Ethylene/propylene copolymerization catalyzed by half-titanocenes containing monodentate anionic nitrogen ligands: effect of ligands on catalytic behaviour

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Electronic Supplementary Information (ESI)

Additional data for polymerization

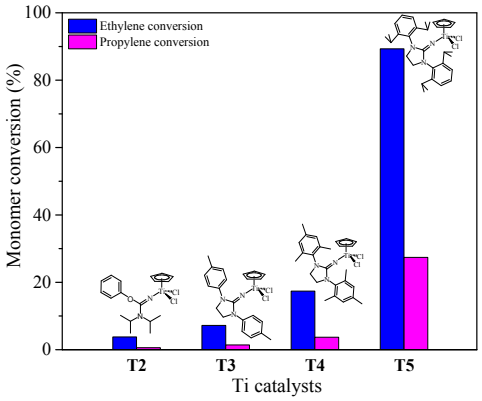

Fig. S1 The ethylene and propylene conversion in ethylene/propylene copolymerization using the **T2**-**T5**/MAO catalytic systems. ([M] = 140 g/L, P/E = 2 (molar ratio), [Ti]/[M] = 1.3 × 10^{-5}, Al/Ti = 1000 (molar ratio), T= 80 °C, t_p = 30 min.)

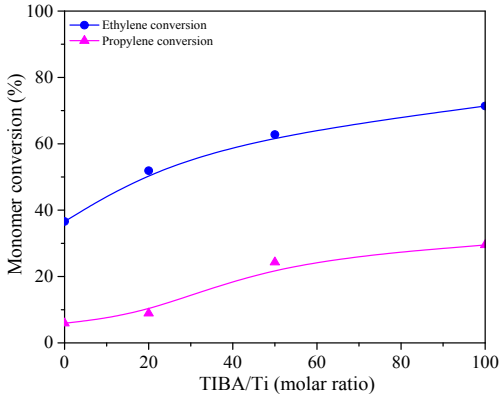

Fig. S2 Effect of TIBA/Ti molar ratio on ethylene and propylene conversion in ethylene/propylene copolymerization using the **T6**/TIBA/MMAO catalytic system. ([M] = 140 g/L, P/E = 2 (molar ratio), [Ti]/[M] = 1.3 × 10^{-5}, Al/Ti = 1000 (molar ratio), T = 50 °C, t_p = 30 min.)

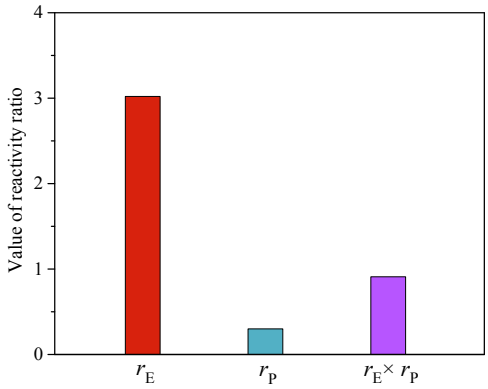

Fig. S3 The reactivity ratio of **T6**/TIBA/MMAO catalytic system. ([M] = 140 g/L, P/E = 2 (molar ratio), [Ti]/[M] = 1.3 × 10^{-6}, TIBA/Ti = 50, MMAO/Ti = 1000 (molar ratio), T = 50 °C, t_p = 30 min.)

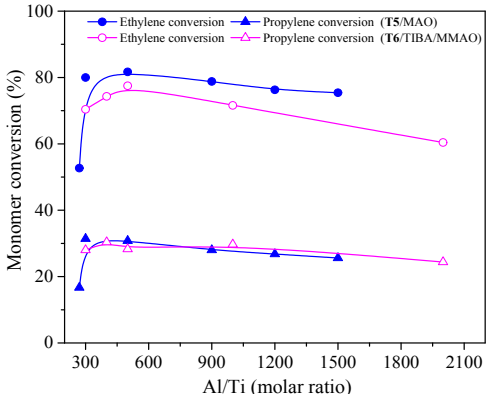

Fig. S4 Effect of Al/Ti molar ratio on ethylene and propylene conversion in ethylene/propylene copolymerization using the **T5**/MAO and **T6/**TIBA/MMAO catalytic systems**.** (**T5**/MAO: [M] = 140 g/L, P/E = 2 (molar ratio), [Ti]/[M] = 1.3 × 10^{-5}, T = 80 °C, t_p = 30 min; **T6**/TIBA/MMAO: [M] = 140 g/L, P/E = 2 (molar ratio), [Ti]/[M] = 1.3 × 10^{-5}, TIBA/Ti = 100, T = 50 °C, t_p =30 min.)

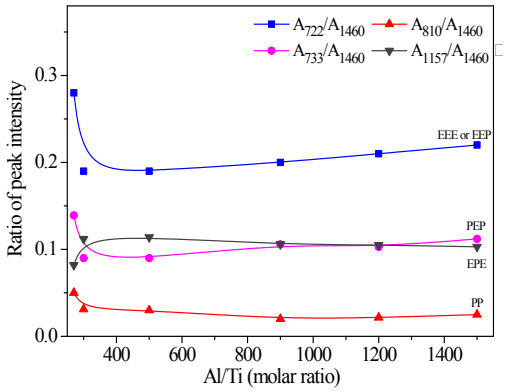

Fig. S5 Effect of Al/Ti molar ratio on the ratio of peak intensity of ethylene/propylene copolymers prepared by **T5**/MAO catalytic system. ([M] = 140 g/L, P/E = 2 (molar ratio), [Ti]/[M] = 1.3 × 10^{-5}, T = 80°C, t_p = 30 min.)

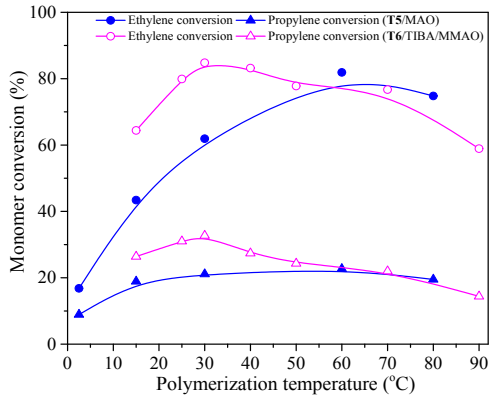

Fig. S6 Effect of polymerization temperature on ethylene and propylene conversion in ethylene/propylene copolymerization using the **T5**/MAO and **T6/**TIBA/MMAO catalytic systems**.** (**T5**/MAO: [M] = 80 g/L, P/E = 2 (molar ratio), [Ti]/[M] = 4.7 × 10^{-6}, Al/Ti = 2000 (molar ratio), t_p= 30 min; **T6**/TIBA/MMAO: [M] = 140 g/L, P/E = 2 (molar ratio), [Ti]/[M] = 5.3 × 10^{-6}, TIBA/Ti = 100, Al/Ti = 1000 (molar ratio), t_p = 30 min.)

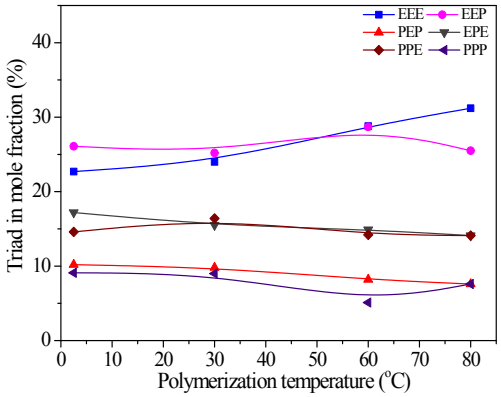

Fig. S7 Effect of polymerization temperature on triads fraction of ethylene-propylene copolymers prepared by **T5**/MAO catalytic system. ([M] = 80 g/L, P/E = 2 (molar ratio), [Ti]/[M] = 4.7 × 10^{-6}, Al/Ti = 2000 (molar ratio), t_p = 30 min.)

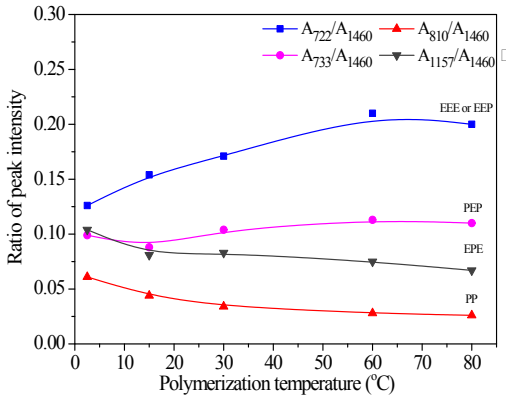

Fig. S8 Effect of polymerization temperature on the ratio of peak intensity of ethylene/propylene copolymers prepared by **T5/**MAO catalytic system. ([M] = 80 g/L, P/E = 2 (molar ratio), [Ti]/[M] = 4.7 × 10^{-6}, Al/Ti = 2000 (molar ratio), t_p = 30 min.)

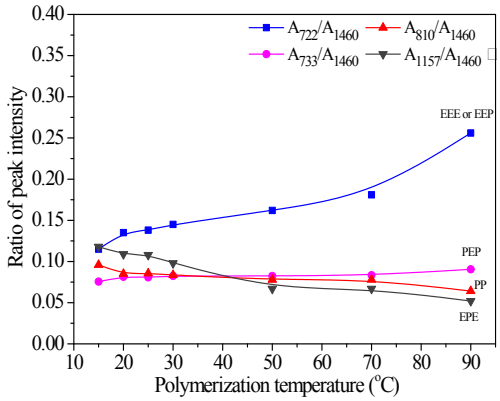

Fig. S9 Effect of polymerization temperature on the ratio of peak intensity of ethylene/propylene copolymers prepared by **T6/**TIBA**/**MMAO catalytic system. (M] = 140 g/L, P/E = 2 (molar ratio), [Ti]/[M] = 5.3 × 10^{-6}, TIBA/Ti = 100, Al/Ti = 1000 (molar ratio), t_p = 30 min.)

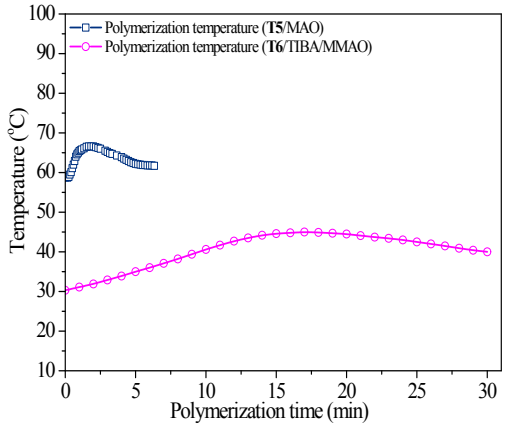

Fig. S10 The variation of polymerization temperature for ethylene/propylene copolymerization using **T5**/MAO and **T6/**TIBA/MMAO catalytic systems at various polymerization time. (**T5**/MAO: [M] = 80 g/L, P/E = 2 (molar ratio), [Ti]/[M] = 4.7 × 10^{-6}, Al/Ti = 2000 (molar ratio), T = 60 °C. **T6**/TIBA/MMAO: [M] = 140 g/L, P/E = 2 (molar ratio), [Ti]/[M] = 5.3 × 10^{-6}, TIBA/Ti = 100, Al/Ti = 1000 (molar ratio), T = 30 °C)

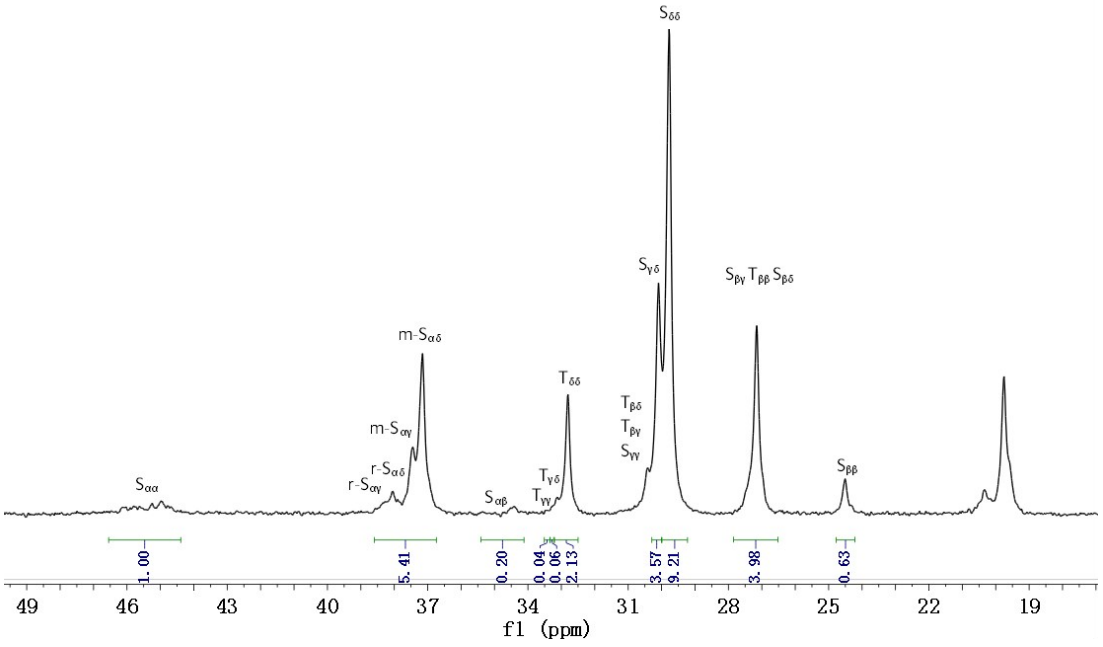

Fig. S11 Representative ^{13}C NMR spectrum of ethylene-propylene copolymer (In Figure 4 and Figure 5) prepared by the **T2**/MAO catalytic system

(In $CDCl_3$, 25 °C).

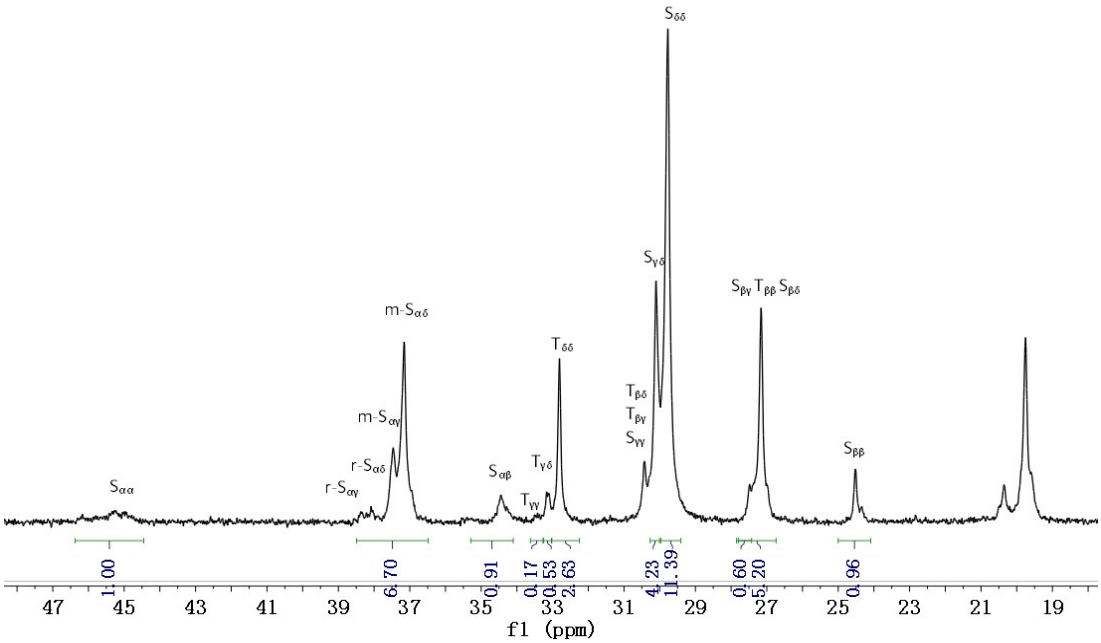

Fig. S12 Representative ^{13}C NMR spectrum of ethylene-propylene copolymer (In Figure 4 and Figure 5) prepared by the **T4**/MAO catalytic system (In $CDCl_3$, 25 °C).

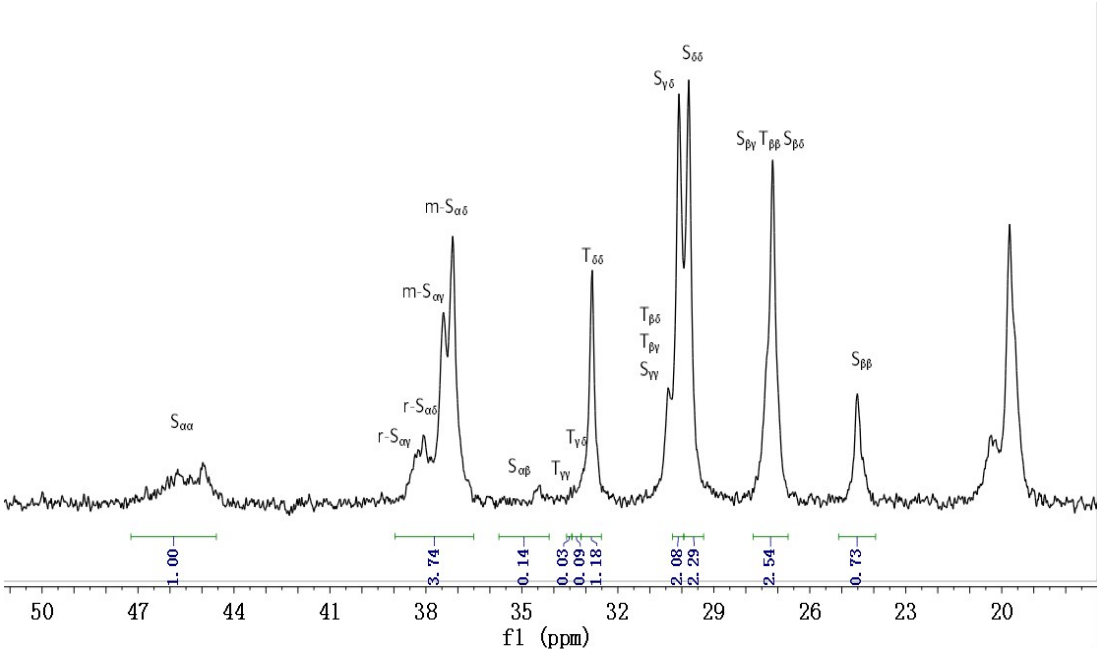

Fig. S13 Representative ^{13}C NMR spectrum of ethylene-propylene copolymer (In Figure 4 and Figure 5) prepared by the **T5**/MAO catalytic system (In $CDCl_3$, 25 °C).

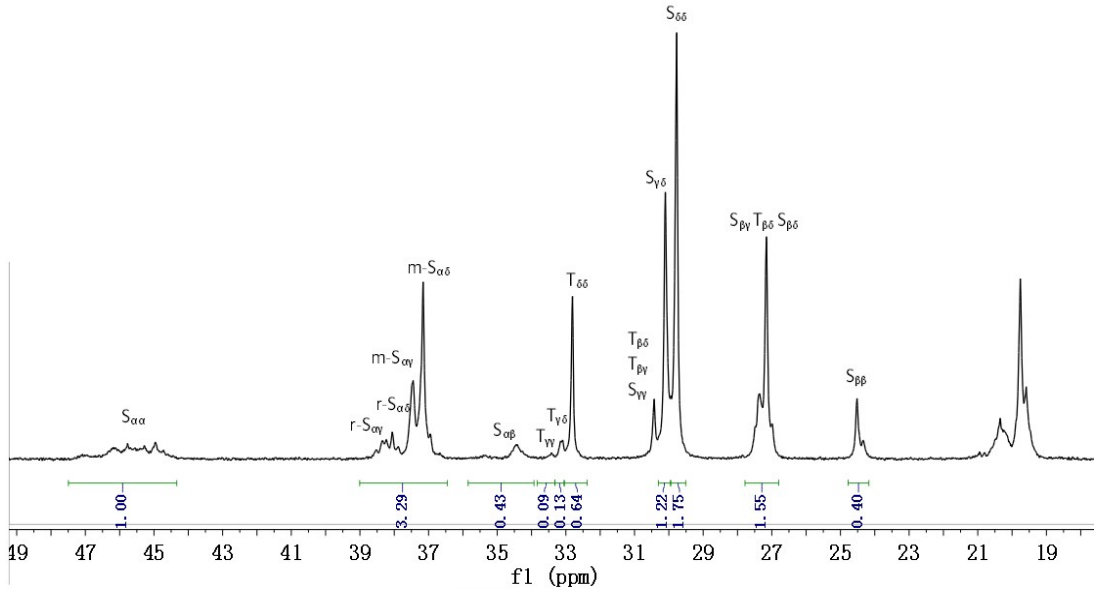

Fig. S14 Representative ^{13}C NMR spectrum of ethylene-propylene copolymer prepared by the **T6**/TIBA/MMAO (TIBA/Ti = 50) catalytic system (In $CDCl_3$, 25 °C).

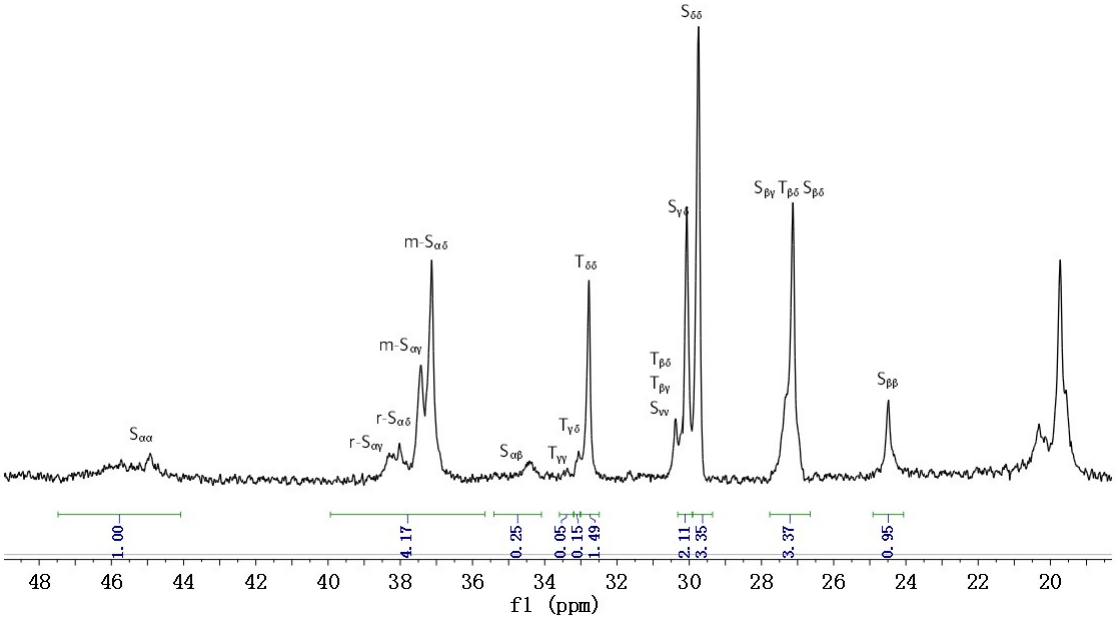

Fig. S15 Representative ^{13}C NMR spectrum of ethylene-propylene copolymer (In Figure 13 and Figure 14, T = 2.5°C) prepared by the **T5**/MAO catalytic system (In $CDCl_3$, 25 °C).

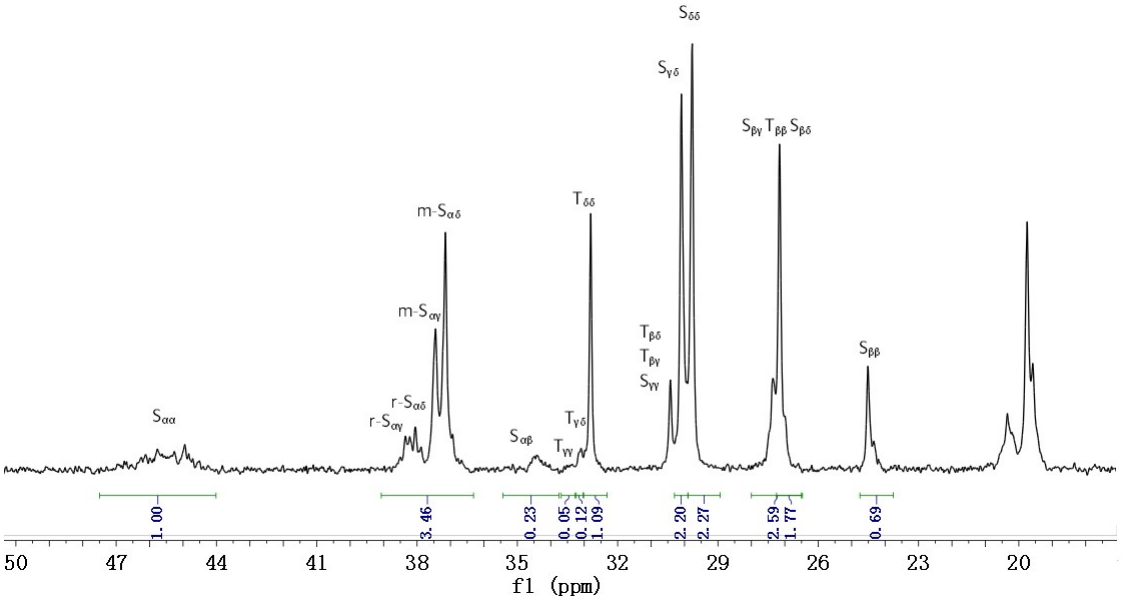

Fig. S16 Representative ^{13}C NMR spectrum of ethylene-propylene copolymer (In Figure 13 and Figure 14, T = 30°C) prepared by the **T5**/MAO catalytic system (In $CDCl_3$, 25 °C).

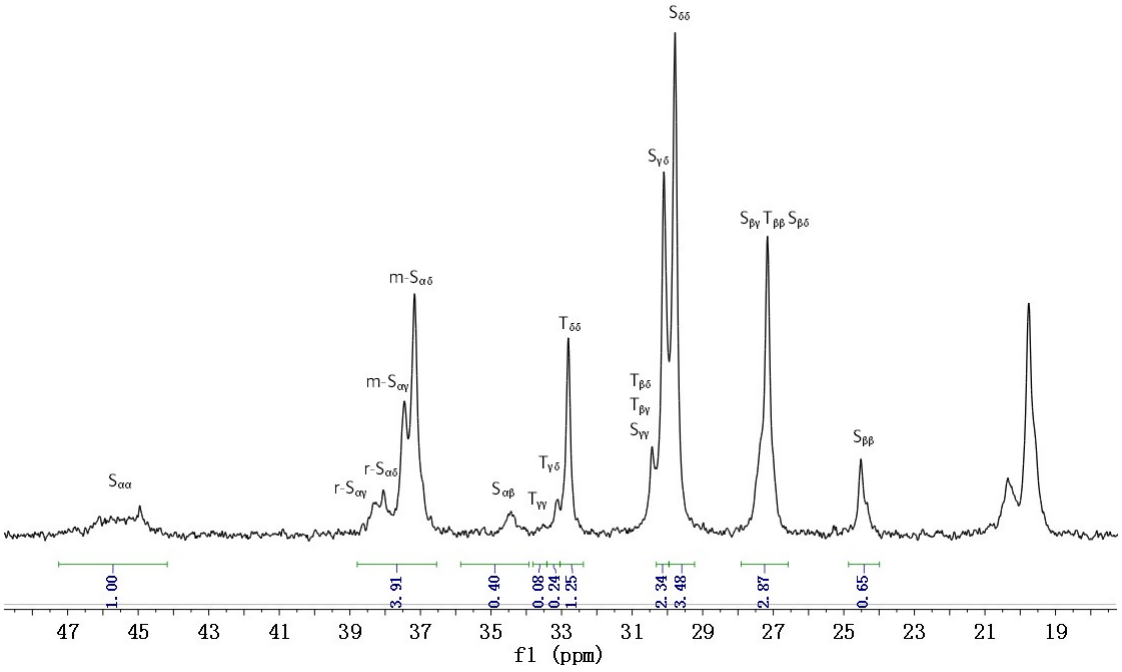

Fig. S17 Representative 1^3C NMR spectrum of ethylene-propylene copolymer (In Figure 13 and Figure 14, T = 60°C) prepared by the **T5**/MAO catalytic system (In $CDCl_3$, 25 °C).

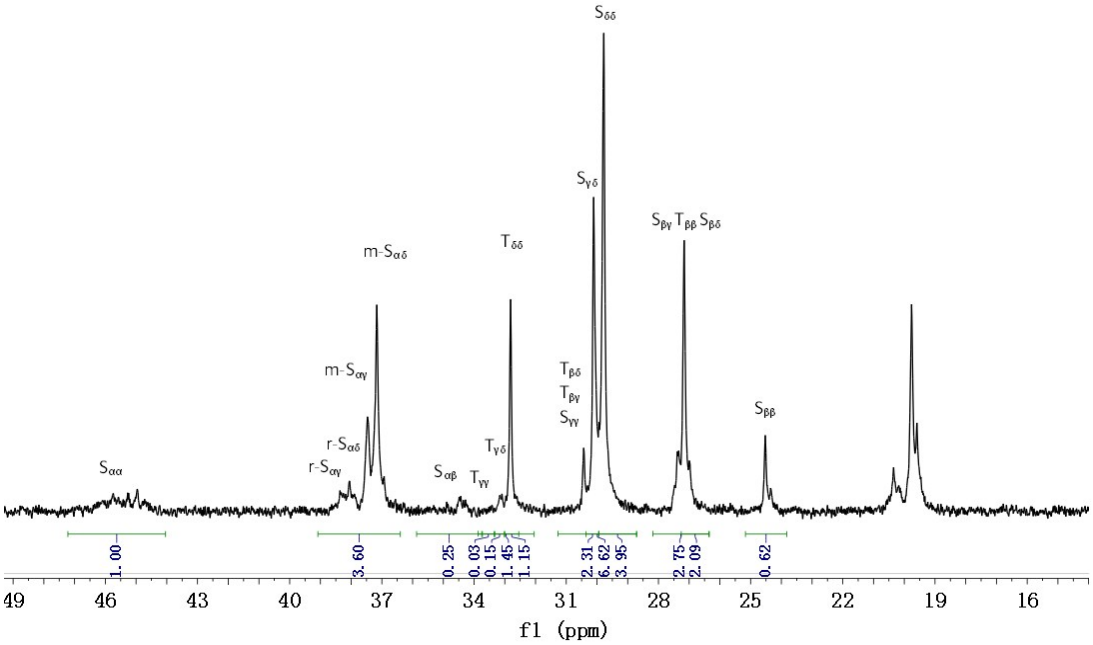

Fig. S18 Representative ^{13}C NMR spectrum of ethylene-propylene copolymer (In Figure 13 and Figure 14, T = 80 °C) prepared by the **T5**/MAO catalytic system (In $CDCl_3$, 25 °C).

The quantitative evaluation of the triad distributions and dyad distributions were calculated follow the analysis method of Cheng H.N [31] and Feng Y. [32] As mentioned above, the $T_{\beta\beta}$ peak overlaps the $S_{\beta\gamma}$ peak. Therefore, the quantitative evaluation of the PPP sequence (calculate by $T_{\beta\beta}$ peak) was hard to calculate directly. According to Cheng H.N, [31] the numerous peaks have the following relationships and proved to be very useful for the purpose of computation and double-checking:

$$S_{\alpha\alpha} = T_{\beta\beta} + 1/2(T_{\beta\gamma} + T_{\beta\delta})$$
$$S_{\alpha\beta} = T_{\beta\gamma} + T_{\gamma\delta} + T_{\gamma\gamma}$$
$$S_{\alpha\gamma} + S_{\alpha\delta} = T_{\beta\delta} + T_{\gamma\delta} + 2T_{\delta\delta}$$

So, the $T_{\beta\beta}$ peak area can be calculated by following equation:

$$T_{\beta\beta} = S_{\alpha\alpha} - 1/2(S_{\alpha\beta} + S_{\alpha\gamma} + S_{\alpha\delta} - 2T_{\gamma\delta} - 2T_{\gamma\gamma} - 2T_{\delta\delta})$$

The triad distributions and dyad distributions were calculatedby following equation:

$$PPP = T_{\beta\beta}$$
$$PPE = T_{\beta\delta}$$
$$EPE = T_{\delta\delta}$$
$$PEP = S_{\beta\beta} = 1/2\, S_{\alpha\gamma}$$
$$EEP = S_{\alpha\delta} = S_{\beta\delta}$$
$$EEE = 1/2\, S_{\delta\delta} + 1/4\, S_{\gamma\delta}$$
$$EE = 1/2\,(S_{\delta\delta} + S_{\beta\delta}) + 1/4\, S_{\gamma\delta}$$
$$PP = S_{\alpha\alpha}$$
$$EP = S_{\alpha\gamma} + S_{\alpha\delta}$$

Herein, the reactivity ratios were calculated by the first-order Markovian statistical model:

$$r_e = 2\,EE\,/\,(EE \times X_e/X_p)$$
$$r_p = (2PP \times X_e/X_p)\,/\,EP$$

EE, EP and PP are dyad distributions calculated by ^{13}C-NMR spectrum. X_e/X_p is the molar ratio of ethylene to propylene.

X-ray Structure Report for T1

Experimental

Single crystals of $C_{14}H_{14}Cl_2N_2OTi$ **[T1]** were recrystallised fromtoluolmounted in inert oil and transferred to the cold gas stream of the diffractometer.

Crystal structure determination of **T1**

Crystal Data. $C_{14}H_{14}Cl_2N_2OTi$, M =345.07, monoclinic, a = 15.3461(11) Å, b = 9.6856(4) Å, c = 20.5438(11) Å, β = 105.618(6)°, U = 2940.8(3) Å^3, T = 106.1, space group $P2_1/c$ (no. 14), Z = 8, μ(Mo Kα) = 0.941, 15847 reflections measured, 5755 unique (R_{int} = 0.0387) which were used in all calculations. The final $wR(F_2)$ was 0.1983 (all data).

Table S1 Crystal data and structure refinement for **T1**

Identification code	**T1**
Empirical formula	$C_{14}H_{14}Cl_2N_2OTi$
Formula weight	345.07
Temperature/K	106.1
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å, b/Å, c/Å	15.3461(11), 9.6856(4), 20.5438(11)
α/°, β/°, γ/°	90.00, 105.618(6), 90.00
Volume/Å^3	2940.8(3)
Z	8
ρ_{calc}/mg mm^{-3}	1.559
μ/mm^{-1}	0.941
F(000)	1408
Crystal size / mm^3	0.55 × 0.23 × 0.14
2Θ range for data collection	5.92 to 52°
Index ranges	-18 ≤ h ≤ 14, -11 ≤ k ≤ 10, -25 ≤ l ≤ 25
Reflections collected	15847

Independent reflections	5755[R(int) = 0.0387 (inf-0.9Å)]
Data/restraints/parameters	5755/12/361
Goodness-of-fit on F^2	1.204
Final R indexes [I>2σ (I) i.e. F_o>4σ (F_o)]	R_1 = 0.0870, wR_2 = 0.1932
Final R indexes [all data]	R_1 = 0.0986, wR_2 = 0.1983
Largest diff. peak/hole / e Å^{-3}	1.794/-0.660
Flack Parameters	N
Completeness	0.998

Table S2 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for **T1**. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
Ti2	2872.0(7)	-2270.7(12)	-689.4(6)	15.8(3)
Cl3	2701.5(12)	-4035.8(18)	-1451.4(9)	27.6(4)
N3	2770(4)	-755(6)	-1252(3)	23.5(12)
N4	2617(4)	1311(6)	-1878(3)	20.3(12)
O2	3950(3)	790(5)	-1170(2)	24.5(10)
C24	1088(5)	272(8)	-2140(4)	27.3(16)
C21	4101(5)	2098(8)	-1472(4)	30.0(16)
C23	1689(4)	1254(7)	-2261(3)	21.0(14)
C22	3225(4)	2408(7)	-2007(3)	20.9(14)
C17	3764(5)	-3586(8)	218(4)	32.7(18)
C27	492(5)	2227(9)	-3157(3)	30.2(17)
C26	-109(5)	1249(9)	-3038(4)	32.9(17)
C25	179(5)	272(9)	-2534(4)	36.1(19)
C20	3078(4)	404(7)	-1415(3)	21.4(14)
C19	4391(4)	-1744(9)	-173(4)	31.9(18)
C16	3513(5)	-2388(8)	496(3)	26.2(16)
C18	4313(5)	-3194(9)	-192(4)	35.2(19)
C28	1383(5)	2237(8)	-2773(3)	25.6(15)
C15	3876(5)	-1245(7)	242(3)	25.1(15)
Ti1	2071.3(7)	2427.8(11)	-4561.1(6)	14.7(3)
Cl4	1515.7(10)	-2250.0(18)	-413.9(8)	24.2(4)
Cl2	2208.4(12)	4402.6(18)	-3917.0(9)	29.4(4)
N1	2309(4)	955(7)	-3935(3)	23.6(13)
C6	2130(4)	-76(8)	-3709(3)	24.0(15)
N2	2704(4)	-949(6)	-3252(3)	22.5(12)
O1	1284(3)	-642(5)	-3875(2)	26.3(11)

C10	4158(5)	128(7)	-3251(4)	26.5(15)
C11	5080(5)	269(8)	-2944(4)	34.5(18)
C8	2210(5)	-2090(8)	-3038(3)	26.3(15)
C14	4058(5)	-1385(8)	-2343(4)	29.3(16)
C9	3641(5)	-722(7)	-2945(3)	23.9(15)
C13	4984(5)	-1176(9)	-2039(4)	35.1(18)
C7	1298(5)	-2017(8)	-3583(4)	30.4(17)
C12	5489(5)	-367(9)	-2343(4)	38.1(19)
Cl1	3381.8(11)	2440.0(17)	-4902.8(10)	27.9(4)
C5	1352(5)	2149(9)	-5726(4)	32.7(18)
C3	573(4)	3143(8)	-5052(4)	27.9(16)
C2	564(4)	1711(7)	-4956(3)	22.4(14)
C1	1052(4)	1095(8)	-5372(4)	26.6(15)
C4	1070(5)	3414(9)	-5529(4)	33.9(19)

Table S3 Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for **T1**.

The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+...+2hka\times b\times U_{12}]$

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Ti2	11.0(5)	19.6(6)	16.2(6)	4.3(4)	2.4(4)	-1.4(5)
Cl3	29.6(9)	22.1(8)	31.6(9)	-1.3(7)	9.2(7)	1.4(7)
N3	14(2)	12(2)	47(3)	5(2)	13(2)	-2(2)
N4	22(3)	18(3)	20(3)	1(2)	4(2)	-1(2)
O2	19(2)	25(3)	28(2)	4(2)	3.0(19)	-3(2)
C24	26(4)	26(4)	27(4)	9(3)	2(3)	0(3)
C21	25(4)	24(4)	39(4)	6(3)	6(3)	-4(3)
C23	19(3)	22(3)	23(3)	-2(3)	8(3)	4(3)
C22	23(3)	20(3)	22(3)	2(3)	11(3)	-2(3)
C17	39(4)	18(4)	30(4)	6(3)	-12(3)	-4(3)
C27	29(4)	42(4)	18(3)	2(3)	3(3)	7(3)
C26	23(4)	43(5)	30(4)	0(3)	2(3)	7(3)
C25	22(4)	46(5)	37(4)	6(4)	3(3)	4(4)
C20	18(3)	23(3)	23(3)	-2(3)	5(3)	2(3)
C19	13(3)	45(5)	32(4)	16(3)	-4(3)	-10(3)
C16	19(3)	38(4)	15(3)	6(3)	-5(3)	-7(3)
C18	21(4)	50(5)	26(4)	-9(4)	-9(3)	17(4)
C28	22(3)	34(4)	21(3)	1(3)	7(3)	0(3)
C15	29(4)	15(3)	24(3)	3(3)	-7(3)	-2(3)
Ti1	12.7(5)	9.1(5)	21.7(6)	1.7(4)	3.6(4)	-1.4(4)
Cl4	15.1(7)	31.6(9)	27.5(8)	-2.5(7)	8.5(6)	-5.7(7)
Cl2	33.7(10)	21.1(8)	31.3(9)	1.6(7)	5.0(7)	-1.3(7)
N1	13(2)	37(3)	20(2)	-10(2)	4(2)	0(2)
C6	16(3)	31(4)	23(3)	-11(3)	2(3)	8(3)
N2	24(3)	21(3)	22(3)	-1(2)	5(2)	-1(2)
O1	23(2)	20(2)	34(3)	3(2)	6(2)	-3(2)

C10	27(4)	24(4)	29(4)	0(3)	7(3)	0(3)
C11	23(4)	33(4)	45(5)	-9(4)	5(3)	-4(3)
C8	29(4)	24(4)	23(3)	2(3)	3(3)	-7(3)
C14	33(4)	28(4)	27(4)	-1(3)	6(3)	6(3)
C9	23(3)	22(4)	26(3)	-6(3)	4(3)	5(3)
C13	37(4)	37(4)	27(4)	-1(3)	3(3)	15(4)
C7	33(4)	22(4)	36(4)	11(3)	10(3)	-6(3)
C12	29(4)	33(4)	45(5)	-8(4)	-3(4)	6(4)
Cl1	21.6(8)	21.0(9)	45.8(11)	3.6(7)	17.1(8)	-2.2(7)
C5	29(4)	48(5)	21(4)	0(3)	8(3)	-11(4)
C3	16(3)	26(4)	36(4)	4(3)	-3(3)	5(3)
C2	14(3)	29(4)	23(3)	0(3)	4(3)	-6(3)
C1	18(3)	27(4)	32(4)	-4(3)	2(3)	-4(3)
C4	21(4)	37(4)	34(4)	19(3)	-8(3)	-11(3)

Table S4 Bond Lengths for **T1**.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Ti2	Cl3	2.285(2)	Ti1	Cl2	2.303(2)
Ti2	N3	1.849(6)	Ti1	N1	1.889(7)
Ti2	C17	2.365(7)	Ti1	Cl1	2.302(2)
Ti2	C19	2.343(7)	Ti1	C5	2.366(7)
Ti2	C16	2.370(6)	Ti1	C3	2.352(7)
Ti2	C18	2.349(7)	Ti1	C2	2.340(6)
Ti2	C15	2.332(7)	Ti1	C1	2.342(7)
Ti2	Cl4	2.2995(19)	Ti1	C4	2.363(7)
N3	C20	1.296(9)	N1	C6	1.165(9)
N4	C23	1.430(8)	C6	N2	1.389(9)
N4	C22	1.484(8)	C6	O1	1.365(8)
N4	C20	1.347(8)	N2	C8	1.472(9)
O2	C21	1.456(8)	N2	C9	1.423(9)
O2	C20	1.350(8)	O1	C7	1.459(8)
C24	C23	1.393(10)	C10	C11	1.392(10)
C24	C25	1.411(10)	C10	C9	1.404(10)
C21	C22	1.519(10)	C11	C12	1.372(11)
C23	C28	1.403(10)	C8	C7	1.541(10)
C17	C16	1.393(11)	C14	C9	1.389(10)
C17	C18	1.395(11)	C14	C13	1.405(11)
C27	C26	1.390(11)	C13	C12	1.365(12)
C27	C28	1.382(10)	C5	C1	1.401(10)
C26	C25	1.386(11)	C5	C4	1.395(12)
C19	C18	1.408(12)	C3	C2	1.401(10)
C19	C15	1.397(11)	C3	C4	1.420(11)
C16	C15	1.401(10)	C2	C1	1.412(10)

Table S5 Bond Angles for **T1**.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
Cl3	Ti2	C17	94.1(2)	Cl2	Ti1	C5	128.4(2)
Cl3	Ti2	C19	112.9(2)	Cl2	Ti1	C3	85.94(19)
Cl3	Ti2	C16	127.4(2)	Cl2	Ti1	C2	111.99(18)
Cl3	Ti2	C18	86.2(2)	Cl2	Ti1	C1	143.78(19)
Cl3	Ti2	C15	144.07(19)	Cl2	Ti1	C4	94.9(2)
Cl3	Ti2	Cl4	103.35(8)	N1	Ti1	Cl2	105.34(18)
N3	Ti2	Cl3	101.0(2)	N1	Ti1	Cl1	100.77(17)
N3	Ti2	C17	148.6(3)	N1	Ti1	C5	123.7(3)
N3	Ti2	C19	91.0(2)	N1	Ti1	C3	120.1(2)
N3	Ti2	C16	128.5(3)	N1	Ti1	C2	90.2(2)
N3	Ti2	C18	119.0(3)	N1	Ti1	C1	92.2(3)
N3	Ti2	C15	95.8(2)	N1	Ti1	C4	147.3(3)
N3	Ti2	Cl4	102.55(17)	Cl1	Ti1	Cl2	102.64(8)
C17	Ti2	C16	34.2(3)	Cl1	Ti1	C5	84.24(19)
C19	Ti2	C17	57.7(3)	Cl1	Ti1	C3	134.5(2)
C19	Ti2	C16	57.2(3)	Cl1	Ti1	C2	139.34(18)
C19	Ti2	C18	34.9(3)	Cl1	Ti1	C1	104.87(18)
C18	Ti2	C17	34.4(3)	Cl1	Ti1	C4	99.5(2)
C18	Ti2	C16	56.9(3)	C3	Ti1	C5	57.6(3)
C15	Ti2	C17	57.9(2)	C3	Ti1	C4	35.1(3)
C15	Ti2	C19	34.8(3)	C2	Ti1	C5	57.8(2)
C15	Ti2	C16	34.7(2)	C2	Ti1	C3	34.7(3)
C15	Ti2	C18	57.9(3)	C2	Ti1	C1	35.1(2)
Cl4	Ti2	C17	100.4(2)	C2	Ti1	C4	58.0(2)
Cl4	Ti2	C19	138.0(2)	C1	Ti1	C5	34.6(3)
Cl4	Ti2	C16	84.28(18)	C1	Ti1	C3	57.9(3)
Cl4	Ti2	C18	134.8(2)	C1	Ti1	C4	57.7(3)
Cl4	Ti2	C15	103.6(2)	C4	Ti1	C5	34.3(3)
C20	N3	Ti2	150.8(5)	C6	N1	Ti1	153.5(5)
C23	N4	C22	120.7(5)	N1	C6	N2	128.1(7)
C20	N4	C23	128.2(6)	N1	C6	O1	123.8(6)
C20	N4	C22	110.9(5)	O1	C6	N2	108.1(6)
C20	O2	C21	109.7(5)	C6	N2	C8	112.0(6)
C23	C24	C25	119.9(7)	C6	N2	C9	125.9(6)
O2	C21	C22	105.6(5)	C9	N2	C8	121.6(6)
C24	C23	N4	122.5(6)	C6	O1	C7	110.9(5)
C24	C23	C28	119.5(6)	C11	C10	C9	118.9(7)
C28	C23	N4	118.0(6)	C12	C11	C10	121.8(8)
N4	C22	C21	101.9(5)	N2	C8	C7	100.9(5)
C16	C17	Ti2	73.1(4)	C9	C14	C13	119.8(7)
C16	C17	C18	107.4(7)	C10	C9	N2	121.2(6)

C18	C17	Ti2	72.1(4)	C14	C9	N2	119.4(6)
C28	C27	C26	120.4(7)	C14	C9	C10	119.3(7)
C25	C26	C27	120.2(7)	C12	C13	C14	120.7(7)
C26	C25	C24	119.7(8)	O1	C7	C8	104.5(6)
N3	C20	N4	126.0(6)	C13	C12	C11	119.4(7)
N3	C20	O2	122.5(6)	C1	C5	Ti1	71.8(4)
N4	C20	O2	111.2(6)	C4	C5	Ti1	72.7(4)
C18	C19	Ti2	72.8(4)	C4	C5	C1	108.6(7)
C15	C19	Ti2	72.2(4)	C2	C3	Ti1	72.2(4)
C15	C19	C18	107.7(7)	C2	C3	C4	107.9(7)
C17	C16	Ti2	72.7(4)	C4	C3	Ti1	72.9(4)
C17	C16	C15	108.9(7)	C3	C2	Ti1	73.1(4)
C15	C16	Ti2	71.2(4)	C3	C2	C1	107.8(6)
C17	C18	Ti2	73.4(4)	C1	C2	Ti1	72.5(4)
C17	C18	C19	108.4(7)	C5	C1	Ti1	73.6(4)
C19	C18	Ti2	72.3(4)	C5	C1	C2	108.0(7)
C27	C28	C23	120.3(7)	C2	C1	Ti1	72.4(4)
C19	C15	Ti2	73.0(4)	C5	C4	Ti1	73.0(4)
C19	C15	C16	107.5(6)	C5	C4	C3	107.7(7)
C16	C15	Ti2	74.2(4)	C3	C4	Ti1	72.1(4)

Table S6 Torsion Angles for **T1**.

A	B	C	D	Angle/°
Ti2	N3	C20	N4	-168.2(7)
Ti2	N3	C20	O2	17.8(14)
Ti2	C17	C16	C15	-62.3(5)
Ti2	C17	C18	C19	64.3(5)
Ti2	C19	C18	C17	-65.1(5)
Ti2	C19	C15	C16	66.8(5)
Ti2	C16	C15	C19	-66.0(5)
Cl3	Ti2	N3	C20	-127.0(10)
Cl3	Ti2	C17	C16	-167.6(4)
Cl3	Ti2	C17	C18	77.1(4)
Cl3	Ti2	C19	C18	-43.0(5)
Cl3	Ti2	C19	C15	-158.8(4)
Cl3	Ti2	C16	C17	15.6(5)
Cl3	Ti2	C16	C15	133.4(4)
Cl3	Ti2	C18	C17	-103.0(4)
Cl3	Ti2	C18	C19	140.9(5)
Cl3	Ti2	C15	C19	34.5(6)
Cl3	Ti2	C15	C16	-79.8(5)
N3	Ti2	C17	C16	73.4(7)
N3	Ti2	C17	C18	-41.9(8)
N3	Ti2	C19	C18	-145.4(5)

N3	Ti2	C19	C15	98.8(4)
N3	Ti2	C16	C17	-140.4(5)
N3	Ti2	C16	C15	-22.7(6)
N3	Ti2	C18	C17	156.6(4)
N3	Ti2	C18	C19	40.5(5)
N3	Ti2	C15	C19	-83.3(4)
N3	Ti2	C15	C16	162.3(4)
N4	C23	C28	C27	180.0(6)
O2	C21	C22	N4	7.8(7)
C24	C23	C28	C27	-0.3(10)
C21	O2	C20	N3	176.8(6)
C21	O2	C20	N4	2.1(8)
C23	N4	C22	C21	177.3(6)
C23	N4	C20	N3	4.2(11)
C23	N4	C20	O2	178.7(6)
C23	C24	C25	C26	0.0(12)
C22	N4	C23	C24	-177.7(6)
C22	N4	C23	C28	2.0(9)
C22	N4	C20	N3	-171.1(6)
C22	N4	C20	O2	3.5(7)
C17	Ti2	N3	C20	-9.7(13)
C17	Ti2	C19	C18	36.9(4)
C17	Ti2	C19	C15	-78.9(5)
C17	Ti2	C16	C15	117.7(6)
C17	Ti2	C18	C19	-116.1(7)
C17	Ti2	C15	C19	78.4(5)
C17	Ti2	C15	C16	-36.0(4)
C17	C16	C15	Ti2	63.3(5)
C17	C16	C15	C19	-2.7(7)
C27	C26	C25	C24	0.0(12)
C26	C27	C28	C23	0.3(11)
C25	C24	C23	N4	179.8(7)
C25	C24	C23	C28	0.1(11)
C20	N4	C23	C24	7.5(11)
C20	N4	C23	C28	-172.8(6)
C20	N4	C22	C21	-7.1(7)
C20	O2	C21	C22	-6.5(7)
C19	Ti2	N3	C20	-13.4(10)
C19	Ti2	C17	C16	77.8(5)
C19	Ti2	C17	C18	-37.5(5)
C19	Ti2	C16	C17	-79.6(5)
C19	Ti2	C16	C15	38.2(4)
C19	Ti2	C18	C17	116.1(7)
C19	Ti2	C15	C16	-114.4(6)

C16	Ti2	N3	C20	33.8(11)
C16	Ti2	C17	C18	-115.3(6)
C16	Ti2	C19	C18	77.7(5)
C16	Ti2	C19	C15	-38.0(4)
C16	Ti2	C18	C17	37.4(4)
C16	Ti2	C18	C19	-78.7(5)
C16	Ti2	C15	C19	114.4(6)
C16	C17	C18	Ti2	-65.1(5)
C16	C17	C18	C19	-0.7(8)
C18	Ti2	N3	C20	-35.3(11)
C18	Ti2	C17	C16	115.3(6)
C18	Ti2	C19	C15	-115.8(6)
C18	Ti2	C16	C17	-37.6(5)
C18	Ti2	C16	C15	80.1(5)
C18	Ti2	C15	C19	37.5(4)
C18	Ti2	C15	C16	-76.9(5)
C18	C17	C16	Ti2	64.4(5)
C18	C17	C16	C15	2.1(8)
C18	C19	C15	Ti2	-64.6(5)
C18	C19	C15	C16	2.2(8)
C28	C27	C26	C25	-0.1(12)
C15	Ti2	N3	C20	21.1(11)
C15	Ti2	C17	C16	36.4(4)
C15	Ti2	C17	C18	-78.8(5)
C15	Ti2	C19	C18	115.8(6)
C15	Ti2	C16	C17	-117.7(6)
C15	Ti2	C18	C17	78.8(5)
C15	Ti2	C18	C19	-37.3(4)
C15	C19	C18	Ti2	64.2(5)
C15	C19	C18	C17	-0.9(8)
Ti1	N1	C6	N2	165.4(8)
Ti1	N1	C6	O1	-13.3(16)
Ti1	C5	C1	C2	64.7(5)
Ti1	C5	C4	C3	-64.1(5)
Ti1	C3	C2	C1	-64.7(5)
Ti1	C3	C4	C5	64.7(5)
Ti1	C2	C1	C5	-65.5(5)
Cl4	Ti2	N3	C20	126.5(10)
Cl4	Ti2	C17	C16	-63.2(4)
Cl4	Ti2	C17	C18	-178.5(4)
Cl4	Ti2	C19	C18	104.5(5)
Cl4	Ti2	C19	C15	-11.3(6)
Cl4	Ti2	C16	C17	118.1(4)
Cl4	Ti2	C16	C15	-124.2(4)

Cl4	Ti2	C18	C17	2.1(6)
Cl4	Ti2	C18	C19	-114.0(5)
Cl4	Ti2	C15	C19	172.3(4)
Cl4	Ti2	C15	C16	57.9(4)
Cl2	Ti1	N1	C6	124.2(11)
Cl2	Ti1	C5	C1	-131.6(4)
Cl2	Ti1	C5	C4	-14.6(5)
Cl2	Ti1	C3	C2	-139.6(4)
Cl2	Ti1	C3	C4	104.6(5)
Cl2	Ti1	C2	C3	44.3(4)
Cl2	Ti1	C2	C1	159.8(4)
Cl2	Ti1	C1	C5	82.8(5)
Cl2	Ti1	C1	C2	-32.7(6)
Cl2	Ti1	C4	C5	168.6(4)
Cl2	Ti1	C4	C3	-75.7(4)
N1	Ti1	C5	C1	27.7(6)
N1	Ti1	C5	C4	144.7(4)
N1	Ti1	C3	C2	-34.2(5)
N1	Ti1	C3	C4	-150.0(5)
N1	Ti1	C2	C3	150.9(4)
N1	Ti1	C2	C1	-93.5(4)
N1	Ti1	C1	C5	-157.2(5)
N1	Ti1	C1	C2	87.3(4)
N1	Ti1	C4	C5	-62.7(7)
N1	Ti1	C4	C3	53.0(7)
N1	C6	N2	C8	174.8(7)
N1	C6	N2	C9	2.3(11)
N1	C6	O1	C7	172.3(7)
C6	N2	C8	C7	15.4(7)
C6	N2	C9	C10	-24.2(10)
C6	N2	C9	C14	157.8(6)
C6	O1	C7	C8	16.1(7)
N2	C6	O1	C7	-6.6(7)
N2	C8	C7	O1	-18.0(7)
O1	C6	N2	C8	-6.4(7)
O1	C6	N2	C9	-178.9(6)
C10	C11	C12	C13	0.8(12)
C11	C10	C9	N2	-177.4(6)
C11	C10	C9	C14	0.7(10)
C8	N2	C9	C10	164.0(6)
C8	N2	C9	C14	-14.1(9)
C14	C13	C12	C11	1.3(12)
C9	N2	C8	C7	-171.7(6)
C9	C10	C11	C12	-1.9(11)

C9	C14	C13	C12	-2.4(11)
C13	C14	C9	N2	179.5(6)
C13	C14	C9	C10	1.3(10)
Cl1	Ti1	N1	C6	-129.4(11)
Cl1	Ti1	C5	C1	126.9(4)
Cl1	Ti1	C5	C4	-116.2(4)
Cl1	Ti1	C3	C2	116.7(4)
Cl1	Ti1	C3	C4	0.8(6)
Cl1	Ti1	C2	C3	-102.1(5)
Cl1	Ti1	C2	C1	13.5(6)
Cl1	Ti1	C1	C5	-55.4(5)
Cl1	Ti1	C1	C2	-171.0(4)
Cl1	Ti1	C4	C5	64.9(4)
Cl1	Ti1	C4	C3	-179.4(4)
C5	Ti1	N1	C6	-39.2(12)
C5	Ti1	C3	C2	78.9(5)
C5	Ti1	C3	C4	-37.0(5)
C5	Ti1	C2	C3	-78.3(5)
C5	Ti1	C2	C1	37.3(4)
C5	Ti1	C1	C2	-115.5(6)
C5	Ti1	C4	C3	115.7(6)
C3	Ti1	N1	C6	29.9(12)
C3	Ti1	C5	C1	-79.2(5)
C3	Ti1	C5	C4	37.8(4)
C3	Ti1	C2	C1	115.6(6)
C3	Ti1	C1	C5	78.2(5)
C3	Ti1	C1	C2	-37.4(4)
C3	Ti1	C4	C5	-115.7(6)
C3	C2	C1	Ti1	65.0(5)
C3	C2	C1	C5	-0.5(8)
C2	Ti1	N1	C6	11.2(12)
C2	Ti1	C5	C1	-37.8(4)
C2	Ti1	C5	C4	79.2(5)
C2	Ti1	C3	C4	-115.9(7)
C2	Ti1	C1	C5	115.5(6)
C2	Ti1	C4	C5	-78.5(5)
C2	Ti1	C4	C3	37.2(4)
C2	C3	C4	Ti1	-64.2(5)
C2	C3	C4	C5	0.6(8)
C1	Ti1	N1	C6	-23.8(12)
C1	Ti1	C5	C4	117.0(6)
C1	Ti1	C3	C2	37.7(4)
C1	Ti1	C3	C4	-78.1(5)
C1	Ti1	C2	C3	-115.6(6)

C1	Ti1	C4	C5	-36.8(4)
C1	Ti1	C4	C3	78.9(5)
C1	C5	C4	Ti1	63.2(5)
C1	C5	C4	C3	-0.9(8)
C4	Ti1	N1	C6	-2.1(14)
C4	Ti1	C5	C1	-117.0(6)
C4	Ti1	C3	C2	115.9(7)
C4	Ti1	C2	C3	-37.5(5)
C4	Ti1	C2	C1	78.0(5)
C4	Ti1	C1	C5	36.5(5)
C4	Ti1	C1	C2	-79.0(5)
C4	C5	C1	Ti1	-63.9(5)
C4	C5	C1	C2	0.9(8)
C4	C3	C2	Ti1	64.6(5)
C4	C3	C2	C1	-0.1(8)

Table S7 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for **T1**.

Atom	*x*	*y*	*z*	U(eq)
H24	1285	-382	-1801	33
H21A	4601	2023	-1675	36
H21B	4235	2823	-1133	36
H22A	2998	3320	-1946	25
H22B	3304	2336	-2458	25
H17	3596	-4483	291	39
H27	295	2879	-3497	36
H26	-708	1250	-3298	39
H25	-224	-382	-2455	43
H19	4726	-1215	-397	38
H16	3162	-2353	800	31
H18	4582	-3788	-437	42
H28	1781	2898	-2854	31
H15	3789	-322	334	30
H10	3889	588	-3652	32
H11	5428	809	-3152	41
H8A	2137	-1936	-2589	32
H8B	2510	-2969	-3048	32
H14	3725	-1965	-2140	35
H13	5257	-1594	-1627	42
H7A	1262	-2724	-3923	36
H7B	798	-2135	-3383	36
H12	6105	-248	-2144	46
H5	1684	2027	-6040	39
H3	302	3800	-4840	33
H2	286	1249	-4670	27

H1	1156	155	-5406	32
H4	1187	4279	-5683	41

X-ray Structure Report for T2

Experimental

Single crystals of $C_{18}H_{24}C_{l2}N_2OTi$ **[T2]** were recrystallised fromtoluol mounted in inert oil and transferred to the cold gas stream of the diffractometer.

Crystal structure determination of[**T2**]

Crystal Data. $C_{18}H_{24}Cl_2N_2OTi$, M =403.19, monoclinic, a = 14.5895(5) Å, b = 10.0182(4) Å, c = 13.9424(5) Å, β = 101.750(3)°, U = 1995.13(12) Å^3, T = 107.1, space group $P2_1/c$ (no. 14), Z = 4, μ(Mo Kα) = 0.704, 9083 reflections measured, 3913 unique (R_{int} = 0.0261) which were used in all calculations. The final $wR(F_2)$ was 0.0777 (all data).

Table S8 Crystal data and structure refinement for **T2**

Identification code	**T2**
Empirical formula	$C_{18}H_{24}Cl_2N_2OTi$
Formula weight	403.19
Temperature / K	107.1
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å, b/Å, c/Å	14.5895(5), 10.0182(4), 13.9424(5)
α/°, β/°, γ/°	90.00, 101.750(3), 90.00
Volume/Å^3	1995.13(12)
Z	4
ρ_{calc}/mg mm^{-3}	1.342
μ/mm^{-1}	0.704
F(000)	840
Crystal size / mm^3	0.35 × 0.34 × 0.30
2Θ range for data collection	6.06 to 52°
Index ranges	-17 ≤ h ≤ 17, -12 ≤ k ≤ 11, -17 ≤ l ≤ 17
Reflections collected	9083
Independent reflections	3913[R(int) = 0.0261 (inf-0.9Å)]
Data/restraints/parameters	3913/0/221
Goodness-of-fit on F^2	1.048
Final R indexes [I>2σ (I) i.e. F_o>4σ (F_o)]	R_1 = 0.0318, wR_2 = 0.0732
Final R indexes [all data]	R_1 = 0.0393, wR_2 = 0.0777
Largest diff. peak/hole / e Å^{-3}	0.281/-0.267
Flack Parameters	N
Completeness	0.998

Table S9 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for **T2** is defined as 1/3 of of the trace

of the orthogonalised U_{ij} tensor.

Atom	*x*	*y*	*z*	U(eq)
Ti1	3138.6(2)	3767.5(3)	637.5(2)	17.5(1)
Cl2	2019.3(3)	5280.1(5)	-70.5(3)	27.68(12)
Cl1	3802.6(3)	3258.9(6)	-680.9(3)	33.05(14)
O1	1382.5(9)	1148.0(13)	1429.7(9)	24.4(3)
N2	2412.7(10)	-70.8(15)	799(1)	18.9(3)
N1	2507.9(9)	2263.8(15)	769.4(10)	18.9(3)
C6	2141.7(12)	1155.8(19)	993.3(12)	18.2(4)
C16	3208.5(12)	-208.8(19)	278.9(13)	21.3(4)
C7	1144.5(11)	2350.6(19)	1851.7(13)	19.9(4)
C13	2021.2(13)	-1325.6(19)	1136.6(13)	24.7(4)
C1	3535.8(14)	4033(2)	2349.3(13)	27.7(5)
C9	398.7(13)	4483(2)	1713.5(15)	28.5(4)
C4	4264.6(13)	5365(2)	1410.9(13)	28.2(5)
C14	1024.9(14)	-1594(2)	574.7(16)	33.6(5)
C10	607.0(13)	4599(2)	2727.2(15)	30.5(5)
C5	3544.7(14)	5315(2)	1942.4(13)	27.3(4)
C18	2976.1(14)	-1156(2)	-590.2(13)	27.9(4)
C8	670.5(12)	3349(2)	1268.5(13)	23.5(4)
C17	4094.5(13)	-618(2)	1002.5(15)	32.7(5)
C11	1074.2(13)	3583(2)	3295.5(14)	30.2(5)
C12	1348.7(12)	2441(2)	2862.8(13)	24.5(4)
C2	4250.5(14)	3284(2)	2068.3(14)	32.2(5)
C3	4700.9(13)	4122(2)	1491.0(14)	33.5(5)
C15	2110.8(17)	-1384(2)	2253.3(15)	36.1(5)

Table S10 Anisotropic Displacement Parameters ($Å^2×10^3$) for **T2**.

The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+...+2hka×b×U_{12}]$

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Ti1	21.52(17)	15.04(18)	16.34(16)	-1.16(13)	4.79(12)	-3.63(13)
Cl2	33.5(2)	18.9(2)	27.9(2)	3.4(2)	-0.15(19)	0.0(2)
Cl1	36.8(3)	39.1(3)	27.8(2)	-12.3(2)	17.3(2)	-13.6(2)
O1	28.2(7)	15.8(7)	33.4(7)	-1.9(6)	15.9(6)	-3.8(6)
N2	24.2(7)	14.7(8)	18.7(7)	1.7(7)	6.5(6)	-0.8(6)
N1	19.2(7)	16.4(8)	21.2(7)	-1.2(7)	4.8(6)	-0.9(6)
C6	19.6(8)	19.1(10)	15.5(8)	-0.3(8)	2.5(6)	-1.1(7)
C16	25.3(9)	16.6(9)	24.1(9)	0.6(8)	9.8(7)	0.7(8)
C7	17.5(8)	17.3(9)	26.0(9)	-2.3(8)	7.1(7)	-3.6(7)
C13	35.1(10)	13.9(9)	27.2(9)	1.4(8)	11.1(8)	-1.9(8)
C1	33.6(10)	32.5(12)	15.8(8)	-2.0(9)	1.9(7)	-11.4(9)
C9	23.4(9)	25.3(11)	36.6(11)	4(1)	5.3(8)	5.1(9)
C4	32.2(10)	29.6(12)	21.2(9)	-1.6(9)	2.0(8)	-17.0(9)
C14	35.9(11)	22.3(11)	45.4(12)	-2.8(10)	14.8(9)	-8.3(9)

C10	27.6(10)	28.1(11)	38.2(11)	-11(1)	12.5(9)	0.6(9)
C5	37.1(10)	23.8(11)	19.3(9)	-7.3(9)	1.5(8)	-0.9(9)
C18	37.3(11)	25.0(11)	23.6(9)	-0.4(9)	11.6(8)	3.8(9)
C8	24.0(9)	25.1(11)	20.8(9)	0.3(8)	3.0(7)	-2.7(8)
C17	26.7(10)	32.4(12)	37.9(11)	-2.9(10)	3.8(8)	0.9(9)
C11	28.9(10)	39.2(13)	22.7(9)	-7(1)	5.9(8)	-3.6(10)
C12	21.1(9)	27.2(11)	24.5(9)	3.9(9)	3.2(7)	1.9(8)
C2	37.9(11)	22.6(11)	28.6(10)	-0.4(9)	-10.6(8)	-0.2(10)
C3	21.4(9)	51.0(15)	26.6(10)	-8.8(11)	1.5(8)	-2.5(10)
C15	58.1(14)	24.2(11)	29.4(10)	8.7(10)	17(1)	4.3(11)

Table S11 Bond Lengths for **T2**.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Ti1	Cl2	2.2980(6)	C16	C17	1.525(3)
Ti1	Cl1	2.3027(5)	C7	C8	1.382(3)
Ti1	N1	1.7941(15)	C7	C12	1.383(2)
Ti1	C1	2.3536(18)	C13	C14	1.528(3)
Ti1	C4	2.3880(19)	C13	C15	1.537(3)
Ti1	C5	2.3718(18)	C1	C5	1.405(3)
Ti1	C2	2.3511(19)	C1	C2	1.404(3)
Ti1	C3	2.3734(19)	C9	C10	1.389(3)
O1	C6	1.368(2)	C9	C8	1.390(3)
O1	C7	1.415(2)	C4	C5	1.404(3)
N2	C6	1.335(2)	C4	C3	1.393(3)
N2	C16	1.495(2)	C10	C11	1.382(3)
N2	C13	1.496(2)	C11	C12	1.390(3)
N1	C6	1.297(2)	C2	C3	1.415(3)
C16	C18	1.522(3)			

Table S12 Bond Angles for **T2**.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
Cl2	Ti1	Cl1	100.41(2)	N2	C6	O1	112.64(15)
Cl2	Ti1	C1	111.58(6)	N1	C6	O1	121.49(16)
Cl2	Ti1	C4	96.62(5)	N1	C6	N2	125.80(15)
Cl2	Ti1	C5	86.74(5)	N2	C16	C18	112.00(14)
Cl2	Ti1	C2	143.86(6)	N2	C16	C17	109.96(14)
Cl2	Ti1	C3	129.98(6)	C18	C16	C17	112.37(16)
Cl1	Ti1	C1	141.06(5)	C8	C7	O1	120.47(15)
Cl1	Ti1	C4	98.41(5)	C8	C7	C12	122.04(18)
Cl1	Ti1	C5	132.61(5)	C12	C7	O1	117.34(17)
Cl1	Ti1	C2	107.57(6)	N2	C13	C14	111.76(15)
Cl1	Ti1	C3	85.19(5)	N2	C13	C15	113.06(16)
N1	Ti1	Cl2	105.27(5)	C14	C13	C15	112.86(17)
N1	Ti1	Cl1	101.76(5)	C5	C1	Ti1	73.41(10)

N1	Ti1	C1	90.95(7)	C2	C1	Ti1	72.54(10)
N1	Ti1	C4	146.79(7)	C2	C1	C5	107.92(18)
N1	Ti1	C5	121.57(7)	C10	C9	C8	119.99(19)
N1	Ti1	C2	91.13(7)	C5	C4	Ti1	72.21(11)
N1	Ti1	C3	122.32(8)	C3	C4	Ti1	72.42(11)
C1	Ti1	C4	57.43(7)	C3	C4	C5	107.71(18)
C1	Ti1	C5	34.59(7)	C11	C10	C9	120.11(19)
C1	Ti1	C3	57.43(7)	C1	C5	Ti1	71.99(11)
C5	Ti1	C4	34.31(7)	C4	C5	Ti1	73.47(11)
C5	Ti1	C3	56.84(7)	C4	C5	C1	108.38(19)
C2	Ti1	C1	34.72(7)	C7	C8	C9	118.85(17)
C2	Ti1	C4	57.50(7)	C10	C11	C12	120.65(18)
C2	Ti1	C5	57.48(7)	C7	C12	C11	118.34(18)
C2	Ti1	C3	34.84(7)	C1	C2	Ti1	72.74(10)
C3	Ti1	C4	34.01(7)	C1	C2	C3	107.38(19)
C6	O1	C7	118.01(14)	C3	C2	Ti1	73.44(11)
C6	N2	C16	118.34(15)	C4	C3	Ti1	73.57(11)
C6	N2	C13	124.17(14)	C4	C3	C2	108.60(18)
C16	N2	C13	117.31(14)	C2	C3	Ti1	71.72(11)
C6	N1	Ti1	171.14(13)				

Table S13 Torsion Angles for **T2**.

A	B	C	D	Angle/°
Ti1	N1	C6	O1	95.6(8)
Ti1	N1	C6	N2	-87.5(9)
Ti1	C1	C5	C4	-64.96(13)
Ti1	C1	C2	C3	65.80(13)
Ti1	C4	C5	C1	64.00(13)
Ti1	C4	C3	C2	-63.62(13)
Ti1	C2	C3	C4	64.82(13)
Cl2	Ti1	N1	C6	-141.3(8)
Cl2	Ti1	C1	C5	-47.07(12)
Cl2	Ti1	C1	C2	-162.55(11)
Cl2	Ti1	C4	C5	74.25(12)
Cl2	Ti1	C4	C3	-169.85(11)
Cl2	Ti1	C5	C1	137.00(12)
Cl2	Ti1	C5	C4	-106.75(12)
Cl2	Ti1	C2	C1	28.22(17)
Cl2	Ti1	C2	C3	-86.54(15)
Cl2	Ti1	C3	C4	13.21(14)
Cl2	Ti1	C3	C2	129.80(12)
Cl1	Ti1	N1	C6	114.3(8)
Cl1	Ti1	C1	C5	95.91(14)
Cl1	Ti1	C1	C2	-19.57(17)

Cl1	Ti1	C4	C5	175.85(11)
Cl1	Ti1	C4	C3	-68.25(12)
Cl1	Ti1	C5	C1	-121.84(11)
Cl1	Ti1	C5	C4	-5.59(15)
Cl1	Ti1	C2	C1	167.24(11)
Cl1	Ti1	C2	C3	52.49(13)
Cl1	Ti1	C3	C4	112.77(11)
Cl1	Ti1	C3	C2	-130.64(13)
O1	C7	C8	C9	176.16(16)
O1	C7	C12	C11	-176.48(15)
N1	Ti1	C1	C5	-153.92(12)
N1	Ti1	C1	C2	90.61(13)
N1	Ti1	C4	C5	-57.14(18)
N1	Ti1	C4	C3	58.76(18)
N1	Ti1	C5	C1	31.06(14)
N1	Ti1	C5	C4	147.32(12)
N1	Ti1	C2	C1	-90.04(13)
N1	Ti1	C2	C3	155.20(13)
N1	Ti1	C3	C4	-146.34(11)
N1	Ti1	C3	C2	-29.75(15)
C6	O1	C7	C8	78.6(2)
C6	O1	C7	C12	-105.63(18)
C6	N2	C16	C18	-130.53(17)
C6	N2	C16	C17	103.77(19)
C6	N2	C13	C14	72.4(2)
C6	N2	C13	C15	-56.3(2)
C16	N2	C6	O1	177.21(13)
C16	N2	C6	N1	0.1(2)
C16	N2	C13	C14	-112.56(17)
C16	N2	C13	C15	118.79(18)
C7	O1	C6	N2	167.37(14)
C7	O1	C6	N1	-15.4(2)
C13	N2	C6	O1	-7.8(2)
C13	N2	C6	N1	175.11(16)
C13	N2	C16	C18	54.1(2)
C13	N2	C16	C17	-71.6(2)
C1	Ti1	N1	C6	-28.6(9)
C1	Ti1	C4	C5	-37.17(12)
C1	Ti1	C4	C3	78.73(13)
C1	Ti1	C5	C4	116.25(18)
C1	Ti1	C2	C3	-114.75(18)
C1	Ti1	C3	C4	-78.73(13)
C1	Ti1	C3	C2	37.86(12)
C1	C2	C3	Ti1	-65.33(13)

C1	C2	C3	C4	-0.5(2)
C9	C10	C11	C12	0.6(3)
C4	Ti1	N1	C6	-11.9(9)
C4	Ti1	C1	C5	36.87(12)
C4	Ti1	C1	C2	-78.61(13)
C4	Ti1	C5	C1	-116.25(18)
C4	Ti1	C2	C1	78.38(13)
C4	Ti1	C2	C3	-36.37(12)
C4	Ti1	C3	C2	116.60(17)
C10	C9	C8	C7	0.2(3)
C10	C11	C12	C7	0.2(3)
C5	Ti1	N1	C6	-45.6(9)
C5	Ti1	C1	C2	-115.48(17)
C5	Ti1	C4	C3	115.90(17)
C5	Ti1	C2	C1	37.43(12)
C5	Ti1	C2	C3	-77.32(14)
C5	Ti1	C3	C4	-37.28(11)
C5	Ti1	C3	C2	79.32(13)
C5	C1	C2	Ti1	-65.41(13)
C5	C1	C2	C3	0.4(2)
C5	C4	C3	Ti1	64.05(13)
C5	C4	C3	C2	0.4(2)
C8	C7	C12	C11	-0.8(3)
C8	C9	C10	C11	-0.8(3)
C12	C7	C8	C9	0.6(3)
C2	Ti1	N1	C6	6.1(9)
C2	Ti1	C1	C5	115.48(17)
C2	Ti1	C4	C5	-78.62(13)
C2	Ti1	C4	C3	37.28(12)
C2	Ti1	C5	C1	-37.57(12)
C2	Ti1	C5	C4	78.68(13)
C2	Ti1	C3	C4	-116.60(17)
C2	C1	C5	Ti1	64.83(13)
C2	C1	C5	C4	-0.1(2)
C3	Ti1	N1	C6	22.6(9)
C3	Ti1	C1	C5	77.48(13)
C3	Ti1	C1	C2	-38.00(13)
C3	Ti1	C4	C5	-115.90(17)
C3	Ti1	C5	C1	-79.31(13)
C3	Ti1	C5	C4	36.94(12)
C3	Ti1	C2	C1	114.75(18)
C3	C4	C5	Ti1	-64.18(13)
C3	C4	C5	C1	-0.2(2)

Table S14 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for **T2**.

Atom	*x*	*y*	*z*	U(eq)
H16	3323	673	23	26
H13	2407	-2056	969	30
H1	3129	3734	2736	33
H9	77	5163	1332	34
H4	4422	6097	1067	34
H14A	616	-902	716	50
H14B	816	-2441	770	50
H14C	1016	-1606	-116	50
H10	432	5363	3024	37
H5	3142	6012	2013	33
H18A	2914	-2047	-359	42
H18B	3469	-1132	-952	42
H18C	2399	-887	-1008	42
H8	536	3263	590	28
H17A	4236	38	1514	49
H17B	4606	-678	667	49
H17C	3999	-1469	1282	49
H11	1206	3664	3974	36
H12	1662	1754	3244	29
H2	4400	2399	2232	39
H3	5204	3884	1212	40
H15A	2734	-1133	2570	54
H15B	1985	-2276	2443	54
H15C	1669	-780	2444	54

X-ray Structure Report for T5

Experimental

Single crystals of $C_{35.5}H_{47}Cl_2N_3Ti$ **[T5]** were recrystallised from toluol mounted in inert oil and transferred to the cold gas stream of the diffractometer.

Crystal structure determination of**T5**

Crystal Data. $C_{35.5}H_{47}Cl_2N_3Ti$, M =634.56, monoclinic, a = 18.8611(10) Å, b = 19.4952(12) Å, c = 19.5123(11) Å, β = 105.765(5)°, U = 6904.8(7) Å^3, T = 106.1, space group P2$_1$/n (no. 14), Z = 8, μ(Mo Kα) = 0.430, 50094 reflections measured, 13543 unique (R_{int} = 0.0351) which were used in all calculations. The final $wR(F_2)$ was 0.0891 (all data).

Table S15 Crystal data and structure refinement for **T5**

Identification code	**T5**
Empirical formula	$C_{35.5}H_{47}Cl_2N_3Ti$
Formula weight	634.56
Temperature/K	106.1
Crystal system	monoclinic

Space group	$P2_1/n$
a/Å, b/Å, c/Å	18.8611(10), 19.4952(12), 19.5123(11)
α/°, β/°, γ/°	90.00, 105.765(5), 90.00
Volume/Å^3	6904.8(7)
Z	8
ρ_{calc}/mg mm^{-3}	1.221
μ/mm^{-1}	0.430
F(000)	2696
Crystal size / mm^3	0.45 × 0.40 × 0.34
2Θ range for data collection	6.48 to 52°
Index ranges	$-23 \le h \le 23$, $-24 \le k \le 23$, $-24 \le l \le 24$
Reflections collected	50094
Independent reflections	13543[R(int) = 0.0351 (inf-0.9Å)]
Data/restraints/parameters	13543/0/765
Goodness-of-fit on F^2	1.021
Final R indexes [I>2σ (I) i.e. F_o>4σ (F_o)]	R_1 = 0.0369, wR_2 = 0.0832
Final R indexes [all data]	R_1 = 0.0486, wR_2 = 0.0891
Largest diff. peak/hole / e Å^{-3}	0.451/-0.366
Flack Parameters	N
Completeness	0.998

Table S16 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for **T5**. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{ij} tensor.

Atom	*x*	*y*	*z*	U(eq)
Ti1	-2170.65(16)	10105.51(16)	8000.99(16)	15.48(8)
Ti2	2444.68(16)	13813.40(16)	8048.61(16)	14.51(8)
Cl2	-1136.9(2)	9417.9(2)	8276.6(3)	25.98(11)
Cl4	3438.3(3)	14542.4(2)	8384.2(3)	27.25(11)
Cl3	1558.7(3)	14471.3(3)	8359.4(2)	26.78(11)
Cl1	-3058.1(3)	9357.6(3)	8149.6(3)	29.82(12)
N4	2172.0(7)	13816.8(7)	7096.1(7)	14.6(3)
N1	-2372.9(7)	10202.5(7)	7057.9(7)	15.4(3)
N5	1630.1(7)	14287.7(7)	5963.5(7)	14.0(3)
N6	2141.3(7)	13267.3(7)	5987.5(7)	13.2(3)
N3	-2449.9(7)	9797.5(7)	5899.7(7)	14.3(3)
C38	1994.4(8)	13783.3(8)	6397.9(9)	12.6(3)
C53	1245.4(9)	14843.1(9)	6188.2(9)	14.5(3)
C62	2356.3(10)	15605.5(9)	6209.3(10)	21.4(4)
C21	-1919.0(9)	9252.5(9)	6089.1(9)	15.0(4)
C6	-2588.5(8)	10263.5(8)	6363.7(9)	12.7(3)
N2	-2990.1(7)	10784.6(7)	5986.1(7)	14.0(3)
C14	-3923.5(9)	11311(1)	6478.6(10)	20.5(4)

C61	12.9(10)	13758.9(10)	6853.5(10)	25.3(4)
C7	-2710.5(10)	10038.2(9)	5160.2(9)	18.8(4)
C54	1580.2(10)	15489.8(9)	6279.9(9)	18.1(4)
C42	2222.1(9)	12038.1(9)	6205.2(9)	17.0(4)
C26	-1166.1(9)	9412.3(9)	6231.3(9)	17.2(4)
C30	-888.4(9)	10143.9(9)	6219.6(9)	19.2(4)
C8	-3217(1)	10631.0(9)	5222.9(9)	18.8(4)
C24	-914(1)	8196.3(10)	6368(1)	25.1(4)
C41	2584.5(9)	12672.3(9)	6237.0(9)	14.2(3)
C45	3749.9(10)	12135.6(11)	6711.7(10)	26.5(4)
C39	1974.4(9)	13476.6(9)	5237.7(9)	16.4(4)
C59	183.7(9)	14015.5(9)	6172.2(10)	18.6(4)
C35	2085.2(11)	12702.7(9)	8263.9(10)	24.6(4)
C50	3752.3(10)	13411.3(10)	6446.8(10)	24.0(4)
C37	3300.0(11)	12959(1)	8632.2(11)	29.4(5)
C46	3353.4(9)	12735.1(10)	6470.1(9)	18.7(4)
C15	-2153.3(10)	12038.7(9)	6128.2(10)	21.7(4)
C23	-1659.7(10)	8053.7(10)	6234.5(10)	22.9(4)
C9	-3262.5(9)	11366.8(9)	6287.3(9)	15.5(4)
C10	-2859.8(10)	11982.0(9)	6360.4(9)	17.6(4)
C55	1177.4(10)	16032.6(10)	6453.3(10)	23.0(4)
C56	476.4(11)	15930.7(10)	6525.4(10)	24.1(4)
C22	-2180.2(10)	8579.3(9)	6086.6(9)	18.3(4)
C44	3406.6(11)	11509(1)	6703.7(10)	26.8(4)
C5	-2396.5(11)	11268.7(10)	8191.9(10)	27.3(4)
C27	-2997.9(10)	8422.1(9)	5946.2(10)	20.8(4)
C40	1459.2(9)	14089.5(9)	5211.5(9)	16.5(4)
C12	-3761.9(11)	12495.4(10)	6873.6(10)	27.7(4)
C18	-4396.7(10)	10667.0(11)	6330.9(11)	26.7(4)
C1	-2736.4(11)	10894.8(11)	8620.6(11)	28.5(5)
C4	-1631.1(11)	11161.8(10)	8445.8(11)	28.1(4)
C57	161.1(10)	15282.2(10)	6439.7(10)	20.9(4)
C13	-4153.1(10)	11888.5(11)	6785.5(11)	28.0(5)
C47	1388.6(10)	11985.1(9)	5916.1(10)	19.4(4)
C34	2222.4(11)	13028.4(10)	8929.2(10)	25.2(4)
C31	-305.6(10)	10328.1(10)	6909.3(10)	26.3(4)
C51	4144.7(11)	13408.0(11)	5851.0(11)	30.5(5)
C36	2758.1(11)	12650.5(9)	8083.3(10)	26.5(4)
C25	-670.4(10)	8865.2(10)	6365.6(10)	21.8(4)
C33	2969.5(11)	13194.2(10)	9155.9(10)	26.9(4)
C43	2650.6(11)	11455.8(10)	6441.5(10)	22.4(4)
C19	-4624.2(11)	10422.0(12)	6986.3(12)	37.1(5)
C63	2878.1(11)	15806.2(11)	6928.2(11)	28.7(5)
C11	-3126(1)	12546.1(10)	6654.6(10)	23.4(4)

C64	2371.9(10)	16136.6(10)	5637.1(10)	26.6(4)
C48	1003.9(10)	12099.9(11)	6503.4(11)	28.4(5)
C3	-1504.2(11)	10737.1(11)	9052.6(10)	29.7(5)
C16	-1475.0(11)	11963.2(12)	6766.5(11)	34.5(5)
C58	539.6(9)	14722.2(9)	6270.6(9)	15.8(4)
C70	639.2(11)	11732.8(14)	9838.6(12)	39.8(6)
C60	-513.1(11)	14016.3(11)	5545.4(11)	30.5(5)
C67	226.7(12)	12340.5(15)	8517.0(13)	45.8(6)
C32	-583.3(11)	10261.3(11)	5576.2(10)	28.8(5)
C28	-3258.3(11)	7884.6(12)	5365.6(12)	37.8(5)
C49	1143.0(12)	11307.2(11)	5532.1(11)	31.5(5)
C2	-2180.9(11)	10565.0(11)	9158.5(10)	29.3(5)
C17	-2118.8(12)	12702.5(10)	5725.2(11)	31.9(5)
C20	-5085.4(11)	10793.6(12)	5704.0(12)	35.9(5)
C65	520.9(11)	11321.1(12)	9240.1(13)	36.1(5)
C69	553.5(12)	12433.0(14)	9779.2(13)	44.2(6)
C29	-3177.1(12)	8193.6(14)	6627.3(12)	41.4(6)
C68	347.8(12)	12742.3(13)	9125.2(15)	45.8(6)
C52	4312.1(11)	13571.7(13)	7154.4(11)	39.1(6)
C66	316.5(11)	11634.7(14)	8577.6(12)	41.0(6)
C71	618.7(15)	10549.9(14)	9301.1(19)	63.8(8)

Table S17 Anisotropic Displacement Parameters ($Å^2×10^3$) for **T5**.

The Anisotropic displacement factor exponent takes the form: $-2π^2[h^2a^{*2}U_{11}+...+2hka×b×U_{12}]$

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Ti1	18.60(16)	17.34(17)	11.01(15)	1.24(13)	4.93(12)	2.87(12)
Ti2	18.54(16)	13.99(16)	10.05(15)	-0.56(12)	2.25(12)	2.21(12)
Cl2	25.3(2)	28.0(3)	23.8(2)	2.6(2)	5.21(19)	10.39(19)
Cl4	27.5(2)	25.4(3)	23.6(2)	0.6(2)	-2.00(19)	-6.71(19)
Cl3	29.5(2)	31.4(3)	19.0(2)	-3.1(2)	6.06(19)	13.1(2)
Cl1	29.1(3)	29.1(3)	34.3(3)	5.7(2)	13.8(2)	-4.0(2)
N4	16.3(7)	13.6(7)	12.8(7)	-0.3(6)	2.4(6)	1.7(6)
N1	17.4(7)	15.8(7)	13.9(7)	-1.2(6)	5.6(6)	2.2(6)
N5	17.0(7)	13.3(7)	11.4(7)	0.2(6)	3.5(6)	2.1(6)
N6	15.1(7)	13.3(7)	10.8(7)	-0.3(6)	2.8(5)	1.5(6)
N3	17.8(7)	14.9(7)	9.6(7)	0.5(6)	2.4(6)	2.8(6)
C38	9.9(8)	13.4(8)	15.2(8)	-0.5(7)	4.5(6)	-2.5(6)
C53	17.3(8)	14.6(9)	10.8(8)	2.0(7)	2.4(7)	3.5(7)
C62	21.9(9)	16.4(9)	24.8(10)	0.2(8)	4.2(8)	-1.7(7)
C21	19.6(9)	16.3(9)	9.2(8)	-1.6(7)	4.2(7)	3.8(7)
C6	11.1(8)	13.3(8)	14.4(8)	-1.2(7)	5.0(6)	-2.9(6)
N2	17.1(7)	14.0(7)	11.0(7)	0.0(6)	4.1(6)	0.7(6)
C14	17.8(9)	23.7(10)	19.1(9)	4.1(8)	3.6(7)	5.0(7)
C61	25.1(10)	26.0(11)	26(1)	2.6(9)	9.0(8)	-4.1(8)

C7	23.8(9)	21.1(9)	10.5(8)	-0.2(7)	2.8(7)	1.3(7)
C54	22.3(9)	17.8(9)	13.0(9)	1.7(7)	2.9(7)	0.6(7)
C42	22.7(9)	17.6(9)	11.0(8)	-0.5(7)	5.3(7)	2.8(7)
C26	20.6(9)	20.1(9)	11.1(8)	-3.3(7)	4.4(7)	0.9(7)
C30	17.1(9)	22.2(10)	19.3(9)	-2.6(8)	6.4(7)	0.0(7)
C8	23.2(9)	20.2(9)	11.5(8)	0.4(7)	1.9(7)	2.5(7)
C24	27.9(10)	22.9(10)	22.6(10)	-0.3(8)	3.8(8)	10.7(8)
C41	18.6(8)	15.7(9)	8.9(8)	-0.4(7)	4.5(7)	3.3(7)
C45	18.1(9)	39.7(12)	20.8(10)	0.3(9)	3.7(8)	9.9(8)
C39	20.8(9)	17.8(9)	10.5(8)	-0.2(7)	3.9(7)	-0.1(7)
C59	16.5(9)	19.5(9)	20.4(9)	-0.8(8)	5.8(7)	-0.1(7)
C35	37.5(11)	15.5(9)	20.3(10)	2.5(8)	6.9(8)	-1.1(8)
C50	16.4(9)	29.7(11)	25(1)	-6.9(9)	4.1(8)	-3.1(8)
C37	29.9(11)	26.9(11)	31.5(11)	13.0(9)	8.2(9)	11.9(9)
C46	17.8(9)	25.3(10)	13.7(9)	-3.8(8)	5.3(7)	1.6(7)
C15	30.1(10)	17.1(9)	20.7(10)	-4.8(8)	11.5(8)	-5.4(8)
C23	30.7(10)	15.4(9)	22.3(10)	-0.6(8)	6.6(8)	1.1(8)
C9	18.5(8)	16.2(9)	11.0(8)	2.4(7)	2.8(7)	6.3(7)
C10	24.7(9)	16.0(9)	11.6(8)	1.9(7)	4.2(7)	2.0(7)
C55	32.9(11)	14.5(9)	20.4(10)	-1.0(8)	5.0(8)	-1.0(8)
C56	32.2(11)	19.7(10)	20.7(10)	-1.5(8)	7.5(8)	9.7(8)
C22	23.3(9)	19.0(9)	12.6(8)	-0.7(7)	5.0(7)	0.8(7)
C44	33.8(11)	25.0(11)	22.5(10)	4.5(9)	9.2(8)	16.2(9)
C5	39.0(11)	20.1(10)	19.5(10)	-3.9(8)	2.6(9)	8.1(9)
C27	22.6(9)	16.5(9)	23.1(10)	-0.3(8)	5.7(8)	-0.6(7)
C40	19.0(9)	20.3(9)	9.6(8)	0.9(7)	2.9(7)	2.5(7)
C12	33.6(11)	25.9(11)	23.5(10)	-1.4(9)	7.4(9)	15.2(9)
C18	18.6(9)	32.0(11)	31.7(11)	2.1(9)	10.4(8)	0.7(8)
C1	30.8(11)	31.5(11)	25.1(10)	-8.6(9)	10.9(9)	9.6(9)
C4	35.1(11)	24.8(11)	23.7(10)	-9.2(9)	6.9(9)	-6.0(9)
C57	18.6(9)	26.3(10)	18.7(9)	0.5(8)	6.5(7)	5.4(8)
C13	21.5(10)	37.3(12)	27.7(11)	2.0(9)	11.2(8)	10.9(9)
C47	22.1(9)	18.1(9)	17.3(9)	0.3(8)	3.9(7)	-4.2(7)
C34	41.1(12)	17.7(10)	21.2(10)	2.0(8)	15.7(9)	1.7(8)
C31	26(1)	28.1(11)	24(1)	-6.1(9)	5.3(8)	-5.5(8)
C51	29.8(11)	36.2(12)	25.0(11)	-3.9(9)	6.9(9)	-9.2(9)
C36	47.5(12)	15.2(9)	19.3(10)	4.1(8)	13.4(9)	12.4(9)
C25	18.8(9)	26.6(10)	19.3(9)	-3.2(8)	3.9(7)	3.6(8)
C33	42.7(12)	20.9(10)	13.5(9)	4.6(8)	1.3(8)	1.3(9)
C43	35.4(11)	15.7(9)	17.3(9)	0.6(8)	9.3(8)	4.3(8)
C19	26.7(11)	47.8(14)	38.3(13)	12.8(11)	11.4(10)	-3.9(10)
C63	26(1)	28.1(11)	27.7(11)	9.2(9)	-0.1(8)	-3.3(8)
C11	33.4(11)	16.2(9)	18.9(9)	1.3(8)	4.4(8)	3.1(8)
C64	25(1)	30.5(11)	23.4(10)	3.9(9)	4.8(8)	-5.6(8)

C48	24.4(10)	34.3(12)	27.3(11)	-4.0(9)	8.3(8)	-0.4(9)
C3	32.7(11)	32.8(12)	19(1)	-8.8(9)	-1.0(8)	7.4(9)
C16	25.6(11)	46.9(14)	33.9(12)	2.9(11)	12.9(9)	-3.5(10)
C58	17.8(8)	17.8(9)	10.3(8)	1.3(7)	1.1(7)	2.0(7)
C70	28.9(11)	60.5(17)	29.1(12)	2.3(11)	6.7(9)	-4.7(11)
C60	26.4(10)	31.7(12)	28.8(11)	-0.6(9)	-0.5(9)	-6.6(9)
C67	27.6(12)	71.0(19)	36.7(14)	16.6(13)	5.2(10)	3.4(12)
C32	31.9(11)	33.4(12)	23.7(10)	0.6(9)	12.2(9)	-5.5(9)
C28	27.8(11)	50.5(15)	33.5(12)	-16.4(11)	5.4(9)	-4.5(10)
C49	36.1(11)	29.6(11)	30.0(11)	-8.5(9)	10.8(9)	-11.2(9)
C2	43.1(12)	32.5(12)	14.8(9)	-1.6(9)	11.8(9)	8.8(9)
C17	50.5(13)	22.7(11)	28.0(11)	-1.5(9)	19.8(10)	-9.8(9)
C20	26.4(11)	46.5(14)	33.9(12)	-0.9(11)	6.7(9)	-6.1(10)
C65	19.9(10)	42.7(13)	45.3(14)	-1.5(11)	8.2(9)	-6.8(9)
C69	33.2(12)	58.2(17)	39.3(14)	-16.1(13)	6.5(10)	-3.4(11)
C29	36.7(12)	59.7(16)	30.3(12)	-8.0(11)	13.4(10)	-15.5(11)
C68	29.5(12)	41.7(14)	63.7(18)	-2.8(13)	8.6(12)	-1.4(10)
C52	29.3(11)	61.8(16)	26.6(11)	-15.9(11)	8.4(9)	-17.3(11)
C66	27.3(11)	60.7(17)	32.9(13)	-14.1(12)	4.7(9)	-3.0(11)
C71	45.6(15)	44.6(16)	98(3)	2.6(16)	14.6(16)	-6.9(12)

Table S18 Bond Lengths for T5.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Ti1	Cl2	2.3061(5)	C30	C32	1.534(2)
Ti1	Cl1	2.2969(6)	C24	C23	1.387(3)
Ti1	N1	1.7849(14)	C24	C25	1.383(3)
Ti1	C5	2.3556(19)	C41	C46	1.402(2)
Ti1	C1	2.3810(18)	C45	C46	1.398(3)
Ti1	C4	2.356(2)	C45	C44	1.381(3)
Ti1	C3	2.430(2)	C39	C40	1.532(2)
Ti1	C2	2.4346(19)	C59	C58	1.522(2)
Ti2	Cl4	2.3008(6)	C59	C60	1.533(3)
Ti2	Cl3	2.3141(5)	C35	C34	1.405(3)
Ti2	N4	1.7888(14)	C35	C36	1.410(3)
Ti2	C35	2.3409(19)	C50	C46	1.525(3)
Ti2	C37	2.3823(19)	C50	C51	1.538(3)
Ti2	C34	2.4210(19)	C50	C52	1.525(3)
Ti2	C36	2.3391(18)	C37	C36	1.400(3)
Ti2	C33	2.4379(18)	C37	C33	1.410(3)
N4	C38	1.313(2)	C15	C10	1.523(2)
N1	C6	1.310(2)	C15	C16	1.531(3)
N5	C38	1.357(2)	C15	C17	1.525(3)
N5	C53	1.437(2)	C23	C22	1.394(3)
N5	C40	1.466(2)	C9	C10	1.406(2)

N6	C38	1.360(2)	C10	C11	1.396(3)
N6	C41	1.435(2)	C55	C56	1.381(3)
N6	C39	1.468(2)	C56	C57	1.388(3)
N3	C21	1.438(2)	C22	C27	1.523(2)
N3	C6	1.357(2)	C44	C43	1.382(3)
N3	C7	1.469(2)	C5	C1	1.391(3)
C53	C54	1.400(2)	C5	C4	1.409(3)
C53	C58	1.404(2)	C27	C28	1.523(3)
C62	C54	1.524(2)	C27	C29	1.524(3)
C62	C63	1.529(3)	C12	C13	1.380(3)
C62	C64	1.529(3)	C12	C11	1.382(3)
C21	C26	1.406(2)	C18	C19	1.532(3)
C21	C22	1.401(2)	C18	C20	1.543(3)
C6	N2	1.359(2)	C1	C2	1.420(3)
N2	C8	1.464(2)	C4	C3	1.411(3)
N2	C9	1.436(2)	C57	C58	1.392(2)
C14	C9	1.399(2)	C47	C48	1.530(3)
C14	C18	1.522(3)	C47	C49	1.528(3)
C14	C13	1.398(3)	C34	C33	1.395(3)
C61	C59	1.534(3)	C3	C2	1.388(3)
C7	C8	1.525(2)	C70	C65	1.384(3)
C54	C55	1.397(3)	C70	C69	1.376(4)
C42	C41	1.406(2)	C67	C68	1.388(4)
C42	C47	1.523(2)	C67	C66	1.387(4)
C42	C43	1.397(2)	C65	C66	1.387(3)
C26	C30	1.522(2)	C65	C71	1.516(3)
C26	C25	1.395(2)	C69	C68	1.369(4)
C30	C31	1.531(3)			

Table S19 Bond Angles for **T5**.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
Cl2	Ti1	C5	134.47(5)	C21	C26	C30	122.56(15)
Cl2	Ti1	C1	136.42(5)	C25	C26	C21	117.18(16)
Cl2	Ti1	C4	99.73(5)	C25	C26	C30	120.23(16)
Cl2	Ti1	C3	83.51(5)	C26	C30	C31	111.99(15)
Cl2	Ti1	C2	102.52(5)	C26	C30	C32	111.06(15)
Cl1	Ti1	Cl2	101.57(2)	C31	C30	C32	110.18(15)
Cl1	Ti1	C5	114.95(5)	N2	C8	C7	102.71(13)
Cl1	Ti1	C1	84.47(6)	C25	C24	C23	120.60(17)
Cl1	Ti1	C4	139.91(5)	C42	C41	N6	117.67(14)
Cl1	Ti1	C3	116.27(5)	C46	C41	N6	119.67(15)
Cl1	Ti1	C2	85.80(5)	C46	C41	C42	122.59(16)
N1	Ti1	Cl2	103.44(5)	C44	C45	C46	121.96(17)
N1	Ti1	Cl1	103.79(5)	N6	C39	C40	102.25(13)

N1	Ti1	C5	93.66(7)	C58	C59	C61	112.03(15)
N1	Ti1	C1	117.08(7)	C58	C59	C60	110.67(15)
N1	Ti1	C4	103.72(7)	C60	C59	C61	110.82(15)
N1	Ti1	C3	137.18(7)	C34	C35	Ti2	76.00(11)
N1	Ti1	C2	149.77(7)	C34	C35	C36	108.13(18)
C5	Ti1	C1	34.14(7)	C36	C35	Ti2	72.40(11)
C5	Ti1	C4	34.79(7)	C46	C50	C51	111.19(15)
C5	Ti1	C3	56.84(7)	C46	C50	C52	112.09(17)
C5	Ti1	C2	56.75(7)	C52	C50	C51	109.15(15)
C1	Ti1	C3	56.23(7)	C36	C37	Ti2	71.08(11)
C1	Ti1	C2	34.26(7)	C36	C37	C33	108.64(18)
C4	Ti1	C1	57.07(7)	C33	C37	Ti2	75.16(11)
C4	Ti1	C3	34.25(7)	C41	C46	C50	122.76(16)
C4	Ti1	C2	56.50(7)	C45	C46	C41	116.59(17)
C3	Ti1	C2	33.16(7)	C45	C46	C50	120.63(16)
Cl4	Ti2	Cl3	99.99(2)	C10	C15	C16	110.87(15)
Cl4	Ti2	C35	140.67(5)	C10	C15	C17	112.23(16)
Cl4	Ti2	C37	84.40(6)	C17	C15	C16	110.96(17)
Cl4	Ti2	C34	118.24(5)	C24	C23	C22	120.85(17)
Cl4	Ti2	C36	114.24(6)	C14	C9	N2	119.45(16)
Cl4	Ti2	C33	87.16(5)	C14	C9	C10	122.35(16)
Cl3	Ti2	C35	101.58(5)	C10	C9	N2	118.18(15)
Cl3	Ti2	C37	134.88(5)	C9	C10	C15	121.59(15)
Cl3	Ti2	C34	83.56(5)	C11	C10	C15	120.43(16)
Cl3	Ti2	C36	136.41(5)	C11	C10	C9	117.98(16)
Cl3	Ti2	C33	100.98(5)	C56	C55	C54	120.95(17)
N4	Ti2	Cl4	105.99(5)	C55	C56	C57	120.63(17)
N4	Ti2	Cl3	104.24(5)	C21	C22	C27	121.81(16)
N4	Ti2	C35	100.04(7)	C23	C22	C21	117.42(16)
N4	Ti2	C37	117.74(7)	C23	C22	C27	120.76(16)
N4	Ti2	C34	133.11(7)	C45	C44	C43	120.28(18)
N4	Ti2	C36	91.88(7)	C1	C5	Ti1	73.93(11)
N4	Ti2	C33	148.83(7)	C1	C5	C4	107.87(18)
C35	Ti2	C37	57.25(7)	C4	C5	Ti1	72.61(11)
C35	Ti2	C34	34.26(6)	C22	C27	C28	112.24(16)
C35	Ti2	C33	56.67(7)	C22	C27	C29	110.83(16)
C37	Ti2	C34	56.23(7)	C28	C27	C29	110.14(17)
C37	Ti2	C33	34.00(7)	N5	C40	C39	101.95(13)
C34	Ti2	C33	33.38(7)	C13	C12	C11	120.17(18)
C36	Ti2	C35	35.07(7)	C14	C18	C19	112.46(17)
C36	Ti2	C37	34.47(7)	C14	C18	C20	110.01(17)
C36	Ti2	C34	57.18(7)	C19	C18	C20	110.19(16)
C36	Ti2	C33	57.04(7)	C5	C1	Ti1	71.93(11)
C38	N4	Ti2	176.43(13)	C5	C1	C2	108.29(18)

C6	N1	Ti1	174.44(12)	C2	C1	Ti1	74.94(11)
C38	N5	C53	124.58(14)	C5	C4	Ti1	72.59(11)
C38	N5	C40	111.75(13)	C5	C4	C3	107.81(18)
C53	N5	C40	120.81(13)	C3	C4	Ti1	75.75(12)
C38	N6	C41	126.23(14)	C56	C57	C58	120.83(17)
C38	N6	C39	110.99(13)	C12	C13	C14	121.75(18)
C41	N6	C39	120.66(13)	C42	C47	C48	111.38(15)
C21	N3	C7	120.81(13)	C42	C47	C49	112.67(16)
C6	N3	C21	124.77(14)	C49	C47	C48	110.59(15)
C6	N3	C7	111.58(14)	C35	C34	Ti2	69.74(11)
N4	C38	N5	123.72(15)	C33	C34	Ti2	73.97(11)
N4	C38	N6	127.74(15)	C33	C34	C35	108.32(17)
N5	C38	N6	108.53(14)	C35	C36	Ti2	72.53(10)
C54	C53	N5	118.05(15)	C37	C36	Ti2	74.45(11)
C54	C53	C58	123.08(16)	C37	C36	C35	107.31(17)
C58	C53	N5	118.80(15)	C24	C25	C26	121.01(17)
C54	C62	C63	110.46(16)	C37	C33	Ti2	70.84(11)
C54	C62	C64	112.07(15)	C34	C33	Ti2	72.65(11)
C64	C62	C63	111.18(15)	C34	C33	C37	107.58(18)
C26	C21	N3	118.85(15)	C44	C43	C42	120.49(18)
C22	C21	N3	118.13(15)	C12	C11	C10	120.67(18)
C22	C21	C26	122.93(16)	C4	C3	Ti1	69.99(11)
N1	C6	N3	124.56(15)	C2	C3	Ti1	73.60(11)
N1	C6	N2	126.84(15)	C2	C3	C4	108.27(18)
N3	C6	N2	108.59(14)	C53	C58	C59	122.50(15)
C6	N2	C8	111.38(14)	C57	C58	C53	117.31(16)
C6	N2	C9	125.30(14)	C57	C58	C59	120.19(15)
C9	N2	C8	122.67(14)	C69	C70	C65	121.0(2)
C9	C14	C18	122.18(16)	C66	C67	C68	119.9(2)
C13	C14	C9	116.99(17)	C1	C2	Ti1	70.80(11)
C13	C14	C18	120.77(16)	C3	C2	Ti1	73.24(11)
N3	C7	C8	102.30(13)	C3	C2	C1	107.72(18)
C53	C54	C62	122.20(16)	C70	C65	C66	118.1(2)
C55	C54	C53	117.21(16)	C70	C65	C71	121.4(2)
C55	C54	C62	120.58(16)	C66	C65	C71	120.5(2)
C41	C42	C47	121.12(15)	C68	C69	C70	120.9(2)
C43	C42	C41	117.98(16)	C69	C68	C67	119.2(2)
C43	C42	C47	120.90(16)	C65	C66	C67	120.9(2)

Table S20 Torsion Angles for **T5**.

A	B	C	D	Angle/°
Ti1	N1	C6	N3	-109.2(13)
Ti1	N1	C6	N2	69.8(14)

Ti1	C5	C1	C2	66.68(14)
Ti1	C5	C4	C3	-68.18(14)
Ti1	C1	C2	C3	64.41(14)
Ti1	C4	C3	C2	-64.11(14)
Ti1	C3	C2	C1	-62.82(14)
Ti2	N4	C38	N5	-174(2)
Ti2	N4	C38	N6	5(2)
Ti2	C35	C34	C33	-64.39(14)
Ti2	C35	C36	C37	66.89(13)
Ti2	C37	C36	C35	-65.60(13)
Ti2	C37	C33	C34	63.82(14)
Ti2	C34	C33	C37	-62.63(13)
Cl2	Ti1	N1	C6	136.1(13)
Cl2	Ti1	C5	C1	-111.17(12)
Cl2	Ti1	C5	C4	3.97(15)
Cl2	Ti1	C1	C5	105.12(12)
Cl2	Ti1	C1	C2	-10.33(16)
Cl2	Ti1	C4	C5	-177.13(11)
Cl2	Ti1	C4	C3	-62.90(12)
Cl2	Ti1	C3	C4	117.99(12)
Cl2	Ti1	C3	C2	-124.96(12)
Cl2	Ti1	C2	C1	172.73(12)
Cl2	Ti1	C2	C3	56.53(12)
Cl4	Ti2	N4	C38	99(2)
Cl4	Ti2	C35	C34	62.24(14)
Cl4	Ti2	C35	C36	-52.32(14)
Cl4	Ti2	C37	C36	-150.65(12)
Cl4	Ti2	C37	C33	93.23(12)
Cl4	Ti2	C34	C35	-140.46(11)
Cl4	Ti2	C34	C33	-23.42(13)
Cl4	Ti2	C36	C35	146.63(10)
Cl4	Ti2	C36	C37	32.34(13)
Cl4	Ti2	C33	C37	-84.19(12)
Cl4	Ti2	C33	C34	159.47(11)
Cl3	Ti2	N4	C38	-156(2)
Cl3	Ti2	C35	C34	-59.72(12)
Cl3	Ti2	C35	C36	-174.28(10)
Cl3	Ti2	C37	C36	110.83(12)
Cl3	Ti2	C37	C33	-5.29(16)
Cl3	Ti2	C34	C35	121.64(12)
Cl3	Ti2	C34	C33	-121.32(11)
Cl3	Ti2	C36	C35	8.15(15)
Cl3	Ti2	C36	C37	-106.14(12)
Cl3	Ti2	C33	C37	176.18(12)

Cl3	Ti2	C33	C34	59.85(11)
Cl1	Ti1	N1	C6	30.4(14)
Cl1	Ti1	C5	C1	28.88(13)
Cl1	Ti1	C5	C4	144.02(11)
Cl1	Ti1	C1	C5	-153.90(12)
Cl1	Ti1	C1	C2	90.65(12)
Cl1	Ti1	C4	C5	-55.82(15)
Cl1	Ti1	C4	C3	58.41(15)
Cl1	Ti1	C3	C4	-142.29(11)
Cl1	Ti1	C3	C2	-25.23(13)
Cl1	Ti1	C2	C1	-86.34(12)
Cl1	Ti1	C2	C3	157.46(12)
N4	Ti2	C35	C34	-166.65(12)
N4	Ti2	C35	C36	78.79(12)
N4	Ti2	C37	C36	-45.51(14)
N4	Ti2	C37	C33	-161.64(12)
N4	Ti2	C34	C35	18.14(16)
N4	Ti2	C34	C33	135.18(12)
N4	Ti2	C36	C35	-104.89(12)
N4	Ti2	C36	C37	140.82(12)
N4	Ti2	C33	C37	32.6(2)
N4	Ti2	C33	C34	-83.74(17)
N1	Ti1	C5	C1	135.94(12)
N1	Ti1	C5	C4	-108.93(12)
N1	Ti1	C1	C5	-51.22(14)
N1	Ti1	C1	C2	-166.67(12)
N1	Ti1	C4	C5	76.34(12)
N1	Ti1	C4	C3	-169.43(12)
N1	Ti1	C3	C4	15.20(17)
N1	Ti1	C3	C2	132.25(13)
N1	Ti1	C2	C1	24.1(2)
N1	Ti1	C2	C3	-92.13(17)
N1	C6	N2	C8	-171.80(16)
N1	C6	N2	C9	-0.9(3)
N5	C53	C54	C62	-5.2(2)
N5	C53	C54	C55	175.94(15)
N5	C53	C58	C59	3.6(2)
N5	C53	C58	C57	-175.56(15)
N6	C41	C46	C45	179.45(15)
N6	C41	C46	C50	-2.3(2)
N6	C39	C40	N5	20.18(16)
N3	C21	C26	C30	2.3(2)
N3	C21	C26	C25	-175.75(15)
N3	C21	C22	C23	176.68(15)

N3	C21	C22	C27	-4.7(2)
N3	C6	N2	C8	7.29(18)
N3	C6	N2	C9	178.17(15)
N3	C7	C8	N2	17.75(17)
C38	N5	C53	C54	103.67(19)
C38	N5	C53	C58	-79.5(2)
C38	N5	C40	C39	-16.40(18)
C38	N6	C41	C42	108.57(19)
C38	N6	C41	C46	-74.3(2)
C38	N6	C39	C40	-19.15(17)
C53	N5	C38	N4	-15.0(2)
C53	N5	C38	N6	165.92(14)
C53	N5	C40	C39	-178.10(14)
C53	C54	C55	C56	-0.4(3)
C62	C54	C55	C56	-179.34(17)
C21	N3	C6	N1	-14.4(3)
C21	N3	C6	N2	166.46(15)
C21	N3	C7	C8	-176.85(14)
C21	C26	C30	C31	126.92(18)
C21	C26	C30	C32	-109.42(19)
C21	C26	C25	C24	-0.9(3)
C21	C22	C27	C28	128.47(19)
C21	C22	C27	C29	-107.9(2)
C6	N3	C21	C26	-74.9(2)
C6	N3	C21	C22	108.43(19)
C6	N3	C7	C8	-15.09(18)
C6	N2	C8	C7	-16.18(18)
C6	N2	C9	C14	-83.5(2)
C6	N2	C9	C10	98.3(2)
N2	C9	C10	C15	0.1(2)
N2	C9	C10	C11	-179.90(15)
C14	C9	C10	C15	-178.10(16)
C14	C9	C10	C11	1.9(3)
C61	C59	C58	C53	119.20(18)
C61	C59	C58	C57	-61.7(2)
C7	N3	C21	C26	84.4(2)
C7	N3	C21	C22	-92.33(19)
C7	N3	C6	N1	-175.32(15)
C7	N3	C6	N2	5.57(19)
C54	C53	C58	C59	-179.74(16)
C54	C53	C58	C57	1.1(2)
C54	C55	C56	C57	1.2(3)
C42	C41	C46	C45	-3.5(3)
C42	C41	C46	C50	174.72(16)

C26	C21	C22	C23	0.1(3)
C26	C21	C22	C27	178.69(16)
C30	C26	C25	C24	-179.05(17)
C8	N2	C9	C14	86.4(2)
C8	N2	C9	C10	-91.8(2)
C24	C23	C22	C21	-0.9(3)
C24	C23	C22	C27	-179.50(17)
C41	N6	C38	N4	-6.1(3)
C41	N6	C38	N5	173.00(14)
C41	N6	C39	C40	176.40(14)
C41	C42	C47	C48	-88.1(2)
C41	C42	C47	C49	146.95(17)
C41	C42	C43	C44	0.6(3)
C45	C44	C43	C42	-2.3(3)
C39	N6	C38	N4	-169.45(16)
C39	N6	C38	N5	9.62(18)
C39	N6	C41	C42	-89.52(19)
C39	N6	C41	C46	87.64(19)
C35	Ti2	N4	C38	-51(2)
C35	Ti2	C37	C36	38.51(11)
C35	Ti2	C37	C33	-77.61(13)
C35	Ti2	C34	C33	117.04(17)
C35	Ti2	C36	C37	-114.29(17)
C35	Ti2	C33	C37	79.46(13)
C35	Ti2	C33	C34	-36.87(11)
C35	C34	C33	Ti2	61.67(13)
C35	C34	C33	C37	-1.0(2)
C37	Ti2	N4	C38	7(2)
C37	Ti2	C35	C34	76.72(13)
C37	Ti2	C35	C36	-37.84(11)
C37	Ti2	C34	C35	-79.96(13)
C37	Ti2	C34	C33	37.08(12)
C37	Ti2	C36	C35	114.29(17)
C37	Ti2	C33	C34	-116.33(18)
C46	C45	C44	C43	1.1(3)
C15	C10	C11	C12	-179.26(17)
C23	C24	C25	C26	0.2(3)
C23	C22	C27	C28	-53.0(2)
C23	C22	C27	C29	70.6(2)
C9	N2	C8	C7	172.66(15)
C9	C14	C18	C19	131.22(19)
C9	C14	C18	C20	-105.5(2)
C9	C14	C13	C12	2.3(3)
C9	C10	C11	C12	0.7(3)

C55	C56	C57	C58	-0.8(3)
C56	C57	C58	C53	-0.3(3)
C56	C57	C58	C59	-179.47(16)
C22	C21	C26	C30	178.86(16)
C22	C21	C26	C25	0.8(3)
C44	C45	C46	C41	1.8(3)
C44	C45	C46	C50	-176.50(17)
C5	Ti1	N1	C6	-86.5(14)
C5	Ti1	C1	C2	-115.45(18)
C5	Ti1	C4	C3	114.23(17)
C5	Ti1	C3	C4	-38.43(12)
C5	Ti1	C3	C2	78.62(13)
C5	Ti1	C2	C1	37.30(12)
C5	Ti1	C2	C3	-78.90(13)
C5	C1	C2	Ti1	-64.70(13)
C5	C1	C2	C3	-0.3(2)
C5	C4	C3	Ti1	66.06(13)
C5	C4	C3	C2	1.9(2)
C40	N5	C38	N4	-175.84(15)
C40	N5	C38	N6	5.04(18)
C40	N5	C53	C54	-97.08(19)
C40	N5	C53	C58	79.8(2)
C18	C14	C9	N2	-4.4(3)
C18	C14	C9	C10	173.77(16)
C18	C14	C13	C12	-174.89(18)
C1	Ti1	N1	C6	-60.5(14)
C1	Ti1	C5	C4	115.14(17)
C1	Ti1	C4	C5	-37.25(12)
C1	Ti1	C4	C3	76.97(13)
C1	Ti1	C3	C4	-79.63(13)
C1	Ti1	C3	C2	37.42(12)
C1	Ti1	C2	C3	-116.20(18)
C1	C5	C4	Ti1	66.07(14)
C1	C5	C4	C3	-2.1(2)
C4	Ti1	N1	C6	-120.2(14)
C4	Ti1	C5	C1	-115.14(17)
C4	Ti1	C1	C5	37.99(12)
C4	Ti1	C1	C2	-77.46(13)
C4	Ti1	C3	C2	117.05(18)
C4	Ti1	C2	C1	79.25(14)
C4	Ti1	C2	C3	-36.95(12)
C4	C5	C1	Ti1	-65.19(13)
C4	C5	C1	C2	1.5(2)
C4	C3	C2	Ti1	61.79(14)

C4	C3	C2	C1	-1.0(2)
C13	C14	C9	N2	178.47(16)
C13	C14	C9	C10	-3.4(3)
C13	C14	C18	C19	-51.7(2)
C13	C14	C18	C20	71.5(2)
C13	C12	C11	C10	-1.8(3)
C47	C42	C41	N6	0.0(2)
C47	C42	C41	C46	-177.06(16)
C47	C42	C43	C44	-179.94(16)
C34	Ti2	N4	C38	-61(2)
C34	Ti2	C35	C36	-114.56(17)
C34	Ti2	C37	C36	79.74(13)
C34	Ti2	C37	C33	-36.38(12)
C34	Ti2	C36	C35	37.54(11)
C34	Ti2	C36	C37	-76.75(13)
C34	Ti2	C33	C37	116.33(18)
C34	C35	C36	Ti2	-68.22(13)
C34	C35	C36	C37	-1.3(2)
C51	C50	C46	C41	-106.8(2)
C51	C50	C46	C45	71.4(2)
C36	Ti2	N4	C38	-17(2)
C36	Ti2	C35	C34	114.56(17)
C36	Ti2	C37	C33	-116.12(18)
C36	Ti2	C34	C35	-38.45(12)
C36	Ti2	C34	C33	78.59(13)
C36	Ti2	C33	C37	37.28(12)
C36	Ti2	C33	C34	-79.05(13)
C36	C35	C34	Ti2	65.82(13)
C36	C35	C34	C33	1.4(2)
C36	C37	C33	Ti2	-63.68(13)
C36	C37	C33	C34	0.1(2)
C25	C26	C30	C31	-55.1(2)
C25	C26	C30	C32	68.6(2)
C25	C24	C23	C22	0.8(3)
C33	Ti2	N4	C38	-13(2)
C33	Ti2	C35	C34	35.90(11)
C33	Ti2	C35	C36	-78.65(12)
C33	Ti2	C37	C36	116.12(18)
C33	Ti2	C34	C35	-117.04(17)
C33	Ti2	C36	C35	77.53(12)
C33	Ti2	C36	C37	-36.76(12)
C33	C37	C36	Ti2	66.34(14)
C33	C37	C36	C35	0.7(2)
C43	C42	C41	N6	179.46(15)

C43	C42	C41	C46	2.4(3)
C43	C42	C47	C48	92.4(2)
C43	C42	C47	C49	-32.5(2)
C63	C62	C54	C53	-113.56(19)
C63	C62	C54	C55	65.3(2)
C11	C12	C13	C14	0.2(3)
C64	C62	C54	C53	121.86(19)
C64	C62	C54	C55	-59.3(2)
C3	Ti1	N1	C6	-128.9(13)
C3	Ti1	C5	C1	-77.32(13)
C3	Ti1	C5	C4	37.81(12)
C3	Ti1	C1	C5	79.26(13)
C3	Ti1	C1	C2	-36.19(12)
C3	Ti1	C4	C5	-114.23(17)
C3	Ti1	C2	C1	116.20(18)
C16	C15	C10	C9	-98.9(2)
C16	C15	C10	C11	81.1(2)
C58	C53	C54	C62	178.14(16)
C58	C53	C54	C55	-0.8(3)
C70	C65	C66	C67	-0.6(3)
C70	C69	C68	C67	-0.1(3)
C60	C59	C58	C53	-116.57(18)
C60	C59	C58	C57	62.5(2)
C2	Ti1	N1	C6	-75.4(14)
C2	Ti1	C5	C1	-37.44(12)
C2	Ti1	C5	C4	77.70(13)
C2	Ti1	C1	C5	115.45(18)
C2	Ti1	C4	C5	-78.48(13)
C2	Ti1	C4	C3	35.75(11)
C2	Ti1	C3	C4	-117.05(18)
C17	C15	C10	C9	136.41(17)
C17	C15	C10	C11	-43.6(2)
C65	C70	C69	C68	0.1(3)
C69	C70	C65	C66	0.3(3)
C69	C70	C65	C71	179.6(2)
C68	C67	C66	C65	0.5(3)
C52	C50	C46	C41	130.73(18)
C52	C50	C46	C45	-51.1(2)
C66	C67	C68	C69	-0.2(3)
C71	C65	C66	C67	-179.9(2

Table S21 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for **T5**.

Atom	*x*	*y*	*z*	U(eq)
H62	2531	15169	6065	26
H61A	-198	13308	6774	38

H61B	-330	14065	6979	38
H61C	460	13743	7234	38
H7A	-2978	9681	4849	23
H7B	-2304	10194	4984	23
H30	-1308	10453	6173	23
H8A	-3142	11023	4944	23
H8B	-3731	10495	5069	23
H24	-575	7839	6460	30
H45	4260	12160	6883	32
H39A	1731	13112	4923	20
H39B	2417	13611	5111	20
H59	535	13695	6057	22
H35	1630	12548	7990	30
H50	3384	13779	6346	29
H37	3795	13002	8649	35
H15	-2148	11657	5803	26
H23	-1814	7602	6244	27
H55	1384	16469	6521	28
H56	213	16300	6632	29
H44	3685	11121	6875	32
H5	-2633	11541	7806	33
H27	-3271	8846	5784	25
H40A	1568	14458	4922	20
H40B	947	13957	5029	20
H12	-3927	12871	7081	33
H18	-4107	10302	6191	32
H1	-3241	10866	8565	34
H4	-1273	11340	8249	34
H57	-309	15221	6496	25
H13	-4581	11863	6934	34
H47	1230	12353	5566	23
H34	1875	13118	9176	30
H31A	-501	10250	7308	40
H31B	-173	10802	6897	40
H31C	123	10047	6955	40
H51A	3789	13339	5400	46
H51B	4500	13044	5934	46
H51C	4389	13839	5847	46
H36	2829	12449	7675	32
H25	-169	8952	6455	26
H33	3207	13419	9576	32
H43	2425	11029	6422	27
H19A	-4192	10339	7371	56
H19B	-4904	10006	6874	56

H19C	-4920	10768	7126	56
H63A	2887	15448	7268	43
H63B	2710	16224	7092	43
H63C	3365	15873	6876	43
H11	-2873	12960	6704	28
H64A	2871	16209	5623	40
H64B	2169	16561	5747	40
H64C	2085	15973	5182	40
H48A	1145	11745	6855	43
H48B	480	12089	6301	43
H48C	1145	12538	6723	43
H3	-1046	10596	9333	36
H16A	-1488	11525	6987	52
H16B	-1475	12321	7105	52
H16C	-1037	11996	6608	52
H70	779	11533	10288	48
H60A	-697	13556	5456	46
H60B	-398	14193	5129	46
H60C	-881	14300	5659	46
H67	85	12544	8069	55
H32A	-159	9976	5618	43
H32B	-446	10734	5561	43
H32C	-954	10147	5147	43
H28A	-3142	8033	4940	57
H28B	-3781	7826	5270	57
H28C	-3016	7457	5521	57
H49A	1416	11227	5190	47
H49B	627	11329	5293	47
H49C	1232	10940	5872	47
H2	-2257	10284	9517	35
H17A	-1708	12685	5523	48
H17B	-2060	13084	6047	48
H17C	-2567	12757	5351	48
H20A	-5381	11147	5831	54
H20B	-5367	10378	5598	54
H20C	-4936	10935	5293	54
H69	636	12700	10189	53
H29A	-2912	7780	6800	62
H29B	-3697	8110	6530	62
H29C	-3036	8547	6981	62
H68	290	13216	9089	55
H52A	4523	14016	7129	59
H52B	4695	13232	7250	59
H52C	4071	13568	7529	59

H66	238	11368	8168	49
H71A	1055	10421	9170	96
H71B	199	10329	8989	96
H71C	664	10411	9783	96