Table 1. Crystal data and structure refinement for compound 11.

Empirical formula	C35 H42 Cl2 N Ta
Formula weight	728.55
Temperature	293(2) K
Wavelength	0.71073 A
Crystal system, space group	Orthorhombic, P b c a
Unit cell dimensions	a = 15.544(2) A alpha = 90 deg. b = 19.634(3) A beta = 90 deg. c = 20.140(7) A gamma = 90 deg.
Volume	6147(2) A^3
Z, Calculated density	8, 1.575 Mg/m^3
Absorption coefficient	3.775 mm^-1
F(000)	2928
Crystal size	0.58 x 0.35 x 0.24 mm
Theta range for data collection	3.18 to 27.50 deg.
Limiting indices	-19<=h<=19, -25<=k<=24, -25<=l<=25
Reflections collected / unique	37934 / 6304 [R(int) = 0.1593]
Completeness to theta = 27.50	89.3 %
Absorption correction	Gaussian
Max. and min. transmission	0.293 and 0.1721
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	6304 / 0 / 323
Goodness-of-fit on F^2	1.060
Final R indices [I>2sigma(I)]	R1 = 0.0730, wR2 = 0.1696
R indices (all data)	R1 = 0.1183, wR2 = 0.1993
Largest diff. peak and hole	1.979 and -1.796 e.A^-3

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for compound 11.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Ta(1)	-232(1)	1562(1)	6949(1)	7(1)
Cl(1)	1161(2)	1711(1)	7490(1)	15(1)
Cl(2)	569(2)	1746(1)	5966(1)	14(1)
N(1)	-507(6)	2425(5)	7442(5)	14(2)
C(11)	255(7)	352(6)	6931(6)	13(2)
C(12)	-44(7)	488(5)	7592(5)	6(2)
C(13)	-937(7)	644(5)	7526(6)	13(2)
C(14)	-1182(7)	566(6)	6851(5)	12(2)
C(15)	-437(7)	372(6)	6487(5)	15(2)
C(16)	-1397(8)	2748(6)	7372(6)	19(2)
C(17)	-1780(9)	2456(6)	6755(6)	24(2)
C(18)	-1381(6)	1959(5)	6421(5)	6(2)
C(19)	-1798(7)	1766(6)	5767(6)	16(2)
C(20)	-1325(8)	1610(5)	5204(6)	16(2)
C(21)	-1726(8)	1474(6)	4599(6)	18(2)
C(22)	-2620(9)	1481(6)	4553(6)	24(3)
C(23)	-3108(8)	1636(6)	5113(6)	19(3)
C(24)	-2701(7)	1773(6)	5702(6)	17(2)
C(25)	82(6)	2847(6)	7847(5)	12(2)
C(26)	151(7)	2752(5)	8510(6)	13(2)
C(27)	718(8)	3170(7)	8886(6)	24(3)
C(28)	1187(7)	3679(6)	8553(7)	21(3)
C(29)	1119(7)	3748(6)	7876(6)	19(3)
C(30)	570(7)	3335(6)	7492(6)	12(2)
C(31)	7857(8)	4673(6)	4903(6)	23(3)
C(32)	7519(9)	4023(7)	4861(6)	23(3)
C(33)	7985(10)	3473(7)	5048(7)	30(3)
C(34)	8805(9)	3566(7)	5304(6)	26(3)
C(35)	9172(9)	4193(7)	5342(7)	29(3)
C(36)	8693(9)	4767(7)	5145(6)	26(3)
C(111)	1179(7)	150(6)	6750(6)	17(3)
C(121)	449(8)	410(7)	8224(7)	27
C(131)	-1548(8)	699(7)	8100(6)	19(3)
C(141)	-2104(7)	489(6)	6638(6)	15(2)
C(151)	-372(8)	194(6)	5777(6)	18(3)
C(161)	-1953(7)	2576(7)	7973(6)	20(3)
C(162)	-1380(8)	3524(6)	7308(7)	25(3)
C(261)	-262(8)	2166(7)	8898(6)	21(3)
C(301)	607(8)	3382(6)	6764(6)	19(3)

Table 3. Bond lengths [A] and angles [deg] for compound 11.

Ta(1)-N(1)	2.010(10)
Ta(1)-C(18)	2.219(10)
Ta(1)-Cl(2)	2.366(3)
Ta(1)-C(13)	2.408(11)
Ta(1)-Cl(1)	2.441(3)
Ta(1)-C(14)	2.458(12)
Ta(1)-C(12)	2.491(11)
Ta(1)-C(11)	2.494(12)
Ta(1)-C(15)	2.535(12)
N(1)-C(25)	1.481(14)
N(1)-C(16)	1.527(15)
C(11)-C(15)	1.400(16)
C(11)-C(12)	1.435(15)
C(11)-C(111)	1.533(15)
C(12)-C(13)	1.427(15)
C(12)-C(121)	1.495(18)
C(13)-C(14)	1.420(16)
C(13)-C(131)	1.501(16)
C(14)-C(15)	1.422(16)
C(14)-C(141)	1.504(15)
C(15)-C(151)	1.476(15)
C(16)-C(17)	1.493(15)
C(16)-C(161)	1.526(17)
C(16)-C(162)	1.529(17)
C(17)-C(18)	1.338(16)
C(18)-C(19)	1.516(15)
C(19)-C(20)	1.385(16)
C(19)-C(24)	1.409(15)
C(20)-C(21)	1.395(16)
C(21)-C(22)	1.393(17)
C(22)-C(23)	1.392(18)
C(23)-C(24)	1.372(16)
C(25)-C(26)	1.352(16)
C(25)-C(30)	1.417(16)
C(26)-C(27)	1.422(16)
C(26)-C(261)	1.533(16)
C(27)-C(28)	1.405(19)
C(28)-C(29)	1.375(18)
C(29)-C(30)	1.408(16)
C(30)-C(301)	1.470(16)
C(31)-C(32)	1.383(18)
C(31)-C(36)	1.400(18)
C(32)-C(33)	1.354(19)
C(33)-C(34)	1.39(2)
C(34)-C(35)	1.361(19)
C(35)-C(36)	1.408(19)
N(1)-Ta(1)-C(18)	76.7(4)
N(1)-Ta(1)-Cl(2)	113.4(3)
C(18)-Ta(1)-Cl(2)	88.2(3)
N(1)-Ta(1)-C(13)	107.2(4)
C(18)-Ta(1)-C(13)	97.4(4)
Cl(2)-Ta(1)-C(13)	139.2(3)
N(1)-Ta(1)-Cl(1)	82.4(3)
C(18)-Ta(1)-Cl(1)	152.3(3)
Cl(2)-Ta(1)-Cl(1)	83.62(10)
C(13)-Ta(1)-Cl(1)	106.1(3)

N(1)-Ta(1)-C(14)	125.6(4)
C(18)-Ta(1)-C(14)	76.0(4)
Cl(2)-Ta(1)-C(14)	111.7(3)
C(13)-Ta(1)-C(14)	33.9(4)
Cl(1)-Ta(1)-C(14)	131.6(3)
N(1)-Ta(1)-C(12)	118.8(4)
C(18)-Ta(1)-C(12)	129.8(4)
Cl(2)-Ta(1)-C(12)	120.1(2)
C(13)-Ta(1)-C(12)	33.8(3)
Cl(1)-Ta(1)-C(12)	76.4(3)
C(14)-Ta(1)-C(12)	55.9(4)
N(1)-Ta(1)-C(11)	151.0(4)
C(18)-Ta(1)-C(11)	124.9(4)
Cl(2)-Ta(1)-C(11)	88.5(3)
C(13)-Ta(1)-C(11)	55.4(4)
Cl(1)-Ta(1)-C(11)	81.4(3)
C(14)-Ta(1)-C(11)	54.8(4)
C(12)-Ta(1)-C(11)	33.5(3)
N(1)-Ta(1)-C(15)	158.7(4)
C(18)-Ta(1)-C(15)	92.7(4)
Cl(2)-Ta(1)-C(15)	84.2(3)
C(13)-Ta(1)-C(15)	55.3(4)
Cl(1)-Ta(1)-C(15)	112.7(3)
C(14)-Ta(1)-C(15)	33.0(4)
C(12)-Ta(1)-C(15)	54.9(4)
C(11)-Ta(1)-C(15)	32.3(4)
C(25)-N(1)-C(16)	112.3(9)
C(25)-N(1)-Ta(1)	127.8(7)
C(16)-N(1)-Ta(1)	119.8(7)
C(15)-C(11)-C(12)	109.7(9)
C(15)-C(11)-C(111)	125.1(10)
C(12)-C(11)-C(111)	124.9(10)
C(15)-C(11)-Ta(1)	75.5(7)
C(12)-C(11)-Ta(1)	73.2(6)
C(111)-C(11)-Ta(1)	122.3(7)
C(13)-C(12)-C(11)	105.6(9)
C(13)-C(12)-C(121)	126.8(10)
C(11)-C(12)-C(121)	127.2(10)
C(13)-C(12)-Ta(1)	69.9(6)
C(11)-C(12)-Ta(1)	73.4(6)
C(121)-C(12)-Ta(1)	126.1(8)
C(14)-C(13)-C(12)	109.0(10)
C(14)-C(13)-C(131)	125.1(10)
C(12)-C(13)-C(131)	124.1(10)
C(14)-C(13)-Ta(1)	75.0(7)
C(12)-C(13)-Ta(1)	76.3(6)
C(131)-C(13)-Ta(1)	127.3(8)
C(13)-C(14)-C(15)	107.7(10)
C(13)-C(14)-C(141)	122.7(10)
C(15)-C(14)-C(141)	127.0(10)
C(13)-C(14)-Ta(1)	71.1(6)
C(15)-C(14)-Ta(1)	76.5(7)
C(141)-C(14)-Ta(1)	132.4(8)
C(11)-C(15)-C(14)	107.7(10)
C(11)-C(15)-C(151)	124.0(10)
C(14)-C(15)-C(151)	128.2(10)
C(11)-C(15)-Ta(1)	72.2(7)
C(14)-C(15)-Ta(1)	70.5(7)
C(151)-C(15)-Ta(1)	124.4(8)
C(17)-C(16)-C(161)	110.4(11)
C(17)-C(16)-N(1)	106.2(9)

C(161)-C(16)-N(1)	110.3(9)
C(17)-C(16)-C(162)	108.6(10)
C(161)-C(16)-C(162)	107.3(10)
N(1)-C(16)-C(162)	114.0(10)
C(18)-C(17)-C(16)	120.9(11)
C(17)-C(18)-C(19)	114.8(10)
C(17)-C(18)-Ta(1)	112.8(8)
C(19)-C(18)-Ta(1)	132.3(7)
C(20)-C(19)-C(24)	117.1(11)
C(20)-C(19)-C(18)	122.6(10)
C(24)-C(19)-C(18)	120.3(10)
C(19)-C(20)-C(21)	121.4(11)
C(22)-C(21)-C(20)	120.0(12)
C(21)-C(22)-C(23)	119.5(12)
C(24)-C(23)-C(22)	119.5(11)
C(23)-C(24)-C(19)	122.5(11)
C(26)-C(25)-C(30)	123.3(10)
C(26)-C(25)-N(1)	121.2(10)
C(30)-C(25)-N(1)	115.6(9)
C(25)-C(26)-C(27)	119.7(11)
C(25)-C(26)-C(261)	124.9(11)
C(27)-C(26)-C(261)	115.0(11)
C(28)-C(27)-C(26)	118.5(12)
C(29)-C(28)-C(27)	120.2(11)
C(28)-C(29)-C(30)	122.2(12)
C(29)-C(30)-C(25)	116.0(11)
C(29)-C(30)-C(301)	119.1(11)
C(25)-C(30)-C(301)	124.5(10)
C(32)-C(31)-C(36)	119.7(12)
C(33)-C(32)-C(31)	121.1(13)
C(32)-C(33)-C(34)	119.3(13)
C(35)-C(34)-C(33)	121.7(13)
C(34)-C(35)-C(36)	119.2(13)
C(31)-C(36)-C(35)	118.9(12)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for compound 11.
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
Ta(1)	4(1)	8(1)	8(1)	0(1)	1(1)	0(1)
Cl(1)	7(1)	17(1)	21(1)	-3(1)	-1(1)	0(1)
Cl(2)	12(1)	15(1)	15(1)	0(1)	6(1)	-2(1)
N(1)	15	14(5)	11(5)	2(4)	-5(4)	-10(4)
C(11)	13(5)	8(5)	19(6)	0(5)	7(5)	-3(5)
C(13)	15(6)	7(5)	18(6)	9(5)	-1(5)	1(5)
C(15)	15(5)	23	7(5)	0(5)	2(4)	-5(5)
C(16)	23	12(6)	21(6)	-7(5)	-14(5)	10(5)
C(17)	45	11(6)	16(6)	-8(5)	-20(6)	5(6)
C(19)	9(5)	26	13(5)	-1(5)	-2(4)	-4(5)
C(20)	24(6)	7(5)	18(6)	-3(5)	4(5)	5(5)
C(21)	18(6)	23	14(6)	11(5)	-4(5)	-6(5)
C(22)	35(8)	16(6)	20(7)	4(5)	-12(6)	-8(6)
C(23)	14(6)	14(6)	27(7)	9(5)	-1(5)	0(5)
C(24)	17(6)	20(6)	13(6)	8(5)	-8(4)	-3(5)
C(25)	4(5)	28	3(5)	0(5)	-3(4)	1(5)
C(26)	7(5)	3(5)	30(7)	-2(5)	6(5)	-1(4)
C(27)	20(6)	30(7)	21(6)	-14(6)	-15(5)	4(6)
C(28)	11(6)	17(6)	34(7)	-13(6)	-6(5)	6(5)
C(29)	11(5)	14(6)	33(7)	7(5)	-8(5)	4(5)
C(30)	7(5)	13(6)	15(5)	-9(5)	0(4)	2(4)
C(31)	25(6)	13(6)	30(7)	14(6)	7(6)	2(6)
C(32)	25(6)	29(7)	15(6)	6(5)	1(5)	-2(6)
C(33)	41(8)	20(7)	29(8)	0(6)	5(6)	-14(7)
C(34)	40(8)	27(7)	10(6)	-7(5)	3(6)	19(7)
C(35)	30(7)	26(7)	30(8)	2(6)	-5(6)	-8(6)
C(36)	32(7)	21(7)	24(7)	1(6)	4(6)	0(6)
C(111)	10(5)	14(6)	27(7)	-1(5)	3(5)	2(5)
C(121)	25	27	29	14	27	14
C(131)	20(6)	24(7)	12(6)	-7(5)	7(5)	-8(6)
C(141)	18(6)	11(6)	16(6)	6(5)	-2(5)	5(5)
C(151)	23(6)	18(6)	15(6)	-10(5)	6(5)	5(5)
C(161)	6(5)	33(7)	21(6)	-19(6)	3(5)	-5(5)
C(162)	10(5)	27	39(8)	-13(6)	-9(5)	8(5)
C(261)	23(6)	24(7)	15(6)	-6(5)	-1(5)	2(6)
C(301)	20(6)	25(7)	12(6)	-4(5)	-3(5)	-2(6)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for compound 11.

	x	y	z	U(eq)
H(17)	-2304	2621	6601	29
H(20)	-728	1596	5231	19
H(21)	-1395	1378	4225	22
H(22)	-2889	1384	4152	29
H(23)	-3705	1646	5088	22
H(24)	-3033	1874	6073	20
H(27)	778	3108	9341	28
H(28)	1544	3969	8792	25
H(29)	1448	4079	7664	23
H(31)	7531	5046	4770	28
H(32)	6963	3963	4702	28
H(33)	7757	3037	5006	36
H(34)	9112	3189	5453	31
H(35)	9733	4243	5496	35
H(36)	8927	5202	5176	31
H(11A)	1535	176	7138	26
H(11B)	1396	455	6417	26
H(11C)	1184	-307	6581	26
H(12A)	1038	305	8125	41
H(12B)	203	49	8482	41
H(12C)	423	828	8472	41
H(13A)	-1228	744	8506	28
H(13B)	-1899	297	8120	28
H(13C)	-1909	1092	8042	28
H(14A)	-2130	448	6163	23
H(14B)	-2426	882	6775	23
H(14C)	-2345	89	6839	23
H(15A)	-926	245	5571	28
H(15B)	-184	-270	5733	28
H(15C)	34	490	5564	28
H(16A)	-1698	2766	8366	30
H(16B)	-1993	2090	8019	30
H(16C)	-2518	2763	7913	30
H(16D)	-1135	3719	7702	38
H(16E)	-1956	3690	7251	38
H(16F)	-1039	3650	6930	38
H(26A)	-120	2208	9360	31
H(26B)	-50	1740	8732	31
H(26C)	-876	2183	8845	31
H(30A)	199	3072	6574	29
H(30B)	1175	3267	6615	29
H(30C)	472	3839	6629	29