Electronic Supplementary Information for Dalton Transactions

Supporting Information For:

Effects of 5,5-Substitution on Dipyrrolylmethane Ligand Isomerization

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A. Structure of $Ti(NMe_2)_2(tmcpm)$ (**3**)

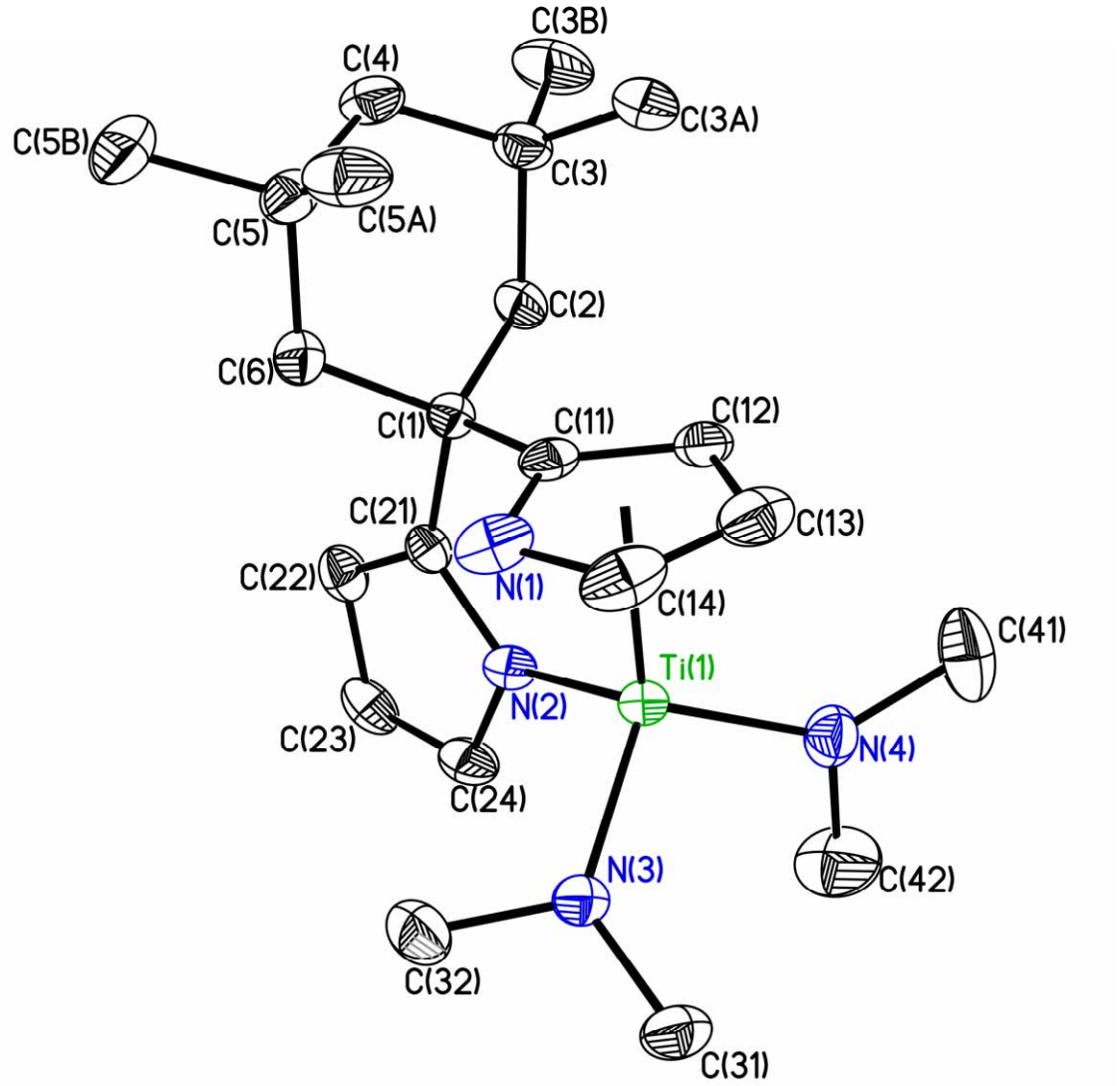


Table 1. Crystal data and structure refinement for TiNMe2tmcpm_0ma.

Identification code	tinme2tmcpm_0ma	
Empirical formula	C22 H36 N4 Ti	
Formula weight	404.45	
Temperature	173(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 21/c	
Unit cell dimensions	a = 21.3114(2) Å	α= 90°.
	b = 8.58140(10) Å	β= 98.1850(10)°.
	c = 12.23980(10) Å	γ = 90°.
Volume	2215.63(4) $Å^3$	
Z	4	
Density (calculated)	1.212 Mg/m^3	
Absorption coefficient	0.400 mm^{-1}	
F(000)	872	
Crystal size	0.53 x 0.40 x 0.24 mm^3	
Theta range for data collection	1.93 to 26.27°.	
Index ranges	-26<=h<=26, -10<=k<=10, -15<=l<=15	
Reflections collected	35590	
Independent reflections	4471 [R(int) = 0.0313]	
Completeness to theta = 25.00°	99.7 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9102 and 0.8161	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4471 / 0 / 252	
Goodness-of-fit on F^2	1.110	
Final R indices [I>2sigma(I)]	R1 = 0.0357, wR2 = 0.0960	
R indices (all data)	R1 = 0.0452, wR2 = 0.1010	
Largest diff. peak and hole	0.330 and -0.292 e.$Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for TiNMe2tmcpm_0ma. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Ti(1)	3395(1)	6919(1)	10173(1)	21(1)
N(1)	2713(1)	5383(2)	10987(1)	36(1)
N(4)	3558(1)	8943(2)	9663(1)	31(1)
N(3)	4198(1)	6259(2)	10904(1)	26(1)
N(2)	3279(1)	5501(2)	8840(1)	23(1)
C(42)	4141(1)	9096(3)	9180(2)	55(1)
C(41)	3203(1)	10401(2)	9533(2)	54(1)
C(5B)	1054(1)	1516(3)	9797(2)	53(1)
C(3B)	517(1)	5976(3)	7358(2)	46(1)
C(5A)	1233(1)	3938(3)	10910(2)	42(1)
C(13)	2602(1)	7988(2)	11137(2)	39(1)
C(3A)	821(1)	6953(2)	9242(2)	39(1)
C(32)	4323(1)	4609(2)	11067(2)	38(1)
C(14)	2847(1)	6657(3)	11674(2)	38(1)
C(31)	4710(1)	7207(2)	11460(2)	35(1)
C(4)	778(1)	4032(2)	8849(2)	32(1)
C(5)	1246(1)	3237(2)	9754(2)	32(1)
C(23)	3497(1)	3853(2)	7515(1)	31(1)
C(3)	949(1)	5645(2)	8449(1)	29(1)
C(24)	3730(1)	5019(2)	8208(1)	29(1)
C(12)	2296(1)	7532(2)	10092(1)	28(1)
C(22)	2865(1)	3577(2)	7711(1)	28(1)
C(6)	1912(1)	3282(2)	9415(1)	26(1)
C(2)	1637(1)	5620(2)	8193(1)	25(1)
C(11)	2359(1)	5932(2)	10035(1)	24(1)
C(21)	2746(1)	4594(2)	8519(1)	21(1)
C(1)	2155(1)	4874(2)	9056(1)	21(1)

Table 3. Bond lengths [Å] and angles [°] for TiNMe2tmcpm_0ma.

Ti(1)-N(4)	1.8950(15)
Ti(1)-N(3)	1.9006(13)
Ti(1)-N(2)	2.0230(13)
Ti(1)-N(1)	2.2922(16)
Ti(1)-C(14)	2.3239(18)
Ti(1)-C(11)	2.3492(15)
Ti(1)-C(13)	2.3785(19)
Ti(1)-C(12)	2.3891(16)
N(1)-C(11)	1.379(2)
N(1)-C(14)	1.384(3)
N(4)-C(42)	1.455(3)
N(4)-C(41)	1.459(2)
N(3)-C(31)	1.451(2)
N(3)-C(32)	1.449(2)
N(2)-C(24)	1.381(2)
N(2)-C(21)	1.387(2)
C(42)-H(42A)	0.9800
C(42)-H(42B)	0.9800
C(42)-H(42C)	0.9800
C(41)-H(41A)	0.9800
C(41)-H(41B)	0.9800
C(41)-H(41C)	0.9800
C(5B)-C(5)	1.536(3)
C(5B)-H(5BA)	0.9800
C(5B)-H(5BB)	0.9800
C(5B)-H(5BC)	0.9800
C(3B)-C(3)	1.537(2)
C(3B)-H(3BA)	0.9800
C(3B)-H(3BB)	0.9800
C(3B)-H(3BC)	0.9800
C(5A)-C(5)	1.541(3)
C(5A)-H(5AA)	0.9800
C(5A)-H(5AB)	0.9800

C(5A)-H(5AC)	0.9800
C(13)-C(14)	1.382(3)
C(13)-C(12)	1.406(2)
C(13)-H(13A)	1.0000
C(3A)-C(3)	1.534(3)
C(3A)-H(3AA)	0.9800
C(3A)-H(3AB)	0.9800
C(3A)-H(3AC)	0.9800
C(32)-H(32A)	0.9800
C(32)-H(32B)	0.9800
C(32)-H(32C)	0.9800
C(14)-H(14A)	1.0000
C(31)-H(31A)	0.9800
C(31)-H(31B)	0.9800
C(31)-H(31C)	0.9800
C(4)-C(3)	1.529(3)
C(4)-C(5)	1.541(2)
C(4)-H(4A)	0.9900
C(4)-H(4B)	0.9900
C(5)-C(6)	1.536(2)
C(23)-C(24)	1.359(3)
C(23)-C(22)	1.421(2)
C(23)-H(23A)	0.9500
C(3)-C(2)	1.542(2)
C(24)-H(24A)	0.9500
C(12)-C(11)	1.383(3)
C(12)-H(12A)	1.0000
C(22)-C(21)	1.370(2)
C(22)-H(22A)	0.9500
C(6)-C(1)	1.547(2)
C(6)-H(6A)	0.9900
C(6)-H(6B)	0.9900
C(2)-C(1)	1.553(2)
C(2)-H(2A)	0.9900
C(2)-H(2B)	0.9900

C(11)-C(1)	1.516(2)
C(21)-C(1)	1.520(2)

N(4)-Ti(1)-N(3)	103.49(6)
N(4)-Ti(1)-N(2)	107.01(6)
N(3)-Ti(1)-N(2)	101.47(6)
N(4)-Ti(1)-N(1)	145.90(6)
N(3)-Ti(1)-N(1)	102.01(6)
N(2)-Ti(1)-N(1)	89.55(5)
N(4)-Ti(1)-C(14)	119.07(7)
N(3)-Ti(1)-C(14)	96.88(6)
N(2)-Ti(1)-C(14)	124.19(6)
N(1)-Ti(1)-C(14)	34.89(6)
N(4)-Ti(1)-C(11)	121.44(6)
N(3)-Ti(1)-C(11)	134.47(6)
N(2)-Ti(1)-C(11)	73.67(5)
N(1)-Ti(1)-C(11)	34.53(5)
C(14)-Ti(1)-C(11)	56.54(6)
N(4)-Ti(1)-C(13)	89.25(7)
N(3)-Ti(1)-C(13)	122.50(7)
N(2)-Ti(1)-C(13)	128.18(6)
N(1)-Ti(1)-C(13)	57.79(7)
C(14)-Ti(1)-C(13)	34.15(7)
C(11)-Ti(1)-C(13)	56.47(6)
N(4)-Ti(1)-C(12)	90.53(6)
N(3)-Ti(1)-C(12)	153.75(6)
N(2)-Ti(1)-C(12)	95.29(5)
N(1)-Ti(1)-C(12)	57.74(6)
C(14)-Ti(1)-C(12)	56.88(6)
C(11)-Ti(1)-C(12)	33.92(6)
C(13)-Ti(1)-C(12)	34.31(6)
C(11)-N(1)-C(14)	106.49(16)
C(11)-N(1)-Ti(1)	75.00(9)
C(14)-N(1)-Ti(1)	73.81(10)
C(42)-N(4)-C(41)	109.76(17)

C(42)-N(4)-Ti(1)	115.08(13)
C(41)-N(4)-Ti(1)	134.83(14)
C(31)-N(3)-C(32)	111.82(14)
C(31)-N(3)-Ti(1)	128.31(12)
C(32)-N(3)-Ti(1)	119.49(11)
C(24)-N(2)-C(21)	106.35(13)
C(24)-N(2)-Ti(1)	128.09(11)
C(21)-N(2)-Ti(1)	124.57(10)
N(4)-C(42)-H(42A)	109.5
N(4)-C(42)-H(42B)	109.5
H(42A)-C(42)-H(42B)	109.5
N(4)-C(42)-H(42C)	109.5
H(42A)-C(42)-H(42C)	109.5
H(42B)-C(42)-H(42C)	109.5
N(4)-C(41)-H(41A)	109.5
N(4)-C(41)-H(41B)	109.5
H(41A)-C(41)-H(41B)	109.5
N(4)-C(41)-H(41C)	109.5
H(41A)-C(41)-H(41C)	109.5
H(41B)-C(41)-H(41C)	109.5
C(5)-C(5B)-H(5BA)	109.5
C(5)-C(5B)-H(5BB)	109.5
H(5BA)-C(5B)-H(5BB)	109.5
C(5)-C(5B)-H(5BC)	109.5
H(5BA)-C(5B)-H(5BC)	109.5
H(5BB)-C(5B)-H(5BC)	109.5
C(3)-C(3B)-H(3BA)	109.5
C(3)-C(3B)-H(3BB)	109.5
H(3BA)-C(3B)-H(3BB)	109.5
C(3)-C(3B)-H(3BC)	109.5
H(3BA)-C(3B)-H(3BC)	109.5
H(3BB)-C(3B)-H(3BC)	109.5
C(5)-C(5A)-H(5AA)	109.5
C(5)-C(5A)-H(5AB)	109.5
H(5AA)-C(5A)-H(5AB)	109.5

C(5)-C(5A)-H(5AC)	109.5
H(5AA)-C(5A)-H(5AC)	109.5
H(5AB)-C(5A)-H(5AC)	109.5
C(14)-C(13)-C(12)	107.30(17)
C(14)-C(13)-Ti(1)	70.76(11)
C(12)-C(13)-Ti(1)	73.26(10)
C(14)-C(13)-H(13A)	126.2
C(12)-C(13)-H(13A)	126.2
Ti(1)-C(13)-H(13A)	126.2
C(3)-C(3A)-H(3AA)	109.5
C(3)-C(3A)-H(3AB)	109.5
H(3AA)-C(3A)-H(3AB)	109.5
C(3)-C(3A)-H(3AC)	109.5
H(3AA)-C(3A)-H(3AC)	109.5
H(3AB)-C(3A)-H(3AC)	109.5
N(3)-C(32)-H(32A)	109.5
N(3)-C(32)-H(32B)	109.5
H(32A)-C(32)-H(32B)	109.5
N(3)-C(32)-H(32C)	109.5
H(32A)-C(32)-H(32C)	109.5
H(32B)-C(32)-H(32C)	109.5
N(1)-C(14)-C(13)	109.48(16)
N(1)-C(14)-Ti(1)	71.31(10)
C(13)-C(14)-Ti(1)	75.09(11)
N(1)-C(14)-H(14A)	125.1
C(13)-C(14)-H(14A)	125.1
Ti(1)-C(14)-H(14A)	125.1
N(3)-C(31)-H(31A)	109.5
N(3)-C(31)-H(31B)	109.5
H(31A)-C(31)-H(31B)	109.5
N(3)-C(31)-H(31C)	109.5
H(31A)-C(31)-H(31C)	109.5
H(31B)-C(31)-H(31C)	109.5
C(3)-C(4)-C(5)	118.11(13)
C(3)-C(4)-H(4A)	107.8

C(5)-C(4)-H(4A)	107.8
C(3)-C(4)-H(4B)	107.8
C(5)-C(4)-H(4B)	107.8
H(4A)-C(4)-H(4B)	107.1
C(6)-C(5)-C(5B)	107.13(16)
C(6)-C(5)-C(5A)	112.12(14)
C(5B)-C(5)-C(5A)	107.73(17)
C(6)-C(5)-C(4)	108.84(15)
C(5B)-C(5)-C(4)	107.60(15)
C(5A)-C(5)-C(4)	113.15(16)
C(24)-C(23)-C(22)	106.85(15)
C(24)-C(23)-H(23A)	126.6
C(22)-C(23)-H(23A)	126.6
C(4)-C(3)-C(3A)	112.83(15)
C(4)-C(3)-C(3B)	107.68(15)
C(3A)-C(3)-C(3B)	106.01(15)
C(4)-C(3)-C(2)	109.24(14)
C(3A)-C(3)-C(2)	113.51(14)
C(3B)-C(3)-C(2)	107.21(14)
C(23)-C(24)-N(2)	110.30(15)
C(23)-C(24)-H(24A)	124.8
N(2)-C(24)-H(24A)	124.8
C(11)-C(12)-C(13)	106.66(16)
C(11)-C(12)-Ti(1)	71.46(9)
C(13)-C(12)-Ti(1)	72.43(10)
C(11)-C(12)-H(12A)	126.5
C(13)-C(12)-H(12A)	126.5
Ti(1)-C(12)-H(12A)	126.5
C(21)-C(22)-C(23)	107.00(15)
C(21)-C(22)-H(22A)	126.5
C(23)-C(22)-H(22A)	126.5
C(5)-C(6)-C(1)	117.33(14)
C(5)-C(6)-H(6A)	108.0
C(1)-C(6)-H(6A)	108.0
C(5)-C(6)-H(6B)	108.0

C(1)-C(6)-H(6B)	108.0
H(6A)-C(6)-H(6B)	107.2
C(3)-C(2)-C(1)	118.14(13)
C(3)-C(2)-H(2A)	107.8
C(1)-C(2)-H(2A)	107.8
C(3)-C(2)-H(2B)	107.8
C(1)-C(2)-H(2B)	107.8
H(2A)-C(2)-H(2B)	107.1
N(1)-C(11)-C(12)	109.99(14)
N(1)-C(11)-C(1)	121.61(15)
C(12)-C(11)-C(1)	128.01(14)
N(1)-C(11)-Ti(1)	70.47(9)
C(12)-C(11)-Ti(1)	74.62(9)
C(1)-C(11)-Ti(1)	115.66(10)
C(22)-C(21)-N(2)	109.50(14)
C(22)-C(21)-C(1)	131.52(15)
N(2)-C(21)-C(1)	118.97(13)
C(11)-C(1)-C(21)	105.96(12)
C(11)-C(1)-C(6)	111.93(13)
C(21)-C(1)-C(6)	108.35(13)
C(11)-C(1)-C(2)	112.75(13)
C(21)-C(1)-C(2)	108.86(12)
C(6)-C(1)-C(2)	108.83(12)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for TiNMe2tmcpm_0ma. The anisotropic displacement factor exponent takes the form: $-2p^2[\ h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Ti(1)	17(1)	22(1)	24(1)	0(1)	1(1)	0(1)
N(1)	27(1)	48(1)	32(1)	1(1)	4(1)	-9(1)
N(4)	34(1)	25(1)	32(1)	2(1)	1(1)	-2(1)
N(3)	22(1)	26(1)	30(1)	2(1)	1(1)	0(1)
N(2)	18(1)	27(1)	26(1)	0(1)	4(1)	1(1)
C(42)	44(1)	65(2)	58(1)	28(1)	12(1)	-8(1)
C(41)	80(2)	26(1)	57(1)	7(1)	9(1)	11(1)
C(5B)	40(1)	41(1)	77(2)	18(1)	9(1)	-11(1)
C(3B)	28(1)	66(2)	42(1)	9(1)	-2(1)	12(1)
C(5A)	28(1)	64(1)	35(1)	12(1)	8(1)	1(1)
C(13)	27(1)	49(1)	45(1)	-24(1)	13(1)	-7(1)
C(3A)	26(1)	38(1)	54(1)	-4(1)	13(1)	4(1)
C(32)	36(1)	34(1)	41(1)	4(1)	-3(1)	7(1)
C(14)	31(1)	56(1)	26(1)	-9(1)	7(1)	-13(1)
C(31)	25(1)	40(1)	38(1)	-1(1)	-4(1)	-4(1)
C(4)	20(1)	37(1)	38(1)	-2(1)	0(1)	-5(1)
C(5)	25(1)	31(1)	40(1)	7(1)	5(1)	-4(1)
C(23)	32(1)	34(1)	28(1)	0(1)	9(1)	13(1)
C(3)	20(1)	33(1)	32(1)	3(1)	1(1)	4(1)
C(24)	21(1)	36(1)	31(1)	2(1)	9(1)	5(1)
C(12)	17(1)	30(1)	35(1)	-8(1)	4(1)	-2(1)
C(22)	32(1)	24(1)	25(1)	-3(1)	1(1)	5(1)
C(6)	26(1)	23(1)	30(1)	3(1)	2(1)	0(1)
C(2)	23(1)	26(1)	24(1)	3(1)	2(1)	4(1)
C(11)	16(1)	31(1)	25(1)	-4(1)	7(1)	-3(1)
C(21)	22(1)	20(1)	20(1)	3(1)	1(1)	3(1)
C(1)	19(1)	21(1)	22(1)	1(1)	2(1)	0(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for TiNMe2tmcpm_0ma.

	x	y	z	U(eq)
H(42A)	4406	9912	9569	83
H(42B)	4038	9375	8398	83
H(42C)	4371	8104	9246	83
H(41A)	3473	11257	9854	82
H(41B)	2829	10322	9912	82
H(41C)	3069	10604	8747	82
H(5BA)	1359	964	10337	79
H(5BB)	1050	1044	9067	79
H(5BC)	630	1440	10015	79
H(3BA)	73	5958	7484	69
H(3BB)	583	5176	6814	69
H(3BC)	618	7003	7080	69
H(5AA)	1494	3301	11463	63
H(5AB)	795	3956	11071	63
H(5AC)	1400	5003	10930	63
H(13A)	2602	9057	11462	47
H(3AA)	375	6922	9356	58
H(3AB)	914	7962	8926	58
H(3AC)	1093	6811	9951	58
H(32A)	4703	4326	10743	57
H(32B)	3960	4009	10709	57
H(32C)	4392	4377	11859	57
H(14A)	3046	6607	12463	45
H(31A)	5097	7010	11135	52
H(31B)	4783	6941	12246	52
H(31C)	4596	8311	11373	52
H(4A)	716	3330	8201	39
H(4B)	364	4119	9123	39
H(23A)	3714	3324	7000	37

H(24A)	4145	5443	8251	35
H(12A)	2040	8215	9536	33
H(22A)	2579	2828	7350	33
H(6A)	1921	2540	8799	32
H(6B)	2216	2897	10045	32
H(2A)	1765	6709	8074	30
H(2B)	1638	5060	7485	30

Table 6. Torsion angles [°] for TiNMe2tmcpm_0ma.

N(4)-Ti(1)-N(1)-C(11)	59.66(15)
N(3)-Ti(1)-N(1)-C(11)	-162.64(10)
N(2)-Ti(1)-N(1)-C(11)	-61.01(10)
C(14)-Ti(1)-N(1)-C(11)	112.57(15)
C(13)-Ti(1)-N(1)-C(11)	76.34(11)
C(12)-Ti(1)-N(1)-C(11)	35.53(9)
N(4)-Ti(1)-N(1)-C(14)	-52.90(15)
N(3)-Ti(1)-N(1)-C(14)	84.79(12)
N(2)-Ti(1)-N(1)-C(14)	-173.58(11)
C(11)-Ti(1)-N(1)-C(14)	-112.57(15)
C(13)-Ti(1)-N(1)-C(14)	-36.23(11)
C(12)-Ti(1)-N(1)-C(14)	-77.03(12)
N(3)-Ti(1)-N(4)-C(42)	43.02(15)
N(2)-Ti(1)-N(4)-C(42)	-63.67(14)
N(1)-Ti(1)-N(4)-C(42)	-179.59(12)
C(14)-Ti(1)-N(4)-C(42)	148.94(13)
C(11)-Ti(1)-N(4)-C(42)	-144.60(13)
C(13)-Ti(1)-N(4)-C(42)	166.35(14)
C(12)-Ti(1)-N(4)-C(42)	-159.37(14)
N(3)-Ti(1)-N(4)-C(41)	-144.37(18)
N(2)-Ti(1)-N(4)-C(41)	108.93(18)
N(1)-Ti(1)-N(4)-C(41)	-7.0(2)
C(14)-Ti(1)-N(4)-C(41)	-38.5(2)
C(11)-Ti(1)-N(4)-C(41)	28.0(2)
C(13)-Ti(1)-N(4)-C(41)	-21.05(19)
C(12)-Ti(1)-N(4)-C(41)	13.24(19)
N(4)-Ti(1)-N(3)-C(31)	29.30(16)
N(2)-Ti(1)-N(3)-C(31)	140.13(14)
N(1)-Ti(1)-N(3)-C(31)	-127.87(15)
C(14)-Ti(1)-N(3)-C(31)	-92.86(15)
C(11)-Ti(1)-N(3)-C(31)	-141.58(14)
C(13)-Ti(1)-N(3)-C(31)	-68.57(17)
C(12)-Ti(1)-N(3)-C(31)	-91.2(2)
N(4)-Ti(1)-N(3)-C(32)	-158.41(13)
N(2)-Ti(1)-N(3)-C(32)	-47.58(14)
N(1)-Ti(1)-N(3)-C(32)	44.42(14)
C(14)-Ti(1)-N(3)-C(32)	79.43(14)
C(11)-Ti(1)-N(3)-C(32)	30.72(17)
C(13)-Ti(1)-N(3)-C(32)	103.72(14)
C(12)-Ti(1)-N(3)-C(32)	81.05(19)
N(4)-Ti(1)-N(2)-C(24)	69.29(15)
N(3)-Ti(1)-N(2)-C(24)	-38.83(15)
N(1)-Ti(1)-N(2)-C(24)	-140.99(14)
C(14)-Ti(1)-N(2)-C(24)	-145.43(14)
C(11)-Ti(1)-N(2)-C(24)	-172.10(15)
C(13)-Ti(1)-N(2)-C(24)	172.18(13)
C(12)-Ti(1)-N(2)-C(24)	161.47(14)
N(4)-Ti(1)-N(2)-C(21)	-123.65(12)
N(3)-Ti(1)-N(2)-C(21)	128.23(12)
N(1)-Ti(1)-N(2)-C(21)	26.06(13)
C(14)-Ti(1)-N(2)-C(21)	21.63(15)
C(11)-Ti(1)-N(2)-C(21)	-5.05(12)
C(13)-Ti(1)-N(2)-C(21)	-20.76(16)
C(12)-Ti(1)-N(2)-C(21)	-31.47(13)

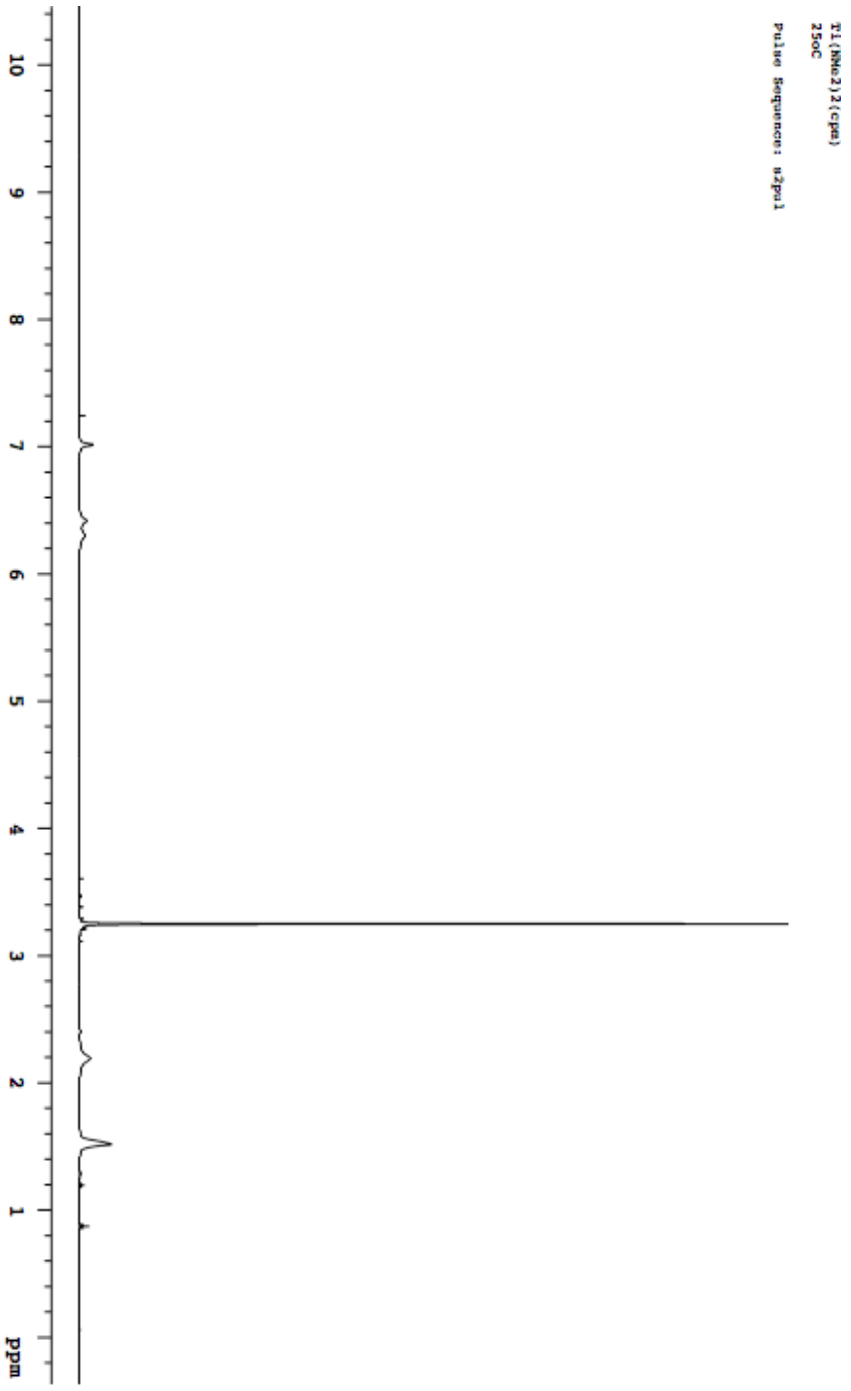
N(4)-Ti(1)-C(13)-C(14)	-152.24(11)
N(3)-Ti(1)-C(13)-C(14)	-46.68(13)
N(2)-Ti(1)-C(13)-C(14)	96.55(12)
N(1)-Ti(1)-C(13)-C(14)	37.02(10)
C(11)-Ti(1)-C(13)-C(14)	78.38(12)
C(12)-Ti(1)-C(13)-C(14)	115.71(16)
N(4)-Ti(1)-C(13)-C(12)	92.04(12)
N(3)-Ti(1)-C(13)-C(12)	-162.39(11)
N(2)-Ti(1)-C(13)-C(12)	-19.17(15)
N(1)-Ti(1)-C(13)-C(12)	-78.69(12)
C(14)-Ti(1)-C(13)-C(12)	-115.71(16)
C(11)-Ti(1)-C(13)-C(12)	-37.34(11)
C(11)-N(1)-C(14)-C(13)	-2.5(2)
Ti(1)-N(1)-C(14)-C(13)	65.93(14)
C(11)-N(1)-C(14)-Ti(1)	-68.46(11)
C(12)-C(13)-C(14)-N(1)	1.1(2)
Ti(1)-C(13)-C(14)-N(1)	-63.51(13)
C(12)-C(13)-C(14)-Ti(1)	64.65(12)
N(4)-Ti(1)-C(14)-N(1)	149.23(10)
N(3)-Ti(1)-C(14)-N(1)	-101.14(11)
N(2)-Ti(1)-C(14)-N(1)	7.77(13)
C(11)-Ti(1)-C(14)-N(1)	38.86(9)
C(13)-Ti(1)-C(14)-N(1)	117.03(15)
C(12)-Ti(1)-C(14)-N(1)	79.71(11)
N(4)-Ti(1)-C(14)-C(13)	32.20(13)
N(3)-Ti(1)-C(14)-C(13)	141.83(11)
N(2)-Ti(1)-C(14)-C(13)	-109.26(11)
N(1)-Ti(1)-C(14)-C(13)	-117.03(15)
C(11)-Ti(1)-C(14)-C(13)	-78.17(11)
C(12)-Ti(1)-C(14)-C(13)	-37.32(10)
C(3)-C(4)-C(5)-C(6)	-50.3(2)
C(3)-C(4)-C(5)-C(5B)	-166.03(17)
C(3)-C(4)-C(5)-C(5A)	75.1(2)
C(5)-C(4)-C(3)-C(3A)	-78.7(2)
C(5)-C(4)-C(3)-C(3B)	164.64(16)
C(5)-C(4)-C(3)-C(2)	48.5(2)
C(22)-C(23)-C(24)-N(2)	0.15(19)
C(21)-N(2)-C(24)-C(23)	-0.16(18)
Ti(1)-N(2)-C(24)-C(23)	168.76(11)
C(14)-C(13)-C(12)-C(11)	0.7(2)
Ti(1)-C(13)-C(12)-C(11)	63.71(11)
C(14)-C(13)-C(12)-Ti(1)	-63.00(13)
N(4)-Ti(1)-C(12)-C(11)	157.07(10)
N(3)-Ti(1)-C(12)-C(11)	-79.81(16)
N(2)-Ti(1)-C(12)-C(11)	49.93(10)
N(1)-Ti(1)-C(12)-C(11)	-36.18(9)
C(14)-Ti(1)-C(12)-C(11)	-77.90(11)
C(13)-Ti(1)-C(12)-C(11)	-115.04(16)
N(4)-Ti(1)-C(12)-C(13)	-87.89(12)
N(3)-Ti(1)-C(12)-C(13)	35.2(2)
N(2)-Ti(1)-C(12)-C(13)	164.98(12)
N(1)-Ti(1)-C(12)-C(13)	78.86(12)
C(14)-Ti(1)-C(12)-C(13)	37.15(12)
C(11)-Ti(1)-C(12)-C(13)	115.04(16)
C(24)-C(23)-C(22)-C(21)	-0.08(19)
C(5B)-C(5)-C(6)-C(1)	166.52(16)

C(5A)-C(5)-C(6)-C(1)	-75.50(19)
C(4)-C(5)-C(6)-C(1)	50.4(2)
C(4)-C(3)-C(2)-C(1)	-47.12(19)
C(3A)-C(3)-C(2)-C(1)	79.74(19)
C(3B)-C(3)-C(2)-C(1)	-163.53(16)
C(14)-N(1)-C(11)-C(12)	3.01(18)
Ti(1)-N(1)-C(11)-C(12)	-64.63(12)
C(14)-N(1)-C(11)-C(1)	176.39(14)
Ti(1)-N(1)-C(11)-C(1)	108.74(14)
C(14)-N(1)-C(11)-Ti(1)	67.64(11)
C(13)-C(12)-C(11)-N(1)	-2.33(18)
Ti(1)-C(12)-C(11)-N(1)	62.03(11)
C(13)-C(12)-C(11)-C(1)	-175.17(15)
Ti(1)-C(12)-C(11)-C(1)	-110.80(15)
C(13)-C(12)-C(11)-Ti(1)	-64.36(12)
N(4)-Ti(1)-C(11)-N(1)	-145.45(10)
N(3)-Ti(1)-C(11)-N(1)	24.14(13)
N(2)-Ti(1)-C(11)-N(1)	114.29(11)
C(14)-Ti(1)-C(11)-N(1)	-39.28(11)
C(13)-Ti(1)-C(11)-N(1)	-80.50(11)
C(12)-Ti(1)-C(11)-N(1)	-118.28(14)
N(4)-Ti(1)-C(11)-C(12)	-27.17(12)
N(3)-Ti(1)-C(11)-C(12)	142.41(10)
N(2)-Ti(1)-C(11)-C(12)	-127.43(10)
N(1)-Ti(1)-C(11)-C(12)	118.28(14)
C(14)-Ti(1)-C(11)-C(12)	79.00(12)
C(13)-Ti(1)-C(11)-C(12)	37.77(10)
N(4)-Ti(1)-C(11)-C(1)	98.03(12)
N(3)-Ti(1)-C(11)-C(1)	-92.39(13)
N(2)-Ti(1)-C(11)-C(1)	-2.23(11)
N(1)-Ti(1)-C(11)-C(1)	-116.53(16)
C(14)-Ti(1)-C(11)-C(1)	-155.80(15)
C(13)-Ti(1)-C(11)-C(1)	162.97(15)
C(12)-Ti(1)-C(11)-C(1)	125.20(16)
C(23)-C(22)-C(21)-N(2)	-0.01(18)
C(23)-C(22)-C(21)-C(1)	178.63(15)
C(24)-N(2)-C(21)-C(22)	0.10(17)
Ti(1)-N(2)-C(21)-C(22)	-169.31(11)
C(24)-N(2)-C(21)-C(1)	-178.74(13)
Ti(1)-N(2)-C(21)-C(1)	11.85(19)
N(1)-C(11)-C(1)-C(21)	-74.38(18)
C(12)-C(11)-C(1)-C(21)	97.71(18)
Ti(1)-C(11)-C(1)-C(21)	7.59(15)
N(1)-C(11)-C(1)-C(6)	43.53(19)
C(12)-C(11)-C(1)-C(6)	-144.38(16)
Ti(1)-C(11)-C(1)-C(6)	125.50(12)
N(1)-C(11)-C(1)-C(2)	166.64(14)
C(12)-C(11)-C(1)-C(2)	-21.3(2)
Ti(1)-C(11)-C(1)-C(2)	-111.39(12)
C(22)-C(21)-C(1)-C(11)	169.67(16)
N(2)-C(21)-C(1)-C(11)	-11.79(18)
C(22)-C(21)-C(1)-C(6)	49.4(2)
N(2)-C(21)-C(1)-C(6)	-132.07(14)
C(22)-C(21)-C(1)-C(2)	-68.8(2)
N(2)-C(21)-C(1)-C(2)	109.73(15)
C(5)-C(6)-C(1)-C(11)	76.07(17)

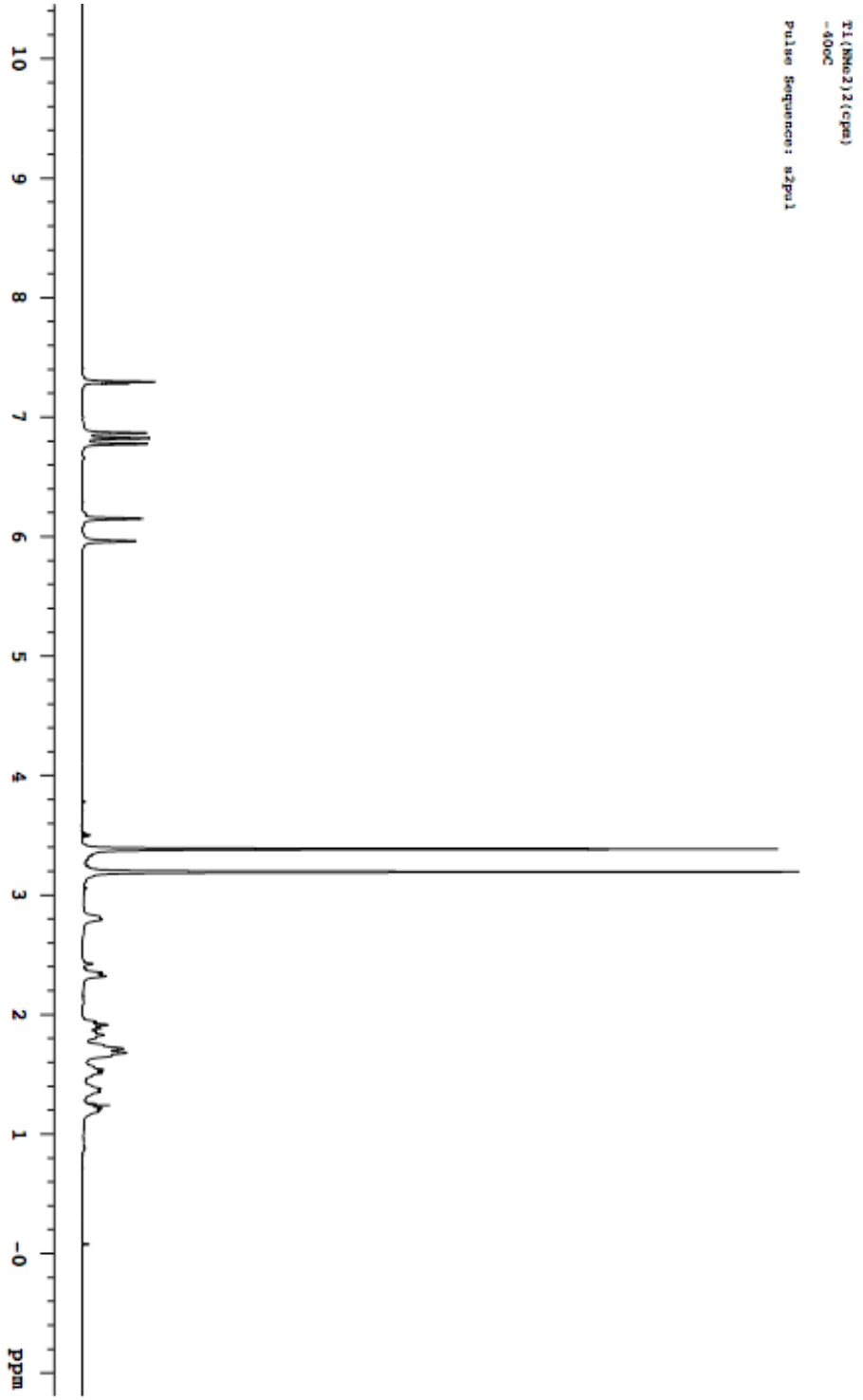
C(5)-C(6)-C(1)-C(21)	-167.45(13)
C(5)-C(6)-C(1)-C(2)	-49.23(19)
C(3)-C(2)-C(1)-C(11)	-77.33(18)
C(3)-C(2)-C(1)-C(21)	165.39(14)
C(3)-C(2)-C(1)-C(6)	47.49(19)

Symmetry transformations used to generate equivalent atoms:

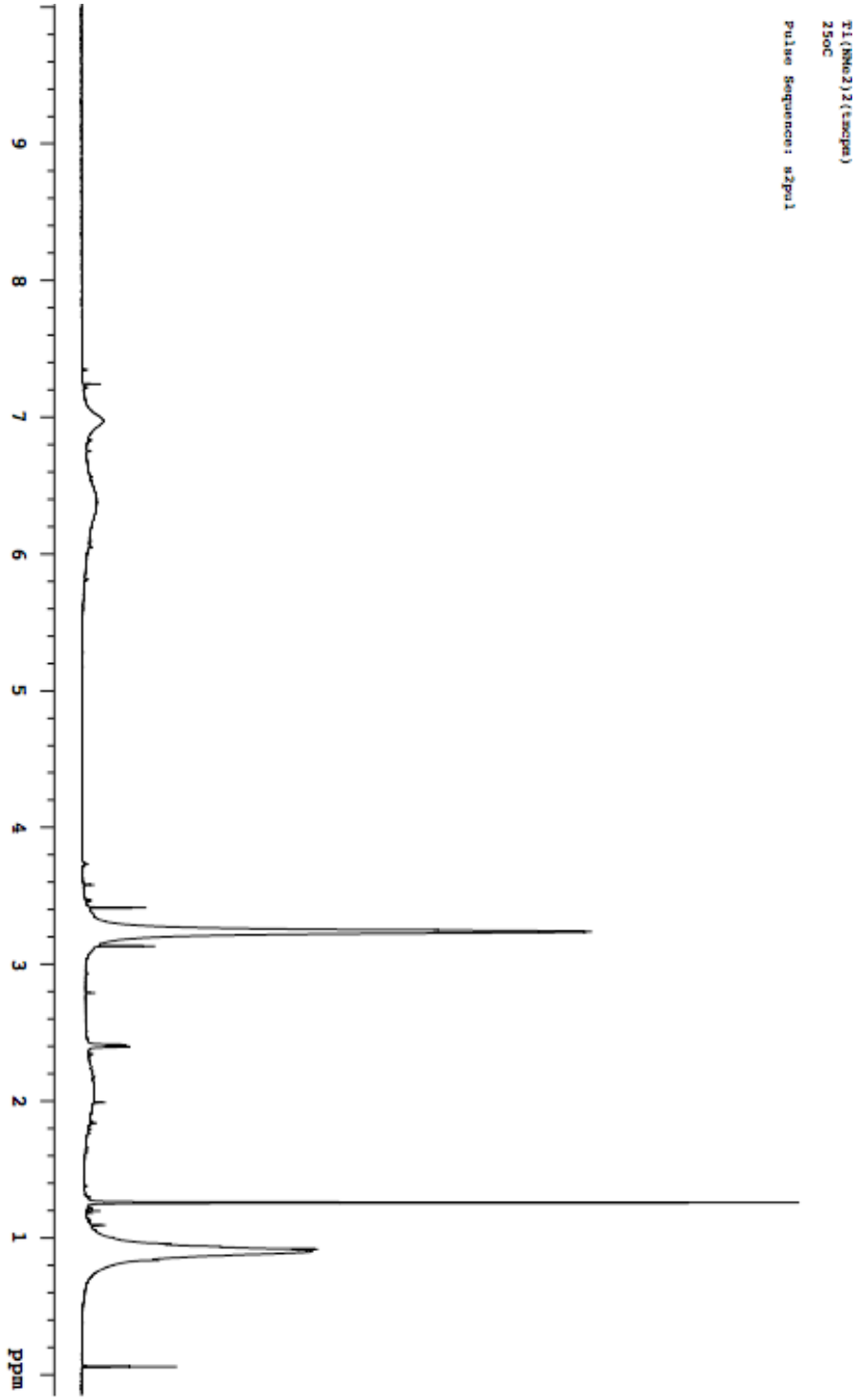
B. ^{1}H NMR Spectra of $Ti(NMe_2)_2(cpm)$ (**2**) 25 °C



C. ^{1}H NMR Spectra of $Ti(NMe_2)_2(cpm)$ (**2**) –40 °C



D. ^{1}H NMR Spectra of Ti(NMe$_2$)$_2$(tmcpm) (**3**) 25 °C



E. ^{1}H NMR Spectra of $Ti(NMe_2)_2$(tmcpm) (**3**) –40 °C