.483	H43A	$H17A^{1}$	2.491
H43A	$H17B^{1}$	2.952	H43A	$H17C^{1}$	3.158
H43B	$C10^{11}$	3.583	H43B	$C23^{1}$	2.947
H43B	$C24^{1}$	3.035	H43B	$C25^{1}$	3.145
H43B	$H1B^{1}$	3.302	H43B	$H10^{11}$	3.344
H43B	$H15A^{11}$	3.392	H43B	$H15C^{11}$	3.338
H43B	$H24^{1}$	3.098	H43B	$H25A^{1}$	3.169
H43B	$H25B^{1}$	2.812	H43C	$C10^{11}$	3.242
H43C	$C15^{11}$	3.559	H43C	$H10^{11}$	2.596
H43C	$H15A^{11}$	2.948	H43C	$H17A^{1}$	3.379

Table S9-12. Intermolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance

Symmetry Operators:

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

X-ray Structure Report

for

$[CpTiCl_2\{(O\text{-}2,4\text{-}^tBu_2C_6H_2)\text{-}6\text{-}CH_2\}]_3N$ (**4**)

April 6, 2017

Experimental

Data Collection

An orange block crystal of $C_{60}H_{81}Cl_6NO_3Ti_3$ having approximate dimensions of 0.120 x 0.080 x 0.070 mm was mounted in a loop. All measurements were made on a Rigaku XtaLAB mini diffractometer using multi-layer mirror monochromated Mo-Kα radiation.

The crystal-to-detector distance was 50.00 mm.

Cell constants and an orientation matrix for data collection corresponded to a R-centered trigonal cell (laue class: -3) with dimensions:

a = 24.4075(13) Å
c = 23.4369(16) Å
V = 12091.4(12) Å^3

For Z = 6 and F.W. = 1220.72, the calculated density is 1.006 g/cm^3. Based on the reflection conditions of:

hkil: -h+k+l = 3n

packing considerations, a statistical analysis of intensity distribution, and the successful solution and refinement of the structure, the space group was determined to be:

R-3(h) (#148)

The data were collected at a temperature of -180 $\pm$ 1^{o}C to a maximum 2θ value of 65.1^o. A total of 540 oscillation images were collected. A sweep of data was done using ω scans from -60.0 to 120.0^o in 1.00^o step, at χ=54.0^o and ϕ = 0.0^o. The exposure rate was 64.0 [sec./^{o}]. The detector swing angle was 30.00^o. A second sweep was performed using ω scans from -60.0 to 120.0^o in 1.00^o step, at χ=54.0^o and ϕ = 120.0^o. The exposure rate was 64.0 [sec./^{o}]. The detector swing angle was 30.00^o. Another sweep was performed using ω scans from -60.0 to 120.0^o in 1.00^o step, at χ=54.0^o and ϕ = 240.0^o. The exposure rate was 64.0 [sec./^{o}]. The detector swing angle

was 30.00°. The crystal-to-detector distance was 50.00 mm. Readout was performed in the 0.073 mm pixel mode.

Data Reduction

Of the 0 reflections were collected, where 0 were unique (R_{int} = 0.1254); equivalent reflections were merged. Data were collected and processed using CrysAlisPro (Rigaku Oxford Diffraction). [1]

The linear absorption coefficient, μ, for Mo-Kα radiation is 5.211 cm^{-1}. An empirical absorption correction was applied which resulted in transmission factors ranging from 0.952 to 0.964. 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 6172 observed reflections and 220 variable parameters and converged (largest parameter shift was 0.00 times its esd) with unweighted and weighted agreement factors of:

$$R1 = \Sigma \, ||Fo| - |Fc|| \, / \, \Sigma \, |Fo| = 0.0750$$

$$wR2 = [\Sigma \, (w \, (Fo^2 - Fc^2)^2) / \Sigma \, w(Fo^2)^2]^{1/2} = 0.2317$$

The goodness of fit[4] was 0.98. Unit weights were used. The maximum and minimum peaks on the final difference Fourier map corresponded to 0.87 and -0.35 $e^-/Å^3$, respectively.

Neutral atom scattering factors were taken from International Tables for Crystallography (IT), Vol. C, Table 6.1.1.4 [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 Version 2014/7[10].

References

(1) CrysAlisPro: Data Collection and Processing Software, Rigaku Corporation (2015). Tokyo 196-8666, Japan.

(2) SHELXT Version 2014/5: Sheldrick, G. M. (2014). Acta Cryst. A70, C1437.

(3) Least Squares function minimized: (SHELXL Version 2014/7)

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

(4) Goodness of fit is defined as:

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

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

(5) International Tables for Crystallography, Vol.C (1992). Ed. A.J.C. Wilson, Kluwer Academic Publishers, Dordrecht, Netherlands, Table 6.1.1.4, pp. 572.

(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 4.2: Crystal Structure Analysis Package, Rigaku Corporation (2000-2015). Tokyo 196-8666, Japan.

(10) SHELXL Version 2014/7: Sheldrick, G. M. (2008). Acta Cryst. A64, 112-122.

EXPERIMENTAL DETAILS

A. Crystal Data

Empirical Formula	$C_{60}H_{81}Cl_6NO_3Ti_3$
Formula Weight	1220.72
Crystal Color, Habit	orange, block
Crystal Dimensions	0.120 X 0.080 X 0.070 mm
Crystal System	trigonal
Lattice Type	R-centered
Lattice Parameters	a = 24.4075(13) Å c = 23.4369(16) Å V = 12091.4(12) $Å^3$
Space Group	R-3 (#148)
Z value	6
D_{calc}	1.006 g/cm^3
F_{000}	3840.00
μ(MoKα)	5.211 cm^{-1}

B. Intensity Measurements

Diffractometer	XtaLAB mini
Radiation	MoKα (λ = 0.71073 Å) multi-layer mirror monochromated
Voltage, Current	50kV, 24mA
Temperature	-180.0^{o}C
Detector Aperture	75.0 mm (diameter)
Data Images	540 exposures
ω oscillation Range (χ=54.0, ϕ=0.0)	-60.0 - 120.0^{o}
Exposure Rate	64.0 sec./^{o}
Detector Swing Angle	30.00^{o}
ω oscillation Range (χ=54.0, ϕ=120.0)	-60.0 - 120.0^{o}
Exposure Rate	64.0 sec./^{o}
Detector Swing Angle	30.00^{o}
ω oscillation Range (χ=54.0, ϕ=240.0)	-60.0 - 120.0^{o}
Exposure Rate	64.0 sec./^{o}
Detector Swing Angle	30.00^{o}
Detector Position	50.00 mm
Pixel Size	0.073 mm
$2\theta_{max}$	55.0^{o}
No. of Reflections Measured	Total: 43023

	Unique: 6172 (R_{int} = 0.1254)
Corrections	Lorentz-polarization Absorption (trans. factors: 0.952 - 0.964)

C. Structure Solution and Refinement

Structure Solution	Direct Methods (SHELXT Version 2014/5)
Refinement	Full-matrix least-squares on F^2
Function Minimized	Σ w $(Fo^2 - Fc^2)^2$
Least Squares Weights	$w = 1/ [\sigma^2(Fo^2) + (0.1174 \cdot P)^2 + 0.0000 \cdot P]$ 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)	6172
No. Variables	220
Reflection/Parameter Ratio	28.05
Residuals: R1 (I>2.00σ(I))	0.0750
Residuals: R (All reflections)	0.1434
Residuals: wR2 (All reflections)	0.2317
Goodness of Fit Indicator	0.984
Max Shift/Error in Final Cycle	0.001
Maximum peak in Final Diff. Map	0.87 $e^-/Å^3$
Minimum peak in Final Diff. Map	-0.35 $e^-/Å^3$

Table S10-1. Atomic coordinates and B_{iso}/B_{eq} and occupancy

atom	x	y	z	B_{eq}	occ
Ti1	0.54550(4)	0.44272(4)	0.76933(3)	3.02(2)	1
Cl1	0.45778(6)	0.43734(6)	0.80772(6)	4.39(3)	1
Cl2	0.59093(5)	0.42821(5)	0.84628(5)	3.77(3)	1
O1	0.51675(12)	0.37056(13)	0.73144(12)	2.83(5)	1
N1	0.66667	0.33333	0.6982(2)	2.42(10)	1/3
C1	0.61930(18)	0.35015(18)	0.71563(17)	2.49(7)	1
C2	0.56262(18)	0.32284(19)	0.67578(17)	2.71(7)	1
C3	0.51099(19)	0.33084(19)	0.68685(17)	2.79(7)	1
C4	0.4547(2)	0.2989(2)	0.65483(18)	3.42(9)	1
C5	0.4556(2)	0.2650(2)	0.6076(2)	3.73(9)	1
C6	0.5086(2)	0.2600(2)	0.59288(18)	3.32(8)	1
C7	0.56014(19)	0.28755(19)	0.62785(17)	2.72(7)	1
C8	0.5069(2)	0.2235(2)	0.5385(2)	4.00(10)	1
C9	0.5673(3)	0.2238(4)	0.5284(3)	7.9(2)	1
C10	0.4507(3)	0.1587(3)	0.5388(3)	8.1(2)	1
C11	0.4980(4)	0.2586(4)	0.4867(3)	7.43(17)	1
C12	0.3947(2)	0.3014(3)	0.6711(2)	4.60(11)	1
C13	0.3777(2)	0.2821(3)	0.7337(2)	4.49(11)	1
C14	0.4040(3)	0.3681(3)	0.6603(3)	5.88(14)	1
C15	0.3382(3)	0.2545(4)	0.6349(3)	7.34(19)	1
C16	0.6027(5)	0.4954(3)	0.6877(4)	7.82(19)	1
C17	0.6412(3)	0.5132(3)	0.7267(4)	6.45(18)	1
C18	0.6279(4)	0.5476(3)	0.7669(3)	7.41(19)	1
C19	0.5717(4)	0.5451(3)	0.7436(4)	7.8(2)	1
C20	0.5617(4)	0.5115(4)	0.6941(4)	7.6(2)	1

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

Table S10-2. Atomic coordinates and B_{iso} involving hydrogen atoms

atom	x	y	z	B_{iso}	occ
H1A	0.63905	0.39680	0.71635	2.989	1
H1B	0.60473	0.33430	0.75478	2.989	1
H5	0.41890	0.24449	0.58432	4.474	1
H7	0.59549	0.28261	0.61937	3.268	1
H9A	0.60259	0.26746	0.52869	9.429	1
H9B	0.57355	0.19968	0.55869	9.429	1
H9C	0.56557	0.20436	0.49139	9.429	1
H10A	0.41244	0.16139	0.54551	9.666	1
H10B	0.44723	0.13835	0.50186	9.666	1
H10C	0.45521	0.13367	0.56916	9.666	1
H11A	0.53404	0.30180	0.48458	8.920	1
H11B	0.49542	0.23597	0.45138	8.920	1
H11C	0.45890	0.26011	0.49173	8.920	1
H13A	0.41284	0.31109	0.75823	5.386	1
H13B	0.33966	0.28398	0.74376	5.386	1
H13C	0.36955	0.23884	0.73924	5.386	1
H14A	0.43985	0.39936	0.68286	7.058	1
H14B	0.41230	0.37857	0.61968	7.058	1
H14C	0.36556	0.36867	0.67154	7.058	1
H15A	0.34751	0.26543	0.59440	8.808	1
H15B	0.33050	0.21155	0.64125	8.808	1
H15C	0.30061	0.25669	0.64577	8.808	1
H16	0.60559	0.47317	0.65299	9.378	1
H17	0.67976	0.50883	0.72719	7.735	1
H18	0.65505	0.57410	0.79915	8.898	1
H19	0.55102	0.56955	0.75617	9.311	1
H20	0.52895	0.50478	0.66500	9.075	1

Table S10-3. Anisotropic displacement parameters

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Ti1	0.0409(5)	0.0360(5)	0.0420(5)	0.0224(4)	0.0008(4)	0.0022(3)
Cl1	0.0534(8)	0.0602(8)	0.0634(8)	0.0361(7)	0.0062(6)	-0.0047(6)
Cl2	0.0500(7)	0.0417(6)	0.0462(7)	0.0191(5)	-0.0094(5)	0.0000(5)
O1	0.0315(15)	0.0401(16)	0.0411(16)	0.0219(13)	-0.0016(12)	-0.0006(13)
N1	0.0276(18)	0.0276(18)	0.037(3)	0.0138(9)	0.00000	0.00000
C1	0.031(2)	0.031(2)	0.037(2)	0.0188(18)	-0.0009(17)	0.0005(17)
C2	0.031(2)	0.035(2)	0.037(2)	0.0174(18)	-0.0006(18)	0.0057(18)
C3	0.035(2)	0.037(2)	0.035(2)	0.0183(19)	0.0013(18)	0.0030(18)
C4	0.032(2)	0.061(3)	0.037(2)	0.024(2)	-0.0052(19)	-0.005(2)
C5	0.034(2)	0.066(3)	0.041(3)	0.025(2)	-0.006(2)	-0.007(2)
C6	0.043(3)	0.046(3)	0.034(2)	0.020(2)	-0.0029(19)	-0.009(2)
C7	0.029(2)	0.036(2)	0.037(2)	0.0145(18)	0.0030(18)	0.0037(18)
C8	0.042(3)	0.061(3)	0.039(3)	0.019(2)	-0.004(2)	-0.016(2)
C9	0.061(4)	0.148(7)	0.088(5)	0.050(4)	-0.015(3)	-0.066(5)
C10	0.067(4)	0.091(5)	0.117(6)	0.016(4)	0.012(4)	-0.054(4)
C11	0.110(6)	0.123(6)	0.058(4)	0.065(5)	-0.006(4)	-0.018(4)
C12	0.045(3)	0.083(4)	0.055(3)	0.039(3)	-0.013(2)	-0.015(3)
C13	0.038(3)	0.071(3)	0.063(3)	0.028(3)	-0.000(2)	-0.010(3)
C14	0.075(4)	0.115(5)	0.066(4)	0.072(4)	-0.015(3)	-0.014(4)
C15	0.053(3)	0.149(7)	0.093(5)	0.062(4)	-0.031(3)	-0.058(5)
C16	0.126(6)	0.066(4)	0.075(4)	0.026(4)	0.027(5)	0.011(4)
C17	0.056(4)	0.055(4)	0.135(7)	0.029(3)	0.039(4)	0.054(4)
C18	0.115(5)	0.037(3)	0.053(3)	-0.019(3)	-0.014(4)	0.010(3)
C19	0.114(5)	0.061(4)	0.150(6)	0.067(4)	0.082(5)	0.047(4)
C20	0.079(4)	0.089(5)	0.095(5)	0.023(3)	-0.027(4)	0.049(4)

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 S10-4. Bond lengths (Å)

atom	atom	distance	atom	atom	distance
Ti1	Cl1	2.2649(19)	Ti1	Cl2	2.2361(16)
Ti1	O1	1.774(3)	Ti1	C16	2.339(8)
Ti1	C17	2.323(7)	Ti1	C18	2.336(5)
Ti1	C19	2.328(8)	Ti1	C20	2.328(9)
O1	C3	1.384(5)	N1	C1	1.465(5)
N1	C1[1]	1.465(5)	N1	C1[2]	1.465(5)
C1	C2	1.519(6)	C2	C3	1.393(7)
C2	C7	1.398(6)	C3	C4	1.409(6)
C4	C5	1.388(7)	C4	C12	1.542(9)
C5	C6	1.402(8)	C6	C7	1.364(6)
C6	C8	1.545(7)	C8	C9	1.489(10)
C8	C10	1.488(7)	C8	C11	1.563(10)
C12	C13	1.536(7)	C12	C14	1.551(10)
C12	C15	1.534(7)	C16	C17	1.223(13)
C16	C20	1.254(17)	C17	C18	1.403(12)
C18	C19	1.449(14)	C19	C20	1.370(13)

Symmetry Operators:

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

Table S10-5. Bond lengths involving hydrogens (Å)

atom	atom	distance	atom	atom	distance
C1	H1A	0.990	C1	H1B	0.990
C5	H5	0.950	C7	H7	0.950
C9	H9A	0.980	C9	H9B	0.980
C9	H9C	0.980	C10	H10A	0.980
C10	H10B	0.980	C10	H10C	0.980
C11	H11A	0.980	C11	H11B	0.980
C11	H11C	0.980	C13	H13A	0.980
C13	H13B	0.980	C13	H13C	0.980
C14	H14A	0.980	C14	H14B	0.980
C14	H14C	0.980	C15	H15A	0.980
C15	H15B	0.980	C15	H15C	0.980
C16	H16	1.000	C17	H17	1.000
C18	H18	1.000	C19	H19	1.000
C20	H20	1.000			

Table S10-6. Bond angles (°)

atom	atom	atom	angle	atom	atom	atom	angle
Cl1	Ti1	Cl2	101.52(6)	Cl1	Ti1	O1	104.37(10)
Cl1	Ti1	C16	130.1(3)	Cl1	Ti1	C17	141.7(2)
Cl1	Ti1	C18	110.2(2)	Cl1	Ti1	C19	84.8(3)
Cl1	Ti1	C20	99.1(3)	Cl2	Ti1	O1	103.17(12)
Cl2	Ti1	C16	122.7(3)	Cl2	Ti1	C17	94.0(2)
Cl2	Ti1	C18	88.3(2)	Cl2	Ti1	C19	119.1(2)
Cl2	Ti1	C20	143.73(18)	O1	Ti1	C16	88.1(2)
O1	Ti1	C17	105.8(2)	O1	Ti1	C18	140.6(2)
O1	Ti1	C19	134.1(3)	O1	Ti1	C20	100.2(2)
C16	Ti1	C17	30.4(3)	C16	Ti1	C18	55.0(2)
C16	Ti1	C19	55.2(4)	C16	Ti1	C20	31.2(4)
C17	Ti1	C18	35.0(3)	C17	Ti1	C19	57.2(3)
C17	Ti1	C20	52.7(3)	C18	Ti1	C19	36.2(3)
C18	Ti1	C20	56.5(2)	C19	Ti1	C20	34.2(3)
Ti1	O1	C3	157.6(2)	C1	N1	C1[1]	112.5(2)
C1	N1	C1[2]	112.5(2)	C1[1]	N1	C1[2]	112.5(2)
N1	C1	C2	112.3(4)	C1	C2	C3	120.9(4)
C1	C2	C7	120.9(4)	C3	C2	C7	118.2(4)
O1	C3	C2	117.2(3)	O1	C3	C4	121.3(5)
C2	C3	C4	121.5(4)	C3	C4	C5	116.9(5)
C3	C4	C12	121.9(4)	C5	C4	C12	121.2(4)
C4	C5	C6	122.6(4)	C5	C6	C7	118.2(4)
C5	C6	C8	119.6(4)	C7	C6	C8	122.1(5)
C2	C7	C6	122.1(5)	C6	C8	C9	112.8(4)
C6	C8	C10	110.7(4)	C6	C8	C11	107.1(5)
C9	C8	C10	113.1(6)	C9	C8	C11	106.5(5)
C10	C8	C11	106.2(5)	C4	C12	C13	110.0(5)
C4	C12	C14	111.0(4)	C4	C12	C15	110.6(5)
C13	C12	C14	110.6(5)	C13	C12	C15	107.2(4)
C14	C12	C15	107.3(6)	Ti1	C16	C17	74.1(5)
Ti1	C16	C20	73.9(6)	C17	C16	C20	113.0(9)
Ti1	C17	C16	75.5(5)	Ti1	C17	C18	73.0(4)
C16	C17	C18	110.4(9)	Ti1	C18	C17	72.0(3)
Ti1	C18	C19	71.6(4)	C17	C18	C19	102.6(6)
Ti1	C19	C18	72.2(4)	Ti1	C19	C20	72.9(5)
C18	C19	C20	103.1(9)	Ti1	C20	C16	74.9(6)
Ti1	C20	C19	72.9(5)	C16	C20	C19	110.9(8)

Table S10-6. Bond angles (°) (continued)

atom	atom	atom	angle	atom	atom	atom	angle

Symmetry Operators:

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

Table S10-7. Bond angles involving hydrogens (°)

atom	atom	atom	angle	atom	atom	atom	angle
N1	C1	H1A	109.2	N1	C1	H1B	109.2
C2	C1	H1A	109.1	C2	C1	H1B	109.1
H1A	C1	H1B	107.9	C4	C5	H5	118.7
C6	C5	H5	118.7	C2	C7	H7	118.9
C6	C7	H7	118.9	C8	C9	H9A	109.5
C8	C9	H9B	109.5	C8	C9	H9C	109.5
H9A	C9	H9B	109.5	H9A	C9	H9C	109.5
H9B	C9	H9C	109.5	C8	C10	H10A	109.5
C8	C10	H10B	109.5	C8	C10	H10C	109.5
H10A	C10	H10B	109.5	H10A	C10	H10C	109.5
H10B	C10	H10C	109.5	C8	C11	H11A	109.5
C8	C11	H11B	109.5	C8	C11	H11C	109.5
H11A	C11	H11B	109.5	H11A	C11	H11C	109.5
H11B	C11	H11C	109.5	C12	C13	H13A	109.5
C12	C13	H13B	109.5	C12	C13	H13C	109.5
H13A	C13	H13B	109.5	H13A	C13	H13C	109.5
H13B	C13	H13C	109.5	C12	C14	H14A	109.5
C12	C14	H14B	109.5	C12	C14	H14C	109.5
H14A	C14	H14B	109.5	H14A	C14	H14C	109.5
H14B	C14	H14C	109.5	C12	C15	H15A	109.5
C12	C15	H15B	109.5	C12	C15	H15C	109.5
H15A	C15	H15B	109.5	H15A	C15	H15C	109.5
H15B	C15	H15C	109.5	Ti1	C16	H16	123.4
C17	C16	H16	123.5	C20	C16	H16	123.4
Ti1	C17	H17	124.6	C16	C17	H17	124.6
C18	C17	H17	124.6	Ti1	C18	H18	128.2
C17	C18	H18	128.2	C19	C18	H18	128.2
Ti1	C19	H19	127.9	C18	C19	H19	127.9
C20	C19	H19	127.9	Ti1	C20	H20	124.4
C16	C20	H20	124.4	C19	C20	H20	124.4

Table S10-8. Torsion Angles(o)
(Those having bond angles > 160 or < 20 degrees are excluded.)

atom1	atom2	atom3	atom4	angle	atom1	atom2	atom3	atom4	angle
Cl1	Ti1	O1	C3	136.6(6)	Cl1	Ti1	C16	C17	126.3(4)
Cl1	Ti1	C16	C20	6.0(4)	Cl1	Ti1	C17	C16	-84.0(5)
Cl1	Ti1	C17	C18	33.1(6)	Cl1	Ti1	C18	C17	-158.9(2)
Cl1	Ti1	C18	C19	-48.4(3)	Cl1	Ti1	C19	C18	135.2(3)
Cl1	Ti1	C19	C20	-114.5(4)	Cl1	Ti1	C20	C16	-175.3(3)
Cl1	Ti1	C20	C19	66.6(3)	Cl2	Ti1	O1	C3	-117.7(6)
Cl2	Ti1	C16	C17	-21.9(6)	Cl2	Ti1	C16	C20	-142.2(3)
Cl2	Ti1	C17	C16	161.7(4)	Cl2	Ti1	C17	C18	-81.2(3)
Cl2	Ti1	C18	C17	99.5(3)	Cl2	Ti1	C18	C19	-150.0(2)
Cl2	Ti1	C19	C18	34.9(5)	Cl2	Ti1	C19	C20	145.2(3)
Cl2	Ti1	C20	C16	60.7(6)	Cl2	Ti1	C20	C19	-57.3(6)
O1	Ti1	C16	C17	-126.4(5)	O1	Ti1	C16	C20	113.3(3)
C16	Ti1	O1	C3	5.5(7)	O1	Ti1	C17	C16	56.8(4)
O1	Ti1	C17	C18	173.9(3)	C17	Ti1	O1	C3	-19.6(7)
O1	Ti1	C18	C17	-9.3(6)	O1	Ti1	C18	C19	101.2(4)
C18	Ti1	O1	C3	-14.0(9)	O1	Ti1	C19	C18	-119.8(3)
O1	Ti1	C19	C20	-9.4(6)	C19	Ti1	O1	C3	39.8(8)
O1	Ti1	C20	C16	-68.8(3)	O1	Ti1	C20	C19	173.1(3)
C20	Ti1	O1	C3	34.4(7)	C16	Ti1	C17	C16	-0.0(5)
C16	Ti1	C17	C18	117.1(8)	C17	Ti1	C16	C17	-0.0(4)
C17	Ti1	C16	C20	-120.3(7)	C16	Ti1	C18	C17	-33.4(4)
C16	Ti1	C18	C19	77.1(4)	C18	Ti1	C16	C17	38.6(4)
C18	Ti1	C16	C20	-81.7(4)	C16	Ti1	C19	C18	-76.5(5)
C16	Ti1	C19	C20	33.8(4)	C19	Ti1	C16	C17	83.1(5)
C19	Ti1	C16	C20	-37.2(4)	C16	Ti1	C20	C16	-0.0(3)
C16	Ti1	C20	C19	-118.0(6)	C20	Ti1	C16	C17	120.3(7)
C20	Ti1	C16	C20	-0.0(3)	C17	Ti1	C18	C17	0.0(4)
C17	Ti1	C18	C19	110.5(5)	C18	Ti1	C17	C16	-117.1(7)
C18	Ti1	C17	C18	-0.0(4)	C17	Ti1	C19	C18	-39.8(4)
C17	Ti1	C19	C20	70.6(4)	C19	Ti1	C17	C16	-76.0(5)
C19	Ti1	C17	C18	41.2(4)	C17	Ti1	C20	C16	33.3(3)
C17	Ti1	C20	C19	-84.7(4)	C20	Ti1	C17	C16	-34.2(4)
C20	Ti1	C17	C18	83.0(4)	C18	Ti1	C19	C18	0.0(3)
C18	Ti1	C19	C20	110.4(6)	C19	Ti1	C18	C17	-110.5(6)
C19	Ti1	C18	C19	-0.0(4)	C18	Ti1	C20	C16	76.4(4)
C18	Ti1	C20	C19	-41.6(3)	C20	Ti1	C18	C17	-71.3(4)
C20	Ti1	C18	C19	39.2(3)	C19	Ti1	C20	C16	118.0(6)

Table S10-8. Torsion angles (°) (continued)

atom1	atom2	atom3	atom4	angle	atom1	atom2	atom3	atom4	angle
C19	Ti1	C20	C19	0.0(4)	C20	Ti1	C19	C18	-110.4(7)
C20	Ti1	C19	C20	0.0(4)	Ti1	O1	C3	C2	68.1(10)
Ti1	O1	C3	C4	-113.2(7)	C1	N1	C1[1]	C2[1]	151.6(3)
C1[1]	N1	C1	C2	-79.9(4)	C1	N1	C1[2]	C2[2]	-79.9(4)
C1[2]	N1	C1	C2	151.6(3)	C1[1]	N1	C1[2]	C2[2]	151.6(3)
C1[2]	N1	C1[1]	C2[1]	-79.9(4)	N1	C1	C2	C3	176.7(3)
N1	C1	C2	C7	-1.6(5)	C1	C2	C3	O1	7.3(5)
C1	C2	C3	C4	-171.4(3)	C1	C2	C7	C6	176.8(3)
C3	C2	C7	C6	-1.5(6)	C7	C2	C3	O1	-174.3(3)
C7	C2	C3	C4	6.9(6)	O1	C3	C4	C5	173.9(3)
O1	C3	C4	C12	-5.9(6)	C2	C3	C4	C5	-7.4(6)
C2	C3	C4	C12	172.8(4)	C3	C4	C5	C6	2.5(7)
C3	C4	C12	C13	-53.0(6)	C3	C4	C12	C14	69.8(6)
C3	C4	C12	C15	-171.2(4)	C5	C4	C12	C13	127.2(5)
C5	C4	C12	C14	-110.0(5)	C5	C4	C12	C15	9.0(7)
C12	C4	C5	C6	-177.6(4)	C4	C5	C6	C7	2.6(7)
C4	C5	C6	C8	-177.8(4)	C5	C6	C7	C2	-3.2(6)
C5	C6	C8	C9	178.8(4)	C5	C6	C8	C10	-53.4(6)
C5	C6	C8	C11	61.9(5)	C7	C6	C8	C9	-1.6(6)
C7	C6	C8	C10	126.1(4)	C7	C6	C8	C11	-118.5(5)
C8	C6	C7	C2	177.3(4)	Ti1	C16	C17	Ti1	0.00(3)
Ti1	C16	C17	C18	-65.2(4)	Ti1	C16	C20	Ti1	0.000(18)
Ti1	C16	C20	C19	64.6(5)	C17	C16	C20	Ti1	-64.4(6)
C17	C16	C20	C19	0.2(9)	C20	C16	C17	Ti1	64.3(6)
C20	C16	C17	C18	-1.0(9)	Ti1	C17	C18	Ti1	-0.00(3)
Ti1	C17	C18	C19	-65.6(3)	C16	C17	C18	Ti1	66.9(5)
C16	C17	C18	C19	1.2(7)	Ti1	C18	C19	Ti1	-0.00(2)
Ti1	C18	C19	C20	-66.9(4)	C17	C18	C19	Ti1	65.9(4)
C17	C18	C19	C20	-1.0(6)	Ti1	C19	C20	Ti1	0.00(3)
Ti1	C19	C20	C16	-65.8(5)	C18	C19	C20	Ti1	66.4(5)
C18	C19	C20	C16	0.6(8)					

Symmetry Operators:

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

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

Table S10-9. Intramolecular contacts less than 3.60 Å

atom	atom	distance	atom	atom	distance
O1	C1	2.810(6)	O1	C12	2.948(5)
O1	C13	2.977(5)	O1	C14	3.193(8)
N1	C2[1]	2.478(5)	N1	C2[2]	2.478(5)
N1	C7	2.797(5)	N1	C7[1]	2.797(5)
N1	C7[2]	2.797(5)	C1	C2[2]	3.148(6)
C1	C7[2]	3.196(6)	C2	C5	2.771(6)
C3	C6	2.783(7)	C3	C13	3.056(7)
C3	C14	3.227(10)	C3	C16	3.487(8)
C4	C7	2.795(8)	C5	C10	3.007(10)
C5	C11	3.047(8)	C5	C14	3.552(11)
C5	C15	2.819(9)	C7	C9	2.856(9)
C7	C11	3.560(7)			

Symmetry Operators:

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

Table S10-10. Intramolecular contacts less than 3.60 Å involving hydrogens

atom	atom	distance	atom	atom	distance
Ti1	H1A	3.251	Ti1	H13A	3.236
Ti1	H14A	3.024	Cl1	H13A	2.943
Cl1	H14A	3.035	Cl1	H19	3.116
Cl2	H1A	3.484	Cl2	H1B	3.277
Cl2	H17	3.478	Cl2	H18	3.283
O1	H1A	2.745	O1	H1B	2.756
O1	H13A	2.292	O1	H13C	3.424
O1	H14A	2.575	O1	H16	2.987
O1	H20	3.503	N1	H1A[1]	2.020
N1	H1A[2]	2.020	N1	H1B[1]	2.020
N1	H1B[2]	2.020	N1	H7	2.411
N1	H7[1]	2.411	N1	H7[2]	2.411
C1	H1A[1]	2.461	C1	H1A[2]	3.255
C1	H1B[1]	2.849	C1	H1B[2]	2.517
C1	H7	2.681	C1	H7[2]	2.719
C1	H16	3.505	C1	H17	3.396
C2	H1A[1]	2.775	C2	H7[2]	2.983
C2	H9B[2]	3.523	C2	H16	3.317
C2	H17[1]	3.431	C3	H1A	2.794
C3	H1B	2.754	C3	H5	3.245
C3	H7	3.251	C3	H13A	2.760
C3	H13C	3.273	C3	H14A	2.954
C3	H14B	3.528	C3	H16	3.164
C4	H13A	2.704	C4	H13B	3.368
C4	H13C	2.709	C4	H14A	2.732
C4	H14B	2.747	C4	H14C	3.390
C4	H15A	2.717	C4	H15B	2.716
C4	H15C	3.373	C5	H7	3.233
C5	H10A	2.638	C5	H10C	3.326
C5	H11A	3.326	C5	H11C	2.721
C5	H14B	3.436	C5	H15A	2.661
C5	H15B	2.769	C6	H9A	2.672
C6	H9B	2.767	C6	H9C	3.365
C6	H10A	2.624	C6	H10B	3.341
C6	H10C	2.738	C6	H11A	2.690
C6	H11B	3.355	C6	H11C	2.664
C7	H1A	3.160	C7	H1A[1]	2.791

Table S10-10. Intramolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
C7	H1B	3.177	C7	H5	3.226
C7	H7[1]	3.575	C7	H7[2]	2.991
C7	H9A	2.688	C7	H9A[2]	3.503
C7	H9B	2.835	C7	H9B[2]	3.355
C7	H10C	3.597	C7	H11A	3.467
C7	H16[1]	3.502	C7	H17[1]	3.401
C8	H5	2.672	C8	H7	2.689
C9	H7	2.467	C9	H9A[1]	3.562
C9	H10A	3.319	C9	H10B	2.686
C9	H10C	2.686	C9	H11A	2.625
C9	H11A[1]	3.263	C9	H11B	2.637
C9	H11C	3.298	C9	H16[1]	3.502
C10	H5	2.784	C10	H9A	3.318
C10	H9B	2.686	C10	H9C	2.686
C10	H11A	3.294	C10	H11B	2.624
C10	H11C	2.624	C10	H16[1]	3.497
C11	H5	2.901	C11	H9A	2.642
C11	H9B	3.312	C11	H9C	2.583
C11	H10A	2.633	C11	H10B	2.577
C11	H10C	3.307	C12	H5	2.688
C13	H14A	2.752	C13	H14B	3.379
C13	H14C	2.703	C13	H15A	3.328
C13	H15B	2.647	C13	H15C	2.647
C14	H13A	2.749	C14	H13B	2.699
C14	H13C	3.382	C14	H15A	2.667
C14	H15B	3.342	C14	H15C	2.649
C14	H20	3.204	C15	H5	2.413
C15	H13A	3.327	C15	H13B	2.647
C15	H13C	2.647	C15	H14A	3.339
C15	H14B	2.662	C15	H14C	2.662
C16	H1A	3.028	C16	H10C[2]	3.219
C16	H14A	3.463	C16	H18	3.112
C16	H19	3.118	C17	H1A	2.827
C17	H19	3.199	C17	H20	3.012
C18	H16	3.120	C18	H20	3.179
C19	H16	3.119	C19	H17	3.196
C20	H14A	2.875	C20	H17	3.016

Table S10-10. Intramolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
C20	H18	3.179	H1A	H1A[1]	3.420
H1A	H1A[2]	3.420	H1A	H1B[1]	3.571
H1A	H1B[2]	2.403	H1A	H7	3.332
H1A	H7[2]	2.521	H1A	H16	2.805
H1A	H17	2.411	H1B	H1B[1]	2.639
H1B	H1B[2]	2.639	H1B	H7	3.381
H1B	H17[1]	3.598	H5	H10A	2.156
H5	H10B	3.566	H5	H10C	3.260
H5	H11A	3.375	H5	H11C	2.331
H5	H14B	3.457	H5	H15A	2.060
H5	H15B	2.312	H5	H15C	3.370
H7	H7[1]	2.683	H7	H7[2]	2.683
H7	H9A	2.179	H7	H9A[2]	3.239
H7	H9B	2.307	H7	H9B[2]	3.505
H7	H9C	3.433	H7	H16[1]	3.275
H9A	H9A[1]	2.748	H9A	H9A[2]	2.748
H9A	H10B	3.571	H9A	H10C	3.572
H9A	H11A	2.444	H9A	H11A[1]	3.043
H9A	H11B	2.950	H9A	H11C	3.529
H9B	H10A	3.572	H9B	H10B	2.984
H9B	H10C	2.519	H9B	H11A	3.544
H9B	H11A[1]	3.238	H9B	H11B	3.526
H9B	H16[1]	2.647	H9C	H10A	3.572
H9C	H10B	2.519	H9C	H10C	2.984
H9C	H11A	2.847	H9C	H11A[1]	2.961
H9C	H11B	2.393	H9C	H11C	3.489
H10A	H11A	3.524	H10A	H11B	2.932
H10A	H11C	2.439	H10B	H11A	3.481
H10B	H11B	2.379	H10B	H11C	2.850
H10C	H11B	3.517	H10C	H11C	3.542
H10C	H16[1]	2.640	H13A	H14A	2.603
H13A	H14C	3.009	H13A	H15B	3.546
H13A	H15C	3.546	H13B	H14A	3.010
H13B	H14B	3.583	H13B	H14C	2.496
H13B	H15A	3.547	H13B	H15B	2.924
H13B	H15C	2.448	H13C	H14C	3.588
H13C	H15A	3.547	H13C	H15B	2.448

Table S10-10. Intramolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
H13C	H15C	2.925	H14A	H15A	3.563
H14A	H15C	3.549	H14A	H16	3.579
H14A	H20	2.435	H14B	H15A	2.472
H14B	H15B	3.567	H14B	H15C	2.923
H14B	H20	3.155	H14C	H15A	2.950
H14C	H15B	3.558	H14C	H15C	2.453
H16	H17	2.342	H16	H20	2.370
H17	H18	2.590	H18	H19	2.682
H19	H20	2.550			

Symmetry Operators:

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

Table S10-11. Intermolecular contacts less than 3.60 Å

atom	atom	distance	atom	atom	distance
Cl2	O1[1]	3.288(3)	Cl2	C3[1]	3.532(4)
O1	Cl2[2]	3.288(3)	C3	Cl2[2]	3.532(4)
C15	C17[3]	3.489(9)	C15	C18[3]	3.408(10)
C17	C15[4]	3.489(9)	C18	C15[4]	3.408(10)

Symmetry Operators:

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

Table S10-12. Intermolecular contacts less than 3.60 Å involving hydrogens

atom	atom	distance	atom	atom	distance
Cl1	H5[1]	3.441	Cl1	H10A[1]	3.584
Cl1	H11C[1]	3.158	Cl1	H15A[1]	3.060
Cl1	H18[2]	2.839	Cl2	H1B[3]	2.818
Cl2	H13A[3]	3.256	Cl2	H13C[3]	3.456
Cl2	H17[2]	3.001	C10	H13B[4]	3.097
C10	H13C[4]	3.508	C10	H19[5]	3.430
C13	H10A[4]	3.132	C13	H10C[4]	3.585
C13	H18[2]	3.271	C15	H15B[4]	3.484
C15	H17[6]	3.515	C15	H18[6]	3.332
C16	H15C[7]	3.075	C17	H15C[7]	2.720
C18	H13A[3]	3.343	C18	H15A[7]	3.179
C18	H15C[7]	2.777	C19	H15C[7]	3.250
C20	H15C[7]	3.362	H1B	Cl2[2]	2.818
H5	Cl1[5]	3.441	H5	H13C[4]	3.378
H10A	Cl1[5]	3.584	H10A	C13[4]	3.132
H10A	H13B[4]	2.681	H10A	H13C[4]	2.700
H10A	H19[5]	3.170	H10B	H13B[4]	3.344
H10B	H19[5]	2.805	H10C	C13[4]	3.585
H10C	H13B[4]	2.796	H10C	H13C[4]	3.529
H10C	H15C[4]	3.368	H11B	H19[5]	3.326
H11C	Cl1[5]	3.158	H11C	H19[5]	3.557
H13A	Cl2[2]	3.256	H13A	C18[2]	3.343
H13A	H18[2]	2.573	H13B	C10[4]	3.097
H13B	H10A[4]	2.681	H13B	H10B[4]	3.344
H13B	H10C[4]	2.796	H13B	H18[2]	3.302
H13C	Cl2[2]	3.456	H13C	C10[4]	3.508
H13C	H5[4]	3.378	H13C	H10A[4]	2.700
H13C	H10C[4]	3.529	H13C	H15B[4]	2.779
H13C	H18[2]	3.480	H15A	Cl1[5]	3.060
H15A	C18[6]	3.179	H15A	H18[6]	2.837
H15B	C15[4]	3.484	H15B	H13C[4]	2.779
H15B	H15B[4]	2.558	H15B	H17[6]	3.448
H15C	C16[6]	3.075	H15C	C17[6]	2.720
H15C	C18[6]	2.777	H15C	C19[6]	3.250
H15C	C20[6]	3.362	H15C	H10C[4]	3.368
H15C	H16[6]	3.545	H15C	H17[6]	2.908
H15C	H18[6]	2.972	H16	H15C[7]	3.545

Table S10-12. Intermolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
H17	Cl2[3]	3.001	H17	C15[7]	3.515
H17	H15B[7]	3.448	H17	H15C[7]	2.908
H18	Cl1[3]	2.839	H18	C13[3]	3.271
H18	C15[7]	3.332	H18	H13A[3]	2.573
H18	H13B[3]	3.302	H18	H13C[3]	3.480
H18	H15A[7]	2.837	H18	H15C[7]	2.972
H19	C10[1]	3.430	H19	H10A[1]	3.170
H19	H10B[1]	2.805	H19	H11B[1]	3.326
H19	H11C[1]	3.557			

Symmetry Operators:

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

X-ray Structure Report

for

[Cp*$TiCl_2${(O-2,4-^{t}$Bu_2$$C_6H_2$)-6-$CH_2$}]$_3$N (**5**)

April 7, 2017

Experimental

Data Collection

A red block crystal of $C_{75}H_{111}Cl_6NO_3Ti_3$ having approximate dimensions of 0.230 x 0.190 x 0.100 mm was mounted on a glass fiber. All measurements were made on a Rigaku XtaLAB mini diffractometer using multi-layer mirror monochromated Mo-Kα radiation.

The crystal-to-detector distance was 50.00 mm.

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

a = 17.5836(9) Å
b = 22.4075(10) Å β = 94.814(4)^o
c = 21.6663(10) Å
V = 8506.5(7) Å^3

For Z = 4 and F.W. = 1431.12, the calculated density is 1.117 g/cm^3. The reflection conditions of:

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

uniquely determine the space group to be:

$P2_1/n$ (#14)

The data were collected at a temperature of -180 $\pm$ 1^{o}C to a maximum 2θ value of 65.3^o. A total of 540 oscillation images were collected. A sweep of data was done using ω scans from -60.0 to 120.0^o in 1.00^o step, at χ=54.0^o and ϕ = 0.0^o. The exposure rate was 32.0 [sec./^{o}]. The detector swing angle was 30.00^o. A second sweep was performed using ω scans from -60.0 to 120.0^o in 1.00^o step, at χ=54.0^o and ϕ = 120.0^o. The exposure rate was 32.0 [sec./^{o}]. The detector swing angle was 30.00^o. Another sweep was performed using ω scans from -60.0 to 120.0^o in 1.00^o step, at χ=54.0^o and ϕ = 240.0^o. The exposure rate was 32.0 [sec./^{o}]. The detector swing angle was 30.00^o. The crystal-to-detector distance was 50.00 mm. Readout was performed

in the 0.073 mm pixel mode.

Data Reduction

Of the 89388 reflections were collected, where 19531 were unique (R_{int} = 0.1354); equivalent reflections were merged. Data were collected and processed using CrysAlisPro (Rigaku Oxford Diffraction). [1]

The linear absorption coefficient, μ, for Mo-Kα radiation is 5.028 cm^{-1}. An empirical absorption correction was applied which resulted in transmission factors ranging from 0.929 to 0.951. 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 19531 observed reflections and 793 variable parameters and converged (largest parameter shift was 0.00 times its esd) with unweighted and weighted agreement factors of:

$$R1 = \Sigma \, ||Fo| - |Fc|| \, / \, \Sigma \, |Fo| = 0.0757$$

$$wR2 = [\, \Sigma \, (\, w \, (Fo^2 - Fc^2)^2 \,) / \, \Sigma \, w(Fo^2)^2]^{1/2} = 0.2209$$

The goodness of fit[4] was 0.94. Unit weights were used. The maximum and minimum peaks on the final difference Fourier map corresponded to 1.23 and -0.55 $e^-/Å^3$, respectively.

Neutral atom scattering factors were taken from International Tables for Crystallography (IT), Vol. C, Table 6.1.1.4 [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 Version 2014/7[10].

References

(1) CrysAlisPro: Data Collection and Processing Software, Rigaku Corporation (2015). Tokyo 196-8666, Japan.

(2) SHELXT: Sheldrick, G. M. (2014). Acta Cryst. A70, C1437.

(3) Least Squares function minimized: (SHELXL Version 2014/7)

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

(4) Goodness of fit is defined as:

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

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

(5) International Tables for Crystallography, Vol.C (1992). Ed. A.J.C. Wilson, Kluwer Academic Publishers, Dordrecht, Netherlands, Table 6.1.1.4, pp. 572.

(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 4.2: Crystal Structure Analysis Package, Rigaku Corporation (2000-2015). Tokyo 196-8666, Japan.

(10) SHELXL Version 2014/7: Sheldrick, G. M. (2008). Acta Cryst. A64, 112-122.

EXPERIMENTAL DETAILS

A. Crystal Data

Empirical Formula	$C_{75}H_{111}Cl_6NO_3Ti_3$
Formula Weight	1431.12
Crystal Color, Habit	red, block
Crystal Dimensions	0.230 X 0.190 X 0.100 mm
Crystal System	monoclinic
Lattice Type	Primitive
Lattice Parameters	a = 17.5836(9) Å b = 22.4075(10) Å c = 21.6663(10) Å β = 94.814(4) ^{o} V = 8506.5(7) Å^3
Space Group	$P2_1/n$ (#14)
Z value	4
D_{calc}	1.117 g/cm^3
F_{000}	3040.00
μ(MoKα)	5.028 cm^{-1}

B. Intensity Measurements

Diffractometer	XtaLAB mini
Radiation	MoKα (λ = 0.71073 Å) multi-layer mirror monochromated
Voltage, Current	50kV, 24mA
Temperature	-180.0^{o}C
Detector Aperture	75.0 mm (diameter)
Data Images	540 exposures
ω oscillation Range (χ=54.0, ϕ=0.0)	-60.0 - 120.0^{o}
Exposure Rate	32.0 sec./^{o}
Detector Swing Angle	30.00^{o}
ω oscillation Range (χ=54.0, ϕ=120.0)	-60.0 - 120.0^{o}
Exposure Rate	32.0 sec./^{o}
Detector Swing Angle	30.00^{o}
ω oscillation Range (χ=54.0, ϕ=240.0)	-60.0 - 120.0^{o}
Exposure Rate	32.0 sec./^{o}
Detector Swing Angle	30.00^{o}
Detector Position	50.00 mm
Pixel Size	0.073 mm
$2\theta_{max}$	55.0^{o}
No. of Reflections Measured	Total: 89388

	Unique: 19531 (R_{int} = 0.1354)
Corrections	Lorentz-polarization Absorption (trans. factors: 0.929 - 0.951)

C. Structure Solution and Refinement

Structure Solution	Direct Methods (SHELXT)
Refinement	Full-matrix least-squares on F^2
Function Minimized	Σ w $(Fo^2 - Fc^2)^2$
Least Squares Weights	$w = 1/ [\sigma^2(Fo^2) + (0.1099 \cdot P)^2 + 0.0000 \cdot P]$ 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)	19531
No. Variables	793
Reflection/Parameter Ratio	24.63
Residuals: R1 (I>2.00σ(I))	0.0757
Residuals: R (All reflections)	0.1382
Residuals: wR2 (All reflections)	0.2209
Goodness of Fit Indicator	0.945
Max Shift/Error in Final Cycle	0.001
Maximum peak in Final Diff. Map	1.23 $e^-/Å^3$
Minimum peak in Final Diff. Map	-0.55 $e^-/Å^3$

Table S11-1. Atomic coordinates and B_{iso}/B_{eq}

atom	x	y	z	B_{eq}
Ti1	0.48107(4)	0.07514(3)	0.25411(4)	1.319(14)
Ti2	0.65054(5)	0.29990(4)	0.47561(4)	1.480(15)
Ti3	0.81685(4)	0.25585(3)	0.19045(4)	1.433(15)
Cl1	0.58178(7)	0.09334(5)	0.32349(5)	2.24(2)
Cl2	0.42210(7)	0.00010(5)	0.30188(6)	2.26(2)
Cl3	0.70457(7)	0.23047(5)	0.41751(5)	2.10(2)
Cl4	0.75169(7)	0.33116(6)	0.53902(6)	2.47(2)
Cl5	0.88700(7)	0.19674(5)	0.13181(6)	2.34(2)
Cl6	0.78373(7)	0.19132(5)	0.26341(6)	2.08(2)
O1	0.42014(16)	0.13792(12)	0.26351(13)	1.39(5)
O2	0.63557(17)	0.36217(13)	0.42411(13)	1.58(5)
O3	0.73059(16)	0.26516(13)	0.14145(13)	1.44(5)
N1	0.54732(19)	0.29758(15)	0.25114(16)	1.27(6)
C1	0.5093(2)	0.23923(18)	0.2472(2)	1.32(7)
C2	0.4263(2)	0.24401(18)	0.25743(19)	1.27(7)
C3	0.3826(3)	0.19179(19)	0.26434(19)	1.50(8)
C4	0.3035(2)	0.19508(18)	0.27205(19)	1.23(7)
C5	0.2728(3)	0.2523(2)	0.2748(2)	1.65(8)
C6	0.3141(3)	0.3043(2)	0.2698(2)	1.76(8)
C7	0.3912(3)	0.2985(2)	0.2599(2)	1.76(8)
C8	0.2797(3)	0.3672(2)	0.2740(2)	2.04(9)
C9	0.2893(3)	0.4024(2)	0.2144(3)	3.23(11)
C10	0.3219(3)	0.4003(2)	0.3291(3)	3.54(12)
C11	0.1958(3)	0.3653(2)	0.2833(3)	2.85(10)
C12	0.2541(2)	0.1399(2)	0.2804(2)	1.68(8)
C13	0.2594(3)	0.0969(2)	0.2252(2)	1.94(8)
C14	0.2807(3)	0.1084(2)	0.3415(2)	2.48(9)
C15	0.1693(3)	0.1558(2)	0.2819(2)	2.27(9)
C16	0.4784(3)	0.09386(18)	0.1473(2)	1.38(7)
C17	0.5569(3)	0.09116(19)	0.1696(2)	1.54(8)
C18	0.5738(3)	0.03206(19)	0.1910(2)	1.58(8)
C19	0.5068(3)	-0.00175(19)	0.1811(2)	1.73(8)
C20	0.4473(3)	0.03569(19)	0.1549(2)	1.50(8)
C21	0.4371(3)	0.1461(2)	0.1173(2)	1.93(8)
C22	0.6163(3)	0.1393(2)	0.1662(2)	2.13(9)
C23	0.6503(3)	0.0107(2)	0.2144(2)	2.36(9)
C24	0.4999(3)	-0.0676(2)	0.1921(2)	2.48(9)

Table S11-1. Atomic coordinates and B_{iso}/B_{eq} (continued)

atom	x	y	z	B_{eq}
C25	0.3692(3)	0.0163(2)	0.1314(2)	2.50(9)
C26	0.5634(2)	0.31545(18)	0.31551(19)	1.26(7)
C27	0.5791(2)	0.38069(19)	0.32259(19)	1.39(7)
C28	0.6161(3)	0.40291(19)	0.3782(2)	1.39(7)
C29	0.6340(3)	0.4643(2)	0.3850(2)	1.90(8)
C30	0.6126(3)	0.5009(2)	0.3342(2)	2.12(9)
C31	0.5759(3)	0.4806(2)	0.2789(2)	1.83(8)
C32	0.5598(3)	0.4203(2)	0.2749(2)	1.79(8)
C33	0.5580(3)	0.5239(2)	0.2246(2)	2.74(9)
C34	0.5066(5)	0.4986(3)	0.1751(4)	7.00(18)
C35	0.6333(4)	0.5387(4)	0.1950(4)	6.08(16)
C36	0.5329(4)	0.5832(3)	0.2450(3)	4.38(13)
C37	0.6765(3)	0.4900(2)	0.4438(2)	2.32(9)
C38	0.7578(3)	0.4630(2)	0.4510(2)	2.88(11)
C39	0.6872(4)	0.5576(2)	0.4404(3)	3.96(14)
C40	0.6338(3)	0.4761(2)	0.5008(2)	2.87(10)
C41	0.5240(2)	0.3028(2)	0.5019(2)	1.47(7)
C42	0.5354(3)	0.2454(2)	0.4776(2)	1.81(8)
C43	0.5896(3)	0.2152(2)	0.5178(2)	2.13(9)
C44	0.6129(3)	0.2536(2)	0.5677(2)	2.02(8)
C45	0.5724(3)	0.3082(2)	0.5572(2)	1.71(8)
C46	0.4679(3)	0.3486(2)	0.4756(2)	2.16(9)
C47	0.4905(3)	0.2166(2)	0.4230(2)	2.39(9)
C48	0.6144(3)	0.1513(2)	0.5117(3)	3.05(11)
C49	0.6678(3)	0.2377(3)	0.6211(2)	2.96(10)
C50	0.5755(3)	0.3598(2)	0.6017(2)	2.21(9)
C51	0.6181(2)	0.2962(2)	0.21945(19)	1.36(7)
C52	0.6034(2)	0.29802(18)	0.1498(2)	1.39(7)
C53	0.6614(2)	0.28179(18)	0.11246(19)	1.19(7)
C54	0.6479(3)	0.28041(19)	0.0472(2)	1.57(8)
C55	0.5756(3)	0.2987(2)	0.0226(2)	1.89(8)
C56	0.5174(3)	0.3165(2)	0.0587(2)	1.70(8)
C57	0.5326(3)	0.31592(19)	0.1229(2)	1.45(7)
C58	0.4393(3)	0.3345(3)	0.0277(2)	2.84(9)
C59	0.3857(4)	0.3551(4)	0.0717(3)	5.52(15)
C60	0.4068(4)	0.2787(3)	-0.0072(4)	5.79(15)
C61	0.4479(4)	0.3833(4)	-0.0203(4)	6.37(17)

Table S11-1. Atomic coordinates and B_{iso}/B_{eq} (continued)

atom	x	y	z	B_{eq}
C62	0.7066(3)	0.2574(2)	0.0040(2)	1.88(8)
C63	0.7233(3)	0.1920(2)	0.0188(2)	2.29(9)
C64	0.6769(3)	0.2616(2)	-0.0640(2)	2.79(10)
C65	0.7803(3)	0.2951(2)	0.0120(2)	2.46(9)
C66	0.8344(3)	0.35913(19)	0.1985(2)	1.97(8)
C67	0.9019(3)	0.3349(2)	0.1767(2)	2.36(9)
C68	0.9374(3)	0.2989(2)	0.2250(3)	2.49(10)
C69	0.8933(3)	0.3000(2)	0.2751(2)	1.92(8)
C70	0.8291(2)	0.33754(19)	0.2603(2)	1.53(8)
C71	0.7811(3)	0.4016(2)	0.1638(3)	3.11(11)
C72	0.9343(4)	0.3493(3)	0.1179(3)	4.52(15)
C73	1.0117(3)	0.2651(3)	0.2249(4)	4.79(16)
C74	0.9115(4)	0.2723(3)	0.3372(3)	3.50(12)
C75	0.7737(3)	0.3559(2)	0.3049(2)	2.49(10)

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

Table S11-2. Atomic coordinates and B_{iso} involving hydrogen atoms

atom	x	y	z	B_{iso}
H1A	0.53462	0.21217	0.27871	1.585
H1B	0.51464	0.22164	0.20590	1.585
H5	0.21995	0.25581	0.28043	1.979
H7	0.42030	0.33362	0.25467	2.115
H9A	0.34354	0.40427	0.20719	3.876
H9B	0.26106	0.38238	0.17933	3.876
H9C	0.26944	0.44290	0.21852	3.876
H10A	0.37661	0.40177	0.32346	4.253
H10B	0.30197	0.44099	0.33128	4.253
H10C	0.31402	0.37907	0.36760	4.253
H11A	0.18813	0.34306	0.32122	3.417
H11B	0.17661	0.40612	0.28702	3.417
H11C	0.16823	0.34559	0.24783	3.417
H13A	0.22767	0.06168	0.23081	2.330
H13B	0.24139	0.11720	0.18663	2.330
H13C	0.31258	0.08449	0.22305	2.330
H14A	0.24898	0.07306	0.34668	2.971
H14B	0.33415	0.09617	0.34060	2.971
H14C	0.27603	0.13580	0.37623	2.971
H15A	0.13979	0.11936	0.28723	2.725
H15B	0.16299	0.18306	0.31646	2.725
H15C	0.15102	0.17522	0.24287	2.725
H21A	0.47137	0.18059	0.11812	2.317
H21B	0.42014	0.13615	0.07429	2.317
H21C	0.39262	0.15568	0.13989	2.317
H22A	0.59177	0.17603	0.15015	2.554
H22B	0.64118	0.14659	0.20766	2.554
H22C	0.65447	0.12642	0.13853	2.554
H23A	0.68619	0.04426	0.21662	2.829
H23B	0.64791	-0.00649	0.25576	2.829
H23C	0.66754	-0.01975	0.18627	2.829
H24A	0.44696	-0.08016	0.18153	2.973
H24B	0.53364	-0.08924	0.16611	2.973
H24C	0.51439	-0.07646	0.23579	2.973
H25A	0.33961	0.05098	0.11583	2.998
H25B	0.37272	-0.01263	0.09780	2.998
H25C	0.34387	-0.00237	0.16511	2.998

Table S11-2. Atomic coordinates and B_{iso} involving hydrogens/B_{eq} (continued)

atom	x	y	z	B_{eq}
H26A	0.60808	0.29283	0.33380	1.514
H26B	0.51915	0.30498	0.33881	1.514
H30	0.62393	0.54230	0.33777	2.549
H32	0.53423	0.40534	0.23771	2.150
H34A	0.52584	0.45953	0.16336	8.395
H34B	0.45564	0.49399	0.18961	8.395
H34C	0.50388	0.52529	0.13917	8.395
H35A	0.67013	0.55595	0.22650	7.298
H35B	0.65450	0.50201	0.17869	7.298
H35C	0.62280	0.56734	0.16121	7.298
H36A	0.56923	0.59811	0.27816	5.262
H36B	0.53045	0.61097	0.20998	5.262
H36C	0.48221	0.57967	0.26042	5.262
H38A	0.75420	0.41939	0.45345	3.461
H38B	0.78524	0.47407	0.41522	3.461
H38C	0.78525	0.47829	0.48895	3.461
H39A	0.71452	0.56748	0.40416	4.756
H39B	0.63717	0.57713	0.43689	4.756
H39C	0.71678	0.57148	0.47804	4.756
H40A	0.62637	0.43290	0.50386	3.440
H40B	0.66368	0.49043	0.53810	3.440
H40C	0.58407	0.49607	0.49695	3.440
H46A	0.47174	0.38451	0.50138	2.596
H46B	0.47932	0.35869	0.43331	2.596
H46C	0.41609	0.33234	0.47482	2.596
H47A	0.45651	0.24626	0.40197	2.866
H47B	0.52584	0.20140	0.39403	2.866
H47C	0.46021	0.18359	0.43752	2.866
H48A	0.65262	0.14144	0.54565	3.665
H48B	0.57011	0.12493	0.51336	3.665
H48C	0.63647	0.14591	0.47200	3.665
H49A	0.67439	0.27191	0.64928	3.551
H49B	0.64812	0.20363	0.64317	3.551
H49C	0.71709	0.22724	0.60605	3.551
H50A	0.61413	0.35181	0.63604	2.653
H50B	0.58894	0.39628	0.58024	2.653
H50C	0.52556	0.36479	0.61798	2.653

Table S11-2. Atomic coordinates and B_{iso} involving hydrogens/B_{eq} (continued)

atom	x	y	z	B_{eq}
H51A	0.64678	0.25942	0.23150	1.629
H51B	0.65024	0.33076	0.23326	1.629
H55	0.56547	0.29898	-0.02115	2.264
H57	0.49412	0.32794	0.14853	1.742
H59A	0.37969	0.32407	0.10279	6.624
H59B	0.40552	0.39154	0.09230	6.624
H59C	0.33603	0.36353	0.04938	6.624
H60A	0.44274	0.26517	-0.03639	6.951
H60B	0.39902	0.24682	0.02264	6.951
H60C	0.35786	0.28871	-0.02987	6.951
H61A	0.48356	0.37004	-0.04986	7.649
H61B	0.39808	0.39165	-0.04233	7.649
H61C	0.46758	0.41966	0.00058	7.649
H63A	0.74255	0.18811	0.06240	2.751
H63B	0.67636	0.16862	0.01115	2.751
H63C	0.76179	0.17719	-0.00761	2.751
H64A	0.66565	0.30330	-0.07470	3.352
H64B	0.71567	0.24629	-0.08983	3.352
H64C	0.63024	0.23772	-0.07107	3.352
H65A	0.80132	0.29357	0.05534	2.955
H65B	0.81784	0.27903	-0.01461	2.955
H65C	0.76869	0.33656	0.00037	2.955
H71A	0.73912	0.41140	0.18905	3.734
H71B	0.80869	0.43811	0.15470	3.734
H71C	0.76056	0.38307	0.12495	3.734
H72A	0.98109	0.32617	0.11460	5.420
H72B	0.89720	0.33942	0.08310	5.420
H72C	0.94624	0.39204	0.11680	5.420
H73A	1.03301	0.27051	0.18490	5.750
H73B	1.04793	0.28021	0.25809	5.750
H73C	1.00250	0.22252	0.23165	5.750
H74A	0.86990	0.28033	0.36346	4.196
H74B	0.91754	0.22914	0.33251	4.196
H74C	0.95906	0.28938	0.35651	4.196
H75A	0.73462	0.38170	0.28386	2.992
H75B	0.74943	0.32042	0.32087	2.992
H75C	0.80055	0.37781	0.33931	2.992

Table S11-3. Anisotropic displacement parameters

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Ti1	0.0195(4)	0.0149(4)	0.0157(4)	0.0019(3)	0.0013(3)	0.0001(3)
Ti2	0.0202(4)	0.0212(4)	0.0148(4)	-0.0000(3)	0.0015(3)	0.0003(3)
Ti3	0.0163(4)	0.0178(4)	0.0202(4)	0.0010(3)	0.0006(3)	-0.0023(3)
Cl1	0.0267(6)	0.0328(7)	0.0242(6)	0.0065(5)	-0.0066(5)	-0.0041(5)
Cl2	0.0373(7)	0.0214(6)	0.0281(6)	-0.0002(5)	0.0094(5)	0.0060(5)
Cl3	0.0271(6)	0.0297(6)	0.0238(6)	0.0069(5)	0.0059(5)	-0.0014(5)
Cl4	0.0272(6)	0.0423(7)	0.0229(6)	-0.0042(6)	-0.0050(5)	0.0016(5)
Cl5	0.0252(6)	0.0289(6)	0.0346(7)	0.0073(5)	0.0018(5)	-0.0112(5)
Cl6	0.0257(6)	0.0235(6)	0.0286(6)	-0.0033(5)	-0.0035(5)	0.0059(5)
O1	0.0164(15)	0.0158(15)	0.0207(16)	0.0004(12)	0.0034(13)	0.0008(13)
O2	0.0239(17)	0.0203(16)	0.0156(16)	-0.0018(13)	0.0010(13)	-0.0012(13)
O3	0.0183(16)	0.0170(16)	0.0198(16)	0.0004(13)	0.0040(13)	0.0012(12)
N1	0.0133(18)	0.0169(19)	0.0181(19)	-0.0013(15)	0.0012(15)	-0.0023(15)
C1	0.016(2)	0.012(2)	0.022(2)	0.0006(17)	-0.0008(18)	-0.0028(17)
C2	0.015(2)	0.015(2)	0.017(2)	0.0002(17)	0.0003(18)	-0.0021(17)
C3	0.024(2)	0.022(2)	0.010(2)	0.0047(19)	0.0001(18)	-0.0015(17)
C4	0.017(2)	0.018(2)	0.013(2)	-0.0007(18)	0.0028(17)	-0.0006(17)
C5	0.018(2)	0.026(3)	0.018(2)	0.0037(19)	-0.0008(18)	0.0009(19)
C6	0.022(2)	0.020(2)	0.025(3)	0.006(2)	0.001(2)	-0.0043(19)
C7	0.020(2)	0.019(2)	0.028(3)	-0.0003(19)	0.002(2)	-0.004(2)
C8	0.024(3)	0.018(2)	0.036(3)	0.005(2)	0.007(2)	-0.008(2)
C9	0.043(3)	0.026(3)	0.054(4)	0.016(3)	0.007(3)	0.004(3)
C10	0.044(3)	0.032(3)	0.056(4)	0.014(3)	-0.011(3)	-0.026(3)
C11	0.023(3)	0.029(3)	0.056(4)	0.011(2)	0.005(3)	-0.010(3)
C12	0.014(2)	0.026(2)	0.025(2)	-0.0018(19)	0.0051(19)	-0.002(2)
C13	0.022(2)	0.022(2)	0.030(3)	-0.0032(19)	-0.003(2)	-0.006(2)
C14	0.029(3)	0.034(3)	0.032(3)	0.002(2)	0.005(2)	0.007(2)
C15	0.022(3)	0.035(3)	0.030(3)	0.004(2)	0.004(2)	-0.000(2)
C16	0.020(2)	0.015(2)	0.017(2)	0.0030(18)	0.0020(18)	0.0001(17)
C17	0.023(2)	0.019(2)	0.017(2)	0.0046(19)	0.0064(19)	-0.0042(18)
C18	0.021(2)	0.018(2)	0.021(2)	0.0090(19)	0.0038(19)	0.0014(18)
C19	0.034(3)	0.016(2)	0.017(2)	0.003(2)	0.006(2)	-0.0016(18)
C20	0.023(2)	0.019(2)	0.015(2)	0.0002(19)	0.0023(19)	-0.0011(18)
C21	0.030(3)	0.022(2)	0.020(2)	0.006(2)	-0.002(2)	0.0024(19)
C22	0.020(2)	0.026(3)	0.036(3)	0.000(2)	0.012(2)	0.002(2)
C23	0.026(3)	0.027(3)	0.036(3)	0.015(2)	0.003(2)	0.002(2)
C24	0.047(3)	0.018(2)	0.030(3)	0.003(2)	0.009(2)	-0.002(2)

Table S11-3. Anisotropic displacement parameters (continued)

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
C25	0.032(3)	0.033(3)	0.029(3)	0.000(2)	-0.001(2)	-0.010(2)
C26	0.016(2)	0.018(2)	0.013(2)	-0.0023(17)	0.0002(18)	-0.0024(17)
C27	0.017(2)	0.021(2)	0.016(2)	-0.0001(18)	0.0028(18)	-0.0038(18)
C28	0.021(2)	0.016(2)	0.017(2)	-0.0021(18)	0.0046(18)	0.0013(17)
C29	0.036(3)	0.019(2)	0.018(2)	-0.005(2)	0.002(2)	-0.0033(19)
C30	0.045(3)	0.011(2)	0.025(3)	-0.002(2)	0.007(2)	-0.0048(19)
C31	0.033(3)	0.020(2)	0.017(2)	0.000(2)	0.003(2)	-0.0011(19)
C32	0.025(2)	0.022(2)	0.020(2)	0.005(2)	-0.003(2)	-0.0014(19)
C33	0.055(3)	0.022(2)	0.025(3)	0.004(2)	-0.005(2)	0.0075(19)
C34	0.137(5)	0.049(4)	0.069(4)	-0.018(4)	-0.056(4)	0.010(3)
C35	0.077(3)	0.084(5)	0.074(4)	0.023(3)	0.030(3)	0.037(4)
C36	0.074(4)	0.042(3)	0.047(3)	0.029(3)	-0.013(3)	0.003(2)
C37	0.052(3)	0.016(2)	0.020(2)	-0.011(2)	0.003(2)	-0.0043(19)
C38	0.047(3)	0.035(3)	0.026(3)	-0.026(3)	-0.005(3)	0.003(2)
C39	0.098(5)	0.023(3)	0.029(3)	-0.017(3)	-0.002(3)	-0.007(2)
C40	0.058(4)	0.029(3)	0.022(3)	-0.006(3)	0.003(3)	-0.008(2)
C41	0.016(2)	0.024(2)	0.016(2)	-0.0029(19)	0.0037(18)	0.0042(18)
C42	0.028(3)	0.023(2)	0.020(2)	-0.002(2)	0.012(2)	-0.0023(19)
C43	0.036(3)	0.019(2)	0.027(3)	-0.001(2)	0.009(2)	0.004(2)
C44	0.028(3)	0.032(3)	0.018(2)	0.005(2)	0.009(2)	0.010(2)
C45	0.025(2)	0.023(2)	0.018(2)	0.000(2)	0.009(2)	0.0017(19)
C46	0.018(2)	0.033(3)	0.032(3)	0.003(2)	0.003(2)	-0.002(2)
C47	0.033(3)	0.031(3)	0.028(3)	-0.015(2)	0.008(2)	0.001(2)
C48	0.054(4)	0.026(3)	0.038(3)	0.006(3)	0.018(3)	0.007(2)
C49	0.039(3)	0.043(3)	0.031(3)	0.012(3)	0.006(3)	0.013(2)
C50	0.036(3)	0.037(3)	0.011(2)	0.002(2)	0.003(2)	-0.000(2)
C51	0.016(2)	0.021(2)	0.014(2)	0.0020(18)	0.0006(18)	-0.0022(18)
C52	0.018(2)	0.013(2)	0.021(2)	-0.0006(17)	-0.0058(19)	0.0024(17)
C53	0.015(2)	0.014(2)	0.016(2)	-0.0019(17)	0.0005(18)	0.0013(17)
C54	0.029(3)	0.014(2)	0.017(2)	0.0015(19)	-0.001(2)	0.0029(17)
C55	0.033(3)	0.025(3)	0.014(2)	-0.003(2)	0.002(2)	0.0034(19)
C56	0.021(2)	0.020(2)	0.022(2)	-0.0007(19)	-0.004(2)	0.0017(19)
C57	0.016(2)	0.020(2)	0.018(2)	0.0013(18)	-0.0007(18)	-0.0015(18)
C58	0.022(3)	0.054(3)	0.029(3)	0.007(2)	-0.0103(19)	0.0081(19)
C59	0.047(4)	0.109(5)	0.053(3)	0.030(4)	0.002(3)	-0.003(3)
C60	0.058(4)	0.079(3)	0.077(4)	0.006(3)	-0.031(3)	-0.018(3)
C61	0.062(4)	0.094(4)	0.085(4)	0.020(4)	0.002(3)	0.053(4)

Table S11-3. Anisotropic displacement parameters (continued)

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
C62	0.030(3)	0.028(3)	0.015(2)	0.005(2)	0.006(2)	-0.0010(19)
C63	0.040(3)	0.024(3)	0.023(3)	0.008(2)	0.004(2)	-0.005(2)
C64	0.051(3)	0.039(3)	0.017(2)	0.009(3)	0.009(2)	0.002(2)
C65	0.043(3)	0.025(3)	0.028(3)	0.004(2)	0.018(2)	0.001(2)
C66	0.035(3)	0.011(2)	0.027(3)	-0.008(2)	-0.003(2)	0.0006(19)
C67	0.031(3)	0.030(3)	0.030(3)	-0.019(2)	0.014(2)	-0.006(2)
C68	0.014(2)	0.033(3)	0.047(3)	-0.007(2)	0.001(2)	-0.021(2)
C69	0.021(2)	0.024(2)	0.027(3)	0.001(2)	-0.004(2)	-0.003(2)
C70	0.017(2)	0.018(2)	0.024(2)	-0.0037(18)	0.0042(19)	-0.0054(19)
C71	0.054(4)	0.015(2)	0.046(3)	-0.004(2)	-0.016(3)	0.001(2)
C72	0.056(4)	0.061(4)	0.059(4)	-0.038(3)	0.031(3)	-0.016(3)
C73	0.019(3)	0.075(5)	0.086(5)	0.001(3)	-0.004(3)	-0.042(4)
C74	0.055(4)	0.034(3)	0.039(3)	-0.008(3)	-0.019(3)	0.001(3)
C75	0.026(3)	0.043(3)	0.025(3)	-0.009(2)	0.000(2)	-0.019(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 S11-4. Bond lengths (Å)

atom	atom	distance	atom	atom	distance
Ti1	Cl1	2.2616(14)	Ti1	Cl2	2.2702(14)
Ti1	O1	1.790(3)	Ti1	C16	2.348(4)
Ti1	C17	2.381(5)	Ti1	C18	2.415(5)
Ti1	C19	2.407(4)	Ti1	C20	2.353(4)
Ti2	Cl3	2.2602(15)	Ti2	Cl4	2.2653(15)
Ti2	O2	1.792(3)	Ti2	C41	2.343(4)
Ti2	C42	2.368(5)	Ti2	C43	2.398(5)
Ti2	C44	2.391(5)	Ti2	C45	2.335(5)
Ti3	Cl5	2.2700(15)	Ti3	Cl6	2.2546(15)
Ti3	O3	1.789(3)	Ti3	C66	2.339(4)
Ti3	C67	2.353(5)	Ti3	C68	2.391(5)
Ti3	C69	2.395(5)	Ti3	C70	2.373(4)
O1	C3	1.377(5)	O2	C28	1.371(5)
O3	C53	1.373(5)	N1	C1	1.468(5)
N1	C26	1.456(5)	N1	C51	1.471(6)
C1	C2	1.498(6)	C2	C3	1.415(6)
C2	C7	1.373(6)	C3	C4	1.417(6)
C4	C5	1.394(6)	C4	C12	1.530(6)
C5	C6	1.382(6)	C6	C7	1.395(6)
C6	C8	1.541(6)	C8	C9	1.534(8)
C8	C10	1.542(7)	C8	C11	1.506(7)
C12	C13	1.545(7)	C12	C14	1.540(7)
C12	C15	1.536(6)	C16	C17	1.425(6)
C16	C20	1.428(6)	C16	C21	1.497(6)
C17	C18	1.426(6)	C17	C22	1.506(6)
C18	C19	1.401(6)	C18	C23	1.477(6)
C19	C20	1.422(6)	C19	C24	1.502(6)
C20	C25	1.489(6)	C26	C27	1.493(6)
C27	C28	1.412(6)	C27	C32	1.382(6)
C28	C29	1.417(6)	C29	C30	1.398(6)
C29	C37	1.534(6)	C30	C31	1.390(6)
C31	C32	1.383(6)	C31	C33	1.537(7)
C33	C34	1.456(9)	C33	C35	1.554(10)
C33	C36	1.479(8)	C37	C38	1.547(8)
C37	C39	1.528(7)	C37	C40	1.530(8)
C41	C42	1.411(6)	C41	C45	1.415(6)
C41	C46	1.501(6)	C42	C43	1.409(7)

Table S11-4. Bond lengths (Å) (continued)

atom	atom	distance	atom	atom	distance
C42	C47	1.510(7)	C43	C44	1.416(7)
C43	C48	1.505(7)	C44	C45	1.425(7)
C44	C49	1.486(7)	C45	C50	1.503(7)
C51	C52	1.510(6)	C52	C53	1.402(6)
C52	C57	1.389(6)	C53	C54	1.414(6)
C54	C55	1.398(6)	C54	C62	1.539(7)
C55	C56	1.397(7)	C56	C57	1.395(6)
C56	C58	1.531(7)	C58	C59	1.471(9)
C58	C60	1.546(9)	C58	C61	1.526(10)
C62	C63	1.524(7)	C62	C64	1.523(6)
C62	C65	1.545(7)	C66	C67	1.422(7)
C66	C70	1.434(7)	C66	C71	1.493(7)
C67	C68	1.424(7)	C67	C72	1.475(8)
C68	C69	1.386(7)	C68	C73	1.511(7)
C69	C70	1.423(6)	C69	C74	1.492(7)
C70	C75	1.487(7)			

Table S11-5. Bond lengths involving hydrogens (Å)

atom	atom	distance	atom	atom	distance
C1	H1A	0.990	C1	H1B	0.990
C5	H5	0.950	C7	H7	0.950
C9	H9A	0.980	C9	H9B	0.980
C9	H9C	0.980	C10	H10A	0.980
C10	H10B	0.980	C10	H10C	0.980
C11	H11A	0.980	C11	H11B	0.980
C11	H11C	0.980	C13	H13A	0.980
C13	H13B	0.980	C13	H13C	0.980
C14	H14A	0.980	C14	H14B	0.980
C14	H14C	0.980	C15	H15A	0.980
C15	H15B	0.980	C15	H15C	0.980
C21	H21A	0.980	C21	H21B	0.980
C21	H21C	0.980	C22	H22A	0.980
C22	H22B	0.980	C22	H22C	0.980
C23	H23A	0.980	C23	H23B	0.980
C23	H23C	0.980	C24	H24A	0.980
C24	H24B	0.980	C24	H24C	0.980
C25	H25A	0.980	C25	H25B	0.980
C25	H25C	0.980	C26	H26A	0.990
C26	H26B	0.990	C30	H30	0.950
C32	H32	0.950	C34	H34A	0.980
C34	H34B	0.980	C34	H34C	0.980
C35	H35A	0.980	C35	H35B	0.980
C35	H35C	0.980	C36	H36A	0.980
C36	H36B	0.980	C36	H36C	0.980
C38	H38A	0.980	C38	H38B	0.980
C38	H38C	0.980	C39	H39A	0.980
C39	H39B	0.980	C39	H39C	0.980
C40	H40A	0.980	C40	H40B	0.980
C40	H40C	0.980	C46	H46A	0.980
C46	H46B	0.980	C46	H46C	0.980
C47	H47A	0.980	C47	H47B	0.980
C47	H47C	0.980	C48	H48A	0.980
C48	H48B	0.980	C48	H48C	0.980
C49	H49A	0.980	C49	H49B	0.980
C49	H49C	0.980	C50	H50A	0.980
C50	H50B	0.980	C50	H50C	0.980

Table S11-5. Bond lengths involving hydrogens (Å) (continued)

atom	atom	distance	atom	atom	distance
C51	H51A	0.990	C51	H51B	0.990
C55	H55	0.950	C57	H57	0.950
C59	H59A	0.980	C59	H59B	0.980
C59	H59C	0.980	C60	H60A	0.980
C60	H60B	0.980	C60	H60C	0.980
C61	H61A	0.980	C61	H61B	0.980
C61	H61C	0.980	C63	H63A	0.980
C63	H63B	0.980	C63	H63C	0.980
C64	H64A	0.980	C64	H64B	0.980
C64	H64C	0.980	C65	H65A	0.980
C65	H65B	0.980	C65	H65C	0.980
C71	H71A	0.980	C71	H71B	0.980
C71	H71C	0.980	C72	H72A	0.980
C72	H72B	0.980	C72	H72C	0.980
C73	H73A	0.980	C73	H73B	0.980
C73	H73C	0.980	C74	H74A	0.980
C74	H74B	0.980	C74	H74C	0.980
C75	H75A	0.980	C75	H75B	0.980
C75	H75C	0.980			

Table S11-6. Bond angles (°)

atom	atom	atom	angle	atom	atom	atom	angle
Cl1	Ti1	Cl2	101.11(5)	Cl1	Ti1	O1	103.02(10)
Cl1	Ti1	C16	124.93(11)	Cl1	Ti1	C17	91.49(11)
Cl1	Ti1	C18	85.43(11)	Cl1	Ti1	C19	112.69(12)
Cl1	Ti1	C20	142.96(12)	Cl2	Ti1	O1	103.27(10)
Cl2	Ti1	C16	127.55(11)	Cl2	Ti1	C17	140.26(11)
Cl2	Ti1	C18	108.53(11)	Cl2	Ti1	C19	83.55(11)
Cl2	Ti1	C20	92.76(11)	O1	Ti1	C16	90.52(14)
O1	Ti1	C17	110.38(14)	O1	Ti1	C18	144.82(14)
O1	Ti1	C19	141.68(14)	O1	Ti1	C20	106.95(14)
C16	Ti1	C17	35.07(15)	C16	Ti1	C18	58.15(15)
C16	Ti1	C19	57.98(14)	C16	Ti1	C20	35.37(15)
C17	Ti1	C18	34.59(15)	C17	Ti1	C19	56.93(15)
C17	Ti1	C20	57.93(15)	C18	Ti1	C19	33.78(15)
C18	Ti1	C20	57.55(15)	C19	Ti1	C20	34.74(15)
Cl3	Ti2	Cl4	101.85(6)	Cl3	Ti2	O2	103.64(11)
Cl3	Ti2	C41	127.33(12)	Cl3	Ti2	C42	93.16(12)
Cl3	Ti2	C43	83.66(13)	Cl3	Ti2	C44	108.96(13)
Cl3	Ti2	C45	141.08(12)	Cl4	Ti2	O2	101.75(11)
Cl4	Ti2	C41	123.88(12)	Cl4	Ti2	C42	141.03(12)
Cl4	Ti2	C43	111.52(12)	Cl4	Ti2	C44	83.47(12)
Cl4	Ti2	C45	89.91(12)	O2	Ti2	C41	92.09(15)
O2	Ti2	C42	109.37(15)	O2	Ti2	C43	143.76(16)
O2	Ti2	C44	145.17(16)	O2	Ti2	C45	110.11(15)
C41	Ti2	C42	34.84(16)	C41	Ti2	C43	57.72(16)
C41	Ti2	C44	58.31(16)	C41	Ti2	C45	35.22(15)
C42	Ti2	C43	34.39(16)	C42	Ti2	C44	57.60(16)
C42	Ti2	C45	57.93(16)	C43	Ti2	C44	34.39(16)
C43	Ti2	C45	57.64(16)	C44	Ti2	C45	35.07(16)
Cl5	Ti3	Cl6	101.69(5)	Cl5	Ti3	O3	102.08(11)
Cl5	Ti3	C66	122.97(13)	Cl5	Ti3	C67	89.26(13)
Cl5	Ti3	C68	84.35(13)	Cl5	Ti3	C69	111.91(12)
Cl5	Ti3	C70	141.47(11)	Cl6	Ti3	O3	103.58(10)
Cl6	Ti3	C66	128.52(13)	Cl6	Ti3	C67	140.89(13)
Cl6	Ti3	C68	108.26(14)	Cl6	Ti3	C69	83.66(12)
Cl6	Ti3	C70	93.60(12)	O3	Ti3	C66	91.65(15)
O3	Ti3	C67	110.68(15)	O3	Ti3	C68	145.49(16)
O3	Ti3	C69	143.10(15)	O3	Ti3	C70	108.39(14)

Table S11-6. Bond angles (°) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
C66	Ti3	C67	35.26(18)	C66	Ti3	C68	57.98(17)
C66	Ti3	C69	58.15(16)	C66	Ti3	C70	35.43(16)
C67	Ti3	C68	34.92(17)	C67	Ti3	C69	57.61(17)
C67	Ti3	C70	58.37(17)	C68	Ti3	C69	33.66(18)
C68	Ti3	C70	57.21(16)	C69	Ti3	C70	34.71(15)
Ti1	O1	C3	169.3(3)	Ti2	O2	C28	169.8(3)
Ti3	O3	C53	167.9(3)	C1	N1	C26	110.5(3)
C1	N1	C51	110.7(3)	C26	N1	C51	110.5(3)
N1	C1	C2	111.9(3)	C1	C2	C3	120.1(4)
C1	C2	C7	121.1(4)	C3	C2	C7	118.8(4)
O1	C3	C2	117.3(4)	O1	C3	C4	121.6(4)
C2	C3	C4	121.1(4)	C3	C4	C5	116.1(4)
C3	C4	C12	123.0(4)	C5	C4	C12	120.8(4)
C4	C5	C6	124.3(4)	C5	C6	C7	117.3(4)
C5	C6	C8	123.7(4)	C7	C6	C8	119.0(4)
C2	C7	C6	122.3(4)	C6	C8	C9	110.4(4)
C6	C8	C10	108.6(4)	C6	C8	C11	112.1(4)
C9	C8	C10	109.0(4)	C9	C8	C11	107.8(4)
C10	C8	C11	108.8(4)	C4	C12	C13	109.9(4)
C4	C12	C14	109.7(4)	C4	C12	C15	112.1(4)
C13	C12	C14	110.2(4)	C13	C12	C15	106.5(4)
C14	C12	C15	108.3(4)	Ti1	C16	C17	73.7(2)
Ti1	C16	C20	72.5(2)	Ti1	C16	C21	122.4(3)
C17	C16	C20	107.0(4)	C17	C16	C21	127.0(4)
C20	C16	C21	125.9(4)	Ti1	C17	C16	71.2(3)
Ti1	C17	C18	74.0(3)	Ti1	C17	C22	125.5(3)
C16	C17	C18	108.6(4)	C16	C17	C22	127.5(4)
C18	C17	C22	123.7(4)	Ti1	C18	C17	71.4(3)
Ti1	C18	C19	72.8(3)	Ti1	C18	C23	125.1(3)
C17	C18	C19	107.7(4)	C17	C18	C23	124.8(4)
C19	C18	C23	127.4(4)	Ti1	C19	C18	73.4(3)
Ti1	C19	C20	70.6(2)	Ti1	C19	C24	125.3(3)
C18	C19	C20	108.8(4)	C18	C19	C24	125.9(4)
C20	C19	C24	125.2(4)	Ti1	C20	C16	72.1(2)
Ti1	C20	C19	74.7(2)	Ti1	C20	C25	125.2(3)
C16	C20	C19	108.0(4)	C16	C20	C25	125.3(4)
C19	C20	C25	126.2(4)	N1	C26	C27	112.8(3)

Table S11-6. Bond angles (°) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
C26	C27	C28	120.1(4)	C26	C27	C32	121.3(4)
C28	C27	C32	118.6(4)	O2	C28	C27	116.9(4)
O2	C28	C29	122.2(4)	C27	C28	C29	120.9(4)
C28	C29	C30	116.4(4)	C28	C29	C37	122.6(4)
C30	C29	C37	120.9(4)	C29	C30	C31	124.2(4)
C30	C31	C32	116.9(4)	C30	C31	C33	120.3(4)
C32	C31	C33	122.8(4)	C27	C32	C31	123.0(4)
C31	C33	C34	113.1(5)	C31	C33	C35	108.8(5)
C31	C33	C36	112.6(4)	C34	C33	C35	106.1(6)
C34	C33	C36	112.8(5)	C35	C33	C36	102.6(5)
C29	C37	C38	108.5(4)	C29	C37	C39	112.6(4)
C29	C37	C40	110.8(4)	C38	C37	C39	106.1(5)
C38	C37	C40	110.5(4)	C39	C37	C40	108.2(4)
Ti2	C41	C42	73.5(3)	Ti2	C41	C45	72.1(3)
Ti2	C41	C46	122.3(3)	C42	C41	C45	107.4(4)
C42	C41	C46	126.2(4)	C45	C41	C46	126.3(4)
Ti2	C42	C41	71.6(3)	Ti2	C42	C43	74.0(3)
Ti2	C42	C47	126.7(3)	C41	C42	C43	108.5(4)
C41	C42	C47	126.9(4)	C43	C42	C47	124.1(4)
Ti2	C43	C42	71.6(3)	Ti2	C43	C44	72.5(3)
Ti2	C43	C48	125.3(4)	C42	C43	C44	108.5(4)
C42	C43	C48	126.0(4)	C44	C43	C48	125.3(4)
Ti2	C44	C43	73.1(3)	Ti2	C44	C45	70.3(3)
Ti2	C44	C49	123.1(3)	C43	C44	C45	106.9(4)
C43	C44	C49	125.2(4)	C45	C44	C49	127.8(4)
Ti2	C45	C41	72.7(3)	Ti2	C45	C44	74.6(3)
Ti2	C45	C50	123.7(3)	C41	C45	C44	108.6(4)
C41	C45	C50	126.6(4)	C44	C45	C50	124.5(4)
N1	C51	C52	112.7(3)	C51	C52	C53	119.9(4)
C51	C52	C57	120.0(4)	C53	C52	C57	120.1(4)
O3	C53	C52	117.8(4)	O3	C53	C54	121.3(4)
C52	C53	C54	120.9(4)	C53	C54	C55	116.5(4)
C53	C54	C62	123.4(4)	C55	C54	C62	120.0(4)
C54	C55	C56	123.8(4)	C55	C56	C57	117.8(4)
C55	C56	C58	120.2(4)	C57	C56	C58	122.0(4)
C52	C57	C56	120.8(4)	C56	C58	C59	113.5(5)
C56	C58	C60	106.4(5)	C56	C58	C61	110.6(5)

Table S11-6. Bond angles (°) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
C59	C58	C60	109.9(5)	C59	C58	C61	108.8(6)
C60	C58	C61	107.5(5)	C54	C62	C63	108.7(4)
C54	C62	C64	112.0(4)	C54	C62	C65	110.4(4)
C63	C62	C64	107.8(4)	C63	C62	C65	110.9(4)
C64	C62	C65	107.0(4)	Ti3	C66	C67	72.9(3)
Ti3	C66	C70	73.6(2)	Ti3	C66	C71	121.3(3)
C67	C66	C70	107.6(4)	C67	C66	C71	125.7(5)
C70	C66	C71	126.7(5)	Ti3	C67	C66	71.8(3)
Ti3	C67	C68	74.0(3)	Ti3	C67	C72	124.8(4)
C66	C67	C68	107.4(4)	C66	C67	C72	126.7(5)
C68	C67	C72	125.6(5)	Ti3	C68	C67	71.1(3)
Ti3	C68	C69	73.3(3)	Ti3	C68	C73	122.8(4)
C67	C68	C69	109.0(4)	C67	C68	C73	127.5(5)
C69	C68	C73	123.5(5)	Ti3	C69	C68	73.0(3)
Ti3	C69	C70	71.8(3)	Ti3	C69	C74	125.7(3)
C68	C69	C70	108.6(4)	C68	C69	C74	127.4(5)
C70	C69	C74	123.8(5)	Ti3	C70	C66	71.0(2)
Ti3	C70	C69	73.5(3)	Ti3	C70	C75	126.8(3)
C66	C70	C69	107.3(4)	C66	C70	C75	127.7(4)
C69	C70	C75	124.6(4)				

Table S11-7. Bond angles involving hydrogens (°)

atom	atom	atom	angle	atom	atom	atom	angle
N1	C1	H1A	109.2	N1	C1	H1B	109.2
C2	C1	H1A	109.2	C2	C1	H1B	109.2
H1A	C1	H1B	107.9	C4	C5	H5	117.9
C6	C5	H5	117.9	C2	C7	H7	118.9
C6	C7	H7	118.9	C8	C9	H9A	109.5
C8	C9	H9B	109.5	C8	C9	H9C	109.5
H9A	C9	H9B	109.5	H9A	C9	H9C	109.5
H9B	C9	H9C	109.5	C8	C10	H10A	109.5
C8	C10	H10B	109.5	C8	C10	H10C	109.5
H10A	C10	H10B	109.5	H10A	C10	H10C	109.5
H10B	C10	H10C	109.5	C8	C11	H11A	109.5
C8	C11	H11B	109.5	C8	C11	H11C	109.5
H11A	C11	H11B	109.5	H11A	C11	H11C	109.5
H11B	C11	H11C	109.5	C12	C13	H13A	109.5
C12	C13	H13B	109.5	C12	C13	H13C	109.5
H13A	C13	H13B	109.5	H13A	C13	H13C	109.5
H13B	C13	H13C	109.5	C12	C14	H14A	109.5
C12	C14	H14B	109.5	C12	C14	H14C	109.5
H14A	C14	H14B	109.5	H14A	C14	H14C	109.5
H14B	C14	H14C	109.5	C12	C15	H15A	109.5
C12	C15	H15B	109.5	C12	C15	H15C	109.5
H15A	C15	H15B	109.5	H15A	C15	H15C	109.5
H15B	C15	H15C	109.5	C16	C21	H21A	109.5
C16	C21	H21B	109.5	C16	C21	H21C	109.5
H21A	C21	H21B	109.5	H21A	C21	H21C	109.5
H21B	C21	H21C	109.5	C17	C22	H22A	109.5
C17	C22	H22B	109.5	C17	C22	H22C	109.5
H22A	C22	H22B	109.5	H22A	C22	H22C	109.5
H22B	C22	H22C	109.5	C18	C23	H23A	109.5
C18	C23	H23B	109.5	C18	C23	H23C	109.5
H23A	C23	H23B	109.5	H23A	C23	H23C	109.5
H23B	C23	H23C	109.5	C19	C24	H24A	109.5
C19	C24	H24B	109.5	C19	C24	H24C	109.5
H24A	C24	H24B	109.5	H24A	C24	H24C	109.5
H24B	C24	H24C	109.5	C20	C25	H25A	109.5
C20	C25	H25B	109.5	C20	C25	H25C	109.5
H25A	C25	H25B	109.5	H25A	C25	H25C	109.5

Table S11-7. Bond angles involving hydrogens (°) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
H25B	C25	H25C	109.5	N1	C26	H26A	109.0
N1	C26	H26B	109.0	C27	C26	H26A	109.0
C27	C26	H26B	109.0	H26A	C26	H26B	107.8
C29	C30	H30	117.9	C31	C30	H30	117.9
C27	C32	H32	118.5	C31	C32	H32	118.5
C33	C34	H34A	109.5	C33	C34	H34B	109.5
C33	C34	H34C	109.5	H34A	C34	H34B	109.5
H34A	C34	H34C	109.5	H34B	C34	H34C	109.5
C33	C35	H35A	109.5	C33	C35	H35B	109.5
C33	C35	H35C	109.5	H35A	C35	H35B	109.5
H35A	C35	H35C	109.5	H35B	C35	H35C	109.5
C33	C36	H36A	109.5	C33	C36	H36B	109.5
C33	C36	H36C	109.5	H36A	C36	H36B	109.5
H36A	C36	H36C	109.5	H36B	C36	H36C	109.5
C37	C38	H38A	109.5	C37	C38	H38B	109.5
C37	C38	H38C	109.5	H38A	C38	H38B	109.5
H38A	C38	H38C	109.5	H38B	C38	H38C	109.5
C37	C39	H39A	109.5	C37	C39	H39B	109.5
C37	C39	H39C	109.5	H39A	C39	H39B	109.5
H39A	C39	H39C	109.5	H39B	C39	H39C	109.5
C37	C40	H40A	109.5	C37	C40	H40B	109.5
C37	C40	H40C	109.5	H40A	C40	H40B	109.5
H40A	C40	H40C	109.5	H40B	C40	H40C	109.5
C41	C46	H46A	109.5	C41	C46	H46B	109.5
C41	C46	H46C	109.5	H46A	C46	H46B	109.5
H46A	C46	H46C	109.5	H46B	C46	H46C	109.5
C42	C47	H47A	109.5	C42	C47	H47B	109.5
C42	C47	H47C	109.5	H47A	C47	H47B	109.5
H47A	C47	H47C	109.5	H47B	C47	H47C	109.5
C43	C48	H48A	109.5	C43	C48	H48B	109.5
C43	C48	H48C	109.5	H48A	C48	H48B	109.5
H48A	C48	H48C	109.5	H48B	C48	H48C	109.5
C44	C49	H49A	109.5	C44	C49	H49B	109.5
C44	C49	H49C	109.5	H49A	C49	H49B	109.5
H49A	C49	H49C	109.5	H49B	C49	H49C	109.5
C45	C50	H50A	109.5	C45	C50	H50B	109.5
C45	C50	H50C	109.5	H50A	C50	H50B	109.5

Table S11-7. Bond angles involving hydrogens (°) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
H50A	C50	H50C	109.5	H50B	C50	H50C	109.5
N1	C51	H51A	109.1	N1	C51	H51B	109.1
C52	C51	H51A	109.1	C52	C51	H51B	109.0
H51A	C51	H51B	107.8	C54	C55	H55	118.1
C56	C55	H55	118.1	C52	C57	H57	119.6
C56	C57	H57	119.6	C58	C59	H59A	109.5
C58	C59	H59B	109.5	C58	C59	H59C	109.5
H59A	C59	H59B	109.5	H59A	C59	H59C	109.5
H59B	C59	H59C	109.5	C58	C60	H60A	109.5
C58	C60	H60B	109.5	C58	C60	H60C	109.5
H60A	C60	H60B	109.5	H60A	C60	H60C	109.5
H60B	C60	H60C	109.5	C58	C61	H61A	109.5
C58	C61	H61B	109.5	C58	C61	H61C	109.5
H61A	C61	H61B	109.5	H61A	C61	H61C	109.5
H61B	C61	H61C	109.5	C62	C63	H63A	109.5
C62	C63	H63B	109.5	C62	C63	H63C	109.5
H63A	C63	H63B	109.5	H63A	C63	H63C	109.5
H63B	C63	H63C	109.5	C62	C64	H64A	109.5
C62	C64	H64B	109.5	C62	C64	H64C	109.5
H64A	C64	H64B	109.5	H64A	C64	H64C	109.5
H64B	C64	H64C	109.5	C62	C65	H65A	109.5
C62	C65	H65B	109.5	C62	C65	H65C	109.5
H65A	C65	H65B	109.5	H65A	C65	H65C	109.5
H65B	C65	H65C	109.5	C66	C71	H71A	109.5
C66	C71	H71B	109.5	C66	C71	H71C	109.5
H71A	C71	H71B	109.5	H71A	C71	H71C	109.5
H71B	C71	H71C	109.5	C67	C72	H72A	109.5
C67	C72	H72B	109.5	C67	C72	H72C	109.5
H72A	C72	H72B	109.5	H72A	C72	H72C	109.5
H72B	C72	H72C	109.5	C68	C73	H73A	109.5
C68	C73	H73B	109.5	C68	C73	H73C	109.5
H73A	C73	H73B	109.5	H73A	C73	H73C	109.5
H73B	C73	H73C	109.5	C69	C74	H74A	109.5
C69	C74	H74B	109.5	C69	C74	H74C	109.5
H74A	C74	H74B	109.5	H74A	C74	H74C	109.5
H74B	C74	H74C	109.5	C70	C75	H75A	109.5
C70	C75	H75B	109.5	C70	C75	H75C	109.5

Table S11-7. Bond angles involving hydrogens (°) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
H75A	C75	H75B	109.5	H75A	C75	H75C	109.5
H75B	C75	H75C	109.5				

Table S11-8. Torsion Angles(O)
(Those having bond angles > 160 or < 20 degrees are excluded.)

atom1	atom2	atom3	atom4	angle	atom1	atom2	atom3	atom4	angle
Cl1	Ti1	C16	C17	20.0(2)	Cl1	Ti1	C16	C20	134.27(12)
Cl1	Ti1	C16	C21	-103.8(3)	Cl1	Ti1	C17	C16	-163.67(15)
Cl1	Ti1	C17	C18	79.73(15)	Cl1	Ti1	C17	C22	-40.5(3)
Cl1	Ti1	C18	C17	-99.33(15)	Cl1	Ti1	C18	C19	144.64(17)
Cl1	Ti1	C18	C23	20.6(3)	Cl1	Ti1	C19	C18	-38.70(19)
Cl1	Ti1	C19	C20	-156.26(13)	Cl1	Ti1	C19	C24	83.8(3)
Cl1	Ti1	C20	C16	-77.0(2)	Cl1	Ti1	C20	C19	38.1(3)
Cl1	Ti1	C20	C25	161.91(16)	Cl2	Ti1	C16	C17	-126.37(13)
Cl2	Ti1	C16	C20	-12.1(2)	Cl2	Ti1	C16	C21	109.8(2)
Cl2	Ti1	C17	C16	86.9(2)	Cl2	Ti1	C17	C18	-29.7(3)
Cl2	Ti1	C17	C22	-149.97(19)	Cl2	Ti1	C18	C17	160.48(12)
Cl2	Ti1	C18	C19	44.44(18)	Cl2	Ti1	C18	C23	-79.6(3)
Cl2	Ti1	C19	C18	-138.08(16)	Cl2	Ti1	C19	C20	104.37(17)
Cl2	Ti1	C19	C24	-15.5(3)	Cl2	Ti1	C20	C16	170.39(15)
Cl2	Ti1	C20	C19	-74.52(16)	Cl2	Ti1	C20	C25	49.3(3)
O1	Ti1	C16	C17	126.38(17)	O1	Ti1	C16	C20	-119.39(18)
O1	Ti1	C16	C21	2.5(3)	O1	Ti1	C17	C16	-59.18(19)
O1	Ti1	C17	C18	-175.78(15)	O1	Ti1	C17	C22	64.0(3)
O1	Ti1	C18	C17	6.9(3)	O1	Ti1	C18	C19	-109.2(2)
O1	Ti1	C18	C23	126.8(3)	O1	Ti1	C19	C18	118.6(2)
O1	Ti1	C19	C20	1.1(3)	O1	Ti1	C19	C24	-118.8(3)
O1	Ti1	C20	C16	65.6(2)	O1	Ti1	C20	C19	-179.29(16)
O1	Ti1	C20	C25	-55.5(3)	C16	Ti1	C17	C16	-0.00(17)
C16	Ti1	C17	C18	-116.6(3)	C16	Ti1	C17	C22	123.1(4)
C17	Ti1	C16	C17	-0.00(18)	C17	Ti1	C16	C20	114.2(3)
C17	Ti1	C16	C21	-123.9(4)	C16	Ti1	C18	C17	37.21(16)
C16	Ti1	C18	C19	-78.8(2)	C16	Ti1	C18	C23	157.2(4)
C18	Ti1	C16	C17	-36.70(16)	C18	Ti1	C16	C20	77.53(19)
C18	Ti1	C16	C21	-160.6(3)	C16	Ti1	C19	C18	79.4(2)
C16	Ti1	C19	C20	-38.19(17)	C16	Ti1	C19	C24	-158.1(4)
C19	Ti1	C16	C17	-76.74(19)	C19	Ti1	C16	C20	37.49(17)
C19	Ti1	C16	C21	159.4(3)	C16	Ti1	C20	C16	-0.00(18)
C16	Ti1	C20	C19	115.1(3)	C16	Ti1	C20	C25	-121.1(4)
C20	Ti1	C16	C17	-114.2(3)	C20	Ti1	C16	C20	-0.00(18)
C20	Ti1	C16	C21	121.9(4)	C17	Ti1	C18	C17	-0.00(18)
C17	Ti1	C18	C19	-116.0(3)	C17	Ti1	C18	C23	120.0(4)
C18	Ti1	C17	C16	116.6(3)	C18	Ti1	C17	C18	-0.00(18)

Table S11-8. Torsion angles (°) (continued)

atom1	atom2	atom3	atom4	angle	atom1	atom2	atom3	atom4	angle
C18	Ti1	C17	C22	-120.3(4)	C17	Ti1	C19	C18	37.50(16)
C17	Ti1	C19	C20	-80.1(2)	C17	Ti1	C19	C24	160.1(4)
C19	Ti1	C17	C16	80.0(2)	C19	Ti1	C17	C18	-36.60(16)
C19	Ti1	C17	C22	-156.9(4)	C17	Ti1	C20	C16	-38.19(16)
C17	Ti1	C20	C19	76.9(2)	C17	Ti1	C20	C25	-159.3(4)
C20	Ti1	C17	C16	38.53(16)	C20	Ti1	C17	C18	-78.07(19)
C20	Ti1	C17	C22	161.7(4)	C18	Ti1	C19	C18	0.00(19)
C18	Ti1	C19	C20	-117.6(3)	C18	Ti1	C19	C24	122.6(4)
C19	Ti1	C18	C17	116.0(3)	C19	Ti1	C18	C19	0.00(18)
C19	Ti1	C18	C23	-124.0(4)	C18	Ti1	C20	C16	-79.4(2)
C18	Ti1	C20	C19	35.74(16)	C18	Ti1	C20	C25	159.6(4)
C20	Ti1	C18	C17	79.3(2)	C20	Ti1	C18	C19	-36.77(16)
C20	Ti1	C18	C23	-160.8(4)	C19	Ti1	C20	C16	-115.1(3)
C19	Ti1	C20	C19	-0.00(19)	C19	Ti1	C20	C25	123.8(4)
C20	Ti1	C19	C18	117.6(3)	C20	Ti1	C19	C20	0.00(19)
C20	Ti1	C19	C24	-119.9(4)	Cl3	Ti2	C41	C42	13.0(2)
Cl3	Ti2	C41	C45	128.04(14)	Cl3	Ti2	C41	C46	-109.9(3)
Cl3	Ti2	C42	C41	-169.71(15)	Cl3	Ti2	C42	C43	73.95(17)
Cl3	Ti2	C42	C47	-47.0(3)	Cl3	Ti2	C43	C42	-105.11(18)
Cl3	Ti2	C43	C44	137.84(19)	Cl3	Ti2	C43	C48	16.5(3)
Cl3	Ti2	C44	C43	-44.9(2)	Cl3	Ti2	C44	C45	-160.46(13)
Cl3	Ti2	C44	C49	76.5(3)	Cl3	Ti2	C45	C41	-85.4(2)
Cl3	Ti2	C45	C44	30.2(3)	Cl3	Ti2	C45	C50	151.69(18)
Cl4	Ti2	C41	C42	-132.43(13)	Cl4	Ti2	C41	C45	-17.4(2)
Cl4	Ti2	C41	C46	104.7(3)	Cl4	Ti2	C42	C41	77.0(2)
Cl4	Ti2	C42	C43	-39.3(3)	Cl4	Ti2	C42	C47	-160.23(19)
Cl4	Ti2	C43	C42	154.63(14)	Cl4	Ti2	C43	C44	37.6(2)
Cl4	Ti2	C43	C48	-83.8(3)	Cl4	Ti2	C44	C43	-145.18(18)
Cl4	Ti2	C44	C45	99.22(17)	Cl4	Ti2	C44	C49	-23.8(3)
Cl4	Ti2	C45	C41	165.66(16)	Cl4	Ti2	C45	C44	-78.72(16)
Cl4	Ti2	C45	C50	42.7(3)	O2	Ti2	C41	C42	121.91(18)
O2	Ti2	C41	C45	-123.02(18)	O2	Ti2	C41	C46	-0.9(3)
O2	Ti2	C42	C41	-64.1(2)	O2	Ti2	C42	C43	179.59(16)
O2	Ti2	C42	C47	58.7(3)	O2	Ti2	C43	C42	-0.6(4)
O2	Ti2	C43	C44	-117.7(2)	O2	Ti2	C43	C48	120.9(3)
O2	Ti2	C44	C43	113.6(3)	O2	Ti2	C44	C45	-2.0(4)
O2	Ti2	C44	C49	-125.0(3)	O2	Ti2	C45	C41	63.2(2)

Table S11-8. Torsion angles (°) (continued)

atom1	atom2	atom3	atom4	angle	atom1	atom2	atom3	atom4	angle
O2	Ti2	C45	C44	178.78(16)	O2	Ti2	C45	C50	-59.8(3)
C41	Ti2	C42	C41	-0.00(18)	C41	Ti2	C42	C43	-116.3(3)
C41	Ti2	C42	C47	122.8(4)	C42	Ti2	C41	C42	0.00(19)
C42	Ti2	C41	C45	115.1(3)	C42	Ti2	C41	C46	-122.8(4)
C41	Ti2	C43	C42	37.26(17)	C41	Ti2	C43	C44	-79.8(2)
C41	Ti2	C43	C48	158.9(4)	C43	Ti2	C41	C42	-36.78(17)
C43	Ti2	C41	C45	78.3(2)	C43	Ti2	C41	C46	-159.6(3)
C41	Ti2	C44	C43	77.9(2)	C41	Ti2	C44	C45	-37.68(17)
C41	Ti2	C44	C49	-160.7(4)	C44	Ti2	C41	C42	-77.6(2)
C44	Ti2	C41	C45	37.51(17)	C44	Ti2	C41	C46	159.6(4)
C41	Ti2	C45	C41	0.00(19)	C41	Ti2	C45	C44	115.6(3)
C41	Ti2	C45	C50	-122.9(4)	C45	Ti2	C41	C42	-115.1(3)
C45	Ti2	C41	C45	-0.00(19)	C45	Ti2	C41	C46	122.1(4)
C42	Ti2	C43	C42	-0.0(2)	C42	Ti2	C43	C44	-117.1(4)
C42	Ti2	C43	C48	121.6(5)	C43	Ti2	C42	C41	116.3(3)
C43	Ti2	C42	C43	-0.0(2)	C43	Ti2	C42	C47	-120.9(5)
C42	Ti2	C44	C43	36.57(17)	C42	Ti2	C44	C45	-79.0(2)
C42	Ti2	C44	C49	158.0(4)	C44	Ti2	C42	C41	79.8(2)
C44	Ti2	C42	C43	-36.56(18)	C44	Ti2	C42	C47	-157.5(4)
C42	Ti2	C45	C41	-37.63(17)	C42	Ti2	C45	C44	78.0(2)
C42	Ti2	C45	C50	-160.6(4)	C45	Ti2	C42	C41	38.05(17)
C45	Ti2	C42	C43	-78.3(2)	C45	Ti2	C42	C47	160.8(4)
C43	Ti2	C44	C43	0.0(2)	C43	Ti2	C44	C45	-115.6(3)
C43	Ti2	C44	C49	121.4(5)	C44	Ti2	C43	C42	117.1(4)
C44	Ti2	C43	C44	0.0(2)	C44	Ti2	C43	C48	-121.3(5)
C43	Ti2	C45	C41	-78.5(2)	C43	Ti2	C45	C44	37.08(17)
C43	Ti2	C45	C50	158.5(4)	C45	Ti2	C43	C42	79.2(2)
C45	Ti2	C43	C44	-37.84(18)	C45	Ti2	C43	C48	-159.2(4)
C44	Ti2	C45	C41	-115.6(3)	C44	Ti2	C45	C44	0.00(19)
C44	Ti2	C45	C50	121.5(4)	C45	Ti2	C44	C43	115.6(3)
C45	Ti2	C44	C45	0.00(19)	C45	Ti2	C44	C49	-123.0(5)
Cl5	Ti3	C66	C67	-19.3(2)	Cl5	Ti3	C66	C70	-134.17(14)
Cl5	Ti3	C66	C71	102.5(3)	Cl5	Ti3	C67	C66	163.92(17)
Cl5	Ti3	C67	C68	-81.17(18)	Cl5	Ti3	C67	C72	41.4(3)
Cl5	Ti3	C68	C67	96.84(19)	Cl5	Ti3	C68	C69	-145.6(2)
Cl5	Ti3	C68	C73	-26.2(3)	Cl5	Ti3	C69	C68	37.3(2)
Cl5	Ti3	C69	C70	154.16(14)	Cl5	Ti3	C69	C74	-86.9(3)

Table S11-8. Torsion angles (°) (continued)

atom1	atom2	atom3	atom4	angle	atom1	atom2	atom3	atom4	angle
Cl5	Ti3	C70	C66	75.0(2)	Cl5	Ti3	C70	C69	-40.5(3)
Cl5	Ti3	C70	C75	-161.64(17)	Cl6	Ti3	C66	C67	126.31(15)
Cl6	Ti3	C66	C70	11.4(3)	Cl6	Ti3	C66	C71	-111.9(3)
Cl6	Ti3	C67	C66	-88.3(2)	Cl6	Ti3	C67	C68	26.6(3)
Cl6	Ti3	C67	C72	149.2(2)	Cl6	Ti3	C68	C67	-162.69(15)
Cl6	Ti3	C68	C69	-45.1(2)	Cl6	Ti3	C68	C73	74.3(4)
Cl6	Ti3	C69	C68	137.37(18)	Cl6	Ti3	C69	C70	-105.75(17)
Cl6	Ti3	C69	C74	13.2(3)	Cl6	Ti3	C70	C66	-171.07(14)
Cl6	Ti3	C70	C69	73.42(16)	Cl6	Ti3	C70	C75	-47.7(3)
O3	Ti3	C66	C67	-124.84(19)	O3	Ti3	C66	C70	120.27(19)
O3	Ti3	C66	C71	-3.1(3)	O3	Ti3	C67	C66	61.3(2)
O3	Ti3	C67	C68	176.19(17)	O3	Ti3	C67	C72	-61.2(4)
O3	Ti3	C68	C67	-6.3(4)	O3	Ti3	C68	C69	111.2(3)
O3	Ti3	C68	C73	-129.3(3)	O3	Ti3	C69	C68	-118.4(2)
O3	Ti3	C69	C70	-1.5(4)	O3	Ti3	C69	C74	117.4(3)
O3	Ti3	C70	C66	-65.48(19)	O3	Ti3	C70	C69	179.02(16)
O3	Ti3	C70	C75	57.9(3)	C66	Ti3	C67	C66	-0.0(2)
C66	Ti3	C67	C68	114.9(4)	C66	Ti3	C67	C72	-122.5(5)
C67	Ti3	C66	C67	0.0(2)	C67	Ti3	C66	C70	-114.9(3)
C67	Ti3	C66	C71	121.8(5)	C66	Ti3	C68	C67	-38.14(19)
C66	Ti3	C68	C69	79.4(2)	C66	Ti3	C68	C73	-161.1(4)
C68	Ti3	C66	C67	37.8(2)	C68	Ti3	C66	C70	-77.1(2)
C68	Ti3	C66	C71	159.5(4)	C66	Ti3	C69	C68	-78.9(2)
C66	Ti3	C69	C70	38.02(19)	C66	Ti3	C69	C74	157.0(4)
C69	Ti3	C66	C67	77.7(2)	C69	Ti3	C66	C70	-37.24(18)
C69	Ti3	C66	C71	-160.6(4)	C66	Ti3	C70	C66	-0.0(2)
C66	Ti3	C70	C69	-115.5(3)	C66	Ti3	C70	C75	123.3(4)
C70	Ti3	C66	C67	114.9(3)	C70	Ti3	C66	C70	-0.00(17)
C70	Ti3	C66	C71	-123.3(5)	C67	Ti3	C68	C67	-0.0(2)
C67	Ti3	C68	C69	117.5(4)	C67	Ti3	C68	C73	-123.0(5)
C68	Ti3	C67	C66	-114.9(4)	C68	Ti3	C67	C68	-0.0(2)
C68	Ti3	C67	C72	122.6(5)	C67	Ti3	C69	C68	-36.95(19)
C67	Ti3	C69	C70	79.9(2)	C67	Ti3	C69	C74	-161.1(4)
C69	Ti3	C67	C66	-79.3(2)	C69	Ti3	C67	C68	35.59(18)
C69	Ti3	C67	C72	158.2(4)	C67	Ti3	C70	C66	37.96(17)
C67	Ti3	C70	C69	-77.5(2)	C67	Ti3	C70	C75	161.3(4)
C70	Ti3	C67	C66	-38.14(17)	C70	Ti3	C67	C68	76.8(2)

Table S11-8. Torsion angles (°) (continued)

atom1	atom2	atom3	atom4	angle	atom1	atom2	atom3	atom4	angle
C70	Ti3	C67	C72	-160.6(4)	C68	Ti3	C69	C68	-0.0(2)
C68	Ti3	C69	C70	116.9(4)	C68	Ti3	C69	C74	-124.2(5)
C69	Ti3	C68	C67	-117.5(4)	C69	Ti3	C68	C69	-0.0(2)
C69	Ti3	C68	C73	119.5(5)	C68	Ti3	C70	C66	79.5(2)
C68	Ti3	C70	C69	-36.02(19)	C68	Ti3	C70	C75	-157.2(4)
C70	Ti3	C68	C67	-80.4(2)	C70	Ti3	C68	C69	37.17(18)
C70	Ti3	C68	C73	156.6(4)	C69	Ti3	C70	C66	115.5(3)
C69	Ti3	C70	C69	0.0(2)	C69	Ti3	C70	C75	-121.2(4)
C70	Ti3	C69	C68	-116.9(3)	C70	Ti3	C69	C70	0.00(19)
C70	Ti3	C69	C74	118.9(5)	C1	N1	C26	C27	-162.1(3)
C26	N1	C1	C2	78.1(4)	C1	N1	C51	C52	76.0(4)
C51	N1	C1	C2	-159.2(3)	C26	N1	C51	C52	-161.2(3)
C51	N1	C26	C27	75.0(4)	N1	C1	C2	C3	-170.9(3)
N1	C1	C2	C7	9.5(5)	C1	C2	C3	O1	2.3(6)
C1	C2	C3	C4	-178.0(3)	C1	C2	C7	C6	-179.5(4)
C3	C2	C7	C6	0.9(6)	C7	C2	C3	O1	-178.1(4)
C7	C2	C3	C4	1.7(6)	O1	C3	C4	C5	177.3(3)
O1	C3	C4	C12	0.4(6)	C2	C3	C4	C5	-2.4(6)
C2	C3	C4	C12	-179.3(3)	C3	C4	C5	C6	0.8(6)
C3	C4	C12	C13	-56.7(5)	C3	C4	C12	C14	64.7(5)
C3	C4	C12	C15	-174.9(3)	C5	C4	C12	C13	126.6(4)
C5	C4	C12	C14	-112.1(4)	C5	C4	C12	C15	8.3(5)
C12	C4	C5	C6	177.8(3)	C4	C5	C6	C7	1.6(6)
C4	C5	C6	C8	-179.0(4)	C5	C6	C7	C2	-2.5(6)
C5	C6	C8	C9	-120.9(4)	C5	C6	C8	C10	119.6(4)
C5	C6	C8	C11	-0.7(6)	C7	C6	C8	C9	58.5(5)
C7	C6	C8	C10	-61.0(5)	C7	C6	C8	C11	178.7(4)
C8	C6	C7	C2	178.1(4)	Ti1	C16	C17	Ti1	0.000(17)
Ti1	C16	C17	C18	65.0(3)	Ti1	C16	C17	C22	-120.8(4)
Ti1	C16	C20	Ti1	-0.000(18)	Ti1	C16	C20	C19	-66.7(2)
Ti1	C16	C20	C25	121.0(4)	C17	C16	C20	Ti1	66.2(3)
C17	C16	C20	C19	-0.4(5)	C17	C16	C20	C25	-172.8(4)
C20	C16	C17	Ti1	-65.4(3)	C20	C16	C17	C18	-0.4(5)
C20	C16	C17	C22	173.8(4)	C21	C16	C17	Ti1	118.7(5)
C21	C16	C17	C18	-176.3(4)	C21	C16	C17	C22	-2.1(7)
C21	C16	C20	Ti1	-117.8(4)	C21	C16	C20	C19	175.5(4)
C21	C16	C20	C25	3.2(7)	Ti1	C17	C18	Ti1	-0.000(18)

Table S11-8. Torsion angles (°) (continued)

atom1	atom2	atom3	atom4	angle	atom1	atom2	atom3	atom4	angle
Ti1	C17	C18	C19	64.3(3)	Ti1	C17	C18	C23	-120.3(4)
C16	C17	C18	Ti1	-63.2(3)	C16	C17	C18	C19	1.1(5)
C16	C17	C18	C23	176.5(4)	C22	C17	C18	Ti1	122.3(4)
C22	C17	C18	C19	-173.4(4)	C22	C17	C18	C23	2.0(7)
Ti1	C18	C19	Ti1	-0.000(19)	Ti1	C18	C19	C20	62.1(3)
Ti1	C18	C19	C24	-121.8(4)	C17	C18	C19	Ti1	-63.4(3)
C17	C18	C19	C20	-1.3(5)	C17	C18	C19	C24	174.8(4)
C23	C18	C19	Ti1	121.4(5)	C23	C18	C19	C20	-176.6(4)
C23	C18	C19	C24	-0.5(7)	Ti1	C19	C20	Ti1	0.000(19)
Ti1	C19	C20	C16	64.9(2)	Ti1	C19	C20	C25	-122.8(4)
C18	C19	C20	Ti1	-63.9(3)	C18	C19	C20	C16	1.1(5)
C18	C19	C20	C25	173.4(4)	C24	C19	C20	Ti1	120.0(5)
C24	C19	C20	C16	-175.0(4)	C24	C19	C20	C25	-2.8(7)
N1	C26	C27	C28	-162.1(3)	N1	C26	C27	C32	16.2(5)
C26	C27	C28	O2	-0.5(6)	C26	C27	C28	C29	177.7(3)
C26	C27	C32	C31	-177.5(4)	C28	C27	C32	C31	0.8(7)
C32	C27	C28	O2	-178.9(4)	C32	C27	C28	C29	-0.7(6)
O2	C28	C29	C30	178.5(4)	O2	C28	C29	C37	0.2(7)
C27	C28	C29	C30	0.3(6)	C27	C28	C29	C37	-177.9(4)
C28	C29	C30	C31	-0.1(7)	C28	C29	C37	C38	64.2(6)
C28	C29	C37	C39	-178.6(4)	C28	C29	C37	C40	-57.3(6)
C30	C29	C37	C38	-113.9(5)	C30	C29	C37	C39	3.2(7)
C30	C29	C37	C40	124.5(5)	C37	C29	C30	C31	178.1(4)
C29	C30	C31	C32	0.3(7)	C29	C30	C31	C33	-177.2(4)
C30	C31	C32	C27	-0.7(7)	C30	C31	C33	C34	-168.5(4)
C30	C31	C33	C35	73.9(5)	C30	C31	C33	C36	-39.2(6)
C32	C31	C33	C34	14.1(7)	C32	C31	C33	C35	-103.5(5)
C32	C31	C33	C36	143.4(4)	C33	C31	C32	C27	176.8(4)
Ti2	C41	C42	Ti2	-0.00(2)	Ti2	C41	C42	C43	65.3(3)
Ti2	C41	C42	C47	-122.5(4)	Ti2	C41	C45	Ti2	-0.00(2)
Ti2	C41	C45	C44	-66.5(3)	Ti2	C41	C45	C50	119.5(4)
C42	C41	C45	Ti2	65.6(3)	C42	C41	C45	C44	-1.0(5)
C42	C41	C45	C50	-174.9(4)	C45	C41	C42	Ti2	-64.6(3)
C45	C41	C42	C43	0.7(5)	C45	C41	C42	C47	172.9(4)
C46	C41	C42	Ti2	118.3(5)	C46	C41	C42	C43	-176.4(4)
C46	C41	C42	C47	-4.2(7)	C46	C41	C45	Ti2	-117.3(5)
C46	C41	C45	C44	176.2(4)	C46	C41	C45	C50	2.2(7)

Table S11-8. Torsion angles (°) (continued)

atom1	atom2	atom3	atom4	angle	atom1	atom2	atom3	atom4	angle
Ti2	C42	C43	Ti2	-0.00(2)	Ti2	C42	C43	C44	63.6(3)
Ti2	C42	C43	C48	-120.7(4)	C41	C42	C43	Ti2	-63.8(3)
C41	C42	C43	C44	-0.2(5)	C41	C42	C43	C48	175.5(4)
C47	C42	C43	Ti2	123.8(5)	C47	C42	C43	C44	-172.6(4)
C47	C42	C43	C48	3.0(8)	Ti2	C43	C44	Ti2	0.00(2)
Ti2	C43	C44	C45	62.6(3)	Ti2	C43	C44	C49	-118.9(4)
C42	C43	C44	Ti2	-63.0(4)	C42	C43	C44	C45	-0.5(5)
C42	C43	C44	C49	178.0(4)	C48	C43	C44	Ti2	121.3(5)
C48	C43	C44	C45	-176.2(4)	C48	C43	C44	C49	2.3(8)
Ti2	C44	C45	Ti2	0.00(2)	Ti2	C44	C45	C41	65.3(3)
Ti2	C44	C45	C50	-120.6(4)	C43	C44	C45	Ti2	-64.4(3)
C43	C44	C45	C41	0.9(5)	C43	C44	C45	C50	175.0(4)
C49	C44	C45	Ti2	117.1(5)	C49	C44	C45	C41	-177.6(4)
C49	C44	C45	C50	-3.5(8)	N1	C51	C52	C53	-163.6(3)
N1	C51	C52	C57	16.6(5)	C51	C52	C53	O3	-0.6(6)
C51	C52	C53	C54	177.0(3)	C51	C52	C57	C56	-178.4(3)
C53	C52	C57	C56	1.8(6)	C57	C52	C53	O3	179.2(3)
C57	C52	C53	C54	-3.2(6)	O3	C53	C54	C55	-179.6(3)
O3	C53	C54	C62	3.4(6)	C52	C53	C54	C55	2.9(6)
C52	C53	C54	C62	-174.1(3)	C53	C54	C55	C56	-1.4(6)
C53	C54	C62	C63	61.3(5)	C53	C54	C62	C64	-179.6(4)
C53	C54	C62	C65	-60.5(5)	C55	C54	C62	C63	-115.6(4)
C55	C54	C62	C64	3.5(6)	C55	C54	C62	C65	122.6(4)
C62	C54	C55	C56	175.7(4)	C54	C55	C56	C57	0.0(7)
C54	C55	C56	C58	-178.7(4)	C55	C56	C57	C52	-0.2(6)
C55	C56	C58	C59	-176.9(4)	C55	C56	C58	C60	62.1(5)
C55	C56	C58	C61	-54.3(6)	C57	C56	C58	C59	4.5(7)
C57	C56	C58	C60	-116.5(4)	C57	C56	C58	C61	127.0(4)
C58	C56	C57	C52	178.5(4)	Ti3	C66	C67	Ti3	0.00(2)
Ti3	C66	C67	C68	-66.0(3)	Ti3	C66	C67	C72	120.3(4)
Ti3	C66	C70	Ti3	0.000(18)	Ti3	C66	C70	C69	65.1(2)
Ti3	C66	C70	C75	-122.3(4)	C67	C66	C70	Ti3	-65.5(3)
C67	C66	C70	C69	-0.4(5)	C67	C66	C70	C75	172.2(4)
C70	C66	C67	Ti3	65.9(3)	C70	C66	C67	C68	-0.1(5)
C70	C66	C67	C72	-173.8(4)	C71	C66	C67	Ti3	-116.6(5)
C71	C66	C67	C68	177.4(4)	C71	C66	C67	C72	3.7(7)
C71	C66	C70	Ti3	117.1(5)	C71	C66	C70	C69	-177.8(4)

Table S11-8. Torsion angles (°) (continued)

atom1	atom2	atom3	atom4	angle	atom1	atom2	atom3	atom4	angle
C71	C66	C70	C75	-5.2(7)	Ti3	C67	C68	Ti3	0.00(2)
Ti3	C67	C68	C69	-64.0(3)	Ti3	C67	C68	C73	117.3(5)
C66	C67	C68	Ti3	64.5(3)	C66	C67	C68	C69	0.6(5)
C66	C67	C68	C73	-178.2(4)	C72	C67	C68	Ti3	-121.7(5)
C72	C67	C68	C69	174.4(5)	C72	C67	C68	C73	-4.4(8)
Ti3	C68	C69	Ti3	-0.000(18)	Ti3	C68	C69	C70	-63.4(3)
Ti3	C68	C69	C74	122.3(4)	C67	C68	C69	Ti3	62.5(3)
C67	C68	C69	C70	-0.8(5)	C67	C68	C69	C74	-175.2(4)
C73	C68	C69	Ti3	-118.7(5)	C73	C68	C69	C70	178.0(4)
C73	C68	C69	C74	3.6(8)	Ti3	C69	C70	Ti3	0.00(2)
Ti3	C69	C70	C66	-63.4(2)	Ti3	C69	C70	C75	123.7(4)
C68	C69	C70	Ti3	64.2(3)	C68	C69	C70	C66	0.8(5)
C68	C69	C70	C75	-172.2(4)	C74	C69	C70	Ti3	-121.2(5)
C74	C69	C70	C66	175.4(4)	C74	C69	C70	C75	2.4(7)

Table S11-9. Intramolecular contacts less than 3.60 Å

atom	atom	distance	atom	atom	distance
Cl1	C23	3.308(5)	Cl2	C24	3.221(5)
Cl3	C48	3.220(6)	Cl4	C38	3.522(6)
Cl4	C49	3.188(6)	Cl4	C50	3.544(5)
Cl5	C72	3.538(7)	Cl5	C73	3.237(6)
Cl6	C74	3.209(6)	O1	C1	2.798(5)
O1	C12	2.973(5)	O1	C13	3.021(5)
O1	C14	3.162(6)	O1	C21	3.211(5)
O2	C26	2.783(5)	O2	C37	2.976(5)
O2	C38	3.138(6)	O2	C40	3.048(6)
O2	C46	3.252(6)	O3	C22	3.531(6)
O3	C51	2.795(5)	O3	C62	2.978(5)
O3	C63	3.116(6)	O3	C65	3.081(6)
O3	C71	3.209(6)	N1	C7	2.768(6)
N1	C32	2.802(6)	N1	C57	2.799(6)
C1	C22	3.492(7)	C1	C52	3.085(6)
C1	C57	3.250(6)	C2	C5	2.763(6)
C2	C26	3.073(6)	C3	C6	2.799(6)
C3	C13	3.102(6)	C3	C14	3.162(7)
C3	C21	3.553(6)	C4	C7	2.809(6)
C5	C10	3.599(7)	C5	C11	2.885(7)
C5	C14	3.533(7)	C5	C15	2.838(7)
C7	C9	3.049(7)	C7	C10	3.039(7)
C7	C26	3.186(6)	C13	C25	3.431(7)
C21	C22	3.243(7)	C21	C25	3.169(7)
C22	C23	3.104(7)	C22	C52	3.581(6)
C22	C53	3.513(6)	C23	C24	3.178(7)
C24	C25	3.167(7)	C26	C47	3.530(7)
C27	C30	2.765(6)	C27	C51	3.050(6)
C27	C75	3.520(7)	C28	C31	2.813(6)
C28	C38	3.136(7)	C28	C40	3.114(7)
C28	C75	3.471(7)	C29	C32	2.801(6)
C30	C35	3.183(9)	C30	C36	2.940(8)
C30	C38	3.543(7)	C30	C39	2.850(7)
C32	C34	2.879(9)	C32	C35	3.476(9)
C32	C51	3.230(6)	C46	C47	3.205(7)
C46	C50	3.201(6)	C47	C48	3.142(7)
C48	C49	3.144(7)	C49	C50	3.189(7)

Table S11-9. Intramolecular contacts less than 3.60 Å (continued)

atom	atom	distance	atom	atom	distance
C51	C75	3.443(6)	C52	C55	2.759(6)
C53	C56	2.807(6)	C53	C63	3.118(6)
C53	C65	3.157(7)	C53	C71	3.532(7)
C54	C57	2.827(6)	C55	C60	3.018(9)
C55	C61	3.025(9)	C55	C63	3.536(7)
C55	C64	2.818(7)	C57	C59	2.863(8)
C57	C60	3.534(8)	C71	C72	3.173(9)
C71	C75	3.236(8)	C72	C73	3.204(9)
C73	C74	3.126(9)	C74	C75	3.096(8)

Table S11-10. Intramolecular contacts less than 3.60 Å involving hydrogens

atom	atom	distance	atom	atom	distance
Ti1	H1A	3.243	Ti1	H1B	3.510
Ti1	H13C	2.990	Ti1	H14B	3.350
Ti1	H21C	3.340	Ti1	H22B	3.461
Ti1	H23B	3.455	Ti1	H24C	3.476
Ti1	H25C	3.431	Ti2	H26A	3.104
Ti2	H38A	3.297	Ti2	H40A	3.079
Ti2	H46B	3.343	Ti2	H47B	3.486
Ti2	H48C	3.460	Ti2	H49C	3.384
Ti2	H50B	3.375	Ti3	H51A	3.192
Ti3	H51B	3.566	Ti3	H63A	3.332
Ti3	H65A	3.037	Ti3	H71C	3.299
Ti3	H72B	3.386	Ti3	H73C	3.394
Ti3	H74B	3.472	Ti3	H75B	3.471
Cl1	H1A	2.930	Cl1	H22B	3.042
Cl1	H23A	3.264	Cl1	H23B	2.966
Cl1	H47B	3.069	Cl1	H48C	3.485
Cl2	H13C	3.106	Cl2	H14B	2.819
Cl2	H24A	3.227	Cl2	H24C	2.831
Cl2	H25C	3.161	Cl3	H26A	2.758
Cl3	H47B	3.208	Cl3	H48A	3.598
Cl3	H48C	2.580	Cl3	H74A	3.412
Cl3	H75B	3.057	Cl4	H38A	2.713
Cl4	H38C	3.536	Cl4	H40A	3.217
Cl4	H49A	3.140	Cl4	H49C	2.837
Cl4	H50A	3.367	Cl4	H50B	3.398
Cl5	H63A	2.848	Cl5	H65A	3.050
Cl5	H72A	3.375	Cl5	H72B	3.376
Cl5	H73A	3.186	Cl5	H73C	2.898
Cl6	H22B	2.870	Cl6	H51A	2.885
Cl6	H74A	3.228	Cl6	H74B	2.811
Cl6	H75B	3.226	O1	H1A	2.611
O1	H1B	2.861	O1	H13B	3.463
O1	H13C	2.345	O1	H14B	2.525
O1	H21A	3.482	O1	H21C	2.711
O1	H47B	3.549	O2	H26A	2.513
O2	H26B	2.935	O2	H38A	2.485
O2	H40A	2.360	O2	H40C	3.543

Table S11-10. Intramolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
O2	H46A	3.487	O2	H46B	2.772
O2	H75B	3.262	O2	H75C	3.579
O3	H22A	3.172	O3	H22B	3.459
O3	H22C	3.383	O3	H51A	2.545
O3	H51B	2.930	O3	H63A	2.453
O3	H65A	2.413	O3	H65C	3.563
O3	H71A	3.435	O3	H71C	2.724
N1	H7	2.382	N1	H32	2.441
N1	H57	2.435	C1	H7	2.644
C1	H21A	3.112	C1	H21C	3.510
C1	H22A	3.007	C1	H22B	3.280
C1	H26A	2.726	C1	H26B	2.466
C1	H47A	3.557	C1	H47B	3.281
C1	H51A	2.511	C1	H51B	3.250
C1	H57	2.915	C2	H21A	3.487
C2	H21C	3.240	C2	H26B	2.675
C2	H47A	3.133	C2	H47B	3.444
C2	H57	3.316	C3	H1A	2.704
C3	H1B	2.817	C3	H5	3.244
C3	H7	3.257	C3	H13B	3.330
C3	H13C	2.813	C3	H14B	2.878
C3	H14C	3.424	C3	H21C	2.835
C3	H47A	3.380	C4	H13A	3.363
C4	H13B	2.706	C4	H13C	2.706
C4	H14A	3.357	C4	H14B	2.697
C4	H14C	2.697	C4	H15A	3.380
C4	H15B	2.738	C4	H15C	2.738
C4	H21C	3.491	C5	H7	3.229
C5	H9B	3.570	C5	H10C	3.520
C5	H11A	2.759	C5	H11C	2.812
C5	H13B	3.597	C5	H14C	3.410
C5	H15B	2.691	C5	H15C	2.792
C6	H9A	2.692	C6	H9B	2.733
C6	H9C	3.370	C6	H10A	2.668
C6	H10B	3.355	C6	H10C	2.702
C6	H11A	2.706	C6	H11B	3.369
C6	H11C	2.732	C7	H1A	3.179

Table S11-10. Intramolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
C7	H1B	3.079	C7	H5	3.225
C7	H9A	2.731	C7	H9B	3.337
C7	H10A	2.715	C7	H10C	3.328
C7	H26B	2.714	C7	H32	3.534
C7	H47A	3.402	C7	H57	3.204
C7	H59A	3.441	C8	H5	2.717
C8	H7	2.651	C9	H7	2.847
C9	H10A	2.708	C9	H10B	2.668
C9	H10C	3.353	C9	H11A	3.314
C9	H11B	2.633	C9	H11C	2.634
C9	H59A	3.478	C9	H59B	3.484
C10	H7	2.880	C10	H9A	2.701
C10	H9B	3.355	C10	H9C	2.671
C10	H11A	2.672	C10	H11B	2.643
C10	H11C	3.333	C10	H46B	3.546
C11	H5	2.492	C11	H9A	3.309
C11	H9B	2.640	C11	H9C	2.640
C11	H10A	3.326	C11	H10B	2.666
C11	H10C	2.666	C12	H5	2.666
C13	H14A	2.708	C13	H14B	2.726
C13	H14C	3.376	C13	H15A	2.638
C13	H15B	3.329	C13	H15C	2.643
C13	H21C	3.371	C13	H25A	3.036
C13	H25C	3.028	C14	H13A	2.710
C14	H13B	3.375	C14	H13C	2.726
C14	H15A	2.664	C14	H15B	2.682
C14	H15C	3.346	C15	H5	2.412
C15	H13A	2.630	C15	H13B	2.656
C15	H13C	3.327	C15	H14A	2.654
C15	H14B	3.345	C15	H14C	2.694
C16	H1B	3.175	C16	H13C	3.470
C16	H22A	2.711	C16	H22B	3.266
C16	H22C	3.202	C16	H25A	2.658
C16	H25B	3.156	C16	H25C	3.248
C17	H1B	3.133	C17	H21A	2.691
C17	H21B	3.199	C17	H21C	3.246
C17	H23A	2.631	C17	H23B	3.214

Table S11-10. Intramolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
C17	H23C	3.158	C18	H22A	3.367
C18	H22B	2.837	C18	H22C	2.837
C18	H24A	3.356	C18	H24B	2.848
C18	H24C	2.848	C19	H23A	3.346
C19	H23B	2.847	C19	H23C	2.847
C19	H25A	3.368	C19	H25B	2.857
C19	H25C	2.857	C20	H13C	3.094
C20	H21A	3.378	C20	H21B	2.865
C20	H21C	2.865	C20	H24A	2.659
C20	H24B	3.184	C20	H24C	3.230
C21	H1B	2.823	C21	H13C	3.576
C21	H22A	2.834	C21	H25A	2.733
C21	H60B	3.086	C22	H1A	3.356
C22	H1B	2.757	C22	H21A	2.826
C22	H23A	2.648	C22	H51A	3.068
C22	H63A	3.467	C23	H22B	3.051
C23	H22C	3.074	C23	H24B	3.156
C23	H24C	3.151	C24	H23B	3.155
C24	H23C	3.150	C24	H25B	3.150
C24	H25C	3.120	C25	H13A	3.573
C25	H13B	3.471	C25	H13C	2.757
C25	H21B	3.120	C25	H21C	3.154
C25	H24A	2.733	C26	H1A	2.486
C26	H1B	3.233	C26	H7	2.770
C26	H32	2.649	C26	H46B	3.205
C26	H47A	3.167	C26	H47B	3.170
C26	H51A	2.737	C26	H51B	2.467
C26	H75A	3.477	C26	H75B	3.266
C27	H7	3.222	C27	H10A	3.593
C27	H46B	3.127	C27	H51B	2.640
C27	H75A	2.927	C27	H75B	3.289
C28	H26A	2.647	C28	H26B	2.865
C28	H30	3.250	C28	H32	3.258
C28	H38A	2.832	C28	H38B	3.409
C28	H40A	2.794	C28	H40C	3.396
C28	H46B	2.945	C28	H75A	3.076
C28	H75B	3.308	C28	H75C	3.464

Table S11-10. Intramolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
C29	H38A	2.675	C29	H38B	2.694
C29	H38C	3.352	C29	H39A	2.724
C29	H39B	2.765	C29	H39C	3.384
C29	H40A	2.683	C29	H40B	3.365
C29	H40C	2.741	C29	H75A	3.466
C30	H32	3.221	C30	H35A	2.896
C30	H35B	3.509	C30	H36A	2.578
C30	H36C	3.212	C30	H38B	3.429
C30	H39A	2.697	C30	H39B	2.809
C31	H34A	2.625	C31	H34B	2.760
C31	H34C	3.335	C31	H35A	2.682
C31	H35B	2.712	C31	H35C	3.362
C31	H36A	2.635	C31	H36B	3.346
C31	H36C	2.773	C31	H75A	3.558
C32	H7	3.130	C32	H10A	3.496
C32	H26A	3.213	C32	H26B	3.044
C32	H30	3.216	C32	H34A	2.594
C32	H34B	2.988	C32	H35B	3.325
C32	H51B	2.759	C32	H57	3.547
C32	H75A	3.184	C33	H30	2.656
C33	H32	2.708	C34	H32	2.516
C34	H35A	3.258	C34	H35B	2.596
C34	H35C	2.596	C34	H36A	3.279
C34	H36B	2.652	C34	H36C	2.652
C34	H59B	3.406	C35	H30	3.112
C35	H34A	2.640	C35	H34B	3.273
C35	H34C	2.504	C35	H36A	2.575
C35	H36B	2.470	C35	H36C	3.247
C35	H71A	3.413	C36	H30	2.627
C36	H34A	3.284	C36	H34B	2.646
C36	H34C	2.646	C36	H35A	2.554
C36	H35B	3.234	C36	H35C	2.531
C37	H30	2.674	C38	H39A	2.639
C38	H39B	3.320	C38	H39C	2.616
C38	H40A	2.747	C38	H40B	2.683
C38	H40C	3.373	C38	H75C	3.220
C39	H30	2.426	C39	H38A	3.317

Table S11-10. Intramolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
C39	H38B	2.632	C39	H38C	2.633
C39	H40A	3.330	C39	H40B	2.657
C39	H40C	2.657	C40	H38A	2.741
C40	H38B	3.370	C40	H38C	2.697
C40	H39A	3.330	C40	H39B	2.657
C40	H39C	2.657	C40	H46A	3.513
C40	H50B	2.648	C41	H26B	3.527
C41	H40A	3.424	C41	H47A	2.696
C41	H47B	3.261	C41	H47C	3.174
C41	H50A	3.376	C41	H50B	2.872
C41	H50C	2.872	C42	H26B	3.280
C42	H46A	3.366	C42	H46B	2.860
C42	H46C	2.860	C42	H48A	3.367
C42	H48B	2.860	C42	H48C	2.860
C43	H47A	3.358	C43	H47B	2.835
C43	H47C	2.835	C43	H49A	3.353
C43	H49B	2.835	C43	H49C	2.835
C44	H48A	2.662	C44	H48B	3.181
C44	H48C	3.231	C44	H50A	2.651
C44	H50B	3.239	C44	H50C	3.167
C45	H40A	3.197	C45	H46A	2.675
C45	H46B	3.228	C45	H46C	3.194
C45	H49A	2.695	C45	H49B	3.213
C45	H49C	3.231	C46	H10C	3.493
C46	H26B	3.315	C46	H40A	3.380
C46	H47A	2.790	C46	H50B	3.163
C46	H50C	3.187	C47	H1A	3.285
C47	H26A	3.404	C47	H26B	2.766
C47	H46B	3.198	C47	H46C	3.153
C47	H48B	3.091	C47	H48C	3.125
C48	H47B	3.084	C48	H47C	3.118
C48	H49B	3.092	C48	H49C	3.118
C49	H48A	2.707	C49	H50A	2.753
C50	H40A	2.881	C50	H46A	2.775
C50	H49A	2.767	C51	H1A	2.769
C51	H1B	2.469	C51	H22A	3.099
C51	H22B	3.389	C51	H26A	2.500

Table S11-10. Intramolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
C51	H26B	3.242	C51	H32	2.900
C51	H57	2.656	C51	H71A	3.444
C51	H75A	3.055	C51	H75B	3.099
C52	H1B	2.676	C52	H21A	3.538
C52	H22A	2.741	C52	H32	3.358
C52	H71A	3.540	C52	H71C	3.436
C53	H22A	2.820	C53	H22C	3.531
C53	H51A	2.661	C53	H51B	2.860
C53	H55	3.249	C53	H57	3.274
C53	H63A	2.807	C53	H63B	3.379
C53	H65A	2.857	C53	H65C	3.425
C53	H71A	3.560	C53	H71C	2.861
C54	H22A	3.433	C54	H63A	2.657
C54	H63B	2.684	C54	H63C	3.342
C54	H64A	2.734	C54	H64B	3.379
C54	H64C	2.729	C54	H65A	2.704
C54	H65B	3.375	C54	H65C	2.736
C54	H71C	3.390	C55	H57	3.253
C55	H60A	2.675	C55	H60B	3.315
C55	H61A	2.686	C55	H61C	3.322
C55	H63B	3.430	C55	H64A	2.743
C55	H64C	2.690	C55	H65C	3.571
C56	H21A	3.429	C56	H59A	2.682
C56	H59B	2.733	C56	H59C	3.348
C56	H60A	2.614	C56	H60B	2.665
C56	H60C	3.321	C56	H61A	2.663
C56	H61B	3.355	C56	H61C	2.741
C57	H1B	2.809	C57	H21A	3.217
C57	H22A	3.340	C57	H32	3.192
C57	H34A	3.340	C57	H51A	3.221
C57	H51B	3.046	C57	H55	3.244
C57	H59A	2.694	C57	H59B	2.838
C57	H60B	3.432	C58	H55	2.659
C58	H57	2.716	C59	H9A	3.277
C59	H9B	3.386	C59	H57	2.499
C59	H60A	3.309	C59	H60B	2.668
C59	H60C	2.668	C59	H61A	3.283

Table S11-10. Intramolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
C59	H61B	2.629	C59	H61C	2.629
C60	H55	2.869	C60	H59A	2.670
C60	H59B	3.324	C60	H59C	2.630
C60	H61A	2.661	C60	H61B	2.644
C60	H61C	3.335	C61	H55	2.802
C61	H59A	3.294	C61	H59B	2.616
C61	H59C	2.616	C61	H60A	2.671
C61	H60B	3.331	C61	H60C	2.644
C62	H55	2.663	C63	H22C	3.298
C63	H64A	3.318	C63	H64B	2.643
C63	H64C	2.643	C63	H65A	2.740
C63	H65B	2.701	C63	H65C	3.368
C64	H55	2.389	C64	H63A	3.318
C64	H63B	2.643	C64	H63C	2.643
C64	H65A	3.322	C64	H65B	2.645
C64	H65C	2.645	C65	H63A	2.739
C65	H63B	3.372	C65	H63C	2.691
C65	H64A	2.645	C65	H64B	2.634
C65	H64C	3.326	C65	H71C	3.184
C65	H72B	2.655	C66	H51B	3.445
C66	H65A	3.436	C66	H72A	3.359
C66	H72B	2.850	C66	H72C	2.850
C66	H75A	2.703	C66	H75B	3.269
C66	H75C	3.186	C67	H65A	3.181
C67	H71A	3.367	C67	H71B	2.852
C67	H71C	2.852	C67	H73A	2.712
C67	H73B	3.232	C67	H73C	3.245
C68	H72A	2.645	C68	H72B	3.227
C68	H72C	3.153	C68	H74A	3.343
C68	H74B	2.850	C68	H74C	2.850
C69	H73A	3.331	C69	H73B	2.809
C69	H73C	2.809	C69	H75A	3.356
C69	H75B	2.831	C69	H75C	2.831
C70	H51B	3.154	C70	H71A	2.686
C70	H71B	3.209	C70	H71C	3.240
C70	H74A	2.624	C70	H74B	3.219
C70	H74C	3.152	C71	H35B	3.201

Table S11-10. Intramolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
C71	H51B	3.265	C71	H65A	3.413
C71	H72B	3.124	C71	H72C	3.164
C71	H75A	2.827	C72	H65A	2.887
C72	H71B	3.126	C72	H71C	3.164
C72	H73A	2.796	C73	H72A	2.768
C73	H74B	3.078	C73	H74C	3.119
C74	H73B	3.068	C74	H73C	3.107
C74	H75B	3.040	C74	H75C	3.067
C75	H26A	3.344	C75	H38A	3.562
C75	H38B	3.561	C75	H51A	3.404
C75	H51B	2.622	C75	H71A	2.821
C75	H74A	2.642	H1A	H7	3.397
H1A	H22A	3.145	H1A	H22B	2.920
H1A	H26A	2.470	H1A	H26B	2.481
H1A	H47A	3.196	H1A	H47B	2.528
H1A	H51A	2.529	H1A	H51B	3.536
H1B	H7	3.234	H1B	H21A	2.191
H1B	H21C	2.884	H1B	H22A	2.149
H1B	H22B	2.787	H1B	H26A	3.487
H1B	H26B	3.428	H1B	H51A	2.491
H1B	H51B	3.432	H1B	H57	2.697
H5	H11A	2.236	H5	H11B	3.459
H5	H11C	2.295	H5	H14C	3.488
H5	H15A	3.375	H5	H15B	2.098
H5	H15C	2.286	H7	H9A	2.270
H7	H9B	3.306	H7	H10A	2.310
H7	H10C	3.359	H7	H26B	2.495
H7	H32	2.618	H7	H57	2.737
H7	H59A	3.315	H9A	H10A	2.538
H9A	H10B	2.961	H9A	H11B	3.530
H9A	H11C	3.530	H9A	H32	3.363
H9A	H34B	2.863	H9A	H57	3.481
H9A	H59A	2.999	H9A	H59B	2.814
H9A	H59C	3.531	H9B	H10B	3.561
H9B	H11A	3.540	H9B	H11B	2.918
H9B	H11C	2.440	H9B	H59A	3.064
H9B	H59B	3.295	H9B	H59C	3.235

Table S11-10. Intramolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
H9C	H10A	2.975	H9C	H10B	2.462
H9C	H10C	3.559	H9C	H11A	3.540
H9C	H11B	2.440	H9C	H11C	2.918
H9C	H34B	3.573	H10A	H11A	3.562
H10A	H11B	3.540	H10A	H26B	3.310
H10A	H32	3.465	H10A	H46B	3.023
H10B	H11A	2.966	H10B	H11B	2.456
H10B	H11C	3.557	H10C	H11A	2.487
H10C	H11B	2.923	H10C	H11C	3.571
H10C	H46B	3.161	H10C	H46C	3.002
H13A	H14A	2.520	H13A	H14B	3.002
H13A	H14C	3.600	H13A	H15A	2.423
H13A	H15B	3.534	H13A	H15C	2.901
H13A	H25A	3.311	H13A	H25C	2.958
H13B	H14A	3.598	H13B	H15A	2.932
H13B	H15B	3.556	H13B	H15C	2.455
H13B	H21C	3.048	H13B	H25A	2.825
H13B	H25C	3.284	H13C	H14A	2.999
H13C	H14B	2.557	H13C	H15A	3.533
H13C	H15C	3.549	H13C	H21C	2.863
H13C	H25A	2.524	H13C	H25C	2.405
H14A	H15A	2.451	H14A	H15B	2.937
H14A	H15C	3.552	H14B	H15A	3.553
H14B	H15B	3.586	H14B	H47C	3.518
H14C	H15A	2.969	H14C	H15B	2.513
H14C	H15C	3.591	H14C	H47C	3.560
H21A	H22A	2.174	H21A	H22B	3.505
H21A	H22C	3.434	H21A	H57	3.384
H21A	H59A	3.599	H21A	H60B	2.767
H21B	H22A	3.431	H21B	H25A	2.583
H21B	H25B	3.484	H21B	H60B	2.733
H21C	H22A	3.520	H21C	H25A	2.562
H21C	H60B	3.269	H22A	H51A	2.692
H22A	H63A	3.400	H22A	H63B	3.473
H22B	H23A	2.428	H22B	H23B	3.584
H22B	H51A	2.581	H22C	H23A	2.531
H22C	H23C	3.437	H22C	H63A	2.731

Table S11-10. Intramolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
H22C	H63B	2.973	H23B	H24B	3.255
H23B	H24C	2.826	H23C	H24B	2.826
H23C	H24C	3.241	H24A	H25B	2.624
H24A	H25C	2.518	H24B	H25B	3.527
H26A	H32	3.453	H26A	H46B	3.574
H26A	H47A	3.322	H26A	H47B	2.882
H26A	H51A	2.488	H26A	H51B	2.508
H26A	H75A	3.239	H26A	H75B	2.599
H26B	H32	3.166	H26B	H46B	2.524
H26B	H47A	2.252	H26B	H47B	2.609
H26B	H51A	3.516	H26B	H51B	3.429
H30	H35A	2.626	H30	H36A	1.987
H30	H36B	3.460	H30	H36C	3.003
H30	H38B	3.521	H30	H39A	2.131
H30	H39B	2.278	H30	H39C	3.391
H32	H34A	2.013	H32	H34B	2.588
H32	H34C	3.446	H32	H35B	3.355
H32	H51B	2.645	H32	H57	2.648
H34A	H35A	3.520	H34A	H35B	2.451
H34A	H35C	2.959	H34A	H36B	3.540
H34A	H36C	3.540	H34A	H57	3.013
H34A	H59B	2.936	H34B	H35B	3.529
H34B	H35C	3.467	H34B	H36A	3.531
H34B	H36B	2.949	H34B	H36C	2.477
H34B	H59B	3.191	H34C	H35A	3.416
H34C	H35B	2.764	H34C	H35C	2.307
H34C	H36A	3.531	H34C	H36B	2.477
H34C	H36C	2.949	H34C	H59B	3.565
H35A	H36A	2.372	H35A	H36B	2.745
H35A	H36C	3.485	H35A	H71A	3.576
H35B	H36A	3.474	H35B	H36B	3.380
H35B	H71A	2.516	H35B	H71B	3.148
H35B	H71C	3.507	H35C	H36A	2.861
H35C	H36B	2.235	H35C	H36C	3.420
H36A	H39B	3.576	H38A	H39A	3.537
H38A	H39C	3.520	H38A	H40A	2.598
H38A	H40B	2.987	H38A	H75C	2.826

Table S11-10. Intramolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
H38B	H39A	2.436	H38B	H39B	3.541
H38B	H39C	2.888	H38B	H40B	3.570
H38B	H75A	3.571	H38B	H75C	2.739
H38C	H39A	2.921	H38C	H39B	3.530
H38C	H39C	2.412	H38C	H40A	3.016
H38C	H40B	2.482	H38C	H40C	3.578
H39A	H40B	3.555	H39A	H40C	3.555
H39B	H40A	3.554	H39B	H40B	2.937
H39B	H40C	2.463	H39C	H40A	3.554
H39C	H40B	2.463	H39C	H40C	2.937
H40A	H46A	2.923	H40A	H46B	3.335
H40A	H50A	3.414	H40A	H50B	2.007
H40A	H50C	3.510	H40B	H50B	2.686
H40C	H46A	3.192	H40C	H50B	2.870
H46A	H50B	2.578	H46A	H50C	2.659
H46B	H47A	2.631	H46C	H47A	2.628
H46C	H47C	3.531	H46C	H50C	3.585
H47B	H48B	3.145	H47B	H48C	2.763
H47C	H48B	2.762	H47C	H48C	3.239
H48A	H49B	2.538	H48A	H49C	2.539
H48B	H49B	3.501	H49A	H50A	2.088
H49A	H50B	3.447	H49A	H50C	3.368
H49B	H50A	3.375	H49C	H50A	3.419
H51A	H57	3.462	H51A	H75A	3.299
H51A	H75B	2.879	H51B	H57	3.172
H51B	H71A	2.622	H51B	H71C	3.378
H51B	H75A	2.106	H51B	H75B	2.479
H51B	H75C	3.515	H55	H60A	2.285
H55	H60B	3.361	H55	H61A	2.201
H55	H61B	3.600	H55	H61C	3.261
H55	H63B	3.549	H55	H64A	2.191
H55	H64B	3.353	H55	H64C	2.135
H57	H59A	2.169	H57	H59B	2.371
H57	H59C	3.461	H57	H60B	3.574
H59A	H60A	3.553	H59A	H60B	2.495
H59A	H60C	2.975	H59A	H61B	3.529
H59A	H61C	3.529	H59B	H60B	3.575

Table S11-10. Intramolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
H59B	H60C	3.556	H59B	H61A	3.509
H59B	H61B	2.909	H59B	H61C	2.429
H59C	H60A	3.524	H59C	H60B	2.917
H59C	H60C	2.453	H59C	H61A	3.509
H59C	H61B	2.429	H59C	H61C	2.909
H60A	H61A	2.481	H60A	H61B	2.941
H60A	H61C	3.572	H60A	H64C	3.497
H60B	H61A	3.563	H60B	H61B	3.537
H60C	H61A	2.925	H60C	H61B	2.434
H60C	H61C	3.543	H63A	H64B	3.541
H63A	H64C	3.541	H63A	H65A	2.589
H63A	H65B	3.010	H63B	H64A	3.542
H63B	H64B	2.924	H63B	H64C	2.447
H63B	H65B	3.585	H63C	H64A	3.542
H63C	H64B	2.447	H63C	H64C	2.923
H63C	H65A	2.997	H63C	H65B	2.495
H63C	H65C	3.577	H64A	H65A	3.542
H64A	H65B	2.927	H64A	H65C	2.447
H64B	H65A	3.534	H64B	H65B	2.435
H64B	H65C	2.911	H64C	H65B	3.544
H64C	H65C	3.549	H65A	H71C	2.644
H65A	H72A	3.390	H65A	H72B	2.022
H65A	H72C	3.545	H65B	H72B	2.786
H65C	H71C	2.908	H65C	H72B	2.765
H71A	H75A	2.167	H71A	H75B	3.501
H71A	H75C	3.427	H71B	H72B	3.182
H71B	H72C	2.815	H71B	H75A	3.426
H71C	H72B	2.814	H71C	H72C	3.291
H71C	H75A	3.511	H72A	H73A	2.116
H72A	H73B	3.390	H72A	H73C	3.436
H72B	H73A	3.474	H72C	H73A	3.397
H73B	H74B	3.128	H73B	H74C	2.755
H73C	H74B	2.753	H73C	H74C	3.239
H74A	H75B	2.412	H74A	H75C	2.535
H74B	H75B	3.586	H74C	H75C	3.415

Table S11-11. Intermolecular contacts less than 3.60 Å

atom	atom	distance	atom	atom	distance
Cl4	C21[1]	3.582(5)	C21	Cl4[2]	3.582(5)
C24	C69[3]	3.550(7)	C39	C63[4]	3.477(7)
C60	C74[2]	3.568(10)	C63	C39[3]	3.477(7)
C69	C24[4]	3.550(7)	C74	C60[1]	3.568(10)

Symmetry Operators:

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

Table S11-12. Intermolecular contacts less than 3.60 Å involving hydrogens

atom	atom	distance	atom	atom	distance
Cl2	H9C[1]	3.596	Cl2	H11B[1]	3.255
Cl3	H60C[2]	2.869	Cl4	H13B[2]	3.420
Cl4	H21B[2]	3.084	Cl4	H21C[2]	3.177
Cl4	H25A[2]	3.421	Cl4	H60B[2]	3.169
Cl5	H30[3]	3.531	Cl5	H36A[3]	3.005
Cl5	H39A[3]	3.457	Cl5	H39B[3]	3.078
Cl5	H46C[4]	3.542	Cl5	H50C[4]	2.837
Cl6	H35A[3]	3.143	Cl6	H35C[3]	3.555
Cl6	H36A[3]	3.500	C4	H49A[5]	3.429
C5	H49A[5]	3.145	C5	H49B[5]	3.586
C5	H64B[6]	3.179	C11	H24A[7]	2.949
C11	H25C[7]	3.264	C11	H49B[5]	3.448
C11	H73B[8]	3.235	C13	H50A[5]	3.279
C14	H64A[6]	3.453	C15	H36C[1]	3.231
C15	H49A[5]	3.305	C15	H50A[5]	3.231
C15	H64A[6]	3.246	C15	H64B[6]	3.581
C15	H73B[8]	3.522	C15	H73C[8]	3.389
C23	H35A[3]	3.458	C23	H38B[3]	3.222
C23	H71A[3]	3.526	C23	H71B[3]	3.297
C23	H75A[3]	3.527	C23	H75C[3]	3.338
C24	H11B[1]	3.227	C24	H74C[3]	3.468
C25	H11B[1]	3.178	C25	H38C[5]	3.310
C35	H23A[9]	3.569	C36	H15A[7]	3.163
C36	H50C[10]	3.426	C36	H73C[9]	3.232
C38	H23C[9]	3.373	C39	H46A[10]	3.417
C39	H63A[9]	3.177	C39	H63B[9]	3.553
C39	H63C[9]	3.144	C42	H72A[6]	3.574
C43	H72A[6]	3.094	C44	H72A[6]	3.161
C44	H73A[6]	3.051	C45	H73A[6]	3.402
C46	H39B[10]	3.221	C47	H65B[6]	3.428
C48	H72A[6]	3.406	C49	H5[2]	3.500
C49	H9B[2]	3.343	C49	H11C[2]	3.320
C49	H15C[2]	3.314	C49	H72A[6]	3.574
C49	H73A[6]	2.848	C50	H13B[2]	3.355
C50	H15C[2]	3.324	C50	H36C[10]	3.507
C50	H73A[6]	3.543	C60	H74A[5]	3.118
C60	H74B[5]	3.499	C60	H74C[5]	3.515

Table S11-12. Intermolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
C61	H34C[11]	3.452	C61	H35C[11]	3.385
C63	H39A[3]	3.385	C63	H39C[3]	2.897
C64	H5[4]	3.538	C64	H11A[4]	3.436
C64	H14C[4]	3.223	C64	H15B[4]	2.865
C65	H14C[4]	3.320	C66	H23B[9]	3.177
C66	H24C[9]	3.247	C67	H24C[9]	3.040
C68	H24B[9]	3.451	C68	H24C[9]	3.020
C69	H24B[9]	3.026	C69	H24C[9]	3.227
C70	H23B[9]	3.539	C70	H23C[9]	3.400
C70	H24B[9]	3.227	C70	H24C[9]	3.355
C71	H23B[9]	2.911	C72	H48B[4]	3.474
C73	H11C[12]	3.293	C73	H15C[12]	3.169
C73	H49A[4]	3.512	C73	H49B[4]	3.177
C74	H24B[9]	3.251	C74	H60A[2]	2.873
C74	H60C[2]	3.392	C75	H23C[9]	2.972
H5	C49[5]	3.500	H5	C64[6]	3.538
H5	H49A[5]	2.953	H5	H49B[5]	3.261
H5	H64B[6]	2.819	H5	H73B[8]	3.072
H9B	C49[5]	3.343	H9B	H48A[5]	3.374
H9B	H49B[5]	2.830	H9B	H49C[5]	2.991
H9C	Cl2[7]	3.596	H9C	H13A[7]	2.878
H9C	H14A[7]	3.245	H9C	H25C[7]	3.560
H10B	H13A[7]	3.046	H10B	H25C[7]	2.868
H10B	H40B[10]	3.232	H10C	H40B[10]	3.570
H10C	H63C[6]	3.187	H10C	H64B[6]	3.464
H11A	C64[6]	3.436	H11A	H24A[7]	2.930
H11A	H25C[7]	3.525	H11A	H64B[6]	2.793
H11A	H64C[6]	3.187	H11A	H73B[8]	3.060
H11B	Cl2[7]	3.255	H11B	C24[7]	3.227
H11B	C25[7]	3.178	H11B	H24A[7]	2.351
H11B	H24C[7]	3.376	H11B	H25B[7]	3.265
H11B	H25C[7]	2.339	H11C	C49[5]	3.320
H11C	C73[8]	3.293	H11C	H24A[7]	3.120
H11C	H49A[5]	3.397	H11C	H49B[5]	2.520
H11C	H73A[8]	3.130	H11C	H73B[8]	2.598
H13A	H9C[1]	2.878	H13A	H10B[1]	3.046
H13A	H50A[5]	3.357	H13B	Cl4[5]	3.420

Table S11-12. Intermolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
H13B	C50[5]	3.355	H13B	H49A[5]	2.838
H13B	H50A[5]	2.506	H13B	H50B[5]	3.399
H14A	H9C[1]	3.245	H14C	C64[6]	3.223
H14C	C65[6]	3.320	H14C	H64A[6]	2.666
H14C	H64B[6]	2.963	H14C	H65B[6]	3.080
H14C	H65C[6]	2.774	H15A	C36[1]	3.163
H15A	H34B[1]	3.332	H15A	H36B[1]	3.005
H15A	H36C[1]	2.467	H15A	H50A[5]	3.332
H15A	H64A[6]	3.454	H15A	H73C[8]	3.483
H15B	C64[6]	2.865	H15B	H64A[6]	2.374
H15B	H64B[6]	2.678	H15B	H64C[6]	3.107
H15B	H73B[8]	3.163	H15B	H73C[8]	3.354
H15C	C49[5]	3.314	H15C	C50[5]	3.324
H15C	C73[8]	3.169	H15C	H36C[1]	3.170
H15C	H49A[5]	2.413	H15C	H49B[5]	3.467
H15C	H50A[5]	2.428	H15C	H50C[5]	3.463
H15C	H73A[8]	3.163	H15C	H73B[8]	3.005
H15C	H73C[8]	2.810	H21B	Cl4[5]	3.084
H21C	Cl4[5]	3.177	H22C	H39A[3]	2.875
H23A	C35[3]	3.569	H23A	H35A[3]	2.729
H23A	H35B[3]	3.581	H23A	H38B[3]	3.336
H23A	H39A[3]	3.307	H23B	C66[3]	3.177
H23B	C70[3]	3.539	H23B	C71[3]	2.911
H23B	H35A[3]	3.484	H23B	H71A[3]	2.892
H23B	H71B[3]	2.375	H23B	H75A[3]	3.403
H23B	H75C[3]	3.478	H23C	C38[3]	3.373
H23C	C70[3]	3.400	H23C	C75[3]	2.972
H23C	H38B[3]	2.419	H23C	H39A[3]	3.556
H23C	H71A[3]	3.410	H23C	H71B[3]	3.563
H23C	H75A[3]	2.840	H23C	H75C[3]	2.438
H24A	C11[1]	2.949	H24A	H11A[1]	2.930
H24A	H11B[1]	2.351	H24A	H11C[1]	3.120
H24A	H73B[3]	3.390	H24A	H74C[3]	3.491
H24B	C68[3]	3.451	H24B	C69[3]	3.026
H24B	C70[3]	3.227	H24B	C74[3]	3.251
H24B	H74A[3]	3.466	H24B	H74C[3]	2.769
H24B	H75C[3]	3.019	H24C	C66[3]	3.247

Table S11-12. Intermolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
H24C	C67[3]	3.040	H24C	C68[3]	3.020
H24C	C69[3]	3.227	H24C	C70[3]	3.355
H24C	H11B[1]	3.376	H24C	H72C[3]	3.287
H24C	H73B[3]	3.400	H25A	Cl4[5]	3.421
H25A	H38C[5]	2.909	H25A	H40B[5]	3.520
H25B	H11B[1]	3.265	H25B	H38C[5]	2.813
H25C	C11[1]	3.264	H25C	H9C[1]	3.560
H25C	H10B[1]	2.868	H25C	H11A[1]	3.525
H25C	H11B[1]	2.339	H30	Cl5[9]	3.531
H30	H50C[10]	3.548	H34B	H15A[7]	3.332
H34C	C61[11]	3.452	H34C	H61A[11]	3.060
H34C	H61B[11]	3.383	H34C	H61C[11]	3.346
H35A	Cl6[9]	3.143	H35A	C23[9]	3.458
H35A	H23A[9]	2.729	H35A	H23B[9]	3.484
H35B	H23A[9]	3.581	H35C	Cl6[9]	3.555
H35C	C61[11]	3.385	H35C	H61A[11]	3.245
H35C	H61B[11]	2.730	H36A	Cl5[9]	3.005
H36A	Cl6[9]	3.500	H36A	H50C[10]	3.027
H36A	H73C[9]	3.060	H36B	H15A[7]	3.005
H36B	H61A[11]	3.483	H36B	H73C[9]	2.882
H36B	H74B[9]	2.973	H36C	C15[7]	3.231
H36C	C50[10]	3.507	H36C	H15A[7]	2.467
H36C	H15C[7]	3.170	H36C	H50A[10]	3.301
H36C	H50C[10]	2.927	H36C	H73C[9]	3.216
H38B	C23[9]	3.222	H38B	H23A[9]	3.336
H38B	H23C[9]	2.419	H38C	C25[2]	3.310
H38C	H25A[2]	2.909	H38C	H25B[2]	2.813
H39A	Cl5[9]	3.457	H39A	C63[9]	3.385
H39A	H22C[9]	2.875	H39A	H23A[9]	3.307
H39A	H23C[9]	3.556	H39A	H63A[9]	2.883
H39A	H63B[9]	3.405	H39A	H63C[9]	3.329
H39B	Cl5[9]	3.078	H39B	C46[10]	3.221
H39B	H46A[10]	2.574	H39B	H46C[10]	2.992
H39B	H50C[10]	3.275	H39B	H63A[9]	3.264
H39B	H63C[9]	3.174	H39C	C63[9]	2.897
H39C	H46A[10]	3.522	H39C	H46C[10]	3.398
H39C	H63A[9]	2.866	H39C	H63B[9]	2.872

Table S11-12. Intermolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
H39C	H63C^{9}	2.474	H40B	H10B^{10}	3.232
H40B	H10C^{10}	3.570	H40B	H25A^{2}	3.520
H40C	H40C^{10}	2.976	H40C	H46A^{10}	2.851
H46A	C39^{10}	3.417	H46A	H39B^{10}	2.574
H46A	H39C^{10}	3.522	H46A	H40C^{10}	2.851
H46C	Cl5^{6}	3.542	H46C	H39B^{10}	2.992
H46C	H39C^{10}	3.398	H46C	H63C^{6}	2.779
H46C	H65B^{6}	3.055	H47A	H65B^{6}	3.205
H47C	H65B^{6}	2.912	H47C	H72B^{6}	3.468
H48A	H9B^{2}	3.374	H48A	H59C^{2}	3.221
H48A	H72A^{6}	3.551	H48B	C72^{6}	3.474
H48B	H72A^{6}	3.006	H48B	H72B^{6}	3.597
H48B	H72C^{6}	3.276	H49A	C4^{2}	3.429
H49A	C5^{2}	3.145	H49A	C15^{2}	3.305
H49A	C73^{6}	3.512	H49A	H5^{2}	2.953
H49A	H11C^{2}	3.397	H49A	H13B^{2}	2.838
H49A	H15C^{2}	2.413	H49A	H73A^{6}	2.829
H49A	H73B^{6}	3.570	H49B	C5^{2}	3.586
H49B	C11^{2}	3.448	H49B	C73^{6}	3.177
H49B	H5^{2}	3.261	H49B	H9B^{2}	2.830
H49B	H11C^{2}	2.520	H49B	H15C^{2}	3.467
H49B	H72A^{6}	3.025	H49B	H73A^{6}	2.357
H49B	H73B^{6}	3.189	H49C	H9B^{2}	2.991
H49C	H59A^{2}	3.088	H49C	H59C^{2}	3.233
H50A	C13^{2}	3.279	H50A	C15^{2}	3.231
H50A	H13A^{2}	3.357	H50A	H13B^{2}	2.506
H50A	H15A^{2}	3.332	H50A	H15C^{2}	2.428
H50A	H36C^{10}	3.301	H50A	H73A^{6}	3.305
H50A	H73C^{6}	3.406	H50B	H13B^{2}	3.399
H50C	Cl5^{6}	2.837	H50C	C36^{10}	3.426
H50C	H15C^{2}	3.463	H50C	H30^{10}	3.548
H50C	H36A^{10}	3.027	H50C	H36C^{10}	2.927
H50C	H39B^{10}	3.275	H50C	H73A^{6}	3.358
H50C	H73C^{6}	3.198	H59A	H49C^{5}	3.088
H59C	H48A^{5}	3.221	H59C	H49C^{5}	3.233
H60A	C74^{5}	2.873	H60A	H74A^{5}	2.631
H60A	H74B^{5}	2.841	H60A	H74C^{5}	2.659

Table S11-12. Intermolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
H60B	Cl4^{5}	3.169	H60B	H74A^{5}	3.497
H60C	Cl3^{5}	2.869	H60C	C74^{5}	3.392
H60C	H74A^{5}	2.804	H60C	H74B^{5}	3.268
H61A	H34C^{11}	3.060	H61A	H35C^{11}	3.245
H61A	H36B^{11}	3.483	H61A	H74B^{5}	3.505
H61B	H34C^{11}	3.383	H61B	H35C^{11}	2.730
H61C	H34C^{11}	3.346	H63A	C39^{3}	3.177
H63A	H39A^{3}	2.883	H63A	H39B^{3}	3.264
H63A	H39C^{3}	2.866	H63B	C39^{3}	3.553
H63B	H39A^{3}	3.405	H63B	H39C^{3}	2.872
H63C	C39^{3}	3.144	H63C	H10C^{4}	3.187
H63C	H39A^{3}	3.329	H63C	H39B^{3}	3.174
H63C	H39C^{3}	2.474	H63C	H46C^{4}	2.779
H64A	C14^{4}	3.453	H64A	C15^{4}	3.246
H64A	H14C^{4}	2.666	H64A	H15A^{4}	3.454
H64A	H15B^{4}	2.374	H64B	C5^{4}	3.179
H64B	C15^{4}	3.581	H64B	H5^{4}	2.819
H64B	H10C^{4}	3.464	H64B	H11A^{4}	2.793
H64B	H14C^{4}	2.963	H64B	H15B^{4}	2.678
H64C	H11A^{4}	3.187	H64C	H15B^{4}	3.107
H64C	H74C^{5}	3.331	H65B	C47^{4}	3.428
H65B	H14C^{4}	3.080	H65B	H46C^{4}	3.055
H65B	H47A^{4}	3.205	H65B	H47C^{4}	2.912
H65C	H14C^{4}	2.774	H71A	C23^{9}	3.526
H71A	H23B^{9}	2.892	H71A	H23C^{9}	3.410
H71B	C23^{9}	3.297	H71B	H23B^{9}	2.375
H71B	H23C^{9}	3.563	H72A	C42^{4}	3.574
H72A	C43^{4}	3.094	H72A	C44^{4}	3.161
H72A	C48^{4}	3.406	H72A	C49^{4}	3.574
H72A	H48A^{4}	3.551	H72A	H48B^{4}	3.006
H72A	H49B^{4}	3.025	H72B	H47C^{4}	3.468
H72B	H48B^{4}	3.597	H72C	H24C^{9}	3.287
H72C	H48B^{4}	3.276	H73A	C44^{4}	3.051
H73A	C45^{4}	3.402	H73A	C49^{4}	2.848
H73A	C50^{4}	3.543	H73A	H11C^{12}	3.130
H73A	H15C^{12}	3.163	H73A	H49A^{4}	2.829
H73A	H49B^{4}	2.357	H73A	H50A^{4}	3.305

Table S11-12. Intermolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
H73A	H50C[4]	3.358	H73B	C11[12]	3.235
H73B	C15[12]	3.522	H73B	H5[12]	3.072
H73B	H11A[12]	3.060	H73B	H11C[12]	2.598
H73B	H15B[12]	3.163	H73B	H15C[12]	3.005
H73B	H24A[9]	3.390	H73B	H24C[9]	3.400
H73B	H49A[4]	3.570	H73B	H49B[4]	3.189
H73C	C15[12]	3.389	H73C	C36[3]	3.232
H73C	H15A[12]	3.483	H73C	H15B[12]	3.354
H73C	H15C[12]	2.810	H73C	H36A[3]	3.060
H73C	H36B[3]	2.882	H73C	H36C[3]	3.216
H73C	H50A[4]	3.406	H73C	H50C[4]	3.198
H74A	C60[2]	3.118	H74A	H24B[9]	3.466
H74A	H60A[2]	2.631	H74A	H60B[2]	3.497
H74A	H60C[2]	2.804	H74B	C60[2]	3.499
H74B	H36B[3]	2.973	H74B	H60A[2]	2.841
H74B	H60C[2]	3.268	H74B	H61A[2]	3.505
H74C	C24[9]	3.468	H74C	C60[2]	3.515
H74C	H24A[9]	3.491	H74C	H24B[9]	2.769
H74C	H60A[2]	2.659	H74C	H64C[2]	3.331
H75A	C23[9]	3.527	H75A	H23B[9]	3.403
H75A	H23C[9]	2.840	H75C	C23[9]	3.338
H75C	H23B[9]	3.478	H75C	H23C[9]	2.438
H75C	H24B[9]	3.019			

Symmetry Operators:

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

X-ray Structure Report

for

[(1,2,4-$Me_3C_5H_2$)$TiCl_2${(O-2,4-$^tBu_2C_6H_2$)-6-CH_2}]$_3$N (**7**)

February 17, 2016

Experimental

Data Collection

A red plate crystal of $C_{69}H_{99}Cl_6NO_3Ti_3$ having approximate dimensions of 0.330 x 0.130 x 0.050 mm was mounted on a glass fiber. All measurements were made on a Rigaku XtaLAB mini diffractometer using multi-layer mirror monochromated Mo-Kα radiation.

The crystal-to-detector distance was 50.00 mm.

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

a = 13.2258(6) Å
b = 22.4804(11) Å β = 99.642(4)^o
c = 24.4338(12) Å
V = 7162.1(6) Å^3

For Z = 4 and F.W. = 1346.96, the calculated density is 1.249 g/cm^3. The reflection conditions of:

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

uniquely determine the space group to be:

$P2_1/n$ (#14)

The data were collected at a temperature of -180 $\pm$ 1^{o}C to a maximum 2θ value of 65.2^o. A total of 540 oscillation images were collected. A sweep of data was done using ω scans from -60.0 to 120.0^o in 1.00^o step, at χ=54.0^o and ϕ = 0.0^o. The exposure rate was 16.0 [sec./^{o}]. The detector swing angle was 30.00^o. A second sweep was performed using ω scans from -60.0 to 120.0^o in 1.00^o step, at χ=54.0^o and ϕ = 120.0^o. The exposure rate was 16.0 [sec./^{o}]. The detector swing angle was 30.00^o. Another sweep was performed using ω scans from -60.0 to 120.0^o in 1.00^o step, at χ=54.0^o and ϕ = 240.0^o. The exposure rate was 16.0 [sec./^{o}]. The detector swing angle

was 30.00°. The crystal-to-detector distance was 50.00 mm. Readout was performed in the 0.073 mm pixel mode.

Data Reduction

Of the 0 reflections were collected, where 0 were unique (R_{int} = 0.1157); equivalent reflections were merged. Data were collected and processed using CrysAlisPro (Rigaku Oxford Diffraction). [1]

The linear absorption coefficient, μ, for Mo-Kα radiation is 5.929 cm^{-1}. An empirical absorption correction was applied which resulted in transmission factors ranging from 0.936 to 0.971. 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 16446 observed reflections and 739 variable parameters and converged (largest parameter shift was 0.00 times its esd) with unweighted and weighted agreement factors of:

$$R1 = \Sigma \, ||Fo| - |Fc|| \, / \, \Sigma \, |Fo| = 0.0571$$

$$wR2 = [\Sigma \, (w \, (Fo^2 - Fc^2)^2) / \Sigma \, w(Fo^2)^2]^{1/2} = 0.1330$$

The goodness of fit[4] was 1.01. Unit weights were used. The maximum and minimum peaks on the final difference Fourier map corresponded to 0.47 and -0.59 $e^-/Å^3$, respectively.

Neutral atom scattering factors were taken from International Tables for Crystallography (IT), Vol. C, Table 6.1.1.4 [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 Version 2014/7[10].

References

(1) CrysAlisPro: Data Collection and Processing Software, Rigaku Corporation (2015). Tokyo 196-8666, Japan.

(2) SHELXT: Sheldrick, G. M. (2014). Acta Cryst. A70, C1437.

(3) Least Squares function minimized: (SHELXL Version 2014/7)

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

(4) Goodness of fit is defined as:

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

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

(5) International Tables for Crystallography, Vol.C (1992). Ed. A.J.C. Wilson, Kluwer Academic Publishers, Dordrecht, Netherlands, Table 6.1.1.4, pp. 572.

(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 4.2: Crystal Structure Analysis Package, Rigaku Corporation (2000-2015). Tokyo 196-8666, Japan.

(10) SHELXL Version 2014/7: Sheldrick, G. M. (2008). Acta Cryst. A64, 112-122.

EXPERIMENTAL DETAILS

A. Crystal Data

Empirical Formula	$C_{69}H_{99}Cl_6NO_3Ti_3$
Formula Weight	1346.96
Crystal Color, Habit	red, plate
Crystal Dimensions	0.330 X 0.130 X 0.050 mm
Crystal System	monoclinic
Lattice Type	Primitive
Lattice Parameters	a = 13.2258(6) Å b = 22.4804(11) Å c = 24.4338(12) Å β = 99.642(4) ^{o} V = 7162.1(6) Å^3
Space Group	$P2_1/n$ (#14)
Z value	4
D_{calc}	1.249 g/cm^3
F_{000}	2848.00
μ(MoKα)	5.929 cm^{-1}

B. Intensity Measurements

Diffractometer	XtaLAB mini
Radiation	MoKα (λ = 0.71073 Å) multi-layer mirror monochromated
Voltage, Current	50kV, 24mA
Temperature	-180.0^{o}C
Detector Aperture	75.0 mm (diameter)
Data Images	540 exposures
ω oscillation Range (χ=54.0, ϕ=0.0)	-60.0 - 120.0^{o}
Exposure Rate	16.0 sec./^{o}
Detector Swing Angle	30.00^{o}
ω oscillation Range (χ=54.0, ϕ=120.0)	-60.0 - 120.0^{o}
Exposure Rate	16.0 sec./^{o}
Detector Swing Angle	30.00^{o}
ω oscillation Range (χ=54.0, ϕ=240.0)	-60.0 - 120.0^{o}
Exposure Rate	16.0 sec./^{o}
Detector Swing Angle	30.00^{o}
Detector Position	50.00 mm
Pixel Size	0.073 mm
$2\theta_{max}$	55.0^{o}
No. of Reflections Measured	Total: 75160

	Unique: 16446 (R_{int} = 0.1157)
Corrections	Lorentz-polarization Absorption (trans. factors: 0.936 - 0.971)

C. Structure Solution and Refinement

Structure Solution	Direct Methods (SHELXT)
Refinement	Full-matrix least-squares on F^2
Function Minimized	Σ w (Fo^2 - Fc^2)^2
Least Squares Weights	w = 1/ [$\sigma^2(Fo^2)$ + (0.0399 · P)^2 + 5.5057 · 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)	16446
No. Variables	739
Reflection/Parameter Ratio	22.25
Residuals: R1 (I>2.00σ(I))	0.0571
Residuals: R (All reflections)	0.1132
Residuals: wR2 (All reflections)	0.1330
Goodness of Fit Indicator	1.012
Max Shift/Error in Final Cycle	0.001
Maximum peak in Final Diff. Map	0.47 e^-/Å^3
Minimum peak in Final Diff. Map	-0.59 e^-/Å^3

Table S12-1. Atomic coordinates and B_{iso}/B_{eq}

atom	x	y	z	B_{eq}
Ti1	0.87213(4)	0.80126(3)	0.12163(2)	1.160(10)
Ti2	0.97466(4)	0.61217(3)	0.34628(2)	1.236(11)
Ti3	0.74388(5)	0.86571(3)	0.41457(3)	1.625(12)
Cl1	0.99463(7)	0.77997(4)	0.07021(4)	2.231(17)
Cl2	0.96031(6)	0.79098(4)	0.20809(3)	1.916(16)
Cl3	1.02344(7)	0.70625(4)	0.33600(4)	2.018(16)
Cl4	1.08453(6)	0.58496(4)	0.42370(4)	2.078(17)
Cl5	0.75121(8)	0.95782(4)	0.45159(4)	2.91(2)
Cl6	0.87265(7)	0.86880(5)	0.36488(4)	2.768(19)
O1	0.79022(16)	0.73798(9)	0.11262(9)	1.27(4)
O2	0.85303(16)	0.61947(9)	0.36921(9)	1.16(4)
O3	0.63185(16)	0.86951(10)	0.36197(9)	1.44(4)
N1	0.65644(19)	0.72527(11)	0.25601(10)	1.08(5)
C1	0.6853(2)	0.74466(14)	0.20344(13)	1.21(5)
C2	0.6597(2)	0.69900(14)	0.15813(13)	1.20(5)
C3	0.7113(2)	0.69792(14)	0.11255(13)	1.16(5)
C4	0.6872(3)	0.65629(14)	0.06946(13)	1.39(6)
C5	0.6116(3)	0.61473(15)	0.07592(14)	1.55(6)
C6	0.5609(3)	0.61266(15)	0.12119(13)	1.48(6)
C7	0.5853(2)	0.65639(14)	0.16139(13)	1.27(6)
C8	0.7452(3)	0.65284(15)	0.01998(14)	1.73(6)
C9	0.8549(3)	0.63252(17)	0.04285(15)	2.34(7)
C10	0.7458(3)	0.71207(15)	-0.01075(14)	1.88(6)
C11	0.6972(3)	0.60673(16)	-0.02272(14)	2.11(7)
C12	0.4877(3)	0.56259(15)	0.13127(14)	1.76(6)
C13	0.4613(3)	0.52132(16)	0.08110(15)	2.36(7)
C14	0.5409(3)	0.52469(17)	0.17995(15)	2.61(8)
C15	0.3889(3)	0.58808(18)	0.14646(15)	2.54(8)
C16	0.7280(2)	0.86019(14)	0.09024(14)	1.42(6)
C17	0.8034(3)	0.87368(15)	0.05831(14)	1.54(6)
C18	0.8881(3)	0.90196(15)	0.09244(14)	1.54(6)
C19	0.8655(3)	0.90450(14)	0.14634(14)	1.49(6)
C20	0.7678(3)	0.87780(14)	0.14515(14)	1.52(6)
C21	0.6240(3)	0.83499(16)	0.06916(15)	1.86(6)
C22	0.9815(3)	0.92685(17)	0.07406(15)	2.21(7)
C23	0.9284(3)	0.93278(16)	0.19607(15)	2.14(7)
C24	0.7264(2)	0.67868(15)	0.28134(13)	1.27(6)

Table S12-1. Atomic coordinates and B_{iso}/B_{eq} (continued)

atom	x	y	z	B_{eq}
C25	0.6846(2)	0.64650(14)	0.32698(13)	1.17(5)
C26	0.7498(2)	0.61914(14)	0.37104(13)	1.14(5)
C27	0.7117(2)	0.59396(14)	0.41597(13)	1.16(5)
C28	0.6049(2)	0.59445(15)	0.41277(14)	1.51(6)
C29	0.5372(2)	0.61831(15)	0.36860(13)	1.39(6)
C30	0.5798(2)	0.64494(14)	0.32638(14)	1.36(6)
C31	0.7821(2)	0.56736(15)	0.46659(13)	1.39(6)
C32	0.8403(3)	0.51408(15)	0.44835(14)	1.79(6)
C33	0.7216(3)	0.54585(17)	0.51079(14)	2.15(7)
C34	0.8569(3)	0.61518(16)	0.49371(14)	1.86(6)
C35	0.4202(3)	0.61496(16)	0.36423(14)	1.71(6)
C36	0.3815(3)	0.5688(2)	0.3199(2)	3.93(10)
C37	0.3879(3)	0.5975(2)	0.41835(17)	3.93(11)
C38	0.3700(3)	0.67446(19)	0.34701(19)	3.35(9)
C39	0.8994(3)	0.54080(15)	0.28095(14)	1.48(6)
C40	0.9278(3)	0.59113(15)	0.25252(13)	1.49(6)
C41	1.0362(3)	0.59525(15)	0.26113(14)	1.52(6)
C42	1.0732(3)	0.54943(16)	0.29801(14)	1.82(6)
C43	0.9899(3)	0.51517(15)	0.31012(14)	1.47(6)
C44	0.7930(3)	0.51637(16)	0.27834(15)	2.01(6)
C45	1.0976(3)	0.63793(16)	0.23330(15)	2.09(7)
C46	0.9980(3)	0.45959(15)	0.34411(16)	2.16(7)
C47	0.6571(2)	0.77508(14)	0.29402(13)	1.23(5)
C48	0.5601(2)	0.81130(14)	0.28467(13)	1.34(6)
C49	0.5500(2)	0.85854(15)	0.32060(13)	1.29(6)
C50	0.4601(3)	0.89308(15)	0.31465(14)	1.60(6)
C51	0.3826(3)	0.87810(15)	0.27042(14)	1.68(6)
C52	0.3887(3)	0.83123(15)	0.23414(14)	1.57(6)
C53	0.4790(2)	0.79778(15)	0.24256(13)	1.38(6)
C54	0.4464(3)	0.94505(16)	0.35349(14)	1.97(6)
C55	0.5274(3)	0.99252(16)	0.34941(15)	2.34(7)
C56	0.3410(3)	0.97493(19)	0.33832(17)	2.99(8)
C57	0.4549(3)	0.92216(18)	0.41329(15)	2.69(8)
C58	0.3012(3)	0.81415(16)	0.18719(15)	1.89(6)
C59	0.2513(3)	0.75716(18)	0.20365(17)	2.77(8)
C60	0.3413(3)	0.8034(2)	0.13313(15)	3.08(8)
C61	0.2196(3)	0.86243(19)	0.17714(19)	3.72(10)

Table S12-1. Atomic coordinates and B_{iso}/B_{eq} (continued)

atom	x	y	z	B_{eq}
C62	0.6704(3)	0.78726(16)	0.45876(14)	2.10(7)
C63	0.7575(3)	0.76564(16)	0.43893(15)	2.27(7)
C64	0.8473(3)	0.79146(16)	0.46874(15)	2.19(7)
C65	0.8142(3)	0.83275(17)	0.50518(14)	2.13(7)
C66	0.7058(3)	0.82995(17)	0.50002(15)	2.25(7)
C67	0.5626(3)	0.76742(18)	0.44038(15)	2.67(8)
C68	0.9554(3)	0.77637(19)	0.46501(17)	3.07(8)
C69	0.6439(3)	0.86309(19)	0.53630(16)	2.85(8)

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

Table S12-2. Atomic coordinates and B_{iso} involving hydrogen atoms

atom	x	y	z	B_{iso}
H1A	0.75991	0.75275	0.20930	1.450
H1B	0.64913	0.78223	0.19152	1.450
H5	0.59365	0.58600	0.04744	1.859
H7	0.54981	0.65709	0.19212	1.519
H9A	0.85277	0.59457	0.06235	2.808
H9B	0.89316	0.62751	0.01210	2.808
H9C	0.88889	0.66252	0.06869	2.808
H10A	0.77611	0.74294	0.01526	2.259
H10B	0.78646	0.70801	-0.04061	2.259
H10C	0.67537	0.72322	-0.02660	2.259
H11A	0.69533	0.56795	-0.00460	2.531
H11B	0.62724	0.61897	-0.03845	2.531
H11C	0.73832	0.60376	-0.05245	2.531
H13A	0.52467	0.50496	0.07134	2.829
H13B	0.41786	0.48875	0.09027	2.829
H13C	0.42464	0.54383	0.04956	2.829
H14A	0.60444	0.50805	0.17074	3.129
H14B	0.55693	0.54957	0.21321	3.129
H14C	0.49527	0.49224	0.18700	3.129
H15A	0.40569	0.61451	0.17859	3.046
H15B	0.35218	0.61058	0.11490	3.046
H15C	0.34540	0.55550	0.15562	3.046
H17	0.79499	0.86965	0.01704	1.844
H20	0.72915	0.87682	0.17699	1.820
H21A	0.58651	0.82983	0.10020	2.238
H21B	0.58608	0.86226	0.04186	2.238
H21C	0.63132	0.79637	0.05163	2.238
H22A	0.97851	0.91907	0.03436	2.652
H22B	0.98448	0.96986	0.08069	2.652
H22C	1.04272	0.90798	0.09506	2.652
H23A	0.89385	0.92780	0.22827	2.565
H23B	0.99600	0.91381	0.20358	2.565
H23C	0.93652	0.97527	0.18897	2.565
H24A	0.79339	0.69672	0.29678	1.527
H24B	0.73777	0.64972	0.25245	1.527
H28	0.57718	0.57743	0.44261	1.815
H30	0.53557	0.66263	0.29614	1.629

Table S12-2. Atomic coordinates and B_{iso} involving hydrogens/B_{eq} (continued)

atom	x	y	z	B_{eq}
H32A	0.87990	0.52676	0.41989	2.152
H32B	0.88701	0.49816	0.48040	2.152
H32C	0.79137	0.48317	0.43306	2.152
H33A	0.68354	0.57926	0.52319	2.581
H33B	0.67340	0.51475	0.49511	2.581
H33C	0.76903	0.52974	0.54245	2.581
H34A	0.89736	0.63015	0.46650	2.238
H34B	0.81825	0.64802	0.50663	2.238
H34C	0.90295	0.59791	0.52532	2.238
H36A	0.40253	0.58025	0.28476	4.718
H36B	0.41064	0.52984	0.33154	4.718
H36C	0.30651	0.56670	0.31491	4.718
H37A	0.41903	0.55917	0.43070	4.716
H37B	0.41076	0.62790	0.44645	4.716
H37C	0.31307	0.59402	0.41308	4.716
H38A	0.38940	0.68719	0.31184	4.019
H38B	0.29528	0.67032	0.34237	4.019
H38C	0.39297	0.70420	0.37573	4.019
H40	0.87998	0.61561	0.22548	1.793
H42	1.14729	0.53964	0.31035	2.186
H44A	0.74380	0.54248	0.25539	2.416
H44B	0.78943	0.47645	0.26201	2.416
H44C	0.77643	0.51425	0.31590	2.416
H45A	1.05132	0.66510	0.20979	2.511
H45B	1.14297	0.66083	0.26148	2.511
H45C	1.13893	0.61589	0.21037	2.511
H46A	1.07004	0.45214	0.35972	2.587
H46B	0.95830	0.46417	0.37432	2.587
H46C	0.97083	0.42600	0.32058	2.587
H47A	0.71553	0.80139	0.29023	1.473
H47B	0.66825	0.75967	0.33252	1.473
H51	0.32197	0.90153	0.26489	2.020
H53	0.48521	0.76495	0.21887	1.657
H55A	0.51856	1.02567	0.37422	2.809
H55B	0.59589	0.97531	0.36026	2.809
H55C	0.51970	1.00705	0.31112	2.809
H56A	0.28697	0.94563	0.34052	3.586

Table S12-2. Atomic coordinates and B_{iso} involving hydrogens/B_{eq} (continued)

atom	x	y	z	B_{eq}
H56B	0.33552	1.00752	0.36430	3.586
H56C	0.33327	0.99072	0.30046	3.586
H57A	0.40229	0.89181	0.41494	3.224
H57B	0.52296	0.90479	0.42520	3.224
H57C	0.44479	0.95528	0.43789	3.224
H59A	0.30291	0.72552	0.21029	3.322
H59B	0.22271	0.76417	0.23758	3.322
H59C	0.19633	0.74518	0.17365	3.322
H60A	0.39402	0.77234	0.13881	3.699
H60B	0.28462	0.79058	0.10439	3.699
H60C	0.37086	0.84024	0.12139	3.699
H61A	0.19284	0.86999	0.21156	4.469
H61B	0.24972	0.89903	0.16520	4.469
H61C	0.16349	0.84937	0.14820	4.469
H63	0.75655	0.73218	0.41189	2.727
H65	0.86029	0.85675	0.53349	2.557
H67A	0.51702	0.78960	0.46077	3.204
H67B	0.54266	0.77483	0.40050	3.204
H67C	0.55713	0.72480	0.44777	3.204
H68A	0.95654	0.74625	0.43613	3.680
H68B	0.99112	0.81219	0.45567	3.680
H68C	0.98964	0.76072	0.50078	3.680
H69A	0.68893	0.88981	0.56105	3.417
H69B	0.59063	0.88642	0.51304	3.417
H69C	0.61174	0.83468	0.55850	3.417

Table S12-3. Anisotropic displacement parameters

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Ti1	0.0122(3)	0.0167(3)	0.0150(3)	-0.0009(2)	0.0018(2)	-0.0007(2)
Ti2	0.0104(3)	0.0187(3)	0.0175(3)	0.0004(3)	0.0013(2)	0.0027(3)
Ti3	0.0189(3)	0.0191(3)	0.0219(3)	0.0000(3)	-0.0021(3)	-0.0024(3)
Cl1	0.0208(5)	0.0340(5)	0.0330(5)	-0.0041(4)	0.0133(4)	-0.0097(4)
Cl2	0.0211(4)	0.0286(5)	0.0204(4)	-0.0003(4)	-0.0042(3)	0.0033(4)
Cl3	0.0285(5)	0.0221(5)	0.0268(5)	-0.0065(4)	0.0068(4)	-0.0003(4)
Cl4	0.0155(4)	0.0391(5)	0.0226(5)	0.0033(4)	-0.0020(3)	0.0068(4)
Cl5	0.0426(6)	0.0223(5)	0.0398(6)	0.0019(4)	-0.0100(5)	-0.0080(4)
Cl6	0.0204(5)	0.0402(6)	0.0454(6)	-0.0057(4)	0.0077(4)	-0.0018(5)
O1	0.0147(12)	0.0158(12)	0.0181(12)	-0.0032(10)	0.0040(9)	-0.0008(10)
O2	0.0115(11)	0.0175(12)	0.0151(12)	0.0009(9)	0.0026(9)	0.0017(9)
O3	0.0173(12)	0.0182(12)	0.0183(12)	0.0024(10)	0.0004(10)	-0.0013(10)
N1	0.0147(14)	0.0168(14)	0.0097(13)	0.0013(11)	0.0028(11)	0.0017(11)
C1	0.0159(17)	0.0174(17)	0.0132(16)	-0.0035(14)	0.0040(13)	0.0011(13)
C2	0.0135(16)	0.0182(17)	0.0128(16)	0.0007(14)	-0.0014(13)	0.0010(14)
C3	0.0128(16)	0.0138(16)	0.0172(17)	0.0002(13)	0.0021(13)	0.0008(13)
C4	0.0187(17)	0.0176(17)	0.0157(17)	-0.0014(14)	0.0010(14)	-0.0003(14)
C5	0.0219(18)	0.0181(18)	0.0167(18)	-0.0010(15)	-0.0032(14)	-0.0020(14)
C6	0.0161(17)	0.0211(18)	0.0169(17)	-0.0037(14)	-0.0033(14)	0.0034(14)
C7	0.0157(17)	0.0182(17)	0.0141(17)	-0.0017(14)	0.0023(13)	0.0014(14)
C8	0.0212(19)	0.0238(19)	0.0205(19)	-0.0024(15)	0.0033(14)	-0.0086(15)
C9	0.027(2)	0.036(2)	0.027(2)	0.0018(18)	0.0058(16)	-0.0124(18)
C10	0.028(2)	0.028(2)	0.0168(18)	-0.0083(17)	0.0071(15)	-0.0049(15)
C11	0.033(2)	0.030(2)	0.0191(19)	-0.0046(17)	0.0084(16)	-0.0092(16)
C12	0.0234(19)	0.0210(19)	0.0197(19)	-0.0078(15)	-0.0047(15)	0.0044(15)
C13	0.036(2)	0.024(2)	0.027(2)	-0.0151(18)	-0.0021(17)	0.0026(17)
C14	0.038(2)	0.027(2)	0.030(2)	-0.0122(18)	-0.0066(18)	0.0083(17)
C15	0.028(2)	0.043(2)	0.024(2)	-0.0187(19)	-0.0010(16)	0.0058(18)
C16	0.0143(17)	0.0144(17)	0.0241(19)	0.0010(14)	-0.0005(14)	0.0039(14)
C17	0.0187(18)	0.0220(19)	0.0167(18)	0.0010(15)	-0.0002(14)	0.0065(14)
C18	0.0175(17)	0.0183(18)	0.0220(19)	-0.0035(14)	0.0008(14)	0.0056(14)
C19	0.0173(17)	0.0130(17)	0.0254(19)	0.0010(14)	0.0013(14)	0.0007(14)
C20	0.0180(17)	0.0160(18)	0.0243(19)	0.0026(14)	0.0053(14)	-0.0007(14)
C21	0.0162(18)	0.025(2)	0.028(2)	-0.0010(15)	-0.0007(15)	0.0027(16)
C22	0.025(2)	0.028(2)	0.031(2)	-0.0068(17)	0.0041(16)	0.0083(17)
C23	0.023(2)	0.024(2)	0.033(2)	-0.0002(16)	0.0021(16)	-0.0055(17)
C24	0.0109(16)	0.0210(18)	0.0173(17)	0.0006(14)	0.0047(13)	0.0018(14)

Table S12-3. Anisotropic displacement parameters (continued)

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
C25	0.0121(16)	0.0176(17)	0.0150(17)	0.0020(13)	0.0031(13)	0.0010(13)
C26	0.0096(15)	0.0172(17)	0.0163(17)	0.0020(13)	0.0018(13)	-0.0025(13)
C27	0.0141(16)	0.0172(17)	0.0121(16)	-0.0003(14)	0.0007(13)	-0.0010(13)
C28	0.0154(17)	0.0258(19)	0.0168(18)	0.0011(15)	0.0044(14)	0.0030(15)
C29	0.0115(16)	0.0219(18)	0.0193(18)	0.0006(14)	0.0019(13)	0.0023(14)
C30	0.0106(16)	0.0204(18)	0.0190(18)	0.0007(14)	-0.0020(13)	0.0036(14)
C31	0.0139(17)	0.0232(19)	0.0144(17)	0.0009(14)	-0.0015(13)	0.0027(14)
C32	0.0187(18)	0.0235(19)	0.0242(19)	0.0018(15)	-0.0014(15)	0.0066(15)
C33	0.0172(18)	0.041(2)	0.022(2)	0.0004(17)	-0.0009(15)	0.0122(17)
C34	0.0211(19)	0.032(2)	0.0164(18)	0.0009(16)	-0.0006(14)	0.0010(16)
C35	0.0120(17)	0.031(2)	0.0224(19)	0.0011(15)	0.0028(14)	0.0072(16)
C36	0.017(2)	0.061(3)	0.071(3)	-0.011(2)	0.007(2)	-0.022(3)
C37	0.017(2)	0.095(4)	0.039(3)	0.010(2)	0.0098(18)	0.035(3)
C38	0.0141(19)	0.047(3)	0.066(3)	0.0073(19)	0.0050(19)	0.015(2)
C39	0.0152(17)	0.0209(18)	0.0209(18)	-0.0019(14)	0.0053(14)	-0.0047(14)
C40	0.0183(18)	0.0210(18)	0.0170(18)	-0.0004(15)	0.0015(14)	-0.0019(14)
C41	0.0196(18)	0.0214(18)	0.0181(18)	0.0016(15)	0.0066(14)	0.0006(14)
C42	0.0154(17)	0.029(2)	0.026(2)	0.0022(16)	0.0063(14)	-0.0018(16)
C43	0.0180(17)	0.0198(18)	0.0187(18)	0.0030(14)	0.0052(14)	-0.0007(14)
C44	0.0194(18)	0.026(2)	0.032(2)	-0.0062(16)	0.0054(16)	-0.0069(17)
C45	0.026(2)	0.023(2)	0.033(2)	-0.0031(16)	0.0112(17)	0.0014(17)
C46	0.029(2)	0.0187(19)	0.036(2)	0.0046(16)	0.0101(17)	0.0044(16)
C47	0.0138(16)	0.0197(18)	0.0125(16)	0.0031(14)	0.0003(13)	-0.0004(13)
C48	0.0165(17)	0.0184(18)	0.0162(17)	-0.0011(14)	0.0033(13)	0.0043(14)
C49	0.0106(16)	0.0227(18)	0.0154(17)	-0.0023(14)	0.0014(13)	0.0048(14)
C50	0.0192(18)	0.0204(18)	0.0214(19)	0.0022(15)	0.0037(14)	0.0042(15)
C51	0.0170(17)	0.025(2)	0.0228(19)	0.0024(15)	0.0059(14)	0.0056(15)
C52	0.0155(17)	0.0243(19)	0.0194(18)	-0.0032(15)	0.0010(14)	0.0072(15)
C53	0.0137(16)	0.0208(18)	0.0182(17)	-0.0035(14)	0.0033(13)	0.0044(14)
C54	0.026(2)	0.028(2)	0.0207(19)	0.0102(17)	0.0043(15)	0.0038(16)
C55	0.040(2)	0.0196(19)	0.029(2)	0.0053(17)	0.0042(18)	0.0002(16)
C56	0.033(2)	0.048(3)	0.034(2)	0.018(2)	0.0061(18)	-0.004(2)
C57	0.036(2)	0.042(2)	0.027(2)	0.011(2)	0.0136(18)	0.0022(19)
C58	0.0147(17)	0.025(2)	0.030(2)	-0.0020(15)	-0.0036(15)	0.0104(16)
C59	0.024(2)	0.037(2)	0.039(2)	-0.0107(18)	-0.0089(17)	0.0078(19)
C60	0.029(2)	0.059(3)	0.024(2)	-0.011(2)	-0.0079(17)	0.004(2)
C61	0.029(2)	0.040(3)	0.061(3)	0.003(2)	-0.026(2)	0.003(2)

Table S12-3. Anisotropic displacement parameters (continued)

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
C62	0.032(2)	0.028(2)	0.0164(18)	-0.0067(17)	-0.0035(16)	0.0056(16)
C63	0.043(2)	0.0172(19)	0.021(2)	0.0010(17)	-0.0110(17)	0.0012(15)
C64	0.032(2)	0.026(2)	0.022(2)	0.0063(17)	-0.0064(16)	-0.0023(16)
C65	0.030(2)	0.031(2)	0.0160(18)	-0.0011(17)	-0.0075(15)	-0.0055(16)
C66	0.033(2)	0.031(2)	0.0193(19)	-0.0027(18)	-0.0031(16)	0.0046(16)
C67	0.041(2)	0.039(2)	0.020(2)	-0.015(2)	-0.0001(17)	0.0055(17)
C68	0.035(2)	0.041(3)	0.036(2)	0.015(2)	-0.0087(19)	-0.007(2)
C69	0.030(2)	0.054(3)	0.023(2)	-0.001(2)	0.0011(17)	-0.0042(19)

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 S12-4. Bond lengths (Å)

atom	atom	distance	atom	atom	distance
Ti1	Cl1	2.2615(12)	Ti1	Cl2	2.2475(8)
Ti1	O1	1.779(2)	Ti1	C16	2.343(3)
Ti1	C17	2.324(3)	Ti1	C18	2.393(3)
Ti1	C19	2.403(3)	Ti1	C20	2.337(3)
Ti2	Cl3	2.2376(11)	Ti2	Cl4	2.2679(10)
Ti2	O2	1.797(2)	Ti2	C39	2.362(3)
Ti2	C40	2.320(3)	Ti2	C41	2.388(4)
Ti2	C42	2.365(4)	Ti2	C43	2.374(3)
Ti3	Cl5	2.2552(11)	Ti3	Cl6	2.2521(13)
Ti3	O3	1.793(2)	Ti3	C62	2.361(4)
Ti3	C63	2.326(4)	Ti3	C64	2.409(4)
Ti3	C65	2.372(3)	Ti3	C66	2.369(4)
O1	C3	1.379(4)	O2	C26	1.374(4)
O3	C49	1.374(4)	N1	C1	1.466(4)
N1	C24	1.464(4)	N1	C47	1.454(4)
C1	C2	1.506(4)	C2	C3	1.400(5)
C2	C7	1.385(4)	C3	C4	1.405(4)
C4	C5	1.397(5)	C4	C8	1.538(5)
C5	C6	1.387(5)	C6	C7	1.389(4)
C6	C12	1.532(5)	C8	C9	1.535(5)
C8	C10	1.529(5)	C8	C11	1.531(5)
C12	C13	1.530(5)	C12	C14	1.535(5)
C12	C15	1.529(5)	C16	C17	1.399(5)
C16	C20	1.413(5)	C16	C21	1.497(4)
C17	C18	1.429(4)	C18	C19	1.400(5)
C18	C22	1.491(5)	C19	C20	1.421(5)
C19	C23	1.495(5)	C24	C25	1.509(5)
C25	C26	1.403(4)	C25	C30	1.384(4)
C26	C27	1.402(5)	C27	C28	1.401(5)
C27	C31	1.539(4)	C28	C29	1.390(4)
C29	C30	1.391(5)	C29	C35	1.535(5)
C31	C32	1.530(5)	C31	C33	1.526(5)
C31	C34	1.534(5)	C35	C36	1.525(6)
C35	C37	1.508(6)	C35	C38	1.521(5)
C39	C40	1.411(5)	C39	C43	1.409(4)
C39	C44	1.502(5)	C40	C41	1.416(5)
C41	C42	1.402(5)	C41	C45	1.493(5)

Table S12-4. Bond lengths (Å) (continued)

atom	atom	distance	atom	atom	distance
C42	C43	1.416(5)	C43	C46	1.494(5)
C47	C48	1.504(4)	C48	C49	1.399(5)
C48	C53	1.390(4)	C49	C50	1.407(5)
C50	C51	1.400(4)	C50	C54	1.535(5)
C51	C52	1.388(5)	C52	C53	1.398(5)
C52	C58	1.535(4)	C54	C55	1.527(5)
C54	C56	1.536(5)	C54	C57	1.535(5)
C58	C59	1.526(5)	C58	C60	1.523(6)
C58	C61	1.522(5)	C62	C63	1.409(6)
C62	C66	1.414(5)	C62	C67	1.490(5)
C63	C64	1.411(5)	C64	C65	1.406(5)
C64	C68	1.486(6)	C65	C66	1.419(5)
C66	C69	1.501(6)			

Table S12-5. Bond lengths involving hydrogens (Å)

atom	atom	distance	atom	atom	distance
C1	H1A	0.990	C1	H1B	0.990
C5	H5	0.950	C7	H7	0.950
C9	H9A	0.980	C9	H9B	0.980
C9	H9C	0.980	C10	H10A	0.980
C10	H10B	0.980	C10	H10C	0.980
C11	H11A	0.980	C11	H11B	0.980
C11	H11C	0.980	C13	H13A	0.980
C13	H13B	0.980	C13	H13C	0.980
C14	H14A	0.980	C14	H14B	0.980
C14	H14C	0.980	C15	H15A	0.980
C15	H15B	0.980	C15	H15C	0.980
C17	H17	1.000	C20	H20	1.000
C21	H21A	0.980	C21	H21B	0.980
C21	H21C	0.980	C22	H22A	0.980
C22	H22B	0.980	C22	H22C	0.980
C23	H23A	0.980	C23	H23B	0.980
C23	H23C	0.980	C24	H24A	0.990
C24	H24B	0.990	C28	H28	0.950
C30	H30	0.950	C32	H32A	0.980
C32	H32B	0.980	C32	H32C	0.980
C33	H33A	0.980	C33	H33B	0.980
C33	H33C	0.980	C34	H34A	0.980
C34	H34B	0.980	C34	H34C	0.980
C36	H36A	0.980	C36	H36B	0.980
C36	H36C	0.980	C37	H37A	0.980
C37	H37B	0.980	C37	H37C	0.980
C38	H38A	0.980	C38	H38B	0.980
C38	H38C	0.980	C40	H40	1.000
C42	H42	1.000	C44	H44A	0.980
C44	H44B	0.980	C44	H44C	0.980
C45	H45A	0.980	C45	H45B	0.980
C45	H45C	0.980	C46	H46A	0.980
C46	H46B	0.980	C46	H46C	0.980
C47	H47A	0.990	C47	H47B	0.990
C51	H51	0.950	C53	H53	0.950
C55	H55A	0.980	C55	H55B	0.980
C55	H55C	0.980	C56	H56A	0.980

Table S12-5. Bond lengths involving hydrogens (Å) (continued)

atom	atom	distance	atom	atom	distance
C56	H56B	0.980	C56	H56C	0.980
C57	H57A	0.980	C57	H57B	0.980
C57	H57C	0.980	C59	H59A	0.980
C59	H59B	0.980	C59	H59C	0.980
C60	H60A	0.980	C60	H60B	0.980
C60	H60C	0.980	C61	H61A	0.980
C61	H61B	0.980	C61	H61C	0.980
C63	H63	1.000	C65	H65	1.000
C67	H67A	0.980	C67	H67B	0.980
C67	H67C	0.980	C68	H68A	0.980
C68	H68B	0.980	C68	H68C	0.980
C69	H69A	0.980	C69	H69B	0.980
C69	H69C	0.980			

Table S12-6. Bond angles (°)

atom	atom	atom	angle	atom	atom	atom	angle
Cl1	Ti1	Cl2	101.14(4)	Cl1	Ti1	O1	103.89(8)
Cl1	Ti1	C16	123.86(9)	Cl1	Ti1	C17	90.86(9)
Cl1	Ti1	C18	85.83(9)	Cl1	Ti1	C19	113.81(9)
Cl1	Ti1	C20	143.13(9)	Cl2	Ti1	O1	104.09(8)
Cl2	Ti1	C16	129.17(9)	Cl2	Ti1	C17	141.39(9)
Cl2	Ti1	C18	108.63(8)	Cl2	Ti1	C19	84.16(8)
Cl2	Ti1	C20	94.55(8)	O1	Ti1	C16	88.07(10)
O1	Ti1	C17	108.40(10)	O1	Ti1	C18	143.29(10)
O1	Ti1	C19	139.11(11)	O1	Ti1	C20	104.28(11)
C16	Ti1	C17	34.89(12)	C16	Ti1	C18	58.35(11)
C16	Ti1	C19	58.27(11)	C16	Ti1	C20	35.16(11)
C17	Ti1	C18	35.23(11)	C17	Ti1	C19	57.59(11)
C17	Ti1	C20	57.77(12)	C18	Ti1	C19	33.93(12)
C18	Ti1	C20	57.47(12)	C19	Ti1	C20	34.84(11)
Cl3	Ti2	Cl4	101.07(4)	Cl3	Ti2	O2	103.81(8)
Cl3	Ti2	C39	131.52(9)	Cl3	Ti2	C40	96.67(9)
Cl3	Ti2	C41	84.60(9)	Cl3	Ti2	C42	108.32(9)
Cl3	Ti2	C43	141.48(9)	Cl4	Ti2	O2	104.27(7)
Cl4	Ti2	C39	121.26(9)	Cl4	Ti2	C40	142.80(9)
Cl4	Ti2	C41	114.80(8)	Cl4	Ti2	C42	85.72(8)
Cl4	Ti2	C43	88.87(8)	O2	Ti2	C39	88.57(11)
O2	Ti2	C40	102.81(11)	O2	Ti2	C41	137.70(10)
O2	Ti2	C42	143.77(11)	O2	Ti2	C43	109.64(11)
C39	Ti2	C40	35.07(12)	C39	Ti2	C41	57.97(12)
C39	Ti2	C42	57.52(12)	C39	Ti2	C43	34.62(11)
C40	Ti2	C41	34.98(11)	C40	Ti2	C42	57.60(11)
C40	Ti2	C43	58.02(11)	C41	Ti2	C42	34.30(11)
C41	Ti2	C43	57.79(12)	C42	Ti2	C43	34.76(12)
Cl5	Ti3	Cl6	101.67(5)	Cl5	Ti3	O3	102.62(8)
Cl5	Ti3	C62	119.72(10)	Cl5	Ti3	C63	142.09(10)
Cl5	Ti3	C64	115.69(9)	Cl5	Ti3	C65	85.91(10)
Cl5	Ti3	C66	87.67(10)	Cl6	Ti3	O3	102.76(8)
Cl6	Ti3	C62	132.54(10)	Cl6	Ti3	C63	97.75(11)
Cl6	Ti3	C64	84.63(10)	Cl6	Ti3	C65	107.42(10)
Cl6	Ti3	C66	141.01(10)	O3	Ti3	C62	90.53(11)
O3	Ti3	C63	104.39(12)	O3	Ti3	C64	138.74(12)
O3	Ti3	C65	146.24(12)	O3	Ti3	C66	112.07(12)

Table S12-6. Bond angles (°) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
C62	Ti3	C63	34.97(14)	C62	Ti3	C64	58.03(13)
C62	Ti3	C65	57.77(12)	C62	Ti3	C66	34.78(12)
C63	Ti3	C64	34.61(12)	C63	Ti3	C65	57.16(13)
C63	Ti3	C66	57.66(14)	C64	Ti3	C65	34.20(13)
C64	Ti3	C66	57.70(13)	C65	Ti3	C66	34.83(13)
Ti1	O1	C3	165.4(2)	Ti2	O2	C26	163.0(2)
Ti3	O3	C49	166.7(2)	C1	N1	C24	110.1(2)
C1	N1	C47	110.9(2)	C24	N1	C47	110.2(2)
N1	C1	C2	112.5(3)	C1	C2	C3	121.1(3)
C1	C2	C7	120.2(3)	C3	C2	C7	118.6(3)
O1	C3	C2	117.2(3)	O1	C3	C4	120.9(3)
C2	C3	C4	121.9(3)	C3	C4	C5	116.0(3)
C3	C4	C8	122.8(3)	C5	C4	C8	121.0(3)
C4	C5	C6	124.3(3)	C5	C6	C7	117.0(3)
C5	C6	C12	123.8(3)	C7	C6	C12	119.0(3)
C2	C7	C6	122.1(3)	C4	C8	C9	107.1(3)
C4	C8	C10	112.7(3)	C4	C8	C11	111.4(3)
C9	C8	C10	110.8(3)	C9	C8	C11	107.8(3)
C10	C8	C11	106.9(3)	C6	C12	C13	112.5(3)
C6	C12	C14	108.2(3)	C6	C12	C15	110.7(3)
C13	C12	C14	107.3(3)	C13	C12	C15	109.4(3)
C14	C12	C15	108.6(3)	Ti1	C16	C17	71.81(18)
Ti1	C16	C20	72.20(18)	Ti1	C16	C21	123.3(2)
C17	C16	C20	106.4(3)	C17	C16	C21	126.2(3)
C20	C16	C21	127.4(3)	Ti1	C17	C16	73.30(19)
Ti1	C17	C18	75.06(19)	C16	C17	C18	109.5(3)
Ti1	C18	C17	69.71(19)	Ti1	C18	C19	73.42(19)
Ti1	C18	C22	124.3(2)	C17	C18	C19	107.3(3)
C17	C18	C22	126.8(3)	C19	C18	C22	125.9(3)
Ti1	C19	C18	72.64(19)	Ti1	C19	C20	70.02(18)
Ti1	C19	C23	125.2(2)	C18	C19	C20	107.5(3)
C18	C19	C23	127.2(3)	C20	C19	C23	125.2(3)
Ti1	C20	C16	72.64(19)	Ti1	C20	C19	75.14(19)
C16	C20	C19	109.3(3)	N1	C24	C25	111.8(3)
C24	C25	C26	121.6(3)	C24	C25	C30	119.6(3)
C26	C25	C30	118.8(3)	O2	C26	C25	117.3(3)
O2	C26	C27	121.1(3)	C25	C26	C27	121.5(3)

Table S12-6. Bond angles (°) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
C26	C27	C28	116.4(3)	C26	C27	C31	122.5(3)
C28	C27	C31	121.1(3)	C27	C28	C29	124.0(3)
C28	C29	C30	116.9(3)	C28	C29	C35	123.1(3)
C30	C29	C35	119.9(3)	C25	C30	C29	122.2(3)
C27	C31	C32	109.7(3)	C27	C31	C33	111.9(3)
C27	C31	C34	109.5(3)	C32	C31	C33	107.9(3)
C32	C31	C34	110.8(3)	C33	C31	C34	107.0(3)
C29	C35	C36	107.3(3)	C29	C35	C37	112.4(3)
C29	C35	C38	111.4(3)	C36	C35	C37	109.6(3)
C36	C35	C38	108.8(3)	C37	C35	C38	107.3(3)
Ti2	C39	C40	70.81(18)	Ti2	C39	C43	73.15(19)
Ti2	C39	C44	124.2(2)	C40	C39	C43	107.6(3)
C40	C39	C44	126.7(3)	C43	C39	C44	125.6(3)
Ti2	C40	C39	74.12(19)	Ti2	C40	C41	75.16(19)
C39	C40	C41	109.0(3)	Ti2	C41	C40	69.86(19)
Ti2	C41	C42	72.0(2)	Ti2	C41	C45	125.8(2)
C40	C41	C42	106.4(3)	C40	C41	C45	126.1(3)
C42	C41	C45	127.4(3)	Ti2	C42	C41	73.7(2)
Ti2	C42	C43	73.0(2)	C41	C42	C43	109.5(3)
Ti2	C43	C39	72.23(19)	Ti2	C43	C42	72.3(2)
Ti2	C43	C46	124.3(2)	C39	C43	C42	107.3(3)
C39	C43	C46	126.8(3)	C42	C43	C46	125.8(3)
N1	C47	C48	114.0(2)	C47	C48	C49	119.0(3)
C47	C48	C53	121.8(3)	C49	C48	C53	119.2(3)
O3	C49	C48	116.8(3)	O3	C49	C50	121.7(3)
C48	C49	C50	121.5(3)	C49	C50	C51	116.3(3)
C49	C50	C54	122.8(3)	C51	C50	C54	120.9(3)
C50	C51	C52	124.2(3)	C51	C52	C53	117.0(3)
C51	C52	C58	123.4(3)	C53	C52	C58	119.6(3)
C48	C53	C52	121.7(3)	C50	C54	C55	109.6(3)
C50	C54	C56	112.3(3)	C50	C54	C57	109.6(3)
C55	C54	C56	107.3(3)	C55	C54	C57	110.9(3)
C56	C54	C57	107.2(3)	C52	C58	C59	108.5(3)
C52	C58	C60	111.1(3)	C52	C58	C61	111.6(3)
C59	C58	C60	108.9(3)	C59	C58	C61	108.3(3)
C60	C58	C61	108.3(3)	Ti3	C62	C63	71.2(2)
Ti3	C62	C66	72.9(2)	Ti3	C62	C67	122.2(2)

Table S12-6. Bond angles (°) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
C63	C62	C66	106.7(3)	C63	C62	C67	126.1(3)
C66	C62	C67	127.2(4)	Ti3	C63	C62	73.8(2)
Ti3	C63	C64	75.9(2)	C62	C63	C64	110.3(3)
Ti3	C64	C63	69.5(2)	Ti3	C64	C65	71.5(2)
Ti3	C64	C68	126.0(3)	C63	C64	C65	105.9(3)
C63	C64	C68	127.6(3)	C65	C64	C68	126.5(3)
Ti3	C65	C64	74.3(2)	Ti3	C65	C66	72.5(2)
C64	C65	C66	109.4(3)	Ti3	C66	C62	72.3(2)
Ti3	C66	C65	72.7(2)	Ti3	C66	C69	124.7(3)
C62	C66	C65	107.6(3)	C62	C66	C69	127.6(3)
C65	C66	C69	124.6(3)				

Table S12-7. Bond angles involving hydrogens (°)

atom	atom	atom	angle	atom	atom	atom	angle
N1	C1	H1A	109.1	N1	C1	H1B	109.1
C2	C1	H1A	109.1	C2	C1	H1B	109.1
H1A	C1	H1B	107.9	C4	C5	H5	117.9
C6	C5	H5	117.9	C2	C7	H7	118.9
C6	C7	H7	118.9	C8	C9	H9A	109.5
C8	C9	H9B	109.5	C8	C9	H9C	109.5
H9A	C9	H9B	109.5	H9A	C9	H9C	109.5
H9B	C9	H9C	109.5	C8	C10	H10A	109.5
C8	C10	H10B	109.5	C8	C10	H10C	109.5
H10A	C10	H10B	109.5	H10A	C10	H10C	109.5
H10B	C10	H10C	109.5	C8	C11	H11A	109.5
C8	C11	H11B	109.5	C8	C11	H11C	109.5
H11A	C11	H11B	109.5	H11A	C11	H11C	109.5
H11B	C11	H11C	109.5	C12	C13	H13A	109.5
C12	C13	H13B	109.5	C12	C13	H13C	109.5
H13A	C13	H13B	109.5	H13A	C13	H13C	109.5
H13B	C13	H13C	109.5	C12	C14	H14A	109.5
C12	C14	H14B	109.5	C12	C14	H14C	109.5
H14A	C14	H14B	109.5	H14A	C14	H14C	109.5
H14B	C14	H14C	109.5	C12	C15	H15A	109.5
C12	C15	H15B	109.5	C12	C15	H15C	109.5
H15A	C15	H15B	109.5	H15A	C15	H15C	109.5
H15B	C15	H15C	109.5	Ti1	C17	H17	125.0
C16	C17	H17	125.0	C18	C17	H17	125.0
Ti1	C20	H20	125.1	C16	C20	H20	125.1
C19	C20	H20	125.1	C16	C21	H21A	109.5
C16	C21	H21B	109.5	C16	C21	H21C	109.5
H21A	C21	H21B	109.5	H21A	C21	H21C	109.5
H21B	C21	H21C	109.5	C18	C22	H22A	109.5
C18	C22	H22B	109.5	C18	C22	H22C	109.5
H22A	C22	H22B	109.5	H22A	C22	H22C	109.5
H22B	C22	H22C	109.5	C19	C23	H23A	109.5
C19	C23	H23B	109.5	C19	C23	H23C	109.5
H23A	C23	H23B	109.5	H23A	C23	H23C	109.5
H23B	C23	H23C	109.5	N1	C24	H24A	109.3
N1	C24	H24B	109.3	C25	C24	H24A	109.3
C25	C24	H24B	109.3	H24A	C24	H24B	107.9

Table S12-7. Bond angles involving hydrogens (°) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
C27	C28	H28	118.0	C29	C28	H28	118.0
C25	C30	H30	118.9	C29	C30	H30	118.9
C31	C32	H32A	109.5	C31	C32	H32B	109.5
C31	C32	H32C	109.5	H32A	C32	H32B	109.5
H32A	C32	H32C	109.4	H32B	C32	H32C	109.5
C31	C33	H33A	109.5	C31	C33	H33B	109.5
C31	C33	H33C	109.5	H33A	C33	H33B	109.5
H33A	C33	H33C	109.5	H33B	C33	H33C	109.5
C31	C34	H34A	109.5	C31	C34	H34B	109.5
C31	C34	H34C	109.5	H34A	C34	H34B	109.5
H34A	C34	H34C	109.5	H34B	C34	H34C	109.5
C35	C36	H36A	109.5	C35	C36	H36B	109.5
C35	C36	H36C	109.5	H36A	C36	H36B	109.5
H36A	C36	H36C	109.5	H36B	C36	H36C	109.5
C35	C37	H37A	109.5	C35	C37	H37B	109.5
C35	C37	H37C	109.5	H37A	C37	H37B	109.5
H37A	C37	H37C	109.5	H37B	C37	H37C	109.5
C35	C38	H38A	109.5	C35	C38	H38B	109.5
C35	C38	H38C	109.5	H38A	C38	H38B	109.5
H38A	C38	H38C	109.5	H38B	C38	H38C	109.5
Ti2	C40	H40	125.1	C39	C40	H40	125.1
C41	C40	H40	125.1	Ti2	C42	H42	125.1
C41	C42	H42	125.1	C43	C42	H42	125.1
C39	C44	H44A	109.5	C39	C44	H44B	109.5
C39	C44	H44C	109.5	H44A	C44	H44B	109.5
H44A	C44	H44C	109.5	H44B	C44	H44C	109.5
C41	C45	H45A	109.5	C41	C45	H45B	109.5
C41	C45	H45C	109.5	H45A	C45	H45B	109.5
H45A	C45	H45C	109.5	H45B	C45	H45C	109.5
C43	C46	H46A	109.5	C43	C46	H46B	109.5
C43	C46	H46C	109.5	H46A	C46	H46B	109.5
H46A	C46	H46C	109.5	H46B	C46	H46C	109.5
N1	C47	H47A	108.7	N1	C47	H47B	108.7
C48	C47	H47A	108.8	C48	C47	H47B	108.8
H47A	C47	H47B	107.7	C50	C51	H51	117.9
C52	C51	H51	117.9	C48	C53	H53	119.1
C52	C53	H53	119.1	C54	C55	H55A	109.5

Table S12-7. Bond angles involving hydrogens (°) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
C54	C55	H55B	109.5	C54	C55	H55C	109.5
H55A	C55	H55B	109.5	H55A	C55	H55C	109.5
H55B	C55	H55C	109.5	C54	C56	H56A	109.5
C54	C56	H56B	109.5	C54	C56	H56C	109.5
H56A	C56	H56B	109.5	H56A	C56	H56C	109.5
H56B	C56	H56C	109.5	C54	C57	H57A	109.5
C54	C57	H57B	109.5	C54	C57	H57C	109.5
H57A	C57	H57B	109.5	H57A	C57	H57C	109.5
H57B	C57	H57C	109.5	C58	C59	H59A	109.5
C58	C59	H59B	109.5	C58	C59	H59C	109.5
H59A	C59	H59B	109.5	H59A	C59	H59C	109.5
H59B	C59	H59C	109.5	C58	C60	H60A	109.5
C58	C60	H60B	109.5	C58	C60	H60C	109.5
H60A	C60	H60B	109.5	H60A	C60	H60C	109.5
H60B	C60	H60C	109.5	C58	C61	H61A	109.5
C58	C61	H61B	109.5	C58	C61	H61C	109.5
H61A	C61	H61B	109.5	H61A	C61	H61C	109.5
H61B	C61	H61C	109.5	Ti3	C63	H63	124.5
C62	C63	H63	124.5	C64	C63	H63	124.5
Ti3	C65	H65	125.1	C64	C65	H65	125.1
C66	C65	H65	125.1	C62	C67	H67A	109.5
C62	C67	H67B	109.5	C62	C67	H67C	109.5
H67A	C67	H67B	109.5	H67A	C67	H67C	109.5
H67B	C67	H67C	109.5	C64	C68	H68A	109.5
C64	C68	H68B	109.5	C64	C68	H68C	109.5
H68A	C68	H68B	109.5	H68A	C68	H68C	109.5
H68B	C68	H68C	109.5	C66	C69	H69A	109.5
C66	C69	H69B	109.5	C66	C69	H69C	109.5
H69A	C69	H69B	109.5	H69A	C69	H69C	109.5
H69B	C69	H69C	109.5				

Table S12-8. Torsion Angles(O)
(Those having bond angles > 160 or < 20 degrees are excluded.)

atom1	atom2	atom3	atom4	angle	atom1	atom2	atom3	atom4	angle
Cl1	Ti1	C16	C17	-21.44(16)	Cl1	Ti1	C16	C20	-136.08(10)
Cl1	Ti1	C16	C21	100.4(2)	Cl1	Ti1	C17	C16	162.33(12)
Cl1	Ti1	C17	C18	-81.53(13)	Cl1	Ti1	C18	C17	97.43(13)
Cl1	Ti1	C18	C19	-146.45(12)	Cl1	Ti1	C18	C22	-23.9(2)
Cl1	Ti1	C19	C18	37.05(14)	Cl1	Ti1	C19	C20	153.72(9)
Cl1	Ti1	C19	C23	-86.6(2)	Cl1	Ti1	C20	C16	73.72(18)
Cl1	Ti1	C20	C19	-42.5(2)	Cl2	Ti1	C16	C17	126.43(11)
Cl2	Ti1	C16	C20	11.79(18)	Cl2	Ti1	C16	C21	-111.7(2)
Cl2	Ti1	C17	C16	-88.50(16)	Cl2	Ti1	C17	C18	27.6(2)
Cl2	Ti1	C18	C17	-162.21(10)	Cl2	Ti1	C18	C19	-46.09(14)
Cl2	Ti1	C18	C22	76.4(2)	Cl2	Ti1	C19	C18	136.67(12)
Cl2	Ti1	C19	C20	-106.66(12)	Cl2	Ti1	C19	C23	13.0(2)
Cl2	Ti1	C20	C16	-170.86(12)	Cl2	Ti1	C20	C19	72.95(12)
O1	Ti1	C16	C17	-126.91(14)	O1	Ti1	C16	C20	118.45(14)
O1	Ti1	C16	C21	-5.1(2)	O1	Ti1	C17	C16	57.38(16)
O1	Ti1	C17	C18	173.52(13)	O1	Ti1	C18	C17	-10.3(3)
O1	Ti1	C18	C19	105.80(19)	O1	Ti1	C18	C22	-131.7(2)
O1	Ti1	C19	C18	-118.52(16)	O1	Ti1	C19	C20	-1.8(2)
O1	Ti1	C19	C23	117.8(2)	O1	Ti1	C20	C16	-65.06(15)
O1	Ti1	C20	C19	178.75(12)	C16	Ti1	C17	C16	-0.00(13)
C16	Ti1	C17	C18	116.1(2)	C17	Ti1	C16	C17	-0.00(14)
C17	Ti1	C16	C20	-114.6(2)	C17	Ti1	C16	C21	121.8(3)
C16	Ti1	C18	C17	-37.10(13)	C16	Ti1	C18	C19	79.02(16)
C16	Ti1	C18	C22	-158.5(3)	C18	Ti1	C16	C17	37.46(12)
C18	Ti1	C16	C20	-77.18(15)	C18	Ti1	C16	C21	159.3(3)
C16	Ti1	C19	C18	-79.27(15)	C16	Ti1	C19	C20	37.41(13)
C16	Ti1	C19	C23	157.0(3)	C19	Ti1	C16	C17	77.58(15)
C19	Ti1	C16	C20	-37.07(13)	C19	Ti1	C16	C21	-160.6(3)
C16	Ti1	C20	C16	-0.00(14)	C16	Ti1	C20	C19	-116.2(2)
C20	Ti1	C16	C17	114.6(2)	C20	Ti1	C16	C20	0.00(14)
C20	Ti1	C16	C21	-123.5(3)	C17	Ti1	C18	C17	0.00(15)
C17	Ti1	C18	C19	116.1(3)	C17	Ti1	C18	C22	-121.4(3)
C18	Ti1	C17	C16	-116.1(3)	C18	Ti1	C17	C18	0.00(15)
C17	Ti1	C19	C18	-37.84(13)	C17	Ti1	C19	C20	78.83(15)
C17	Ti1	C19	C23	-161.5(3)	C19	Ti1	C17	C16	-79.72(16)
C19	Ti1	C17	C18	36.42(13)	C17	Ti1	C20	C16	37.92(13)
C17	Ti1	C20	C19	-78.26(15)	C20	Ti1	C17	C16	-38.22(13)

Table S12-8. Torsion angles (°) (continued)

atom1	atom2	atom3	atom4	angle	atom1	atom2	atom3	atom4	angle
C20	Ti1	C17	C18	77.92(15)	C18	Ti1	C19	C18	0.00(14)
C18	Ti1	C19	C20	116.7(2)	C18	Ti1	C19	C23	-123.7(3)
C19	Ti1	C18	C17	-116.1(2)	C19	Ti1	C18	C19	-0.00(13)
C19	Ti1	C18	C22	122.5(3)	C18	Ti1	C20	C16	79.91(15)
C18	Ti1	C20	C19	-36.27(12)	C20	Ti1	C18	C17	-78.85(15)
C20	Ti1	C18	C19	37.27(12)	C20	Ti1	C18	C22	159.8(3)
C19	Ti1	C20	C16	116.2(2)	C19	Ti1	C20	C19	-0.00(14)
C20	Ti1	C19	C18	-116.7(2)	C20	Ti1	C19	C20	-0.00(14)
C20	Ti1	C19	C23	119.6(3)	Cl3	Ti2	C39	C40	7.68(19)
Cl3	Ti2	C39	C43	123.84(11)	Cl3	Ti2	C39	C44	-114.2(2)
Cl3	Ti2	C40	C39	-174.22(11)	Cl3	Ti2	C40	C41	70.59(13)
Cl3	Ti2	C41	C40	-109.78(12)	Cl3	Ti2	C41	C42	134.33(12)
Cl3	Ti2	C41	C45	10.8(2)	Cl3	Ti2	C42	C41	-48.61(14)
Cl3	Ti2	C42	C43	-165.56(9)	Cl3	Ti2	C43	C39	-93.08(16)
Cl3	Ti2	C43	C42	22.3(2)	Cl3	Ti2	C43	C46	144.09(15)
Cl4	Ti2	C39	C40	-139.20(9)	Cl4	Ti2	C39	C43	-23.04(18)
Cl4	Ti2	C39	C44	98.9(2)	Cl4	Ti2	C40	C39	67.5(2)
Cl4	Ti2	C40	C41	-47.7(2)	Cl4	Ti2	C41	C40	150.49(9)
Cl4	Ti2	C41	C42	34.61(15)	Cl4	Ti2	C41	C45	-88.9(2)
Cl4	Ti2	C42	C41	-148.87(13)	Cl4	Ti2	C42	C43	94.18(12)
Cl4	Ti2	C43	C39	160.45(13)	Cl4	Ti2	C43	C42	-84.13(11)
Cl4	Ti2	C43	C46	37.6(2)	O2	Ti2	C39	C40	114.94(14)
O2	Ti2	C39	C43	-128.90(15)	O2	Ti2	C39	C44	-6.9(2)
O2	Ti2	C40	C39	-68.37(14)	O2	Ti2	C40	C41	176.44(12)
O2	Ti2	C41	C40	-5.2(2)	O2	Ti2	C41	C42	-121.06(15)
O2	Ti2	C41	C45	115.4(2)	O2	Ti2	C42	C41	102.7(2)
O2	Ti2	C42	C43	-14.3(2)	O2	Ti2	C43	C39	55.69(16)
O2	Ti2	C43	C42	171.11(11)	O2	Ti2	C43	C46	-67.1(2)
C39	Ti2	C40	C39	-0.00(14)	C39	Ti2	C40	C41	-115.2(2)
C40	Ti2	C39	C40	0.00(14)	C40	Ti2	C39	C43	116.2(3)
C40	Ti2	C39	C44	-121.9(3)	C39	Ti2	C41	C40	37.83(12)
C39	Ti2	C41	C42	-78.06(15)	C39	Ti2	C41	C45	158.4(3)
C41	Ti2	C39	C40	-37.73(13)	C41	Ti2	C39	C43	78.43(16)
C41	Ti2	C39	C44	-159.6(3)	C39	Ti2	C42	C41	79.49(15)
C39	Ti2	C42	C43	-37.46(12)	C42	Ti2	C39	C40	-78.54(16)
C42	Ti2	C39	C43	37.62(13)	C42	Ti2	C39	C44	159.6(3)
C39	Ti2	C43	C39	0.00(15)	C39	Ti2	C43	C42	115.4(3)

Table S12-8. Torsion angles (°) (continued)

atom1	atom2	atom3	atom4	angle	atom1	atom2	atom3	atom4	angle
C39	Ti2	C43	C46	-122.8(3)	C43	Ti2	C39	C40	-116.2(3)
C43	Ti2	C39	C43	-0.00(15)	C43	Ti2	C39	C44	122.0(3)
C40	Ti2	C41	C40	0.00(14)	C40	Ti2	C41	C42	-115.9(2)
C40	Ti2	C41	C45	120.6(3)	C41	Ti2	C40	C39	115.2(2)
C41	Ti2	C40	C41	0.00(14)	C40	Ti2	C42	C41	37.65(13)
C40	Ti2	C42	C43	-79.30(15)	C42	Ti2	C40	C39	78.29(16)
C42	Ti2	C40	C41	-36.90(13)	C40	Ti2	C43	C39	-37.45(13)
C40	Ti2	C43	C42	77.97(15)	C40	Ti2	C43	C46	-160.3(3)
C43	Ti2	C40	C39	36.95(13)	C43	Ti2	C40	C41	-78.24(15)
C41	Ti2	C42	C41	0.00(14)	C41	Ti2	C42	C43	-117.0(2)
C42	Ti2	C41	C40	115.9(2)	C42	Ti2	C41	C42	-0.00(14)
C42	Ti2	C41	C45	-123.5(3)	C41	Ti2	C43	C39	-79.00(15)
C41	Ti2	C43	C42	36.42(12)	C41	Ti2	C43	C46	158.2(3)
C43	Ti2	C41	C40	78.97(15)	C43	Ti2	C41	C42	-36.92(12)
C43	Ti2	C41	C45	-160.5(3)	C42	Ti2	C43	C39	-115.4(2)
C42	Ti2	C43	C42	-0.00(14)	C42	Ti2	C43	C46	121.7(3)
C43	Ti2	C42	C41	117.0(2)	C43	Ti2	C42	C43	-0.00(13)
Cl5	Ti3	C62	C63	-140.25(10)	Cl5	Ti3	C62	C66	-25.29(18)
Cl5	Ti3	C62	C67	98.3(2)	Cl5	Ti3	C63	C62	64.7(2)
Cl5	Ti3	C63	C64	-51.8(3)	Cl5	Ti3	C64	C63	147.62(11)
Cl5	Ti3	C64	C65	31.92(18)	Cl5	Ti3	C64	C68	-90.2(2)
Cl5	Ti3	C65	C64	-151.46(14)	Cl5	Ti3	C65	C66	91.80(14)
Cl5	Ti3	C66	C62	158.20(14)	Cl5	Ti3	C66	C65	-86.19(14)
Cl5	Ti3	C66	C69	34.3(2)	Cl6	Ti3	C62	C63	6.91(19)
Cl6	Ti3	C62	C66	121.87(12)	Cl6	Ti3	C62	C67	-114.5(2)
Cl6	Ti3	C63	C62	-174.87(12)	Cl6	Ti3	C63	C64	68.69(15)
Cl6	Ti3	C64	C63	-112.00(14)	Cl6	Ti3	C64	C65	132.31(14)
Cl6	Ti3	C64	C68	10.2(2)	Cl6	Ti3	C65	C64	-50.50(16)
Cl6	Ti3	C65	C66	-167.24(11)	Cl6	Ti3	C66	C62	-96.04(17)
Cl6	Ti3	C66	C65	19.6(2)	Cl6	Ti3	C66	C69	140.09(17)
O3	Ti3	C62	C63	114.86(14)	O3	Ti3	C62	C66	-130.18(15)
O3	Ti3	C62	C67	-6.6(2)	O3	Ti3	C63	C62	-69.51(16)
O3	Ti3	C63	C64	174.05(15)	O3	Ti3	C64	C63	-8.8(3)
O3	Ti3	C64	C65	-124.45(17)	O3	Ti3	C64	C68	113.5(2)
O3	Ti3	C65	C64	101.8(2)	O3	Ti3	C65	C66	-14.9(3)
O3	Ti3	C66	C62	55.53(18)	O3	Ti3	C66	C65	171.13(13)
O3	Ti3	C66	C69	-68.3(3)	C62	Ti3	C63	C62	0.00(14)

Table S12-8. Torsion angles (°) (continued)

atom1	atom2	atom3	atom4	angle	atom1	atom2	atom3	atom4	angle
C62	Ti3	C63	C64	-116.4(3)	C63	Ti3	C62	C63	0.00(15)
C63	Ti3	C62	C66	115.0(3)	C63	Ti3	C62	C67	-121.4(3)
C62	Ti3	C64	C63	37.23(14)	C62	Ti3	C64	C65	-78.46(17)
C62	Ti3	C64	C68	159.4(3)	C64	Ti3	C62	C63	-36.83(13)
C64	Ti3	C62	C66	78.13(16)	C64	Ti3	C62	C67	-158.2(3)
C62	Ti3	C65	C64	79.28(17)	C62	Ti3	C65	C66	-37.46(14)
C65	Ti3	C62	C63	-77.45(16)	C65	Ti3	C62	C66	37.51(14)
C65	Ti3	C62	C67	161.1(3)	C62	Ti3	C66	C62	0.00(16)
C62	Ti3	C66	C65	115.6(3)	C62	Ti3	C66	C69	-123.9(4)
C66	Ti3	C62	C63	-115.0(3)	C66	Ti3	C62	C66	0.00(16)
C66	Ti3	C62	C67	123.6(4)	C63	Ti3	C64	C63	-0.00(18)
C63	Ti3	C64	C65	-115.7(3)	C63	Ti3	C64	C68	122.2(4)
C64	Ti3	C63	C62	116.4(3)	C64	Ti3	C63	C64	0.00(17)
C63	Ti3	C65	C64	37.53(15)	C63	Ti3	C65	C66	-79.21(18)
C65	Ti3	C63	C62	79.36(17)	C65	Ti3	C63	C64	-37.08(15)
C63	Ti3	C66	C62	-37.96(14)	C63	Ti3	C66	C65	77.65(17)
C63	Ti3	C66	C69	-161.8(3)	C66	Ti3	C63	C62	37.75(14)
C66	Ti3	C63	C64	-78.69(17)	C64	Ti3	C65	C64	-0.00(16)
C64	Ti3	C65	C66	-116.7(3)	C65	Ti3	C64	C63	115.7(3)
C65	Ti3	C64	C65	-0.00(16)	C65	Ti3	C64	C68	-122.1(4)
C64	Ti3	C66	C62	-79.17(17)	C64	Ti3	C66	C65	36.43(14)
C64	Ti3	C66	C69	157.0(3)	C66	Ti3	C64	C63	78.57(18)
C66	Ti3	C64	C65	-37.12(14)	C66	Ti3	C64	C68	-159.2(3)
C65	Ti3	C66	C62	-115.6(3)	C65	Ti3	C66	C65	-0.00(16)
C65	Ti3	C66	C69	120.5(4)	C66	Ti3	C65	C64	116.7(3)
C66	Ti3	C65	C66	-0.00(16)	C1	N1	C24	C25	-165.3(2)
C24	N1	C1	C2	72.6(3)	C1	N1	C47	C48	83.4(3)
C47	N1	C1	C2	-165.2(2)	C24	N1	C47	C48	-154.4(2)
C47	N1	C24	C25	72.1(3)	N1	C1	C2	C3	-156.8(2)
N1	C1	C2	C7	22.1(4)	C1	C2	C3	O1	3.8(4)
C1	C2	C3	C4	-178.9(2)	C1	C2	C7	C6	-178.5(2)
C3	C2	C7	C6	0.4(4)	C7	C2	C3	O1	-175.2(2)
C7	C2	C3	C4	2.2(4)	O1	C3	C4	C5	174.9(2)
O1	C3	C4	C8	-0.6(4)	C2	C3	C4	C5	-2.4(4)
C2	C3	C4	C8	-177.9(2)	C3	C4	C5	C6	0.0(4)
C3	C4	C8	C9	66.8(4)	C3	C4	C8	C10	-55.3(4)
C3	C4	C8	C11	-175.5(3)	C5	C4	C8	C9	-108.5(3)

Table S12-8. Torsion angles (°) (continued)

atom1	atom2	atom3	atom4	angle	atom1	atom2	atom3	atom4	angle
C5	C4	C8	C10	129.4(3)	C5	C4	C8	C11	9.2(4)
C8	C4	C5	C6	175.6(3)	C4	C5	C6	C7	2.4(5)
C4	C5	C6	C12	-172.4(3)	C5	C6	C7	C2	-2.6(4)
C5	C6	C12	C13	-10.4(4)	C5	C6	C12	C14	107.9(3)
C5	C6	C12	C15	-133.1(3)	C7	C6	C12	C13	174.9(2)
C7	C6	C12	C14	-66.7(4)	C7	C6	C12	C15	52.2(4)
C12	C6	C7	C2	172.4(2)	Ti1	C16	C17	Ti1	0.000(15)
Ti1	C16	C17	C18	-66.94(19)	Ti1	C16	C20	Ti1	0.000(16)
Ti1	C16	C20	C19	66.78(18)	C17	C16	C20	Ti1	-64.2(2)
C17	C16	C20	C19	2.6(3)	C20	C16	C17	Ti1	64.4(2)
C20	C16	C17	C18	-2.5(3)	C21	C16	C17	Ti1	-118.4(3)
C21	C16	C17	C18	174.7(3)	C21	C16	C20	Ti1	118.7(3)
C21	C16	C20	C19	-174.5(3)	Ti1	C17	C18	Ti1	-0.000(14)
Ti1	C17	C18	C19	-64.31(19)	Ti1	C17	C18	C22	118.3(3)
C16	C17	C18	Ti1	65.8(2)	C16	C17	C18	C19	1.5(4)
C16	C17	C18	C22	-175.9(3)	Ti1	C18	C19	Ti1	0.000(13)
Ti1	C18	C19	C20	-61.71(17)	Ti1	C18	C19	C23	121.4(3)
C17	C18	C19	Ti1	61.9(2)	C17	C18	C19	C20	0.2(3)
C17	C18	C19	C23	-176.7(3)	C22	C18	C19	Ti1	-120.7(3)
C22	C18	C19	C20	177.6(3)	C22	C18	C19	C23	0.7(5)
Ti1	C19	C20	Ti1	-0.000(12)	Ti1	C19	C20	C16	-65.16(18)
C18	C19	C20	Ti1	63.4(2)	C18	C19	C20	C16	-1.7(3)
C23	C19	C20	Ti1	-119.6(3)	C23	C19	C20	C16	175.2(3)
N1	C24	C25	C26	-153.3(2)	N1	C24	C25	C30	25.2(4)
C24	C25	C26	O2	-4.1(4)	C24	C25	C26	C27	174.1(3)
C24	C25	C30	C29	-177.0(3)	C26	C25	C30	C29	1.4(5)
C30	C25	C26	O2	177.5(3)	C30	C25	C26	C27	-4.3(4)
O2	C26	C27	C28	-178.1(2)	O2	C26	C27	C31	2.2(4)
C25	C26	C27	C28	3.7(4)	C25	C26	C27	C31	-175.9(3)
C26	C27	C28	C29	-0.4(5)	C26	C27	C31	C32	-63.3(4)
C26	C27	C31	C33	177.1(3)	C26	C27	C31	C34	58.5(4)
C28	C27	C31	C32	117.1(3)	C28	C27	C31	C33	-2.6(4)
C28	C27	C31	C34	-121.1(3)	C31	C27	C28	C29	179.3(3)
C27	C28	C29	C30	-2.3(5)	C27	C28	C29	C35	176.1(3)
C28	C29	C30	C25	1.7(5)	C28	C29	C35	C36	-106.2(3)
C28	C29	C35	C37	14.4(4)	C28	C29	C35	C38	134.8(3)
C30	C29	C35	C36	72.2(4)	C30	C29	C35	C37	-167.2(3)

Table S12-8. Torsion angles (°) (continued)

atom1	atom2	atom3	atom4	angle	atom1	atom2	atom3	atom4	angle
C30	C29	C35	C38	-46.8(4)	C35	C29	C30	C25	-176.7(3)
Ti2	C39	C40	Ti2	0.000(14)	Ti2	C39	C40	C41	67.69(18)
Ti2	C39	C43	Ti2	-0.000(14)	Ti2	C39	C43	C42	-64.27(19)
Ti2	C39	C43	C46	120.0(3)	C40	C39	C43	Ti2	62.8(2)
C40	C39	C43	C42	-1.5(4)	C40	C39	C43	C46	-177.2(3)
C43	C39	C40	Ti2	-64.4(2)	C43	C39	C40	C41	3.3(4)
C44	C39	C40	Ti2	118.9(4)	C44	C39	C40	C41	-173.4(3)
C44	C39	C43	Ti2	-120.4(4)	C44	C39	C43	C42	175.3(3)
C44	C39	C43	C46	-0.4(6)	Ti2	C40	C41	Ti2	-0.000(17)
Ti2	C40	C41	C42	63.11(19)	Ti2	C40	C41	C45	-120.3(3)
C39	C40	C41	Ti2	-67.0(2)	C39	C40	C41	C42	-3.9(4)
C39	C40	C41	C45	172.7(3)	Ti2	C41	C42	Ti2	-0.000(14)
Ti2	C41	C42	C43	64.7(2)	C40	C41	C42	Ti2	-61.7(2)
C40	C41	C42	C43	3.0(4)	C45	C41	C42	Ti2	121.7(4)
C45	C41	C42	C43	-173.6(3)	Ti2	C42	C43	Ti2	-0.000(12)
Ti2	C42	C43	C39	64.24(19)	Ti2	C42	C43	C46	-120.0(3)
C41	C42	C43	Ti2	-65.2(3)	C41	C42	C43	C39	-1.0(4)
C41	C42	C43	C46	174.8(3)	N1	C47	C48	C49	176.8(2)
N1	C47	C48	C53	-0.9(4)	C47	C48	C49	O3	1.4(4)
C47	C48	C49	C50	-178.5(3)	C47	C48	C53	C52	179.5(3)
C49	C48	C53	C52	1.9(5)	C53	C48	C49	O3	179.1(3)
C53	C48	C49	C50	-0.8(5)	O3	C49	C50	C51	179.1(3)
O3	C49	C50	C54	-0.1(5)	C48	C49	C50	C51	-1.0(5)
C48	C49	C50	C54	179.8(3)	C49	C50	C51	C52	1.8(5)
C49	C50	C54	C55	61.4(4)	C49	C50	C54	C56	-179.4(3)
C49	C50	C54	C57	-60.4(4)	C51	C50	C54	C55	-117.7(3)
C51	C50	C54	C56	1.4(4)	C51	C50	C54	C57	120.4(3)
C54	C50	C51	C52	-178.9(3)	C50	C51	C52	C53	-0.8(5)
C50	C51	C52	C58	177.7(3)	C51	C52	C53	C48	-1.1(5)
C51	C52	C58	C59	-106.2(4)	C51	C52	C58	C60	134.1(3)
C51	C52	C58	C61	13.2(5)	C53	C52	C58	C59	72.3(4)
C53	C52	C58	C60	-47.4(4)	C53	C52	C58	C61	-168.4(3)
C58	C52	C53	C48	-179.7(3)	Ti3	C62	C63	Ti3	-0.000(17)
Ti3	C62	C63	C64	67.8(2)	Ti3	C62	C66	Ti3	0.000(17)
Ti3	C62	C66	C65	-64.6(2)	Ti3	C62	C66	C69	120.6(3)
C63	C62	C66	Ti3	63.6(2)	C63	C62	C66	C65	-1.0(4)
C63	C62	C66	C69	-175.8(3)	C66	C62	C63	Ti3	-64.8(3)

Table S12-8. Torsion angles (°) (continued)

atom1	atom2	atom3	atom4	angle	atom1	atom2	atom3	atom4	angle
C66	C62	C63	C64	3.0(4)	C67	C62	C63	Ti3	116.6(4)
C67	C62	C63	C64	-175.6(3)	C67	C62	C66	Ti3	-117.8(4)
C67	C62	C66	C65	177.6(3)	C67	C62	C66	C69	2.8(6)
Ti3	C63	C64	Ti3	-0.000(19)	Ti3	C63	C64	C65	62.6(2)
Ti3	C63	C64	C68	-120.3(3)	C62	C63	C64	Ti3	-66.5(3)
C62	C63	C64	C65	-3.9(4)	C62	C63	C64	C68	173.2(3)
Ti3	C64	C65	Ti3	0.000(17)	Ti3	C64	C65	C66	64.5(2)
C63	C64	C65	Ti3	-61.3(2)	C63	C64	C65	C66	3.2(4)
C68	C64	C65	Ti3	121.5(4)	C68	C64	C65	C66	-173.9(3)
Ti3	C65	C66	Ti3	-0.000(17)	Ti3	C65	C66	C62	64.3(2)
Ti3	C65	C66	C69	-120.6(3)	C64	C65	C66	Ti3	-65.7(3)
C64	C65	C66	C62	-1.4(4)	C64	C65	C66	C69	173.6(3)

Table S12-9. Intramolecular contacts less than 3.60 Å

atom	atom	distance	atom	atom	distance
Cl1	C22	3.309(4)	Cl2	C23	3.223(4)
Cl3	C45	3.232(4)	Cl4	C46	3.506(4)
Cl5	C69	3.438(4)	Cl6	C68	3.256(4)
O1	C1	2.811(4)	O1	C8	2.948(4)
O1	C9	3.122(4)	O1	C10	3.029(4)
O1	C21	3.152(4)	O2	C24	2.825(4)
O2	C31	2.943(4)	O2	C32	3.080(4)
O2	C34	3.035(4)	O2	C44	3.216(4)
O3	C47	2.749(4)	O3	C54	2.962(4)
O3	C55	3.083(4)	O3	C57	3.072(5)
O3	C67	3.219(5)	N1	C7	2.811(4)
N1	C30	2.798(4)	N1	C53	2.830(4)
C1	C20	3.563(5)	C1	C48	3.166(5)
C1	C53	3.264(5)	C2	C5	2.757(5)
C2	C24	3.027(4)	C3	C6	2.795(5)
C3	C9	3.123(5)	C3	C10	3.138(5)
C3	C21	3.397(5)	C4	C7	2.806(5)
C5	C9	3.471(5)	C5	C11	2.835(5)
C5	C13	2.908(5)	C5	C14	3.497(5)
C7	C14	3.067(5)	C7	C15	2.987(5)
C7	C24	3.239(4)	C22	C23	3.178(5)
C24	C40	3.478(5)	C25	C28	2.759(5)
C25	C44	3.549(5)	C25	C47	3.006(4)
C26	C29	2.802(4)	C26	C32	3.134(4)
C26	C34	3.095(4)	C26	C44	3.351(5)
C27	C30	2.805(4)	C28	C32	3.578(5)
C28	C33	2.841(5)	C28	C36	3.459(5)
C28	C37	2.897(5)	C30	C36	3.114(5)
C30	C38	2.978(5)	C30	C47	3.240(5)
C44	C46	3.178(5)	C47	C63	3.573(5)
C48	C51	2.760(5)	C49	C52	2.807(4)
C49	C55	3.119(5)	C49	C57	3.116(5)
C49	C67	3.553(5)	C50	C53	2.811(5)
C51	C55	3.574(5)	C51	C56	2.846(6)
C51	C59	3.481(5)	C51	C61	2.885(5)
C53	C59	3.138(5)	C53	C60	2.976(5)
C67	C69	3.230(5)			

Table S12-10. Intramolecular contacts less than 3.60 Å involving hydrogens

atom	atom	distance	atom	atom	distance
Ti1	H1A	3.008	Ti1	H9C	3.398
Ti1	H10A	2.997	Ti1	H21C	3.355
Ti1	H22C	3.429	Ti1	H23B	3.464
Ti2	H24A	3.139	Ti2	H32A	3.041
Ti2	H34A	3.293	Ti2	H44C	3.409
Ti2	H45B	3.463	Ti2	H46B	3.411
Ti3	H47A	3.329	Ti3	H47B	3.167
Ti3	H55B	3.285	Ti3	H57B	3.103
Ti3	H67B	3.327	Ti3	H68B	3.471
Ti3	H69B	3.427	Cl1	H9C	2.985
Cl1	H10A	3.090	Cl1	H17	3.402
Cl1	H22A	3.245	Cl1	H22C	2.987
Cl2	H1A	2.791	Cl2	H20	3.587
Cl2	H23A	3.259	Cl2	H23B	2.807
Cl2	H45A	3.073	Cl3	H24A	3.041
Cl3	H45A	3.299	Cl3	H45B	2.797
Cl3	H68A	2.881	Cl4	H32A	2.993
Cl4	H34A	3.020	Cl4	H42	3.189
Cl4	H46A	3.361	Cl4	H46B	3.308
Cl5	H55B	2.796	Cl5	H57B	3.209
Cl5	H65	3.206	Cl5	H69A	3.303
Cl5	H69B	3.226	Cl6	H47A	2.945
Cl6	H68A	3.347	Cl6	H68B	2.798
O1	H1A	2.484	O1	H1B	3.065
O1	H9A	3.595	O1	H9C	2.490
O1	H10A	2.357	O1	H10C	3.501
O1	H21A	3.368	O1	H21C	2.704
O2	H24A	2.510	O2	H24B	3.077
O2	H32A	2.420	O2	H32C	3.594
O2	H34A	2.363	O2	H34B	3.523
O2	H40	3.590	O2	H44A	3.387
O2	H44C	2.806	O2	H63	3.095
O2	H68A	3.453	O3	H47A	2.700
O3	H47B	2.639	O3	H55B	2.424
O3	H55C	3.562	O3	H57A	3.530
O3	H57B	2.416	O3	H67A	3.548
O3	H67B	2.680	N1	H7	2.457

Table S12-10. Intramolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
N1	H30	2.455	N1	H53	2.462
C1	H7	2.645	C1	H20	3.116
C1	H21A	3.261	C1	H24A	2.705
C1	H24B	2.488	C1	H47A	2.449
C1	H47B	3.217	C1	H53	2.773
C2	H21A	3.336	C2	H21C	3.373
C2	H24A	3.549	C2	H24B	2.609
C2	H53	3.298	C3	H1A	2.648
C3	H1B	2.919	C3	H5	3.233
C3	H7	3.252	C3	H9A	3.343
C3	H9C	2.854	C3	H10A	2.845
C3	H10C	3.401	C3	H21A	3.382
C3	H21C	2.776	C3	H24B	3.547
C4	H9A	2.623	C4	H9B	3.329
C4	H9C	2.675	C4	H10A	2.730
C4	H10B	3.390	C4	H10C	2.770
C4	H11A	2.701	C4	H11B	2.754
C4	H11C	3.376	C4	H21C	3.247
C5	H7	3.227	C5	H9A	3.294
C5	H11A	2.633	C5	H11B	2.838
C5	H13A	2.716	C5	H13C	2.921
C5	H14A	3.347	C6	H13A	2.717
C6	H13B	3.381	C6	H13C	2.766
C6	H14A	2.663	C6	H14B	2.666
C6	H14C	3.337	C6	H15A	2.674
C6	H15B	2.739	C6	H15C	3.360
C7	H1A	3.239	C7	H1B	3.008
C7	H5	3.220	C7	H14A	3.349
C7	H14B	2.769	C7	H15A	2.653
C7	H15B	3.269	C7	H24B	2.745
C7	H30	3.467	C7	H53	3.210
C8	H5	2.678	C9	H10A	2.733
C9	H10B	2.691	C9	H10C	3.365
C9	H11A	2.662	C9	H11B	3.332
C9	H11C	2.649	C10	H9A	3.365
C10	H9B	2.712	C10	H9C	2.712
C10	H11A	3.317	C10	H11B	2.635

Table S12-10. Intramolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
C10	H11C	2.635	C10	H21C	2.997
C11	H5	2.412	C11	H9A	2.683
C11	H9B	2.631	C11	H9C	3.330
C11	H10A	3.317	C11	H10B	2.635
C11	H10C	2.635	C12	H5	2.720
C12	H7	2.644	C13	H5	2.517
C13	H14A	2.661	C13	H14B	3.325
C13	H14C	2.633	C13	H15A	3.345
C13	H15B	2.682	C13	H15C	2.682
C14	H7	2.992	C14	H13A	2.664
C14	H13B	2.628	C14	H13C	3.325
C14	H15A	2.694	C14	H15B	3.340
C14	H15C	2.646	C14	H44A	3.017
C15	H7	2.718	C15	H13A	3.345
C15	H13B	2.682	C15	H13C	2.682
C15	H14A	3.339	C15	H14B	2.671
C15	H14C	2.671	C15	H36A	3.358
C16	H1B	3.339	C16	H10A	3.332
C17	H10A	3.122	C17	H20	3.215
C17	H21A	3.352	C17	H21B	2.847
C17	H21C	2.847	C17	H22A	2.683
C17	H22B	3.205	C17	H22C	3.235
C18	H20	3.235	C18	H23A	3.358
C18	H23B	2.861	C18	H23C	2.861
C19	H17	3.237	C19	H22A	3.346
C19	H22B	2.838	C19	H22C	2.838
C20	H1A	3.229	C20	H1B	2.993
C20	H17	3.215	C20	H21A	2.690
C20	H21B	3.199	C20	H21C	3.232
C20	H23A	2.652	C20	H23B	3.219
C20	H23C	3.182	C21	H1B	3.182
C21	H10A	3.309	C21	H10C	3.575
C21	H17	2.882	C21	H20	2.921
C22	H17	2.920	C22	H23B	3.152
C22	H23C	3.159	C23	H20	2.886
C23	H22B	3.145	C23	H22C	3.153
C24	H1A	2.516	C24	H1B	3.245

Table S12-10. Intramolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
C24	H7	2.956	C24	H30	2.634
C24	H40	2.988	C24	H44A	3.143
C24	H47A	2.773	C24	H47B	2.407
C24	H63	3.370	C25	H7	3.482
C25	H44A	3.098	C25	H44C	3.240
C25	H47B	2.559	C25	H63	2.874
C26	H24A	2.649	C26	H24B	2.956
C26	H28	3.238	C26	H30	3.255
C26	H32A	2.831	C26	H32C	3.415
C26	H34A	2.791	C26	H34B	3.349
C26	H44A	3.299	C26	H44C	2.767
C26	H47B	3.419	C26	H63	2.726
C27	H32A	2.678	C27	H32B	3.357
C27	H32C	2.709	C27	H33A	2.727
C27	H33B	2.738	C27	H33C	3.380
C27	H34A	2.683	C27	H34B	2.706
C27	H34C	3.359	C27	H44C	3.259
C27	H63	3.168	C28	H30	3.231
C28	H32C	3.489	C28	H33A	2.745
C28	H33B	2.733	C28	H34B	3.536
C28	H36B	3.308	C28	H37A	2.689
C28	H37B	2.924	C28	H67C	3.146
C29	H36A	2.623	C29	H36B	2.659
C29	H36C	3.322	C29	H37A	2.703
C29	H37B	2.743	C29	H37C	3.368
C29	H38A	2.689	C29	H38B	3.365
C29	H38C	2.740	C29	H67C	3.061
C30	H7	3.249	C30	H14B	3.472
C30	H24A	3.246	C30	H24B	2.983
C30	H28	3.225	C30	H36A	2.802
C30	H36B	3.437	C30	H38A	2.660
C30	H38C	3.215	C30	H47B	2.825
C30	H63	3.470	C30	H67B	3.514
C30	H67C	3.523	C31	H28	2.685
C32	H33A	3.326	C32	H33B	2.650
C32	H33C	2.651	C32	H34A	2.732
C32	H34B	3.364	C32	H34C	2.693

Table S12-10. Intramolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
C32	H44C	3.205	C32	H46B	2.813
C33	H28	2.421	C33	H32A	3.325
C33	H32B	2.651	C33	H32C	2.652
C33	H34A	3.318	C33	H34B	2.639
C33	H34C	2.639	C34	H32A	2.735
C34	H32B	2.688	C34	H32C	3.365
C34	H33A	2.643	C34	H33B	3.319
C34	H33C	2.631	C34	H63	3.433
C35	H28	2.713	C35	H30	2.664
C35	H67C	3.508	C36	H30	3.055
C36	H37A	2.678	C36	H37B	3.328
C36	H37C	2.648	C36	H38A	2.672
C36	H38B	2.649	C36	H38C	3.328
C37	H28	2.514	C37	H36A	3.325
C37	H36B	2.667	C37	H36C	2.667
C37	H38A	3.295	C37	H38B	2.621
C37	H38C	2.621	C38	H30	2.706
C38	H36A	2.684	C38	H36B	3.327
C38	H36C	2.640	C38	H37A	3.298
C38	H37B	2.617	C38	H37C	2.617
C38	H59A	3.503	C38	H67B	3.319
C38	H67C	3.380	C39	H24B	3.249
C39	H32A	3.462	C39	H42	3.236
C39	H46A	3.364	C39	H46B	2.861
C39	H46C	2.861	C40	H24A	3.257
C40	H24B	2.838	C40	H42	3.223
C40	H44A	2.680	C40	H44B	3.193
C40	H44C	3.230	C40	H45A	2.663
C40	H45B	3.223	C40	H45C	3.182
C42	H40	3.220	C42	H45A	3.359
C42	H45B	2.863	C42	H45C	2.863
C42	H46A	2.661	C42	H46B	3.226
C42	H46C	3.176	C43	H32A	3.269
C43	H40	3.238	C43	H44A	3.362
C43	H44B	2.850	C43	H44C	2.850
C44	H14A	3.312	C44	H14B	3.343
C44	H24B	3.125	C44	H32A	3.465

Table S12-10. Intramolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
C44	H40	2.910	C44	H46B	3.152
C44	H46C	3.148	C45	H40	2.897
C45	H42	2.906	C46	H32A	3.019
C46	H42	2.892	C46	H44B	3.150
C46	H44C	3.145	C47	H1A	2.707
C47	H1B	2.494	C47	H24A	2.513
C47	H24B	3.237	C47	H30	3.001
C47	H53	2.682	C47	H63	3.112
C47	H67B	3.221	C48	H1B	2.809
C48	H30	3.374	C48	H67B	2.992
C49	H47A	2.746	C49	H47B	2.705
C49	H51	3.241	C49	H53	3.260
C49	H55B	2.829	C49	H55C	3.366
C49	H57A	3.346	C49	H57B	2.837
C49	H67B	2.725	C50	H55A	3.350
C50	H55B	2.686	C50	H55C	2.686
C50	H56A	2.742	C50	H56B	3.387
C50	H56C	2.749	C50	H57A	2.686
C50	H57B	2.703	C50	H57C	3.357
C50	H67B	3.449	C51	H53	3.236
C51	H55C	3.475	C51	H56A	2.750
C51	H56C	2.745	C51	H57A	3.511
C51	H59B	3.333	C51	H61A	2.682
C51	H61B	2.899	C52	H59A	2.656
C52	H59B	2.676	C52	H59C	3.337
C52	H60A	2.690	C52	H60B	3.364
C52	H60C	2.733	C52	H61A	2.700
C52	H61B	2.739	C52	H61C	3.369
C53	H1B	2.771	C53	H7	3.575
C53	H30	3.343	C53	H38A	3.335
C53	H47A	3.150	C53	H47B	3.160
C53	H51	3.230	C53	H59A	2.841
C53	H59B	3.456	C53	H60A	2.658
C53	H60C	3.210	C54	H51	2.675
C55	H56A	3.322	C55	H56B	2.645
C55	H56C	2.645	C55	H57A	3.364
C55	H57B	2.713	C55	H57C	2.713

Table S12-10. Intramolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
C56	H51	2.419	C56	H55A	2.626
C56	H55B	3.324	C56	H55C	2.660
C56	H57A	2.673	C56	H57B	3.328
C56	H57C	2.623	C57	H55A	2.703
C57	H55B	2.719	C57	H55C	3.365
C57	H56A	2.655	C57	H56B	2.641
C57	H56C	3.328	C57	H67A	3.253
C57	H67B	3.541	C57	H69B	2.889
C58	H51	2.714	C58	H53	2.667
C59	H38A	3.344	C59	H53	3.058
C59	H60A	2.681	C59	H60B	2.645
C59	H60C	3.330	C59	H61A	2.668
C59	H61B	3.324	C59	H61C	2.637
C60	H21A	3.521	C60	H53	2.725
C60	H59A	2.682	C60	H59B	3.330
C60	H59C	2.646	C60	H61A	3.321
C60	H61B	2.650	C60	H61C	2.650
C61	H51	2.496	C61	H59A	3.323
C61	H59B	2.654	C61	H59C	2.653
C61	H60A	3.321	C61	H60B	2.650
C61	H60C	2.650	C62	H47B	3.142
C62	H57B	3.304	C62	H65	3.248
C62	H69A	3.379	C62	H69B	2.883
C62	H69C	2.883	C63	H34A	3.569
C63	H34B	3.151	C63	H47B	2.673
C63	H65	3.214	C63	H67A	3.355
C63	H67B	2.846	C63	H67C	2.846
C63	H68A	2.681	C63	H68B	3.223
C63	H68C	3.189	C64	H34B	3.394
C65	H63	3.210	C65	H68A	3.352
C65	H68B	2.846	C65	H68C	2.847
C65	H69A	2.648	C65	H69B	3.229
C65	H69C	3.168	C66	H57B	3.246
C66	H63	3.225	C66	H67A	2.678
C66	H67B	3.217	C66	H67C	3.200
C67	H38C	2.891	C67	H47B	3.188
C67	H57A	3.501	C67	H57B	3.144

Table S12-10. Intramolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
C67	H63	2.880	C67	H69B	3.198
C67	H69C	3.226	C68	H34A	3.377
C68	H63	2.905	C68	H65	2.890
C69	H57B	3.058	C69	H65	2.878
C69	H67A	2.813	H1A	H7	3.483
H1A	H20	2.909	H1A	H24A	2.456
H1A	H24B	2.582	H1A	H40	3.460
H1A	H47A	2.416	H1A	H47B	3.432
H1B	H7	3.106	H1B	H20	2.428
H1B	H21A	2.488	H1B	H21C	3.401
H1B	H24A	3.508	H1B	H24B	3.447
H1B	H47A	2.463	H1B	H47B	3.449
H1B	H53	2.405	H1B	H60A	3.411
H5	H9A	3.391	H5	H11A	2.040
H5	H11B	2.337	H5	H11C	3.368
H5	H13A	2.161	H5	H13B	3.478
H5	H13C	2.437	H5	H14A	3.467
H7	H14A	3.485	H7	H14B	2.470
H7	H15A	2.109	H7	H15B	3.136
H7	H15C	3.537	H7	H24B	2.674
H7	H30	2.583	H7	H53	2.688
H7	H60A	3.429	H9A	H10B	3.586
H9A	H11A	2.496	H9A	H11B	3.578
H9A	H11C	2.963	H9B	H10A	3.029
H9B	H10B	2.513	H9B	H10C	3.593
H9B	H11A	2.906	H9B	H11B	3.532
H9B	H11C	2.426	H9C	H10A	2.558
H9C	H10B	2.967	H9C	H11A	3.570
H9C	H11C	3.535	H10A	H11B	3.536
H10A	H11C	3.535	H10A	H17	2.859
H10A	H21C	2.544	H10B	H11A	3.535
H10B	H11B	2.912	H10B	H11C	2.433
H10C	H11A	3.535	H10C	H11B	2.433
H10C	H11C	2.912	H10C	H21C	2.659
H11A	H13A	3.456	H13A	H14A	2.482
H13A	H14B	3.565	H13A	H14C	2.930
H13A	H15B	3.576	H13A	H15C	3.576

Table S12-10. Intramolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
H13B	H14A	2.919	H13B	H14B	3.525
H13B	H14C	2.414	H13B	H15A	3.577
H13B	H15B	2.965	H13B	H15C	2.496
H13C	H14A	3.565	H13C	H14C	3.528
H13C	H15A	3.577	H13C	H15B	2.496
H13C	H15C	2.965	H14A	H15A	3.584
H14A	H15C	3.548	H14A	H44A	2.645
H14A	H44B	3.104	H14B	H15A	2.506
H14B	H15B	3.578	H14B	H15C	2.916
H14B	H24B	3.308	H14B	H30	3.292
H14B	H36A	2.983	H14B	H44A	2.518
H14B	H44B	3.514	H14B	H44C	3.594
H14C	H15A	2.987	H14C	H15B	3.556
H14C	H15C	2.456	H14C	H36A	3.479
H15A	H30	3.274	H15A	H36A	2.713
H15A	H59A	3.005	H15C	H36A	3.168
H17	H21B	2.931	H17	H21C	2.954
H17	H22A	2.638	H17	H22B	3.531
H20	H21A	2.648	H20	H21B	3.535
H20	H23A	2.591	H20	H23B	3.578
H20	H23C	3.498	H20	H47A	3.276
H21A	H60A	3.138	H21A	H60C	2.992
H22B	H23B	3.236	H22B	H23C	2.825
H22C	H23B	2.825	H22C	H23C	3.257
H24A	H30	3.492	H24A	H40	2.888
H24A	H47A	2.563	H24A	H47B	2.447
H24A	H63	3.040	H24B	H30	3.055
H24B	H40	2.230	H24B	H44A	2.413
H24B	H44C	3.417	H24B	H47A	3.557
H24B	H47B	3.374	H28	H32C	3.576
H28	H33A	2.220	H28	H33B	2.169
H28	H33C	3.386	H28	H36B	3.370
H28	H37A	2.103	H28	H37B	2.492
H28	H37C	3.467	H28	H67C	3.328
H30	H36A	2.538	H30	H36B	3.587
H30	H38A	2.107	H30	H38B	3.551
H30	H38C	3.073	H30	H47B	2.847

Table S12-10. Intramolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
H30	H53	2.980	H30	H67B	3.577
H32A	H33B	3.548	H32A	H33C	3.549
H32A	H34A	2.582	H32A	H34C	3.004
H32A	H44C	2.691	H32A	H46A	3.541
H32A	H46B	2.164	H32B	H33A	3.550
H32B	H33B	2.931	H32B	H33C	2.456
H32B	H34A	2.992	H32B	H34B	3.575
H32B	H34C	2.490	H32B	H46B	3.002
H32C	H33A	3.550	H32C	H33B	2.455
H32C	H33C	2.931	H32C	H34C	3.577
H32C	H44C	2.921	H32C	H46B	2.860
H33A	H34A	3.541	H33A	H34B	2.443
H33A	H34C	2.924	H33B	H34B	3.542
H33B	H34C	3.536	H33C	H34A	3.532
H33C	H34B	2.907	H33C	H34C	2.431
H34A	H63	3.111	H34A	H68A	2.858
H34A	H68C	3.235	H34B	H63	2.995
H34B	H68A	3.499	H34B	H68C	3.418
H36A	H37A	3.567	H36A	H37C	3.545
H36A	H38A	2.507	H36A	H38B	2.960
H36A	H38C	3.580	H36B	H37A	2.495
H36B	H37B	3.569	H36B	H37C	2.929
H36B	H38A	3.575	H36B	H38B	3.536
H36C	H37A	2.973	H36C	H37B	3.555
H36C	H37C	2.463	H36C	H38A	2.928
H36C	H38B	2.436	H36C	H38C	3.536
H37A	H38B	3.521	H37A	H38C	3.521
H37B	H38A	3.516	H37B	H38B	2.900
H37B	H38C	2.418	H37B	H67C	2.911
H37C	H38A	3.516	H37C	H38B	2.418
H37C	H38C	2.900	H38A	H53	3.284
H38A	H59A	2.694	H38A	H59B	3.132
H38A	H67B	3.348	H38B	H59A	3.475
H38B	H59B	3.332	H38C	H67A	3.091
H38C	H67B	2.531	H38C	H67C	2.597
H40	H44A	2.631	H40	H44B	3.518
H40	H45A	2.610	H40	H45B	3.589

Table S12-10. Intramolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
H40	H45C	3.506	H42	H45B	2.971
H42	H45C	2.971	H42	H46A	2.604
H42	H46B	3.589	H42	H46C	3.497
H44B	H46B	3.247	H44B	H46C	2.818
H44C	H46B	2.818	H44C	H46C	3.234
H47A	H53	3.348	H47A	H63	3.318
H47B	H53	3.367	H47B	H63	2.179
H47B	H67B	2.561	H47B	H67C	3.477
H51	H55C	3.571	H51	H56A	2.213
H51	H56B	3.386	H51	H56C	2.180
H51	H59B	3.378	H51	H61A	2.091
H51	H61B	2.464	H51	H61C	3.449
H53	H59A	2.544	H53	H59B	3.577
H53	H60A	2.126	H53	H60B	3.565
H53	H60C	3.101	H55A	H56A	3.529
H55A	H56B	2.427	H55A	H56C	2.897
H55A	H57A	3.595	H55A	H57B	2.986
H55A	H57C	2.527	H55B	H56B	3.536
H55B	H56C	3.552	H55B	H57B	2.544
H55B	H57C	3.011	H55C	H56A	3.555
H55C	H56B	2.947	H55C	H56C	2.463
H55C	H57C	3.600	H56A	H57A	2.483
H56A	H57B	3.564	H56A	H57C	2.898
H56B	H57A	2.951	H56B	H57B	3.530
H56B	H57C	2.415	H56C	H57A	3.570
H56C	H57C	3.525	H57A	H67A	2.875
H57A	H67B	3.272	H57A	H69B	3.157
H57B	H67A	2.737	H57B	H67B	3.003
H57B	H69B	2.221	H57C	H69B	2.881
H59A	H60A	2.513	H59A	H60B	2.947
H59A	H60C	3.582	H59A	H61A	3.561
H59A	H61C	3.538	H59B	H60A	3.581
H59B	H60B	3.536	H59B	H61A	2.477
H59B	H61B	3.558	H59B	H61C	2.912
H59C	H60A	2.946	H59C	H60B	2.435
H59C	H60C	3.537	H59C	H61A	2.958
H59C	H61B	3.543	H59C	H61C	2.444

Table S12-10. Intramolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
H60A	H61B	3.547	H60A	H61C	3.547
H60B	H61A	3.547	H60B	H61B	2.932
H60B	H61C	2.456	H60C	H61A	3.547
H60C	H61B	2.456	H60C	H61C	2.932
H63	H67B	2.956	H63	H67C	2.920
H63	H68A	2.631	H63	H68B	3.591
H63	H68C	3.520	H65	H68B	2.952
H65	H68C	2.947	H65	H69A	2.579
H65	H69B	3.580	H65	H69C	3.478
H67A	H69B	2.627	H67A	H69C	2.701

Table S12-11. Intermolecular contacts less than 3.60 Å

atom	atom	distance	atom	atom	distance
C40	C55[1]	3.459(5)	C41	C55[1]	3.546(5)
C45	C59[2]	3.512(5)	C55	C40[3]	3.459(5)
C55	C41[3]	3.546(5)	C59	C45[4]	3.512(5)

Symmetry Operators:

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

Table S12-12. Intermolecular contacts less than 3.60 Å involving hydrogens

atom	atom	distance	atom	atom	distance
Cl1	H59C[1]	3.443	Cl1	H61C[1]	3.103
Cl1	H67A[2]	3.154	Cl1	H67C[2]	3.236
Cl1	H69C[2]	3.045	Cl2	H59B[1]	3.477
Cl2	H59C[1]	3.520	Cl2	H61A[1]	3.540
Cl2	H61C[1]	3.522	Cl4	H17[3]	3.444
Cl4	H21B[3]	3.118	Cl4	H32B[4]	2.971
Cl4	H33C[4]	3.248	Cl4	H37C[1]	3.083
Cl5	H5[5]	3.535	Cl5	H9A[5]	3.362
Cl5	H11A[5]	2.828	Cl5	H13A[5]	3.283
Cl5	H13C[3]	3.025	Cl6	H13A[5]	3.596
Cl6	H14A[5]	3.277	C4	H68B[6]	3.541
C4	H68C[6]	3.414	C5	H65[6]	3.373
C5	H68B[6]	3.507	C5	H68C[6]	3.580
C6	H65[6]	3.194	C8	H68B[6]	3.551
C9	H55A[7]	3.397	C9	H57A[2]	3.334
C9	H57C[2]	3.593	C9	H69B[2]	3.345
C9	H69C[2]	3.434	C10	H68B[6]	3.376
C10	H68C[6]	3.501	C11	H13B[8]	2.967
C11	H57A[2]	3.326	C11	H68B[6]	3.248
C12	H65[6]	3.238	C13	H11A[8]	3.243
C13	H11B[8]	3.464	C13	H65[6]	3.183
C14	H23A[7]	3.142	C14	H23C[7]	3.356
C15	H56B[9]	3.449	C15	H65[6]	2.992
C15	H69A[6]	3.122	C16	H32C[5]	2.826
C17	H32C[5]	2.786	C17	H33B[5]	3.462
C17	H37B[2]	3.284	C18	H32C[5]	2.977
C18	H33B[5]	3.329	C19	H32C[5]	3.138
C19	H44C[5]	3.323	C20	H32C[5]	3.062
C20	H44B[5]	3.348	C20	H44C[5]	3.293
C20	H46B[5]	3.530	C20	H46C[5]	3.566
C21	H32C[5]	3.517	C21	H34C[6]	3.305
C21	H46B[5]	3.468	C21	H68C[6]	3.096
C22	H28[5]	3.481	C22	H33A[2]	3.134
C22	H33B[5]	3.130	C22	H36B[5]	3.408
C22	H37A[5]	3.263	C22	H37A[2]	3.476
C22	H37B[2]	3.337	C22	H61C[1]	3.264
C23	H14B[5]	3.421	C23	H14C[5]	3.163

Table S12-12. Intermolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
C23	H36B^{5}	3.199	C23	H44B^{5}	3.361
C23	H44C^{5}	3.242	C28	H22B^{7}	3.055
C29	H22B^{7}	3.588	C29	H23C^{7}	3.550
C32	H21B^{7}	3.546	C33	H22A^{10}	3.451
C33	H22C^{10}	3.542	C33	H37A^{11}	3.460
C34	H21B^{3}	3.104	C34	H60C^{3}	3.252
C36	H22B^{7}	3.542	C36	H23C^{7}	3.231
C36	H42^{12}	3.137	C37	H17^{10}	2.977
C37	H22A^{10}	2.910	C37	H22B^{7}	3.327
C37	H33B^{11}	3.474	C38	H45B^{12}	3.373
C39	H55C^{7}	2.754	C40	H55C^{7}	2.614
C41	H55C^{7}	2.675	C41	H56C^{7}	3.411
C42	H36C^{1}	3.068	C42	H55C^{7}	2.903
C42	H56C^{7}	3.171	C43	H55C^{7}	2.949
C44	H20^{7}	3.351	C44	H23A^{7}	3.157
C44	H23C^{7}	3.394	C44	H55C^{7}	3.574
C45	H36C^{1}	3.511	C45	H38B^{1}	3.483
C45	H55C^{7}	3.417	C45	H56C^{7}	3.566
C45	H59A^{1}	3.475	C45	H59B^{1}	3.278
C45	H59C^{1}	3.206	C46	H20^{7}	3.497
C46	H21A^{7}	3.481	C46	H34C^{4}	3.488
C46	H60C^{7}	3.229	C51	H46C^{5}	3.362
C52	H46C^{5}	3.258	C53	H46C^{5}	3.387
C55	H9A^{5}	3.358	C56	H15C^{13}	3.083
C56	H45C^{5}	3.411	C57	H9B^{10}	2.899
C57	H11C^{10}	3.170	C59	H45A^{12}	3.382
C59	H45B^{12}	3.069	C59	H45C^{12}	3.522
C60	H34B^{6}	3.244	C60	H46A^{5}	3.539
C61	H22C^{12}	2.995	C61	H23B^{12}	3.337
C65	H13C^{3}	3.237	C65	H15B^{3}	2.935
C66	H15B^{3}	3.405	C68	H10C^{3}	2.883
C68	H11B^{3}	3.283	C68	H21C^{3}	3.305
C69	H9B^{10}	3.276	C69	H15B^{3}	3.139
H1B	H46C^{5}	3.591	H5	Cl5^{7}	3.535
H5	H65^{6}	3.308	H5	H68B^{6}	3.330
H9A	Cl5^{7}	3.362	H9A	C55^{7}	3.358
H9A	H55A^{7}	2.610	H9A	H55B^{7}	3.285

Table S12-12. Intermolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
H9A	H69B^{2}	3.578	H9B	C57^{2}	2.899
H9B	C69^{2}	3.276	H9B	H57A^{2}	2.436
H9B	H57B^{2}	3.034	H9B	H57C^{2}	2.763
H9B	H67A^{2}	2.901	H9B	H69B^{2}	2.627
H9B	H69C^{2}	3.044	H9C	H55A^{7}	3.512
H9C	H67A^{2}	3.533	H9C	H69B^{2}	3.375
H9C	H69C^{2}	3.000	H10B	H38C^{2}	3.320
H10B	H57A^{2}	3.020	H10B	H67A^{2}	3.044
H10C	C68^{6}	2.883	H10C	H68A^{6}	2.965
H10C	H68B^{6}	2.531	H10C	H68C^{6}	2.676
H11A	Cl5^{7}	2.828	H11A	C13^{8}	3.243
H11A	H13A^{8}	3.496	H11A	H13B^{8}	2.683
H11A	H13C^{8}	3.075	H11B	C13^{8}	3.464
H11B	C68^{6}	3.283	H11B	H13A^{8}	3.450
H11B	H13B^{8}	2.751	H11B	H68B^{6}	2.360
H11B	H68C^{6}	3.483	H11C	C57^{2}	3.170
H11C	H13B^{8}	2.968	H11C	H56A^{2}	3.008
H11C	H56B^{2}	3.595	H11C	H57A^{2}	2.434
H11C	H57C^{2}	3.081	H13A	Cl5^{7}	3.283
H13A	Cl6^{7}	3.596	H13A	H11A^{8}	3.496
H13A	H11B^{8}	3.450	H13A	H13A^{8}	3.445
H13A	H13C^{8}	3.323	H13B	C11^{8}	2.967
H13B	H11A^{8}	2.683	H13B	H11B^{8}	2.751
H13B	H11C^{8}	2.968	H13B	H56A^{9}	3.560
H13C	Cl5^{6}	3.025	H13C	C65^{6}	3.237
H13C	H11A^{8}	3.075	H13C	H13A^{8}	3.323
H13C	H65^{6}	2.400	H13C	H69A^{6}	3.509
H14A	Cl6^{7}	3.277	H14A	H23A^{7}	3.054
H14B	C23^{7}	3.421	H14B	H23A^{7}	3.106
H14B	H23C^{7}	2.905	H14C	C23^{7}	3.163
H14C	H23A^{7}	2.742	H14C	H23B^{7}	3.188
H14C	H23C^{7}	3.038	H15A	H65^{6}	3.554
H15B	C65^{6}	2.935	H15B	C66^{6}	3.405
H15B	C69^{6}	3.139	H15B	H56B^{9}	3.494
H15B	H65^{6}	2.140	H15B	H69A^{6}	2.333
H15B	H69C^{6}	3.472	H15C	C56^{9}	3.083
H15C	H45C^{12}	3.509	H15C	H56A^{9}	3.038

Table S12-12. Intermolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
H15C	H56B^{9}	2.595	H15C	H56C^{9}	3.115
H15C	H69A^{6}	3.087	H17	Cl4^{6}	3.444
H17	C37^{2}	2.977	H17	H32C^{5}	3.126
H17	H33B^{5}	3.308	H17	H37A^{2}	3.296
H17	H37B^{2}	2.491	H17	H37C^{2}	2.717
H20	C44^{5}	3.351	H20	C46^{5}	3.497
H20	H32C^{5}	3.574	H20	H44B^{5}	2.724
H20	H44C^{5}	3.096	H20	H46B^{5}	3.245
H20	H46C^{5}	2.876	H21A	C46^{5}	3.481
H21A	H34C^{6}	3.224	H21A	H46B^{5}	3.160
H21A	H46C^{5}	3.080	H21A	H68C^{6}	3.262
H21B	Cl4^{6}	3.118	H21B	C32^{5}	3.546
H21B	C34^{6}	3.104	H21B	H32B^{5}	3.134
H21B	H32C^{5}	3.171	H21B	H34A^{6}	2.848
H21B	H34B^{6}	3.510	H21B	H34C^{6}	2.550
H21B	H46B^{5}	3.192	H21B	H68C^{6}	3.138
H21C	C68^{6}	3.305	H21C	H68A^{6}	3.470
H21C	H68C^{6}	2.434	H22A	C33^{2}	3.451
H22A	C37^{2}	2.910	H22A	H28^{2}	2.778
H22A	H33A^{2}	2.771	H22A	H33B^{5}	2.949
H22A	H33B^{2}	3.257	H22A	H37A^{5}	3.478
H22A	H37A^{2}	2.570	H22A	H37B^{2}	2.426
H22A	H37C^{2}	3.389	H22B	C28^{5}	3.055
H22B	C29^{5}	3.588	H22B	C36^{5}	3.542
H22B	C37^{5}	3.327	H22B	H28^{5}	2.585
H22B	H33A^{2}	3.371	H22B	H33B^{5}	2.741
H22B	H33B^{2}	3.533	H22B	H36B^{5}	2.710
H22B	H37A^{5}	2.420	H22C	C33^{2}	3.542
H22C	C61^{1}	2.995	H22C	H33A^{2}	2.780
H22C	H36B^{5}	3.276	H22C	H37A^{5}	3.509
H22C	H61A^{1}	3.299	H22C	H61B^{1}	2.983
H22C	H61C^{1}	2.297	H23A	C14^{5}	3.142
H23A	C44^{5}	3.157	H23A	H14A^{5}	3.054
H23A	H14B^{5}	3.106	H23A	H14C^{5}	2.742
H23A	H44A^{5}	3.219	H23A	H44B^{5}	2.706
H23A	H44C^{5}	3.033	H23B	C61^{1}	3.337
H23B	H14C^{5}	3.188	H23B	H36B^{5}	3.069

Table S12-12. Intermolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
H23B	H61A[1]	2.760	H23B	H61C[1]	3.137
H23C	C14[5]	3.356	H23C	C29[5]	3.550
H23C	C36[5]	3.231	H23C	C44[5]	3.394
H23C	H14B[5]	2.905	H23C	H14C[5]	3.038
H23C	H36A[5]	3.171	H23C	H36B[5]	2.486
H23C	H44A[5]	3.302	H23C	H44B[5]	3.401
H23C	H44C[5]	2.933	H28	C22[7]	3.481
H28	H22A[10]	2.778	H28	H22B[7]	2.585
H32B	Cl4[4]	2.971	H32B	H21B[7]	3.134
H32B	H32B[4]	2.983	H32B	H34C[4]	3.540
H32C	C16[7]	2.826	H32C	C17[7]	2.786
H32C	C18[7]	2.977	H32C	C19[7]	3.138
H32C	C20[7]	3.062	H32C	C21[7]	3.517
H32C	H17[7]	3.126	H32C	H20[7]	3.574
H32C	H21B[7]	3.171	H33A	C22[10]	3.134
H33A	H22A[10]	2.771	H33A	H22B[10]	3.371
H33A	H22C[10]	2.780	H33A	H61B[3]	3.468
H33A	H61C[3]	3.499	H33B	C17[7]	3.462
H33B	C18[7]	3.329	H33B	C22[7]	3.130
H33B	C37[11]	3.474	H33B	H17[7]	3.308
H33B	H22A[7]	2.949	H33B	H22A[10]	3.257
H33B	H22B[7]	2.741	H33B	H22B[10]	3.533
H33B	H37A[11]	2.878	H33B	H37C[11]	3.303
H33C	Cl4[4]	3.248	H33C	H37A[11]	3.340
H33C	H37C[11]	3.240	H33C	H46A[4]	2.951
H33C	H61B[3]	3.447	H34A	H21B[3]	2.848
H34B	C60[3]	3.244	H34B	H21B[3]	3.510
H34B	H60B[3]	2.857	H34B	H60C[3]	2.786
H34C	C21[3]	3.305	H34C	C46[4]	3.488
H34C	H21A[3]	3.224	H34C	H21B[3]	2.550
H34C	H32B[4]	3.540	H34C	H46A[4]	2.991
H34C	H46B[4]	3.134	H34C	H60C[3]	2.821
H36A	H23C[7]	3.171	H36B	C22[7]	3.408
H36B	C23[7]	3.199	H36B	H22B[7]	2.710
H36B	H22C[7]	3.276	H36B	H23B[7]	3.069
H36B	H23C[7]	2.486	H36B	H42[12]	3.441
H36C	C42[12]	3.068	H36C	C45[12]	3.511

Table S12-12. Intermolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
H36C	H42[12]	2.177	H36C	H45B[12]	3.149
H36C	H45C[12]	3.281	H36C	H56C[9]	3.541
H37A	C22[7]	3.263	H37A	C22[10]	3.476
H37A	C33[11]	3.460	H37A	H17[10]	3.296
H37A	H22A[7]	3.478	H37A	H22A[10]	2.570
H37A	H22B[7]	2.420	H37A	H22C[7]	3.509
H37A	H33B[11]	2.878	H37A	H33C[11]	3.340
H37B	C17[10]	3.284	H37B	C22[10]	3.337
H37B	H17[10]	2.491	H37B	H22A[10]	2.426
H37C	Cl4[12]	3.083	H37C	H17[10]	2.717
H37C	H22A[10]	3.389	H37C	H33B[11]	3.303
H37C	H33C[11]	3.240	H37C	H42[12]	3.280
H38A	H45B[12]	3.338	H38B	C45[12]	3.483
H38B	H42[12]	3.544	H38B	H45B[12]	2.584
H38C	H10B[10]	3.320	H40	H55A[7]	3.594
H40	H55C[7]	2.986	H42	C36[1]	3.137
H42	H36B[1]	3.441	H42	H36C[1]	2.177
H42	H37C[1]	3.280	H42	H38B[1]	3.544
H42	H55C[7]	3.468	H42	H56C[7]	2.973
H42	H61B[7]	3.454	H44A	H23A[7]	3.219
H44A	H23C[7]	3.302	H44B	C20[7]	3.348
H44B	C23[7]	3.361	H44B	H20[7]	2.724
H44B	H23A[7]	2.706	H44B	H23C[7]	3.401
H44B	H55B[7]	3.570	H44B	H55C[7]	3.398
H44C	C19[7]	3.323	H44C	C20[7]	3.293
H44C	C23[7]	3.242	H44C	H20[7]	3.096
H44C	H23A[7]	3.033	H44C	H23C[7]	2.933
H45A	C59[1]	3.382	H45A	H59A[1]	3.592
H45A	H59B[1]	3.169	H45A	H59C[1]	2.875
H45B	C38[1]	3.373	H45B	C59[1]	3.069
H45B	H36C[1]	3.149	H45B	H38A[1]	3.338
H45B	H38B[1]	2.584	H45B	H59A[1]	3.007
H45B	H59B[1]	2.656	H45B	H59C[1]	3.034
H45C	C56[7]	3.411	H45C	C59[1]	3.522
H45C	H15C[1]	3.509	H45C	H36C[1]	3.281
H45C	H55A[7]	3.359	H45C	H55C[7]	3.209
H45C	H56B[7]	3.096	H45C	H56C[7]	2.856

Table S12-12. Intermolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
H45C	H59A[1]	3.283	H45C	H59B[1]	3.540
H45C	H59C[1]	3.171	H46A	C60[7]	3.539
H46A	H33C[4]	2.951	H46A	H34C[4]	2.991
H46A	H60C[7]	2.652	H46A	H61B[7]	2.822
H46B	C20[7]	3.530	H46B	C21[7]	3.468
H46B	H20[7]	3.245	H46B	H21A[7]	3.160
H46B	H21B[7]	3.192	H46B	H34C[4]	3.134
H46B	H60C[7]	3.578	H46C	C20[7]	3.566
H46C	C51[7]	3.362	H46C	C52[7]	3.258
H46C	C53[7]	3.387	H46C	H1B[7]	3.591
H46C	H20[7]	2.876	H46C	H21A[7]	3.080
H46C	H60C[7]	3.019	H55A	C9[5]	3.397
H55A	H9A[5]	2.610	H55A	H9C[5]	3.512
H55A	H40[5]	3.594	H55A	H45C[5]	3.359
H55B	H9A[5]	3.285	H55B	H44B[5]	3.570
H55C	C39[5]	2.754	H55C	C40[5]	2.614
H55C	C41[5]	2.675	H55C	C42[5]	2.903
H55C	C43[5]	2.949	H55C	C44[5]	3.574
H55C	C45[5]	3.417	H55C	H40[5]	2.986
H55C	H42[5]	3.468	H55C	H44B[5]	3.398
H55C	H45C[5]	3.209	H56A	H11C[10]	3.008
H56A	H13B[13]	3.560	H56A	H15C[13]	3.038
H56B	C15[13]	3.449	H56B	H11C[10]	3.595
H56B	H15B[13]	3.494	H56B	H15C[13]	2.595
H56B	H45C[5]	3.096	H56B	H69A[14]	2.993
H56C	C41[5]	3.411	H56C	C42[5]	3.171
H56C	C45[5]	3.566	H56C	H15C[13]	3.115
H56C	H36C[13]	3.541	H56C	H42[5]	2.973
H56C	H45C[5]	2.856	H57A	C9[10]	3.334
H57A	C11[10]	3.326	H57A	H9B[10]	2.436
H57A	H10B[10]	3.020	H57A	H11C[10]	2.434
H57B	H9B[10]	3.034	H57C	C9[10]	3.593
H57C	H9B[10]	2.763	H57C	H11C[10]	3.081
H59A	C45[12]	3.475	H59A	H45A[12]	3.592
H59A	H45B[12]	3.007	H59A	H45C[12]	3.283
H59B	Cl2[12]	3.477	H59B	C45[12]	3.278
H59B	H45A[12]	3.169	H59B	H45B[12]	2.656

Table S12-12. Intermolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
H59B	H45C[12]	3.540	H59C	Cl1[12]	3.443
H59C	Cl2[12]	3.520	H59C	C45[12]	3.206
H59C	H45A[12]	2.875	H59C	H45B[12]	3.034
H59C	H45C[12]	3.171	H59C	H69C[6]	3.367
H60B	H34B[6]	2.857	H60C	C34[6]	3.252
H60C	C46[5]	3.229	H60C	H34B[6]	2.786
H60C	H34C[6]	2.821	H60C	H46A[5]	2.652
H60C	H46B[5]	3.578	H60C	H46C[5]	3.019
H61A	Cl2[12]	3.540	H61A	H22C[12]	3.299
H61A	H23B[12]	2.760	H61B	H22C[12]	2.983
H61B	H33A[6]	3.468	H61B	H33C[6]	3.447
H61B	H42[5]	3.454	H61B	H46A[5]	2.822
H61C	Cl1[12]	3.103	H61C	Cl2[12]	3.522
H61C	C22[12]	3.264	H61C	H22C[12]	2.297
H61C	H23B[12]	3.137	H61C	H33A[6]	3.499
H65	C5[3]	3.373	H65	C6[3]	3.194
H65	C12[3]	3.238	H65	C13[3]	3.183
H65	C15[3]	2.992	H65	H5[3]	3.308
H65	H13C[3]	2.400	H65	H15A[3]	3.554
H65	H15B[3]	2.140	H67A	Cl1[10]	3.154
H67A	H9B[10]	2.901	H67A	H9C[10]	3.533
H67A	H10B[10]	3.044	H67C	Cl1[10]	3.236
H68A	H10C[3]	2.965	H68A	H21C[3]	3.470
H68B	C4[3]	3.541	H68B	C5[3]	3.507
H68B	C8[3]	3.551	H68B	C10[3]	3.376
H68B	C11[3]	3.248	H68B	H5[3]	3.330
H68B	H10C[3]	2.531	H68B	H11B[3]	2.360
H68C	C4[3]	3.414	H68C	C5[3]	3.580
H68C	C10[3]	3.501	H68C	C21[3]	3.096
H68C	H10C[3]	2.676	H68C	H11B[3]	3.483
H68C	H21A[3]	3.262	H68C	H21B[3]	3.138
H68C	H21C[3]	2.434	H69A	C15[3]	3.122
H69A	H13C[3]	3.509	H69A	H15B[3]	2.333
H69A	H15C[3]	3.087	H69A	H56B[14]	2.993
H69B	C9[10]	3.345	H69B	H9A[10]	3.578
H69B	H9B[10]	2.627	H69B	H9C[10]	3.375
H69C	Cl1[10]	3.045	H69C	C9[10]	3.434

Table S12-12. Intermolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
H69C	H9B[10]	3.044	H69C	H9C[10]	3.000
H69C	H15B[3]	3.472	H69C	H59C[3]	3.367

Symmetry Operators:

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

X-ray Structure Report

for

[Cp*TiMe$_2${(O-2,4-^{t}Bu$_2$C$_6$H$_2$)-6-CH$_2$}]$_3$N (**9**)

July 5, 2016

Experimental

Data Collection

An orange block crystal of $C_{81}H_{129}NO_3Ti_3$ having approximate dimensions of 0.108 x 0.090 x 0.046 mm was mounted on a glass fiber. All measurements were made on a Rigaku XtaLAB P200 diffractometer using multi-layer mirror monochromated Mo-Kα radiation.

The crystal-to-detector distance was 45.00 mm.

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

a = 19.9129(4) Å
b = 19.9654(3) Å β = 98.7979(19)^o
c = 20.1690(4) Å
V = 7924.2(3) Å^3

For Z = 4 and F.W. = 1308.62, the calculated density is 1.097 g/cm^3. The reflection conditions of:

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

uniquely determine the space group to be:

$P2_1/n$ (#14)

The data were collected at a temperature of -180 $\pm$ 1^{o}C to a maximum 2θ value of 61.4^o. A total of 720 oscillation images were collected. A sweep of data was done using ω scans from -105.0 to 75.0^o in 0.50^o step, at χ=45.0^o and ϕ = 0.0^o. The exposure rate was 128.0 [sec./^{o}]. The detector swing angle was -15.00^o. A second sweep was performed using ω scans from -105.0 to 75.0^o in 0.50^o step, at χ=45.0^o and ϕ = 90.0^o. The exposure rate was 128.0 [sec./^{o}]. The detector swing angle was -15.00^o. The crystal-to-detector distance was 45.00 mm. Readout was performed in the 0.172 mm pixel mode.

Data Reduction

Of the 0 reflections were collected, where 0 were unique (R_{int} = 0.0458); equivalent reflections were merged. Data were collected and processed using CrysAlisPro (Rigaku Oxford Diffraction). [1]

The linear absorption coefficient, μ, for Mo-Kα radiation is 3.388 cm^{-1}. An empirical absorption correction was applied which resulted in transmission factors ranging from 0.892 to 0.985. 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 17594 observed reflections and 805 variable parameters and converged (largest parameter shift was 0.00 times its esd) with unweighted and weighted agreement factors of:

$$R1 = \Sigma \, ||Fo| - |Fc|| \, / \, \Sigma \, |Fo| = 0.0579$$

$$wR2 = [\, \Sigma \, (\, w \, (Fo^2 - Fc^2)^2 \,) / \, \Sigma \, w(Fo^2)^2]^{1/2} = 0.1774$$

The goodness of fit[4] was 1.01. Unit weights were used. The maximum and minimum peaks on the final difference Fourier map corresponded to 0.70 and -0.54 $e^-/Å^3$, respectively.

Neutral atom scattering factors were taken from International Tables for Crystallography (IT), Vol. C, Table 6.1.1.4 [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 Version 2014/7[10].

References

(1) CrysAlisPro: Data Collection and Processing Software, Rigaku Corporation (2015). Tokyo 196-8666, Japan.

(2) SHELXT Version 2014/5: Sheldrick, G. M. (2014). Acta Cryst. A70, C1437.

(3) Least Squares function minimized: (SHELXL Version 2014/7)

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

(4) Goodness of fit is defined as:

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

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

(5) International Tables for Crystallography, Vol.C (1992). Ed. A.J.C. Wilson, Kluwer Academic Publishers, Dordrecht, Netherlands, Table 6.1.1.4, pp. 572.

(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 4.2: Crystal Structure Analysis Package, Rigaku Corporation (2000-2015). Tokyo 196-8666, Japan.

(10) SHELXL Version 2014/7: Sheldrick, G. M. (2008). Acta Cryst. A64, 112-122.

EXPERIMENTAL DETAILS

A. Crystal Data

Empirical Formula	$C_{81}H_{129}NO_3Ti_3$
Formula Weight	1308.62
Crystal Color, Habit	orange, block
Crystal Dimensions	0.108 X 0.090 X 0.046 mm
Crystal System	monoclinic
Lattice Type	Primitive
Lattice Parameters	a = 19.9129(4) Å b = 19.9654(3) Å c = 20.1690(4) Å β = 98.7979(19) ^{o} V = 7924.2(3) Å^3
Space Group	$P2_1/n$ (#14)
Z value	4
D_{calc}	1.097 g/cm^3
F_{000}	2848.00
μ(MoKα)	3.388 cm^{-1}

B. Intensity Measurements

Diffractometer	XtaLAB P200
Radiation	MoKα (λ = 0.71073 Å) multi-layer mirror monochromated
Voltage, Current	50kV, 24mA
Temperature	-180.0^{o}C
Detector Aperture	83.8 x 70.0 mm
Data Images	720 exposures
ω oscillation Range (χ=45.0, ϕ=0.0)	-105.0 - 75.0^{o}
Exposure Rate	128.0 sec./^{o}
Detector Swing Angle	-15.00^{o}
ω oscillation Range (χ=45.0, ϕ=90.0)	-105.0 - 75.0^{o}
Exposure Rate	128.0 sec./^{o}
Detector Swing Angle	-15.00^{o}
Detector Position	45.00 mm
Pixel Size	0.172 mm
$2\theta_{max}$	55.0^{o}
No. of Reflections Measured	Total: 65232 Unique: 17594 (R_{int} = 0.0458)
Corrections	Lorentz-polarization Absorption (trans. factors: 0.892 - 0.985)

C. Structure Solution and Refinement

Structure Solution	Direct Methods (SHELXT Version 2014/5)
Refinement	Full-matrix least-squares on F^2
Function Minimized	Σ w $(Fo^2 - Fc^2)^2$
Least Squares Weights	$w = 1/ [\sigma^2(Fo^2) + (0.0987 \cdot P)^2 + 9.4361 \cdot P]$ 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)	17594
No. Variables	805
Reflection/Parameter Ratio	21.86
Residuals: R1 (I>2.00σ(I))	0.0579
Residuals: R (All reflections)	0.0738
Residuals: wR2 (All reflections)	0.1774
Goodness of Fit Indicator	1.008
Max Shift/Error in Final Cycle	0.001
Maximum peak in Final Diff. Map	0.70 $e^-/Å^3$
Minimum peak in Final Diff. Map	-0.54 $e^-/Å^3$

Table S13-1. Atomic coordinates and B_{iso}/B_{eq}

atom	x	y	z	B_{eq}
Ti1	0.51189(2)	0.53696(2)	0.80883(2)	1.449(8)
Ti2	0.38246(2)	0.74257(2)	0.52058(2)	1.896(9)
Ti3	0.23200(2)	0.78453(2)	0.84358(2)	2.138(10)
O1	0.56716(8)	0.59880(7)	0.77837(8)	1.43(3)
O2	0.38485(8)	0.82087(8)	0.56738(8)	1.70(3)
O3	0.31436(9)	0.79177(9)	0.89587(8)	1.90(3)
N1	0.46332(10)	0.78258(9)	0.76986(9)	1.39(3)
C1	0.49686(11)	0.71843(11)	0.78711(12)	1.46(3)
C2	0.56817(11)	0.71698(11)	0.76961(11)	1.31(3)
C3	0.60027(12)	0.77616(11)	0.75657(11)	1.44(3)
C4	0.66531(12)	0.77651(11)	0.73918(11)	1.49(3)
C5	0.69755(12)	0.71491(11)	0.73597(11)	1.52(3)
C6	0.66790(11)	0.65357(11)	0.74903(11)	1.38(3)
C7	0.60183(11)	0.65562(10)	0.76621(11)	1.29(3)
C8	0.70527(12)	0.58741(11)	0.74233(12)	1.58(4)
C9	0.66657(14)	0.54737(12)	0.68303(13)	2.13(4)
C10	0.71094(13)	0.54745(12)	0.80823(13)	2.03(4)
C11	0.77812(13)	0.59833(12)	0.72830(15)	2.28(4)
C12	0.69744(12)	0.84386(11)	0.72412(12)	1.77(4)
C13	0.65517(16)	0.87582(14)	0.66235(15)	2.99(5)
C14	0.69725(15)	0.89052(13)	0.78468(14)	2.50(5)
C15	0.77069(14)	0.83611(13)	0.71128(15)	2.50(5)
C16	0.41694(13)	0.54836(13)	0.74587(13)	2.23(4)
C17	0.53980(14)	0.44702(12)	0.76293(13)	2.27(4)
C18	0.54111(13)	0.56763(12)	0.92306(12)	1.91(4)
C19	0.46942(13)	0.57327(12)	0.90735(12)	1.98(4)
C20	0.44202(13)	0.50791(12)	0.89187(12)	1.97(4)
C21	0.49687(13)	0.46216(11)	0.89926(12)	1.84(4)
C22	0.55811(13)	0.49878(12)	0.91783(12)	1.83(4)
C23	0.62740(13)	0.46798(13)	0.93317(14)	2.35(4)
C24	0.49088(14)	0.38733(12)	0.89464(14)	2.35(4)
C25	0.36819(14)	0.49069(15)	0.87749(15)	2.79(5)
C26	0.42673(17)	0.63484(14)	0.91146(16)	2.68(5)
C27	0.59092(15)	0.62362(13)	0.94310(13)	2.43(5)
C28	0.44177(12)	0.78790(11)	0.69720(11)	1.52(4)
C29	0.43477(11)	0.86012(11)	0.67391(11)	1.42(3)
C30	0.45830(12)	0.91215(11)	0.71731(11)	1.58(4)

Table S13-1. Atomic coordinates and B_{iso}/B_{eq} (continued)

atom	x	y	z	B_{eq}
C31	0.44960(13)	0.97879(12)	0.69776(12)	1.84(4)
C32	0.41449(13)	0.99153(12)	0.63391(12)	1.98(4)
C33	0.38917(12)	0.94131(12)	0.58818(12)	1.83(4)
C34	0.40318(12)	0.87426(11)	0.60867(11)	1.56(4)
C35	0.34551(14)	0.95877(13)	0.52056(13)	2.29(4)
C36	0.27657(14)	0.92353(15)	0.51770(14)	2.75(5)
C37	0.33206(17)	1.03405(15)	0.51315(16)	3.25(6)
C38	0.38088(15)	0.93641(16)	0.46149(13)	2.72(5)
C39	0.47549(14)	1.03649(12)	0.74549(13)	2.27(4)
C40	0.51479(18)	1.01166(15)	0.81225(15)	3.34(6)
C41	0.4149(2)	1.07719(17)	0.76212(19)	4.17(7)
C42	0.5216(2)	1.0818(2)	0.71242(17)	4.61(8)
C43	0.29267(15)	0.75619(16)	0.45033(15)	3.06(5)
C44	0.34185(16)	0.67051(14)	0.58196(14)	2.86(5)
C45	0.49896(15)	0.71030(16)	0.52701(14)	2.83(5)
C46	0.46034(17)	0.65233(15)	0.50658(16)	3.27(6)
C47	0.42250(16)	0.66656(16)	0.44239(15)	3.08(5)
C48	0.43813(15)	0.73242(16)	0.42500(14)	2.81(5)
C49	0.48554(14)	0.75904(15)	0.47756(14)	2.71(5)
C50	0.52086(16)	0.82657(17)	0.47982(17)	3.36(6)
C51	0.41261(18)	0.7656(2)	0.35875(15)	3.84(6)
C52	0.3775(2)	0.61706(19)	0.40028(19)	4.39(7)
C53	0.4655(2)	0.58547(18)	0.5415(2)	4.78(8)
C54	0.55353(17)	0.7158(2)	0.58807(16)	4.03(7)
C55	0.40611(12)	0.79304(12)	0.80584(11)	1.59(4)
C56	0.42788(12)	0.81186(11)	0.87888(11)	1.57(4)
C57	0.49376(12)	0.83109(12)	0.90294(12)	1.81(4)
C58	0.51467(13)	0.84485(13)	0.97088(12)	2.11(4)
C59	0.46681(14)	0.83537(14)	1.01400(12)	2.27(4)
C60	0.39976(13)	0.81557(12)	0.99282(12)	2.00(4)
C61	0.37991(12)	0.80703(12)	0.92288(12)	1.66(4)
C62	0.35178(14)	0.79933(14)	1.04370(13)	2.38(4)
C63	0.32815(16)	0.72599(14)	1.03385(14)	2.72(5)
C64	0.38725(16)	0.80582(17)	1.11674(13)	3.03(5)
C65	0.29004(15)	0.84710(16)	1.03409(14)	2.88(5)
C66	0.58737(14)	0.86765(16)	0.99854(14)	2.75(5)
C67	0.58397(19)	0.9376(2)	1.0299(2)	4.67(8)

Table S13-1. Atomic coordinates and B_{iso}/B_{eq} (continued)

atom	x	y	z	B_{eq}
C68	0.61926(18)	0.8185(2)	1.05315(18)	4.54(8)
C69	0.63299(17)	0.8712(2)	0.94495(16)	3.91(7)
C70	0.17516(15)	0.73121(18)	0.90764(17)	3.45(6)
C71	0.24490(15)	0.70104(15)	0.78119(17)	3.15(5)
C72	0.22593(14)	0.88665(14)	0.78173(16)	2.67(5)
C73	0.19311(15)	0.89818(14)	0.83786(15)	2.81(5)
C74	0.13470(14)	0.85720(14)	0.83080(14)	2.66(5)
C75	0.13138(14)	0.82031(14)	0.77091(15)	2.63(5)
C76	0.18878(15)	0.83851(13)	0.73977(14)	2.68(5)
C77	0.20328(19)	0.81483(17)	0.67241(16)	3.73(6)
C78	0.28578(16)	0.92730(16)	0.7658(2)	3.90(7)
C79	0.07628(16)	0.77140(16)	0.74448(18)	3.40(6)
C80	0.08106(17)	0.85898(19)	0.87654(17)	3.75(6)
C81	0.2141(2)	0.94940(17)	0.89150(19)	4.12(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 S13-2. Atomic coordinates and B_{iso} involving hydrogen atoms

atom	x	y	z	B_{iso}
H1A	0.46973	0.68206	0.76271	1.750
H1B	0.49892	0.71020	0.83579	1.750
H3	0.57730	0.81749	0.75957	1.734
H5	0.74200	0.71445	0.72431	1.829
H9A	0.69011	0.50493	0.67833	2.555
H9B	0.62025	0.53828	0.69145	2.555
H9C	0.66477	0.57348	0.64165	2.555
H10A	0.73489	0.50525	0.80346	2.441
H10B	0.73621	0.57378	0.84481	2.441
H10C	0.66532	0.53787	0.81836	2.441
H11A	0.80001	0.55484	0.72441	2.736
H11B	0.77696	0.62329	0.68631	2.736
H11C	0.80389	0.62381	0.76524	2.736
H13A	0.60806	0.88098	0.67017	3.582
H13B	0.67402	0.91988	0.65420	3.582
H13C	0.65637	0.84706	0.62317	3.582
H14A	0.65058	0.89608	0.79367	2.995
H14B	0.72527	0.87096	0.82411	2.995
H14C	0.71579	0.93426	0.77489	2.995
H15A	0.79811	0.81568	0.75058	3.003
H15B	0.77165	0.80743	0.67200	3.003
H15C	0.78930	0.88024	0.70302	3.003
H16A	0.38422	0.51639	0.75936	2.673
H16B	0.40016	0.59408	0.74999	2.673
H16C	0.42261	0.53988	0.69919	2.673
H17A	0.51274	0.40965	0.77605	2.724
H17B	0.53132	0.45211	0.71404	2.724
H17C	0.58815	0.43797	0.77762	2.724
H23A	0.66135	0.50332	0.94465	2.816
H23B	0.62873	0.43710	0.97112	2.816
H23C	0.63743	0.44339	0.89379	2.816
H24A	0.53637	0.36735	0.90163	2.820
H24B	0.46520	0.37095	0.92911	2.820
H24C	0.46715	0.37481	0.85018	2.820
H25A	0.34115	0.53188	0.87490	3.343
H25B	0.35877	0.46672	0.83467	3.343
H25C	0.35622	0.46217	0.91346	3.343

Table S13-2. Atomic coordinates and B_{iso} involving hydrogens/B_{eq} (continued)

atom	x	y	z	B_{eq}
H27A	0.63719	0.60549	0.95104	2.919
H27B	0.58726	0.65696	0.90707	2.919
H27C	0.58068	0.64481	0.98424	2.919
H28A	0.39758	0.76487	0.68498	1.827
H28B	0.47543	0.76497	0.67373	1.827
H30	0.48074	0.90193	0.76115	1.891
H32	0.40725	1.03690	0.62050	2.378
H36A	0.28368	0.87508	0.52233	3.305
H36B	0.25379	0.93986	0.55432	3.305
H36C	0.24825	0.93315	0.47460	3.305
H37A	0.37533	1.05786	0.51480	3.895
H37B	0.30336	1.04290	0.47009	3.895
H37C	0.30890	1.04962	0.54981	3.895
H38A	0.39015	0.88823	0.46493	3.259
H38B	0.35126	0.94590	0.41911	3.259
H38C	0.42373	0.96087	0.46285	3.259
H40A	0.48556	0.98223	0.83427	4.007
H40B	0.55508	0.98680	0.80384	4.007
H40C	0.52885	1.05008	0.84132	4.007
H41A	0.38490	1.04799	0.78351	5.008
H41B	0.43133	1.11376	0.79274	5.008
H41C	0.38958	1.09581	0.72071	5.008
H42A	0.56043	1.05596	0.70175	5.533
H42B	0.49630	1.10045	0.67105	5.533
H42C	0.53806	1.11840	0.74309	5.533
H43A	0.28512	0.71674	0.42123	3.677
H43B	0.25386	0.76217	0.47434	3.677
H43C	0.29758	0.79595	0.42298	3.677
H44A	0.33911	0.62678	0.55965	3.438
H44B	0.37150	0.66718	0.62534	3.438
H44C	0.29632	0.68450	0.58906	3.438
H50A	0.50303	0.85231	0.43960	4.030
H50B	0.51251	0.85115	0.51982	4.030
H50C	0.56984	0.81984	0.48151	4.030
H51A	0.38003	0.73603	0.33166	4.606
H51B	0.39027	0.80797	0.36674	4.606
H51C	0.45097	0.77447	0.33481	4.606

Table S13-2. Atomic coordinates and B_{iso} involving hydrogens/B_{eq} (continued)

atom	x	y	z	B_{eq}
H52A	0.37596	0.57514	0.42527	5.273
H52B	0.33155	0.63552	0.38948	5.273
H52C	0.39580	0.60831	0.35867	5.273
H53A	0.43293	0.55422	0.51670	5.741
H53B	0.51164	0.56780	0.54336	5.741
H53C	0.45520	0.59088	0.58720	5.741
H54A	0.55321	0.67530	0.61551	4.832
H54B	0.59807	0.72056	0.57357	4.832
H54C	0.54459	0.75501	0.61459	4.832
H55A	0.37867	0.75152	0.80359	1.903
H55B	0.37690	0.82904	0.78335	1.903
H57	0.52560	0.83506	0.87256	2.167
H59	0.48079	0.84287	1.06058	2.730
H63A	0.30518	0.71969	0.98772	3.259
H63B	0.36764	0.69619	1.04233	3.259
H63C	0.29662	0.71547	1.06523	3.259
H64A	0.35492	0.79507	1.14725	3.630
H64B	0.42573	0.77473	1.12452	3.630
H64C	0.40368	0.85179	1.12496	3.630
H65A	0.26656	0.84385	0.98782	3.453
H65B	0.25877	0.83455	1.06508	3.453
H65C	0.30562	0.89321	1.04328	3.453
H67A	0.55460	0.93595	1.06468	5.599
H67B	0.62974	0.95165	1.04995	5.599
H67C	0.56540	0.96962	0.99508	5.599
H68A	0.59041	0.81548	1.08829	5.445
H68B	0.62316	0.77412	1.03325	5.445
H68C	0.66450	0.83446	1.07269	5.445
H69A	0.61346	0.90241	0.90966	4.693
H69B	0.67817	0.88700	0.96500	4.693
H69C	0.63683	0.82666	0.92556	4.693
H70A	0.12875	0.72409	0.88447	4.135
H70B	0.19676	0.68780	0.91929	4.135
H70C	0.17380	0.75719	0.94864	4.135
H71A	0.20254	0.69284	0.75057	3.774
H71B	0.28151	0.71049	0.75513	3.774
H71C	0.25660	0.66132	0.80914	3.774

Table S13-2. Atomic coordinates and B_{iso} involving hydrogens/B_{eq} (continued)

atom	x	y	z	B_{eq}
H77A	0.16946	0.78125	0.65439	4.475
H77B	0.20104	0.85293	0.64151	4.475
H77C	0.24877	0.79493	0.67754	4.475
H78A	0.30004	0.91026	0.72452	4.681
H78B	0.27241	0.97440	0.75957	4.681
H78C	0.32359	0.92353	0.80288	4.681
H79A	0.08572	0.75244	0.70204	4.080
H79B	0.07484	0.73533	0.77718	4.080
H79C	0.03238	0.79456	0.73698	4.080
H80A	0.09610	0.88856	0.91470	4.495
H80B	0.03831	0.87586	0.85158	4.495
H80C	0.07406	0.81369	0.89291	4.495
H81A	0.18321	0.94750	0.92487	4.943
H81B	0.26060	0.94001	0.91332	4.943
H81C	0.21232	0.99415	0.87132	4.943
H26A	0.4544(16)	0.6742(17)	0.9256(15)	2.6(6)
H26B	0.4001(16)	0.6436(15)	0.8678(17)	2.5(6)
H26C	0.396(2)	0.629(2)	0.940(2)	5.6(10)

Table S13-3. Anisotropic displacement parameters

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Ti1	0.0205(2)	0.01470(19)	0.0209(2)	-0.00340(15)	0.00641(16)	0.00136(14)
Ti2	0.0257(3)	0.0262(2)	0.0200(2)	-0.00084(17)	0.00294(17)	-0.00376(16)
Ti3	0.0201(2)	0.0285(2)	0.0335(3)	0.00007(17)	0.00693(19)	0.00611(18)
O1	0.0204(8)	0.0143(7)	0.0209(8)	-0.0021(6)	0.0075(6)	0.0014(6)
O2	0.0228(9)	0.0248(8)	0.0172(8)	0.0012(7)	0.0036(7)	-0.0012(6)
O3	0.0211(9)	0.0282(9)	0.0245(8)	0.0022(7)	0.0087(7)	0.0026(7)
N1	0.0197(10)	0.0169(9)	0.0172(9)	0.0039(7)	0.0059(7)	0.0019(7)
C1	0.0174(11)	0.0162(10)	0.0229(11)	0.0005(8)	0.0067(9)	0.0037(8)
C2	0.0168(11)	0.0160(10)	0.0176(10)	-0.0003(8)	0.0045(8)	0.0007(8)
C3	0.0212(12)	0.0143(10)	0.0204(11)	0.0014(8)	0.0063(9)	0.0012(8)
C4	0.0215(12)	0.0164(10)	0.0192(11)	-0.0031(8)	0.0048(9)	0.0021(8)
C5	0.0182(11)	0.0197(11)	0.0211(11)	-0.0020(8)	0.0061(9)	0.0003(8)
C6	0.0198(11)	0.0158(10)	0.0176(10)	0.0006(8)	0.0048(9)	0.0008(8)
C7	0.0190(11)	0.0144(10)	0.0157(10)	-0.0024(8)	0.0030(8)	0.0015(8)
C8	0.0192(11)	0.0158(10)	0.0262(12)	0.0015(8)	0.0074(9)	0.0010(8)
C9	0.0340(14)	0.0200(11)	0.0284(13)	0.0028(10)	0.0094(11)	-0.0046(9)
C10	0.0263(13)	0.0212(11)	0.0309(13)	0.0056(9)	0.0078(10)	0.0054(9)
C11	0.0238(13)	0.0213(12)	0.0448(15)	0.0037(9)	0.0157(11)	0.0010(10)
C12	0.0246(12)	0.0165(10)	0.0278(12)	-0.0046(9)	0.0089(10)	0.0009(9)
C13	0.0451(17)	0.0301(14)	0.0369(15)	-0.0124(12)	0.0022(13)	0.0143(12)
C14	0.0369(15)	0.0207(12)	0.0404(15)	-0.0084(10)	0.0161(12)	-0.0061(10)
C15	0.0345(15)	0.0225(12)	0.0419(15)	-0.0071(10)	0.0181(12)	-0.0006(11)
C16	0.0260(13)	0.0298(13)	0.0287(13)	-0.0053(10)	0.0037(10)	0.0031(10)
C17	0.0376(15)	0.0210(12)	0.0295(13)	-0.0095(10)	0.0109(11)	-0.0020(10)
C18	0.0347(14)	0.0203(11)	0.0188(11)	-0.0051(10)	0.0083(10)	0.0019(9)
C19	0.0343(14)	0.0216(11)	0.0220(11)	-0.0004(10)	0.0133(10)	0.0037(9)
C20	0.0275(13)	0.0252(12)	0.0245(12)	-0.0027(10)	0.0119(10)	0.0057(9)
C21	0.0297(13)	0.0188(11)	0.0231(11)	-0.0056(9)	0.0092(10)	0.0038(9)
C22	0.0292(13)	0.0206(11)	0.0204(11)	-0.0037(9)	0.0061(10)	0.0043(9)
C23	0.0285(14)	0.0290(13)	0.0306(13)	-0.0032(10)	0.0013(11)	0.0077(10)
C24	0.0355(15)	0.0203(12)	0.0345(14)	-0.0047(10)	0.0087(11)	0.0051(10)
C25	0.0280(14)	0.0366(15)	0.0445(16)	-0.0045(11)	0.0160(12)	0.0100(12)
C26	0.0462(17)	0.0248(13)	0.0369(15)	0.0048(12)	0.0256(14)	0.0069(11)
C27	0.0414(16)	0.0249(12)	0.0261(13)	-0.0081(11)	0.0049(11)	0.0004(10)
C28	0.0238(12)	0.0169(10)	0.0174(10)	0.0018(8)	0.0040(9)	0.0001(8)
C29	0.0190(11)	0.0185(10)	0.0174(10)	0.0027(8)	0.0062(9)	0.0008(8)
C30	0.0227(12)	0.0198(11)	0.0184(10)	0.0030(9)	0.0061(9)	0.0003(8)

Table S13-3. Anisotropic displacement parameters (continued)

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
C31	0.0284(13)	0.0187(11)	0.0249(12)	0.0004(9)	0.0105(10)	-0.0004(9)
C32	0.0300(13)	0.0192(11)	0.0274(12)	0.0038(9)	0.0084(10)	0.0057(9)
C33	0.0238(12)	0.0264(12)	0.0204(11)	0.0052(9)	0.0065(9)	0.0055(9)
C34	0.0195(12)	0.0212(11)	0.0199(11)	0.0011(9)	0.0076(9)	0.0004(8)
C35	0.0332(14)	0.0308(13)	0.0223(12)	0.0071(11)	0.0021(11)	0.0075(10)
C36	0.0273(14)	0.0439(16)	0.0326(14)	0.0087(12)	0.0018(11)	0.0069(12)
C37	0.0487(19)	0.0377(16)	0.0344(15)	0.0108(13)	-0.0020(13)	0.0132(12)
C38	0.0350(15)	0.0472(16)	0.0208(12)	0.0022(12)	0.0035(11)	0.0098(11)
C39	0.0386(15)	0.0186(11)	0.0294(13)	-0.0012(10)	0.0068(11)	-0.0010(9)
C40	0.064(2)	0.0282(14)	0.0319(15)	-0.0016(13)	0.0001(14)	-0.0061(11)
C41	0.066(2)	0.0347(17)	0.057(2)	0.0095(15)	0.0057(18)	-0.0160(15)
C42	0.080(3)	0.058(2)	0.0376(17)	-0.038(2)	0.0104(17)	-0.0045(15)
C43	0.0318(16)	0.0458(17)	0.0366(15)	-0.0022(13)	-0.0017(12)	-0.0091(13)
C44	0.0473(18)	0.0291(14)	0.0325(14)	-0.0081(12)	0.0064(13)	-0.0055(11)
C45	0.0319(15)	0.0499(17)	0.0269(13)	0.0096(12)	0.0077(11)	-0.0142(12)
C46	0.0516(19)	0.0347(15)	0.0410(16)	0.0130(13)	0.0165(14)	-0.0020(12)
C47	0.0395(17)	0.0427(16)	0.0357(15)	-0.0037(13)	0.0084(13)	-0.0207(13)
C48	0.0330(15)	0.0492(17)	0.0264(13)	0.0033(12)	0.0106(12)	-0.0030(12)
C49	0.0279(14)	0.0428(16)	0.0344(14)	0.0024(12)	0.0117(12)	-0.0101(12)
C50	0.0312(16)	0.0513(18)	0.0480(18)	-0.0037(13)	0.0151(14)	-0.0090(14)
C51	0.047(2)	0.071(2)	0.0281(15)	0.0019(17)	0.0077(14)	0.0052(15)
C52	0.061(2)	0.054(2)	0.053(2)	-0.0132(17)	0.0131(17)	-0.0262(17)
C53	0.081(3)	0.0415(19)	0.062(2)	0.0210(18)	0.019(2)	0.0011(16)
C54	0.0368(18)	0.084(3)	0.0314(16)	0.0220(17)	0.0027(13)	-0.0115(16)
C55	0.0190(12)	0.0217(11)	0.0205(11)	0.0021(9)	0.0058(9)	0.0006(8)
C56	0.0235(12)	0.0199(11)	0.0176(10)	0.0039(9)	0.0078(9)	0.0015(8)
C57	0.0234(12)	0.0263(12)	0.0206(11)	0.0030(9)	0.0085(9)	0.0004(9)
C58	0.0248(13)	0.0336(13)	0.0220(12)	0.0023(10)	0.0039(10)	-0.0020(10)
C59	0.0317(14)	0.0373(14)	0.0182(11)	0.0041(11)	0.0064(10)	-0.0036(10)
C60	0.0289(13)	0.0271(12)	0.0219(12)	0.0063(10)	0.0107(10)	0.0013(9)
C61	0.0193(12)	0.0221(11)	0.0228(11)	0.0051(9)	0.0072(9)	0.0014(9)
C62	0.0339(15)	0.0358(14)	0.0235(12)	0.0061(11)	0.0127(11)	0.0010(10)
C63	0.0421(16)	0.0380(15)	0.0260(13)	0.0015(12)	0.0146(12)	0.0065(11)
C64	0.0447(17)	0.0501(17)	0.0241(13)	0.0035(14)	0.0177(12)	-0.0006(12)
C65	0.0358(16)	0.0456(16)	0.0316(14)	0.0091(13)	0.0169(12)	-0.0019(12)
C66	0.0287(14)	0.0500(17)	0.0255(13)	-0.0014(12)	0.0036(11)	-0.0057(12)
C67	0.046(2)	0.070(3)	0.061(2)	-0.0137(18)	0.0097(17)	-0.027(2)

Table S13-3. Anisotropic displacement parameters (continued)

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
C68	0.0397(19)	0.087(3)	0.0431(19)	-0.0004(18)	-0.0027(15)	0.0103(18)
C69	0.0337(17)	0.079(3)	0.0361(16)	-0.0112(16)	0.0043(13)	-0.0084(16)
C70	0.0246(15)	0.0553(19)	0.0524(19)	-0.0017(13)	0.0099(13)	0.0192(15)
C71	0.0292(15)	0.0333(15)	0.0550(19)	-0.0036(12)	0.0001(13)	-0.0044(13)
C72	0.0247(14)	0.0275(13)	0.0490(17)	0.0063(10)	0.0051(12)	0.0093(12)
C73	0.0345(16)	0.0303(14)	0.0394(15)	0.0081(11)	-0.0026(12)	0.0009(11)
C74	0.0302(15)	0.0370(15)	0.0351(14)	0.0094(11)	0.0082(12)	0.0070(11)
C75	0.0285(14)	0.0297(14)	0.0402(15)	0.0033(11)	0.0001(12)	0.0038(11)
C76	0.0415(16)	0.0262(13)	0.0356(15)	0.0113(11)	0.0111(12)	0.0067(11)
C77	0.064(2)	0.0384(17)	0.0425(17)	0.0138(15)	0.0198(16)	0.0043(13)
C78	0.0331(16)	0.0318(15)	0.084(3)	0.0028(13)	0.0107(16)	0.0192(16)
C79	0.0384(17)	0.0359(16)	0.0533(19)	-0.0001(13)	0.0020(14)	0.0052(14)
C80	0.0410(18)	0.061(2)	0.0437(18)	0.0103(15)	0.0168(14)	0.0050(15)
C81	0.059(2)	0.0373(17)	0.055(2)	0.0087(15)	-0.0092(17)	-0.0061(15)

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 S13-4. Bond lengths (Å)

atom	atom	distance	atom	atom	distance
Ti1	O1	1.8221(16)	Ti1	C16	2.122(2)
Ti1	C17	2.133(3)	Ti1	C18	2.369(2)
Ti1	C19	2.388(3)	Ti1	C20	2.406(3)
Ti1	C21	2.411(2)	Ti1	C22	2.375(2)
Ti2	O2	1.8230(17)	Ti2	C43	2.122(3)
Ti2	C44	2.136(3)	Ti2	C45	2.392(3)
Ti2	C46	2.422(3)	Ti2	C47	2.410(3)
Ti2	C48	2.375(3)	Ti2	C49	2.370(3)
Ti3	O3	1.8149(17)	Ti3	C70	2.129(4)
Ti3	C71	2.128(3)	Ti3	C72	2.384(3)
Ti3	C73	2.395(3)	Ti3	C74	2.403(3)
Ti3	C75	2.403(3)	Ti3	C76	2.395(3)
O1	C7	1.369(3)	O2	C34	1.367(3)
O3	C61	1.370(3)	N1	C1	1.462(3)
N1	C28	1.467(3)	N1	C55	1.456(3)
C1	C2	1.515(3)	C2	C3	1.388(3)
C2	C7	1.403(3)	C3	C4	1.393(3)
C4	C5	1.393(3)	C4	C12	1.539(3)
C5	C6	1.402(3)	C6	C7	1.411(3)
C6	C8	1.532(3)	C8	C9	1.543(3)
C8	C10	1.539(3)	C8	C11	1.535(4)
C12	C13	1.532(4)	C12	C14	1.537(4)
C12	C15	1.528(4)	C18	C19	1.419(4)
C18	C22	1.423(3)	C18	C27	1.508(4)
C19	C20	1.430(3)	C19	C26	1.504(4)
C20	C21	1.414(3)	C20	C25	1.494(4)
C21	C22	1.422(3)	C21	C24	1.501(3)
C22	C23	1.499(4)	C28	C29	1.516(3)
C29	C30	1.393(3)	C29	C34	1.398(3)
C30	C31	1.391(3)	C31	C32	1.392(3)
C31	C39	1.539(3)	C32	C33	1.403(3)
C33	C34	1.416(3)	C33	C35	1.541(3)
C35	C36	1.536(4)	C35	C37	1.530(4)
C35	C38	1.540(4)	C39	C40	1.533(4)
C39	C41	1.535(5)	C39	C42	1.516(5)
C45	C46	1.416(4)	C45	C49	1.390(4)
C45	C54	1.517(4)	C46	C47	1.423(4)

Table S13-4. Bond lengths (Å) (continued)

atom	atom	distance	atom	atom	distance
C46	C53	1.506(5)	C47	C48	1.408(5)
C47	C52	1.506(5)	C48	C49	1.411(4)
C48	C51	1.509(4)	C49	C50	1.518(4)
C55	C56	1.518(3)	C56	C57	1.382(3)
C56	C61	1.403(4)	C57	C58	1.397(3)
C58	C59	1.398(4)	C58	C66	1.539(4)
C59	C60	1.395(4)	C60	C61	1.416(3)
C60	C62	1.540(4)	C62	C63	1.542(4)
C62	C64	1.539(4)	C62	C65	1.545(4)
C66	C67	1.538(5)	C66	C68	1.538(5)
C66	C69	1.516(5)	C72	C73	1.410(5)
C72	C76	1.413(4)	C72	C78	1.517(5)
C73	C74	1.411(4)	C73	C81	1.501(5)
C74	C75	1.408(4)	C74	C80	1.515(5)
C75	C76	1.433(4)	C75	C79	1.504(4)
C76	C77	1.508(4)			

Table S13-5. Bond lengths involving hydrogens (Å)

atom	atom	distance	atom	atom	distance
C1	H1A	0.990	C1	H1B	0.990
C3	H3	0.950	C5	H5	0.950
C9	H9A	0.980	C9	H9B	0.980
C9	H9C	0.980	C10	H10A	0.980
C10	H10B	0.980	C10	H10C	0.980
C11	H11A	0.980	C11	H11B	0.980
C11	H11C	0.980	C13	H13A	0.980
C13	H13B	0.980	C13	H13C	0.980
C14	H14A	0.980	C14	H14B	0.980
C14	H14C	0.980	C15	H15A	0.980
C15	H15B	0.980	C15	H15C	0.980
C16	H16A	0.980	C16	H16B	0.980
C16	H16C	0.980	C17	H17A	0.980
C17	H17B	0.980	C17	H17C	0.980
C23	H23A	0.980	C23	H23B	0.980
C23	H23C	0.980	C24	H24A	0.980
C24	H24B	0.980	C24	H24C	0.980
C25	H25A	0.980	C25	H25B	0.980
C25	H25C	0.980	C26	H26A	0.98(3)
C26	H26B	0.97(3)	C26	H26C	0.92(5)
C27	H27A	0.980	C27	H27B	0.980
C27	H27C	0.980	C28	H28A	0.990
C28	H28B	0.990	C30	H30	0.950
C32	H32	0.950	C36	H36A	0.980
C36	H36B	0.980	C36	H36C	0.980
C37	H37A	0.980	C37	H37B	0.980
C37	H37C	0.980	C38	H38A	0.980
C38	H38B	0.980	C38	H38C	0.980
C40	H40A	0.980	C40	H40B	0.980
C40	H40C	0.980	C41	H41A	0.980
C41	H41B	0.980	C41	H41C	0.980
C42	H42A	0.980	C42	H42B	0.980
C42	H42C	0.980	C43	H43A	0.980
C43	H43B	0.980	C43	H43C	0.980
C44	H44A	0.980	C44	H44B	0.980
C44	H44C	0.980	C50	H50A	0.980
C50	H50B	0.980	C50	H50C	0.980

Table S13-5. Bond lengths involving hydrogens (Å) (continued)

atom	atom	distance	atom	atom	distance
C51	H51A	0.980	C51	H51B	0.980
C51	H51C	0.980	C52	H52A	0.980
C52	H52B	0.980	C52	H52C	0.980
C53	H53A	0.980	C53	H53B	0.980
C53	H53C	0.980	C54	H54A	0.980
C54	H54B	0.980	C54	H54C	0.980
C55	H55A	0.990	C55	H55B	0.990
C57	H57	0.950	C59	H59	0.950
C63	H63A	0.980	C63	H63B	0.980
C63	H63C	0.980	C64	H64A	0.980
C64	H64B	0.980	C64	H64C	0.980
C65	H65A	0.980	C65	H65B	0.980
C65	H65C	0.980	C67	H67A	0.980
C67	H67B	0.980	C67	H67C	0.980
C68	H68A	0.980	C68	H68B	0.980
C68	H68C	0.980	C69	H69A	0.980
C69	H69B	0.980	C69	H69C	0.980
C70	H70A	0.980	C70	H70B	0.980
C70	H70C	0.980	C71	H71A	0.980
C71	H71B	0.980	C71	H71C	0.980
C77	H77A	0.980	C77	H77B	0.980
C77	H77C	0.980	C78	H78A	0.980
C78	H78B	0.980	C78	H78C	0.980
C79	H79A	0.980	C79	H79B	0.980
C79	H79C	0.980	C80	H80A	0.980
C80	H80B	0.980	C80	H80C	0.980
C81	H81A	0.980	C81	H81B	0.980
C81	H81C	0.980			

Table S13-6. Bond angles (°)

atom	atom	atom	angle	atom	atom	atom	angle
O1	Ti1	C16	104.74(9)	O1	Ti1	C17	102.31(9)
O1	Ti1	C18	94.68(8)	O1	Ti1	C19	112.57(8)
O1	Ti1	C20	147.29(8)	O1	Ti1	C21	145.69(8)
O1	Ti1	C22	111.16(8)	C16	Ti1	C17	95.63(10)
C16	Ti1	C18	128.17(10)	C16	Ti1	C19	93.95(10)
C16	Ti1	C20	83.41(9)	C16	Ti1	C21	108.47(10)
C16	Ti1	C22	140.51(10)	C17	Ti1	C18	126.75(9)
C17	Ti1	C19	139.98(9)	C17	Ti1	C20	108.42(10)
C17	Ti1	C21	82.97(9)	C17	Ti1	C22	92.39(9)
C18	Ti1	C19	34.70(9)	C18	Ti1	C20	57.83(8)
C18	Ti1	C21	57.64(8)	C18	Ti1	C22	34.92(8)
C19	Ti1	C20	34.71(8)	C19	Ti1	C21	57.17(8)
C19	Ti1	C22	57.57(9)	C20	Ti1	C21	34.14(8)
C20	Ti1	C22	57.45(9)	C21	Ti1	C22	34.56(8)
O2	Ti2	C43	100.86(10)	O2	Ti2	C44	105.05(10)
O2	Ti2	C45	104.75(9)	O2	Ti2	C46	137.04(9)
O2	Ti2	C47	153.33(10)	O2	Ti2	C48	121.00(10)
O2	Ti2	C49	96.61(9)	C43	Ti2	C44	96.79(12)
C43	Ti2	C45	141.43(11)	C43	Ti2	C46	120.44(11)
C43	Ti2	C47	88.46(11)	C43	Ti2	C48	85.36(11)
C43	Ti2	C49	115.22(11)	C44	Ti2	C45	103.72(11)
C44	Ti2	C46	82.67(12)	C44	Ti2	C47	98.49(11)
C44	Ti2	C48	132.69(11)	C44	Ti2	C49	137.00(11)
C45	Ti2	C46	34.20(11)	C45	Ti2	C47	56.69(10)
C45	Ti2	C48	56.75(10)	C45	Ti2	C49	33.93(10)
C46	Ti2	C47	34.26(10)	C46	Ti2	C48	56.98(11)
C46	Ti2	C49	56.96(11)	C47	Ti2	C48	34.21(11)
C47	Ti2	C49	57.06(10)	C48	Ti2	C49	34.60(9)
O3	Ti3	C70	101.79(10)	O3	Ti3	C71	103.06(10)
O3	Ti3	C72	101.83(9)	O3	Ti3	C73	102.08(9)
O3	Ti3	C74	131.03(9)	O3	Ti3	C75	157.79(9)
O3	Ti3	C76	130.11(9)	C70	Ti3	C71	95.20(13)
C70	Ti3	C72	139.14(12)	C70	Ti3	C73	107.76(12)
C70	Ti3	C74	82.66(11)	C70	Ti3	C75	92.74(11)
C70	Ti3	C76	127.04(11)	C71	Ti3	C72	111.20(12)
C71	Ti3	C73	141.38(11)	C71	Ti3	C74	125.31(10)
C71	Ti3	C75	92.12(11)	C71	Ti3	C76	83.99(11)

Table S13-6. Bond angles (°) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
C72	Ti3	C73	34.32(11)	C72	Ti3	C74	56.76(10)
C72	Ti3	C75	57.02(9)	C72	Ti3	C76	34.39(9)
C73	Ti3	C74	34.22(10)	C73	Ti3	C75	57.02(9)
C73	Ti3	C76	57.39(10)	C74	Ti3	C75	34.06(10)
C74	Ti3	C76	57.20(10)	C75	Ti3	C76	34.75(10)
Ti1	O1	C7	165.63(15)	Ti2	O2	C34	165.28(15)
Ti3	O3	C61	166.02(16)	C1	N1	C28	110.77(18)
C1	N1	C55	111.77(18)	C28	N1	C55	110.85(17)
N1	C1	C2	111.82(19)	C1	C2	C3	120.2(2)
C1	C2	C7	120.0(2)	C3	C2	C7	119.8(2)
C2	C3	C4	121.7(2)	C3	C4	C5	117.4(2)
C3	C4	C12	119.0(2)	C5	C4	C12	123.6(2)
C4	C5	C6	123.5(2)	C5	C6	C7	117.1(2)
C5	C6	C8	120.8(2)	C7	C6	C8	122.02(19)
O1	C7	C2	117.2(2)	O1	C7	C6	122.30(19)
C2	C7	C6	120.5(2)	C6	C8	C9	108.86(18)
C6	C8	C10	110.1(2)	C6	C8	C11	112.28(19)
C9	C8	C10	111.26(19)	C9	C8	C11	107.7(2)
C10	C8	C11	106.62(19)	C4	C12	C13	109.33(19)
C4	C12	C14	108.7(2)	C4	C12	C15	112.42(19)
C13	C12	C14	109.0(2)	C13	C12	C15	108.9(2)
C14	C12	C15	108.3(2)	Ti1	C18	C19	73.39(14)
Ti1	C18	C22	72.79(14)	Ti1	C18	C27	120.39(17)
C19	C18	C22	107.6(2)	C19	C18	C27	126.8(2)
C22	C18	C27	125.6(2)	Ti1	C19	C18	71.91(15)
Ti1	C19	C20	73.34(15)	Ti1	C19	C26	124.68(18)
C18	C19	C20	108.3(2)	C18	C19	C26	127.6(2)
C20	C19	C26	123.9(2)	Ti1	C20	C19	71.95(15)
Ti1	C20	C21	73.12(15)	Ti1	C20	C25	125.22(18)
C19	C20	C21	107.7(2)	C19	C20	C25	125.7(2)
C21	C20	C25	126.4(2)	Ti1	C21	C20	72.74(14)
Ti1	C21	C22	71.35(14)	Ti1	C21	C24	125.99(18)
C20	C21	C22	108.2(2)	C20	C21	C24	125.7(2)
C22	C21	C24	125.8(2)	Ti1	C22	C18	72.29(13)
Ti1	C22	C21	74.10(13)	Ti1	C22	C23	122.47(18)
C18	C22	C21	108.2(2)	C18	C22	C23	127.1(2)
C21	C22	C23	124.7(2)	N1	C28	C29	112.17(18)

Table S13-6. Bond angles (°) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
C28	C29	C30	120.56(19)	C28	C29	C34	119.38(19)
C30	C29	C34	120.1(2)	C29	C30	C31	121.3(2)
C30	C31	C32	117.4(2)	C30	C31	C39	121.6(2)
C32	C31	C39	121.0(2)	C31	C32	C33	123.8(2)
C32	C33	C34	116.7(2)	C32	C33	C35	121.2(2)
C34	C33	C35	122.1(2)	O2	C34	C29	117.11(19)
O2	C34	C33	122.47(19)	C29	C34	C33	120.4(2)
C33	C35	C36	108.0(2)	C33	C35	C37	112.0(2)
C33	C35	C38	110.9(2)	C36	C35	C37	107.7(2)
C36	C35	C38	110.5(2)	C37	C35	C38	107.6(2)
C31	C39	C40	112.6(2)	C31	C39	C41	109.5(2)
C31	C39	C42	109.9(2)	C40	C39	C41	107.0(3)
C40	C39	C42	108.5(2)	C41	C39	C42	109.3(3)
Ti2	C45	C46	74.05(18)	Ti2	C45	C49	72.19(17)
Ti2	C45	C54	126.4(2)	C46	C45	C49	109.1(2)
C46	C45	C54	125.8(3)	C49	C45	C54	124.6(3)
Ti2	C46	C45	71.75(18)	Ti2	C46	C47	72.44(18)
Ti2	C46	C53	127.1(3)	C45	C46	C47	106.9(3)
C45	C46	C53	126.4(3)	C47	C46	C53	126.2(3)
Ti2	C47	C46	73.30(18)	Ti2	C47	C48	71.51(18)
Ti2	C47	C52	123.7(2)	C46	C47	C48	107.9(3)
C46	C47	C52	124.6(3)	C48	C47	C52	127.4(3)
Ti2	C48	C47	74.28(18)	Ti2	C48	C49	72.53(17)
Ti2	C48	C51	123.1(2)	C47	C48	C49	108.2(2)
C47	C48	C51	125.0(3)	C49	C48	C51	126.6(3)
Ti2	C49	C45	73.88(18)	Ti2	C49	C48	72.87(17)
Ti2	C49	C50	122.4(2)	C45	C49	C48	108.0(3)
C45	C49	C50	124.3(2)	C48	C49	C50	127.6(3)
N1	C55	C56	112.96(18)	C55	C56	C57	121.6(2)
C55	C56	C61	118.4(2)	C57	C56	C61	119.9(2)
C56	C57	C58	121.6(2)	C57	C58	C59	117.0(2)
C57	C58	C66	122.4(2)	C59	C58	C66	120.5(2)
C58	C59	C60	124.0(2)	C59	C60	C61	116.6(2)
C59	C60	C62	121.2(2)	C61	C60	C62	122.1(2)
O3	C61	C56	117.6(2)	O3	C61	C60	121.8(2)
C56	C61	C60	120.6(2)	C60	C62	C63	108.8(2)
C60	C62	C64	112.3(2)	C60	C62	C65	110.5(2)

Table S13-6. Bond angles (°) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
C63	C62	C64	106.8(2)	C63	C62	C65	110.4(2)
C64	C62	C65	107.9(2)	C58	C66	C67	108.6(2)
C58	C66	C68	109.5(3)	C58	C66	C69	112.9(2)
C67	C66	C68	108.9(3)	C67	C66	C69	108.6(3)
C68	C66	C69	108.3(3)	Ti3	C72	C73	73.27(17)
Ti3	C72	C76	73.24(16)	Ti3	C72	C78	126.18(19)
C73	C72	C76	109.1(3)	C73	C72	C78	124.0(3)
C76	C72	C78	126.4(3)	Ti3	C73	C72	72.41(16)
Ti3	C73	C74	73.20(16)	Ti3	C73	C81	123.9(2)
C72	C73	C74	107.5(2)	C72	C73	C81	125.3(3)
C74	C73	C81	127.0(3)	Ti3	C74	C73	72.58(16)
Ti3	C74	C75	72.98(16)	Ti3	C74	C80	125.5(2)
C73	C74	C75	108.6(3)	C73	C74	C80	124.9(3)
C75	C74	C80	126.2(3)	Ti3	C75	C74	72.95(15)
Ti3	C75	C76	72.31(15)	Ti3	C75	C79	121.20(19)
C74	C75	C76	107.9(2)	C74	C75	C79	125.4(3)
C76	C75	C79	126.6(3)	Ti3	C76	C72	72.37(16)
Ti3	C76	C75	72.94(16)	Ti3	C76	C77	123.6(2)
C72	C76	C75	106.8(3)	C72	C76	C77	126.7(3)
C75	C76	C77	126.2(3)				

Table S13-7. Bond angles involving hydrogens (°)

atom	atom	atom	angle	atom	atom	atom	angle
N1	C1	H1A	109.2	N1	C1	H1B	109.2
C2	C1	H1A	109.3	C2	C1	H1B	109.3
H1A	C1	H1B	107.9	C2	C3	H3	119.2
C4	C3	H3	119.2	C4	C5	H5	118.3
C6	C5	H5	118.2	C8	C9	H9A	109.5
C8	C9	H9B	109.5	C8	C9	H9C	109.5
H9A	C9	H9B	109.5	H9A	C9	H9C	109.5
H9B	C9	H9C	109.5	C8	C10	H10A	109.5
C8	C10	H10B	109.5	C8	C10	H10C	109.5
H10A	C10	H10B	109.5	H10A	C10	H10C	109.5
H10B	C10	H10C	109.5	C8	C11	H11A	109.5
C8	C11	H11B	109.5	C8	C11	H11C	109.5
H11A	C11	H11B	109.5	H11A	C11	H11C	109.5
H11B	C11	H11C	109.5	C12	C13	H13A	109.5
C12	C13	H13B	109.5	C12	C13	H13C	109.5
H13A	C13	H13B	109.5	H13A	C13	H13C	109.5
H13B	C13	H13C	109.5	C12	C14	H14A	109.5
C12	C14	H14B	109.5	C12	C14	H14C	109.5
H14A	C14	H14B	109.5	H14A	C14	H14C	109.5
H14B	C14	H14C	109.5	C12	C15	H15A	109.5
C12	C15	H15B	109.5	C12	C15	H15C	109.5
H15A	C15	H15B	109.5	H15A	C15	H15C	109.5
H15B	C15	H15C	109.5	Ti1	C16	H16A	109.5
Ti1	C16	H16B	109.5	Ti1	C16	H16C	109.5
H16A	C16	H16B	109.5	H16A	C16	H16C	109.5
H16B	C16	H16C	109.5	Ti1	C17	H17A	109.5
Ti1	C17	H17B	109.5	Ti1	C17	H17C	109.5
H17A	C17	H17B	109.5	H17A	C17	H17C	109.5
H17B	C17	H17C	109.5	C22	C23	H23A	109.5
C22	C23	H23B	109.5	C22	C23	H23C	109.5
H23A	C23	H23B	109.5	H23A	C23	H23C	109.5
H23B	C23	H23C	109.5	C21	C24	H24A	109.5
C21	C24	H24B	109.5	C21	C24	H24C	109.5
H24A	C24	H24B	109.5	H24A	C24	H24C	109.5
H24B	C24	H24C	109.5	C20	C25	H25A	109.5
C20	C25	H25B	109.5	C20	C25	H25C	109.5
H25A	C25	H25B	109.5	H25A	C25	H25C	109.5

Table S13-7. Bond angles involving hydrogens (°) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
H25B	C25	H25C	109.5	C19	C26	H26A	112.1(19)
C19	C26	H26B	109.4(19)	C19	C26	H26C	112(3)
H26A	C26	H26B	109(3)	H26A	C26	H26C	108(3)
H26B	C26	H26C	106(3)	C18	C27	H27A	109.5
C18	C27	H27B	109.5	C18	C27	H27C	109.5
H27A	C27	H27B	109.5	H27A	C27	H27C	109.5
H27B	C27	H27C	109.5	N1	C28	H28A	109.2
N1	C28	H28B	109.2	C29	C28	H28A	109.2
C29	C28	H28B	109.2	H28A	C28	H28B	107.9
C29	C30	H30	119.3	C31	C30	H30	119.3
C31	C32	H32	118.1	C33	C32	H32	118.1
C35	C36	H36A	109.5	C35	C36	H36B	109.5
C35	C36	H36C	109.5	H36A	C36	H36B	109.5
H36A	C36	H36C	109.5	H36B	C36	H36C	109.5
C35	C37	H37A	109.5	C35	C37	H37B	109.5
C35	C37	H37C	109.5	H37A	C37	H37B	109.5
H37A	C37	H37C	109.5	H37B	C37	H37C	109.5
C35	C38	H38A	109.5	C35	C38	H38B	109.5
C35	C38	H38C	109.5	H38A	C38	H38B	109.5
H38A	C38	H38C	109.5	H38B	C38	H38C	109.5
C39	C40	H40A	109.5	C39	C40	H40B	109.5
C39	C40	H40C	109.5	H40A	C40	H40B	109.5
H40A	C40	H40C	109.5	H40B	C40	H40C	109.5
C39	C41	H41A	109.5	C39	C41	H41B	109.5
C39	C41	H41C	109.5	H41A	C41	H41B	109.5
H41A	C41	H41C	109.5	H41B	C41	H41C	109.5
C39	C42	H42A	109.5	C39	C42	H42B	109.5
C39	C42	H42C	109.5	H42A	C42	H42B	109.5
H42A	C42	H42C	109.5	H42B	C42	H42C	109.5
Ti2	C43	H43A	109.5	Ti2	C43	H43B	109.5
Ti2	C43	H43C	109.5	H43A	C43	H43B	109.5
H43A	C43	H43C	109.5	H43B	C43	H43C	109.5
Ti2	C44	H44A	109.5	Ti2	C44	H44B	109.5
Ti2	C44	H44C	109.5	H44A	C44	H44B	109.5
H44A	C44	H44C	109.5	H44B	C44	H44C	109.5
C49	C50	H50A	109.5	C49	C50	H50B	109.5
C49	C50	H50C	109.5	H50A	C50	H50B	109.5

Table S13-7. Bond angles involving hydrogens (°) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
H50A	C50	H50C	109.5	H50B	C50	H50C	109.5
C48	C51	H51A	109.5	C48	C51	H51B	109.5
C48	C51	H51C	109.5	H51A	C51	H51B	109.5
H51A	C51	H51C	109.5	H51B	C51	H51C	109.5
C47	C52	H52A	109.5	C47	C52	H52B	109.5
C47	C52	H52C	109.5	H52A	C52	H52B	109.5
H52A	C52	H52C	109.5	H52B	C52	H52C	109.5
C46	C53	H53A	109.5	C46	C53	H53B	109.5
C46	C53	H53C	109.5	H53A	C53	H53B	109.5
H53A	C53	H53C	109.5	H53B	C53	H53C	109.5
C45	C54	H54A	109.5	C45	C54	H54B	109.5
C45	C54	H54C	109.5	H54A	C54	H54B	109.5
H54A	C54	H54C	109.5	H54B	C54	H54C	109.5
N1	C55	H55A	109.0	N1	C55	H55B	109.0
C56	C55	H55A	109.0	C56	C55	H55B	109.0
H55A	C55	H55B	107.8	C56	C57	H57	119.2
C58	C57	H57	119.2	C58	C59	H59	118.0
C60	C59	H59	118.0	C62	C63	H63A	109.5
C62	C63	H63B	109.5	C62	C63	H63C	109.5
H63A	C63	H63B	109.5	H63A	C63	H63C	109.5
H63B	C63	H63C	109.5	C62	C64	H64A	109.5
C62	C64	H64B	109.5	C62	C64	H64C	109.5
H64A	C64	H64B	109.5	H64A	C64	H64C	109.5
H64B	C64	H64C	109.5	C62	C65	H65A	109.5
C62	C65	H65B	109.5	C62	C65	H65C	109.5
H65A	C65	H65B	109.5	H65A	C65	H65C	109.5
H65B	C65	H65C	109.5	C66	C67	H67A	109.5
C66	C67	H67B	109.5	C66	C67	H67C	109.5
H67A	C67	H67B	109.5	H67A	C67	H67C	109.5
H67B	C67	H67C	109.5	C66	C68	H68A	109.5
C66	C68	H68B	109.5	C66	C68	H68C	109.5
H68A	C68	H68B	109.5	H68A	C68	H68C	109.5
H68B	C68	H68C	109.5	C66	C69	H69A	109.5
C66	C69	H69B	109.5	C66	C69	H69C	109.5
H69A	C69	H69B	109.5	H69A	C69	H69C	109.5
H69B	C69	H69C	109.5	Ti3	C70	H70A	109.5
Ti3	C70	H70B	109.5	Ti3	C70	H70C	109.5

Table S13-7. Bond angles involving hydrogens (°) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
H70A	C70	H70B	109.5	H70A	C70	H70C	109.5
H70B	C70	H70C	109.5	Ti3	C71	H71A	109.5
Ti3	C71	H71B	109.5	Ti3	C71	H71C	109.5
H71A	C71	H71B	109.5	H71A	C71	H71C	109.5
H71B	C71	H71C	109.5	C76	C77	H77A	109.5
C76	C77	H77B	109.5	C76	C77	H77C	109.5
H77A	C77	H77B	109.5	H77A	C77	H77C	109.5
H77B	C77	H77C	109.5	C72	C78	H78A	109.5
C72	C78	H78B	109.5	C72	C78	H78C	109.5
H78A	C78	H78B	109.5	H78A	C78	H78C	109.5
H78B	C78	H78C	109.4	C75	C79	H79A	109.5
C75	C79	H79B	109.5	C75	C79	H79C	109.5
H79A	C79	H79B	109.5	H79A	C79	H79C	109.5
H79B	C79	H79C	109.5	C74	C80	H80A	109.5
C74	C80	H80B	109.5	C74	C80	H80C	109.5
H80A	C80	H80B	109.5	H80A	C80	H80C	109.5
H80B	C80	H80C	109.5	C73	C81	H81A	109.5
C73	C81	H81B	109.5	C73	C81	H81C	109.5
H81A	C81	H81B	109.5	H81A	C81	H81C	109.5
H81B	C81	H81C	109.5				

Table S13-8. Torsion Angles(O)
(Those having bond angles > 160 or < 20 degrees are excluded.)

atom1	atom2	atom3	atom4	angle	atom1	atom2	atom3	atom4	angle
O1	Ti1	C18	C19	123.94(10)	O1	Ti1	C18	C22	-121.03(10)
O1	Ti1	C18	C27	0.58(16)	O1	Ti1	C19	C18	-63.56(11)
O1	Ti1	C19	C20	-179.80(8)	O1	Ti1	C19	C26	60.14(18)
O1	Ti1	C20	C19	0.34(19)	O1	Ti1	C20	C21	-115.30(13)
O1	Ti1	C20	C25	121.73(16)	O1	Ti1	C21	C20	119.91(13)
O1	Ti1	C21	C22	3.11(19)	O1	Ti1	C21	C24	-118.09(16)
O1	Ti1	C22	C18	66.32(12)	O1	Ti1	C22	C21	-178.12(9)
O1	Ti1	C22	C23	-56.82(17)	C16	Ti1	C18	C19	11.05(16)
C16	Ti1	C18	C22	126.08(12)	C16	Ti1	C18	C27	-112.31(17)
C16	Ti1	C19	C18	-171.31(11)	C16	Ti1	C19	C20	72.45(11)
C16	Ti1	C19	C26	-47.61(17)	C16	Ti1	C20	C19	-106.76(11)
C16	Ti1	C20	C21	137.61(11)	C16	Ti1	C20	C25	14.64(16)
C16	Ti1	C21	C20	-44.92(12)	C16	Ti1	C21	C22	-161.72(10)
C16	Ti1	C21	C24	77.08(19)	C16	Ti1	C22	C18	-87.67(16)
C16	Ti1	C22	C21	27.89(19)	C16	Ti1	C22	C23	149.19(15)
C17	Ti1	C18	C19	-126.90(12)	C17	Ti1	C18	C22	-11.87(17)
C17	Ti1	C18	C27	109.74(16)	C17	Ti1	C19	C18	85.10(16)
C17	Ti1	C19	C20	-31.14(18)	C17	Ti1	C19	C26	-151.19(15)
C17	Ti1	C20	C19	159.48(10)	C17	Ti1	C20	C21	43.85(12)
C17	Ti1	C20	C25	-79.12(17)	C17	Ti1	C21	C20	-138.53(11)
C17	Ti1	C21	C22	104.67(11)	C17	Ti1	C21	C24	-16.53(17)
C17	Ti1	C22	C18	170.50(12)	C17	Ti1	C22	C21	-73.94(12)
C17	Ti1	C22	C23	47.36(17)	C18	Ti1	C19	C18	0.00(10)
C18	Ti1	C19	C20	-116.24(17)	C18	Ti1	C19	C26	123.7(2)
C19	Ti1	C18	C19	0.00(10)	C19	Ti1	C18	C22	115.03(18)
C19	Ti1	C18	C27	-123.4(2)	C18	Ti1	C20	C19	37.10(9)
C18	Ti1	C20	C21	-78.53(11)	C18	Ti1	C20	C25	158.5(2)
C20	Ti1	C18	C19	-37.12(9)	C20	Ti1	C18	C22	77.91(11)
C20	Ti1	C18	C27	-160.48(19)	C18	Ti1	C21	C20	79.11(11)
C18	Ti1	C21	C22	-37.68(9)	C18	Ti1	C21	C24	-158.9(2)
C21	Ti1	C18	C19	-77.74(11)	C21	Ti1	C18	C22	37.28(10)
C21	Ti1	C18	C27	158.9(2)	C18	Ti1	C22	C18	0.00(11)
C18	Ti1	C22	C21	115.56(19)	C18	Ti1	C22	C23	-123.1(2)
C22	Ti1	C18	C19	-115.03(19)	C22	Ti1	C18	C22	-0.00(11)
C22	Ti1	C18	C27	121.6(2)	C19	Ti1	C20	C19	-0.00(10)
C19	Ti1	C20	C21	-115.63(17)	C19	Ti1	C20	C25	121.4(2)
C20	Ti1	C19	C18	116.24(17)	C20	Ti1	C19	C20	-0.00(10)

Table S13-8. Torsion angles (°) (continued)

atom1	atom2	atom3	atom4	angle	atom1	atom2	atom3	atom4	angle
C20	Ti1	C19	C26	-120.1(2)	C19	Ti1	C21	C20	37.66(9)
C19	Ti1	C21	C22	-79.14(11)	C19	Ti1	C21	C24	159.7(2)
C21	Ti1	C19	C18	79.22(11)	C21	Ti1	C19	C20	-37.02(9)
C21	Ti1	C19	C26	-157.1(2)	C19	Ti1	C22	C18	-37.67(10)
C19	Ti1	C22	C21	77.89(12)	C19	Ti1	C22	C23	-160.81(19)
C22	Ti1	C19	C18	37.92(9)	C22	Ti1	C19	C20	-78.32(11)
C22	Ti1	C19	C26	161.6(2)	C20	Ti1	C21	C20	0.00(10)
C20	Ti1	C21	C22	-116.80(17)	C20	Ti1	C21	C24	122.0(2)
C21	Ti1	C20	C19	115.63(17)	C21	Ti1	C20	C21	-0.00(10)
C21	Ti1	C20	C25	-123.0(2)	C20	Ti1	C22	C18	-79.10(12)
C20	Ti1	C22	C21	36.47(9)	C20	Ti1	C22	C23	157.76(19)
C22	Ti1	C20	C19	78.71(11)	C22	Ti1	C20	C21	-36.92(9)
C22	Ti1	C20	C25	-159.9(2)	C21	Ti1	C22	C18	-115.56(19)
C21	Ti1	C22	C21	0.00(10)	C21	Ti1	C22	C23	121.3(2)
C22	Ti1	C21	C20	116.80(17)	C22	Ti1	C21	C22	0.00(11)
C22	Ti1	C21	C24	-121.2(2)	O2	Ti2	C45	C46	163.56(10)
O2	Ti2	C45	C49	-79.74(12)	O2	Ti2	C45	C54	40.5(2)
O2	Ti2	C46	C45	-23.7(2)	O2	Ti2	C46	C47	-138.81(11)
O2	Ti2	C46	C53	98.6(2)	O2	Ti2	C47	C46	88.5(2)
O2	Ti2	C47	C48	-27.5(3)	O2	Ti2	C47	C52	-150.62(15)
O2	Ti2	C48	C47	166.02(8)	O2	Ti2	C48	C49	50.62(15)
O2	Ti2	C48	C51	-72.1(2)	O2	Ti2	C49	C45	106.68(11)
O2	Ti2	C49	C48	-138.17(11)	O2	Ti2	C49	C50	-14.03(17)
C43	Ti2	C45	C46	-66.5(2)	C43	Ti2	C45	C49	50.3(2)
C43	Ti2	C45	C54	170.49(18)	C43	Ti2	C46	C45	138.47(13)
C43	Ti2	C46	C47	23.34(19)	C43	Ti2	C46	C53	-99.2(2)
C43	Ti2	C47	C46	-160.02(15)	C43	Ti2	C47	C48	84.02(13)
C43	Ti2	C47	C52	-39.1(2)	C43	Ti2	C48	C47	-94.08(13)
C43	Ti2	C48	C49	150.51(14)	C43	Ti2	C48	C51	27.8(2)
C43	Ti2	C49	C45	-148.00(12)	C43	Ti2	C49	C48	-32.84(16)
C43	Ti2	C49	C50	91.29(19)	C44	Ti2	C45	C46	53.64(13)
C44	Ti2	C45	C49	170.34(12)	C44	Ti2	C45	C54	-69.4(2)
C44	Ti2	C46	C45	-127.93(14)	C44	Ti2	C46	C47	116.94(14)
C44	Ti2	C46	C53	-5.6(2)	C44	Ti2	C47	C46	-63.38(14)
C44	Ti2	C47	C48	-179.34(12)	C44	Ti2	C47	C52	57.5(2)
C44	Ti2	C48	C47	0.89(19)	C44	Ti2	C48	C49	-114.52(15)
C44	Ti2	C48	C51	122.8(2)	C44	Ti2	C49	C45	-13.8(2)

Table S13-8. Torsion angles (°) (continued)

atom1	atom2	atom3	atom4	angle	atom1	atom2	atom3	atom4	angle
C44	Ti2	C49	C48	101.33(15)	C44	Ti2	C49	C50	-134.53(17)
C45	Ti2	C46	C45	0.00(12)	C45	Ti2	C46	C47	-115.1(2)
C45	Ti2	C46	C53	122.3(3)	C46	Ti2	C45	C46	0.00(14)
C46	Ti2	C45	C49	116.7(2)	C46	Ti2	C45	C54	-123.1(3)
C45	Ti2	C47	C46	37.51(12)	C45	Ti2	C47	C48	-78.45(14)
C45	Ti2	C47	C52	158.4(3)	C47	Ti2	C45	C46	-37.58(11)
C47	Ti2	C45	C49	79.12(14)	C47	Ti2	C45	C54	-160.6(3)
C45	Ti2	C48	C47	78.24(14)	C45	Ti2	C48	C49	-37.17(12)
C45	Ti2	C48	C51	-159.9(3)	C48	Ti2	C45	C46	-78.78(14)
C48	Ti2	C45	C49	37.92(12)	C48	Ti2	C45	C54	158.2(3)
C45	Ti2	C49	C45	0.00(13)	C45	Ti2	C49	C48	115.2(2)
C45	Ti2	C49	C50	-120.7(3)	C49	Ti2	C45	C46	-116.7(2)
C49	Ti2	C45	C49	0.00(12)	C49	Ti2	C45	C54	120.2(3)
C46	Ti2	C47	C46	0.00(14)	C46	Ti2	C47	C48	-116.0(2)
C46	Ti2	C47	C52	120.9(3)	C47	Ti2	C46	C45	115.1(2)
C47	Ti2	C46	C47	0.00(14)	C47	Ti2	C46	C53	-122.6(3)
C46	Ti2	C48	C47	37.13(11)	C46	Ti2	C48	C49	-78.27(14)
C46	Ti2	C48	C51	159.0(2)	C48	Ti2	C46	C45	78.05(14)
C48	Ti2	C46	C47	-37.08(12)	C48	Ti2	C46	C53	-159.6(3)
C46	Ti2	C49	C45	-36.80(11)	C46	Ti2	C49	C48	78.36(14)
C46	Ti2	C49	C50	-157.5(2)	C49	Ti2	C46	C45	36.50(11)
C49	Ti2	C46	C47	-78.63(14)	C49	Ti2	C46	C53	158.8(3)
C47	Ti2	C48	C47	0.00(12)	C47	Ti2	C48	C49	-115.4(2)
C47	Ti2	C48	C51	121.9(3)	C48	Ti2	C47	C46	116.0(2)
C48	Ti2	C47	C48	0.00(12)	C48	Ti2	C47	C52	-123.2(3)
C47	Ti2	C49	C45	-77.92(14)	C47	Ti2	C49	C48	37.24(11)
C47	Ti2	C49	C50	161.4(2)	C49	Ti2	C47	C46	78.29(14)
C49	Ti2	C47	C48	-37.67(11)	C49	Ti2	C47	C52	-160.8(2)
C48	Ti2	C49	C45	-115.2(2)	C48	Ti2	C49	C48	-0.00(13)
C48	Ti2	C49	C50	124.1(3)	C49	Ti2	C48	C47	115.4(2)
C49	Ti2	C48	C49	-0.00(13)	C49	Ti2	C48	C51	-122.7(3)
O3	Ti3	C72	C73	-94.16(11)	O3	Ti3	C72	C76	149.24(11)
O3	Ti3	C72	C78	26.0(2)	O3	Ti3	C73	C72	93.33(11)
O3	Ti3	C73	C74	-151.52(11)	O3	Ti3	C73	C81	-27.8(2)
O3	Ti3	C74	C73	38.18(17)	O3	Ti3	C74	C75	154.69(10)
O3	Ti3	C74	C80	-82.7(2)	O3	Ti3	C75	C74	-58.5(3)
O3	Ti3	C75	C76	57.3(3)	O3	Ti3	C75	C79	179.90(16)

Table S13-8. Torsion angles (°) (continued)

atom1	atom2	atom3	atom4	angle	atom1	atom2	atom3	atom4	angle
O3	Ti3	C76	C72	-40.89(18)	O3	Ti3	C76	C75	-155.43(9)
O3	Ti3	C76	C77	82.0(2)	C70	Ti3	C72	C73	30.0(2)
C70	Ti3	C72	C76	-86.6(2)	C70	Ti3	C72	C78	150.18(19)
C70	Ti3	C73	C72	-159.93(12)	C70	Ti3	C73	C74	-44.79(15)
C70	Ti3	C73	C81	78.9(2)	C70	Ti3	C74	C73	137.43(14)
C70	Ti3	C74	C75	-106.05(14)	C70	Ti3	C74	C80	16.60(19)
C70	Ti3	C75	C74	72.60(14)	C70	Ti3	C75	C76	-171.59(14)
C70	Ti3	C75	C79	-49.0(2)	C70	Ti3	C76	C72	125.10(15)
C70	Ti3	C76	C75	10.55(19)	C70	Ti3	C76	C77	-112.0(2)
C71	Ti3	C72	C73	156.64(11)	C71	Ti3	C72	C76	40.04(15)
C71	Ti3	C72	C78	-83.2(2)	C71	Ti3	C73	C72	-36.3(2)
C71	Ti3	C73	C74	78.8(2)	C71	Ti3	C73	C81	-157.45(18)
C71	Ti3	C74	C73	-131.38(13)	C71	Ti3	C74	C75	-14.86(19)
C71	Ti3	C74	C80	107.8(2)	C71	Ti3	C75	C74	167.91(14)
C71	Ti3	C75	C76	-76.27(13)	C71	Ti3	C75	C79	46.4(2)
C71	Ti3	C76	C72	-142.91(14)	C71	Ti3	C76	C75	102.54(12)
C71	Ti3	C76	C77	-20.05(19)	C72	Ti3	C73	C72	-0.00(11)
C72	Ti3	C73	C74	115.1(2)	C72	Ti3	C73	C81	-121.1(3)
C73	Ti3	C72	C73	-0.00(12)	C73	Ti3	C72	C76	-116.6(2)
C73	Ti3	C72	C78	120.2(3)	C72	Ti3	C74	C73	-37.61(11)
C72	Ti3	C74	C75	78.90(14)	C72	Ti3	C74	C80	-158.4(2)
C74	Ti3	C72	C73	37.49(10)	C74	Ti3	C72	C76	-79.11(13)
C74	Ti3	C72	C78	157.7(3)	C72	Ti3	C75	C74	-78.05(14)
C72	Ti3	C75	C76	37.77(11)	C72	Ti3	C75	C79	160.4(2)
C75	Ti3	C72	C73	78.43(13)	C75	Ti3	C72	C76	-38.17(11)
C75	Ti3	C72	C78	-161.4(3)	C72	Ti3	C76	C72	0.00(13)
C72	Ti3	C76	C75	-114.5(2)	C72	Ti3	C76	C77	122.9(3)
C76	Ti3	C72	C73	116.6(2)	C76	Ti3	C72	C76	0.00(13)
C76	Ti3	C72	C78	-123.2(3)	C73	Ti3	C74	C73	0.00(13)
C73	Ti3	C74	C75	116.5(2)	C73	Ti3	C74	C80	-120.8(3)
C74	Ti3	C73	C72	-115.1(2)	C74	Ti3	C73	C74	0.00(12)
C74	Ti3	C73	C81	123.7(3)	C73	Ti3	C75	C74	-36.86(12)
C73	Ti3	C75	C76	78.96(13)	C73	Ti3	C75	C79	-158.4(2)
C75	Ti3	C73	C72	-78.45(13)	C75	Ti3	C73	C74	36.69(11)
C75	Ti3	C73	C81	160.4(3)	C73	Ti3	C76	C72	36.77(11)
C73	Ti3	C76	C75	-77.78(13)	C73	Ti3	C76	C77	159.6(2)
C76	Ti3	C73	C72	-36.84(11)	C76	Ti3	C73	C74	78.30(13)

Table S13-8. Torsion angles (°) (continued)

atom1	atom2	atom3	atom4	angle	atom1	atom2	atom3	atom4	angle
C76	Ti3	C73	C81	-158.0(3)	C74	Ti3	C75	C74	0.00(12)
C74	Ti3	C75	C76	115.8(2)	C74	Ti3	C75	C79	-121.5(3)
C75	Ti3	C74	C73	-116.5(2)	C75	Ti3	C74	C75	0.00(13)
C75	Ti3	C74	C80	122.7(3)	C74	Ti3	C76	C72	77.69(13)
C74	Ti3	C76	C75	-36.86(10)	C74	Ti3	C76	C77	-159.4(2)
C76	Ti3	C74	C73	-78.90(13)	C76	Ti3	C74	C75	37.62(11)
C76	Ti3	C74	C80	160.3(2)	C75	Ti3	C76	C72	114.5(2)
C75	Ti3	C76	C75	-0.00(12)	C75	Ti3	C76	C77	-122.6(3)
C76	Ti3	C75	C74	-115.8(2)	C76	Ti3	C75	C76	-0.00(11)
C76	Ti3	C75	C79	122.6(3)	C1	N1	C28	C29	-155.87(17)
C28	N1	C1	C2	75.2(2)	C1	N1	C55	C56	75.7(2)
C55	N1	C1	C2	-160.66(15)	C28	N1	C55	C56	-160.19(16)
C55	N1	C28	C29	79.5(2)	N1	C1	C2	C3	15.9(3)
N1	C1	C2	C7	-163.74(16)	C1	C2	C3	C4	-178.84(17)
C1	C2	C7	O1	0.8(3)	C1	C2	C7	C6	179.10(17)
C3	C2	C7	O1	-178.83(17)	C3	C2	C7	C6	-0.6(3)
C7	C2	C3	C4	0.8(3)	C2	C3	C4	C5	-0.6(3)
C2	C3	C4	C12	178.90(17)	C3	C4	C5	C6	0.2(3)
C3	C4	C12	C13	-63.4(2)	C3	C4	C12	C14	55.6(2)
C3	C4	C12	C15	175.53(17)	C5	C4	C12	C13	116.1(2)
C5	C4	C12	C14	-124.9(2)	C5	C4	C12	C15	-5.0(3)
C12	C4	C5	C6	-179.31(17)	C4	C5	C6	C7	0.0(3)
C4	C5	C6	C8	177.96(17)	C5	C6	C7	O1	178.32(17)
C5	C6	C7	C2	0.1(3)	C5	C6	C8	C9	-112.9(2)
C5	C6	C8	C10	124.9(2)	C5	C6	C8	C11	6.3(3)
C7	C6	C8	C9	64.9(3)	C7	C6	C8	C10	-57.3(2)
C7	C6	C8	C11	-175.86(17)	C8	C6	C7	O1	0.4(3)
C8	C6	C7	C2	-177.75(17)	Ti1	C18	C19	Ti1	0.000(10)
Ti1	C18	C19	C20	64.81(14)	Ti1	C18	C19	C26	-120.3(2)
Ti1	C18	C22	Ti1	-0.000(10)	Ti1	C18	C22	C21	-65.94(14)
Ti1	C18	C22	C23	117.7(2)	C19	C18	C22	Ti1	65.65(17)
C19	C18	C22	C21	-0.3(3)	C19	C18	C22	C23	-176.6(2)
C22	C18	C19	Ti1	-65.25(17)	C22	C18	C19	C20	-0.4(3)
C22	C18	C19	C26	174.5(2)	C27	C18	C19	Ti1	115.9(3)
C27	C18	C19	C20	-179.3(2)	C27	C18	C19	C26	-4.4(4)
C27	C18	C22	Ti1	-115.4(3)	C27	C18	C22	C21	178.6(2)
C27	C18	C22	C23	2.3(4)	Ti1	C19	C20	Ti1	-0.0

Table S13-8. Torsion angles (°) (continued)

atom1	atom2	atom3	atom4	angle	atom1	atom2	atom3	atom4	angle
Ti1	C19	C20	C21	64.88(14)	Ti1	C19	C20	C25	-120.9(2)
C18	C19	C20	Ti1	-63.88(18)	C18	C19	C20	C21	1.0(3)
C18	C19	C20	C25	175.3(2)	C26	C19	C20	Ti1	121.0(3)
C26	C19	C20	C21	-174.2(2)	C26	C19	C20	C25	0.1(4)
Ti1	C20	C21	Ti1	-0.0	Ti1	C20	C21	C22	62.93(14)
Ti1	C20	C21	C24	-122.3(2)	C19	C20	C21	Ti1	-64.12(17)
C19	C20	C21	C22	-1.2(3)	C19	C20	C21	C24	173.6(2)
C25	C20	C21	Ti1	121.7(3)	C25	C20	C21	C22	-175.4(2)
C25	C20	C21	C24	-0.6(4)	Ti1	C21	C22	Ti1	-0.000(10)
Ti1	C21	C22	C18	64.76(14)	Ti1	C21	C22	C23	-118.8(2)
C20	C21	C22	Ti1	-63.84(17)	C20	C21	C22	C18	0.9(3)
C20	C21	C22	C23	177.4(2)	C24	C21	C22	Ti1	121.4(3)
C24	C21	C22	C18	-173.8(2)	C24	C21	C22	C23	2.6(4)
N1	C28	C29	C30	10.2(3)	N1	C28	C29	C34	-168.58(18)
C28	C29	C30	C31	-177.11(19)	C28	C29	C34	O2	-5.0(3)
C28	C29	C34	C33	172.86(19)	C30	C29	C34	O2	176.3(2)
C30	C29	C34	C33	-5.9(3)	C34	C29	C30	C31	1.6(3)
C29	C30	C31	C32	2.1(4)	C29	C30	C31	C39	-180.0(2)
C30	C31	C32	C33	-1.6(4)	C30	C31	C39	C40	4.0(3)
C30	C31	C39	C41	-114.9(2)	C30	C31	C39	C42	125.1(2)
C32	C31	C39	C40	-178.1(2)	C32	C31	C39	C41	63.0(3)
C32	C31	C39	C42	-57.0(3)	C39	C31	C32	C33	-179.6(2)
C31	C32	C33	C34	-2.5(4)	C31	C32	C33	C35	174.8(2)
C32	C33	C34	O2	-176.1(2)	C32	C33	C34	C29	6.2(3)
C32	C33	C35	C36	-121.2(2)	C32	C33	C35	C37	-2.7(3)
C32	C33	C35	C38	117.6(2)	C34	C33	C35	C36	55.9(3)
C34	C33	C35	C37	174.4(2)	C34	C33	C35	C38	-65.3(3)
C35	C33	C34	O2	6.7(4)	C35	C33	C34	C29	-171.0(2)
Ti2	C45	C46	Ti2	0.000(10)	Ti2	C45	C46	C47	64.41(19)
Ti2	C45	C46	C53	-123.2(3)	Ti2	C45	C49	Ti2	0.0
Ti2	C45	C49	C48	-65.42(17)	Ti2	C45	C49	C50	118.5(3)
C46	C45	C49	Ti2	65.4(2)	C46	C45	C49	C48	-0.0(3)
C46	C45	C49	C50	-176.1(3)	C49	C45	C46	Ti2	-64.2(2)
C49	C45	C46	C47	0.2(3)	C49	C45	C46	C53	172.7(3)
C54	C45	C46	Ti2	123.7(3)	C54	C45	C46	C47	-171.9(3)
C54	C45	C46	C53	0.5(5)	C54	C45	C49	Ti2	-122.4(3)
C54	C45	C49	C48	172.2(3)	C54	C45	C49	C50	-3.8(5)

Table S13-8. Torsion angles (°) (continued)

atom1	atom2	atom3	atom4	angle	atom1	atom2	atom3	atom4	angle
Ti2	C46	C47	Ti2	0.000(10)	Ti2	C46	C47	C48	63.61(19)
Ti2	C46	C47	C52	-119.8(3)	C45	C46	C47	Ti2	-64.0(2)
C45	C46	C47	C48	-0.3(4)	C45	C46	C47	C52	176.3(3)
C53	C46	C47	Ti2	123.6(4)	C53	C46	C47	C48	-172.8(3)
C53	C46	C47	C52	3.8(6)	Ti2	C47	C48	Ti2	0.0
Ti2	C47	C48	C49	65.10(18)	Ti2	C47	C48	C51	-119.7(3)
C46	C47	C48	Ti2	-64.8(2)	C46	C47	C48	C49	0.3(3)
C46	C47	C48	C51	175.5(3)	C52	C47	C48	Ti2	118.7(4)
C52	C47	C48	C49	-176.2(3)	C52	C47	C48	C51	-1.0(5)
Ti2	C48	C49	Ti2	-0.0	Ti2	C48	C49	C45	66.09(17)
Ti2	C48	C49	C50	-118.0(3)	C47	C48	C49	Ti2	-66.3(2)
C47	C48	C49	C45	-0.2(3)	C47	C48	C49	C50	175.7(3)
C51	C48	C49	Ti2	118.6(3)	C51	C48	C49	C45	-175.3(3)
C51	C48	C49	C50	0.6(5)	N1	C55	C56	C57	13.3(3)
N1	C55	C56	C61	-164.35(17)	C55	C56	C57	C58	-176.43(18)
C55	C56	C61	O3	-6.2(3)	C55	C56	C61	C60	171.79(18)
C57	C56	C61	O3	176.09(19)	C57	C56	C61	C60	-5.9(3)
C61	C56	C57	C58	1.2(3)	C56	C57	C58	C59	2.8(3)
C56	C57	C58	C66	-178.78(19)	C57	C58	C59	C60	-2.4(4)
C57	C58	C66	C67	118.8(2)	C57	C58	C66	C68	-122.4(2)
C57	C58	C66	C69	-1.7(4)	C59	C58	C66	C67	-62.9(3)
C59	C58	C66	C68	55.9(3)	C59	C58	C66	C69	176.6(2)
C66	C58	C59	C60	179.2(2)	C58	C59	C60	C61	-2.1(4)
C58	C59	C60	C62	173.9(2)	C59	C60	C61	O3	-175.9(2)
C59	C60	C61	C56	6.2(3)	C59	C60	C62	C63	-119.6(2)
C59	C60	C62	C64	-1.6(3)	C59	C60	C62	C65	119.0(2)
C61	C60	C62	C63	56.1(3)	C61	C60	C62	C64	174.2(2)
C61	C60	C62	C65	-65.3(3)	C62	C60	C61	O3	8.2(4)
C62	C60	C61	C56	-169.7(2)	Ti3	C72	C73	Ti3	0.0
Ti3	C72	C73	C74	-65.31(16)	Ti3	C72	C73	C81	119.6(2)
Ti3	C72	C76	Ti3	0.000(11)	Ti3	C72	C76	C75	65.31(15)
Ti3	C72	C76	C77	-119.2(2)	C73	C72	C76	Ti3	-65.0(2)
C73	C72	C76	C75	0.3(3)	C73	C72	C76	C77	175.8(2)
C76	C72	C73	Ti3	65.0(2)	C76	C72	C73	C74	-0.3(3)
C76	C72	C73	C81	-175.5(2)	C78	C72	C73	Ti3	-122.7(3)
C78	C72	C73	C74	172.0(2)	C78	C72	C73	C81	-3.2(4)
C78	C72	C76	Ti3	122.9(3)	C78	C72	C76	C75	-171.7(2)

Table S13-8. Torsion angles (°) (continued)

atom1	atom2	atom3	atom4	angle	atom1	atom2	atom3	atom4	angle
C78	C72	C76	C77	3.7(4)	Ti3	C73	C74	Ti3	0.000(10)
Ti3	C73	C74	C75	-64.56(16)	Ti3	C73	C74	C80	121.6(2)
C72	C73	C74	Ti3	64.78(19)	C72	C73	C74	C75	0.2(3)
C72	C73	C74	C80	-173.6(2)	C81	C73	C74	Ti3	-120.2(3)
C81	C73	C74	C75	175.2(3)	C81	C73	C74	C80	1.4(4)
Ti3	C74	C75	Ti3	-0.000(10)	Ti3	C74	C75	C76	-64.33(15)
Ti3	C74	C75	C79	116.5(2)	C73	C74	C75	Ti3	64.30(19)
C73	C74	C75	C76	-0.0(3)	C73	C74	C75	C79	-179.2(2)
C80	C74	C75	Ti3	-121.9(3)	C80	C74	C75	C76	173.7(2)
C80	C74	C75	C79	-5.4(4)	Ti3	C75	C76	Ti3	-0.000(10)
Ti3	C75	C76	C72	-64.92(15)	Ti3	C75	C76	C77	119.6(2)
C74	C75	C76	Ti3	64.75(19)	C74	C75	C76	C72	-0.2(3)
C74	C75	C76	C77	-175.7(2)	C79	C75	C76	Ti3	-116.1(3)
C79	C75	C76	C72	178.9(2)	C79	C75	C76	C77	3.4(4)

Table S13-9. Intramolecular contacts less than 3.60 Å

atom	atom	distance	atom	atom	distance
O1	C1	2.788(3)	O1	C8	2.959(3)
O1	C9	3.136(3)	O1	C10	3.014(3)
O1	C27	3.321(3)	O2	C28	2.769(3)
O2	C35	2.976(3)	O2	C36	3.032(3)
O2	C38	3.136(3)	O2	C50	3.454(4)
O3	C55	2.766(3)	O3	C62	2.964(3)
O3	C63	3.051(3)	O3	C65	3.105(3)
N1	C3	2.784(3)	N1	C30	2.792(3)
N1	C57	2.831(3)	C1	C26	3.478(4)
C1	C56	3.094(3)	C1	C57	3.250(3)
C2	C5	2.763(3)	C2	C28	3.058(3)
C3	C6	2.809(3)	C3	C13	3.066(4)
C3	C14	2.988(4)	C3	C28	3.208(3)
C3	C54	3.592(4)	C4	C7	2.816(3)
C5	C9	3.537(3)	C5	C11	2.845(3)
C5	C13	3.585(4)	C5	C15	2.906(4)
C7	C9	3.132(3)	C7	C10	3.089(3)
C10	C23	3.594(4)	C16	C25	3.179(4)
C17	C24	3.196(4)	C23	C24	3.153(4)
C23	C27	3.204(4)	C24	C25	3.176(4)
C25	C26	3.141(4)	C26	C27	3.242(4)
C26	C56	3.596(4)	C26	C61	3.579(4)
C29	C32	2.756(3)	C29	C55	3.109(3)
C30	C33	2.814(3)	C30	C40	2.867(4)
C30	C41	3.558(4)	C30	C55	3.239(3)
C31	C34	2.816(3)	C32	C36	3.593(4)
C32	C37	2.850(4)	C32	C41	3.099(4)
C32	C42	3.046(5)	C34	C36	3.046(3)
C34	C38	3.185(3)	C38	C50	3.521(4)
C43	C51	3.241(5)	C43	C52	3.480(5)
C44	C53	3.197(5)	C50	C51	3.237(4)
C50	C54	3.106(5)	C51	C52	3.189(6)
C52	C53	3.171(5)	C53	C54	3.197(5)
C56	C59	2.757(3)	C57	C60	2.815(4)
C57	C67	3.591(5)	C57	C69	2.886(4)
C58	C61	2.813(3)	C59	C63	3.590(4)
C59	C64	2.856(4)	C59	C67	3.079(5)

Table S13-9. Intramolecular contacts less than 3.60 Å (continued)

atom	atom	distance	atom	atom	distance
C59	C68	3.036(4)	C61	C63	3.065(4)
C61	C65	3.178(4)	C70	C80	3.171(5)
C71	C77	3.179(5)	C77	C78	3.216(5)
C77	C79	3.223(5)	C78	C81	3.125(6)
C79	C80	3.175(5)	C80	C81	3.182(5)

Table S13-10. Intramolecular contacts less than 3.60 Å involving hydrogens

atom	atom	distance	atom	atom	distance
Ti1	H1A	3.118	Ti1	H1B	3.517
Ti1	H9B	3.439	Ti1	H10C	3.032
Ti1	H23C	3.371	Ti1	H24C	3.492
Ti1	H25B	3.467	Ti1	H27B	3.318
Ti1	H26B	3.42(3)	Ti2	H28A	3.313
Ti2	H28B	3.379	Ti2	H36A	3.300
Ti2	H38A	3.129	Ti2	H50B	3.379
Ti2	H51B	3.392	Ti2	H52B	3.430
Ti2	H53C	3.533	Ti2	H54C	3.494
Ti3	H55A	3.215	Ti3	H55B	3.415
Ti3	H63A	3.310	Ti3	H65A	3.119
Ti3	H77C	3.422	Ti3	H78C	3.487
Ti3	H79B	3.357	Ti3	H80C	3.490
Ti3	H81B	3.420	O1	H1A	2.538
O1	H1B	2.935	O1	H9B	2.494
O1	H10B	3.464	O1	H10C	2.339
O1	H16B	3.288	O1	H16C	3.288
O1	H17B	3.238	O1	H17C	3.238
O1	H27A	3.550	O1	H27B	2.816
O1	H54A	3.594	O2	H28A	2.599
O2	H28B	2.814	O2	H36A	2.344
O2	H36B	3.509	O2	H38A	2.481
O2	H43B	3.194	O2	H43C	3.194
O2	H44B	3.309	O2	H44C	3.309
O2	H50B	2.914	O2	H54C	3.439
O3	H55A	2.545	O3	H55B	2.849
O3	H63A	2.375	O3	H63B	3.540
O3	H65A	2.443	O3	H70B	3.218
O3	H70C	3.218	O3	H71B	3.248
O3	H71C	3.248	O3	H78C	3.252
O3	H81B	3.185	O3	H26B	3.50(3)
N1	H3	2.413	N1	H30	2.418
N1	H57	2.478	C1	H3	2.657
C1	H16B	3.161	C1	H27B	3.044
C1	H28A	2.787	C1	H28B	2.445
C1	H55A	2.515	C1	H55B	3.246
C1	H57	2.901	C1	H26A	3.17(3)

Table S13-10. Intramolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
C1	H26B	3.09(3)	C2	H27B	2.991
C2	H28B	2.641	C2	H54A	3.187
C2	H54C	3.182	C2	H57	3.336
C3	H1A	3.225	C3	H1B	3.057
C3	H5	3.235	C3	H13A	2.743
C3	H13C	3.378	C3	H14A	2.658
C3	H14B	3.255	C3	H28B	2.784
C3	H30	3.471	C3	H54A	3.495
C3	H54C	2.939	C3	H57	3.183
C3	H69C	3.522	C4	H13A	2.665
C4	H13B	3.354	C4	H13C	2.713
C4	H14A	2.663	C4	H14B	2.700
C4	H14C	3.351	C4	H15A	2.733
C4	H15B	2.753	C4	H15C	3.386
C4	H54B	3.582	C4	H54C	3.229
C5	H3	3.241	C5	H9C	3.412
C5	H10B	3.582	C5	H11B	2.708
C5	H11C	2.785	C5	H13C	3.498
C5	H14B	3.588	C5	H15A	2.822
C5	H15B	2.799	C5	H54A	3.557
C5	H54B	3.561	C6	H9A	3.351
C6	H9B	2.685	C6	H9C	2.685
C6	H10A	3.362	C6	H10B	2.705
C6	H10C	2.705	C6	H11A	3.384
C6	H11B	2.743	C6	H11C	2.743
C6	H54A	3.282	C7	H1A	2.673
C7	H1B	2.870	C7	H3	3.268
C7	H5	3.257	C7	H9B	2.840
C7	H9C	3.396	C7	H10B	3.324
C7	H10C	2.797	C7	H27B	2.900
C7	H54A	3.071	C8	H5	2.680
C9	H10A	2.729	C9	H10B	3.386
C9	H10C	2.740	C9	H11A	2.665
C9	H11B	2.663	C9	H11C	3.342
C9	H17B	3.432	C9	H17C	3.429
C9	H54A	3.540	C10	H9A	2.725
C10	H9B	2.746	C10	H9C	3.385

Table S13-10. Intramolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
C10	H11A	2.635	C10	H11B	3.325
C10	H11C	2.644	C10	H17C	3.267
C10	H23A	3.186	C10	H23C	3.195
C11	H5	2.425	C11	H9A	2.650
C11	H9B	3.340	C11	H9C	2.681
C11	H10A	2.625	C11	H10B	2.657
C11	H10C	3.324	C12	H3	2.652
C12	H5	2.732	C13	H3	2.922
C13	H14A	2.695	C13	H14B	3.348
C13	H14C	2.671	C13	H15A	3.341
C13	H15B	2.673	C13	H15C	2.673
C13	H54C	3.308	C14	H3	2.778
C14	H13A	2.696	C14	H13B	2.667
C14	H13C	3.349	C14	H15A	2.676
C14	H15B	3.338	C14	H15C	2.653
C14	H40B	3.492	C14	H69A	3.237
C14	H69C	3.492	C15	H5	2.518
C15	H13A	3.340	C15	H13B	2.674
C15	H13C	2.674	C15	H14A	3.336
C15	H14B	2.667	C15	H14C	2.666
C16	H1A	2.870	C16	H17A	3.365
C16	H17B	3.121	C16	H25A	3.219
C16	H25B	2.800	C16	H44B	3.418
C16	H53C	3.505	C16	H26B	3.17(3)
C17	H9B	2.945	C17	H10C	3.152
C17	H16A	3.384	C17	H16C	3.101
C17	H23C	3.030	C17	H24A	3.228
C17	H24C	2.837	C18	H1B	3.384
C18	H10C	3.539	C18	H23A	2.693
C18	H23B	3.203	C18	H23C	3.244
C18	H26A	2.75(3)	C18	H26B	3.24(3)
C18	H26C	3.21(5)	C19	H1B	3.188
C19	H16A	3.395	C19	H16B	3.288
C19	H25A	2.669	C19	H25B	3.247
C19	H25C	3.178	C19	H27A	3.384
C19	H27B	2.881	C19	H27C	2.881
C20	H16A	2.749	C20	H16B	3.334

Table S13-10. Intramolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
C20	H17A	3.506	C20	H24A	3.366
C20	H24B	2.855	C20	H24C	2.854
C20	H26A	3.39(3)	C20	H26B	2.86(3)
C20	H26C	2.82(4)	C21	H16A	3.497
C21	H17A	2.759	C21	H17C	3.305
C21	H23A	3.365	C21	H23B	2.843
C21	H23C	2.843	C21	H25A	3.366
C21	H25B	2.859	C21	H25C	2.859
C22	H10C	3.241	C22	H17A	3.372
C22	H17C	3.217	C22	H24A	2.671
C22	H24B	3.181	C22	H24C	3.242
C22	H27A	2.673	C22	H27B	3.224
C22	H27C	3.211	C23	H10C	2.901
C23	H17C	3.172	C23	H24A	2.716
C23	H27A	2.772	C24	H17A	2.535
C24	H17C	3.427	C24	H23B	3.099
C24	H23C	3.128	C24	H25B	3.150
C24	H25C	3.143	C25	H16A	2.505
C25	H16B	3.432	C25	H24B	3.149
C25	H24C	3.142	C25	H26B	3.13(3)
C25	H26C	3.06(4)	C26	H1A	3.378
C26	H1B	2.708	C26	H16B	3.320
C26	H25A	2.700	C26	H27B	3.242
C26	H27C	3.196	C26	H55A	3.231
C26	H63A	3.498	C26	H63B	3.287
C27	H1B	3.133	C27	H10C	3.549
C27	H23A	2.779	C27	H68B	3.520
C27	H26A	2.87(3)	C28	H1A	2.509
C28	H1B	3.247	C28	H3	2.859
C28	H30	2.673	C28	H44B	3.041
C28	H54C	2.906	C28	H55A	2.745
C28	H55B	2.459	C29	H3	3.204
C29	H13A	3.488	C29	H54C	3.379
C29	H55B	2.714	C29	H78A	3.175
C30	H3	3.049	C30	H13A	3.324
C30	H28A	3.208	C30	H28B	3.101
C30	H32	3.231	C30	H40A	2.725

Table S13-10. Intramolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
C30	H40B	2.820	C30	H41A	3.446
C30	H42A	3.560	C30	H55B	2.796
C30	H57	3.562	C30	H78A	3.177
C30	H78C	3.412	C31	H40A	2.738
C31	H40B	2.764	C31	H40C	3.391
C31	H41A	2.691	C31	H41B	3.358
C31	H41C	2.696	C31	H42A	2.683
C31	H42B	2.685	C31	H42C	3.349
C31	H78A	3.395	C32	H30	3.239
C32	H36B	3.509	C32	H37A	2.750
C32	H37C	2.748	C32	H38C	3.536
C32	H41A	3.356	C32	H41C	2.813
C32	H42A	3.280	C32	H42B	2.751
C32	H78A	3.527	C33	H36A	2.659
C33	H36B	2.678	C33	H36C	3.344
C33	H37A	2.749	C33	H37B	3.385
C33	H37C	2.730	C33	H38A	2.705
C33	H38B	3.379	C33	H38C	2.747
C33	H50B	3.494	C33	H78A	3.548
C34	H28A	2.684	C34	H28B	2.824
C34	H30	3.270	C34	H32	3.256
C34	H36A	2.725	C34	H36B	3.282
C34	H38A	2.884	C34	H38C	3.489
C34	H50B	3.059	C34	H78A	3.415
C35	H32	2.693	C36	H37A	3.332
C36	H37B	2.654	C36	H37C	2.654
C36	H38A	2.735	C36	H38B	2.696
C36	H38C	3.370	C36	H43B	3.351
C36	H43C	3.249	C36	H77B	3.411
C37	H32	2.437	C37	H36A	3.330
C37	H36B	2.655	C37	H36C	2.655
C37	H38A	3.332	C37	H38B	2.658
C37	H38C	2.658	C38	H36A	2.735
C38	H36B	3.371	C38	H36C	2.695
C38	H37A	2.662	C38	H37B	2.649
C38	H37C	3.334	C38	H43C	3.290
C38	H50A	3.043	C38	H50B	3.195

Table S13-10. Intramolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
C38	H51B	3.221	C39	H30	2.705
C39	H32	2.675	C40	H30	2.471
C40	H41A	2.663	C40	H41B	2.621
C40	H41C	3.323	C40	H42A	2.682
C40	H42B	3.327	C40	H42C	2.627
C40	H69A	3.361	C41	H32	2.949
C41	H40A	2.659	C41	H40B	3.323
C41	H40C	2.625	C41	H42A	3.339
C41	H42B	2.670	C41	H42C	2.671
C41	H78B	3.495	C42	H32	2.853
C42	H40A	3.324	C42	H40B	2.658
C42	H40C	2.658	C42	H41A	3.335
C42	H41B	2.675	C42	H41C	2.675
C43	H36A	2.803	C43	H38A	3.260
C43	H44A	3.431	C43	H44C	3.134
C43	H51A	3.192	C43	H51B	2.948
C43	H52B	2.864	C44	H28A	2.897
C44	H28B	3.543	C44	H43A	3.394
C44	H43B	3.157	C44	H53A	3.338
C44	H53C	2.750	C45	H28B	3.255
C45	H44B	3.558	C45	H50A	3.346
C45	H50B	2.831	C45	H50C	2.831
C45	H53A	3.376	C45	H53B	2.871
C45	H53C	2.871	C46	H44A	2.833
C46	H44B	3.202	C46	H52A	2.654
C46	H52B	3.227	C46	H52C	3.186
C46	H54A	2.686	C46	H54B	3.173
C46	H54C	3.263	C47	H43A	2.883
C47	H43C	3.566	C47	H44A	3.191
C47	H51A	2.655	C47	H51B	3.227
C47	H51C	3.170	C47	H53A	2.688
C47	H53B	3.175	C47	H53C	3.264
C48	H38A	3.387	C48	H43A	3.052
C48	H43C	3.067	C48	H50A	2.715
C48	H50B	3.256	C48	H50C	3.211
C48	H52A	3.376	C48	H52B	2.880
C48	H52C	2.880	C49	H38A	3.190

Table S13-10. Intramolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
C49	H51A	3.375	C49	H51B	2.873
C49	H51C	2.873	C49	H54A	3.347
C49	H54B	2.834	C49	H54C	2.834
C50	H38A	2.853	C50	H38C	3.293
C50	H51B	3.207	C50	H51C	3.214
C50	H54B	3.087	C50	H54C	3.043
C51	H38A	3.327	C51	H43A	3.157
C51	H43C	2.863	C51	H50A	2.828
C51	H52B	3.169	C51	H52C	3.159
C52	H43A	2.786	C52	H44A	3.422
C52	H51A	2.753	C52	H53A	2.741
C53	H16C	3.536	C53	H44A	2.725
C53	H44B	3.161	C53	H52A	2.727
C53	H54A	2.775	C54	H13C	3.335
C54	H28B	2.681	C54	H50B	3.086
C54	H50C	3.042	C54	H53B	3.164
C54	H53C	3.169	C55	H1A	2.758
C55	H1B	2.485	C55	H28A	2.482
C55	H28B	3.232	C55	H30	2.856
C55	H57	2.683	C55	H71B	3.024
C55	H78A	3.401	C55	H78C	3.076
C55	H26A	3.42(3)	C55	H26B	3.24(3)
C56	H1B	2.693	C56	H30	3.278
C56	H78C	3.265	C56	H26A	2.93(3)
C56	H26B	3.41(3)	C57	H1B	2.777
C57	H3	3.560	C57	H30	3.165
C57	H40A	3.314	C57	H55A	3.223
C57	H55B	3.085	C57	H59	3.238
C57	H67C	3.511	C57	H68B	3.573
C57	H69A	2.762	C57	H69C	2.817
C57	H26A	3.28(3)	C58	H67A	2.657
C58	H67B	3.350	C58	H67C	2.704
C58	H68A	2.671	C58	H68B	2.723
C58	H68C	3.360	C58	H69A	2.731
C58	H69B	3.382	C58	H69C	2.750
C59	H57	3.245	C59	H63B	3.506
C59	H64B	2.768	C59	H64C	2.749

Table S13-10. Intramolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
C59	H65C	3.545	C59	H67A	2.754
C59	H67C	3.378	C59	H68A	2.708
C59	H68B	3.312	C60	H63A	2.676
C60	H63B	2.699	C60	H63C	3.356
C60	H64A	3.394	C60	H64B	2.751
C60	H64C	2.751	C60	H65A	2.699
C60	H65B	3.377	C60	H65C	2.745
C60	H26A	3.38(3)	C61	H55A	2.646
C61	H55B	2.840	C61	H57	3.265
C61	H59	3.249	C61	H63A	2.750
C61	H63B	3.308	C61	H65A	2.873
C61	H65C	3.485	C61	H78C	3.420
C61	H81B	3.548	C61	H26A	3.03(3)
C61	H26B	3.49(3)	C61	H26C	3.58(4)
C62	H59	2.684	C63	H64A	2.654
C63	H64B	2.642	C63	H64C	3.332
C63	H65A	2.749	C63	H65B	2.696
C63	H65C	3.378	C63	H70B	3.304
C63	H70C	3.343	C63	H26C	3.15(5)
C64	H59	2.438	C64	H63A	3.331
C64	H63B	2.649	C64	H63C	2.649
C64	H65A	3.347	C64	H65B	2.673
C64	H65C	2.673	C65	H63A	2.743
C65	H63B	3.379	C65	H63C	2.701
C65	H64A	2.656	C65	H64B	3.348
C65	H64C	2.687	C65	H70C	3.214
C65	H81A	3.459	C65	H81B	3.046
C66	H57	2.727	C66	H59	2.670
C67	H59	2.927	C67	H68A	2.701
C67	H68B	3.353	C67	H68C	2.670
C67	H69A	2.675	C67	H69B	2.646
C67	H69C	3.334	C68	H59	2.826
C68	H67A	2.703	C68	H67B	2.669
C68	H67C	3.353	C68	H69A	3.331
C68	H69B	2.655	C68	H69C	2.655
C69	H14A	3.163	C69	H14B	3.269
C69	H57	2.504	C69	H67A	3.330

Table S13-10. Intramolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
C69	H67B	2.666	C69	H67C	2.666
C69	H68A	3.327	C69	H68B	2.660
C69	H68C	2.660	C70	H63A	2.844
C70	H65A	3.176	C70	H71A	3.384
C70	H71C	3.084	C70	H79B	3.052
C70	H80A	3.527	C70	H80C	2.583
C71	H55A	2.819	C71	H70A	3.373
C71	H70B	3.093	C71	H77A	3.192
C71	H77C	2.818	C71	H79A	3.479
C71	H79B	3.444	C71	H26B	3.50(3)
C72	H55B	3.214	C72	H77A	3.377
C72	H77B	2.875	C72	H77C	2.876
C72	H81A	3.359	C72	H81B	2.845
C72	H81C	2.845	C73	H65A	3.333
C73	H78A	3.363	C73	H78B	2.840
C73	H78C	2.840	C73	H80A	2.662
C73	H80B	3.168	C73	H80C	3.241
C74	H70A	2.879	C74	H70C	3.111
C74	H79A	3.361	C74	H79B	2.849
C74	H79C	2.849	C74	H81A	2.687
C74	H81B	3.242	C74	H81C	3.185
C75	H70A	2.996	C75	H71A	2.972
C75	H77A	2.693	C75	H77B	3.204
C75	H77C	3.258	C75	H80A	3.374
C75	H80B	2.870	C75	H80C	2.870
C76	H71A	2.926	C76	H71B	3.141
C76	H78A	2.695	C76	H78B	3.177
C76	H78C	3.265	C76	H79A	2.696
C76	H79B	3.238	C76	H79C	3.228
C77	H71A	2.902	C77	H71B	2.959
C77	H78A	2.798	C77	H79A	2.796
C78	H41A	3.101	C78	H55B	2.659
C78	H77B	3.168	C78	H77C	3.208
C78	H81B	3.103	C78	H81C	3.067
C79	H70A	3.009	C79	H71A	2.950
C79	H77A	2.795	C79	H80B	3.176
C79	H80C	3.117	C80	H70A	2.852

Table S13-10. Intramolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
C80	H70C	2.972	C80	H79B	3.170
C80	H79C	3.112	C80	H81A	2.758
C81	H65A	2.947	C81	H65C	3.499
C81	H78B	3.102	C81	H78C	3.067
C81	H80A	2.749	H1A	H3	3.456
H1A	H16B	2.228	H1A	H16C	3.196
H1A	H27B	3.482	H1A	H28A	2.563
H1A	H28B	2.457	H1A	H44B	3.152
H1A	H55A	2.520	H1A	H55B	3.527
H1A	H26A	3.350	H1A	H26B	2.812
H1B	H3	3.181	H1B	H16B	3.346
H1B	H27B	2.349	H1B	H27C	3.439
H1B	H28A	3.555	H1B	H28B	3.410
H1B	H55A	2.522	H1B	H55B	3.445
H1B	H57	2.632	H1B	H26A	2.254
H1B	H26B	2.539	H1B	H26C	3.550
H3	H13A	2.360	H3	H13C	3.424
H3	H14A	2.181	H3	H14B	3.216
H3	H14C	3.588	H3	H28B	2.672
H3	H30	2.561	H3	H40B	3.541
H3	H54C	3.154	H3	H57	2.663
H3	H69A	3.448	H3	H69C	3.381
H5	H9C	3.505	H5	H11A	3.389
H5	H11B	2.133	H5	H11C	2.272
H5	H15A	2.331	H5	H15B	2.258
H5	H15C	3.486	H9A	H10A	2.545
H9A	H10C	3.013	H9A	H11A	2.454
H9A	H11B	2.918	H9A	H11C	3.553
H9A	H17B	3.511	H9A	H17C	3.341
H9B	H10A	3.029	H9B	H10C	2.580
H9B	H11A	3.555	H9B	H11B	3.568
H9B	H17B	2.559	H9B	H17C	2.789
H9B	H53B	3.460	H9B	H54A	3.315
H9C	H11A	2.967	H9C	H11B	2.485
H9C	H11C	3.576	H9C	H53B	3.375
H9C	H54A	2.998	H9C	H54B	3.423
H10A	H11A	2.416	H10A	H11B	3.528

Table S13-10. Intramolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
H10A	H11C	2.900	H10A	H17C	3.186
H10A	H23A	3.396	H10A	H23C	3.113
H10B	H11A	2.932	H10B	H11B	3.556
H10B	H11C	2.460	H10B	H23A	3.029
H10B	H23C	3.495	H10B	H27A	3.189
H10C	H11A	3.529	H10C	H11C	3.551
H10C	H17B	3.572	H10C	H17C	2.575
H10C	H23A	2.652	H10C	H23C	2.538
H10C	H27A	3.123	H10C	H27B	3.482
H13A	H14A	2.523	H13A	H14B	3.593
H13A	H14C	2.968	H13A	H15B	3.568
H13A	H15C	3.568	H13A	H28B	3.522
H13A	H30	3.375	H13A	H50B	3.377
H13A	H54C	2.957	H13B	H14A	2.959
H13B	H14B	3.559	H13B	H14C	2.466
H13B	H15A	3.570	H13B	H15B	2.956
H13B	H15C	2.485	H13C	H14A	3.594
H13C	H14C	3.562	H13C	H15A	3.570
H13C	H15B	2.485	H13C	H15C	2.956
H13C	H50B	3.276	H13C	H50C	3.150
H13C	H54B	2.893	H13C	H54C	2.871
H14A	H15A	3.570	H14A	H15C	3.552
H14A	H30	3.347	H14A	H40B	2.657
H14A	H57	3.379	H14A	H69A	2.562
H14A	H69B	3.420	H14A	H69C	3.049
H14B	H15A	2.486	H14B	H15B	3.569
H14B	H15C	2.929	H14B	H69A	3.083
H14B	H69B	3.142	H14B	H69C	3.029
H14C	H15A	2.963	H14C	H15B	3.558
H14C	H15C	2.461	H14C	H40B	3.501
H16A	H17A	3.308	H16A	H17B	3.447
H16A	H25A	2.622	H16A	H25B	1.945
H16A	H25C	3.417	H16A	H26B	3.336
H16B	H25A	3.190	H16B	H25B	3.239
H16B	H44B	2.887	H16B	H55A	3.373
H16B	H71B	3.327	H16B	H71C	3.527
H16B	H26B	2.574	H16C	H17A	3.396

Table S13-10. Intramolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
H16C	H17B	2.766	H16C	H25B	3.504
H16C	H44A	3.502	H16C	H44B	3.041
H16C	H53C	2.647	H17A	H23C	3.233
H17A	H24A	2.643	H17A	H24B	3.452
H17A	H24C	1.990	H17B	H24C	3.554
H17C	H23C	2.400	H17C	H24A	3.177
H17C	H24C	3.258	H23A	H27A	2.104
H23A	H27B	3.438	H23A	H27C	3.404
H23B	H24A	2.549	H23B	H24B	3.496
H23B	H27A	3.394	H23C	H24A	2.545
H23C	H27A	3.436	H24B	H25B	3.247
H24B	H25C	2.814	H24C	H25B	2.814
H24C	H25C	3.227	H25A	H71C	3.254
H25A	H26B	2.535	H25A	H26C	2.503
H25C	H26C	3.449	H27B	H68B	3.450
H27B	H69C	3.533	H27B	H26A	2.751
H27C	H68B	2.846	H27C	H26A	2.676
H28A	H30	3.437	H28A	H44B	2.309
H28A	H44C	3.032	H28A	H54C	3.449
H28A	H55A	2.492	H28A	H55B	2.449
H28A	H71B	3.086	H28A	H77C	3.005
H28B	H30	3.247	H28B	H44B	2.903
H28B	H54A	2.746	H28B	H54B	3.513
H28B	H54C	1.965	H28B	H55A	3.491
H28B	H55B	3.421	H30	H40A	2.171
H30	H40B	2.327	H30	H40C	3.436
H30	H41A	3.551	H30	H55B	2.622
H30	H57	2.649	H30	H78A	3.565
H30	H78C	3.390	H32	H37A	2.170
H32	H37B	3.403	H32	H37C	2.254
H32	H38C	3.583	H32	H41A	3.392
H32	H41C	2.410	H32	H42A	3.257
H32	H42B	2.289	H36A	H37B	3.552
H36A	H37C	3.552	H36A	H38A	2.580
H36A	H38B	3.000	H36A	H43B	2.489
H36A	H43C	2.600	H36A	H77B	3.145
H36B	H37A	3.554	H36B	H37B	2.934

Table S13-10. Intramolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
H36B	H37C	2.459	H36B	H38B	3.583
H36B	H77B	2.788	H36B	H78A	3.466
H36C	H37A	3.554	H36C	H37B	2.459
H36C	H37C	2.934	H36C	H38A	2.999
H36C	H38B	2.495	H36C	H38C	3.581
H36C	H43B	3.416	H36C	H43C	3.141
H37A	H38A	3.558	H37A	H38B	2.944
H37A	H38C	2.467	H37B	H38A	3.548
H37B	H38B	2.453	H37B	H38C	2.925
H37C	H38B	3.554	H37C	H38C	3.560
H38A	H43C	2.652	H38A	H50A	2.486
H38A	H50B	2.624	H38A	H51B	2.548
H38B	H43C	3.184	H38B	H50A	3.523
H38B	H51B	3.091	H38C	H50A	2.764
H38C	H50B	2.936	H40A	H41A	2.482
H40A	H41B	2.913	H40A	H41C	3.564
H40A	H42A	3.571	H40A	H42C	3.529
H40A	H57	3.111	H40A	H67C	3.396
H40A	H69A	3.186	H40A	H78C	3.399
H40B	H41A	3.566	H40B	H41B	3.518
H40B	H42A	2.495	H40B	H42B	3.568
H40B	H42C	2.897	H40B	H57	3.419
H40B	H69A	2.826	H40C	H41A	2.925
H40C	H41B	2.401	H40C	H41C	3.518
H40C	H42A	2.979	H40C	H42B	3.542
H40C	H42C	2.435	H40C	H67C	3.469
H40C	H69A	3.567	H41A	H42B	3.564
H41A	H42C	3.564	H41A	H78A	3.349
H41A	H78B	2.661	H41A	H78C	2.822
H41B	H42A	3.571	H41B	H42B	2.956
H41B	H42C	2.486	H41C	H42A	3.571
H41C	H42B	2.486	H41C	H42C	2.956
H41C	H78B	3.535	H43A	H44A	3.355
H43A	H44C	3.419	H43A	H51A	2.833
H43A	H51B	3.101	H43A	H52A	3.351
H43A	H52B	2.019	H43A	H52C	3.462
H43B	H44A	3.501	H43B	H44C	2.806

Table S13-10. Intramolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
H43B	H52B	3.539	H43C	H51A	2.906
H43C	H51B	2.322	H43C	H52B	3.364
H44A	H52A	3.091	H44A	H52B	3.417
H44A	H53A	2.614	H44A	H53C	2.403
H44B	H53A	3.493	H44B	H53C	2.466
H44B	H71B	3.499	H44C	H71B	3.446
H44C	H77A	3.587	H44C	H77C	3.076
H50A	H51B	2.641	H50A	H51C	2.699
H50B	H54B	3.211	H50B	H54C	2.715
H50C	H54B	2.715	H50C	H54C	3.090
H51A	H52B	2.581	H51A	H52C	2.616
H51C	H52C	3.550	H52A	H53A	2.055
H52A	H53B	3.320	H52A	H53C	3.417
H52B	H53A	3.422	H52C	H53A	3.339
H53B	H54A	2.653	H53B	H54B	3.509
H53C	H54A	2.576	H55A	H57	3.469
H55A	H71B	2.189	H55A	H71C	3.041
H55A	H77C	3.449	H55A	H26A	3.095
H55A	H26B	2.516	H55B	H57	3.223
H55B	H71B	3.034	H55B	H77C	3.140
H55B	H78A	2.413	H55B	H78B	3.560
H55B	H78C	2.229	H57	H69A	2.242
H57	H69B	3.471	H57	H69C	2.314
H59	H64A	3.404	H59	H64B	2.269
H59	H64C	2.165	H59	H65C	3.595
H59	H67A	2.363	H59	H67C	3.416
H59	H68A	2.237	H59	H68B	3.272
H63A	H64A	3.553	H63A	H64B	3.544
H63A	H65A	2.596	H63A	H65B	2.998
H63A	H70B	2.462	H63A	H70C	2.719
H63A	H26A	3.515	H63A	H26C	2.825
H63B	H64A	2.933	H63B	H64B	2.441
H63B	H64C	3.547	H63B	H65B	3.584
H63B	H26A	3.156	H63B	H26C	2.587
H63C	H64A	2.454	H63C	H64B	2.915
H63C	H64C	3.552	H63C	H65A	3.013
H63C	H65B	2.494	H63C	H65C	3.584

Table S13-10. Intramolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
H63C	H70B	3.337	H63C	H70C	3.232
H64A	H65A	3.557	H64A	H65B	2.462
H64A	H65C	2.928	H64B	H65B	3.563
H64B	H65C	3.578	H64B	H68A	3.561
H64C	H65A	3.581	H64C	H65B	2.973
H64C	H65C	2.495	H65A	H70C	2.566
H65A	H81A	2.829	H65A	H81B	2.430
H65B	H70C	3.090	H65C	H81A	3.323
H65C	H81B	2.798	H67A	H68A	2.533
H67A	H68C	2.969	H67A	H69A	3.566
H67A	H69B	3.545	H67B	H68A	2.964
H67B	H68B	3.561	H67B	H68C	2.463
H67B	H69A	2.966	H67B	H69B	2.457
H67B	H69C	3.557	H67C	H68C	3.561
H67C	H69A	2.488	H67C	H69B	2.924
H67C	H69C	3.570	H68A	H69B	3.550
H68A	H69C	3.550	H68B	H69A	3.559
H68B	H69B	2.939	H68B	H69C	2.464
H68C	H69A	3.559	H68C	H69B	2.464
H68C	H69C	2.938	H70A	H71A	3.325
H70A	H71C	3.398	H70A	H79B	2.275
H70A	H79C	3.573	H70A	H80A	3.420
H70A	H80B	3.535	H70A	H80C	2.115
H70B	H71A	3.424	H70B	H71C	2.729
H70B	H79B	3.589	H70B	H80C	3.489
H70C	H80A	3.069	H70C	H80C	2.408
H71A	H77A	2.631	H71A	H77C	2.754
H71A	H79A	2.662	H71A	H79B	2.809
H71B	H77A	3.117	H71B	H77C	2.325
H71B	H26B	3.299	H71C	H26B	2.942
H71C	H26C	3.589	H77A	H79A	2.127
H77A	H79B	3.457	H77A	H79C	3.419
H77B	H78A	2.644	H77B	H78B	3.541
H77B	H79A	3.413	H77C	H78A	2.636
H77C	H79A	3.464	H78B	H81B	3.220
H78B	H81C	2.737	H78C	H81B	2.738
H78C	H81C	3.121	H79B	H80B	3.315

Table S13-10. Intramolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
H79B	H80C	2.812	H79C	H80B	2.812
H79C	H80C	3.151	H80A	H81A	2.080
H80A	H81B	3.437	H80A	H81C	3.344
H80B	H81A	3.354	H80C	H81A	3.442

Table S13-11. Intermolecular contacts less than 3.60 Å involving hydrogens

atom	atom	distance	atom	atom	distance
C8	H14C[1]	3.480	C9	H14C[1]	3.271
C9	H52A[2]	3.302	C9	H52C[2]	3.405
C10	H13B[1]	3.432	C10	H14C[1]	3.285
C10	H15C[1]	3.346	C10	H36C[3]	3.346
C10	H38B[3]	3.304	C11	H14C[1]	3.279
C11	H42A[1]	3.414	C11	H64A[4]	3.210
C11	H65B[4]	3.520	C12	H10A[5]	3.569
C13	H10A[5]	3.389	C13	H37B[6]	3.335
C14	H9A[5]	3.208	C14	H10A[5]	3.312
C14	H11A[5]	3.287	C14	H52B[3]	3.188
C15	H10A[5]	3.390	C15	H17C[5]	3.449
C15	H51A[3]	3.331	C15	H63C[4]	3.236
C15	H64A[4]	3.465	C16	H81C[7]	3.394
C17	H52C[2]	3.137	C17	H79C[7]	3.366
C17	H80B[7]	2.945	C18	H24B[8]	3.244
C19	H23B[8]	3.367	C19	H24B[8]	3.536
C20	H23B[8]	3.467	C23	H25C[8]	3.363
C23	H36C[3]	3.126	C23	H37B[3]	3.476
C23	H63B[8]	3.314	C23	H26C[8]	3.29(5)
C24	H27C[8]	3.078	C24	H63B[8]	3.352
C24	H79A[7]	3.532	C24	H79C[7]	3.212
C25	H23B[8]	3.369	C25	H36B[7]	3.137
C25	H77B[7]	3.074	C26	H23B[8]	3.113
C26	H24B[8]	3.587	C27	H24B[8]	2.964
C27	H25C[8]	3.388	C27	H36C[3]	3.301
C36	H10B[9]	3.457	C36	H23A[9]	2.921
C36	H25C[10]	3.262	C36	H27A[9]	2.950
C37	H13B[6]	3.483	C37	H23A[9]	3.547
C37	H50C[6]	3.503	C37	H70B[10]	3.442
C38	H10B[9]	3.436	C40	H64C[11]	3.323
C40	H67A[11]	3.196	C41	H67A[11]	3.463
C41	H71A[10]	3.268	C41	H79A[10]	3.573
C41	H79B[10]	3.269	C42	H11C[5]	3.535
C42	H50A[6]	3.303	C42	H51B[6]	3.365
C42	H51C[6]	3.098	C43	H69C[9]	3.484
C44	H68C[9]	3.509	C45	H80C[4]	3.319
C46	H80A[4]	3.597	C46	H80C[4]	3.526

Table S13-11. Intermolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
C47	H80B[4]	3.268	C47	H80C[4]	3.344
C48	H80B[4]	3.428	C48	H80C[4]	3.021
C49	H80C[4]	3.009	C50	H37A[6]	3.089
C50	H42B[6]	3.344	C50	H70A[4]	3.256
C50	H80C[4]	3.550	C51	H11C[9]	3.445
C51	H15A[9]	3.327	C51	H42B[6]	3.337
C51	H42C[6]	3.341	C51	H80C[4]	3.555
C52	H9A[2]	3.099	C52	H14B[9]	3.191
C52	H15A[9]	3.458	C52	H17B[2]	3.435
C52	H80B[4]	3.492	C53	H53B[2]	3.569
C63	H15B[12]	3.230	C63	H23B[8]	3.373
C63	H24A[8]	3.372	C64	H11B[12]	3.121
C64	H15B[12]	3.527	C64	H40C[11]	3.369
C64	H42C[11]	3.348	C65	H11B[12]	3.176
C67	H67C[11]	3.475	C68	H44C[3]	3.490
C68	H77A[3]	2.917	C68	H79A[3]	3.476
C69	H43A[3]	3.597	C69	H43B[3]	3.578
C70	H50C[12]	2.935	C71	H41C[7]	3.399
C72	H16A[10]	3.413	C72	H25B[10]	3.115
C73	H16A[10]	3.296	C74	H17A[10]	3.525
C75	H17A[10]	3.389	C75	H24C[10]	3.087
C76	H24C[10]	3.426	C76	H25B[10]	3.044
C77	H24C[10]	3.562	C77	H25B[10]	3.269
C77	H25C[10]	3.526	C77	H68B[9]	3.494
C78	H25B[10]	3.350	C79	H17A[10]	3.272
C79	H24C[10]	2.855	C79	H41B[7]	3.234
C79	H51C[12]	3.431	C80	H17A[10]	3.496
C80	H17B[10]	3.248	C81	H16C[10]	3.535
H5	H51A[3]	3.376	H5	H64A[4]	2.929
H5	H65B[4]	3.422	H9A	C14[1]	3.208
H9A	C52[2]	3.099	H9A	H14B[1]	3.166
H9A	H14C[1]	2.419	H9A	H15C[1]	3.434
H9A	H52A[2]	2.795	H9A	H52B[2]	3.121
H9A	H52C[2]	2.864	H9B	H52A[2]	3.276
H9B	H52C[2]	3.097	H9C	H52A[2]	3.309
H9C	H65B[4]	3.185	H10A	C12[1]	3.569
H10A	C13[1]	3.389	H10A	C14[1]	3.312

Table S13-11. Intermolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
H10A	C15[1]	3.390	H10A	H13B[1]	2.540
H10A	H14C[1]	2.438	H10A	H15C[1]	2.542
H10A	H37B[3]	3.560	H10A	H38B[3]	3.179
H10B	C36[3]	3.457	H10B	C38[3]	3.436
H10B	H13B[1]	3.553	H10B	H36C[3]	2.596
H10B	H37B[3]	3.545	H10B	H38B[3]	2.569
H10B	H43C[3]	3.187	H10C	H15C[1]	3.321
H10C	H36C[3]	3.376	H11A	C14[1]	3.287
H11A	H14A[1]	3.355	H11A	H14C[1]	2.428
H11A	H40B[1]	3.317	H11A	H42A[1]	2.945
H11A	H42C[1]	3.434	H11B	C64[4]	3.121
H11B	C65[4]	3.176	H11B	H64A[4]	2.462
H11B	H64C[4]	3.017	H11B	H65B[4]	2.559
H11B	H65C[4]	3.043	H11C	C42[1]	3.535
H11C	C51[3]	3.445	H11C	H38B[3]	3.400
H11C	H42A[1]	3.005	H11C	H42C[1]	3.179
H11C	H43C[3]	3.581	H11C	H51A[3]	3.362
H11C	H51B[3]	2.816	H11C	H64A[4]	3.172
H13B	C10[5]	3.432	H13B	C37[6]	3.483
H13B	H10A[5]	2.540	H13B	H10B[5]	3.553
H13B	H37A[6]	3.429	H13B	H37B[6]	2.717
H13B	H38B[6]	3.065	H13C	H37A[6]	3.348
H13C	H37B[6]	3.077	H13C	H63C[4]	3.424
H14A	H11A[5]	3.355	H14B	C52[3]	3.191
H14B	H9A[5]	3.166	H14B	H43A[3]	2.758
H14B	H52A[3]	3.529	H14B	H52B[3]	2.320
H14B	H52C[3]	3.386	H14C	C8[5]	3.480
H14C	C9[5]	3.271	H14C	C10[5]	3.285
H14C	C11[5]	3.279	H14C	H9A[5]	2.419
H14C	H10A[5]	2.438	H14C	H11A[5]	2.428
H14C	H52B[3]	3.312	H15A	C51[3]	3.327
H15A	C52[3]	3.458	H15A	H17C[5]	3.436
H15A	H43A[3]	3.550	H15A	H51A[3]	2.363
H15A	H52B[3]	2.945	H15A	H52C[3]	3.089
H15A	H64A[4]	3.352	H15B	C63[4]	3.230
H15B	C64[4]	3.527	H15B	H63B[4]	3.468
H15B	H63C[4]	2.328	H15B	H64A[4]	2.728

Table S13-11. Intermolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
H15B	H65B^{4}	3.547	H15C	C10^{5}	3.346
H15C	H9A^{5}	3.434	H15C	H10A^{5}	2.542
H15C	H10C^{5}	3.321	H15C	H17C^{5}	2.673
H15C	H23C^{5}	2.899	H15C	H52C^{3}	3.517
H15C	H63C^{4}	3.394	H16A	C72^{7}	3.413
H16A	C73^{7}	3.296	H16A	H78B^{7}	3.196
H16A	H81C^{7}	3.048	H16C	C81^{7}	3.535
H16C	H80B^{7}	3.553	H16C	H81A^{7}	3.534
H16C	H81C^{7}	2.984	H17A	C74^{7}	3.525
H17A	C75^{7}	3.389	H17A	C79^{7}	3.272
H17A	C80^{7}	3.496	H17A	H52C^{2}	3.513
H17A	H79C^{7}	2.467	H17A	H80B^{7}	2.705
H17B	C52^{2}	3.435	H17B	C80^{7}	3.248
H17B	H52C^{2}	2.522	H17B	H79C^{7}	3.586
H17B	H80A^{7}	3.574	H17B	H80B^{7}	2.330
H17C	C15^{1}	3.449	H17C	H15A^{1}	3.436
H17C	H15C^{1}	2.673	H17C	H52C^{2}	2.963
H17C	H80B^{7}	3.558	H23A	C36^{3}	2.921
H23A	C37^{3}	3.547	H23A	H25C^{8}	3.015
H23A	H36B^{3}	2.885	H23A	H36C^{3}	2.156
H23A	H37B^{3}	2.944	H23A	H37C^{3}	3.513
H23B	C19^{8}	3.367	H23B	C20^{8}	3.467
H23B	C25^{8}	3.369	H23B	C26^{8}	3.113
H23B	C63^{8}	3.373	H23B	H25A^{8}	3.133
H23B	H25C^{8}	3.056	H23B	H36C^{3}	3.511
H23B	H37B^{3}	3.503	H23B	H63A^{8}	3.448
H23B	H63B^{8}	2.677	H23B	H63C^{8}	3.516
H23B	H26C^{8}	2.332	H23C	H15C^{1}	2.899
H23C	H36C^{3}	3.536	H23C	H37B^{3}	3.436
H23C	H63B^{8}	3.078	H23C	H63C^{8}	3.484
H24A	C63^{8}	3.372	H24A	H27C^{8}	3.526
H24A	H63B^{8}	2.425	H24A	H64B^{8}	3.003
H24A	H79C^{7}	3.261	H24A	H26A^{8}	3.558
H24A	H26C^{8}	3.264	H24B	C18^{8}	3.244
H24B	C19^{8}	3.536	H24B	C26^{8}	3.587
H24B	C27^{8}	2.964	H24B	H27A^{8}	3.425
H24B	H27C^{8}	2.116	H24B	H63B^{8}	3.553

Table S13-11. Intermolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
H24B	H68B[8]	3.531	H24B	H77A[7]	3.443
H24B	H77B[7]	3.417	H24B	H79A[7]	3.578
H24B	H26A[8]	3.244	H24B	H26C[8]	3.512
H24C	C75[7]	3.087	H24C	C76[7]	3.426
H24C	C77[7]	3.562	H24C	C79[7]	2.855
H24C	H77A[7]	3.290	H24C	H77B[7]	3.407
H24C	H79A[7]	2.801	H24C	H79C[7]	2.380
H25A	H23B[8]	3.133	H25A	H36B[7]	3.133
H25A	H37C[7]	3.570	H25A	H78B[7]	3.451
H25B	C72[7]	3.115	H25B	C76[7]	3.044
H25B	C77[7]	3.269	H25B	C78[7]	3.350
H25B	H36B[7]	3.444	H25B	H77B[7]	2.643
H25B	H78A[7]	3.397	H25B	H78B[7]	2.990
H25C	C23[8]	3.363	H25C	C27[8]	3.388
H25C	C36[7]	3.262	H25C	C77[7]	3.526
H25C	H23A[8]	3.015	H25C	H23B[8]	3.056
H25C	H27A[8]	3.033	H25C	H27C[8]	3.099
H25C	H36B[7]	2.420	H25C	H36C[7]	3.346
H25C	H77B[7]	2.627	H27A	C36[3]	2.950
H27A	H24B[8]	3.425	H27A	H25C[8]	3.033
H27A	H36A[3]	3.073	H27A	H36B[3]	3.012
H27A	H36C[3]	2.322	H27A	H43B[3]	3.502
H27C	C24[8]	3.078	H27C	H24A[8]	3.526
H27C	H24B[8]	2.116	H27C	H25C[8]	3.099
H32	H50A[6]	3.196	H32	H50C[6]	3.593
H36A	H27A[9]	3.073	H36B	C25[10]	3.137
H36B	H23A[9]	2.885	H36B	H25A[10]	3.133
H36B	H25B[10]	3.444	H36B	H25C[10]	2.420
H36B	H27A[9]	3.012	H36C	C10[9]	3.346
H36C	C23[9]	3.126	H36C	C27[9]	3.301
H36C	H10B[9]	2.596	H36C	H10C[9]	3.376
H36C	H23A[9]	2.156	H36C	H23B[9]	3.511
H36C	H23C[9]	3.536	H36C	H25C[10]	3.346
H36C	H27A[9]	2.322	H37A	C50[6]	3.089
H37A	H13B[6]	3.429	H37A	H13C[6]	3.348
H37A	H50A[6]	3.041	H37A	H50B[6]	3.042
H37A	H50C[6]	2.671	H37A	H70B[10]	3.338

Table S13-11. Intermolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
H37B	C13^{6}	3.335	H37B	C23^{9}	3.476
H37B	H10A^{9}	3.560	H37B	H10B^{9}	3.545
H37B	H13B^{6}	2.717	H37B	H13C^{6}	3.077
H37B	H23A^{9}	2.944	H37B	H23B^{9}	3.503
H37B	H23C^{9}	3.436	H37C	H23A^{9}	3.513
H37C	H25A^{10}	3.570	H37C	H70B^{10}	2.834
H38B	C10^{9}	3.304	H38B	H10A^{9}	3.179
H38B	H10B^{9}	2.569	H38B	H11C^{9}	3.400
H38B	H13B^{6}	3.065	H38B	H42A^{6}	3.217
H38C	H38C^{6}	3.539	H38C	H42A^{6}	3.399
H38C	H42B^{6}	3.556	H40A	H67A^{11}	2.821
H40B	H11A^{5}	3.317	H40B	H64C^{11}	3.572
H40C	C64^{11}	3.369	H40C	H59^{11}	2.939
H40C	H64C^{11}	2.414	H40C	H67A^{11}	2.720
H41A	H67A^{11}	3.131	H41A	H67B^{11}	3.416
H41A	H71A^{10}	3.391	H41B	C79^{10}	3.234
H41B	H59^{11}	3.314	H41B	H64C^{11}	3.515
H41B	H67A^{11}	3.014	H41B	H68A^{11}	2.874
H41B	H71A^{10}	3.106	H41B	H79A^{10}	2.793
H41B	H79B^{10}	2.800	H41C	C71^{10}	3.399
H41C	H70A^{10}	3.310	H41C	H70B^{10}	3.580
H41C	H71A^{10}	2.789	H41C	H71C^{10}	3.164
H41C	H79A^{10}	3.495	H41C	H79B^{10}	2.873
H42A	C11^{5}	3.414	H42A	H11A^{5}	2.945
H42A	H11C^{5}	3.005	H42A	H38B^{6}	3.217
H42A	H38C^{6}	3.399	H42A	H50A^{6}	3.461
H42A	H51B^{6}	3.266	H42A	H51C^{6}	3.465
H42B	C50^{6}	3.344	H42B	C51^{6}	3.337
H42B	H38C^{6}	3.556	H42B	H50A^{6}	2.425
H42B	H50C^{6}	3.535	H42B	H51B^{6}	3.091
H42B	H51C^{6}	2.719	H42B	H70A^{10}	3.563
H42B	H79B^{10}	3.287	H42C	C51^{6}	3.341
H42C	C64^{11}	3.348	H42C	H11A^{5}	3.434
H42C	H11C^{5}	3.179	H42C	H51B^{6}	3.174
H42C	H51C^{6}	2.683	H42C	H64A^{11}	3.313
H42C	H64B^{11}	3.408	H42C	H64C^{11}	2.800
H42C	H79B^{10}	3.223	H43A	C69^{9}	3.597

Table S13-11. Intermolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
H43A	H14B^{9}	2.758	H43A	H15A^{9}	3.550
H43A	H69B^{9}	3.191	H43A	H69C^{9}	3.091
H43B	C69^{9}	3.578	H43B	H27A^{9}	3.502
H43B	H68B^{9}	3.107	H43B	H68C^{9}	3.450
H43B	H69B^{9}	3.330	H43B	H69C^{9}	2.974
H43C	H10B^{9}	3.187	H43C	H11C^{9}	3.581
H44A	H69B^{9}	3.481	H44A	H81C^{7}	3.230
H44C	C68^{9}	3.490	H44C	H68B^{9}	3.557
H44C	H68C^{9}	2.622	H44C	H69B^{9}	3.469
H50A	C42^{6}	3.303	H50A	H32^{6}	3.196
H50A	H37A^{6}	3.041	H50A	H42A^{6}	3.461
H50A	H42B^{6}	2.425	H50A	H70A^{4}	3.268
H50B	H37A^{6}	3.042	H50C	C37^{6}	3.503
H50C	C70^{4}	2.935	H50C	H32^{6}	3.593
H50C	H37A^{6}	2.671	H50C	H42B^{6}	3.535
H50C	H70A^{4}	2.584	H50C	H70B^{4}	2.993
H50C	H70C^{4}	2.740	H50C	H80C^{4}	3.218
H51A	C15^{9}	3.331	H51A	H5^{9}	3.376
H51A	H11C^{9}	3.362	H51A	H15A^{9}	2.363
H51B	C42^{6}	3.365	H51B	H11C^{9}	2.816
H51B	H42A^{6}	3.266	H51B	H42B^{6}	3.091
H51B	H42C^{6}	3.174	H51C	C42^{6}	3.098
H51C	C79^{4}	3.431	H51C	H42A^{6}	3.465
H51C	H42B^{6}	2.719	H51C	H42C^{6}	2.683
H51C	H70A^{4}	3.529	H51C	H79B^{4}	2.890
H51C	H79C^{4}	3.066	H51C	H80B^{4}	3.459
H51C	H80C^{4}	3.098	H52A	C9^{2}	3.302
H52A	H9A^{2}	2.795	H52A	H9B^{2}	3.276
H52A	H9C^{2}	3.309	H52A	H14B^{9}	3.529
H52B	C14^{9}	3.188	H52B	H9A^{2}	3.121
H52B	H14B^{9}	2.320	H52B	H14C^{9}	3.312
H52B	H15A^{9}	2.945	H52C	C9^{2}	3.405
H52C	C17^{2}	3.137	H52C	H9A^{2}	2.864
H52C	H9B^{2}	3.097	H52C	H14B^{9}	3.386
H52C	H15A^{9}	3.089	H52C	H15C^{9}	3.517
H52C	H17A^{2}	3.513	H52C	H17B^{2}	2.522
H52C	H17C^{2}	2.963	H52C	H80B^{4}	2.881

Table S13-11. Intermolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
H53A	H53A^{2}	3.581	H53A	H53B^{2}	3.005
H53A	H81A^{7}	3.480	H53B	C53^{2}	3.569
H53B	H53A^{2}	3.005	H53B	H53B^{2}	3.218
H53B	H80A^{4}	3.414	H54B	H65B^{4}	3.413
H54B	H70C^{4}	3.160	H59	H40C^{11}	2.939
H59	H41B^{11}	3.314	H63A	H23B^{8}	3.448
H63B	C23^{8}	3.314	H63B	C24^{8}	3.352
H63B	H15B^{12}	3.468	H63B	H23B^{8}	2.677
H63B	H23C^{8}	3.078	H63B	H24A^{8}	2.425
H63B	H24B^{8}	3.553	H63C	C15^{12}	3.236
H63C	H13C^{12}	3.424	H63C	H15B^{12}	2.328
H63C	H15C^{12}	3.394	H63C	H23B^{8}	3.516
H63C	H23C^{8}	3.484	H64A	C11^{12}	3.210
H64A	C15^{12}	3.465	H64A	H5^{12}	2.929
H64A	H11B^{12}	2.462	H64A	H11C^{12}	3.172
H64A	H15A^{12}	3.352	H64A	H15B^{12}	2.728
H64A	H42C^{11}	3.313	H64B	H24A^{8}	3.003
H64B	H42C^{11}	3.408	H64B	H79A^{3}	3.371
H64B	H79C^{3}	3.177	H64C	C40^{11}	3.323
H64C	H11B^{12}	3.017	H64C	H40B^{11}	3.572
H64C	H40C^{11}	2.414	H64C	H41B^{11}	3.515
H64C	H42C^{11}	2.800	H65B	C11^{12}	3.520
H65B	H5^{12}	3.422	H65B	H9C^{12}	3.185
H65B	H11B^{12}	2.559	H65B	H15B^{12}	3.547
H65B	H54B^{12}	3.413	H65C	H11B^{12}	3.043
H67A	C40^{11}	3.196	H67A	C41^{11}	3.463
H67A	H40A^{11}	2.821	H67A	H40C^{11}	2.720
H67A	H41A^{11}	3.131	H67A	H41B^{11}	3.014
H67A	H67C^{11}	3.136	H67B	H41A^{11}	3.416
H67B	H81B^{11}	3.082	H67B	H81C^{11}	3.472
H67C	C67^{11}	3.475	H67C	H67A^{11}	3.136
H67C	H67C^{11}	2.907	H68A	H41B^{11}	2.874
H68A	H77A^{3}	2.710	H68A	H79A^{3}	2.679
H68B	C77^{3}	3.494	H68B	H24B^{8}	3.531
H68B	H43B^{3}	3.107	H68B	H44C^{3}	3.557
H68B	H77A^{3}	2.712	H68B	H77B^{3}	3.546
H68C	C44^{3}	3.509	H68C	H43B^{3}	3.450

Table S13-11. Intermolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
H68C	H44C[3]	2.622	H68C	H71A[3]	3.593
H68C	H77A[3]	2.831	H68C	H77C[3]	3.588
H69B	H43A[3]	3.191	H69B	H43B[3]	3.330
H69B	H44A[3]	3.481	H69B	H44C[3]	3.469
H69C	C43[3]	3.484	H69C	H43A[3]	3.091
H69C	H43B[3]	2.974	H70A	C50[12]	3.256
H70A	H41C[7]	3.310	H70A	H42B[7]	3.563
H70A	H50A[12]	3.268	H70A	H50C[12]	2.584
H70A	H51C[12]	3.529	H70B	C37[7]	3.442
H70B	H37A[7]	3.338	H70B	H37C[7]	2.834
H70B	H41C[7]	3.580	H70B	H50C[12]	2.993
H70C	H50C[12]	2.740	H70C	H54B[12]	3.160
H71A	C41[7]	3.268	H71A	H41A[7]	3.391
H71A	H41B[7]	3.106	H71A	H41C[7]	2.789
H71A	H68C[9]	3.593	H71C	H41C[7]	3.164
H77A	C68[9]	2.917	H77A	H24B[10]	3.443
H77A	H24C[10]	3.290	H77A	H68A[9]	2.710
H77A	H68B[9]	2.712	H77A	H68C[9]	2.831
H77B	C25[10]	3.074	H77B	H24B[10]	3.417
H77B	H24C[10]	3.407	H77B	H25B[10]	2.643
H77B	H25C[10]	2.627	H77B	H68B[9]	3.546
H77C	H68C[9]	3.588	H78A	H25B[10]	3.397
H78B	H16A[10]	3.196	H78B	H25A[10]	3.451
H78B	H25B[10]	2.990	H79A	C24[10]	3.532
H79A	C41[7]	3.573	H79A	C68[9]	3.476
H79A	H24B[10]	3.578	H79A	H24C[10]	2.801
H79A	H41B[7]	2.793	H79A	H41C[7]	3.495
H79A	H64B[9]	3.371	H79A	H68A[9]	2.679
H79B	C41[7]	3.269	H79B	H41B[7]	2.800
H79B	H41C[7]	2.873	H79B	H42B[7]	3.287
H79B	H42C[7]	3.223	H79B	H51C[12]	2.890
H79C	C17[10]	3.366	H79C	C24[10]	3.212
H79C	H17A[10]	2.467	H79C	H17B[10]	3.586
H79C	H24A[10]	3.261	H79C	H24C[10]	2.380
H79C	H51C[12]	3.066	H79C	H64B[9]	3.177
H80A	C46[12]	3.597	H80A	H17B[10]	3.574
H80A	H53B[12]	3.414	H80B	C17[10]	2.945

Table S13-11. Intermolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
H80B	C47[12]	3.268	H80B	C48[12]	3.428
H80B	C52[12]	3.492	H80B	H16C[10]	3.553
H80B	H17A[10]	2.705	H80B	H17B[10]	2.330
H80B	H17C[10]	3.558	H80B	H51C[12]	3.459
H80B	H52C[12]	2.881	H80C	C45[12]	3.319
H80C	C46[12]	3.526	H80C	C47[12]	3.344
H80C	C48[12]	3.021	H80C	C49[12]	3.009
H80C	C50[12]	3.550	H80C	C51[12]	3.555
H80C	H50C[12]	3.218	H80C	H51C[12]	3.098
H81A	H16C[10]	3.534	H81A	H53A[10]	3.480
H81B	H67B[11]	3.082	H81C	C16[10]	3.394
H81C	H16A[10]	3.048	H81C	H16C[10]	2.984
H81C	H44A[10]	3.230	H81C	H67B[11]	3.472
H26A	H24A[8]	3.558	H26A	H24B[8]	3.244
H26C	C23[8]	3.29(5)	H26C	H23B[8]	2.332
H26C	H24A[8]	3.264	H26C	H24B[8]	3.512

Symmetry Operators:

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