1. Crystal data and structure refinement for Cp*Ta(NptBu3)Cl3 1

Identification code test
Empirical formula $C_{22}H_{42}Cl_3NPTa$
Formula weight 638.84
Temperature 293(2) K
Wavelength 0.71073 A
Crystal system orthorhombic
Space group P2(1)2(1)2(1)
Unit cell dimensions
a = 8.6056(9) A alpha = 90^o
b = 14.8186(16) A beta = 90^o
c = 20.613(4) A gamma = 90^o
Volume, Z 2628.6(6) A^3, 4
Density (calculated) 1.614 Mg/m^3
Absorption coefficient 4.556 mm^-1
F(000) 1280
θ range for data collection 1.69 to 24.98^o
Limiting indices -9<h<2, -4<k<16, -1<l<19
Reflections collected 3564
Independent reflections 1561 (Rint = 0.0934)
Completeness to q = 24.98^o 54.2 %
Refinement method Full-matrix least-squares on F^2
Data / restraints / parameters 1561 / 0 / 138
Goodness-of-fit on F^2 1.432
Final R indices [I>2s(I)] R1 = 0.0499, wR2 = 0.1519
R indices (all data) R1 = 0.0540, wR2 = 0.1550
Absolute structure parameter 0.29(3)
Largest diff. peak and hole 1.055 and -1.486 eA^-3

2. Atomic coordinates [x 10^4] and equivalent isotropic displacement parameters [A^2 x 10^3]

	x	y	z	U(eq)
Ta(1)	7618(1)	6601(1)	1587(1)	25(1)
Cl(1)	5786(6)	5690(5)	968(3)	58(2)
Cl(2)	5492(6)	7668(4)	1427(3)	50(2)
Cl(3)	8444(6)	5074(3)	1882(3)	47(1)
P(1)	7131(6)	6959(3)	3217(2)	30(1)
N(1)	7580(13)	6854(9)	2476(6)	25(3)
C(1)	9410(30)	6319(16)	693(12)	51(5)
C(2)	8590(20)	7122(13)	481(10)	40(5)
C(3)	8880(30)	7837(16)	919(13)	53(6)
C(4)	9960(30)	7477(14)	1381(10)	39(5)
C(5)	10340(20)	6629(14)	1225(10)	41(4)
C(6)	9540(40)	5483(19)	343(15)	85(9)
C(7)	7460(30)	7189(17)	-94(13)	71(7)
C(8)	8480(30)	8790(20)	880(14)	79(8)
C(9)	10740(30)	8126(18)	1866(13)	70(7)
C(10)	11610(30)	6085(16)	1515(11)	51(5)
C(11)	6310(20)	8111(15)	3385(11)	43(4)
C(12)	6300(30)	8369(17)	4090(13)	63(6)
C(13)	4610(30)	8134(17)	3113(11)	57(6)
C(14)	7230(30)	8797(15)	2938(12)	58(5)
C(15)	5660(30)	6058(15)	3426(13)	50(5)
C(16)	4510(30)	5985(18)	2852(14)	62(7)
C(17)	4760(20)	6262(15)	4053(11)	44(5)
C(18)	6400(30)	5092(17)	3470(13)	61(6)
C(19)	8910(30)	6844(17)	3717(12)	55(6)
C(20)	9980(30)	6085(18)	3393(14)	66(6)

C(21)	9960(40)	7632(19)	3688(14)	69(7)
C(22)	8680(30)	6554(18)	4397(14)	70(7)

3. Bond lengths [A] and angles [^o]

Ta(1)-N(1)	1.870(13)	C(2)-C(3)	1.41(3)
Ta(1)-C(4)	2.43(2)	C(2)-C(7)	1.54(3)
Ta(1)-Cl(2)	2.440(5)	C(3)-C(4)	1.43(3)
Ta(1)-C(5)	2.458(19)	C(3)-C(8)	1.45(4)
Ta(1)-Cl(1)	2.437(5)	C(4)-C(5)	1.34(3)
Ta(1)-Cl(3)	2.449(5)	C(4)-C(9)	1.54(3)
Ta(1)-C(1)	2.44(2)	C(5)-C(10)	1.49(3)
Ta(1)-C(3)	2.54(2)	C(11)-C(12)	1.50(3)
Ta(1)-C(2)	2.55(2)	C(11)-C(13)	1.56(3)
P(1)-N(1)	1.585(14)	C(11)-C(14)	1.59(3)
P(1)-C(11)	1.88(2)	C(15)-C(18)	1.57(3)
P(1)-C(19)	1.85(2)	C(15)-C(17)	1.54(3)
P(1)-C(15)	1.89(2)	C(15)-C(16)	1.55(4)
C(1)-C(2)	1.45(3)	C(19)-C(21)	1.48(4)
C(1)-C(5)	1.43(3)	C(19)-C(22)	1.48(4)
C(1)-C(6)	1.44(4)	C(19)-C(20)	1.60(3)

N(1)-Ta(1)-C(4)	94.5(6)	C(11)-P(1)-C(19)	107.0(10)
N(1)-Ta(1)-Cl(2)	89.4(4)	N(1)-P(1)-C(15)	108.3(9)
C(4)-Ta(1)-Cl(2)	104.6(5)	C(11)-P(1)-C(15)	110.3(9)
N(1)-Ta(1)-C(5)	108.1(6)	C(19)-P(1)-C(15)	111.3(10)
C(4)-Ta(1)-C(5)	31.7(7)	P(1)-N(1)-Ta(1)	165.7(8)
Cl(2)-Ta(1)-C(5)	131.4(5)	C(2)-C(1)-C(5)	103.8(19)
N(1)-Ta(1)-Cl(1)	127.8(4)	C(2)-C(1)-C(6)	126(2)
C(4)-Ta(1)-Cl(1)	137.7(5)	C(5)-C(1)-C(6)	128(2)
Cl(2)-Ta(1)-Cl(1)	78.7(2)	C(2)-C(1)-Ta(1)	77.2(13)
C(5)-Ta(1)-Cl(1)	117.8(5)	C(5)-C(1)-Ta(1)	73.7(13)
N(1)-Ta(1)-Cl(3)	87.0(4)	C(6)-C(1)-Ta(1)	125.0(19)
C(4)-Ta(1)-Cl(3)	107.2(5)	C(1)-C(2)-C(3)	109.6(18)
Cl(2)-Ta(1)-Cl(3)	148.22(19)	C(1)-C(2)-C(7)	126.4(17)
C(5)-Ta(1)-Cl(3)	79.3(5)	C(3)-C(2)-C(7)	123.8(19)
Cl(1)-Ta(1)-Cl(3)	78.8(2)	C(1)-C(2)-Ta(1)	69.1(12)
N(1)-Ta(1)-C(1)	141.7(7)	C(3)-C(2)-Ta(1)	73.3(14)
C(4)-Ta(1)-C(1)	55.6(7)	C(7)-C(2)-Ta(1)	120.1(15)
Cl(2)-Ta(1)-C(1)	118.9(6)	C(4)-C(3)-C(2)	105(2)
C(5)-Ta(1)-C(1)	33.9(7)	C(4)-C(3)-C(8)	123(2)
Cl(1)-Ta(1)-C(1)	85.4(6)	C(2)-C(3)-C(8)	131(2)
Cl(3)-Ta(1)-C(1)	81.1(6)	C(4)-C(3)-Ta(1)	69.4(13)
N(1)-Ta(1)-C(3)	113.2(7)	C(2)-C(3)-Ta(1)	74.4(14)
C(4)-Ta(1)-C(3)	33.5(7)	C(8)-C(3)-Ta(1)	129.1(19)
Cl(2)-Ta(1)-C(3)	77.3(5)	C(5)-C(4)-C(3)	110(2)
C(5)-Ta(1)-C(3)	54.2(7)	C(5)-C(4)-C(9)	130(2)
Cl(1)-Ta(1)-C(3)	113.1(6)	C(3)-C(4)-C(9)	119(2)
Cl(3)-Ta(1)-C(3)	132.7(6)	C(5)-C(4)-Ta(1)	75.1(13)
C(1)-Ta(1)-C(3)	56.1(8)	C(3)-C(4)-Ta(1)	77.1(13)
N(1)-Ta(1)-C(2)	145.2(6)	C(9)-C(4)-Ta(1)	125.4(16)
C(4)-Ta(1)-C(2)	53.9(7)	C(4)-C(5)-C(1)	110.5(19)
Cl(2)-Ta(1)-C(2)	85.9(5)	C(4)-C(5)-C(10)	126(2)
C(5)-Ta(1)-C(2)	53.9(7)	C(1)-C(5)-C(10)	123.0(19)
Cl(1)-Ta(1)-C(2)	84.9(5)	C(4)-C(5)-Ta(1)	73.1(12)
Cl(3)-Ta(1)-C(2)	114.0(5)	C(1)-C(5)-Ta(1)	72.4(12)
C(1)-Ta(1)-C(2)	33.8(7)	C(10)-C(5)-Ta(1)	124.8(14)
C(3)-Ta(1)-C(2)	32.3(7)	C(12)-C(11)-C(13)	109.8(17)
N(1)-P(1)-C(11)	111.0(9)	C(12)-C(11)-C(14)	113.6(19)
N(1)-P(1)-C(19)	109.0(9)	C(13)-C(11)-C(14)	104.2(19)

C(12)-C(11)-P(1)	114.2(16)	C(16)-C(15)-P(1)	107.8(18)
C(13)-C(11)-P(1)	107.8(16)	C(21)-C(19)-C(22)	110(2)
C(14)-C(11)-P(1)	106.6(15)	C(21)-C(19)-C(20)	100.9(19)
C(18)-C(15)-C(17)	110(2)	C(22)-C(19)-C(20)	106(2)
C(18)-C(15)-C(16)	104(2)	C(21)-C(19)-P(1)	114.1(19)
C(17)-C(15)-C(16)	110(2)	C(22)-C(19)-P(1)	116.3(18)
C(18)-C(15)-P(1)	112.5(15)	C(20)-C(19)-P(1)	107.9(17)
C(17)-C(15)-P(1)	112.9(15)		

Symmetry transformations used to generate equivalent atoms:

4. Anisotropic displacement parameters [A^2 x 10^3]

	U11	U22	U33	U23	U13	U12
Ta(1)	24(1)	33(1)	18(1)	0(1)	0(1)	-2(1)
Cl(1)	46(3)	84(4)	43(5)	-12(3)	-5(2)	-29(3)
Cl(2)	37(3)	69(4)	43(5)	9(2)	-1(2)	20(2)
Cl(3)	59(3)	36(3)	45(5)	-1(2)	9(2)	1(2)
P(1)	38(3)	30(3)	21(4)	4(2)	0(2)	4(2)

5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3)

	x	y	z	U(eq)
H(6A)	8796	5476	-4	127
H(6B)	9336	4988	632	127
H(6C)	10568	5426	168	127
H(7A)	7462	6630	-330	107
H(7B)	7775	7671	-376	107
H(7C)	6428	7307	65	107
H(8A)	7723	8878	546	118
H(8B)	9400	9131	781	118
H(8C)	8069	8985	1289	118
H(9A)	10202	8693	1864	105
H(9B)	11805	8219	1743	105
H(9C)	10701	7870	2294	105
H(10A)	11623	5496	1321	76
H(10B)	11446	6030	1974	76
H(10C)	12589	6378	1437	76
H(12A)	7346	8346	4256	95
H(12B)	5660	7956	4328	95
H(12C)	5904	8970	4136	95
H(13A)	4617	7959	2665	86
H(13B)	4201	8734	3152	86
H(13C)	3973	7724	3356	86
H(14A)	7173	8602	2494	87
H(14B)	8300	8818	3071	87
H(14C)	6783	9388	2977	87
H(16A)	4011	6558	2785	93
H(16B)	3734	5537	2949	93
H(16C)	5059	5814	2467	93
H(17A)	4355	6865	4035	66
H(17B)	5451	6208	4418	66
H(17C)	3922	5841	4100	66
H(18A)	7167	5084	3810	91
H(18B)	6893	4946	3065	91
H(18C)	5610	4656	3562	91
H(20A)	9416	5526	3376	98
H(20B)	10902	6007	3648	98
H(20C)	10256	6267	2962	98
H(21A)	10063	7827	3246	103
H(21B)	10960	7468	3856	103

H(21C)	9533	8114	3944	103
H(22A)	7966	6056	4409	105
H(22B)	8265	7047	4645	105
H(22C)	9658	6371	4579	105

1. Crystal data and structure refinement for Cp*Ta(NPt-Bu$_3$)Me$_3$ 3

Empirical formula $C_{25}H_{51}NPTa$
Formula weight 577.59
Temperature 293(2) K
Wavelength 0.71073 A
Crystal system monoclinic
Space group P2(1)/c
Unit cell dimensions
a = 8.5530(12) A alpha = 90^o
b = 17.7655(15) A beta = 96.635(13)^o
c = 17.775(3) A gamma = 90^o
Volume, Z 2682.7(6) A^3, 4
Density (calculated) 1.430 Mg/m^3
Absorption coefficient 4.167 mm^-1
F(000) 1184
θ range for data collection 1.63 to 25.00^o
Limiting indices -10<h<6, -20<k<21, -21<l<20
Reflections collected 13620
Independent reflections 4689 (Rint = 0.0298)
Completeness to q = 25.00^o 99.2 %
Refinement method Full-matrix least-squares on F^2
Data / restraints / parameters 4689 / 0 / 253
Goodness-of-fit on F^2 0.834
Final R indices [I>2s(I)] R1 = 0.0288, wR2 = 0.0950
R indices (all data) R1 = 0.0313, wR2 = 0.0982
Largest diff. peak and hole 0.572 and -1.433 eA^-3

2. Atomic coordinates [x 10^4] and equivalent isotropic displacement parameters [A^2 x 10^3]

	x	y	z	U(eq)
Ta(1)	1439(1)	7815(1)	1046(1)	38(1)
P(1)	3304(1)	9218(1)	2172(1)	36(1)
N(1)	2592(3)	8584(2)	1611(2)	37(1)
C(1)	599(6)	7293(3)	-268(3)	63(1)
C(2)	1672(6)	7880(2)	-311(2)	53(1)
C(3)	3126(5)	7683(2)	51(2)	45(1)
C(4)	3025(5)	6954(2)	353(2)	52(1)
C(5)	1479(7)	6698(3)	151(3)	69(1)
C(6)	-1065(9)	7238(4)	-618(5)	112(3)
C(7)	1356(8)	8588(3)	-794(3)	88(2)
C(8)	4639(6)	8129(3)	45(3)	70(1)
C(9)	4370(7)	6495(3)	700(3)	84(2)
C(10)	890(9)	5914(3)	322(4)	113(3)
C(11)	1720(5)	9577(2)	2742(2)	52(1)
C(12)	579(6)	10090(3)	2256(3)	73(1)
C(13)	759(6)	8898(3)	2967(3)	68(1)
C(14)	2368(6)	10026(3)	3458(3)	70(1)
C(15)	4049(6)	10016(2)	1607(2)	54(1)
C(16)	2833(7)	10141(2)	898(3)	68(1)
C(17)	5624(6)	9810(3)	1322(3)	70(1)
C(18)	4300(8)	10778(3)	2040(3)	81(2)
C(19)	4991(5)	8805(2)	2834(2)	49(1)
C(20)	4329(6)	8292(3)	3408(3)	68(1)
C(21)	5998(6)	8306(3)	2355(3)	64(1)

C(22)	6061(6)	9397(3)	3260(3)	74(1)
C(23)	-513(5)	8650(3)	728(3)	62(1)
C(24)	-809(8)	7281(3)	1377(4)	80(2)
C(25)	2227(7)	6991(3)	1981(3)	67(1)

3. Bond lengths [A] and angles [^o]

Ta(1)-N(1)	1.902(3)	C(2)-C(3)	1.378(7)
Ta(1)-C(23)	2.257(4)	C(2)-C(7)	1.530(6)
Ta(1)-C(25)	2.259(5)	C(3)-C(4)	1.409(6)
Ta(1)-C(24)	2.280(5)	C(3)-C(8)	1.518(7)
Ta(1)-C(3)	2.421(4)	C(4)-C(5)	1.405(7)
Ta(1)-C(2)	2.447(4)	C(4)-C(9)	1.485(6)
Ta(1)-C(4)	2.467(4)	C(5)-C(10)	1.524(6)
Ta(1)-C(1)	2.540(5)	C(11)-C(12)	1.528(6)
Ta(1)-C(5)	2.546(4)	C(11)-C(13)	1.539(6)
P(1)-N(1)	1.579(3)	C(11)-C(14)	1.549(6)
P(1)-C(15)	1.890(4)	C(15)-C(17)	1.537(7)
P(1)-C(11)	1.894(4)	C(15)-C(16)	1.554(7)
P(1)-C(19)	1.902(4)	C(15)-C(18)	1.560(6)
C(1)-C(2)	1.397(7)	C(19)-C(20)	1.524(6)
C(1)-C(5)	1.451(8)	C(19)-C(22)	1.535(6)
C(1)-C(6)	1.489(8)	C(19)-C(21)	1.556(6)
N(1)-Ta(1)-C(23)	89.04(15)	N(1)-P(1)-C(11)	109.31(17)
N(1)-Ta(1)-C(25)	89.13(16)	C(15)-P(1)-C(11)	109.69(19)
C(23)-Ta(1)-C(25)	139.5(2)	N(1)-P(1)-C(19)	108.98(16)
N(1)-Ta(1)-C(24)	124.31(18)	C(15)-P(1)-C(19)	109.9(2)
C(23)-Ta(1)-C(24)	73.5(2)	C(11)-P(1)-C(19)	109.68(18)
C(25)-Ta(1)-C(24)	74.3(3)	P(1)-N(1)-Ta(1)	169.8(2)
N(1)-Ta(1)-C(3)	97.98(13)	C(2)-C(1)-C(5)	105.4(4)
C(23)-Ta(1)-C(3)	111.52(16)	C(2)-C(1)-C(6)	128.9(6)
C(25)-Ta(1)-C(3)	108.85(18)	C(5)-C(1)-C(6)	125.5(6)
C(24)-Ta(1)-C(3)	137.70(19)	C(2)-C(1)-Ta(1)	70.1(2)
N(1)-Ta(1)-C(2)	112.99(14)	C(5)-C(1)-Ta(1)	73.7(3)
C(23)-Ta(1)-C(2)	82.20(17)	C(6)-C(1)-Ta(1)	124.3(4)
C(25)-Ta(1)-C(2)	134.82(17)	C(3)-C(2)-C(1)	110.4(4)
C(24)-Ta(1)-C(2)	116.1(2)	C(3)-C(2)-C(7)	124.2(5)
C(3)-Ta(1)-C(2)	32.88(16)	C(1)-C(2)-C(7)	124.8(5)
N(1)-Ta(1)-C(4)	115.31(14)	C(3)-C(2)-Ta(1)	72.5(2)
C(23)-Ta(1)-C(4)	135.75(15)	C(1)-C(2)-Ta(1)	77.4(3)
C(25)-Ta(1)-C(4)	80.29(17)	C(7)-C(2)-Ta(1)	124.3(3)
C(24)-Ta(1)-C(4)	113.55(19)	C(2)-C(3)-C(4)	108.6(4)
C(3)-Ta(1)-C(4)	33.49(14)	C(2)-C(3)-C(8)	126.1(4)
C(2)-Ta(1)-C(4)	54.84(14)	C(4)-C(3)-C(8)	124.9(4)
N(1)-Ta(1)-C(1)	145.32(16)	C(2)-C(3)-Ta(1)	74.6(3)
C(23)-Ta(1)-C(1)	83.54(16)	C(4)-C(3)-Ta(1)	75.1(3)
C(25)-Ta(1)-C(1)	117.96(17)	C(8)-C(3)-Ta(1)	122.4(3)
C(24)-Ta(1)-C(1)	85.9(2)	C(5)-C(4)-C(3)	107.3(4)
C(3)-Ta(1)-C(1)	54.62(16)	C(5)-C(4)-C(9)	126.2(5)
C(2)-Ta(1)-C(1)	32.47(16)	C(3)-C(4)-C(9)	125.8(5)
C(4)-Ta(1)-C(1)	55.04(16)	C(5)-C(4)-Ta(1)	76.8(3)
N(1)-Ta(1)-C(5)	147.78(16)	C(3)-C(4)-Ta(1)	71.4(2)
C(23)-Ta(1)-C(5)	114.76(18)	C(9)-C(4)-Ta(1)	125.2(3)
C(25)-Ta(1)-C(5)	86.03(18)	C(4)-C(5)-C(1)	108.3(4)
C(24)-Ta(1)-C(5)	84.83(18)	C(4)-C(5)-C(10)	124.6(6)
C(3)-Ta(1)-C(5)	54.22(14)	C(1)-C(5)-C(10)	127.1(6)
C(2)-Ta(1)-C(5)	53.95(15)	C(4)-C(5)-Ta(1)	70.7(2)
C(4)-Ta(1)-C(5)	32.50(16)	C(1)-C(5)-Ta(1)	73.2(2)
C(1)-Ta(1)-C(5)	33.15(17)	C(10)-C(5)-Ta(1)	124.0(3)
N(1)-P(1)-C(15)	109.27(17)	C(12)-C(11)-C(13)	106.8(4)

C(12)-C(11)-C(14)	107.6(4)	C(16)-C(15)-P(1)	107.6(3)
C(13)-C(11)-C(14)	109.9(4)	C(18)-C(15)-P(1)	115.2(3)
C(12)-C(11)-P(1)	110.4(3)	C(20)-C(19)-C(22)	109.1(4)
C(13)-C(11)-P(1)	108.2(3)	C(20)-C(19)-C(21)	107.3(4)
C(14)-C(11)-P(1)	113.8(3)	C(22)-C(19)-C(21)	108.9(4)
C(17)-C(15)-C(16)	107.3(4)	C(20)-C(19)-P(1)	109.3(3)
C(17)-C(15)-C(18)	107.1(4)	C(22)-C(19)-P(1)	114.0(3)
C(16)-C(15)-C(18)	108.5(4)	C(21)-C(19)-P(1)	108.0(3)
C(17)-C(15)-P(1)	111.0(3)		

Symmetry transformations used to generate equivalent atoms:

4. Anisotropic displacement parameters [A^2 x 10^3]

	U11	U22	U33	U23	U13	U12
Ta(1)	35(1)	39(1)	41(1)	-2(1)	10(1)	-3(1)
P(1)	34(1)	39(1)	36(1)	1(1)	7(1)	1(1)
N(1)	39(2)	37(1)	36(1)	3(1)	8(1)	3(1)
C(1)	44(3)	88(3)	57(3)	-32(2)	6(2)	-1(2)
C(2)	65(3)	58(2)	38(2)	-2(2)	6(2)	7(2)
C(3)	50(2)	49(2)	37(2)	-2(2)	12(2)	1(2)
C(4)	61(3)	50(2)	45(2)	0(2)	18(2)	10(2)
C(5)	96(4)	46(2)	72(3)	-19(2)	44(3)	-28(2)
C(6)	60(4)	173(8)	98(5)	-69(4)	-11(4)	-10(4)
C(7)	126(5)	81(3)	57(3)	22(2)	11(3)	33(3)
C(8)	62(3)	83(3)	68(3)	-13(3)	25(2)	-14(3)
C(9)	98(4)	84(3)	72(3)	14(3)	22(3)	40(3)
C(10)	173(7)	63(3)	116(5)	-34(3)	80(5)	-61(4)
C(11)	48(2)	57(2)	51(2)	-6(2)	13(2)	5(2)
C(12)	62(3)	66(3)	91(3)	-19(2)	4(3)	25(2)
C(13)	51(3)	90(3)	69(3)	1(2)	33(2)	-2(2)
C(14)	74(3)	81(3)	58(3)	-25(2)	16(2)	11(2)
C(15)	67(3)	44(2)	53(2)	1(2)	11(2)	-18(2)
C(16)	98(4)	52(2)	55(2)	15(2)	10(2)	-5(2)
C(17)	69(3)	77(3)	70(3)	4(2)	27(2)	-19(2)
C(18)	107(4)	56(3)	80(3)	-7(2)	11(3)	-24(3)
C(19)	43(2)	58(2)	45(2)	-2(2)	-3(2)	8(2)
C(20)	78(3)	74(3)	50(2)	14(2)	5(2)	15(2)
C(21)	51(3)	72(3)	67(3)	-6(2)	1(2)	18(2)
C(22)	57(3)	97(4)	64(3)	-15(3)	-8(2)	0(3)
C(23)	38(2)	77(3)	69(3)	-17(2)	-6(2)	15(2)
C(24)	67(4)	87(4)	93(4)	-15(3)	40(3)	-27(3)
C(25)	99(4)	48(2)	58(3)	8(2)	27(3)	-8(3)

5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3)

	x	y	z	U(eq)
H(6A)	-1518	6777	-462	168
H(6B)	-1096	7243	-1160	168
H(6C)	-1652	7657	-459	168
H(7A)	246	8636	-944	132
H(7B)	1896	8551	-1237	132
H(7C)	1728	9022	-505	132
H(8A)	5499	7849	304	105
H(8B)	4541	8602	295	105
H(8C)	4835	8216	-469	105
H(9A)	5311	6794	746	125
H(9B)	4505	6066	385	125
H(9C)	4163	6328	1193	125
H(10A)	-221	5884	166	169
H(10B)	1091	5819	856	169

H(10C)	1429	5547	51	169
H(12A)	258	9850	1779	110
H(12B)	1090	10558	2170	110
H(12C)	-329	10184	2514	110
H(13A)	420	8604	2525	102
H(13B)	-145	9073	3190	102
H(13C)	1401	8594	3327	102
H(14A)	3063	10414	3321	105
H(14B)	2933	9692	3817	105
H(14C)	1508	10250	3680	105
H(16A)	1830	10268	1057	102
H(16B)	2735	9688	602	102
H(16C)	3183	10544	599	102
H(17A)	6401	9719	1747	105
H(17B)	5963	10217	1025	105
H(17C)	5492	9364	1016	105
H(18A)	3335	10927	2225	121
H(18B)	4612	11158	1703	121
H(18C)	5106	10720	2459	121
H(20A)	3630	7931	3146	101
H(20B)	3763	8589	3738	101
H(20C)	5177	8033	3701	101
H(21A)	6442	8613	1990	96
H(21B)	5343	7925	2098	96
H(21C)	6829	8072	2682	96
H(22A)	6461	9730	2901	111
H(22B)	6922	9151	3556	111
H(22C)	5467	9682	3588	111
H(23A)	-380	8873	248	93
H(23B)	-481	9037	1108	93
H(23C)	-1510	8397	694	93
H(24A)	-572	6793	1593	120
H(24B)	-1561	7231	935	120
H(24C)	-1239	7595	1742	120
H(25A)	3164	6738	1868	100
H(25B)	1410	6627	2021	100
H(25C)	2440	7256	2452	100

1. Crystal data and structure refinement for Cp*Ta(NptBu$_3$)Cl$_2$(CH$_2$Ph) 5

□
Empirical formula C29H49NPTaCl2
□
Formula weight 694.51
□
Temperature 293(2) K
□
Wavelength 0.71073 &GA
□
Crystal system monoclinic
Space group P2(1)/n
Unit cell dimensions
a = 10.9948(5) A alpha =& 90

b = 19.1989(8) A beta =& 91.8000(10)
c = 15.0970(6) A gamma =& 90
Volume, Z 3185.2(2) A^3, 4
Density (calculated)1.448 Mg/m^3
Absorption coefficient&9&1 3.686 mm^-1

F(000) 1408
Crystal size 0.22 x 0.23 x 0.25 mm
θ range for data collection&5 1.72 to 25.00^o&0
Limiting indices-11 < h< 13, -21 <k<22, -17<l<17
Reflections collected&2&9 16302
Independent reflections 5576 (Rint = 0.0426)
Completeness to θ = 25.00^o 99.6 %
Refinement method&6&9 Full-matrix least-squares on F^2
Data / restraints / parameters 5576 / 0 / 307
Goodness-of-fit on F^2 1.011
Final R indices [I>2s(I)]R1 = 0.0381, wR2 = 0.0955
R indices (all data)R1 = 0.0444, wR2 = 0.0975
Largest diff. peak and hole 1.763 and -3.249 eA^-3

Table 2. Atomic coordinates [x 10&^4&0] and equivalent isotropic displacement parameters [&GA&^2&0 x 10&^3&0]

	x	y	z	U(eq)
Ta	1491(1)	1128(1)	2134(1)	34(1)
Cl(1)	1511(1)	1802(1)	3519(1)	50(1)
Cl(2)	976(1)	1129(1)	538(1)	54(1)
P(1)	4132(1)	2018(1)	1609(1)	39(1)
N(1)	2989(3)	1539(2)	1866(2)	39(1)
C(1)	1443(5)	-134(2)	1805(3)	45(1)
C(2)	2324(5)	-11(3)	2499(4)	50(1)
C(3)	1708(5)	192(2)	3271(3)	49(1)
C(4)	436(5)	183(2)	3055(3)	46(1)
C(5)	271(5)	-24(3)	2161(3)	44(1)
C(6)	1720(6)	-472(3)	921(4)	72(2)
C(7)	3679(5)	-188(3)	2460(6)	80(2)
C(8)	2289(6)	274(3)	4176(4)	76(2)
C(9)	-561(6)	324(3)	3699(4)	69(2)
C(10)	-916(5)	-151(3)	1667(4)	67(2)
C(11)	5137(5)	1508(3)	829(4)	54(1)
C(12)	4301(6)	1089(3)	185(5)	70(2)
C(13)	5938(6)	968(4)	1365(5)	79(2)
C(14)	6001(6)	1968(3)	296(4)	72(2)
C(15)	5010(5)	2256(3)	2670(4)	56(1)
C(16)	5100(5)	1605(4)	3288(4)	69(2)
C(17)	6317(5)	2531(4)	2519(5)	84(2)
C(18)	4317(6)	2830(4)	3195(4)	78(2)
C(19)	3527(5)	2836(3)	1024(4)	52(1)
C(20)	4487(6)	3422(3)	961(4)	70(2)
C(21)	2417(5)	3105(3)	1541(4)	70(2)
C(22)	3044(6)	2658(3)	88(4)	72(2)
C(23)	-427(4)	1619(3)	2086(4)	49(1)
C(24)	-626(4)	2374(3)	1839(4)	49(1)
C(25)	-673(5)	2902(3)	2477(4)	58(1)
C(26)	-967(5)	3575(3)	2260(5)	70(2)
C(27)	-1216(7)	3758(4)	1393(6)	83(2)
C(28)	-1161(6)	3256(4)	751(5)	84(2)
C(29)	-872(5)	2565(3)	959(4)	64(2)

Table 3. Bond lengths [&GA] and angles [&^o&0]

Ta-N(1)	1.882(4)	Ta-C(2)	2.429(5)
Ta-C(23)	2.309(5)	Ta-Cl(2)	2.4572(13)

Ta-Cl(1)	2.4580(12)
Ta-C(1)	2.475(5)
Ta-C(3)	2.492(5)
Ta-C(4)	2.583(5)
Ta-C(5)	2.589(5)
P(1)-N(1)	1.614(4)
P(1)-C(15)	1.900(5)
P(1)-C(19)	1.910(5)
P(1)-C(11)	1.910(5)
C(1)-C(2)	1.425(7)
C(1)-C(5)	1.428(7)
C(1)-C(6)	1.523(7)
C(2)-C(3)	1.420(8)
C(2)-C(7)	1.531(8)
C(3)-C(4)	1.426(7)
C(3)-C(8)	1.498(7)
C(4)-C(5)	1.414(7)
C(4)-C(9)	1.511(7)
C(5)-C(10)	1.502(7)
C(11)-C(14)	1.543(7)
C(11)-C(12)	1.543(8)
C(11)-C(13)	1.568(9)
C(15)-C(17)	1.555(7)
C(15)-C(16)	1.559(8)
C(15)-C(18)	1.568(8)
C(19)-C(22)	1.533(8)
C(19)-C(20)	1.548(7)
C(19)-C(21)	1.558(7)
C(23)-C(24)	1.511(7)
C(24)-C(29)	1.395(8)
C(24)-C(25)	1.401(8)
C(25)-C(26)	1.370(8)
C(26)-C(27)	1.374(10)
C(27)-C(28)	1.371(11)
C(28)-C(29)	1.397(9)

N(1)-Ta-C(23)	128.85(18)
N(1)-Ta-C(2)	95.72(17)
C(23)-Ta-C(2)	135.43(18)
N(1)-Ta-Cl(2)	87.99(12)
C(23)-Ta-Cl(2)	77.69(14)
C(2)-Ta-Cl(2)	107.25(14)
N(1)-Ta-Cl(1)	88.76(12)
C(23)-Ta-Cl(1)	78.22(14)
C(2)-Ta-Cl(1)	106.73(14)
Cl(2)-Ta-Cl(1)	146.02(5)
N(1)-Ta-C(1)	112.36(16)
C(23)-Ta-C(1)	112.30(18)
C(2)-Ta-C(1)	33.78(17)
Cl(2)-Ta-C(1)	78.49(13)
Cl(1)-Ta-C(1)	133.32(12)
N(1)-Ta-C(3)	112.66(17)
C(23)-Ta-C(3)	112.56(18)
C(2)-Ta-C(3)	33.51(18)
Cl(2)-Ta-C(3)	133.58(12)
Cl(1)-Ta-C(3)	78.24(12)
C(1)-Ta-C(3)	55.42(16)
N(1)-Ta-C(4)	145.21(16)
C(23)-Ta-C(4)	83.00(17)
C(2)-Ta-C(4)	54.39(17)
Cl(2)-Ta-C(4)	115.75(12)
Cl(1)-Ta-C(4)	84.48(11)
C(1)-Ta-C(4)	54.07(15)
C(3)-Ta-C(4)	32.58(16)
N(1)-Ta-C(5)	144.99(16)
C(23)-Ta-C(5)	82.86(17)
C(2)-Ta-C(5)	54.44(18)
Cl(2)-Ta-C(5)	84.95(11)
Cl(1)-Ta-C(5)	115.30(11)
C(1)-Ta-C(5)	32.65(16)
C(3)-Ta-C(5)	53.90(16)
C(4)-Ta-C(5)	31.73(15)
N(1)-P(1)-C(15)	108.2(2)
N(1)-P(1)-C(19)	108.5(2)
C(15)-P(1)-C(19)	110.7(3)
N(1)-P(1)-C(11)	109.0(2)
C(15)-P(1)-C(11)	110.8(3)
C(19)-P(1)-C(11)	109.6(2)
P(1)-N(1)-Ta	169.6(3)
C(2)-C(1)-C(5)	107.4(5)
C(2)-C(1)-C(6)	124.4(5)
C(5)-C(1)-C(6)	126.9(5)
C(2)-C(1)-Ta	71.3(3)
C(5)-C(1)-Ta	78.1(3)
C(6)-C(1)-Ta	126.1(4)
C(3)-C(2)-C(1)	108.5(4)
C(3)-C(2)-C(7)	125.7(5)
C(1)-C(2)-C(7)	125.1(6)
C(3)-C(2)-Ta	75.7(3)
C(1)-C(2)-Ta	74.9(3)
C(7)-C(2)-Ta	123.5(4)
C(2)-C(3)-C(4)	107.5(4)
C(2)-C(3)-C(8)	125.2(5)
C(4)-C(3)-C(8)	126.6(5)
C(2)-C(3)-Ta	70.8(3)
C(4)-C(3)-Ta	77.2(3)
C(8)-C(3)-Ta	125.5(4)
C(5)-C(4)-C(3)	108.4(4)
C(5)-C(4)-C(9)	126.2(5)
C(3)-C(4)-C(9)	125.2(5)
C(5)-C(4)-Ta	74.4(3)
C(3)-C(4)-Ta	70.2(3)
C(9)-C(4)-Ta	124.6(3)
C(4)-C(5)-C(1)	108.1(4)
C(4)-C(5)-C(10)	127.1(5)
C(1)-C(5)-C(10)	124.7(5)
C(4)-C(5)-Ta	73.9(3)
C(1)-C(5)-Ta	69.3(3)
C(10)-C(5)-Ta	125.0(4)
C(14)-C(11)-C(12)	109.5(5)
C(14)-C(11)-C(13)	107.6(5)
C(12)-C(11)-C(13)	107.2(5)

C(14)-C(11)-P(1)	113.9(4)	C(22)-C(19)-P(1)	110.4(4)
C(12)-C(11)-P(1)	108.1(4)	C(20)-C(19)-P(1)	113.5(4)
C(13)-C(11)-P(1)	110.3(4)	C(21)-C(19)-P(1)	107.9(4)
C(17)-C(15)-C(16)	108.5(5)	C(24)-C(23)-Ta	121.6(3)
C(17)-C(15)-C(18)	107.5(5)	C(29)-C(24)-C(25)	117.0(5)
C(16)-C(15)-C(18)	106.5(5)	C(29)-C(24)-C(23)	120.5(5)
C(17)-C(15)-P(1)	113.9(4)	C(25)-C(24)-C(23)	122.2(5)
C(16)-C(15)-P(1)	109.5(4)	C(26)-C(25)-C(24)	122.2(6)
C(18)-C(15)-P(1)	110.6(4)	C(25)-C(26)-C(27)	120.4(7)
C(22)-C(19)-C(20)	108.8(5)	C(28)-C(27)-C(26)	118.8(7)
C(22)-C(19)-C(21)	106.3(5)	C(27)-C(28)-C(29)	121.6(7)
C(20)-C(19)-C(21)	109.6(5)	C(24)-C(29)-C(28)	119.9(7)

Table 4. Anisotropic displacement parameters [&GA&^2&0 x 10&^3&0]

	U11	U22	U33	U23	U13	U12
Ta	36(1)	33(1)	35(1)	-1(1)	1(1)	-3(1)
Cl(1)	57(1)	51(1)	44(1)	-12(1)	5(1)	0(1)
Cl(2)	63(1)	59(1)	39(1)	-3(1)	-8(1)	-5(1)
P(1)	39(1)	34(1)	45(1)	-1(1)	5(1)	-3(1)
N(1)	36(2)	40(2)	42(2)	0(2)	4(2)	-4(2)
C(1)	60(3)	23(2)	51(3)	0(2)	6(2)	-2(2)
C(2)	51(3)	28(3)	71(4)	14(2)	3(3)	-1(2)
C(3)	63(3)	32(3)	50(3)	7(2)	-9(2)	-9(2)
C(4)	62(3)	31(3)	46(3)	3(2)	11(2)	-6(2)
C(5)	52(3)	33(3)	48(3)	-2(2)	0(2)	-8(2)
C(6)	102(5)	55(4)	61(4)	-8(3)	23(3)	0(4)
C(7)	59(4)	54(4)	127(6)	23(4)	6(4)	10(3)
C(8)	110(5)	57(4)	61(4)	19(3)	-27(3)	-18(4)
C(9)	86(4)	59(4)	64(4)	4(3)	32(3)	-8(3)
C(10)	62(4)	61(4)	77(4)	-4(3)	-7(3)	-16(3)
C(11)	56(3)	43(3)	64(3)	0(3)	22(3)	-1(2)
C(12)	82(5)	61(4)	69(4)	-19(3)	26(3)	-6(3)
C(13)	60(4)	67(4)	112(6)	7(4)	21(4)	17(3)
C(14)	79(4)	59(4)	80(4)	0(3)	42(3)	-3(3)
C(15)	46(3)	61(4)	60(3)	-6(3)	-5(2)	-15(3)
C(16)	59(3)	79(4)	68(4)	15(3)	-6(3)	-15(3)
C(17)	55(4)	104(6)	93(5)	1(4)	-3(3)	-33(4)
C(18)	73(4)	91(5)	70(4)	-28(4)	3(3)	-28(4)
C(19)	54(3)	37(3)	64(3)	8(2)	6(2)	1(2)
C(20)	80(4)	41(3)	91(5)	3(3)	17(3)	-8(3)
C(21)	65(4)	45(3)	101(5)	9(3)	12(3)	12(3)
C(22)	92(5)	53(4)	69(4)	16(3)	-10(3)	3(3)
C(23)	38(3)	52(3)	58(3)	3(3)	2(2)	-1(2)
C(24)	31(2)	57(3)	59(3)	7(3)	2(2)	-2(2)
C(25)	43(3)	63(4)	66(4)	6(3)	-1(2)	2(3)
C(26)	53(3)	53(4)	103(5)	-2(4)	-2(3)	-4(3)
C(27)	70(5)	57(4)	120(7)	25(4)	-2(4)	3(3)
C(28)	77(5)	88(5)	88(5)	31(4)	-1(4)	13(4)
C(29)	58(3)	68(4)	67(4)	13(3)	-6(3)	10(3)

Table 5. Hydrogen coordinates (x 10&^4&0) and isotropic displacement parameters (&GA&^2&0 x 10&^3&0)

	x	y	z	U(eq)
H(6A)	1634	-968	969	108
H(6B)	2537	-361	766	108
H(6C)	1162	-300	470	108

H(7A)	3804	-666	2628	120
H(7B)	4136	109	2860	120
H(7C)	3948	-119	1868	120
H(8A)	2259	-162	4486	115
H(8B)	1859	622	4498	115
H(8C)	3121	415	4122	115
H(9A)	-809	-106	3962	103
H(9B)	-1244	533	3389	103
H(9C)	-263	635	4154	103
H(10A)	-1187	-617	1780	100
H(10B)	-805	-93	1043	100
H(10C)	-1512	175	1862	100
H(12A)	4789	829	-214	105
H(12B)	3784	1404	-147	105
H(12C)	3809	775	516	105
H(13A)	6438	716	966	119
H(13B)	5420	649	1665	119
H(13C)	6446	1210	1793	119
H(14A)	6477	1680	-80	107
H(14B)	6533	2221	698	107
H(14C)	5532	2291	-60	107
H(16A)	5544	1725	3824	103
H(16B)	5515	1237	2991	103
H(16C)	4297	1453	3428	103
H(17A)	6706	2640	3080	126
H(17B)	6274	2942	2158	126
H(17C)	6778	2180	2226	126
H(18A)	4774	2943	3728	117
H(18B)	3529	2658	3344	117
H(18C)	4225	3239	2834	117
H(20A)	4129	3817	661	106
H(20B)	5165	3257	635	106
H(20C)	4761	3557	1546	106
H(21A)	2097	3517	1259	105
H(21B)	2670	3212	2140	105
H(21C)	1798	2752	1542	105
H(22A)	2745	3074	-198	108
H(22B)	2395	2325	123	108
H(22C)	3689	2464	-248	108
H(23A)	-922	1343	1674	59
H(23B)	-763	1553	2666	59
H(25A)	-499	2792	3067	69
H(26A)	-999	3911	2703	84
H(27A)	-1417	4215	1245	99
H(28A)	-1321	3377	163	101
H(29A)	-843	2232	512	77

1. Crystal data and structure refinement for Cp*Ta(NPt-Bu$_3$)(CHPh)(CH$_2$Ph) 7

Empirical formula $C_{36}H_{55}NPTa$
Formula weight 713.73
Temperature 293(2) K
Wavelength 0.71073 A
Crystal system monoclinic
Space group P2(1)/c
Unit cell dimensions
a = 12.1887(17) A alpha = 90^o
b = 17.329(5) A beta = 103.290(10)^o
c = 16.950(2) A gamma = 90^o
Volume, Z 3484.2(12) A^3, 4

Density (calculated) 1.361 Mg/m^3
Absorption coefficient 3.223 mm^-1
F(000) 1464
θ range for data collection 2.08 to 25.00^o
Limiting indices -14<h<14, -20<k<20, -19<l<20
Reflections collected 17008
Independent reflections 6093 (Rint = 0.0799)
Completeness to q = 25.00^o 99.1 %
Refinement method Full-matrix least-squares on F^2
Data / restraints / parameters 6093 / 0 / 352
Goodness-of-fit on F^2 0.625
Final R indices [I>2s(I)] R1 = 0.0351, wR2 = 0.0857
R indices (all data) R1 = 0.0807, wR2 = 0.1100
Largest diff. peak and hole 0.461 and -0.881 eA^-3

2. Atomic coordinates [x 10^4] and equivalent isotropic displacement parameters [A^2 x 10^3]

	x	y	z	U(eq)
Ta(1)	1977(1)	1602(1)	2288(1)	43(1)
P(1)	-795(1)	1908(1)	1284(1)	49(1)
N(1)	505(4)	1852(3)	1728(3)	49(1)
C(1)	3633(6)	2271(6)	2019(5)	66(2)
C(2)	4087(5)	1881(5)	2734(5)	59(2)
C(3)	3601(6)	2143(4)	3351(4)	54(2)
C(4)	2811(6)	2725(5)	3025(6)	67(2)
C(5)	2881(6)	2821(5)	2200(6)	70(3)
C(6)	4043(9)	2230(8)	1249(5)	121(4)
C(7)	5012(6)	1286(6)	2863(6)	89(3)
C(8)	3925(8)	1960(6)	4235(5)	95(3)
C(9)	2203(9)	3224(6)	3502(9)	131(5)
C(10)	2337(10)	3473(6)	1658(9)	163(8)
C(11)	-1404(6)	2808(5)	1630(5)	69(2)
C(12)	-946(9)	3511(6)	1255(7)	101(4)
C(13)	-2698(7)	2869(7)	1416(6)	100(3)
C(14)	-978(8)	2893(7)	2552(5)	104(4)
C(15)	-906(7)	1962(6)	152(5)	74(2)
C(16)	-2079(7)	2235(7)	-343(5)	106(4)
C(17)	-703(9)	1142(7)	-157(6)	117(4)
C(18)	20(8)	2451(7)	-20(6)	109(4)
C(19)	-1560(7)	1036(5)	1548(6)	79(3)
C(20)	-863(7)	314(6)	1498(7)	107(4)
C(21)	-2767(7)	933(7)	1003(7)	121(4)
C(22)	-1655(8)	1102(7)	2444(7)	113(4)
C(23)	2264(6)	760(5)	1357(4)	62(2)
C(24)	3169(5)	159(4)	1467(4)	52(2)
C(25)	3264(6)	-406(5)	2061(5)	71(2)
C(26)	4063(9)	-966(6)	2133(7)	101(3)
C(27)	4805(7)	-1001(6)	1636(6)	88(3)
C(28)	4729(6)	-454(5)	1057(6)	75(2)
C(29)	3909(6)	105(5)	967(5)	70(2)
C(30)	1789(6)	907(4)	3158(5)	58(2)
C(31)	2124(6)	502(4)	3943(4)	54(2)
C(32)	3156(6)	129(5)	4187(5)	69(2)
C(33)	3440(8)	-251(6)	4938(6)	89(3)
C(34)	2713(9)	-252(6)	5436(6)	88(3)
C(35)	1687(8)	89(5)	5207(5)	80(3)
C(36)	1390(7)	467(5)	4465(5)	66(2)

3. Bond lengths [A] and angles [^o]

Ta(1)-N(1)	1.877(5)
Ta(1)-C(30)	1.957(7)
Ta(1)-C(23)	2.235(7)
Ta(1)-C(5)	2.403(7)
Ta(1)-C(4)	2.407(8)
Ta(1)-C(1)	2.461(7)
Ta(1)-C(3)	2.530(7)
Ta(1)-C(2)	2.555(6)
P(1)-N(1)	1.593(5)
P(1)-C(19)	1.882(9)
P(1)-C(11)	1.877(8)
P(1)-C(15)	1.896(8)
C(1)-C(2)	1.388(10)
C(1)-C(5)	1.404(12)
C(1)-C(6)	1.502(11)
C(2)-C(3)	1.391(10)
C(2)-C(7)	1.506(11)
C(3)-C(4)	1.416(10)
C(3)-C(8)	1.493(10)
C(4)-C(5)	1.431(13)
C(4)-C(9)	1.491(13)
C(5)-C(10)	1.509(11)
C(11)-C(14)	1.538(11)
C(11)-C(13)	1.539(10)
C(11)-C(12)	1.538(13)
C(15)-C(18)	1.494(13)
C(15)-C(17)	1.553(14)
C(15)-C(16)	1.556(10)
C(19)-C(20)	1.526(13)
C(19)-C(22)	1.554(14)
C(19)-C(21)	1.557(10)
C(23)-C(24)	1.497(9)
C(24)-C(29)	1.376(10)
C(24)-C(25)	1.391(11)
C(25)-C(26)	1.360(11)
C(26)-C(27)	1.371(13)
C(27)-C(28)	1.353(12)
C(28)-C(29)	1.374(11)
C(30)-C(31)	1.477(10)
C(31)-C(32)	1.389(10)
C(31)-C(36)	1.397(10)
C(32)-C(33)	1.404(11)
C(33)-C(34)	1.357(13)
C(34)-C(35)	1.357(12)
C(35)-C(36)	1.390(11)

N(1)-Ta(1)-C(30)	105.0(3)
N(1)-Ta(1)-C(23)	94.6(2)
C(30)-Ta(1)-C(23)	101.2(3)
N(1)-Ta(1)-C(5)	99.5(2)
C(30)-Ta(1)-C(5)	136.2(3)
C(23)-Ta(1)-C(5)	112.4(3)
N(1)-Ta(1)-C(4)	108.4(3)
C(30)-Ta(1)-C(4)	102.4(3)
C(23)-Ta(1)-C(4)	141.1(3)
C(5)-Ta(1)-C(4)	34.6(3)
N(1)-Ta(1)-C(1)	121.8(3)
C(30)-Ta(1)-C(1)	132.3(3)
C(23)-Ta(1)-C(1)	84.7(3)
C(5)-Ta(1)-C(1)	33.5(3)
C(4)-Ta(1)-C(1)	56.6(3)
N(1)-Ta(1)-C(3)	140.8(3)
C(30)-Ta(1)-C(3)	84.2(3)
C(23)-Ta(1)-C(3)	121.4(3)
C(5)-Ta(1)-C(3)	54.8(2)
C(4)-Ta(1)-C(3)	33.2(2)
C(1)-Ta(1)-C(3)	54.3(2)
N(1)-Ta(1)-C(2)	152.4(3)
C(30)-Ta(1)-C(2)	100.2(3)
C(23)-Ta(1)-C(2)	91.2(3)
C(5)-Ta(1)-C(2)	53.6(3)
C(4)-Ta(1)-C(2)	54.4(3)
C(1)-Ta(1)-C(2)	32.1(2)
C(3)-Ta(1)-C(2)	31.7(2)
N(1)-P(1)-C(19)	109.4(3)
N(1)-P(1)-C(11)	109.0(3)
C(19)-P(1)-C(11)	109.8(4)
N(1)-P(1)-C(15)	108.2(3)
C(19)-P(1)-C(15)	110.8(4)
C(11)-P(1)-C(15)	109.5(4)
P(1)-N(1)-Ta(1)	169.7(4)
C(2)-C(1)-C(5)	106.8(7)
C(2)-C(1)-C(6)	126.2(9)
C(5)-C(1)-C(6)	125.9(9)
C(2)-C(1)-Ta(1)	77.7(4)
C(5)-C(1)-Ta(1)	71.0(4)
C(6)-C(1)-Ta(1)	126.2(6)
C(3)-C(2)-C(1)	110.1(7)
C(3)-C(2)-C(7)	123.3(8)
C(1)-C(2)-C(7)	126.5(8)
C(3)-C(2)-Ta(1)	73.1(4)
C(1)-C(2)-Ta(1)	70.2(4)
C(7)-C(2)-Ta(1)	125.6(6)
C(2)-C(3)-C(4)	108.0(7)
C(2)-C(3)-C(8)	128.7(8)
C(4)-C(3)-C(8)	122.8(8)
C(2)-C(3)-Ta(1)	75.1(4)
C(4)-C(3)-Ta(1)	68.6(4)
C(8)-C(3)-Ta(1)	128.2(5)
C(3)-C(4)-C(5)	106.0(8)
C(3)-C(4)-C(9)	125.4(10)
C(5)-C(4)-C(9)	127.7(10)
C(3)-C(4)-Ta(1)	78.2(5)
C(5)-C(4)-Ta(1)	72.5(5)
C(9)-C(4)-Ta(1)	123.1(6)
C(1)-C(5)-C(4)	108.9(7)
C(1)-C(5)-C(10)	126.3(11)
C(4)-C(5)-C(10)	124.4(11)
C(1)-C(5)-Ta(1)	75.5(4)
C(4)-C(5)-Ta(1)	72.9(4)
C(10)-C(5)-Ta(1)	123.5(6)
C(14)-C(11)-C(13)	108.7(7)
C(14)-C(11)-C(12)	105.9(8)
C(13)-C(11)-C(12)	107.3(7)
C(14)-C(11)-P(1)	109.4(6)
C(13)-C(11)-P(1)	116.2(6)
C(12)-C(11)-P(1)	108.8(6)
C(18)-C(15)-C(17)	105.5(8)

C(18)-C(15)-C(16)	111.3(8)
C(17)-C(15)-C(16)	107.1(7)
C(18)-C(15)-P(1)	110.2(6)
C(17)-C(15)-P(1)	108.4(7)
C(16)-C(15)-P(1)	113.8(6)
C(20)-C(19)-C(22)	106.3(8)
C(20)-C(19)-C(21)	109.6(8)
C(22)-C(19)-C(21)	108.4(8)
C(20)-C(19)-P(1)	109.4(7)
C(22)-C(19)-P(1)	109.0(7)
C(21)-C(19)-P(1)	113.8(7)
C(24)-C(23)-Ta(1)	126.6(5)
C(29)-C(24)-C(25)	116.1(7)
C(29)-C(24)-C(23)	122.6(7)
C(25)-C(24)-C(23)	121.1(7)
C(26)-C(25)-C(24)	120.4(8)
C(25)-C(26)-C(27)	122.4(9)
C(28)-C(27)-C(26)	118.0(8)
C(27)-C(28)-C(29)	120.1(9)
C(24)-C(29)-C(28)	122.9(8)
C(31)-C(30)-Ta(1)	156.3(5)
C(32)-C(31)-C(36)	117.4(7)
C(32)-C(31)-C(30)	122.1(7)
C(36)-C(31)-C(30)	120.4(7)
C(31)-C(32)-C(33)	120.3(9)
C(34)-C(33)-C(32)	120.3(8)
C(33)-C(34)-C(35)	120.8(9)
C(34)-C(35)-C(36)	119.7(9)
C(35)-C(36)-C(31)	121.4(8)

Symmetry transformations used to generate equivalent atoms:

4. Anisotropic displacement parameters [A^2 x 10^3]

	U11	U22	U33	U23	U13	U12
Ta(1)	38(1)	39(1)	51(1)	4(1)	9(1)	2(1)
P(1)	41(1)	50(1)	55(1)	-2(1)	10(1)	5(1)
N(1)	43(3)	45(4)	60(4)	10(3)	14(3)	7(2)
C(1)	48(4)	95(7)	55(5)	12(5)	12(4)	-18(4)
C(2)	34(3)	67(5)	71(5)	2(4)	2(3)	-6(3)
C(3)	59(4)	48(5)	56(5)	0(4)	20(4)	-11(4)
C(4)	54(4)	46(5)	103(7)	-12(5)	21(4)	-11(4)
C(5)	54(4)	45(5)	97(7)	30(5)	-10(4)	-15(4)
C(6)	114(8)	190(14)	67(7)	10(7)	39(6)	-46(8)
C(7)	40(4)	98(7)	117(8)	-17(6)	-3(5)	13(4)
C(8)	122(8)	106(8)	51(5)	-8(5)	7(5)	-46(7)
C(9)	88(7)	96(9)	219(14)	-81(9)	58(8)	-16(6)
C(10)	119(9)	94(9)	222(15)	98(10)	-69(10)	-40(7)
C(11)	52(4)	79(7)	72(6)	-9(5)	8(4)	20(4)
C(12)	94(7)	61(7)	142(10)	4(6)	15(7)	18(5)
C(13)	65(5)	122(9)	110(8)	-9(7)	16(5)	42(6)
C(14)	99(7)	132(10)	80(7)	-40(6)	18(6)	35(7)
C(15)	63(5)	112(8)	46(5)	-2(5)	11(4)	7(5)
C(16)	67(5)	179(12)	61(6)	3(6)	-8(4)	26(6)
C(17)	103(7)	162(12)	78(7)	-58(7)	0(6)	40(8)
C(18)	88(6)	181(13)	63(6)	28(7)	26(5)	17(7)
C(19)	61(5)	66(6)	106(7)	15(5)	12(5)	-17(4)
C(20)	81(6)	65(7)	161(10)	0(7)	2(6)	-16(5)
C(21)	58(5)	129(11)	162(11)	10(8)	-6(6)	-29(6)
C(22)	73(6)	139(11)	138(10)	51(8)	44(6)	-9(6)
C(23)	65(4)	56(5)	64(5)	-4(4)	10(4)	19(4)
C(24)	48(4)	49(5)	57(4)	-14(4)	8(3)	-2(3)
C(25)	69(5)	57(6)	96(6)	8(5)	35(4)	11(4)
C(26)	119(8)	74(7)	120(8)	39(6)	52(7)	42(6)
C(27)	72(5)	78(7)	117(8)	12(6)	30(6)	30(5)
C(28)	56(4)	82(7)	96(7)	-11(5)	35(4)	15(5)
C(29)	72(5)	77(6)	66(5)	1(4)	24(4)	11(5)
C(30)	49(4)	47(5)	76(5)	7(4)	11(4)	-8(3)
C(31)	56(4)	44(5)	62(5)	8(4)	11(4)	-7(3)
C(32)	53(4)	56(5)	92(6)	13(5)	6(4)	0(4)
C(33)	73(5)	76(7)	102(7)	28(6)	-14(5)	-1(5)
C(34)	97(7)	82(7)	74(6)	18(5)	-4(6)	-23(6)
C(35)	94(6)	82(7)	64(6)	-5(5)	19(5)	-22(5)
C(36)	70(5)	63(6)	62(5)	4(4)	10(4)	-3(4)

5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3)

	x	y	z	U(eq)
H(6A)	4704	2545	1301	181
H(6B)	3464	2415	806	181
H(6C)	4223	1705	1149	181
H(7A)	5730	1537	3029	133
H(7B)	4979	1011	2366	133
H(7C)	4917	930	3276	133
H(8A)	4579	2255	4486	142
H(8B)	4092	1419	4306	142
H(8C)	3313	2088	4480	142
H(9A)	2688	3637	3746	196

H(9B)	1991	2922	3918	196
H(9C)	1540	3433	3149	196
H(10A)	2846	3903	1720	244
H(10B)	1655	3626	1806	244
H(10C)	2166	3304	1104	244
H(12A)	-1253	3975	1427	151
H(12B)	-1159	3475	674	151
H(12C)	-139	3522	1429	151
H(13A)	-2920	3347	1618	150
H(13B)	-3011	2446	1658	150
H(13C)	-2971	2851	838	150
H(14A)	-1289	3353	2730	156
H(14B)	-170	2927	2685	156
H(14C)	-1208	2453	2818	156
H(16A)	-2077	2249	-909	159
H(16B)	-2234	2742	-167	159
H(16C)	-2650	1883	-259	159
H(17A)	-757	1160	-731	176
H(17B)	-1261	794	-45	176
H(17C)	34	966	114	176
H(18A)	-44	2475	-595	164
H(18B)	735	2232	238	164
H(18C)	-36	2963	185	164
H(20A)	-1253	-131	1633	160
H(20B)	-144	359	1873	160
H(20C)	-754	260	958	160
H(21A)	-3108	480	1169	182
H(21B)	-2722	877	448	182
H(21C)	-3216	1377	1055	182
H(22A)	-2046	659	2582	170
H(22B)	-2066	1561	2510	170
H(22C)	-914	1126	2792	170
H(23A)	1559	483	1180	75
H(23B)	2352	1069	898	75
H(25A)	2779	-401	2412	85
H(26A)	4107	-1340	2533	121
H(27A)	5345	-1389	1696	105
H(28A)	5232	-456	719	91
H(29A)	3852	462	550	84
H(30A)	1059	726	2962	69
H(32A)	3661	132	3850	82
H(33A)	4129	-503	5094	107
H(34A)	2921	-489	5940	106
H(35A)	1185	70	5545	96
H(36A)	686	702	4313	79

Crystal data and structure refinement for Cp*Ta(NPt-Bu$_3$)(η^2-CHPhCH$_2$)(CH$_2$Ph) 9

Empirical formula $C_{37}H_{56}NPTa$
Formula weight 726.75
Temperature 293(2) K
Wavelength 0.71073 A
Crystal system triclinic
Space group P-1
Unit cell dimensions
a = 11.668(16) A alpha = 87.37(10)^o
b = 12.359(18) A beta = 71.97(9)^o
c = 13.053(13) A gamma = 74.65(12)^o

Volume, Z 1725(4) A^3, 2
Density (calculated) 1.399 Mg/m^3
Absorption coefficient 3.257 mm^-1
F(000) 746
θ range for data collection 1.64 to 25.00^o
Limiting indices -11<h<13, -14<k<14, -15<l<14
Reflections collected 9115
Independent reflections 5946 (Rint = 0.0199)
Completeness to q = 25.00^o 97.8 %
Refinement method Full-matrix least-squares on F^2
Data / restraints / parameters 5946 / 0 / 361
Goodness-of-fit on F^2 0.746
Final R indices [I>2s(I)] R1 = 0.0281, wR2 = 0.0847
R indices (all data) R1 = 0.0315, wR2 = 0.0883
Largest diff. peak and hole 1.536 and -0.993 eA^-3

2. Atomic coordinates [x 10^4] and equivalent isotropic displacement parameters [A^2 x 10^3]

	x	y	z	U(eq)
Ta(1)	6584(1)	6777(1)	2507(1)	39(1)
P(1)	3462(1)	8298(1)	3266(1)	41(1)
N(1)	4928(3)	7711(3)	2842(3)	44(1)
C(1)	8728(4)	6037(4)	1135(4)	56(1)
C(2)	7882(4)	6802(4)	653(3)	54(1)
C(3)	6930(5)	6275(4)	654(4)	57(1)
C(4)	7153(5)	5232(4)	1167(4)	59(1)
C(5)	8273(5)	5073(4)	1443(4)	60(1)
C(6)	9921(5)	6170(6)	1227(5)	76(2)
C(7)	8091(5)	7842(5)	50(4)	67(1)
C(8)	5988(6)	6664(6)	57(5)	76(2)
C(9)	6444(6)	4346(5)	1222(5)	85(2)
C(10)	8934(6)	4008(5)	1865(5)	84(2)
C(11)	2551(5)	7209(4)	3537(5)	65(1)
C(12)	1158(5)	7659(5)	3659(6)	78(2)
C(13)	2613(6)	6626(6)	4617(6)	93(2)
C(14)	3149(7)	6291(5)	2699(7)	97(2)
C(15)	3113(4)	9131(5)	4552(4)	63(1)
C(16)	3880(5)	8472(6)	5238(5)	82(2)
C(17)	1729(5)	9494(6)	5207(5)	78(2)
C(18)	3609(6)	10203(5)	4262(6)	85(2)
C(19)	2949(5)	9295(5)	2223(4)	63(1)
C(20)	1718(5)	10171(5)	2646(6)	77(2)
C(21)	3964(6)	9867(6)	1659(6)	87(2)
C(22)	2817(7)	8610(6)	1317(5)	88(2)
C(23)	7271(4)	5826(4)	3852(4)	49(1)
C(24)	6263(4)	5463(4)	3657(4)	50(1)
C(25)	7296(4)	6239(4)	4877(4)	47(1)
C(26)	8419(5)	6310(5)	5010(5)	69(1)
C(27)	8516(7)	6635(6)	5967(5)	85(2)
C(28)	7471(7)	6918(6)	6865(5)	85(2)
C(29)	6349(7)	6851(5)	6763(4)	74(2)
C(30)	6264(5)	6513(4)	5798(4)	59(1)
C(31)	7510(4)	7994(4)	2977(3)	49(1)
C(32)	7730(4)	9003(4)	2364(3)	47(1)
C(33)	8923(5)	9191(5)	1980(5)	66(1)
C(34)	9108(6)	10144(6)	1409(5)	73(2)
C(35)	8146(6)	10943(5)	1228(5)	75(2)

C(36)	6963(6)	10780(5)	1591(5)	72(1)
C(37)	6769(5)	9848(4)	2150(4)	59(1)

3. Bond lengths [A] and angles [^o]

Ta(1)-N(1)	1.898(5)	C(11)-C(12)	1.532(7)
Ta(1)-C(24)	2.186(5)	C(11)-C(13)	1.566(9)
Ta(1)-C(31)	2.272(5)	C(15)-C(17)	1.529(7)
Ta(1)-C(23)	2.299(5)	C(15)-C(16)	1.520(8)
Ta(1)-C(3)	2.408(5)	C(15)-C(18)	1.567(8)
Ta(1)-C(2)	2.430(5)	C(19)-C(20)	1.511(8)
Ta(1)-C(4)	2.462(6)	C(19)-C(21)	1.517(8)
Ta(1)-C(1)	2.544(6)	C(19)-C(22)	1.553(9)
Ta(1)-C(5)	2.573(7)	C(23)-C(24)	1.458(6)
P(1)-N(1)	1.597(4)	C(23)-C(25)	1.464(7)
P(1)-C(11)	1.884(5)	C(25)-C(30)	1.391(7)
P(1)-C(15)	1.887(6)	C(25)-C(26)	1.400(7)
P(1)-C(19)	1.920(5)	C(26)-C(27)	1.376(8)
C(1)-C(5)	1.422(8)	C(27)-C(28)	1.382(10)
C(1)-C(2)	1.449(7)	C(28)-C(29)	1.381(10)
C(1)-C(6)	1.485(7)	C(29)-C(30)	1.385(8)
C(2)-C(3)	1.428(7)	C(31)-C(32)	1.488(7)
C(2)-C(7)	1.511(7)	C(32)-C(33)	1.404(7)
C(3)-C(4)	1.425(8)	C(32)-C(37)	1.404(7)
C(3)-C(8)	1.505(7)	C(33)-C(34)	1.395(8)
C(4)-C(5)	1.423(8)	C(34)-C(35)	1.359(9)
C(4)-C(9)	1.524(7)	C(35)-C(36)	1.381(9)
C(5)-C(10)	1.513(8)	C(36)-C(37)	1.367(8)
C(11)-C(14)	1.481(9)		
N(1)-Ta(1)-C(24)	99.4(2)	C(24)-Ta(1)-C(5)	79.8(2)
N(1)-Ta(1)-C(31)	99.1(2)	C(31)-Ta(1)-C(5)	109.5(2)
C(24)-Ta(1)-C(31)	114.38(18)	C(23)-Ta(1)-C(5)	78.43(19)
N(1)-Ta(1)-C(23)	119.75(18)	C(3)-Ta(1)-C(5)	55.20(19)
C(24)-Ta(1)-C(23)	37.83(17)	C(2)-Ta(1)-C(5)	55.32(19)
C(31)-Ta(1)-C(23)	79.11(19)	C(4)-Ta(1)-C(5)	32.72(18)
N(1)-Ta(1)-C(3)	99.47(19)	C(1)-Ta(1)-C(5)	32.27(18)
C(24)-Ta(1)-C(3)	115.7(2)	N(1)-P(1)-C(11)	110.4(2)
C(31)-Ta(1)-C(3)	122.16(19)	N(1)-P(1)-C(15)	108.4(2)
C(23)-Ta(1)-C(3)	132.64(19)	C(11)-P(1)-C(15)	109.5(3)
N(1)-Ta(1)-C(2)	115.40(19)	N(1)-P(1)-C(19)	111.0(2)
C(24)-Ta(1)-C(2)	134.74(19)	C(11)-P(1)-C(19)	108.5(3)
C(31)-Ta(1)-C(2)	88.71(19)	C(15)-P(1)-C(19)	109.0(3)
C(23)-Ta(1)-C(2)	124.68(19)	P(1)-N(1)-Ta(1)	168.7(2)
C(3)-Ta(1)-C(2)	34.34(18)	C(5)-C(1)-C(2)	108.2(4)
N(1)-Ta(1)-C(4)	116.25(19)	C(5)-C(1)-C(6)	124.6(5)
C(24)-Ta(1)-C(4)	83.2(2)	C(2)-C(1)-C(6)	127.0(5)
C(31)-Ta(1)-C(4)	137.78(18)	C(5)-C(1)-Ta(1)	75.0(3)
C(23)-Ta(1)-C(4)	100.6(2)	C(2)-C(1)-Ta(1)	68.8(3)
C(3)-Ta(1)-C(4)	34.01(18)	C(6)-C(1)-Ta(1)	125.5(3)
C(2)-Ta(1)-C(4)	56.4(2)	C(3)-C(2)-C(1)	107.0(4)
N(1)-Ta(1)-C(1)	149.17(17)	C(3)-C(2)-C(7)	124.9(5)
C(24)-Ta(1)-C(1)	107.6(2)	C(1)-C(2)-C(7)	127.0(5)
C(31)-Ta(1)-C(1)	83.1(2)	C(3)-C(2)-Ta(1)	72.0(3)
C(23)-Ta(1)-C(1)	91.0(2)	C(1)-C(2)-Ta(1)	77.4(3)
C(3)-Ta(1)-C(1)	55.63(18)	C(7)-C(2)-Ta(1)	125.6(3)
C(2)-Ta(1)-C(1)	33.78(17)	C(4)-C(3)-C(2)	108.2(4)
C(4)-Ta(1)-C(1)	54.66(19)	C(4)-C(3)-C(8)	125.6(5)
N(1)-Ta(1)-C(5)	148.97(17)	C(2)-C(3)-C(8)	125.4(5)

C(4)-C(3)-Ta(1)	75.1(3)	C(20)-C(19)-C(21)	109.4(5)
C(2)-C(3)-Ta(1)	73.7(3)	C(20)-C(19)-C(22)	106.2(5)
C(8)-C(3)-Ta(1)	124.8(4)	C(21)-C(19)-C(22)	105.1(6)
C(5)-C(4)-C(3)	108.6(5)	C(20)-C(19)-P(1)	115.9(4)
C(5)-C(4)-C(9)	125.5(5)	C(21)-C(19)-P(1)	109.8(4)
C(3)-C(4)-C(9)	125.1(5)	C(22)-C(19)-P(1)	109.8(4)
C(5)-C(4)-Ta(1)	77.9(3)	C(24)-C(23)-C(25)	127.1(4)
C(3)-C(4)-Ta(1)	70.9(3)	C(24)-C(23)-Ta(1)	66.9(3)
C(9)-C(4)-Ta(1)	125.6(4)	C(25)-C(23)-Ta(1)	130.5(3)
C(4)-C(5)-C(1)	107.9(4)	C(23)-C(24)-Ta(1)	75.3(3)
C(4)-C(5)-C(10)	125.5(5)	C(30)-C(25)-C(26)	114.8(5)
C(1)-C(5)-C(10)	126.3(5)	C(30)-C(25)-C(23)	124.4(4)
C(4)-C(5)-Ta(1)	69.3(3)	C(26)-C(25)-C(23)	120.7(4)
C(1)-C(5)-Ta(1)	72.7(3)	C(27)-C(26)-C(25)	123.5(6)
C(10)-C(5)-Ta(1)	128.9(4)	C(26)-C(27)-C(28)	120.4(6)
C(14)-C(11)-C(12)	110.7(5)	C(29)-C(28)-C(27)	117.6(6)
C(14)-C(11)-C(13)	104.6(6)	C(28)-C(29)-C(30)	121.5(6)
C(12)-C(11)-C(13)	105.7(5)	C(25)-C(30)-C(29)	122.1(5)
C(14)-C(11)-P(1)	110.0(4)	C(32)-C(31)-Ta(1)	123.8(3)
C(12)-C(11)-P(1)	115.1(4)	C(33)-C(32)-C(37)	115.1(4)
C(13)-C(11)-P(1)	110.1(4)	C(33)-C(32)-C(31)	121.8(4)
C(17)-C(15)-C(16)	110.5(5)	C(37)-C(32)-C(31)	123.1(4)
C(17)-C(15)-C(18)	108.9(5)	C(32)-C(33)-C(34)	120.9(5)
C(16)-C(15)-C(18)	104.3(5)	C(35)-C(34)-C(33)	121.9(5)
C(17)-C(15)-P(1)	114.5(4)	C(34)-C(35)-C(36)	118.6(5)
C(16)-C(15)-P(1)	109.7(4)	C(37)-C(36)-C(35)	120.1(5)
C(18)-C(15)-P(1)	108.5(4)	C(36)-C(37)-C(32)	123.4(5)

Symmetry transformations used to generate equivalent atoms:

4. Anisotropic displacement parameters [A^2 x 10^3]

	U11	U22	U33	U23	U13	U12
Ta(1)	36(1)	45(1)	33(1)	-2(1)	-7(1)	-7(1)
P(1)	35(1)	46(1)	40(1)	2(1)	-11(1)	-9(1)
N(1)	42(2)	49(2)	40(2)	-1(1)	-12(2)	-11(1)
C(1)	43(2)	73(3)	41(2)	-12(2)	-5(2)	-4(2)
C(2)	53(2)	65(3)	31(2)	-4(2)	-2(2)	-7(2)
C(3)	59(3)	69(3)	37(2)	-14(2)	-12(2)	-8(2)
C(4)	62(3)	58(3)	49(3)	-19(2)	-6(2)	-12(2)
C(5)	61(3)	56(3)	46(3)	-12(2)	-8(2)	4(2)
C(6)	50(3)	107(5)	59(3)	-22(3)	-8(2)	-5(3)
C(7)	74(3)	82(3)	36(2)	-2(2)	-8(2)	-13(3)
C(8)	76(4)	98(4)	52(3)	-5(3)	-26(3)	-10(3)
C(9)	94(5)	78(4)	85(4)	-21(3)	-19(4)	-33(3)
C(10)	86(4)	63(3)	76(4)	-9(3)	-16(3)	16(3)
C(11)	48(3)	52(3)	99(4)	12(3)	-22(3)	-22(2)
C(12)	58(3)	90(4)	101(5)	22(3)	-34(3)	-34(3)
C(13)	68(4)	101(5)	108(5)	46(4)	-25(4)	-28(3)
C(14)	86(4)	72(4)	132(6)	-28(4)	-19(4)	-34(3)
C(15)	40(2)	86(3)	52(3)	-18(2)	-8(2)	-4(2)
C(16)	62(3)	129(5)	52(3)	-7(3)	-22(3)	-10(3)
C(17)	46(3)	104(4)	65(3)	-27(3)	-3(3)	2(3)
C(18)	69(3)	79(4)	100(5)	-36(3)	-15(3)	-18(3)
C(19)	53(3)	73(3)	61(3)	18(2)	-23(2)	-10(2)
C(20)	55(3)	80(4)	94(4)	26(3)	-32(3)	-8(3)
C(21)	67(4)	97(5)	89(5)	51(4)	-23(3)	-16(3)
C(22)	82(4)	122(6)	68(4)	2(4)	-40(3)	-21(4)

C(23)	43(2)	52(2)	45(2)	3(2)	-9(2)	-9(2)
C(24)	51(2)	51(2)	47(2)	5(2)	-16(2)	-11(2)
C(25)	52(2)	44(2)	45(2)	10(2)	-15(2)	-12(2)
C(26)	61(3)	93(4)	60(3)	14(3)	-22(3)	-32(3)
C(27)	92(4)	117(5)	71(4)	15(4)	-37(4)	-55(4)
C(28)	111(5)	94(4)	68(4)	7(3)	-35(4)	-49(4)
C(29)	99(4)	68(3)	43(3)	0(2)	-6(3)	-20(3)
C(30)	57(3)	57(3)	55(3)	3(2)	-11(2)	-9(2)
C(31)	49(2)	61(3)	37(2)	-2(2)	-11(2)	-14(2)
C(32)	45(2)	60(3)	36(2)	-5(2)	-9(2)	-15(2)
C(33)	55(3)	83(4)	75(4)	14(3)	-32(3)	-27(3)
C(34)	76(4)	98(4)	64(3)	17(3)	-26(3)	-51(3)
C(35)	98(4)	65(3)	67(3)	14(3)	-26(3)	-34(3)
C(36)	75(4)	65(3)	65(3)	1(3)	-20(3)	-2(3)
C(37)	51(3)	63(3)	53(3)	-6(2)	-9(2)	-8(2)

5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3)

	x	y	z	U(eq)
H(6A)	10597	5818	608	114
H(6B)	10060	5824	1867	114
H(6C)	9878	6955	1267	114
H(7A)	8641	7628	-669	101
H(7B)	8459	8242	417	101
H(7C)	7306	8315	18	101
H(8A)	6340	6354	-669	114
H(8B)	5769	7469	44	114
H(8C)	5254	6418	414	114
H(9A)	6854	3838	605	128
H(9B)	5604	4706	1229	128
H(9C)	6427	3937	1868	128
H(10A)	9516	3526	1269	126
H(10B)	8331	3629	2278	126
H(10C)	9375	4193	2314	126
H(12A)	770	7050	3795	117
H(12B)	1061	8009	3008	117
H(12C)	770	8201	4252	117
H(13A)	2146	6073	4748	140
H(13B)	2264	7178	5200	140
H(13C)	3468	6268	4563	140
H(14A)	2678	5740	2843	145
H(14B)	3986	5946	2707	145
H(14C)	3170	6591	2004	145
H(16A)	3701	8898	5892	124
H(16B)	4753	8331	4846	124
H(16C)	3670	7771	5410	124
H(17A)	1628	9913	5845	117
H(17B)	1424	8842	5407	117
H(17C)	1267	9956	4780	117
H(18A)	3436	10637	4910	127
H(18B)	3200	10648	3790	127
H(18C)	4494	9981	3909	127
H(20A)	1547	10624	2066	115
H(20B)	1762	10639	3193	115
H(20C)	1063	9807	2949	115
H(21A)	3703	10364	1139	131
H(21B)	4719	9311	1301	131

H(21C)	4113	10290	2181	131
H(22A)	2562	9112	798	132
H(22B)	2203	8204	1625	132
H(22C)	3607	8091	969	132
H(23A)	8063	5267	3520	58
H(24A)	5472	5643	4231	60
H(24B)	6487	4708	3349	60
H(26A)	9139	6127	4419	82
H(27A)	9288	6663	6011	102
H(28A)	7523	7147	7515	102
H(29A)	5633	7037	7357	89
H(30A)	5493	6469	5765	71
H(31A)	7767	7852	3589	59
H(33A)	9599	8672	2109	80
H(34A)	9913	10235	1144	88
H(35A)	8282	11587	867	90
H(36A)	6296	11305	1456	86
H(37A)	5959	9769	2402	70

1. Crystal data and structure refinement for Cp*Ta(NPt-Bu$_3$)(η^2-C$_2$H$_4$)Cl 10

Empirical formula $C_{24}H_{46}ClNPTa$
Formula weight 595.99
Temperature 293(2) K
Wavelength 0.71073 A
Crystal system orthorhombic
Space group Pbca
Unit cell dimensions
a = 16.9128(2) A alpha = 90^o
b = 14.853 A beta = 90^o
c = 21.16780(10) A gamma = 90^o
Volume, Z 5317.51(7) A^3, 8
Density (calculated) 1.489 Mg/m^3
Absorption coefficient 4.305 mm^-1
F(000) 2416
θ range for data collection 1.92 to 25.00^o
Limiting indices -20<h<17, -17<k<17, -25<l<22
Reflections collected 25136
Independent reflections 4676 (Rint = 0.0385)
Completeness to q = 25.00^o 99.8 %
Refinement method Full-matrix least-squares on F^2
Data / restraints / parameters 4676 / 0 / 253
Goodness-of-fit on F^2 1.028
Final R indices [I>2s(I)] R1 = 0.0351, wR2 = 0.0883
R indices (all data) R1 = 0.0454, wR2 = 0.0935
Largest diff. peak and hole 1.553 and -1.425 eA^-3

2. Atomic coordinates [x 10^4] and equivalent isotropic displacement parameters [A^2 x 10^3]

	x	y	z	U(eq)
Ta(1)	1133(1)	3806(1)	3185(1)	44(1)
Cl(1)	-234(1)	4185(2)	3471(1)	109(1)
P(1)	1507(1)	2782(1)	4626(1)	39(1)
N(1)	1363(2)	3180(3)	3931(2)	41(1)
C(1)	1860(3)	3406(6)	2244(3)	74(2)
C(2)	1368(5)	4130(5)	2020(3)	78(2)
C(3)	595(4)	3841(4)	2061(3)	56(1)

C(4)	579(3)	2968(3)	2315(2)	48(1)
C(5)	1359(3)	2675(4)	2416(2)	54(1)
C(6)	2761(4)	3352(10)	2224(4)	163(5)
C(7)	1662(8)	5003(7)	1740(4)	158(6)
C(8)	-124(6)	4394(7)	1865(3)	109(3)
C(9)	-145(4)	2394(6)	2375(4)	90(2)
C(10)	1624(6)	1750(5)	2606(3)	111(3)
C(11)	2603(3)	2622(4)	4741(3)	55(1)
C(12)	2815(4)	2002(5)	5313(3)	83(2)
C(13)	3009(4)	3532(5)	4844(4)	80(2)
C(14)	2964(4)	2231(5)	4133(3)	84(2)
C(15)	962(3)	1664(4)	4684(3)	57(1)
C(16)	813(6)	1344(5)	5362(4)	96(2)
C(17)	1427(5)	933(4)	4318(4)	78(2)
C(18)	165(4)	1768(5)	4338(4)	77(2)
C(19)	1101(3)	3595(4)	5230(3)	54(1)
C(20)	1367(5)	3418(5)	5916(3)	79(2)
C(21)	1350(4)	4573(4)	5040(3)	76(2)
C(22)	197(4)	3574(5)	5211(3)	77(2)
C(23)	1394(8)	5259(5)	3319(4)	127(4)
C(24)	2166(5)	4814(5)	3302(3)	81(3)

3. Bond lengths [A] and angles [^o]

Ta(1)-N(1)	1.873(4)	C(2)-C(7)	1.510(10)
Ta(1)-C(23)	2.220(7)	C(3)-C(4)	1.403(7)
Ta(1)-C(24)	2.313(5)	C(3)-C(8)	1.526(9)
Ta(1)-C(5)	2.370(5)	C(4)-C(5)	1.405(7)
Ta(1)-C(4)	2.413(5)	C(4)-C(9)	1.499(8)
Ta(1)-C(1)	2.416(6)	C(5)-C(10)	1.501(9)
Ta(1)-Cl(1)	2.455(2)	C(11)-C(13)	1.532(8)
Ta(1)-C(2)	2.545(6)	C(11)-C(14)	1.539(9)
Ta(1)-C(3)	2.549(6)	C(11)-C(12)	1.561(8)
P(1)-N(1)	1.603(4)	C(15)-C(16)	1.534(9)
P(1)-C(11)	1.884(5)	C(15)-C(18)	1.543(9)
P(1)-C(19)	1.889(5)	C(15)-C(17)	1.548(9)
P(1)-C(15)	1.903(6)	C(19)-C(22)	1.530(8)
C(1)-C(5)	1.424(9)	C(19)-C(20)	1.542(8)
C(1)-C(2)	1.440(11)	C(19)-C(21)	1.567(8)
C(1)-C(6)	1.527(9)	C(23)-C(24)	1.464(13)
C(2)-C(3)	1.378(9)		

N(1)-Ta(1)-C(23)	109.5(3)	C(24)-Ta(1)-Cl(1)	122.4(2)
N(1)-Ta(1)-C(24)	94.3(2)	C(5)-Ta(1)-Cl(1)	118.88(15)
C(23)-Ta(1)-C(24)	37.6(3)	C(4)-Ta(1)-Cl(1)	86.58(14)
N(1)-Ta(1)-C(5)	101.18(18)	C(1)-Ta(1)-Cl(1)	137.59(15)
C(23)-Ta(1)-C(5)	138.1(3)	N(1)-Ta(1)-C(2)	151.5(2)
C(24)-Ta(1)-C(5)	114.2(3)	C(23)-Ta(1)-C(2)	84.8(3)
N(1)-Ta(1)-C(4)	117.91(18)	C(24)-Ta(1)-C(2)	82.2(2)
C(23)-Ta(1)-C(4)	132.5(3)	C(5)-Ta(1)-C(2)	56.1(2)
C(24)-Ta(1)-C(4)	135.1(2)	C(4)-Ta(1)-C(2)	54.4(2)
C(5)-Ta(1)-C(4)	34.14(17)	C(1)-Ta(1)-C(2)	33.6(3)
N(1)-Ta(1)-C(1)	117.9(2)	Cl(1)-Ta(1)-C(2)	110.0(2)
C(23)-Ta(1)-C(1)	104.1(4)	N(1)-Ta(1)-C(3)	150.60(18)
C(24)-Ta(1)-C(1)	82.1(3)	C(23)-Ta(1)-C(3)	99.8(3)
C(5)-Ta(1)-C(1)	34.6(2)	C(24)-Ta(1)-C(3)	110.9(2)
C(4)-Ta(1)-C(1)	56.0(2)	C(5)-Ta(1)-C(3)	55.26(18)
N(1)-Ta(1)-Cl(1)	95.85(13)	C(4)-Ta(1)-C(3)	32.72(17)
C(23)-Ta(1)-Cl(1)	86.1(4)	C(1)-Ta(1)-C(3)	54.3(2)

Cl(1)-Ta(1)-C(3)	83.61(15)	C(3)-C(4)-Ta(1)	79.0(3)
C(2)-Ta(1)-C(3)	31.4(2)	C(5)-C(4)-Ta(1)	71.3(3)
N(1)-P(1)-C(11)	108.4(2)	C(9)-C(4)-Ta(1)	123.2(4)
N(1)-P(1)-C(19)	109.3(2)	C(4)-C(5)-C(1)	106.5(5)
C(11)-P(1)-C(19)	110.5(3)	C(4)-C(5)-C(10)	127.2(7)
N(1)-P(1)-C(15)	107.9(2)	C(1)-C(5)-C(10)	126.1(7)
C(11)-P(1)-C(15)	111.0(3)	C(4)-C(5)-Ta(1)	74.6(3)
C(19)-P(1)-C(15)	109.8(3)	C(1)-C(5)-Ta(1)	74.4(4)
P(1)-N(1)-Ta(1)	170.9(3)	C(10)-C(5)-Ta(1)	120.9(4)
C(5)-C(1)-C(2)	108.0(5)	C(13)-C(11)-C(14)	105.9(6)
C(5)-C(1)-C(6)	124.1(9)	C(13)-C(11)-C(12)	107.9(5)
C(2)-C(1)-C(6)	127.4(8)	C(14)-C(11)-C(12)	109.6(5)
C(5)-C(1)-Ta(1)	70.9(3)	C(13)-C(11)-P(1)	110.4(4)
C(2)-C(1)-Ta(1)	78.1(4)	C(14)-C(11)-P(1)	109.2(4)
C(6)-C(1)-Ta(1)	122.9(5)	C(12)-C(11)-P(1)	113.6(4)
C(3)-C(2)-C(1)	107.1(6)	C(16)-C(15)-C(18)	109.4(6)
C(3)-C(2)-C(7)	127.2(9)	C(16)-C(15)-C(17)	109.5(6)
C(1)-C(2)-C(7)	125.5(9)	C(18)-C(15)-C(17)	106.1(5)
C(3)-C(2)-Ta(1)	74.4(4)	C(16)-C(15)-P(1)	114.3(5)
C(1)-C(2)-Ta(1)	68.3(3)	C(18)-C(15)-P(1)	107.7(4)
C(7)-C(2)-Ta(1)	126.4(5)	C(17)-C(15)-P(1)	109.5(4)
C(2)-C(3)-C(4)	109.3(6)	C(22)-C(19)-C(20)	108.3(5)
C(2)-C(3)-C(8)	124.9(7)	C(22)-C(19)-C(21)	106.3(5)
C(4)-C(3)-C(8)	125.9(7)	C(20)-C(19)-C(21)	108.8(5)
C(2)-C(3)-Ta(1)	74.2(4)	C(22)-C(19)-P(1)	109.4(4)
C(4)-C(3)-Ta(1)	68.3(3)	C(20)-C(19)-P(1)	115.0(4)
C(8)-C(3)-Ta(1)	123.4(4)	C(21)-C(19)-P(1)	108.7(4)
C(3)-C(4)-C(5)	109.0(5)	C(24)-C(23)-Ta(1)	74.6(4)
C(3)-C(4)-C(9)	125.0(6)	C(23)-C(24)-Ta(1)	67.7(4)
C(5)-C(4)-C(9)	125.3(6)		

Symmetry transformations used to generate equivalent atoms:

4. Anisotropic displacement parameters [A^2 x 10^3]

	U11	U22	U33	U23	U13	U12
Ta(1)	53(1)	41(1)	37(1)	-3(1)	-5(1)	0(1)
Cl(1)	88(1)	160(2)	79(1)	-23(1)	-9(1)	55(1)
P(1)	38(1)	40(1)	40(1)	-2(1)	-2(1)	6(1)
N(1)	38(2)	41(2)	45(2)	-5(2)	2(2)	3(2)
C(1)	44(3)	141(6)	38(3)	-7(4)	1(3)	-7(4)
C(2)	112(6)	83(5)	38(3)	3(3)	-2(4)	-40(4)
C(3)	67(4)	59(3)	42(3)	-2(2)	-11(3)	9(3)
C(4)	48(3)	55(3)	39(3)	-10(2)	-7(2)	-4(2)
C(5)	60(3)	66(4)	38(3)	-10(2)	-5(3)	19(3)
C(6)	42(4)	363(17)	84(6)	-25(9)	4(4)	-11(7)
C(7)	265(15)	133(9)	75(6)	22(5)	-13(7)	-121(10)
C(8)	130(7)	134(8)	63(5)	-4(4)	-26(5)	71(7)
C(9)	74(4)	117(6)	80(5)	-9(4)	-10(4)	-38(4)
C(10)	175(9)	92(5)	66(5)	-30(4)	-29(5)	76(6)
C(11)	45(3)	59(3)	61(3)	-6(3)	-11(3)	10(3)
C(12)	80(5)	85(5)	85(5)	8(4)	-24(4)	25(4)
C(13)	54(4)	87(5)	99(5)	1(4)	-16(4)	-5(3)
C(14)	49(4)	115(6)	87(5)	-13(4)	3(3)	25(4)
C(15)	65(4)	46(3)	59(4)	5(3)	1(3)	-3(3)
C(16)	128(7)	76(5)	84(5)	22(4)	10(5)	-21(5)
C(17)	100(5)	47(3)	87(5)	-10(3)	-9(4)	5(3)
C(18)	56(4)	76(4)	98(5)	0(4)	4(4)	-20(3)
C(19)	69(4)	53(3)	41(3)	-7(2)	0(3)	16(3)

C(20)	108(6)	85(5)	45(3)	-9(3)	-1(4)	22(4)
C(21)	111(5)	51(3)	65(4)	-11(3)	3(4)	16(3)
C(22)	64(4)	97(5)	71(4)	-4(4)	16(3)	27(4)
C(23)	274(15)	42(4)	65(5)	2(3)	-18(7)	-44(6)
C(24)	144(7)	69(4)	30(3)	3(3)	-11(4)	-81(5)

5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3)

	x	y	z	U(eq)
H(6A)	2972	3915	2078	244
H(6B)	2919	2879	1941	244
H(6C)	2959	3227	2640	244
H(7A)	2230	5008	1743	237
H(7B)	1467	5499	1986	237
H(7C)	1476	5057	1313	237
H(8A)	-598	4060	1954	164
H(8B)	-98	4519	1420	164
H(8C)	-131	4949	2096	164
H(9A)	-4	1823	2555	135
H(9B)	-373	2301	1964	135
H(9C)	-523	2689	2643	135
H(10A)	1171	1389	2708	167
H(10B)	1964	1791	2968	167
H(10C)	1907	1476	2262	167
H(12A)	2610	2261	5695	125
H(12B)	3379	1948	5345	125
H(12C)	2586	1417	5250	125
H(13A)	2807	3807	5221	120
H(13B)	2907	3917	4489	120
H(13C)	3569	3442	4886	120
H(14A)	2735	1651	4049	126
H(14B)	3525	2168	4185	126
H(14C)	2857	2628	3786	126
H(16A)	508	1788	5584	144
H(16B)	1309	1257	5574	144
H(16C)	527	785	5354	144
H(17A)	1927	833	4520	117
H(17B)	1512	1129	3892	117
H(17C)	1129	382	4316	117
H(18A)	-151	2212	4550	115
H(18B)	-109	1202	4337	115
H(18C)	258	1956	3910	115
H(20A)	1231	2813	6034	119
H(20B)	1107	3834	6194	119
H(20C)	1929	3497	5947	119
H(21A)	1197	4686	4610	114
H(21B)	1913	4636	5079	114
H(21C)	1093	4998	5312	114
H(22A)	20	3689	4788	116
H(22B)	-10	4027	5489	116
H(22C)	13	2992	5344	116
H(23A)	1272	5648	2964	152
H(23B)	1239	5514	3722	152
H(24A)	2459	4788	3695	97
H(24B)	2493	4923	2933	97

1. Crystal data and structure refinement for [Cp*Ta(NPt-Bu$_3$)(Cl)CH$_2$CH$_2$B(C$_6$F$_5$)$_3$] 22

Empirical formula $C_{42}H_{46}BClF_{15}NPTa$
Formula weight 1107.98
Temperature 293(2) K
Wavelength 0.71073 A
Crystal system monoclinic
Space group P2(1)
Unit cell dimensions
a = 9.667(3) A alpha = 90^o
b = 19.373(7) A beta = 92.20(3)^o
c = 11.920(2) A gamma = 90^o
Volume, Z 2230.6(12) A^3, 2
Density (calculated) 1.650 Mg/m^3
Absorption coefficient 2.654 mm^-1
F(000) 1100
θ range for data collection 2.01 to 25.00^o
Limiting indices -11<h<2, -23<k<18, -9<l<7
Reflections collected 4444
Independent reflections 4100 (Rint = 0.0463)
Completeness to q = 25.00^o 71.4 %
Refinement method Full-matrix least-squares on F^2
Data / restraints / parameters 4100 / 1 / 359
Goodness-of-fit on F^2 1.224
Final R indices [I>2s(I)] R1 = 0.0735, wR2 = 0.1392
R indices (all data) R1 = 0.0915, wR2 = 0.1534
Absolute structure parameter -0.03(2)
Largest diff. peak and hole 0.944 and -1.353 eA^-3

2. Atomic coordinates [x 10^4] and equivalent isotropic displacement parameters [A^2 x 10^3]

	x	y	z	U(eq)
Ta(1)	11878(1)	-957(1)	7596(1)	43(1)
Cl(1)	14026(4)	-1017(8)	8568(5)	70(2)
P(1)	9771(5)	-1420(4)	9740(6)	49(2)
F(1)	12708(15)	-3629(11)	3855(14)	98(6)
F(2)	14224(19)	-3199(15)	2175(18)	129(9)
F(3)	16229(19)	-2238(13)	2482(18)	123(9)
F(4)	16649(19)	-1666(12)	4590(20)	135(9)
F(5)	15027(19)	-1997(13)	6230(20)	112(9)
F(11)	12814(17)	-4506(10)	5628(16)	104(7)
F(12)	14167(19)	-5512(10)	6710(20)	139(9)
F(13)	15850(20)	-5204(14)	8540(20)	176(12)
F(14)	16070(20)	-3907(15)	9230(20)	188(13)
F(15)	14730(20)	-2902(12)	8206(18)	144(10)
F(21)	10932(13)	-2603(9)	4174(13)	70(5)
F(22)	8371(14)	-2954(12)	3757(14)	105(7)
F(23)	6946(13)	-3764(10)	5225(17)	101(7)
F(24)	8346(13)	-4266(9)	7078(17)	94(6)
F(25)	10962(12)	-3967(8)	7490(14)	68(5)
N(1)	10673(13)	-1159(10)	8684(15)	44(6)
C(1)	10850(30)	84(15)	6930(30)	66(8)
C(2)	12200(40)	210(20)	7280(40)	96(14)
C(3)	13070(30)	-47(16)	6560(30)	78(8)
C(4)	12390(30)	-372(16)	5750(30)	74(8)
C(5)	10900(30)	-334(15)	5950(30)	66(8)
C(6)	9630(40)	440(20)	7410(40)	140(15)
C(7)	12670(30)	740(20)	8220(30)	119(13)

C(8)	14700(40)	70(20)	6500(40)	108(16)
C(9)	12870(30)	-686(18)	4680(30)	115(12)
C(10)	9680(30)	-551(17)	5260(30)	100(10)
C(11)	10930(30)	-1977(19)	10690(30)	85(10)
C(12)	10040(40)	-2410(20)	11500(30)	128(14)
C(13)	11990(30)	-1517(16)	11330(30)	89(9)
C(14)	11780(30)	-2450(16)	9970(20)	80(8)
C(15)	9180(30)	-653(15)	10570(30)	78(9)
C(16)	8760(20)	-793(18)	11750(20)	94(10)
C(17)	7970(30)	-290(20)	9900(30)	111(12)
C(18)	10400(30)	-99(19)	10570(30)	97(12)
C(19)	8240(30)	-1929(16)	9060(30)	76(8)
C(20)	8770(30)	-2633(16)	8700(30)	83(9)
C(21)	7070(30)	-2057(16)	9960(30)	82(9)
C(22)	7690(30)	-1528(16)	8090(20)	85(9)
C(23)	11540(30)	-1800(14)	6510(30)	73(9)
C(24)	12400(20)	-2361(14)	7050(20)	43(7)
C(31)	13740(20)	-2816(12)	5140(20)	46(6)
C(32)	13620(30)	-3098(16)	4060(30)	71(8)
C(33)	14500(30)	-2904(17)	3170(30)	78(9)
C(34)	15410(30)	-2416(18)	3350(30)	80(9)
C(35)	15640(30)	-2133(17)	4350(30)	80(9)
C(36)	14770(30)	-2339(14)	5240(30)	63(7)
C(41)	13640(19)	-3648(11)	6860(20)	42(5)
C(42)	13570(20)	-4333(14)	6560(30)	62(7)
C(43)	14290(30)	-4890(20)	7040(30)	84(10)
C(44)	15150(30)	-4714(17)	7980(30)	76(8)
C(45)	15210(40)	-4080(20)	8320(40)	95(12)
C(46)	14550(30)	-3547(17)	7770(30)	74(8)
C(51)	11149(18)	-3298(11)	5830(20)	38(5)
C(52)	10400(20)	-3041(12)	4900(20)	46(5)
C(53)	8970(20)	-3223(14)	4690(20)	58(6)
C(54)	8350(20)	-3621(13)	5390(20)	51(6)
C(55)	8950(20)	-3855(14)	6340(20)	57(7)
C(56)	10380(20)	-3700(11)	6500(20)	42(5)
B(1)	12720(20)	-3030(13)	6220(30)	48(8)

3. Bond lengths [A] and angles [^o]

Ta(1)-N(1)	1.818(16)	F(13)-C(44)	1.33(3)
Ta(1)-C(23)	2.10(3)	F(14)-C(45)	1.38(4)
Ta(1)-C(2)	2.32(4)	F(15)-C(46)	1.36(3)
Ta(1)-Cl(1)	2.342(4)	F(21)-C(52)	1.33(3)
Ta(1)-C(1)	2.37(3)	F(22)-C(53)	1.34(3)
Ta(1)-C(3)	2.47(3)	F(23)-C(54)	1.39(2)
Ta(1)-C(5)	2.46(3)	F(24)-C(55)	1.34(3)
Ta(1)-C(4)	2.54(3)	F(25)-C(56)	1.39(3)
P(1)-N(1)	1.639(18)	C(1)-C(2)	1.38(4)
P(1)-C(15)	1.88(3)	C(1)-C(5)	1.42(4)
P(1)-C(11)	1.90(3)	C(1)-C(6)	1.50(4)
P(1)-C(19)	1.93(3)	C(2)-C(3)	1.33(5)
F(1)-C(32)	1.37(3)	C(2)-C(7)	1.57(5)
F(2)-C(33)	1.34(4)	C(3)-C(4)	1.31(4)
F(3)-C(34)	1.37(4)	C(3)-C(8)	1.59(4)
F(4)-C(35)	1.35(3)	C(4)-C(9)	1.50(4)
F(5)-C(36)	1.37(3)	C(4)-C(5)	1.48(4)
F(11)-C(42)	1.35(3)	C(5)-C(10)	1.47(3)
F(12)-C(43)	1.28(4)	C(11)-C(13)	1.53(4)

C(11)-C(14)	1.52(4)	C(35)-C(36)	1.43(4)
C(11)-C(12)	1.56(5)	C(41)-C(46)	1.38(3)
C(15)-C(16)	1.51(4)	C(41)-C(42)	1.37(3)
C(15)-C(17)	1.56(4)	C(41)-B(1)	1.66(3)
C(15)-C(18)	1.59(4)	C(42)-C(43)	1.39(4)
C(19)-C(22)	1.48(4)	C(43)-C(44)	1.41(4)
C(19)-C(20)	1.52(4)	C(44)-C(45)	1.30(4)
C(19)-C(21)	1.61(4)	C(45)-C(46)	1.37(4)
C(23)-C(24)	1.50(4)	C(51)-C(56)	1.36(3)
C(24)-B(1)	1.67(4)	C(51)-C(52)	1.39(3)
C(31)-C(36)	1.36(3)	C(51)-B(1)	1.66(3)
C(31)-C(32)	1.40(4)	C(52)-C(53)	1.44(3)
C(31)-B(1)	1.70(4)	C(53)-C(54)	1.30(3)
C(32)-C(33)	1.43(4)	C(54)-C(55)	1.34(3)
C(33)-C(34)	1.30(4)	C(55)-C(56)	1.42(3)
C(34)-C(35)	1.33(4)		
N(1)-Ta(1)-C(23)	100.5(10)	C(3)-C(2)-C(1)	111(4)
N(1)-Ta(1)-C(2)	114.7(13)	C(3)-C(2)-C(7)	122(3)
C(23)-Ta(1)-C(2)	132.7(16)	C(1)-C(2)-C(7)	126(4)
N(1)-Ta(1)-Cl(1)	102.5(5)	C(3)-C(2)-Ta(1)	80(3)
C(23)-Ta(1)-Cl(1)	112.4(9)	C(1)-C(2)-Ta(1)	75(2)
C(2)-Ta(1)-Cl(1)	90.5(11)	C(7)-C(2)-Ta(1)	124(3)
N(1)-Ta(1)-C(1)	98.6(9)	C(2)-C(3)-C(4)	110(3)
C(23)-Ta(1)-C(1)	113.6(11)	C(2)-C(3)-C(8)	129(3)
C(2)-Ta(1)-C(1)	34.1(11)	C(4)-C(3)-C(8)	120(3)
Cl(1)-Ta(1)-C(1)	124.1(7)	C(2)-C(3)-Ta(1)	68(2)
N(1)-Ta(1)-C(3)	146.8(10)	C(4)-C(3)-Ta(1)	78(2)
C(23)-Ta(1)-C(3)	108.1(11)	C(8)-C(3)-Ta(1)	127(2)
C(2)-Ta(1)-C(3)	32.1(12)	C(3)-C(4)-C(9)	131(3)
Cl(1)-Ta(1)-C(3)	82.0(7)	C(3)-C(4)-C(5)	109(3)
C(1)-Ta(1)-C(3)	54.7(9)	C(9)-C(4)-C(5)	120(3)
N(1)-Ta(1)-C(5)	115.9(8)	C(3)-C(4)-Ta(1)	72(2)
C(23)-Ta(1)-C(5)	81.1(12)	C(9)-C(4)-Ta(1)	129(2)
C(2)-Ta(1)-C(5)	55.9(13)	C(5)-C(4)-Ta(1)	69.7(17)
Cl(1)-Ta(1)-C(5)	136.5(7)	C(1)-C(5)-C(10)	125(3)
C(1)-Ta(1)-C(5)	34.1(10)	C(1)-C(5)-C(4)	103(2)
C(3)-Ta(1)-C(5)	54.7(9)	C(10)-C(5)-C(4)	131(3)
N(1)-Ta(1)-C(4)	149.9(8)	C(1)-C(5)-Ta(1)	69.6(16)
C(23)-Ta(1)-C(4)	81.0(11)	C(10)-C(5)-Ta(1)	125(2)
C(2)-Ta(1)-C(4)	52.6(14)	C(4)-C(5)-Ta(1)	76.0(16)
Cl(1)-Ta(1)-C(4)	104.5(6)	C(13)-C(11)-C(14)	106(2)
C(1)-Ta(1)-C(4)	54.9(10)	C(13)-C(11)-C(12)	112(3)
C(3)-Ta(1)-C(4)	30.1(9)	C(14)-C(11)-C(12)	111(3)
C(5)-Ta(1)-C(4)	34.3(8)	C(13)-C(11)-P(1)	109(2)
N(1)-P(1)-C(15)	109.8(13)	C(14)-C(11)-P(1)	109(2)
N(1)-P(1)-C(11)	108.3(12)	C(12)-C(11)-P(1)	110(2)
C(15)-P(1)-C(11)	108.6(15)	C(16)-C(15)-C(17)	110(2)
N(1)-P(1)-C(19)	105.0(12)	C(16)-C(15)-C(18)	110(3)
C(15)-P(1)-C(19)	112.3(12)	C(17)-C(15)-C(18)	104(3)
C(11)-P(1)-C(19)	112.7(14)	C(16)-C(15)-P(1)	116(2)
P(1)-N(1)-Ta(1)	171.2(11)	C(17)-C(15)-P(1)	109(2)
C(2)-C(1)-C(5)	107(3)	C(18)-C(15)-P(1)	107(2)
C(2)-C(1)-C(6)	123(3)	C(22)-C(19)-C(20)	111(3)
C(5)-C(1)-C(6)	129(3)	C(22)-C(19)-C(21)	111(2)
C(2)-C(1)-Ta(1)	71(2)	C(20)-C(19)-C(21)	107(3)
C(5)-C(1)-Ta(1)	76.3(17)	C(22)-C(19)-P(1)	108(2)
C(6)-C(1)-Ta(1)	127(2)	C(20)-C(19)-P(1)	108.6(18)

C(21)-C(19)-P(1)	110(2)	F(13)-C(44)-C(43)	120(3)
C(24)-C(23)-Ta(1)	103(2)	C(44)-C(45)-C(46)	123(4)
C(23)-C(24)-B(1)	115(2)	C(44)-C(45)-F(14)	119(3)
C(36)-C(31)-C(32)	112(3)	C(46)-C(45)-F(14)	117(3)
C(36)-C(31)-B(1)	123(2)	F(15)-C(46)-C(45)	117(3)
C(32)-C(31)-B(1)	125(2)	F(15)-C(46)-C(41)	120(3)
F(1)-C(32)-C(31)	119(3)	C(45)-C(46)-C(41)	123(3)
F(1)-C(32)-C(33)	118(3)	C(56)-C(51)-C(52)	113.4(18)
C(31)-C(32)-C(33)	123(3)	C(56)-C(51)-B(1)	122(2)
C(34)-C(33)-F(2)	125(4)	C(52)-C(51)-B(1)	124(2)
C(34)-C(33)-C(32)	119(4)	F(21)-C(52)-C(51)	123.0(18)
F(2)-C(33)-C(32)	116(3)	F(21)-C(52)-C(53)	116(2)
C(33)-C(34)-C(35)	123(4)	C(51)-C(52)-C(53)	121(2)
C(33)-C(34)-F(3)	118(3)	C(54)-C(53)-F(22)	125(2)
C(35)-C(34)-F(3)	120(3)	C(54)-C(53)-C(52)	120(2)
C(34)-C(35)-F(4)	124(3)	F(22)-C(53)-C(52)	115(2)
C(34)-C(35)-C(36)	118(3)	C(53)-C(54)-C(55)	123(2)
F(4)-C(35)-C(36)	118(3)	C(53)-C(54)-F(23)	120(2)
F(5)-C(36)-C(31)	121(3)	C(55)-C(54)-F(23)	117(2)
F(5)-C(36)-C(35)	114(3)	F(24)-C(55)-C(54)	125(2)
C(31)-C(36)-C(35)	125(3)	F(24)-C(55)-C(56)	119(2)
C(46)-C(41)-C(42)	111(2)	C(54)-C(55)-C(56)	116(2)
C(46)-C(41)-B(1)	125(2)	C(51)-C(56)-F(25)	120.1(17)
C(42)-C(41)-B(1)	124(2)	C(51)-C(56)-C(55)	126(2)
F(11)-C(42)-C(41)	118(2)	F(25)-C(56)-C(55)	113(2)
F(11)-C(42)-C(43)	113(3)	C(41)-B(1)-C(24)	113(2)
C(41)-C(42)-C(43)	128(3)	C(41)-B(1)-C(51)	111.8(18)
F(12)-C(43)-C(42)	125(3)	C(24)-B(1)-C(51)	102.7(17)
F(12)-C(43)-C(44)	121(3)	C(41)-B(1)-C(31)	102.0(17)
C(42)-C(43)-C(44)	115(3)	C(24)-B(1)-C(31)	112.8(19)
C(45)-C(44)-F(13)	120(3)	C(51)-B(1)-C(31)	115(2)
C(45)-C(44)-C(43)	119(3)		

Symmetry transformations used to generate equivalent atoms:

4. Anisotropic displacement parameters [A^2 x 10^3]

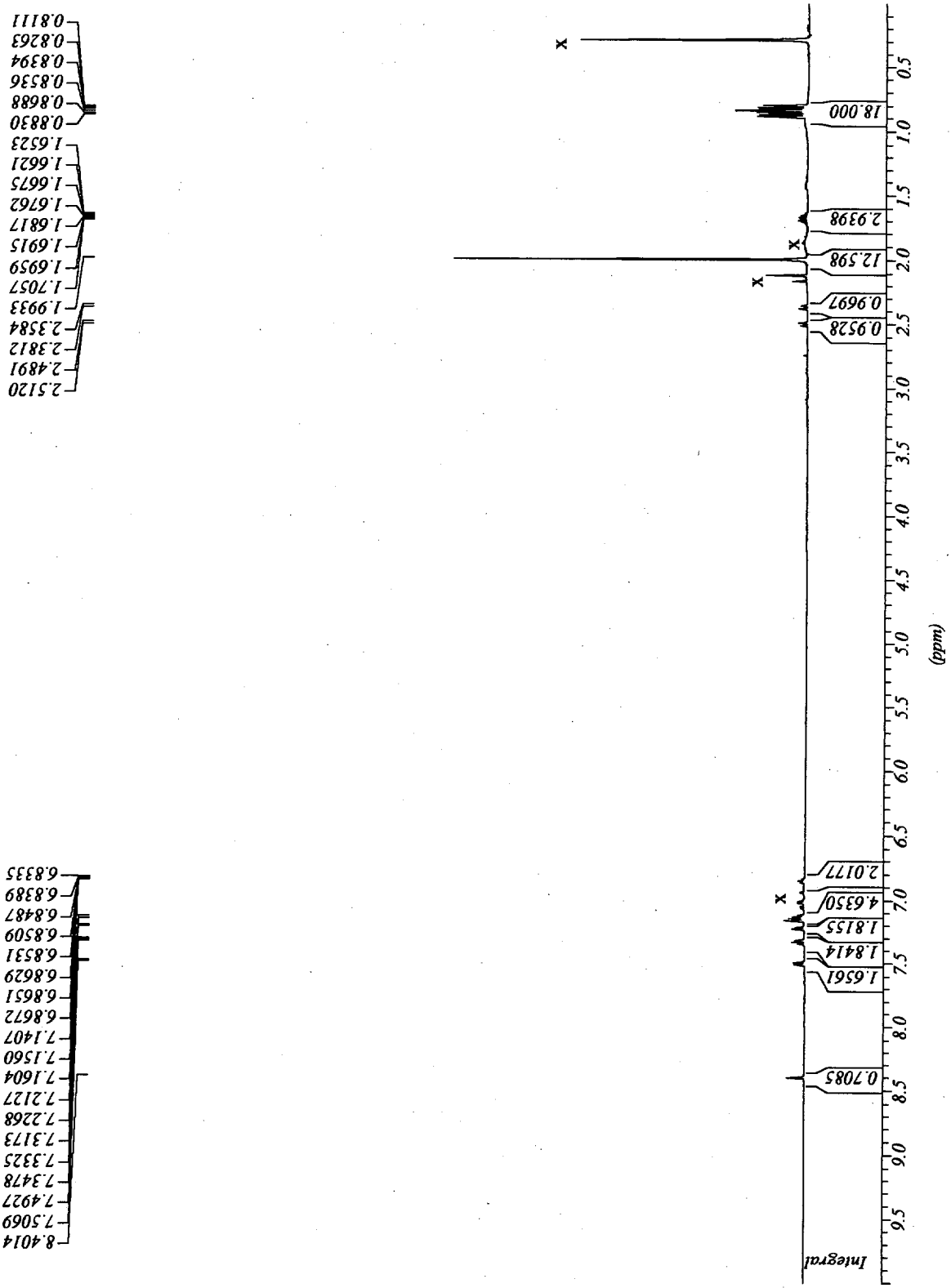
	U11	U22	U33	U23	U13	U12
Ta(1)	36(1)	51(1)	42(1)	9(1)	2(1)	3(1)
Cl(1)	37(2)	93(5)	79(5)	-7(7)	-9(2)	-11(5)
P(1)	41(3)	76(5)	31(6)	-11(4)	3(3)	-11(3)
F(1)	82(10)	150(18)	62(15)	-48(12)	3(9)	-2(10)
F(2)	93(13)	220(30)	76(19)	-34(18)	7(12)	55(15)
F(3)	108(13)	170(20)	90(20)	72(16)	55(13)	35(13)
F(4)	105(14)	140(20)	160(20)	-5(17)	53(13)	-65(14)
F(5)	79(11)	140(20)	112(19)	-29(14)	16(11)	-55(12)
F(11)	115(13)	84(13)	111(18)	-48(11)	-30(11)	15(10)
F(12)	114(14)	71(13)	230(30)	6(15)	21(15)	46(11)
F(13)	122(15)	180(20)	220(30)	130(20)	-14(16)	54(15)
F(14)	180(20)	200(30)	170(30)	60(20)	-130(20)	-20(20)
F(15)	156(17)	121(18)	150(20)	8(15)	-93(16)	-45(14)
F(21)	66(8)	88(12)	57(14)	22(10)	5(8)	14(8)
F(22)	64(9)	200(20)	53(15)	-14(12)	-22(9)	22(11)
F(23)	33(7)	133(16)	140(20)	-27(14)	-13(9)	-5(8)
F(24)	58(8)	86(12)	138(19)	36(12)	12(9)	-15(8)
F(25)	55(7)	87(11)	63(14)	21(9)	5(7)	-5(7)
N(1)	30(7)	72(19)	31(14)	-11(10)	13(7)	3(7)
C(23)	86(19)	43(16)	90(30)	-8(17)	39(19)	-6(14)
C(24)	45(11)	55(17)	30(20)	-1(13)	11(12)	-6(11)

B(1)	50(13)	34(14)	60(30)	3(14)	1(14)	7(11)

5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3)

	x	y	z	U(eq)
H(6A)	9414	851	6971	211
H(6B)	9846	574	8170	211
H(6C)	8844	141	7382	211
H(7A)	12772	1190	7902	179
H(7B)	13544	594	8557	179
H(7C)	11992	756	8789	179
H(8A)	14869	463	6027	162
H(8B)	15119	-331	6187	162
H(8C)	15085	155	7237	162
H(9A)	12977	-330	4126	172
H(9B)	12205	-1017	4403	172
H(9C)	13749	-911	4818	172
H(10A)	9494	-215	4684	150
H(10B)	8896	-589	5726	150
H(10C)	9863	-990	4925	150
H(12A)	10634	-2682	11990	191
H(12B)	9430	-2708	11071	191
H(12C)	9500	-2103	11946	191
H(13A)	12576	-1797	11809	134
H(13B)	11505	-1189	11775	134
H(13C)	12537	-1276	10802	134
H(14A)	12383	-2727	10437	119
H(14B)	12313	-2177	9472	119
H(14C)	11162	-2744	9533	119
H(16A)	8458	-372	12084	140
H(16B)	9537	-975	12181	140
H(16C)	8018	-1123	11736	140
H(17A)	7651	98	10323	167
H(17B)	7227	-607	9763	167
H(17C)	8295	-125	9191	167
H(18A)	10135	301	10985	146
H(18B)	10575	33	9810	146
H(18C)	11223	-295	10912	146
H(20A)	8020	-2887	8346	125
H(20B)	9115	-2882	9351	125
H(20C)	9493	-2573	8186	125
H(21A)	6297	-2288	9604	123
H(21B)	6777	-1622	10255	123
H(21C)	7445	-2337	10566	123
H(22A)	6914	-1765	7746	128
H(22B)	8403	-1479	7551	128
H(22C)	7410	-1079	8332	128
H(23A)	10567	-1927	6464	88
H(23B)	11842	-1697	5763	88
H(24A)	11929	-2530	7701	52
H(24B)	13275	-2164	7316	52

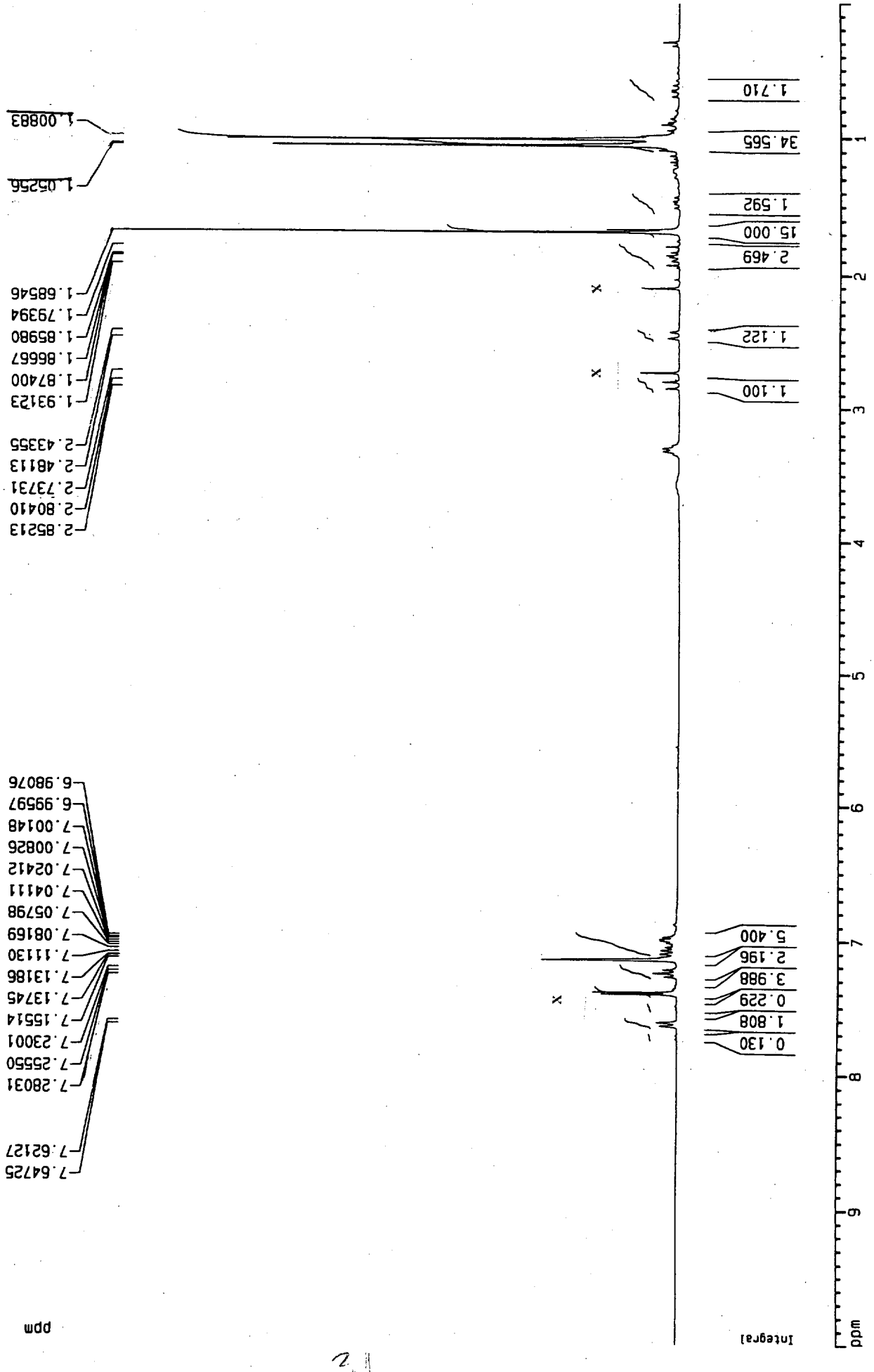
^{1}H NMR (C_6D_6)
Cp*Ta(NP*i*-Pr$_3$)(CHPh)(CH$_2$Ph) **8**
x indicates trace solvent and grease impurities



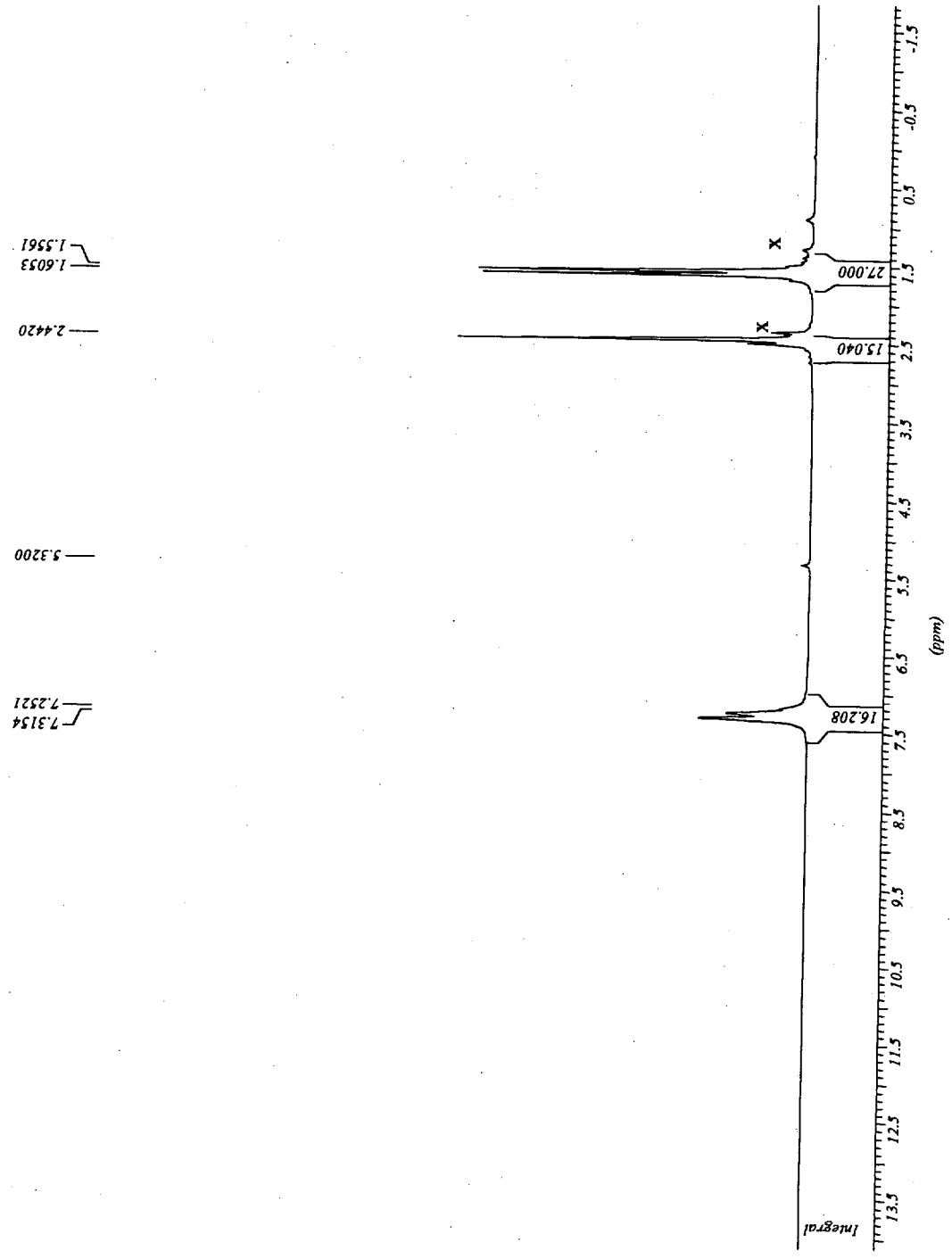
^{1}H NMR (C_6D_6)

Cp*Ta(NP*t*-Bu$_3$)(η^2-CHPhCH$_2$)(CH$_2$Ph) **9**

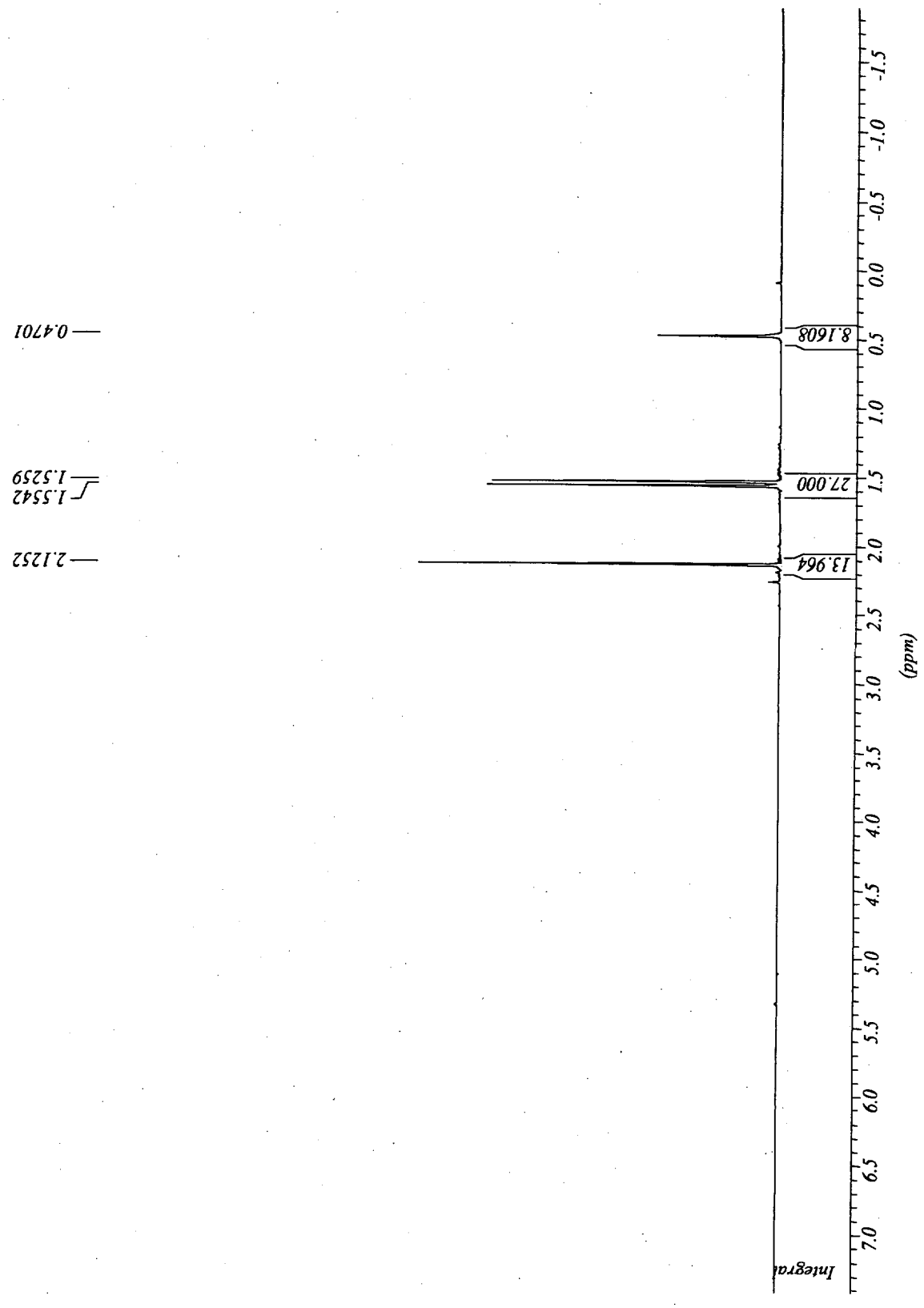
x indicates trace impurities



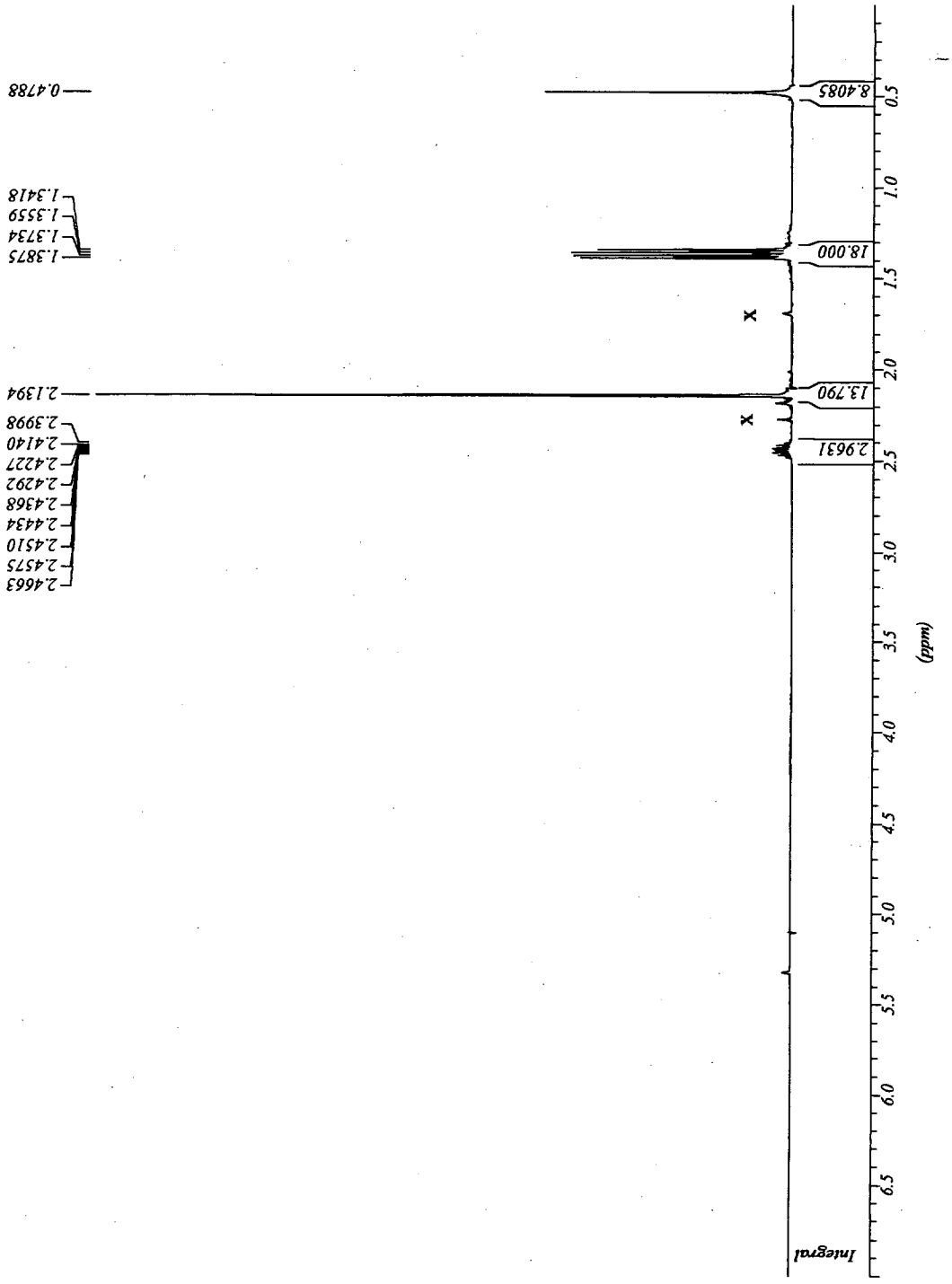
^{1}H NMR (CD_2Cl_2)
$[Cp^*Ta(NPt\text{-}Bu_3)Cl_2][B(C_6F_5)_4]$ **14**
x indicates trace solvent impurities



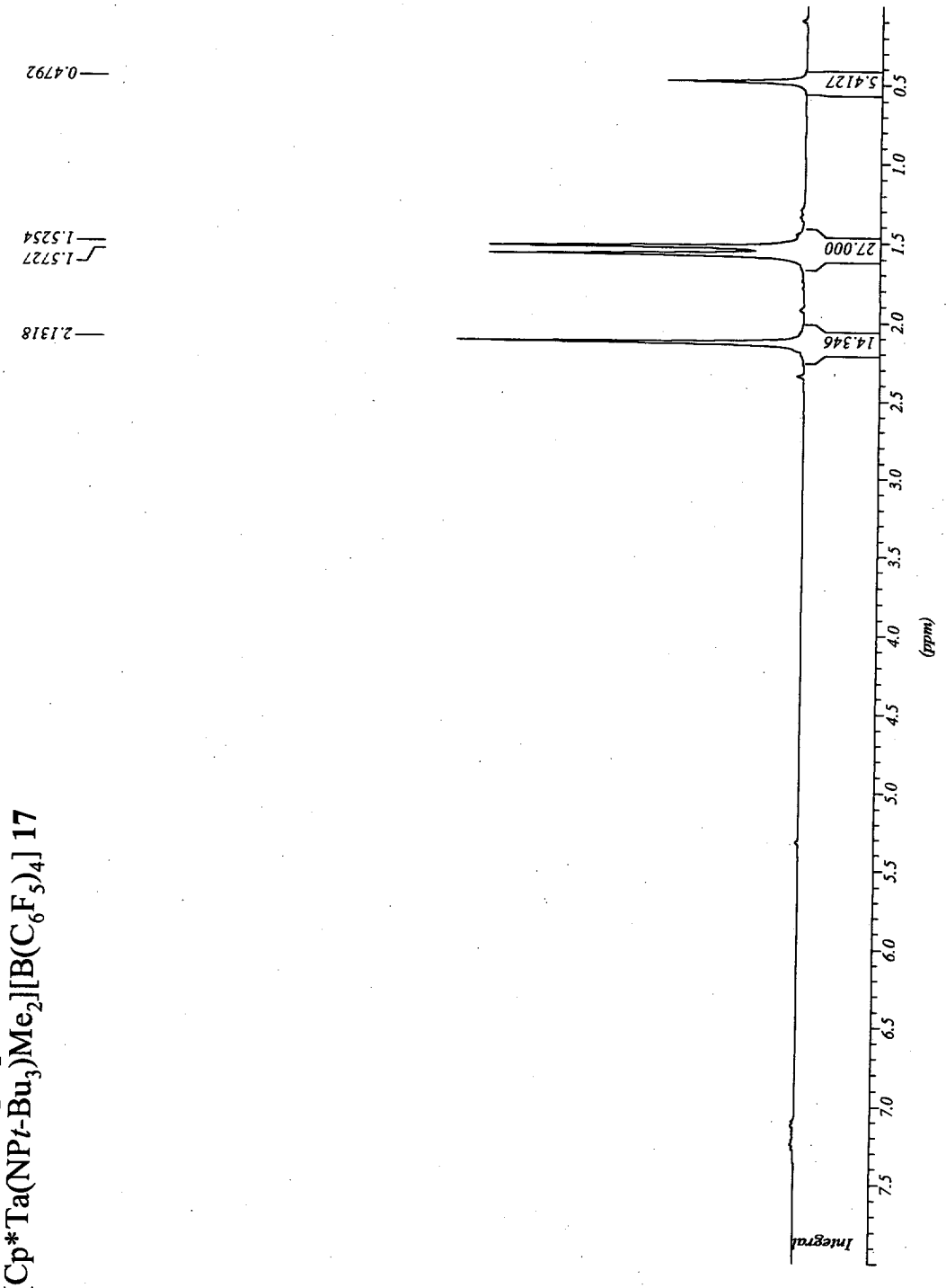
^{1}H NMR (CD_2Cl_2)
$Cp^*Ta(NPt\text{-}Bu_3)Me_2(MeB(C_6F_5)_3)$ **15**



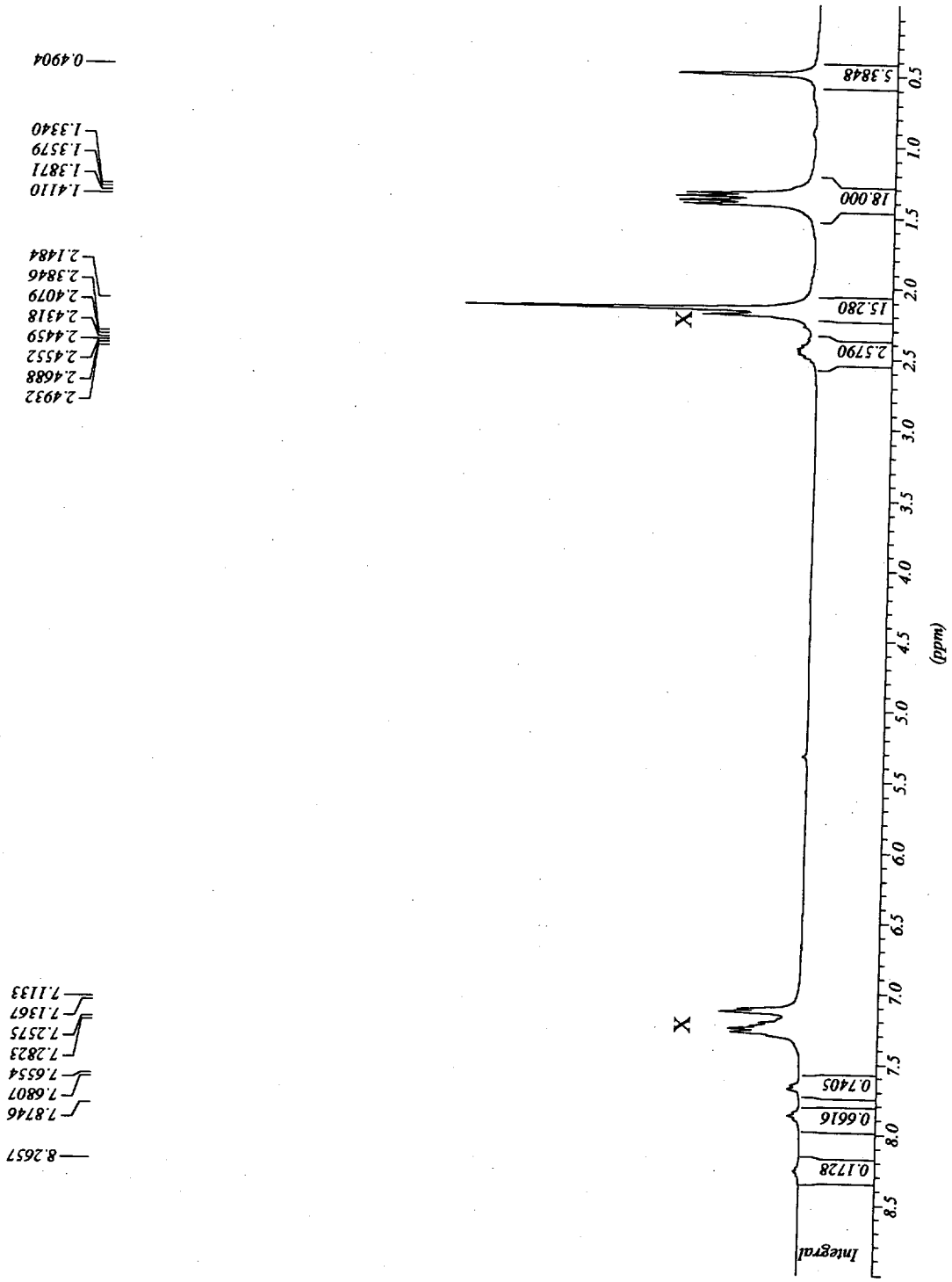
^{1}H NMR (CD_2Cl_2)
Cp*Ta(NP*i*-Pr$_3$)Me$_2$(MeB(C$_6$F$_5$)$_3$) **16**
x indicates trace impurities



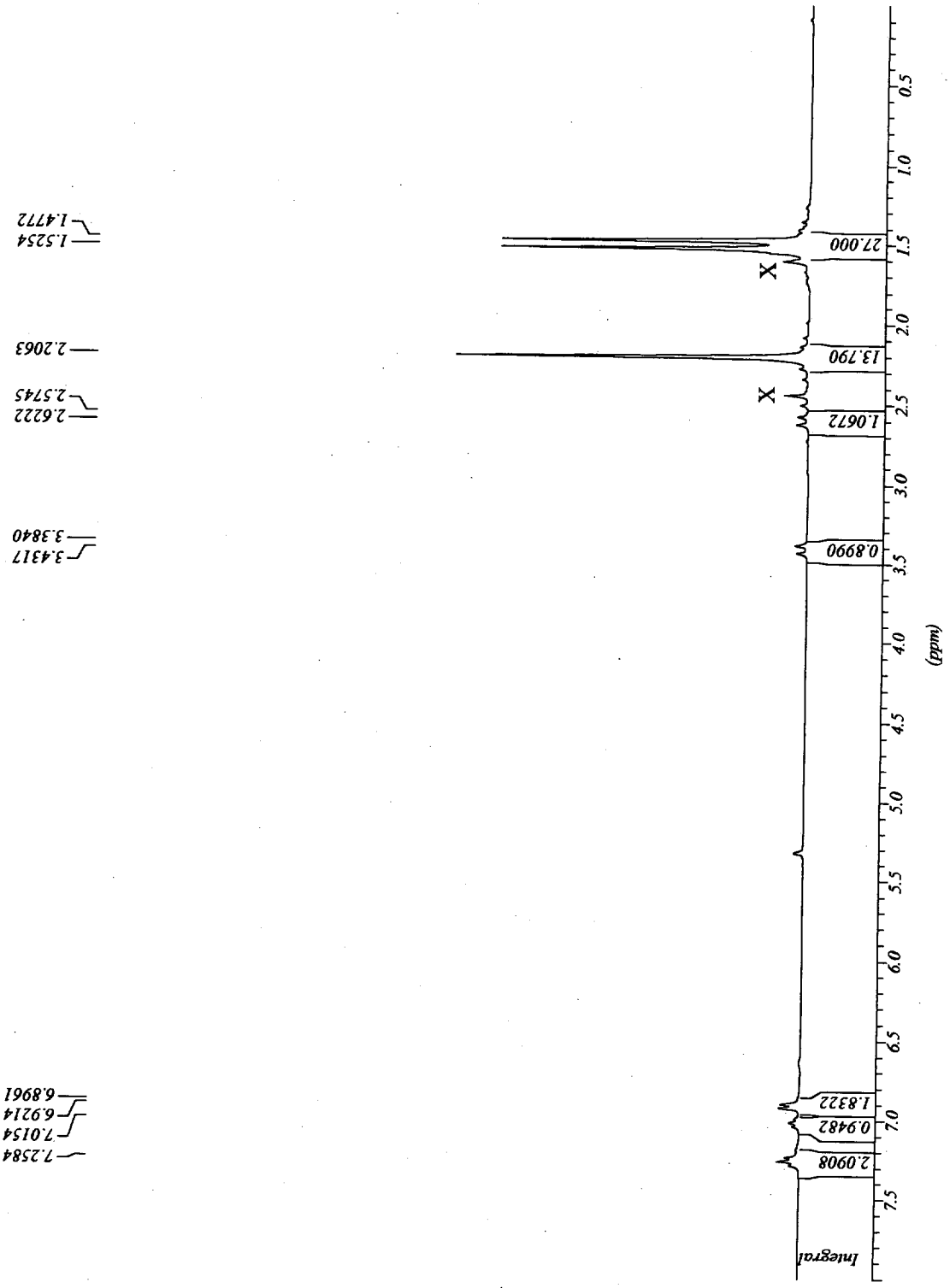
^{1}H NMR (CD_2Cl_2)
[Cp*Ta(NP*t*-Bu_3)Me_2][B(C_6F_5)$_4$] **17**



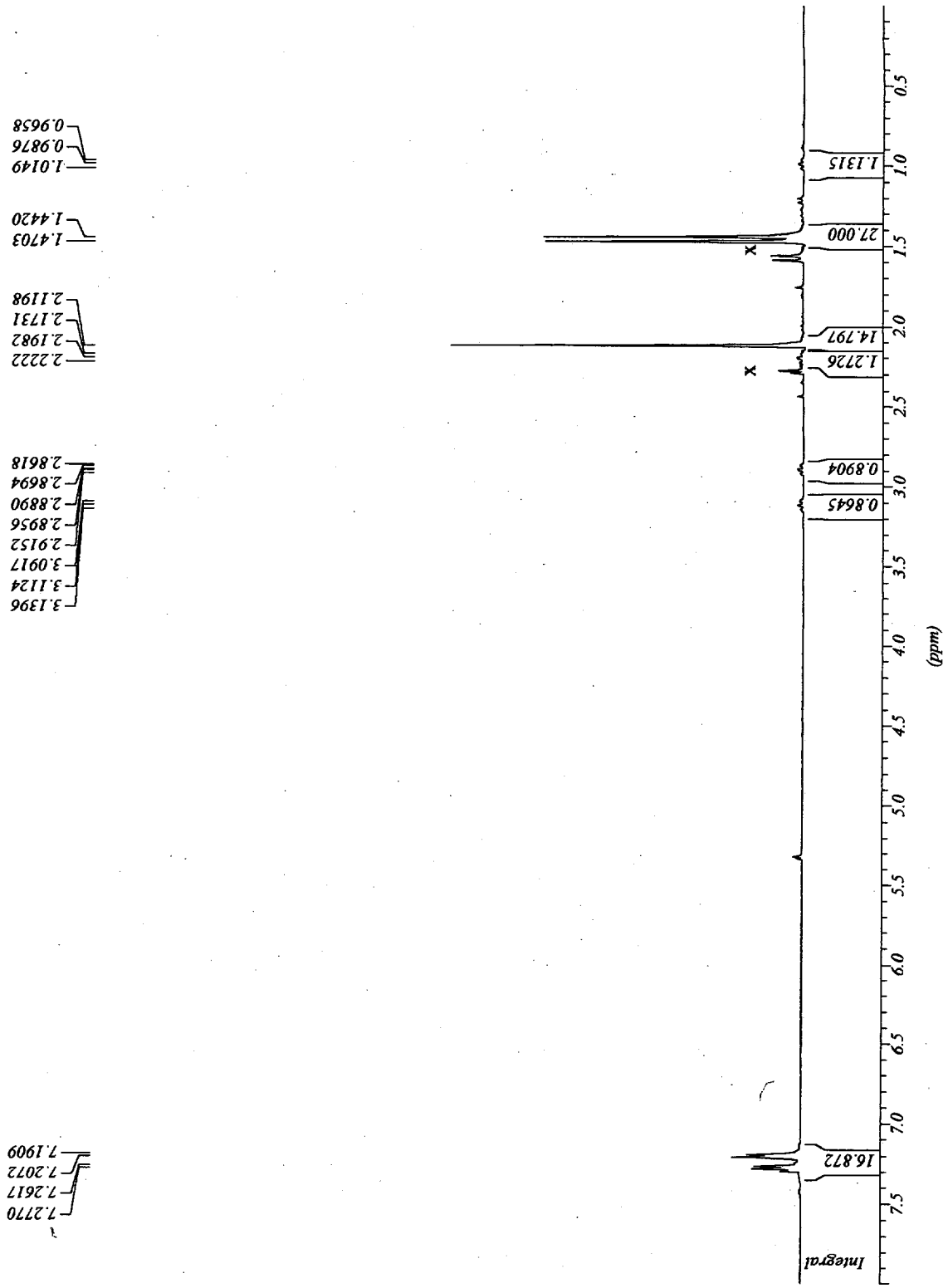
^{1}H NMR (CD_2Cl_2)
$[Cp^*Ta(NPi\text{-}Pr_3)Me_2][B(C_6F_5)_4]$ **18**
x indicates trace solvent impurities



^{1}H NMR (CD_2Cl_2)
[Cp*Ta(NP*t*-Bu$_3$)BnCl][ClB(C_6F_5)$_3$] **19**
x indicates trace impurities



^{1}H NMR (CD_2Cl_2)
[Cp*Ta(NP*t*-Bu_3)(Cl)$CH_2CH_2CPh_3$][$B(C_6F_5)_4$] **20**
x indicates trace impurities



^{1}H NMR (CD_2Cl_2)

$[Cp^*Ta(NPt\text{-}Bu_3)(Cl)CH_2CH_2CPh_3][BF_4]$ **21**

x indicates trace impurities