Supplementary Data for:

A Remarkably Active Non-Metallocene Ethylene Polymerization Catalyst

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Spectroscopic Data

(*t*-Bu$_3$PN)$_2$TiCl$_2$ 1 ^{1}H NMR δ 1.36 (d, $|J^3_{PH}|$ = 13.1 Hz, 54H, PC*Me*$_3$). ^{31}P{^{1}H} NMR δ 32.17. ^{13}C{^{1}H} NMR δ 41.36 (d, $|J^1_{PC}|$ = 46.1 Hz, PCMe$_3$), 29.73. EA Calc'd for: $C_{12}H_{27}Cl_2N_2P_2Ti$; C:37.92; H: 7.16; N: 7.37; Found: ; C: 37.83; H: 7.09; N: 7.28 .

(*t*-Bu$_3$PN)$_2$TiMe$_2$ 2 ^{1}H NMR δ 1.39 (d, $|J^3_{PH}|$ = 12.6 Hz, 54H, PC*Me*$_3$), 0.90 (s, 6H, Ti*Me*$_2$). ^{31}P{^{1}H} NMR δ 25.72. ^{13}C{^{1}H} NMR δ 40.81 (d, $|J^1_{PC}|$ = 47.2 Hz, PCMe$_3$), 36.27 (Ti*Me*$_2$), 29.87. EA Calc'd for: $C_{14}H_{33}N_2P_2Ti$; C: 49.56; H: 9.80; N: 8.26; Found: C: 49.48; H: 9.71; N: 8.16.

[(*t*-Bu$_3$PN)$_2$TiMe(PMe$_3$)][B(C$_6$F$_5$)$_4$] 3 ^{1}H NMR (CD_2Cl_2, 25 °C) δ 1.55 (d, $|J^3_{PH}|$ = 12.4 Hz, 9H, P*Me*$_3$), 1.51 (d, $|J^3_{PH}|$ = 13.2 Hz, 54H, PC*Me*$_3$), 0.80 (s, 3H, Ti*Me*). ^{31}P{^{1}H} NMR (CD_2Cl_2, 25 °C) δ 42.75, -22.78. ^{19}F{^{1}H} NMR (CD_2Cl_2, 25 °C) δ -55.63 (S), -86.36 (t, $|J_{FF}|$ = 20.6 Hz), -90.19 (t, $|J_{FF}|$ = 16.9 Hz). ^{11}B{^{1}H} NMR (CD_2Cl_2, 25 °C) δ -16.98.

(*t*-Bu$_3$PN)$_2$TiMe(μ-Me)B(C$_6$F$_5$)$_3$ 4 ^{1}H NMR (CD_2Cl_2, 25 °C) δ 1.44 (d, $|J^3_{PH}|$ = 13.1 Hz, 54H, PC*Me*$_3$), 0.54 (s, 3H, Ti*Me*), 0.47 (broad singlet, 3H *Me*B). ^{31}P{^{1}H} NMR (CD_2Cl_2, 25 °C) δ 49.75. ^{19}F{^{1}H} NMR (CD_2Cl_2, 25 °C) δ -55.78 (d, $|J_{FF}|$ = 21.5 Hz), -88.07 (t, $|J_{FF}|$ = 19.9 Hz), -90.58 (t, $|J_{FF}|$ = 18.7 Hz). ^{11}B{^{1}H} NMR (CD_2Cl_2, 25 °C) δ -15.27.

Polymerization Screening: These experiments were done in a similar manner and thus a general description is provided. A solution of 10 to 40 μmol of catalyst in 2.0 mL of dry toluene was added to a flask containing 2.0 mL of dry toluene. 500 equivalents of a 10% by weight toluene solution of methylaluminoxane (MAO) were added to the flask. The flask was attached to a Schlenk line with cold trap, a stopwatch was started and the flask was three times evacuated for five seconds and refilled with pre-dried 99.9%

ethylene gas. The solution was rapidly stirred under 1 atmosphere of ethylene at room temperature. The duration of the experiment was limited so as to preclude catalyst from becoming entrained and thus diffusion controlled kinetics. The polymerization was stopped by the injection of a 1.0 N HCl / methanol solution and total reaction time was noted. The polymer was filtered and washed with copious amounts of water and placed on a drying oven for subsequent weighing.

Industrially Relevant Polymerizations Experiments were performed under commercially relevant solution polymerization conditions (160°C and 1500 psi). Cyclohexane, catalyst in toluene (1 mM), and ethylene were continuously added to the reactor and the product continuously removed. Toluene solutions of the catalysts and activators were pumped independently into the reactor. The total flow was 27mL/min. On exiting the reactor nonanoic acid was added to prevent further polymerization. The ethylene conversion was measured by GC reference to an internal standard (propane). Polymer samples were analysed by high temperature GPC.

Crystallographic Data

Data_**(*t*-Bu$_3$PN)$_2$TiCl$_2$ 1**

Table 1. Crystal data and structure refinement

Empirical formula	C24H54Cl2N2P2Ti
Formula weight	551.43
Temperature	293(2) K
Wavelength	0.71073 A
Crystal system	monoclinic
Space group	$P2_1/n$
Unit cell dimensions	
a =13.091(2) A	alpha =90o
b =16.233(3) A	beta =107.04(2)o
c =15.413(4) A	gamma =90o
Volume, Z	3131.4(10), 4
Density (calculated)	1.170 Mg/m3
Absorption coefficient	0.560 mm-1

F(000)	1192
Crystal size	0.20 x 0.22 x 0.15 mm
θ range for data collection	1.80 to 25.00o
Limiting indices	-12<h<17,-21<k<21,-20<l<13
Reflections collected	14650
Independent reflections	5429 (Rint = 0.1309)
Refinement method	Full-matrix least-squares on F2
Data/restraints/parameters	5427 / 0 / 280
Goodness-of-fit on F2	0.743
Final R indices [I>2s(I)]	R1 = 0.0606, wR2 = 0.1466
R indices (all data)	R1 = 0.1278, wR2 = 0.1833
Largest diff. peak and hole	0.324 and -0.520 eA-3

Table 2. Atomic coordinates [x 104] and equivalent isotropic displacement parameters [A2 x 103]

	x	y	z	U(eq)
Ti(1)	4755(1)	2106(1)	1924(1)	35(1)
Cl(1)	5373(1)	3133(1)	1195(1)	80(1)
Cl(2)	3494(1)	1393(1)	836(1)	64(1)
P(1)	6777(1)	783(1)	2733(1)	39(1)
P(2)	3615(1)	3006(1)	3377(1)	35(1)
N(1)	5834(3)	1432(2)	2467(3)	46(1)
N(2)	4124(3)	2550(2)	2701(3)	45(1)
C(1)	6708(4)	125(3)	1701(4)	51(1)
C(2)	5749(5)	-459(4)	1502(5)	85(2)
C(3)	6466(5)	685(4)	854(4)	77(2)
C(4)	7725(5)	-377(4)	1763(5)	88(2)
C(5)	8085(4)	1365(3)	3118(5)	60(2)
C(6)	7957(5)	2080(4)	3743(6)	92(2)
C(7)	8305(5)	1769(5)	2288(6)	101(3)
C(8)	9053(4)	833(4)	3625(6)	94(3)
C(9)	6594(4)	120(4)	3670(4)	62(2)
C(10)	5408(5)	-87(4)	3485(6)	98(3)
C(11)	7249(6)	-706(4)	3817(6)	108(3)
C(12)	6903(6)	577(5)	4562(5)	103(3)
C(13)	4614(4)	3057(3)	4537(4)	56(2)
C(14)	4327(6)	3600(5)	5214(5)	118(3)
C(15)	4816(8)	2196(5)	4941(7)	175(6)
C(16)	5675(5)	3344(7)	4441(6)	158(4)
C(17)	3237(4)	4082(3)	2920(5)	61(2)
C(18)	2600(8)	4026(5)	1945(6)	148(4)
C(19)	2598(7)	4570(4)	3427(6)	130(4)
C(20)	4251(7)	4556(4)	2966(8)	147(5)
C(21)	2390(4)	2415(3)	3416(4)	57(2)
C(22)	1872(6)	2702(5)	4133(7)	121(3)

C(23)	2687(7)	1503(4)	3579(7)	128(4)
C(24)	1566(6)	2429(6)	2498(6)	148(4)

Table 3. Selected bond lengths [A] and angles [o]

Ti(1)-N(1)	1.789(4)
Ti(1)-N(2)	1.792(4)
Ti(1)-Cl(1)	2.288(2)
Ti(1)-Cl(2)	2.292(2)
P(1)-N(1)	1.582(3)
P(1)-C(9)	1.873(6)
P(1)-C(5)	1.893(5)
P(1)-C(1)	1.895(5)
P(2)-N(2)	1.576(4)
P(2)-C(13)	1.883(6)
P(2)-C(21)	1.885(5)
P(2)-C(17)	1.893(5)
C(1)-C(2)	1.531(7)
C(1)-C(4)	1.540(6)
C(1)-C(3)	1.545(8)
C(5)-C(7)	1.538(9)
C(5)-C(8)	1.544(7)
C(5)-C(6)	1.549(8)
C(9)-C(12)	1.510(9)
C(9)-C(10)	1.531(8)
C(9)-C(11)	1.572(7)
C(13)-C(14)	1.494(9)
C(13)-C(16)	1.514(8)
C(13)-C(15)	1.521(9)
C(17)-C(18)	1.493(10)
C(17)-C(20)	1.518(8)
C(17)-C(19)	1.523(8)
C(21)-C(24)	1.507(9)
C(21)-C(22)	1.528(9)
C(21)-C(23)	1.532(8)

N(1)-Ti(1)-N(2)	112.9(2)
N(1)-Ti(1)-Cl(1)	109.34(14)
N(2)-Ti(1)-Cl(1)	109.43(13)
N(1)-Ti(1)-Cl(2)	109.51(13)
N(2)-Ti(1)-Cl(2)	108.54(13)
Cl(1)-Ti(1)-Cl(2)	106.93(7)
N(1)-P(1)-C(9)	108.4(2)
N(1)-P(1)-C(5)	108.3(2)
C(9)-P(1)-C(5)	110.7(3)
N(1)-P(1)-C(1)	108.4(2)
C(9)-P(1)-C(1)	109.7(3)
C(5)-P(1)-C(1)	111.1(2)
N(2)-P(2)-C(13)	109.8(2)
N(2)-P(2)-C(21)	108.1(2)
C(13)-P(2)-C(21)	110.6(3)
N(2)-P(2)-C(17)	107.6(2)
C(13)-P(2)-C(17)	110.2(3)
C(21)-P(2)-C(17)	110.5(2)
P(1)-N(1)-Ti(1)	167.8(3)
P(2)-N(2)-Ti(1)	175.5(2)
C(2)-C(1)-C(4)	109.1(5)
C(2)-C(1)-C(3)	104.0(5)
C(4)-C(1)-C(3)	108.9(5)
C(2)-C(1)-P(1)	110.6(4)
C(4)-C(1)-P(1)	114.8(4)
C(3)-C(1)-P(1)	109.0(4)
C(7)-C(5)-C(8)	109.5(5)
C(7)-C(5)-C(6)	106.2(5)
C(8)-C(5)-C(6)	109.1(5)
C(7)-C(5)-P(1)	109.0(4)
C(8)-C(5)-P(1)	114.4(4)
C(6)-C(5)-P(1)	108.4(4)
C(12)-C(9)-C(10)	105.3(6)
C(12)-C(9)-C(11)	107.4(6)
C(10)-C(9)-C(11)	108.7(5)
C(12)-C(9)-P(1)	111.0(5)
C(10)-C(9)-P(1)	109.6(4)
C(11)-C(9)-P(1)	114.4(4)
C(14)-C(13)-C(16)	108.2(6)
C(14)-C(13)-C(15)	107.8(7)
C(16)-C(13)-C(15)	105.6(7)
C(14)-C(13)-P(2)	116.2(4)
C(16)-C(13)-P(2)	108.8(5)
C(15)-C(13)-P(2)	109.7(4)
C(18)-C(17)-C(20)	107.5(8)
C(18)-C(17)-C(19)	108.6(6)
C(20)-C(17)-C(19)	108.5(6)
C(18)-C(17)-P(2)	109.0(4)
C(20)-C(17)-P(2)	108.7(4)
C(19)-C(17)-P(2)	114.3(5)
C(24)-C(21)-C(22)	109.1(6)

C(24)-C(21)-C(23)	104.3(6)	C(22)-C(21)-P(2)	115.4(4)
C(22)-C(21)-C(23)	108.7(6)	C(23)-C(21)-P(2)	108.7(4)
C(24)-C(21)-P(2)	110.1(5)		

Table 4. Anisotropic displacement parameters [A2 x 103]

	U11	U22	U33	U23	U13	U12
Ti(1)	36(1)	34(1)	34(1)	1(1)	10(1)	2(1)
Cl(1)	90(1)	76(1)	77(1)	19(1)	28(1)	-27(1)
Cl(2)	53(1)	70(1)	59(1)	-14(1)	4(1)	-12(1)
P(1)	34(1)	43(1)	40(1)	-1(1)	13(1)	7(1)
P(2)	34(1)	29(1)	42(1)	-2(1)	10(1)	4(1)
N(1)	40(2)	45(2)	49(3)	-3(2)	8(2)	8(2)
N(2)	48(2)	37(2)	52(3)	-4(2)	16(2)	7(2)
C(1)	55(3)	59(3)	41(4)	-11(3)	16(3)	7(2)
C(2)	68(4)	72(4)	105(7)	-38(4)	11(4)	-3(3)
C(3)	85(4)	104(5)	42(4)	-10(4)	18(3)	10(4)
C(4)	73(4)	108(5)	82(6)	-39(4)	19(4)	35(4)
C(5)	33(2)	65(3)	79(5)	-14(3)	13(3)	-4(2)
C(6)	72(4)	85(4)	113(7)	-44(5)	18(4)	-13(3)
C(7)	71(4)	109(5)	133(8)	0(5)	46(5)	-32(4)
C(8)	39(3)	119(5)	111(7)	-24(5)	0(4)	15(3)
C(9)	69(3)	75(3)	50(4)	20(3)	29(3)	20(3)
C(10)	85(4)	104(5)	121(7)	38(5)	58(5)	-3(4)
C(11)	125(6)	80(4)	134(8)	61(5)	62(6)	48(4)
C(12)	114(6)	142(7)	58(6)	19(5)	35(5)	22(5)
C(13)	42(3)	74(3)	44(4)	-8(3)	3(3)	1(2)
C(14)	94(5)	193(9)	58(6)	-48(6)	8(5)	11(5)
C(15)	205(10)	92(6)	136(10)	21(6)	-96(8)	23(6)
C(16)	53(4)	307(13)	97(8)	-25(8)	-3(4)	-55(6)
C(17)	77(4)	33(2)	78(5)	13(3)	33(4)	19(2)
C(18)	244(11)	100(6)	66(7)	32(5)	-6(7)	71(7)
C(19)	208(9)	70(4)	140(9)	25(5)	96(7)	85(5)
C(20)	147(7)	49(3)	268(14)	47(6)	95(8)	-7(4)
C(21)	50(3)	60(3)	65(4)	-18(3)	24(3)	-20(2)
C(22)	95(5)	124(6)	186(10)	-68(6)	105(6)	-52(4)
C(23)	151(7)	56(4)	209(12)	-1(5)	103(8)	-35(4)
C(24)	81(5)	238(10)	101(8)	0(8)	-11(5)	-87(6)

Table 5. Hydrogen coordinates (x 104) and isotropic displacement parameters (A2 x 103)

	x	Y	z	U(eq)
H(2A)	5113(5)	-148(4)	1463(5)	127
H(2B)	5859(5)	-857(4)	1982(5)	127

H(2C)	5674(5)	-737(4)	938(5)	127
H(3A)	7035(5)	1075(4)	923(4)	116
H(3B)	5807(5)	974(4)	787(4)	116
H(3C)	6404(5)	353(4)	325(4)	116
H(4A)	8329(5)	-14(4)	1888(5)	133
H(4B)	7647(5)	-656(4)	1198(5)	133
H(4C)	7832(5)	-775(4)	2242(5)	133
H(6A)	7817(5)	1859(4)	4274(6)	138
H(6B)	7371(5)	2425(4)	3423(6)	138
H(6C)	8602(5)	2400(4)	3918(6)	138
H(7A)	7703(5)	2100(5)	1972(6)	151
H(7B)	8421(5)	1349(5)	1888(6)	151
H(7C)	8929(5)	2111(5)	2484(6)	151
H(8A)	8916(4)	581(4)	4143(6)	142
H(8B)	9678(4)	1175(4)	3822(6)	142
H(8C)	9169(4)	413(4)	3226(6)	142
H(10A)	5159(5)	-381(4)	2922(6)	146
H(10B)	5006(5)	414(4)	3449(6)	146
H(10C)	5314(5)	-422(4)	3969(6)	146
H(11A)	7070(6)	-1013(4)	3260(6)	162
H(11B)	7078(6)	-1027(4)	4279(6)	162
H(11C)	7999(6)	-583(4)	4001(6)	162
H(12A)	7645(6)	726(5)	4717(5)	154
H(12B)	6785(6)	231(5)	5028(5)	154
H(12C)	6477(6)	1067(5)	4507(5)	154
H(14A)	3655(6)	3427(5)	5285(5)	177
H(14B)	4272(6)	4160(5)	5004(5)	177
H(14C)	4871(6)	3561(5)	5787(5)	177
H(15A)	5002(8)	1834(5)	4519(7)	263
H(15B)	4182(8)	1997(5)	5064(7)	263
H(15C)	5392(8)	2214(5)	5496(7)	263
H(16A)	5873(5)	3003(7)	4008(6)	236
H(16B)	6212(5)	3307(7)	5017(6)	236
H(16C)	5613(5)	3906(7)	4235(6)	236
H(18A)	1951(8)	3728(5)	1894(6)	222
H(18B)	3008(8)	3743(5)	1612(6)	222
H(18C)	2430(8)	4570(5)	1702(6)	222
H(19A)	2999(7)	4611(4)	4056(6)	194
H(19B)	1933(7)	4294(4)	3373(6)	194
H(19C)	2458(7)	5112(4)	3171(6)	194
H(20A)	4679(7)	4603(4)	3588(8)	221
H(20B)	4069(7)	5097(4)	2716(8)	221
H(20C)	4647(7)	4269(4)	2625(8)	221
H(22A)	2394(6)	2694(5)	4719(7)	182
H(22B)	1293(6)	2340(5)	4134(7)	182
H(22C)	1605(6)	3252(5)	3994(7)	182
H(23A)	3214(7)	1441(4)	4158(7)	192

H(23B)	2970(7)	1307(4)	3109(7)	192
H(23C)	2061(7)	1192(4)	3573(7)	192
H(24A)	1887(6)	2250(6)	2045(6)	222
H(24B)	1299(6)	2980(6)	2362(6)	222
H(24C)	987(6)	2068(6)	2502(6)	222

data_**(*t*-Bu$_3$PN)$_2$TiMe$_2$ 2**

Table 1. Crystal data and structure refinement

Empirical formula	C26H60N2P2Ti
Formula weight	510.60
Temperature	93(2) K
Wavelength	0.71073 A
Crystal system	monoclinic
Space group	
Unit cell dimensions	
a =13.1885(3) A	alpha =90o
b =16.4592(4) A	beta =106.5890(10)o
c =15.5549(3) A	gamma =90o
Volume, Z	3235.99(12), 4
Density (calculated)	1.048 Mg/m3
Absorption coefficient	0.378 mm-1
F(000)	1128
Crystal size	? x ? x ? mm
q range for data collection	1.79 to 25.00o
Limiting indices	-17<h<11, -21<k<21,-18<l<20
Reflections collected	15936
Independent reflections	5619 (Rint = 0.0318)
Refinement method	Full-matrix least-squares on F2
Data/restraints/parameters	5619 / 0 / 280
Goodness-of-fit on F2	1.062
Final R indices [I>2s(I)]	R1 = 0.0512, wR2 = 0.1438
R indices (all data)	R1 = 0.0776, wR2 = 0.1597
Largest diff. peak and hole	0.367 and -0.202 eA-3

Table 2. Atomic coordinates [x 104] and equivalent isotropic displacement parameters [A2 x 103]

	x	y	z	U(eq)
Ti(1)	243(1)	2109(1)	3057(1)	42(1)
P(1)	1417(1)	3026(1)	1643(1)	44(1)
P(2)	-1748(1)	770(1)	2279(1)	46(1)
N(1)	921(2)	2579(2)	2307(2)	55(1)
N(2)	-834(2)	1407(2)	2557(2)	56(1)
C(1)	440(3)	3077(3)	489(2)	70(1)
C(2)	730(4)	3633(4)	-183(3)	138(2)

C(3)	294(6)	2228(4)	84(4)	171(3)
C(4)	-629(4)	3329(6)	589(4)	181(3)
C(5)	1774(3)	4098(2)	2074(3)	76(1)
C(6)	2364(6)	4054(4)	3062(4)	163(3)
C(7)	756(5)	4569(3)	1999(5)	152(3)
C(8)	2442(6)	4579(3)	1585(4)	155(3)
C(9)	2647(3)	2460(2)	1592(2)	70(1)
C(10)	3475(4)	2531(6)	2503(4)	180(3)
C(11)	3144(4)	2737(4)	861(4)	144(3)
C(12)	2390(5)	1560(3)	1462(5)	146(3)
C(13)	-3066(3)	1317(2)	1909(3)	72(1)
C(14)	-4017(3)	796(3)	1406(3)	110(2)
C(15)	-3299(4)	1697(4)	2734(3)	117(2)
C(16)	-2953(4)	2039(3)	1300(4)	111(2)
C(17)	-1697(3)	87(2)	3277(2)	59(1)
C(18)	-2684(4)	-433(3)	3195(3)	107(2)
C(19)	-1488(4)	631(3)	4124(2)	92(1)
C(20)	-741(3)	-466(3)	3463(3)	93(1)
C(21)	-1562(3)	117(2)	1328(2)	74(1)
C(22)	-2213(5)	-685(3)	1173(4)	129(2)
C(23)	-1863(4)	606(4)	454(3)	123(2)
C(24)	-390(4)	-78(3)	1519(3)	119(2)
C(25)	1398(3)	1524(2)	4108(2)	70(1)
C(26)	-340(3)	3035(2)	3744(3)	80(1)

Table 3. Selected bond lengths [A] and angles [o]

Ti(1)-N(2)	1.824(2)	C(5)-C(6)	1.514(7)
Ti(1)-N(1)	1.830(2)	C(5)-C(7)	1.526(6)
Ti(1)-C(25)	2.121(3)	C(5)-C(8)	1.537(5)
Ti(1)-C(26)	2.129(3)	C(9)-C(10)	1.527(6)
P(1)-N(1)	1.558(2)	C(9)-C(11)	1.535(5)
P(1)-C(1)	1.889(3)	C(9)-C(12)	1.521(6)
P(1)-C(9)	1.891(4)	C(13)-C(14)	1.536(5)
P(1)-C(5)	1.897(4)	C(13)-C(16)	1.554(5)
P(2)-N(2)	1.564(2)	C(13)-C(15)	1.535(6)
P(2)-C(21)	1.900(3)	C(17)-C(20)	1.514(5)
P(2)-C(13)	1.895(3)	C(17)-C(18)	1.533(5)
P(2)-C(17)	1.903(3)	C(17)-C(19)	1.551(5)
C(1)-C(2)	1.519(6)	C(21)-C(24)	1.523(6)
C(1)-C(4)	1.520(6)	C(21)-C(23)	1.531(6)
C(1)-C(3)	1.522(7)	C(21)-C(22)	1.556(6)
N(2)-Ti(1)-N(1)	117.24(11)	C(25)-Ti(1)-C(26)	102.8(2)
N(2)-Ti(1)-C(25)	109.99(13)	N(1)-P(1)-C(1)	110.4(2)
N(1)-Ti(1)-C(25)	108.01(13)	N(1)-P(1)-C(9)	108.8(2)
N(2)-Ti(1)-C(26)	108.59(14)	C(1)-P(1)-C(9)	110.0(2)
N(1)-Ti(1)-C(26)	109.2(2)	N(1)-P(1)-C(5)	108.3(2)

C(1)-P(1)-C(5)	109.1(2)	C(10)-C(9)-C(12)	105.7(5)
C(9)-P(1)-C(5)	110.1(2)	C(11)-C(9)-C(12)	108.5(4)
N(2)-P(2)-C(21)	109.5(2)	C(10)-C(9)-P(1)	108.6(3)
N(2)-P(2)-C(13)	109.4(2)	C(11)-C(9)-P(1)	116.0(3)
C(21)-P(2)-C(13)	110.1(2)	C(12)-C(9)-P(1)	108.9(3)
N(2)-P(2)-C(17)	109.03(14)	C(14)-C(13)-C(16)	108.8(3)
C(21)-P(2)-C(17)	108.6(2)	C(14)-C(13)-C(15)	108.9(4)
C(13)-P(2)-C(17)	110.1(2)	C(16)-C(13)-C(15)	106.0(4)
P(1)-N(1)-Ti(1)	175.3(2)	C(14)-C(13)-P(2)	115.7(3)
P(2)-N(2)-Ti(1)	171.2(2)	C(16)-C(13)-P(2)	108.0(3)
C(2)-C(1)-C(4)	109.2(4)	C(15)-C(13)-P(2)	109.0(3)
C(2)-C(1)-C(3)	107.2(4)	C(20)-C(17)-C(18)	108.8(3)
C(4)-C(1)-C(3)	106.4(5)	C(20)-C(17)-C(19)	104.3(3)
C(2)-C(1)-P(1)	116.3(3)	C(18)-C(17)-C(19)	109.5(3)
C(4)-C(1)-P(1)	108.4(3)	C(20)-C(17)-P(2)	110.1(2)
C(3)-C(1)-P(1)	108.9(3)	C(18)-C(17)-P(2)	115.5(2)
C(6)-C(5)-C(7)	106.7(5)	C(19)-C(17)-P(2)	107.9(2)
C(6)-C(5)-C(8)	109.0(5)	C(24)-C(21)-C(23)	106.0(4)
C(7)-C(5)-C(8)	108.4(5)	C(24)-C(21)-C(22)	109.6(4)
C(6)-C(5)-P(1)	108.5(3)	C(23)-C(21)-C(22)	108.4(4)
C(7)-C(5)-P(1)	108.8(3)	C(24)-C(21)-P(2)	108.5(3)
C(8)-C(5)-P(1)	115.0(3)	C(23)-C(21)-P(2)	109.6(3)
C(10)-C(9)-C(11)	108.7(5)		
C(22)-C(21)-P(2)	114.3(3)		

Table 4. Anisotropic displacement parameters [A2 x 103]

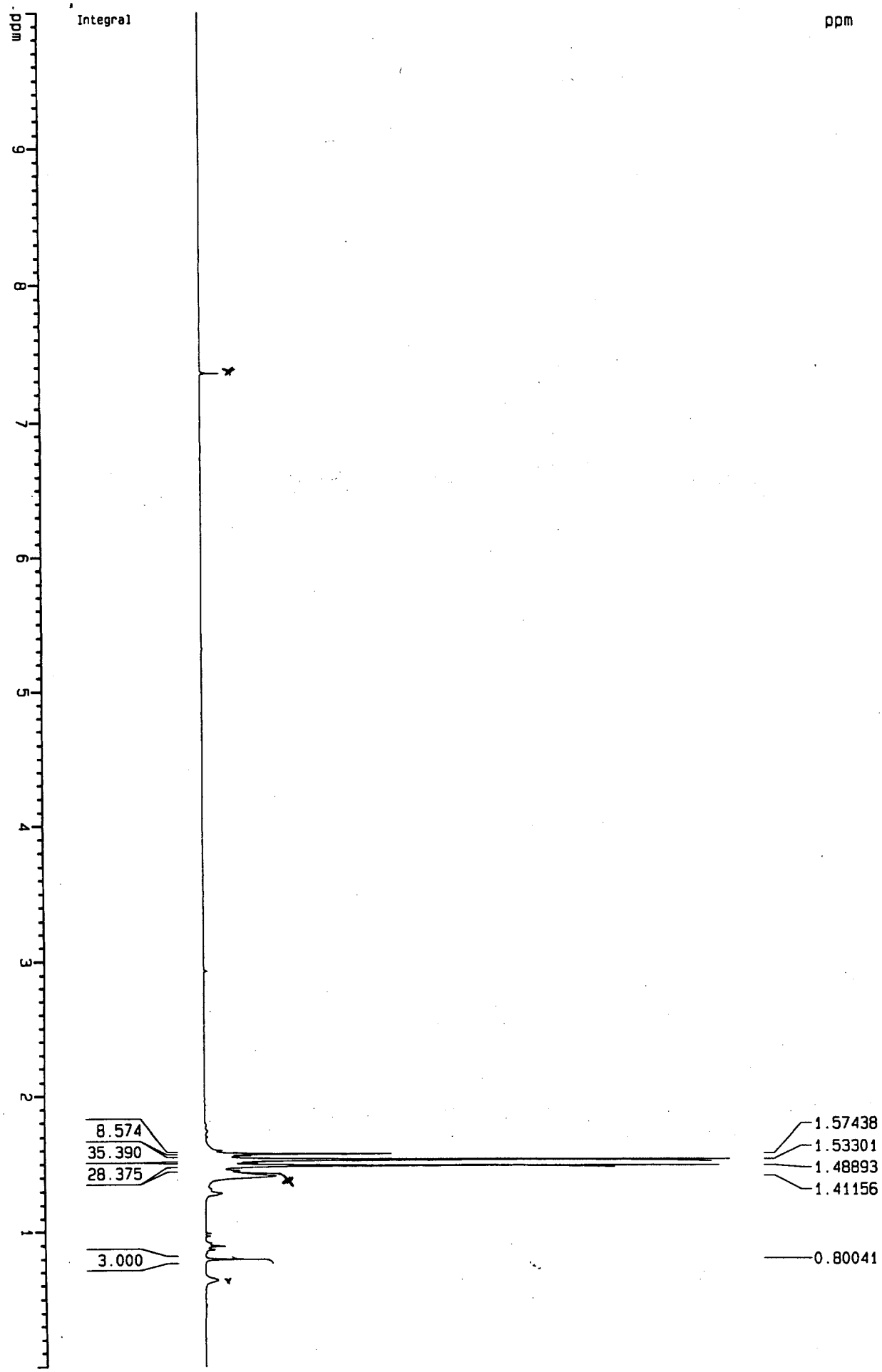
	U11	U22	U33	U23	U13	U12
Ti(1)	45(1)	46(1)	36(1)	1(1)	12(1)	-4(1)
P(1)	42(1)	44(1)	44(1)	5(1)	12(1)	-4(1)
P(2)	42(1)	54(1)	43(1)	2(1)	14(1)	-8(1)
N(1)	61(2)	56(2)	52(2)	4(1)	22(1)	-12(1)
N(2)	54(2)	59(2)	54(2)	4(1)	15(1)	-12(1)
C(1)	56(2)	99(3)	50(2)	14(2)	8(2)	-4(2)
C(2)	104(4)	229(7)	71(3)	59(4)	9(3)	-14(4)
C(3)	200(7)	144(5)	112(4)	-38(4)	-47(4)	-39(5)
C(4)	56(3)	373(11)	102(4)	31(6)	2(3)	57(5)
C(5)	96(3)	54(2)	85(3)	-8(2)	40(2)	-23(2)
C(6)	245(8)	127(5)	89(4)	-40(3)	6(4)	-78(5)
C(7)	180(6)	66(3)	238(7)	-28(4)	102(6)	14(4)
C(8)	241(7)	96(4)	165(5)	-23(3)	120(5)	-93(4)
C(9)	65(2)	79(2)	74(2)	22(2)	32(2)	19(2)
C(10)	91(4)	312(10)	113(4)	28(5)	-9(3)	94(5)
C(11)	121(4)	163(5)	192(6)	3(4)	117(4)	69(4)
C(12)	195(7)	73(3)	203(7)	17(4)	109(6)	52(4)
C(13)	48(2)	83(3)	81(3)	18(2)	12(2)	4(2)

C(14)	54(2)	134(4)	127(4)	24(3)	1(2)	-14(3)
C(15)	88(3)	141(4)	133(4)	2(3)	48(3)	49(3)
C(16)	86(3)	99(3)	135(4)	52(3)	12(3)	20(3)
C(17)	55(2)	65(2)	56(2)	13(2)	15(2)	-12(2)
C(18)	89(3)	128(4)	100(3)	41(3)	21(3)	-45(3)
C(19)	105(3)	122(4)	49(2)	5(2)	24(2)	-14(3)
C(20)	91(3)	91(3)	91(3)	33(2)	19(2)	5(2)
C(21)	78(3)	91(3)	58(2)	-19(2)	30(2)	-17(2)
C(22)	163(5)	112(4)	124(4)	-63(3)	62(4)	-51(4)
C(23)	134(4)	185(6)	57(3)	-2(3)	37(3)	-14(4)
C(24)	107(4)	150(5)	117(4)	-26(4)	60(3)	21(3)
C(25)	65(2)	81(3)	56(2)	7(2)	3(2)	9(2)
C(26)	86(3)	80(3)	79(3)	-12(2)	30(2)	18(2)

Table 5. Hydrogen coordinates (x 104) and isotropic displacement parameters (A2 x 103)

	x	y	z	U(eq)
H(2A)	1400(4)	3471(4)	-255(3)	207
H(2B)	776(4)	4183(4)	31(3)	207
H(2C)	197(4)	3597(4)	-750(3)	207
H(3A)	113(6)	1858(4)	495(4)	257
H(3B)	940(6)	2054(4)	-26(4)	257
H(3C)	-263(6)	2235(4)	-470(4)	257
H(4A)	-816(4)	2978(6)	1012(4)	272
H(4B)	-1155(4)	3290(6)	19(4)	272
H(4C)	-590(4)	3880(6)	800(4)	272
H(6A)	3010(6)	3757(4)	3140(4)	244
H(6B)	1933(6)	3784(4)	3378(4)	244
H(6C)	2523(6)	4594(4)	3295(4)	244
H(7A)	349(5)	4603(3)	1380(5)	229
H(7B)	927(5)	5107(3)	2235(5)	229
H(7C)	350(5)	4295(3)	2334(5)	229
H(8A)	2065(6)	4620(3)	960(4)	232
H(8B)	3101(6)	4303(3)	1651(4)	232
H(8C)	2577(6)	5113(3)	1839(4)	232
H(10A)	3171(4)	2363(6)	2966(4)	270
H(10B)	3707(4)	3085(6)	2603(4)	270
H(10C)	4068(4)	2189(6)	2512(4)	270
H(11A)	2632(4)	2689(4)	284(4)	216
H(11B)	3745(4)	2401(4)	878(4)	216
H(11C)	3366(4)	3292(4)	964(4)	216
H(12A)	1866(5)	1478(3)	897(5)	220
H(12B)	2122(5)	1369(3)	1938(5)	220
H(12C)	3020(5)	1264(3)	1470(5)	220
H(14A)	-4093(3)	347(3)	1777(3)	165

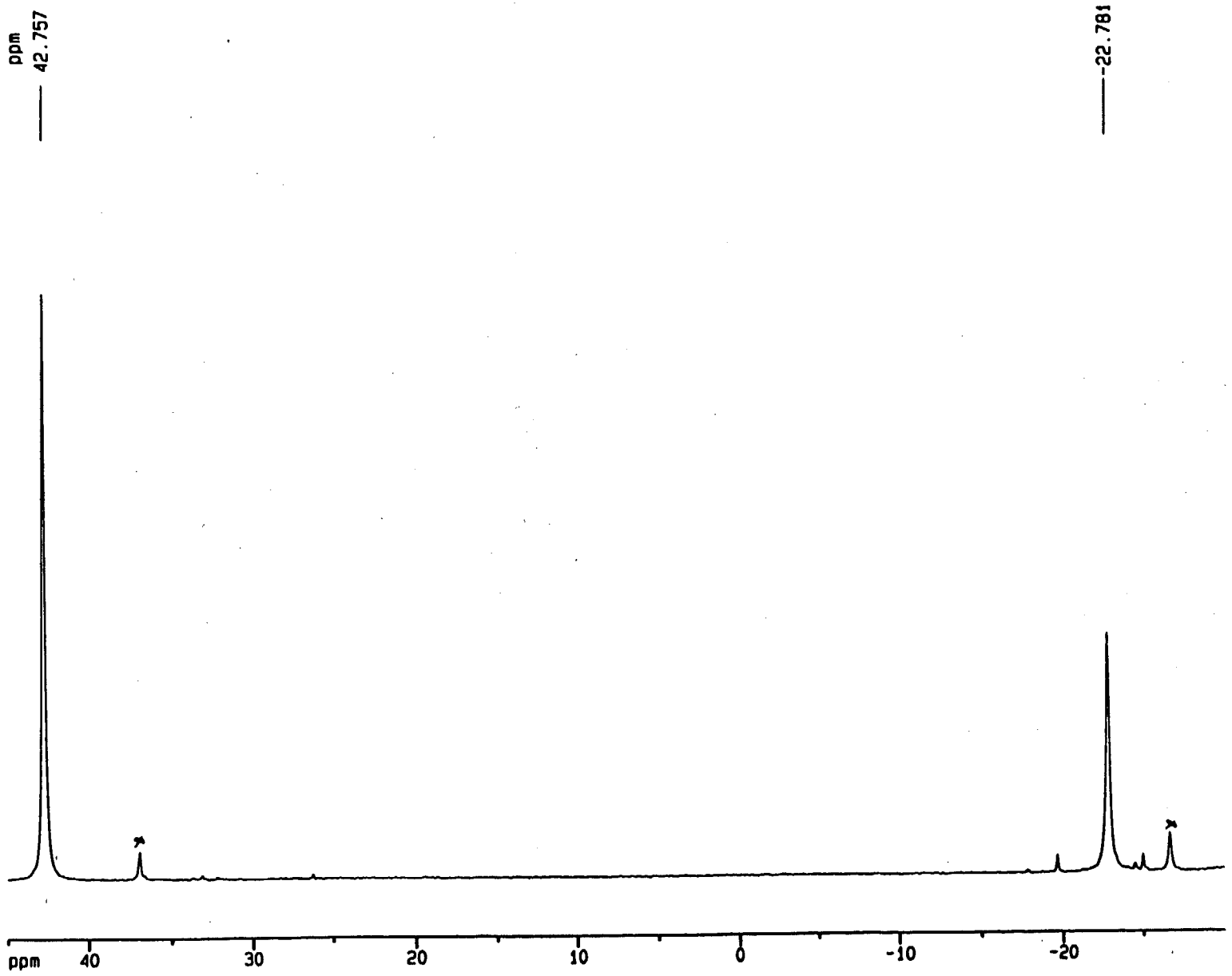
H(14B)	-3904(3)	594(3)	861(3)	165
H(14C)	-4647(3)	1121(3)	1265(3)	165
H(15A)	-2709(4)	2025(4)	3052(3)	175
H(15B)	-3411(4)	1273(4)	3122(3)	175
H(15C)	-3922(4)	2029(4)	2545(3)	175
H(16A)	-2360(4)	2368(3)	1608(4)	166
H(16B)	-3586(4)	2361(3)	1159(4)	166
H(16C)	-2843(4)	1833(3)	756(4)	166
H(18A)	-3296(4)	-88(3)	3077(3)	160
H(18B)	-2608(4)	-724(3)	3745(3)	160
H(18C)	-2768(4)	-813(3)	2711(3)	160
H(19A)	-2065(4)	1004(3)	4056(2)	137
H(19B)	-843(4)	929(3)	4197(2)	137
H(19C)	-1426(4)	296(3)	4642(2)	137
H(20A)	-118(3)	-146(3)	3514(3)	139
H(20B)	-830(3)	-847(3)	2980(3)	139
H(20C)	-669(3)	-755(3)	4014(3)	139
H(22A)	-2953(5)	-560(3)	1037(4)	193
H(22B)	-2004(5)	-1013(3)	1705(4)	193
H(22C)	-2084(5)	-978(3)	681(4)	193
H(23A)	-2602(4)	738(4)	296(3)	185
H(23B)	-1721(4)	288(4)	-17(3)	185
H(23C)	-1454(4)	1097(4)	534(3)	185
H(24A)	-158(4)	-387(3)	2064(3)	178
H(24B)	7(4)	418(3)	1581(3)	178
H(24C)	-280(4)	-390(3)	1031(3)	178
H(25A)	1962(3)	1897(2)	4368(2)	106
H(25B)	1675(3)	1062(2)	3873(2)	106
H(25C)	1080(3)	1348(2)	4560(2)	106
H(26A)	219(3)	3411(2)	4010(3)	121
H(26B)	-595(3)	2795(2)	4206(3)	121
H(26C)	-908(3)	3319(2)	3328(3)	121



NMR Spectra for [(t-Bu$_3$PN)$_2$TiMe(PMe$_3$)][B(C$_6$F$_5$)$_4$] **3**

x denoted minor known impurities (solvent, degradation products)

[(tBu3P=N)2TiMe(PMe3)]+ [B(C6F5)4]-
31P in CD2Cl2
october 15th, 1998



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SOLVENT	CDCl3
NS	104
DS	0
SWH	38535.645 Hz
FIDRES	1.176015 Hz
AQ	0.4252148 sec
RG	7298.2
DW	12.975 usec
DE	4.50 usec
TE	300.0 K
D11	0.03000000 sec
PL12	16.30 dB
CPDPRG2	waltz16
PCPD2	80.00 usec
SFO2	300.1312005 MHz
NUC2	1H
PL2	-6.00 dB
D1	1.00000000 sec
P1	4.40 usec
DE	4.50 usec
SFO1	121.4933527 MHz
NUC1	31P
PL1	-6.00 dB

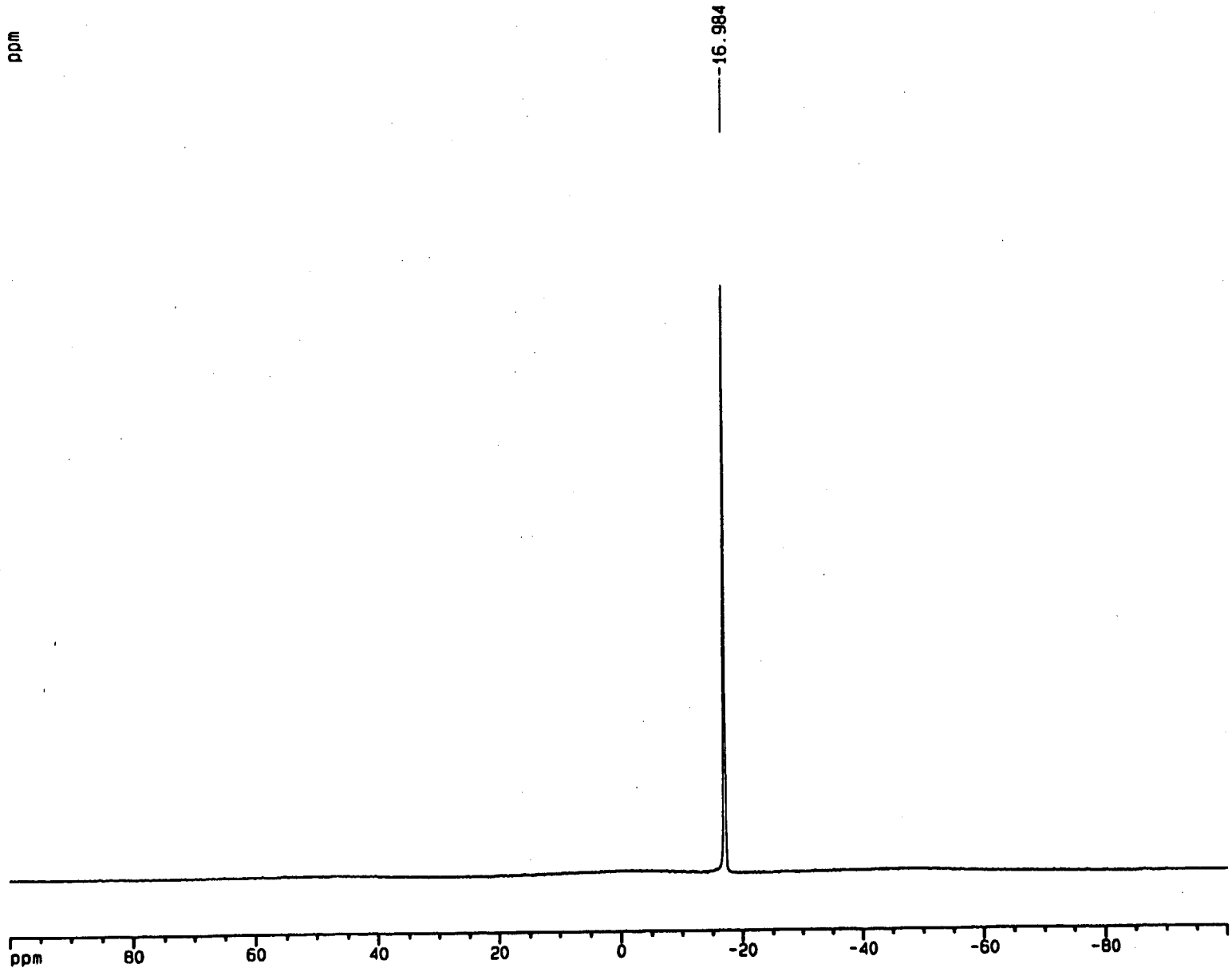
F2 - Processing parameters

SI	16384
SF	121.4947851 MHz
WDW	EM
SSB	0
LB	10.00 Hz
GB	0
PC	1.40

1D NMR plot parameters

CX	20.00 cm
F1P	45.000 ppm
F1	5467.26 Hz
F2P	-30.000 ppm
F2	-3644.84 Hz
PPMCM	3.75000 ppm/cm
HZCM	455.80538 Hz/cm

{(tBu3P=N)2TiMe(PMe3)}+ {B(C6F5)4}-
11B in CD2Cl2
october 15th, 1998



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DS	0
SWH	38535.645 Hz
FIDRES	1.176015 Hz
AQ	0.4252148 sec
RG	574.7
DW	12.975 usec
DE	4.50 usec
TE	300.0 K
D1	1.00000000 sec
P1	4.40 usec
DE	4.50 usec
SFO1	96.2919887 MHz
NUC1	11B
PL1	-6.00 dB

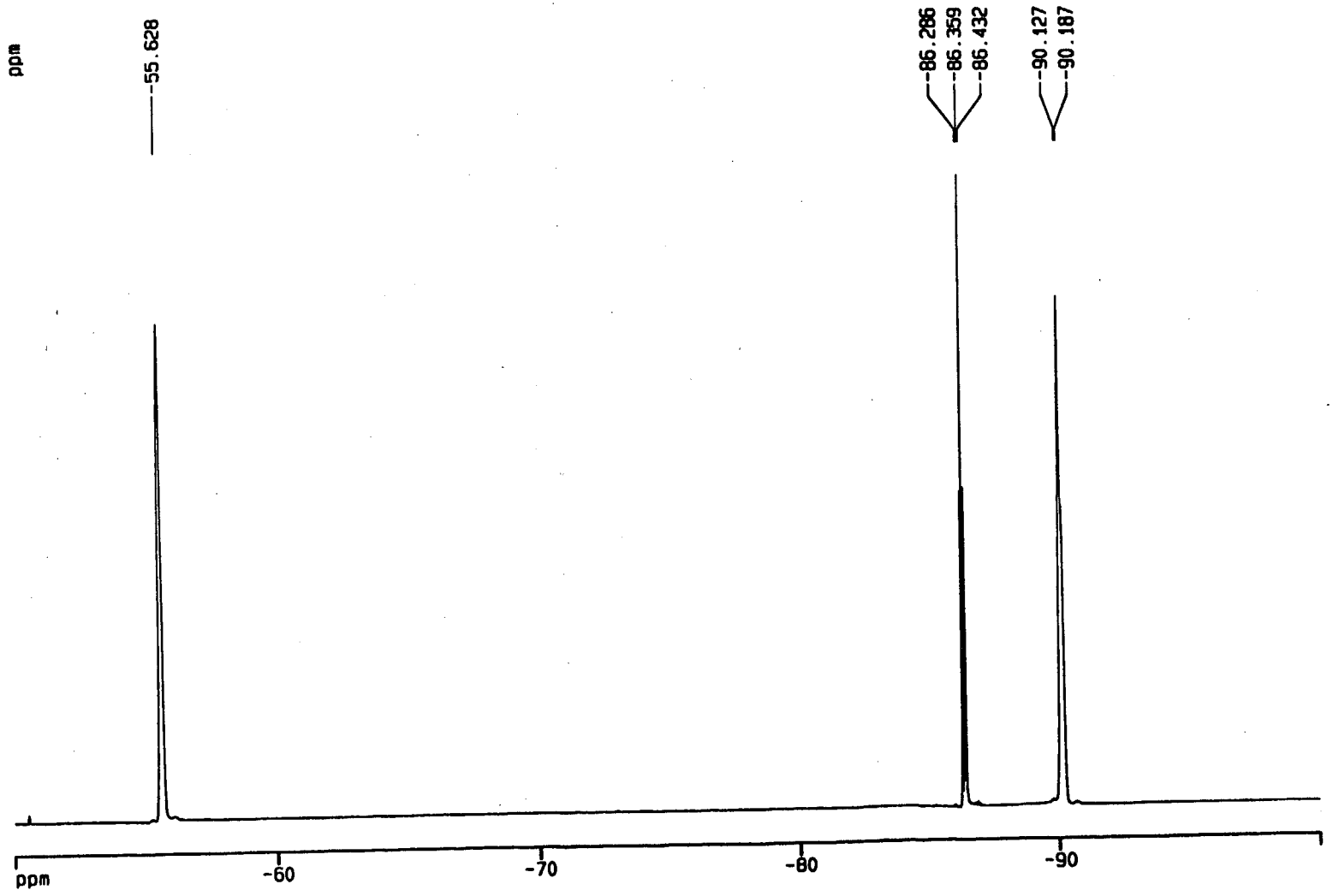
F2 - Processing parameters

SI	16384
SF	96.2936681 MHz
WDW	EM
SSB	0
LB	5.00 Hz
GB	0
PC	1.40

1D NMR plot parameters

CX	20.00 cm
F1P	100.000 ppm
F1	9629.37 Hz
F2P	-100.000 ppm
F2	-9629.37 Hz
PPMCM	10.00000 ppm/cm
HZCM	962.93871 Hz/cm

[(tBu3P=N)2TiMe(PMe3)]+ [B(C6F5)4]-
19F in CD2Cl2
october 15th, 1998



Current Data Parameters

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PROCNO	1

F2 - Acquisition Parameters

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SOLVENT	CDCl3
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DS	0
SWH	56497.176 Hz
FIDRES	3.448314 Hz
AQ	0.1450484 sec
RG	114
DW	8.850 usec
DE	4.50 usec
TE	300.0 K
D1	1.00000000 sec
P1	5.00 usec
DE	4.50 usec
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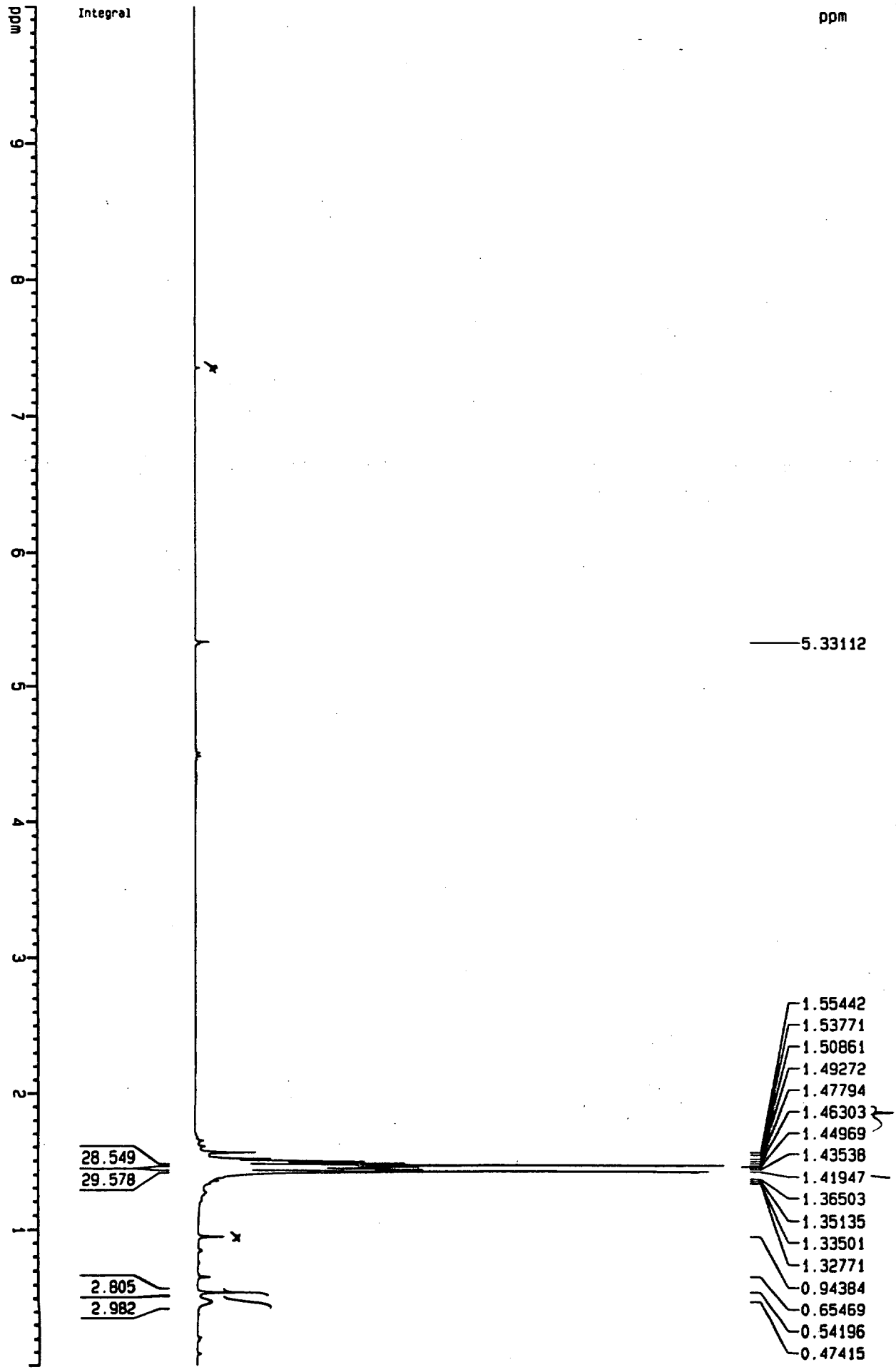
NUC1	19F
PL1	-4.00 dB

F2 - Processing parameters

SI	8192
SF	282.3825555 MHz
WDW	EM
SSB	0
LB	0.50 Hz
GB	0
PC	1.00

1D NMR plot parameters

CX	20.00 cm
F1P	-50.000 ppm
F1	-14119.13 Hz
F2P	-100.000 ppm
F2	-28238.26 Hz
PPMCM	2.50000 ppm/c
HZCM	705.95642 Hz/c

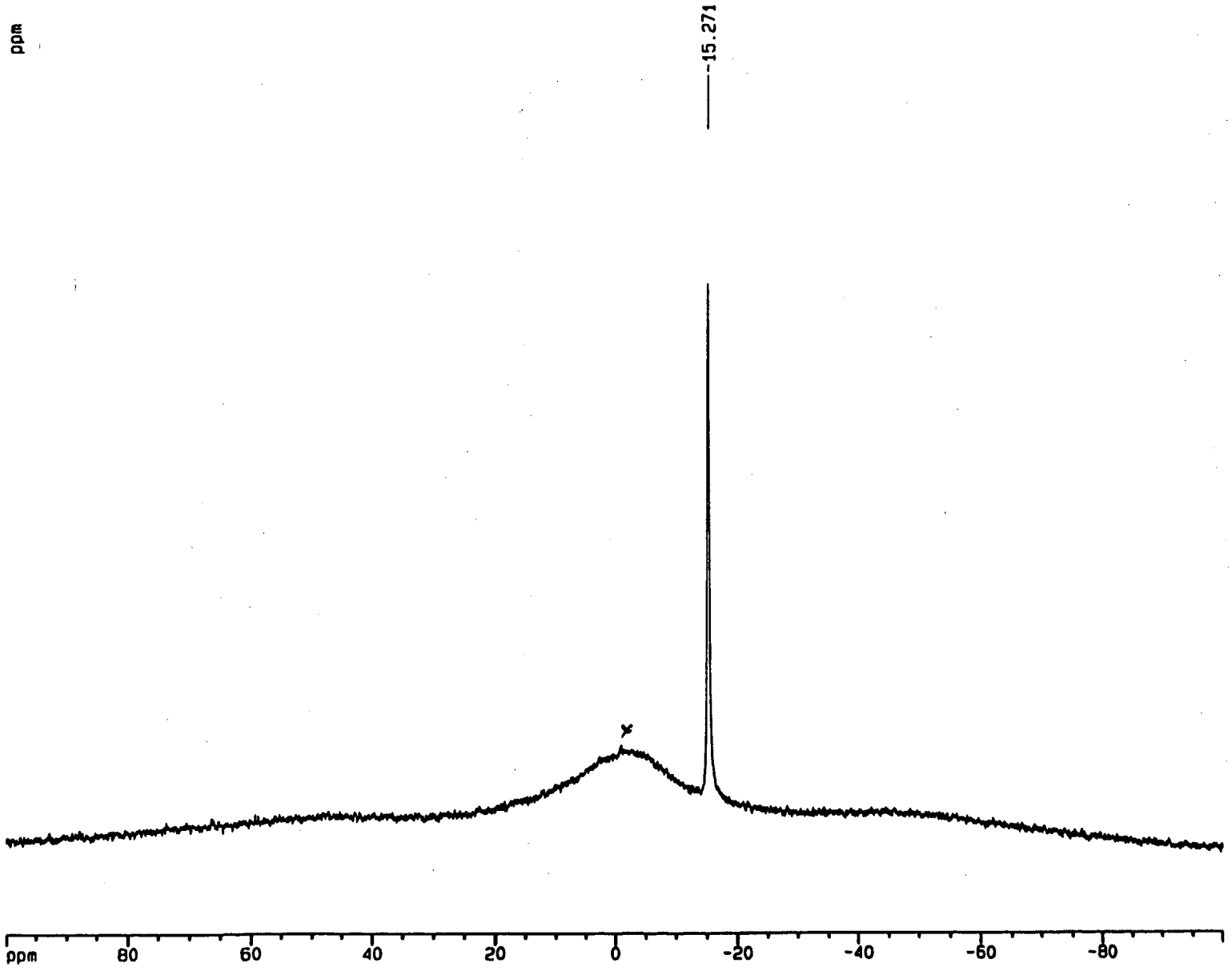


NMR Spectra for (t-$Bu_3PN)_2TiMe(\mu$-Me)$B(C_6F_5)_3$ 4.

x denoted minor known impurities (solvent, degradation products)

october 9th, 1998

(tBu3P=N)2TiMe---Me---Barf
118 in CH2Cl2
october 9th, 1998



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AQ	0.4252148 sec
RG	812.7
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DE	4.50 usec
TE	300.0 K
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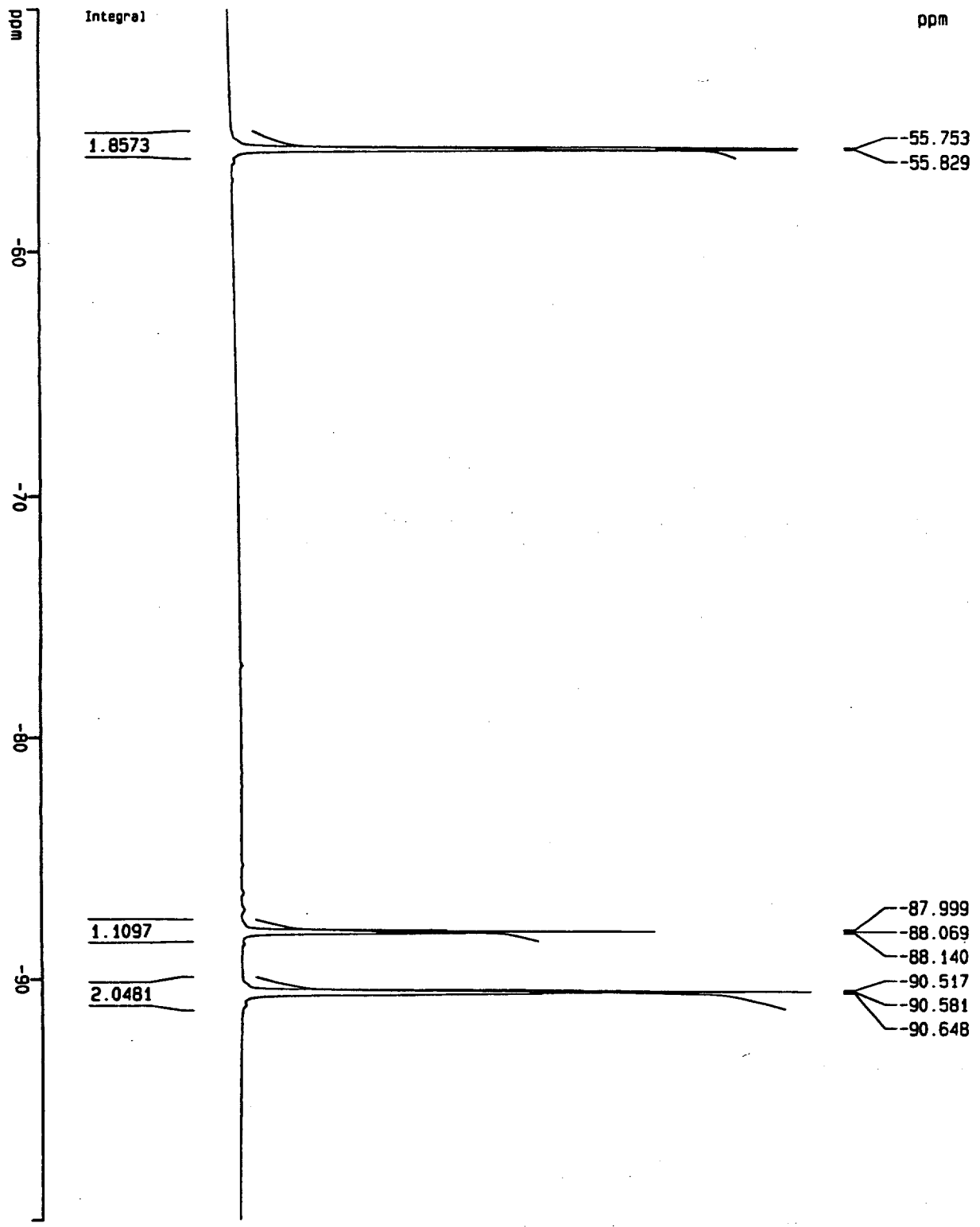
P1	4.40 usec
DE	4.50 usec
SFO1	96.2919887 MHz
NUC1	118
PL1	-6.00 dB

F2 - Processing parameters

SI	16384
SF	96.2936634 MHz
WDW	EM
SSB	0
LB	5.00 Hz
GB	0
PC	1.40

1D NMR plot parameters

CX	20.00 cm
F1P	100.000 ppm
F1	9629.37 Hz
F2P	-100.000 ppm
F2	-9629.37 Hz
PPMCM	10.00000 ppm/cm
HZCM	962.93665 Hz/cm



Current Data Parameters
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PROCNO 1

F2 - Acquisition Parameters
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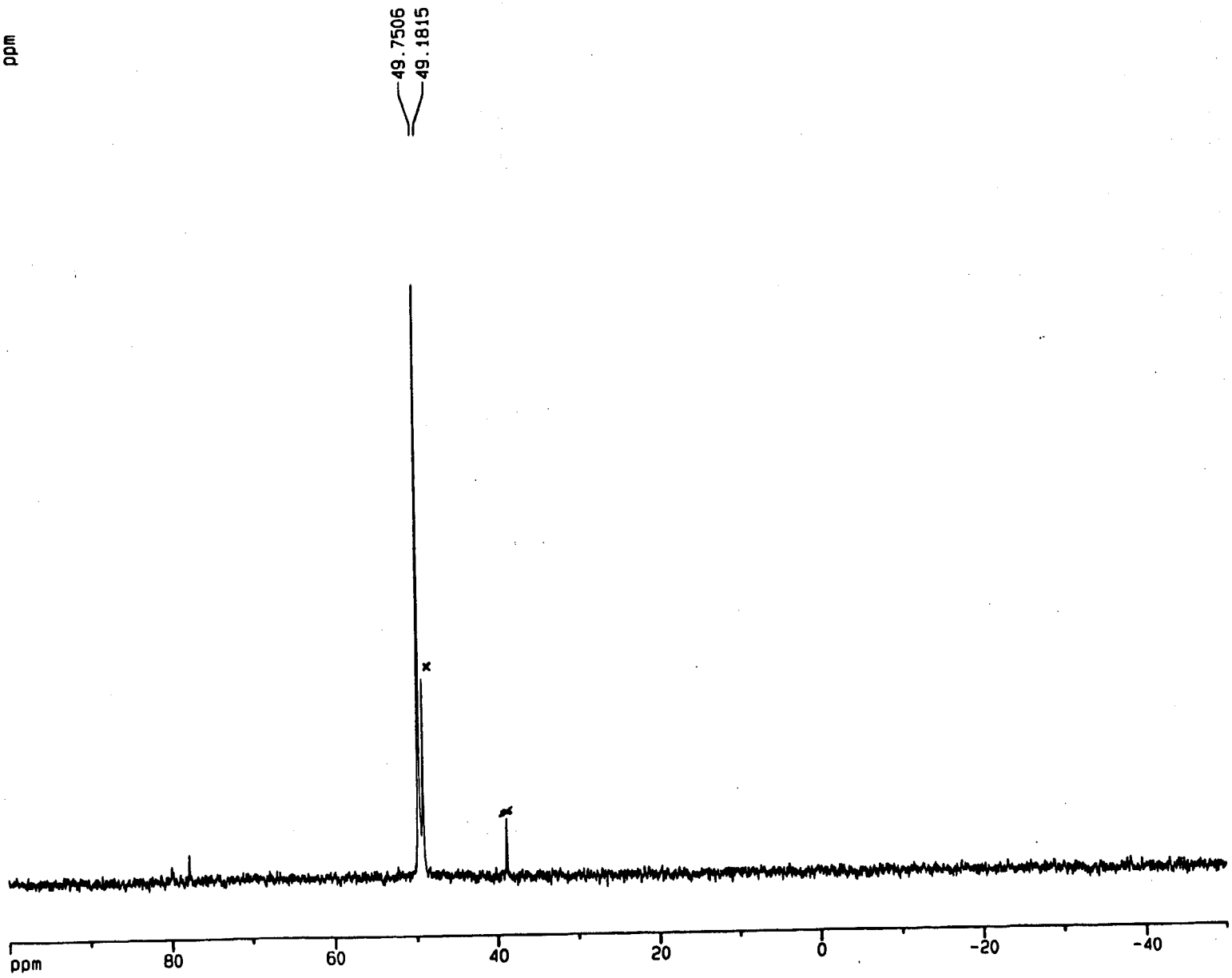
PULPROG zg30
TD 16384
SOLVENT CDCl3
NS 152
DS 0
SWH 56497.176 Hz
FIDRES 3.448314 Hz
AQ 0.1450484 sec
RG 181
DW 8.850 usec
DE 4.50 usec
TE 300.0 K
D1 1.00000000 sec
P1 5.00 usec
DE 4.50 usec
SFO1 282.3682794 MHz
NUC1 19F
PL1 -4.00 dB

F2 - Processing parameters
SI 8192
SF 282.3825348 MHz
WDW EM
SSB 0
LB 5.00 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
F1P -50.000 ppm
F1 -14119.13 Hz
F2P -100.000 ppm
F2 -28238.25 Hz
PPMCM 2.50000 ppm/
HZCM 705.95636 Hz/c

TiMe2(N=P(t-Bu)3)2 + 1.1 Barf in hex/c6d6, 31P in CH2Cl2



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PROCNO	1

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PULPROG	zgdc30
TD	32768
SOLVENT	CDCl3
NS	48
DS	0
SWH	18248.176 Hz
FIDRES	0.556890 Hz
AQ	0.8978932 sec
RG	9195.2
DW	27.400 usec
DE	4.50 usec
TE	300.0 K
D11	0.03000000 sec
PL12	16.30 dB
CPDPRG2	waltz16
PCPD2	80.00 usec
SFO2	300.1312005 MHz
NUC2	1H
PL2	-6.00 dB
D1	1.00000000 sec
P1	4.40 usec
DE	4.50 usec
SFO1	121.4978154 MHz
NUC1	31P
PL1	-6.00 dB

F2 - Processing parameters

SI	16384
SF	121.4947770 MHz
WDW	EM
SSB	0
LB	4.00 Hz
GB	0
PC	1.40

1D NMR plot parameters

CX	20.00 cm
F1P	100.000 ppm
F1	12149.48 Hz
F2P	-50.000 ppm
F2	-6074.74 Hz
PPMCM	7.50000 ppm/cm
HZCM	911.21069 Hz/cm