ORGANOMETALLICS
Organometallics, 1998, 17(19), 4183-4195, DOI:10.1021/om9802966

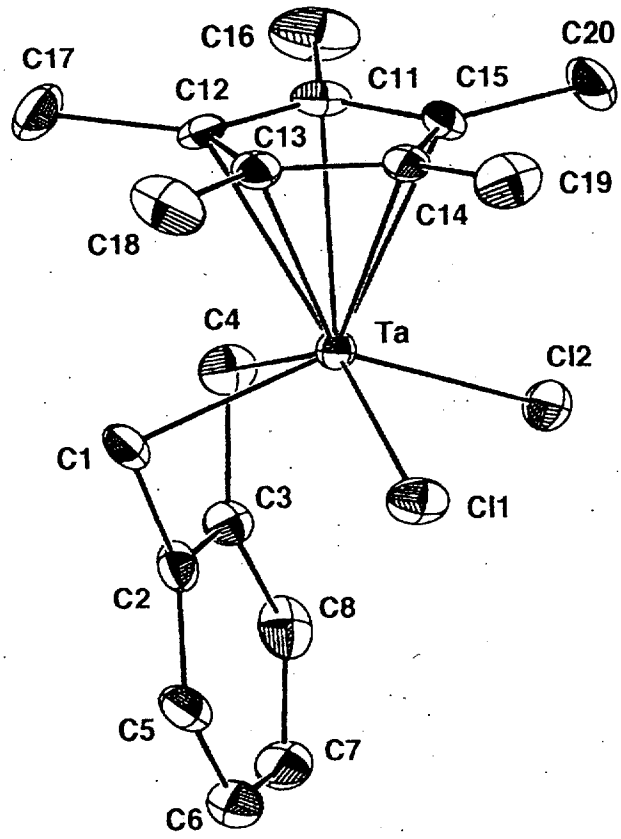

Figure S1. *ORTEP* drawing of **8** with numbering scheme. Hydrogen atoms are omitted for clarity.

Table 1. Atomic coordinates and B_{iso}/B_{eq}

atom	x	y	z	B_{eq}
Ta(1)	0.79360(3)	0.10195(4)	0.23466(2)	2.292(7)
Cl(1)	0.6658(2)	0.2923(3)	0.1472(2)	4.00(6)
Cl(2)	0.9155(2)	0.3023(3)	0.2500(2)	3.98(6)
C(1)	0.6965(7)	0.041(1)	0.3046(7)	3.7(2)
C(2)	0.7421(7)	0.186(1)	0.3670(6)	3.2(2)
C(3)	0.8460(7)	0.185(1)	0.4100(6)	3.4(2)
C(4)	0.8940(7)	0.046(1)	0.3857(6)	3.9(2)
C(5)	0.6905(7)	0.320(1)	0.3804(7)	4.1(3)
C(6)	0.7413(8)	0.442(1)	0.4381(7)	4.6(3)
C(7)	0.8423(9)	0.444(1)	0.4812(7)	5.1(3)
C(8)	0.8955(7)	0.321(1)	0.4663(6)	4.5(3)
C(11)	0.8745(7)	-0.134(1)	0.2047(7)	3.5(2)
C(12)	0.7847(7)	-0.1897(10)	0.2060(7)	3.5(2)
C(13)	0.7058(6)	-0.118(1)	0.1264(6)	3.2(2)
C(14)	0.7473(7)	-0.018(1)	0.0791(6)	3.0(2)
C(15)	0.8500(6)	-0.028(1)	0.1278(6)	2.9(2)
C(16)	0.9783(8)	-0.193(1)	0.2692(8)	7.0(4)
C(17)	0.771(1)	-0.321(1)	0.2725(8)	7.2(4)
C(18)	0.5974(7)	-0.150(1)	0.0963(8)	6.3(3)
C(19)	0.6903(8)	0.066(1)	-0.0158(7)	5.1(3)
C(20)	0.9239(8)	0.042(1)	0.0973(8)	5.7(3)
H(1)	0.6278	0.0493	0.2648	4.4706
H(1')	0.7101	-0.0598	0.3371	4.4706
H(4)	0.9623	0.0603	0.4024	4.6534

Table 1. Atomic coordinates and B_{iso}/B_{eq} (continued)

atom	x	y	z	B_{eq}
H(4')	0.8838	-0.0559	0.4077	4.6534
H(5)	0.6205	0.3236	0.3488	4.8684
H(6)	0.7062	0.5292	0.4491	5.5164
H(7)	0.8761	0.5313	0.5218	6.0784
H(8)	0.9655	0.3263	0.4937	5.4155
H(16)	0.9757	-0.2639	0.3163	8.4062
H(16")	1.0194	-0.1036	0.2996	8.4062
H(16')	1.0045	-0.2494	0.2319	8.4062
H(17)	0.7315	-0.2775	0.3010	8.6860
H(17")	0.8337	-0.3505	0.3210	8.6860
H(17')	0.7394	-0.4129	0.2357	8.6860
H(18)	0.5647	-0.0513	0.0946	7.5473
H(18")	0.5899	-0.2216	0.1405	7.5473
H(18')	0.5693	-0.1979	0.0345	7.5473
H(19)	0.6444	0.1395	-0.0102	6.1244
H(19")	0.6559	-0.0116	-0.0636	6.1244
H(19')	0.7349	0.1240	-0.0329	6.1244
H(20)	0.9567	-0.0428	0.0814	6.7938
H(20")	0.9708	0.1041	0.1481	6.7938
H(20')	0.8910	0.1092	0.0431	6.7938

$$B_{eq} = \frac{8}{3}\pi^2(U_{11}(aa^*)^2 + U_{22}(bb^*)^2 + U_{33}(cc^*)^2 + 2U_{12}aa^*bb^*\cos\gamma + 2U_{13}aa^*cc^*\cos\beta + 2U_{23}bb^*cc^*\cos\alpha)$$

Table 2. Anisotropic Displacement Parameters

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Ta(1)	0.0325(2)	0.0278(2)	0.0270(2)	0.0023(2)	0.0131(1)	0.0013(2)
Cl(1)	0.050(1)	0.050(1)	0.043(1)	0.023(1)	0.012(1)	0.005(1)
Cl(2)	0.052(1)	0.042(1)	0.065(2)	-0.012(1)	0.032(1)	-0.007(1)
C(1)	0.054(6)	0.052(6)	0.054(6)	-0.006(5)	0.041(5)	-0.009(5)
C(2)	0.050(6)	0.046(6)	0.032(5)	-0.011(5)	0.022(4)	-0.002(5)
C(3)	0.062(6)	0.042(5)	0.024(4)	0.005(5)	0.016(4)	0.000(4)
C(4)	0.057(6)	0.049(6)	0.028(5)	0.014(5)	0.006(5)	0.005(4)
C(5)	0.059(6)	0.057(7)	0.051(6)	-0.001(6)	0.036(5)	-0.008(5)
C(6)	0.082(8)	0.050(7)	0.053(7)	0.002(6)	0.039(6)	-0.007(5)
C(7)	0.110(10)	0.047(7)	0.041(6)	-0.009(7)	0.038(7)	-0.015(5)
C(8)	0.062(7)	0.074(8)	0.028(5)	-0.017(6)	0.011(5)	-0.005(5)
C(11)	0.052(6)	0.039(6)	0.043(5)	0.012(5)	0.019(5)	-0.011(5)
C(12)	0.070(7)	0.020(4)	0.050(6)	0.007(5)	0.034(5)	-0.001(4)
C(13)	0.047(5)	0.035(5)	0.044(5)	-0.011(5)	0.024(5)	-0.018(5)
C(14)	0.056(6)	0.032(5)	0.026(4)	-0.004(4)	0.020(4)	-0.010(4)
C(15)	0.047(5)	0.038(5)	0.037(5)	-0.003(4)	0.029(4)	-0.009(4)
C(16)	0.078(8)	0.09(1)	0.074(8)	0.063(8)	0.014(7)	0.006(8)
C(17)	0.20(1)	0.030(6)	0.081(9)	-0.006(8)	0.09(1)	0.006(6)
C(18)	0.054(7)	0.10(1)	0.097(9)	-0.040(7)	0.043(7)	-0.058(8)
C(19)	0.086(8)	0.059(7)	0.032(5)	0.012(6)	0.010(5)	0.000(5)
C(20)	0.087(8)	0.065(8)	0.107(10)	-0.026(6)	0.083(8)	-0.024(7)

The general temperature factor expression:

$$\exp(-2\pi^2(a^{*2}U_{11}h^2 + b^{*2}U_{22}k^2 + c^{*2}U_{33}l^2 + 2a^*b^*U_{12}hk + 2a^*c^*U_{13}hl + 2b^*c^*U_{23}kl))$$

Table 3. Bond Lengths($\AA$)

atom	atom	distance	atom	atom	distance
Ta(1)	Cl(1)	2.400(2)	Ta(1)	Cl(2)	2.405(2)
Ta(1)	C(1)	2.221(8)	Ta(1)	C(4)	2.220(8)
Ta(1)	C(11)	2.448(8)	Ta(1)	C(12)	2.448(8)
Ta(1)	C(13)	2.445(8)	Ta(1)	C(14)	2.420(8)
Ta(1)	C(15)	2.419(8)	C(1)	C(2)	1.51(1)
C(2)	C(3)	1.41(1)	C(2)	C(5)	1.42(1)
C(3)	C(4)	1.49(1)	C(3)	C(8)	1.42(1)
C(5)	C(6)	1.35(1)	C(6)	C(7)	1.37(1)
C(7)	C(8)	1.38(1)	C(11)	C(12)	1.44(1)
C(11)	C(15)	1.39(1)	C(11)	C(16)	1.53(1)
C(12)	C(13)	1.42(1)	C(12)	C(17)	1.57(1)
C(13)	C(14)	1.42(1)	C(13)	C(18)	1.51(1)
C(14)	C(15)	1.40(1)	C(14)	C(19)	1.52(1)
C(15)	C(20)	1.50(1)			

Table 4. Bond Lengths(Å)

atom	atom	distance	atom	atom	distance
C(1)	H(1)	0.95	C(1)	H(1')	0.95
C(4)	H(4)	0.95	C(4)	H(4')	0.95
C(5)	H(5)	0.95	C(6)	H(6)	0.95
C(7)	H(7)	0.95	C(8)	H(8)	0.95
C(16)	H(16)	0.95	C(16)	H(16")	0.95
C(16)	H(16')	0.95	C(17)	H(17)	0.95
C(17)	H(17")	0.95	C(17)	H(17')	0.95
C(18)	H(18)	0.95	C(18)	H(18")	0.95
C(18)	H(18')	0.95	C(19)	H(19)	0.95
C(19)	H(19")	0.95	C(19)	H(19')	0.95
C(20)	H(20)	0.95	C(20)	H(20")	0.95
C(20)	H(20')	0.95			

Table 5. Bond Angles(°)

atom	atom	atom	angle	atom	atom	atom	angle
Cl(1)	Ta(1)	Cl(2)	89.53(9)	Cl(1)	Ta(1)	C(1)	83.8(3)
Cl(1)	Ta(1)	C(4)	138.2(2)	Cl(1)	Ta(1)	C(11)	139.3(2)
Cl(1)	Ta(1)	C(12)	125.3(2)	Cl(1)	Ta(1)	C(13)	92.3(2)
Cl(1)	Ta(1)	C(14)	83.7(2)	Cl(1)	Ta(1)	C(15)	109.7(2)
Cl(2)	Ta(1)	C(1)	137.9(2)	Cl(2)	Ta(1)	C(4)	84.1(3)
Cl(2)	Ta(1)	C(11)	98.6(2)	Cl(2)	Ta(1)	C(12)	132.6(2)
Cl(2)	Ta(1)	C(13)	138.1(2)	Cl(2)	Ta(1)	C(14)	105.1(2)
Cl(2)	Ta(1)	C(15)	84.1(2)	C(1)	Ta(1)	C(4)	74.1(3)
C(1)	Ta(1)	C(11)	113.4(3)	C(1)	Ta(1)	C(12)	82.5(3)
C(1)	Ta(1)	C(13)	83.9(3)	C(1)	Ta(1)	C(14)	115.4(3)
C(1)	Ta(1)	C(15)	137.1(3)	C(4)	Ta(1)	C(11)	82.5(3)
C(4)	Ta(1)	C(12)	86.9(3)	C(4)	Ta(1)	C(13)	119.3(3)
C(4)	Ta(1)	C(14)	137.7(3)	C(4)	Ta(1)	C(15)	110.6(3)
C(11)	Ta(1)	C(12)	34.1(3)	C(11)	Ta(1)	C(13)	55.9(3)
C(11)	Ta(1)	C(14)	55.6(3)	C(11)	Ta(1)	C(15)	33.3(3)
C(12)	Ta(1)	C(13)	33.7(3)	C(12)	Ta(1)	C(14)	56.2(3)
C(12)	Ta(1)	C(15)	56.2(3)	C(13)	Ta(1)	C(14)	33.9(3)
C(13)	Ta(1)	C(15)	56.0(3)	C(14)	Ta(1)	C(15)	33.5(3)
Ta(1)	C(1)	C(2)	85.5(5)	C(1)	C(2)	C(3)	113.7(8)
C(1)	C(2)	C(5)	126.3(8)	C(3)	C(2)	C(5)	120.0(9)
C(2)	C(3)	C(4)	116.5(8)	C(2)	C(3)	C(8)	117.6(9)
C(4)	C(3)	C(8)	125.7(9)	Ta(1)	C(4)	C(3)	85.7(5)
C(2)	C(5)	C(6)	119.8(9)	C(5)	C(6)	C(7)	121.4(10)
C(6)	C(7)	C(8)	120.8(10)	C(3)	C(8)	C(7)	120.2(9)

Table 5. Bond Angles(°) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
Ta(1)	C(11)	C(12)	73.0(5)	Ta(1)	C(11)	C(15)	72.2(5)
Ta(1)	C(11)	C(16)	125.7(7)	C(12)	C(11)	C(15)	108.2(8)
C(12)	C(11)	C(16)	125.9(10)	C(15)	C(11)	C(16)	125.6(10)
Ta(1)	C(12)	C(11)	72.9(5)	Ta(1)	C(12)	C(13)	73.0(5)
Ta(1)	C(12)	C(17)	125.0(6)	C(11)	C(12)	C(13)	106.8(8)
C(11)	C(12)	C(17)	128.7(9)	C(13)	C(12)	C(17)	124.1(9)
Ta(1)	C(13)	C(12)	73.3(5)	Ta(1)	C(13)	C(14)	72.1(5)
Ta(1)	C(13)	C(18)	122.1(6)	C(12)	C(13)	C(14)	107.8(8)
C(12)	C(13)	C(18)	125.4(9)	C(14)	C(13)	C(18)	126.8(9)
Ta(1)	C(14)	C(13)	74.0(5)	Ta(1)	C(14)	C(15)	73.2(5)
Ta(1)	C(14)	C(19)	125.2(6)	C(13)	C(14)	C(15)	108.3(8)
C(13)	C(14)	C(19)	125.6(9)	C(15)	C(14)	C(19)	125.5(8)
Ta(1)	C(15)	C(11)	74.5(5)	Ta(1)	C(15)	C(14)	73.3(5)
Ta(1)	C(15)	C(20)	124.7(6)	C(11)	C(15)	C(14)	108.9(8)
C(11)	C(15)	C(20)	123.7(9)	C(14)	C(15)	C(20)	126.9(9)

Table 6. Bond Angles(°)

atom	atom	atom	angle	atom	atom	atom	angle
Ta(1)	C(1)	H(1)	115.1	Ta(1)	C(1)	H(1')	115.1
C(2)	C(1)	H(1)	115.1	C(2)	C(1)	H(1')	115.1
H(1)	C(1)	H(1')	109.5	Ta(1)	C(4)	H(4)	115.0
Ta(1)	C(4)	H(4')	115.0	C(3)	C(4)	H(4)	115.0
C(3)	C(4)	H(4')	115.0	H(4)	C(4)	H(4')	109.5
C(2)	C(5)	H(5)	120.1	C(6)	C(5)	H(5)	120.1
C(5)	C(6)	H(6)	119.3	C(7)	C(6)	H(6)	119.3
C(6)	C(7)	H(7)	119.6	C(8)	C(7)	H(7)	119.6
C(3)	C(8)	H(8)	119.9	C(7)	C(8)	H(8)	119.9
C(11)	C(16)	H(16)	109.5	C(11)	C(16)	H(16")	109.5
C(11)	C(16)	H(16')	109.5	H(16)	C(16)	H(16")	109.5
H(16)	C(16)	H(16')	109.5	H(16")	C(16)	H(16')	109.5
C(12)	C(17)	H(17)	109.5	C(12)	C(17)	H(17")	109.4
C(12)	C(17)	H(17')	109.5	H(17)	C(17)	H(17")	109.4
H(17)	C(17)	H(17')	109.6	H(17")	C(17)	H(17')	109.4
C(13)	C(18)	H(18)	109.5	C(13)	C(18)	H(18")	109.6
C(13)	C(18)	H(18')	109.5	H(18)	C(18)	H(18")	109.5
H(18)	C(18)	H(18')	109.3	H(18")	C(18)	H(18')	109.5
C(14)	C(19)	H(19)	109.5	C(14)	C(19)	H(19")	109.5
C(14)	C(19)	H(19')	109.5	H(19)	C(19)	H(19")	109.4
H(19)	C(19)	H(19')	109.5	H(19")	C(19)	H(19')	109.5
C(15)	C(20)	H(20)	109.5	C(15)	C(20)	H(20")	109.5
C(15)	C(20)	H(20')	109.5	H(20)	C(20)	H(20")	109.5
H(20)	C(20)	H(20')	109.5	H(20")	C(20)	H(20')	109.5

Table 9. Least Squares Planes

Plane number 1

Atoms defining plane	Distance
Ta(1)	0.0
C(1)	0.0
C(4)	0.0
Additional Atoms	**Distance**
C(2)	-1.328

Plane number 2

Atoms defining plane	Distance
C(1)	0.005(9)
C(2)	-0.008(8)
C(3)	0.008(8)
C(4)	-0.005(9)
Additional Atoms	**Distance**
Ta(1)	-1.717

Plane number 3

Atoms defining plane	Distance
C(2)	0.010(8)
C(3)	0.008(8)
C(5)	-0.023(9)
C(6)	0.01(1)
C(7)	0.02(1)
C(8)	-0.023(9)
Additional Atoms	**Distance**
Ta(1)	-1.788

Plane number 4

Atoms defining plane	Distance
C(11)	-0.008(8)
C(12)	0.008(8)
C(13)	-0.006(8)
C(14)	0.001(8)
C(15)	0.004(8)
Additional Atoms	**Distance**
Ta(1)	2.119

Summary

plane	mean deviation	χ^2
1	0.0000	0.0
2	0.0064	2.3
3	0.0150	16.4
4	0.0054	2.6

Dihedral angles between planes (°)

plane	1	2	3
2	75.67		
3	78.28	2.70	
4	156.31	80.66	78.06

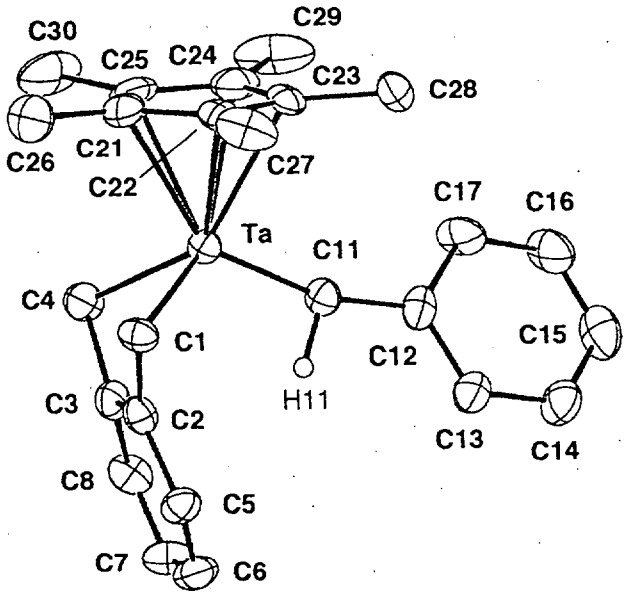

Figure S2. *ORTEP* drawing of **12** with numbering scheme. Hydrogen atoms are omitted for clarity.

Table 1. Atomic coordinates and B_{iso}/B_{eq}

atom	x	y	z	B_{eq}
Ta(1)	0.431(2)	0.16346(1)	0.701(2)	3.080(4)
C(1)	0.328(2)	0.1272(5)	0.809(3)	3.6(2)
C(2)	0.393(2)	0.1822(5)	0.925(3)	3.3(1)
C(3)	0.514(2)	0.1892(6)	0.980(3)	3.7(2)
C(4)	0.574(2)	0.1408(5)	0.915(3)	4.4(2)
C(5)	0.336(2)	0.2364(4)	0.974(3)	3.8(2)
C(6)	0.394(2)	0.2934(5)	1.064(3)	4.5(2)
C(7)	0.512(2)	0.2990(5)	1.117(3)	5.0(2)
C(8)	0.567(2)	0.2497(6)	1.073(3)	4.3(2)
C(11)	0.426(2)	0.2701(4)	0.663(3)	3.5(2)
C(12)	0.429(2)	0.3458(4)	0.602(3)	4.1(1)
C(13)	0.381(2)	0.4078(4)	0.637(3)	4.3(2)
C(14)	0.387(2)	0.4776(5)	0.583(3)	5.2(2)
C(15)	0.439(2)	0.4891(6)	0.495(3)	5.8(2)
C(16)	0.485(2)	0.4297(6)	0.460(3)	6.0(2)
C(17)	0.481(2)	0.3578(5)	0.509(3)	5.2(2)
C(21)	0.406(2)	0.0369(5)	0.596(3)	4.8(2)
C(22)	0.319(2)	0.0841(5)	0.491(2)	3.6(1)
C(23)	0.372(2)	0.1401(5)	0.443(3)	3.6(1)
C(24)	0.494(2)	0.1294(7)	0.516(3)	5.3(2)
C(25)	0.512(2)	0.0653(5)	0.612(3)	5.3(2)
C(26)	0.385(2)	-0.0311(5)	0.667(3)	10.0(6)
C(27)	0.191(2)	0.0752(6)	0.433(3)	6.2(2)
C(28)	0.304(2)	0.1967(6)	0.321(3)	5.3(2)

Table 1. Atomic coordinates and B_{iso}/B_{eq} (continued)

atom	x	y	z	B_{eq}
C(29)	0.581(2)	0.1691(7)	0.488(3)	8.3(4)
C(30)	0.628(2)	0.0287(8)	0.703(3)	9.3(3)
H(1)	0.2494	0.1374	0.7556	4.2935
H(1')	0.3404	0.0760	0.8404	4.2935
H(4)	0.6476	0.1597	0.9282	5.2853
H(4')	0.5833	0.0894	0.9446	5.2853
H(6)	0.361(5)	0.327(3)	1.109(7)	2.3(8)
H(7)	0.554(8)	0.336(5)	1.19(1)	5.7(6)
H(8)	0.651(6)	0.251(4)	1.114(8)	3.6(7)
H(11)	0.415(5)	0.285(3)	0.754(7)	0.2(8)
H(14)	0.3552	0.5194	0.6081	6.2104
H(15)	0.4444	0.5380	0.4602	6.9554
H(26)	0.3461	-0.0166	0.7210	11.9900
H(26")	0.4585	-0.0531	0.7329	11.9900
H(26')	0.3424	-0.0667	0.5940	11.9900
H(27)	0.1614	0.1200	0.4509	7.4014
H(27")	0.1774	0.0340	0.4813	7.4014
H(27')	0.1592	0.0657	0.3303	7.4014
H(28)	0.3584	0.2289	0.3069	6.3018
H(28")	0.2575	0.2260	0.3486	6.3018
H(28')	0.2601	0.1704	0.2326	6.3018
H(29)	0.6573	0.1508	0.5534	9.9678
H(29")	0.5789	0.2216	0.5037	9.9678
H(29')	0.5687	0.1605	0.3894	9.9678

Table 1. Atomic coordinates and B_{iso}/B_{eq} (continued)

atom	x	y	z	B_{eq}
H(30)	0.6306	-0.0204	0.6671	11.1137
H(30")	0.6435	0.0255	0.8034	11.1137
H(30')	0.6889	0.0583	0.6982	11.1137
H(31)	0.2572	0.2319	0.9426	4.5280
H(32)	0.5242	0.4374	0.4000	7.2019
H(33)	0.5146	0.3166	0.4804	6.2760
H(34)	0.3454	0.4018	0.6984	5.1222

$$B_{eq} = \frac{8}{3}\pi^2(U_{11}(aa^*)^2 + U_{22}(bb^*)^2 + U_{33}(cc^*)^2 + 2U_{12}aa^*bb^*\cos\gamma + 2U_{13}aa^*cc^*\cos\beta + 2U_{23}bb^*cc^*\cos\alpha)$$

Table 2. Anisotropic Displacement Parameters

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Ta(1)	0.0394(1)	0.0386(1)	0.0384(1)	0.0012(4)	0.01705(8)	-0.0001(4)
C(1)	0.049(4)	0.050(5)	0.046(4)	-0.009(3)	0.029(3)	-0.004(4)
C(2)	0.041(3)	0.049(4)	0.040(4)	-0.001(3)	0.021(3)	0.007(3)
C(3)	0.039(3)	0.054(4)	0.043(5)	0.012(3)	0.015(3)	0.009(3)
C(4)	0.042(4)	0.077(6)	0.046(3)	0.023(4)	0.017(2)	0.007(4)
C(5)	0.051(4)	0.044(4)	0.060(4)	0.002(3)	0.035(4)	0.000(3)
C(6)	0.070(4)	0.047(4)	0.064(5)	0.002(4)	0.039(4)	-0.011(3)
C(7)	0.069(4)	0.064(5)	0.060(5)	-0.007(4)	0.032(4)	-0.021(4)
C(8)	0.042(4)	0.069(5)	0.046(4)	-0.011(4)	0.016(3)	-0.005(4)
C(11)	0.046(4)	0.042(2)	0.050(6)	-0.005(4)	0.025(6)	0.004(3)
C(12)	0.046(4)	0.037(3)	0.042(3)	-0.005(3)	-0.007(2)	-0.002(3)
C(13)	0.059(5)	0.043(3)	0.059(5)	0.003(3)	0.026(4)	0.003(3)
C(14)	0.080(6)	0.039(4)	0.069(5)	-0.003(4)	0.026(4)	-0.002(4)
C(15)	0.083(6)	0.057(5)	0.070(7)	-0.024(5)	0.025(5)	0.011(5)
C(16)	0.112(8)	0.064(4)	0.075(6)	-0.023(5)	0.062(6)	0.001(5)
C(17)	0.095(7)	0.060(4)	0.080(6)	-0.017(5)	0.071(5)	-0.004(4)
C(21)	0.080(4)	0.048(4)	0.048(4)	0.008(3)	0.021(4)	-0.014(3)
C(22)	0.057(3)	0.044(4)	0.037(4)	-0.017(3)	0.021(3)	-0.016(3)
C(23)	0.061(4)	0.045(4)	0.028(4)	-0.013(3)	0.017(3)	-0.012(3)
C(24)	0.064(4)	0.078(6)	0.047(5)	0.015(4)	0.015(4)	-0.022(4)
C(25)	0.069(4)	0.070(6)	0.057(5)	0.028(4)	0.025(4)	-0.019(4)
C(26)	0.28(3)	0.026(4)	0.11(1)	-0.005(7)	0.13(2)	0.013(5)
C(27)	0.060(4)	0.112(8)	0.068(6)	-0.039(6)	0.033(4)	-0.031(6)
C(28)	0.093(7)	0.058(6)	0.040(5)	0.007(5)	0.022(5)	0.007(4)

Table 2. Anisotropic Displacement Parameters (continued)

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
C(29)	0.102(8)	0.119(10)	0.15(1)	-0.070(7)	0.110(8)	-0.076(9)
C(30)	0.075(6)	0.15(1)	0.083(7)	0.071(7)	0.000(5)	-0.030(7)

The general temperature factor expression:

$$\exp(-2\pi^2(a^{*2}U_{11}h^2 + b^{*2}U_{22}k^2 + c^{*2}U_{33}l^2 + 2a^*b^*U_{12}hk + 2a^*c^*U_{13}hl + 2b^*c^*U_{23}kl))$$

Table 3. Bond Lengths($\AA$)

atom	atom	distance	atom	atom	distance
Ta(1)	C(1)	2.180(9)	Ta(1)	C(4)	2.169(8)
Ta(1)	C(11)	1.925(9)	Ta(1)	C(21)	2.445(9)
Ta(1)	C(22)	2.419(8)	Ta(1)	C(23)	2.415(8)
Ta(1)	C(24)	2.44(1)	Ta(1)	C(25)	2.416(8)
C(1)	C(2)	1.47(1)	C(2)	C(3)	1.42(1)
C(2)	C(5)	1.43(1)	C(3)	C(4)	1.50(1)
C(3)	C(8)	1.39(1)	C(5)	C(6)	1.34(1)
C(6)	C(7)	1.38(1)	C(7)	C(8)	1.33(1)
C(11)	C(12)	1.49(1)	C(12)	C(13)	1.39(1)
C(12)	C(17)	1.41(1)	C(13)	C(14)	1.37(1)
C(14)	C(15)	1.36(1)	C(15)	C(16)	1.34(2)
C(16)	C(17)	1.38(1)	C(21)	C(22)	1.43(1)
C(21)	C(25)	1.40(2)	C(21)	C(26)	1.50(2)
C(22)	C(23)	1.41(1)	C(22)	C(27)	1.50(1)
C(23)	C(24)	1.43(1)	C(23)	C(28)	1.53(1)
C(24)	C(25)	1.45(2)	C(24)	C(29)	1.47(2)
C(25)	C(30)	1.52(1)			

Table 4. Bond Lengths($\AA$)

atom	atom	distance	atom	atom	distance
C(1)	H(1)	0.93	C(1)	H(1')	0.95
C(4)	H(4)	0.97	C(4)	H(4')	0.95
C(5)	H(31)	0.93	C(6)	H(6)	0.96(7)
C(7)	H(7)	0.95(10)	C(8)	H(8)	0.97(8)
C(11)	H(11)	1.03(6)	C(13)	H(34)	0.94
C(14)	H(14)	0.94	C(15)	H(15)	0.95
C(16)	H(32)	0.96	C(17)	H(33)	0.96
C(26)	H(26)	0.94	C(26)	H(26")	0.97
C(26)	H(26')	0.94	C(27)	H(27)	0.94
C(27)	H(27")	0.94	C(27)	H(27')	0.95
C(28)	H(28)	0.96	C(28)	H(28")	0.94
C(28)	H(28')	0.94	C(29)	H(29)	0.97
C(29)	H(29")	0.95	C(29)	H(29')	0.95
C(30)	H(30)	0.95	C(30)	H(30")	0.95
C(30)	H(30')	0.96			

Table 5. Bond Angles(°)

atom	atom	atom	angle	atom	atom	atom	angle
C(1)	Ta(1)	C(4)	83.0(4)	C(1)	Ta(1)	C(11)	114.6(4)
C(1)	Ta(1)	C(21)	87.8(4)	C(1)	Ta(1)	C(22)	90.7(3)
C(1)	Ta(1)	C(23)	122.1(3)	C(1)	Ta(1)	C(24)	144.3(4)
C(1)	Ta(1)	C(25)	116.7(4)	C(4)	Ta(1)	C(11)	108.7(4)
C(4)	Ta(1)	C(21)	98.8(4)	C(4)	Ta(1)	C(22)	132.8(4)
C(4)	Ta(1)	C(23)	140.3(3)	C(4)	Ta(1)	C(24)	107.3(4)
C(4)	Ta(1)	C(25)	85.6(3)	C(11)	Ta(1)	C(21)	146.0(3)
C(11)	Ta(1)	C(22)	116.2(4)	C(11)	Ta(1)	C(23)	89.2(3)
C(11)	Ta(1)	C(24)	94.7(4)	C(11)	Ta(1)	C(25)	127.9(4)
C(21)	Ta(1)	C(22)	34.1(3)	C(21)	Ta(1)	C(23)	56.8(3)
C(21)	Ta(1)	C(24)	57.2(4)	C(21)	Ta(1)	C(25)	33.6(4)
C(22)	Ta(1)	C(23)	34.0(3)	C(22)	Ta(1)	C(24)	56.8(4)
C(22)	Ta(1)	C(25)	56.0(3)	C(23)	Ta(1)	C(24)	34.2(3)
C(23)	Ta(1)	C(25)	56.5(4)	C(24)	Ta(1)	C(25)	34.6(4)
Ta(1)	C(1)	C(2)	87.3(5)	C(1)	C(2)	C(3)	120.4(9)
C(1)	C(2)	C(5)	121.7(7)	C(3)	C(2)	C(5)	117.4(9)
C(2)	C(3)	C(4)	118.7(10)	C(2)	C(3)	C(8)	117.4(9)
C(4)	C(3)	C(8)	122.9(9)	Ta(1)	C(4)	C(3)	87.8(5)
C(2)	C(5)	C(6)	121.6(8)	C(5)	C(6)	C(7)	120.2(9)
C(6)	C(7)	C(8)	119.6(10)	C(3)	C(8)	C(7)	123.7(9)
Ta(1)	C(11)	C(12)	164.8(7)	C(11)	C(12)	C(13)	120.4(9)
C(11)	C(12)	C(17)	122.0(9)	C(13)	C(12)	C(17)	117.6(8)
C(12)	C(13)	C(14)	119.8(9)	C(13)	C(14)	C(15)	122.3(10)
C(14)	C(15)	C(16)	118.4(9)	C(15)	C(16)	C(17)	122.3(9)

Table 5. Bond Angles(°) (continued)

atom	atom	atom	angle
C(12)	C(17)	C(16)	119.5(9)
Ta(1)	C(21)	C(25)	72.1(5)
C(22)	C(21)	C(25)	106.5(9)
C(25)	C(21)	C(26)	128(1)
Ta(1)	C(22)	C(23)	72.9(4)
C(21)	C(22)	C(23)	109.0(8)
C(23)	C(22)	C(27)	124.1(9)
Ta(1)	C(23)	C(24)	74.0(6)
C(22)	C(23)	C(24)	108(1)
C(24)	C(23)	C(28)	127(1)
Ta(1)	C(24)	C(25)	71.7(6)
C(23)	C(24)	C(25)	105(1)
C(25)	C(24)	C(29)	126(1)
Ta(1)	C(25)	C(24)	73.7(6)
C(21)	C(25)	C(24)	110.3(9)
C(24)	C(25)	C(30)	124(1)
Ta(1)	C(21)	C(22)	72.0(5)
Ta(1)	C(21)	C(26)	122.9(9)
C(22)	C(21)	C(26)	125(1)
Ta(1)	C(22)	C(21)	73.9(5)
Ta(1)	C(22)	C(27)	121.8(6)
C(21)	C(22)	C(27)	126.8(9)
Ta(1)	C(23)	C(22)	73.2(5)
Ta(1)	C(23)	C(28)	123.7(7)
C(22)	C(23)	C(28)	123.7(9)
Ta(1)	C(24)	C(23)	71.8(6)
Ta(1)	C(24)	C(29)	126.1(8)
C(23)	C(24)	C(29)	127(1)
Ta(1)	C(25)	C(21)	74.3(5)
Ta(1)	C(25)	C(30)	124.2(7)
C(21)	C(25)	C(30)	124(1)

Table 6. Bond Angles(°)

atom	atom	atom	angle	atom	atom	atom	angle
Ta(1)	C(1)	H(1)	114.4	Ta(1)	C(1)	H(1')	113.8
C(2)	C(1)	H(1)	114.7	C(2)	C(1)	H(1')	114.1
H(1)	C(1)	H(1')	110.9	Ta(1)	C(4)	H(4)	114.9
Ta(1)	C(4)	H(4')	115.4	C(3)	C(4)	H(4)	114.8
C(3)	C(4)	H(4')	115.3	H(4)	C(4)	H(4')	107.9
C(2)	C(5)	H(31)	119.1	C(6)	C(5)	H(31)	119.3
C(5)	C(6)	H(6)	124(4)	C(7)	C(6)	H(6)	114(4)
C(6)	C(7)	H(7)	119(6)	C(8)	C(7)	H(7)	120(6)
C(3)	C(8)	H(8)	115(4)	C(7)	C(8)	H(8)	120(4)
Ta(1)	C(11)	H(11)	94(3)	C(12)	C(11)	H(11)	101(3)
C(12)	C(13)	H(34)	119.8	C(14)	C(13)	H(34)	120.3
C(13)	C(14)	H(14)	119.3	C(15)	C(14)	H(14)	118.4
C(14)	C(15)	H(15)	121.5	C(16)	C(15)	H(15)	120.1
C(15)	C(16)	H(32)	119.1	C(17)	C(16)	H(32)	118.6
C(12)	C(17)	H(33)	120.7	C(16)	C(17)	H(33)	119.8
C(21)	C(26)	H(26)	109.4	C(21)	C(26)	H(26")	108.8
C(21)	C(26)	H(26')	109.4	H(26)	C(26)	H(26")	109.1
H(26)	C(26)	H(26')	111.2	H(26")	C(26)	H(26')	108.9
C(22)	C(27)	H(27)	108.4	C(22)	C(27)	H(27")	108.4
C(22)	C(27)	H(27')	108.3	H(27)	C(27)	H(27")	110.7
H(27)	C(27)	H(27')	110.6	H(27")	C(27)	H(27')	110.4
C(23)	C(28)	H(28)	108.7	C(23)	C(28)	H(28")	109.2
C(23)	C(28)	H(28')	109.1	H(28)	C(28)	H(28")	109.4
H(28)	C(28)	H(28')	109.0	H(28")	C(28)	H(28')	111.3

Table 6. Bond Angles(°) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
C(24)	C(29)	H(29)	110.1	C(24)	C(29)	H(29")	110.4
C(24)	C(29)	H(29')	110.4	H(29)	C(29)	H(29")	108.2
H(29)	C(29)	H(29')	108.1	H(29")	C(29)	H(29')	109.6
C(25)	C(30)	H(30)	110.5	C(25)	C(30)	H(30")	110.5
C(25)	C(30)	H(30')	110.2	H(30)	C(30)	H(30")	109.3
H(30)	C(30)	H(30')	108.1	H(30")	C(30)	H(30')	108.2

Table 9. Least Squares Planes

Plane number 1

Atoms defining plane	Distance
Ta(1)	0.0
C(1)	0.0
C(4)	0.0
Additional Atoms	**Distance**
C(21)	2.412

Plane number 2

Atoms defining plane	Distance
C(1)	0.00(2)
C(2)	0.00(2)
C(3)	0.01(2)
C(4)	0.00(2)
Additional Atoms	**Distance**
Ta(1)	-1.466

Plane number 3

Atoms defining plane	Distance
C(12)	0.00(2)
C(13)	0.00(3)
C(14)	0.00(3)
C(15)	0.00(3)
C(16)	0.00(3)
C(17)	-0.01(3)
Additional Atoms	**Distance**
C(1)	-0.419

Plane number 4

Atoms defining plane	Distance
C(21)	-0.01(2)
C(22)	0.00(2)
C(23)	0.00(2)
C(24)	-0.01(2)
C(25)	0.01(2)
Additional Atoms	**Distance**
Ta(1)	2.103

Summary

plane	mean deviation	χ^2
1	0.0000	0.0
2	0.0047	1.1
3	0.0052	1.9
4	0.0049	1.7

Dihedral angles between planes (°)

plane	1	2	3
2	64.22		
3	106.08	70.55	
4	146.07	81.86	58.73

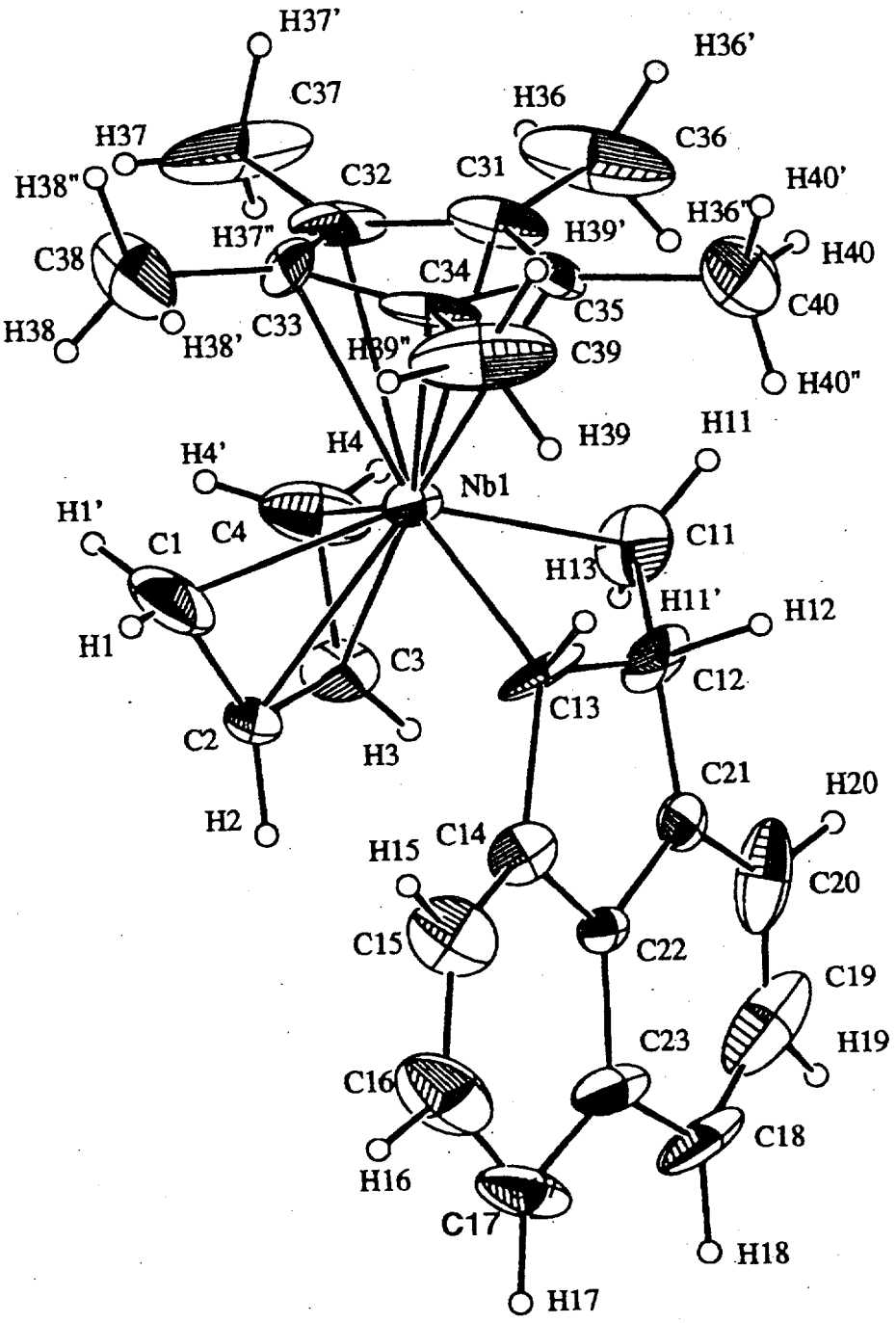

Figure S3. ORTEP drawing of **14** with atom numbering scheme.

Positional parameters and B(eq) for Cp*Nb(BD)(-CH2-ace-)

atom	x	y	z	B(eq)
Nb(1)	0.0566	0.2129	0.9791	6.0122
C(1)	-0.0275	0.2327	1.1317	21.7823
C(2)	0.0163	0.2958	1.1019	8.4361
C(3)	0.1689	0.3023	1.0714	9.1382
C(4)	0.2641	0.2460	1.0860	14.3707
C(11)	0.2218	0.2672	0.8747	12.5053
C(12)	0.0406	0.2900	0.8370	10.3453
C(13)	-0.1179	0.2659	0.8799	9.3992
C(14)	-0.2105	0.3306	0.8960	7.0837
C(15)	-0.3519	0.3423	0.9237	12.4469
C(16)	-0.3974	0.4048	0.9396	15.1950
C(17)	-0.3065	0.4663	0.9192	16.6900
C(18)	-0.0252	0.4956	0.8562	14.4604
C(19)	0.1140	0.4670	0.8256	18.2664
C(20)	0.1455	0.4079	0.8177	15.1904
C(21)	0.0351	0.3625	0.8390	7.1295
C(22)	-0.1102	0.3843	0.8747	5.3617
C(23)	-0.1487	0.4497	0.8824	11.6437
C(31)	0.1987	0.1150	0.9193	10.3734
C(32)	0.1672	0.1048	1.0165	17.0088
C(33)	0.0065	0.0959	1.0203	14.1046
C(34)	-0.0578	0.1105	0.9188	8.5921
C(35)	0.0702	0.1213	0.8591	6.3681
C(36)	0.3618	0.1181	0.8789	23.1986
C(37)	0.2946	0.0879	1.0981	32.3881
C(38)	-0.0910	0.0752	1.1037	41.0621
C(39)	-0.2185	0.1083	0.8565	21.3049
C(40)	0.0722	0.1301	0.7397	17.7418
H(1)	-0.1361	0.2251	1.1383	22.9772
H(1')	0.0324	0.2128	1.1873	22.9772
H(2)	-0.0471	0.3371	1.0950	10.2973
H(3)	0.2208	0.3388	1.0440	12.0606
H(4)	0.3641	0.2457	1.0612	17.2550
H(4')	0.2680	0.2275	1.1555	17.2550
H(11)	0.2785	0.2416	0.8276	15.4486
H(11')	0.2893	0.3007	0.9048	15.4486
H(12)	0.0335	0.2786	0.7635	12.0762
H(13)	-0.1755	0.2366	0.8336	11.6740
H(15)	-0.4216	0.3065	0.9311	14.9318
H(16)	-0.4972	0.4107	0.9687	18.5293
H(17)	-0.3404	0.5103	0.9284	19.6020
H(18)	-0.0486	0.5415	0.8597	14.0722
H(19)	0.1865	0.5052	0.8171	18.2122
H(20)	0.2430	0.4021	0.7853	7.2000
H(36)	0.4368	0.1135	0.9368	27.8357
H(36")	0.3792	0.1594	0.8459	27.8357
H(36')	0.3760	0.0826	0.8322	27.8357
H(37)	0.2406	0.0799	1.1622	39.2278
H(37")	0.3619	0.1240	1.1085	39.2278
H(37')	0.3466	0.0490	1.0810	39.2278

Positional parameters and B(eq) for Cp*Nb(BD)(-CH2-ace-)

atom	x	y	z	B(eq)
H(38)	-0.1116	0.1039	1.1500	39.9563
H(38")	-0.0987	0.0309	1.1121	39.9563
H(38')	-0.2168	0.0795	1.0556	39.9563
H(39)	-0.2363	0.1482	0.8214	22.4366
H(39")	-0.3009	0.1017	0.9047	22.4366
H(39')	-0.2201	0.0716	0.8109	22.4366
H(40)	0.1775	0.1336	0.7213	21.2279
H(40")	0.0146	0.1687	0.7198	21.2279
H(40')	0.0238	0.0919	0.7076	21.2279

Anisotropic Displacement Parameters for Cp*Nb(BD)(-CH2-ace-)

atom	U11	U22	U33	U12	U13	U23
Nb(1)	0.1000	0.0556	0.0684	0.0100	-0.0337	-0.0111
C(1)	0.5369	0.0808	0.2356	-0.0164	0.2477	-0.0631
C(2)	0.1847	0.0514	0.0872	0.0134	0.0322	-0.0153
C(3)	0.1588	0.0607	0.1220	-0.0368	-0.0415	-0.0394
C(4)	0.1531	0.1117	0.2719	0.0106	-0.0696	-0.1031
C(11)	0.1223	0.1492	0.2135	-0.0405	0.0967	0.0478
C(12)	0.1921	0.1132	0.0791	0.0295	-0.0690	0.0329
C(13)	0.1772	0.0381	0.1265	-0.0101	-0.1266	0.0286
C(14)	0.0595	0.0988	0.1066	-0.0055	-0.0329	0.0104
C(15)	0.0616	0.2030	0.2079	0.0099	0.0039	-0.0118
C(16)	0.1065	0.2550	0.2158	0.0888	0.0085	-0.0503
C(17)	0.3113	0.1788	0.1318	0.1772	-0.0950	-0.0644
C(18)	0.3552	0.0383	0.1415	-0.0387	-0.1129	0.0347
C(19)	0.2904	0.2029	0.1896	-0.1024	-0.0840	0.1122
C(20)	0.1587	0.2979	0.1245	-0.1065	0.0425	0.0740
C(21)	0.1055	0.1137	0.0490	0.0381	-0.0188	0.0088
C(22)	0.0970	0.0585	0.0446	0.0098	-0.0277	-0.0015
C(23)	0.2847	0.0578	0.0878	0.0426	-0.0953	-0.0184
C(31)	0.0345	0.0906	0.2656	0.0116	-0.0219	-0.0766
C(32)	0.3769	0.0753	0.1770	0.0773	-0.1335	-0.0956
C(33)	0.3930	0.0362	0.1152	-0.0017	0.0893	0.0403
C(34)	0.0279	0.0413	0.2606	0.0028	0.0379	-0.0383
C(35)	0.0921	0.0782	0.0715	0.0237	0.0033	-0.0225
C(36)	0.0931	0.1624	0.6397	-0.0103	0.1414	-0.1202
C(37)	0.7036	0.1758	0.2995	0.2218	-0.4249	-0.1039
C(38)	1.0829	0.0759	0.4712	-0.0041	0.6575	0.0445
C(39)	0.1149	0.0904	0.5899	-0.0081	-0.1057	-0.0460
C(40)	0.4174	0.1429	0.1161	0.0175	0.0352	-0.0424

Intramolecular Distances Involving the Nonhydrogen Atoms

atom	atom	distance	atom	atom	distance
Nb(1)	C(1)	2.18(3)	C(14)	C(22)	1.41(2)
Nb(1)	C(2)	2.34(2)	C(15)	C(16)	1.33(4)
Nb(1)	C(3)	2.33(2)	C(16)	C(17)	1.49(5)
Nb(1)	C(4)	2.28(2)	C(17)	C(23)	1.49(4)
Nb(1)	C(11)	2.28(2)	C(18)	C(19)	1.39(6)
Nb(1)	C(12)	2.40(2)	C(18)	C(23)	1.45(4)
Nb(1)	C(13)	2.18(1)	C(19)	C(20)	1.22(5)
Nb(1)	C(31)	2.45(2)	C(20)	C(21)	1.35(3)
Nb(1)	C(32)	2.40(3)	C(21)	C(22)	1.41(2)
Nb(1)	C(33)	2.45(2)	C(22)	C(23)	1.36(2)
Nb(1)	C(34)	2.39(2)	C(31)	C(32)	1.32(4)
Nb(1)	C(35)	2.41(2)	C(31)	C(35)	1.31(2)
C(1)	C(2)	1.38(3)	C(31)	C(36)	1.51(3)
C(2)	C(3)	1.38(3)	C(32)	C(33)	1.38(4)
C(3)	C(4)	1.40(3)	C(32)	C(37)	1.51(3)
C(11)	C(12)	1.65(3)	C(33)	C(34)	1.43(3)
C(12)	C(13)	1.56(3)*	C(33)	C(38)	1.46(3)
C(12)	C(21)	1.46(3)	C(34)	C(35)	1.39(3)
C(13)	C(14)	1.54(3)*	C(34)	C(39)	1.54(3)
C(14)	C(15)	1.29(3)*	C(35)	C(40)	1.56(3)

* restrained during refinement

Distances are in angstroms. Estimated standard deviations in the least significant figure are given in parentheses.

Intramolecular Distances Involving the Hydrogen Atoms

atom	atom	distance	atom	atom	distance
C(1)	H(1)	0.943	C(36)	H(36)	0.960
C(1)	H(1')	0.946	C(36)	H(36")	0.948
C(2)	H(2)	0.990	C(36)	H(36')	0.947
C(3)	H(3)	0.934	C(37)	H(37)	0.984
C(4)	H(4)	0.925	C(37)	H(37")	0.928
C(4)	H(4')	0.973	C(37)	H(37')	0.930
C(11)	H(11)	0.949	C(38)	H(38)	0.857
C(11)	H(11')	0.953	C(38)	H(38")	0.898
C(12)	H(12)	0.978	C(38)	H(38')	1.208
C(13)	H(13)	0.955	C(39)	H(39)	0.930
C(15)	H(15)	0.940	C(39)	H(39")	0.973
C(16)	H(16)	0.954	C(39)	H(39')	0.944
C(17)	H(17)	0.940	C(40)	H(40)	0.941
C(18)	H(18)	0.945	C(40)	H(40")	0.944
C(19)	H(19)	0.993	C(40)	H(40')	0.954
C(20)	H(20)	0.956			

Distances are in angstroms. Estimated standard deviations in the least significant figure are given in parentheses.

Intramolecular Bond Angles Involving the Nonhydrogen Atoms

atom	atom	atom	angle	atom	atom	atom	angle
C(1)	Nb(1)	C(2)	35.3(8)	C(3)	Nb(1)	C(32)	116.6(9)
C(1)	Nb(1)	C(3)	62(1)	C(3)	Nb(1)	C(33)	134(1)
C(1)	Nb(1)	C(4)	71(1)	C(3)	Nb(1)	C(34)	168.1(10)
C(1)	Nb(1)	C(11)	134(1)	C(3)	Nb(1)	C(35)	152.1(9)
C(1)	Nb(1)	C(12)	124(1)	C(4)	Nb(1)	C(11)	74(1)
C(1)	Nb(1)	C(13)	101(1)	C(4)	Nb(1)	C(12)	106(1)
C(1)	Nb(1)	C(31)	128(1)	C(4)	Nb(1)	C(13)	133.7(9)
C(1)	Nb(1)	C(32)	97(1)	C(4)	Nb(1)	C(31)	92.8(8)
C(1)	Nb(1)	C(33)	84.7(10)	C(4)	Nb(1)	C(32)	82.0(10)
C(1)	Nb(1)	C(34)	107(1)	C(4)	Nb(1)	C(33)	106(1)
C(1)	Nb(1)	C(35)	139.0(9)	C(4)	Nb(1)	C(34)	137.5(9)
C(2)	Nb(1)	C(3)	34.4(7)	C(4)	Nb(1)	C(35)	123.4(8)
C(2)	Nb(1)	C(4)	61.1(9)	C(11)	Nb(1)	C(12)	41.2(8)
C(2)	Nb(1)	C(11)	100.5(9)	C(11)	Nb(1)	C(13)	80.6(9)
C(2)	Nb(1)	C(12)	93.3(8)	C(11)	Nb(1)	C(31)	82.3(9)
C(2)	Nb(1)	C(13)	86.1(8)	C(11)	Nb(1)	C(32)	107(1)
C(2)	Nb(1)	C(31)	151.3(8)	C(11)	Nb(1)	C(33)	135.0(9)
C(2)	Nb(1)	C(32)	125.1(9)	C(11)	Nb(1)	C(34)	118.1(10)
C(2)	Nb(1)	C(33)	119.9(8)	C(11)	Nb(1)	C(35)	85.9(8)
C(2)	Nb(1)	C(34)	139.7(8)	C(12)	Nb(1)	C(13)	39.5(7)
C(2)	Nb(1)	C(35)	173.2(8)	C(12)	Nb(1)	C(31)	106.4(10)
C(3)	Nb(1)	C(4)	35.3(7)	C(12)	Nb(1)	C(32)	137(1)
C(3)	Nb(1)	C(11)	71.9(10)	C(12)	Nb(1)	C(33)	141(1)
C(3)	Nb(1)	C(12)	84.3(8)	C(12)	Nb(1)	C(34)	107.5(9)
C(3)	Nb(1)	C(13)	99.8(7)	C(12)	Nb(1)	C(35)	90.0(8)
C(3)	Nb(1)	C(31)	125.8(8)	C(13)	Nb(1)	C(31)	122.3(9)

Angles are in degrees. Estimated standard deviations in the least significant figure are given in parentheses.

Intramolecular Bond Angles Involving the Nonhydrogen Atoms cont

atom	atom	atom	angle	atom	atom	atom	angle
C(13)	Nb(1)	C(32)	143.5(7)	C(11)	C(12)	C(13)	127(1)
C(13)	Nb(1)	C(33)	118(1)	C(11)	C(12)	C(21)	107(2)
C(13)	Nb(1)	C(34)	88.7(7)	C(13)	C(12)	C(21)	105(2)
C(13)	Nb(1)	C(35)	92.8(7)	Nb(1)	C(13)	C(12)	77(1)
C(31)	Nb(1)	C(32)	31.5(9)	Nb(1)	C(13)	C(14)	131(1)
C(31)	Nb(1)	C(33)	52.9(9)	C(12)	C(13)	C(14)	104(1)
C(31)	Nb(1)	C(34)	53.5(6)	C(13)	C(14)	C(15)	132(2)
C(31)	Nb(1)	C(35)	31.2(6)	C(13)	C(14)	C(22)	107(1)
C(32)	Nb(1)	C(33)	33.0(9)	C(15)	C(14)	C(22)	119(2)
C(32)	Nb(1)	C(34)	55.6(8)	C(14)	C(15)	C(16)	119(3)
C(32)	Nb(1)	C(35)	53.9(8)	C(15)	C(16)	C(17)	126(3)
C(33)	Nb(1)	C(34)	34.2(9)	C(16)	C(17)	C(23)	110(2)
C(33)	Nb(1)	C(35)	55.0(8)	C(19)	C(18)	C(23)	116(2)
C(34)	Nb(1)	C(35)	33.6(6)	C(18)	C(19)	C(20)	128(4)
Nb(1)	C(1)	C(2)	78(1)	C(19)	C(20)	C(21)	118(4)
Nb(1)	C(2)	C(1)	65(1)	C(12)	C(21)	C(20)	130(2)
Nb(1)	C(2)	C(3)	72(1)	C(12)	C(21)	C(22)	110(2)
C(1)	C(2)	C(3)	116(2)	C(20)	C(21)	C(22)	119(2)
Nb(1)	C(3)	C(2)	73(1)	C(14)	C(22)	C(21)	112(1)
Nb(1)	C(3)	C(4)	70(1)	C(14)	C(22)	C(23)	125(2)
C(2)	C(3)	C(4)	115(2)	C(21)	C(22)	C(23)	122(2)
Nb(1)	C(4)	C(3)	74(1)	C(17)	C(23)	C(18)	127(2)
Nb(1)	C(11)	C(12)	73(1)	C(17)	C(23)	C(22)	117(3)
Nb(1)	C(12)	C(11)	65.4(10)	C(18)	C(23)	C(22)	114(2)*
Nb(1)	C(12)	C(13)	62.6(10)	Nb(1)	C(31)	C(32)	72(1)
Nb(1)	C(12)	C(21)	129(1)	Nb(1)	C(31)	C(35)	72(1)

* restrained during refinement

Angles are in degrees. Estimated standard deviations in the least significant figure are given in parentheses.

Intramolecular Bond Angles Involving the Nonhydrogen Atoms cont

atom	atom	atom	angle	atom	atom	atom	angle
Nb(1)	C(31)	C(36)	123(1)	C(31)	C(35)	C(40)	123(2)
C(32)	C(31)	C(35)	112(2)	C(34)	C(35)	C(40)	128(2)
C(32)	C(31)	C(36)	125(3)				
C(35)	C(31)	C(36)	122(3)				
Nb(1)	C(32)	C(31)	76(1)				
Nb(1)	C(32)	C(33)	75(1)				
Nb(1)	C(32)	C(37)	126(1)				
C(31)	C(32)	C(33)	107(2)				
C(31)	C(32)	C(37)	121(4)				
C(33)	C(32)	C(37)	128(4)				
Nb(1)	C(33)	C(32)	71(1)				
Nb(1)	C(33)	C(34)	70(1)				
Nb(1)	C(33)	C(38)	123(1)				
C(32)	C(33)	C(34)	105(2)				
C(32)	C(33)	C(38)	131(4)				
C(34)	C(33)	C(38)	122(4)				
Nb(1)	C(34)	C(33)	75(1)				
Nb(1)	C(34)	C(35)	74(1)				
Nb(1)	C(34)	C(39)	121(1)				
C(33)	C(34)	C(35)	105(1)				
C(33)	C(34)	C(39)	139(2)				
C(35)	C(34)	C(39)	114(2)				
Nb(1)	C(35)	C(31)	76(1)				
Nb(1)	C(35)	C(34)	72(1)				
Nb(1)	C(35)	C(40)	123(1)				
C(31)	C(35)	C(34)	107(2)				

Angles are in degrees. Estimated standard deviations in the least significant figure are given in parentheses.

Intramolecular Bond Angles Involving the Hydrogen Atoms

atom	atom	atom	angle	atom	atom	atom	angle
Nb(1)	C(1)	H(1)	115.21	C(12)	C(13)	H(13)	112.82
Nb(1)	C(1)	H(1')	115.08	C(14)	C(13)	H(13)	110.91
C(2)	C(1)	H(1)	116.96	C(14)	C(15)	H(15)	119.32
C(2)	C(1)	H(1')	117.31	C(16)	C(15)	H(15)	120.95
H(1)	C(1)	H(1')	110.38	C(15)	C(16)	H(16)	116.80
Nb(1)	C(2)	H(2)	129.30	C(17)	C(16)	H(16)	116.61
C(1)	C(2)	H(2)	129.84	C(16)	C(17)	H(17)	126.34
C(3)	C(2)	H(2)	114.02	C(23)	C(17)	H(17)	122.73
Nb(1)	C(3)	H(3)	126.65	C(19)	C(18)	H(18)	126.87
C(2)	C(3)	H(3)	130.74	C(23)	C(18)	H(18)	116.90
C(4)	C(3)	H(3)	113.89	C(18)	C(19)	H(19)	104.83
Nb(1)	C(4)	H(4)	118.74	C(20)	C(19)	H(19)	126.87
Nb(1)	C(4)	H(4')	115.90	C(19)	C(20)	H(20)	110.74
C(3)	C(4)	H(4)	119.49	C(21)	C(20)	H(20)	129.56
C(3)	C(4)	H(4')	115.06	C(31)	C(36)	H(36)	107.83
H(4)	C(4)	H(4')	109.61	C(31)	C(36)	H(36")	111.27
Nb(1)	C(11)	H(11)	118.30	C(31)	C(36)	H(36')	110.03
Nb(1)	C(11)	H(11')	118.04	H(36)	C(36)	H(36")	108.82
C(12)	C(11)	H(11)	117.30	H(36)	C(36)	H(36')	108.87
C(12)	C(11)	H(11')	116.92	H(36")	C(36)	H(36')	109.96
H(11)	C(11)	H(11')	109.27	C(32)	C(37)	H(37)	106.12
Nb(1)	C(12)	H(12)	126.22	C(32)	C(37)	H(37")	109.71
C(11)	C(12)	H(12)	103.07	C(32)	C(37)	H(37')	110.76
C(13)	C(12)	H(12)	105.49	H(37)	C(37)	H(37")	108.41
C(21)	C(12)	H(12)	104.62	H(37)	C(37)	H(37')	108.32
Nb(1)	C(13)	H(13)	112.11	H(37")	C(37)	H(37')	113.24

Angles are in degrees. Estimated standard deviations in the least significant figure are given in parentheses.

Intramolecular Bond Angles Involving the Hydrogen Atoms cont

atom	atom	atom	angle	atom	atom	atom	angle
C(33)	C(38)	H(38)	118.23				
C(33)	C(38)	H(38")	114.79				
C(33)	C(38)	H(38')	96.87				
H(38)	C(38)	H(38")	124.26				
H(38)	C(38)	H(38')	95.91				
H(38")	C(38)	H(38')	93.74				
C(34)	C(39)	H(39)	110.18				
C(34)	C(39)	H(39")	108.38				
C(34)	C(39)	H(39')	109.25				
H(39)	C(39)	H(39")	109.17				
H(39)	C(39)	H(39')	111.73				
H(39")	C(39)	H(39')	108.06				
C(35)	C(40)	H(40)	108.90				
C(35)	C(40)	H(40")	109.21				
C(35)	C(40)	H(40')	108.28				
H(40)	C(40)	H(40")	110.78				
H(40)	C(40)	H(40')	109.94				
H(40")	C(40)	H(40')	109.68				

Angles are in degrees. Estimated standard deviations in the least significant figure are given in parentheses.

Table of Least-Squares Planes

---------- Plane number 1 ----------

Atoms Defining Plane			Distance	esd
Nb(1)	(	1)	0.0000	
C(1)	(	1)	0.0000	
C(4)	(	1)	0.0000	

Additional Atoms			Distance
C(2)	(	1)	-1.2410

Mean deviation from plane is 0.0000 angstroms
Chi-squared: 0.0

---------- Plane number 2 ----------

Atoms Defining Plane			Distance	esd
C(1)	(	1)	-0.0393	0.0370
C(2)	(	1)	0.0254	0.0205
C(3)	(	1)	-0.0230	0.0195
C(4)	(	1)	0.0239	0.0279

Additional Atoms			Distance
Nb(1)	(	1)	-1.8190

Mean deviation from plane is 0.0279 angstroms
Chi-squared: 3.9

Dihedral angles between least-squares planes

plane	plane	angle
2	1	88.66

---------- Plane number 3 ----------

Atoms Defining Plane			Distance	esd
C(31)	(	1)	0.0238	0.0216
C(32)	(	1)	-0.0495	0.0281
C(33)	(	1)	0.0399	0.0259
C(34)	(	1)	-0.0065	0.0173
C(35)	(	1)	-0.0016	0.0172

Additional Atoms			Distance
Nb(1)	(	1)	-2.1232

Mean deviation from plane is 0.0242 angstroms
Chi-squared: 4.8

Dihedral angles between least-squares planes

plane	plane	angle
3	1	27.50
3	2	116.15

Table of Least-Squares Planes (continued)

---------- Plane number 4 ----------

Atoms Defining Plane			Distance	esd
Nb(1)	(	1)	-0.0000	
C(11)	(	1)	0.0000	
C(13)	(	1)	0.0000	

Additional Atoms			Distance
C(12)	(	1)	-0.0347

Mean deviation from plane is 0.0000 angstroms
Chi-squared: 0.0

Dihedral angles between least-squares planes

plane	plane	angle
4	1	55.23
4	2	143.53
4	3	27.84

---------- Plane number 5 ----------

Atoms Defining Plane			Distance	esd
C(11)	(	1)	0.0000	
C(12)	(	1)	0.0000	
C(13)	(	1)	0.0000	

Additional Atoms			Distance
Nb(1)	(	1)	-0.0837

Mean deviation from plane is 0.0000 angstroms
Chi-squared: 0.0

Dihedral angles between least-squares planes

plane	plane	angle
5	1	58.00
5	2	146.18
5	3	30.65
5	4	2.82

Table of Least-Squares Planes (continued)

---------- Plane number 6 ----------

Atoms Defining Plane			Distance	esd
Nb(1)	(	1)	0.0000	
C(12)	(	1)	0.0000	
C(13)	(	1)	0.0000	

Additional Atoms			Distance
C(22)	(	1)	-1.7728

Mean deviation from plane is 0.0000 angstroms
Chi-squared: 0.0

Dihedral angles between least-squares planes

plane	plane	angle
6	1	55.86
6	2	143.95
6	3	28.56
6	4	1.30
6	5	2.25

---------- Plane number 7 ----------

Atoms Defining Plane			Distance	esd
C(12)	(	1)	-0.0215	0.0174
C(13)	(	1)	0.0280	0.0163
C(14)	(	1)	-0.0334	0.0175
C(21)	(	1)	0.0027	0.0158
C(22)	(	1)	0.0147	0.0140

Additional Atoms			Distance
Nb(1)	(	1)	1.7000

Mean deviation from plane is 0.0200 angstroms
Chi-squared: 7.9

Dihedral angles between least-squares planes

plane	plane	angle
7	1	73.20
7	2	16.38
7	3	100.52
7	4	127.40
7	5	129.97
7	6	127.73

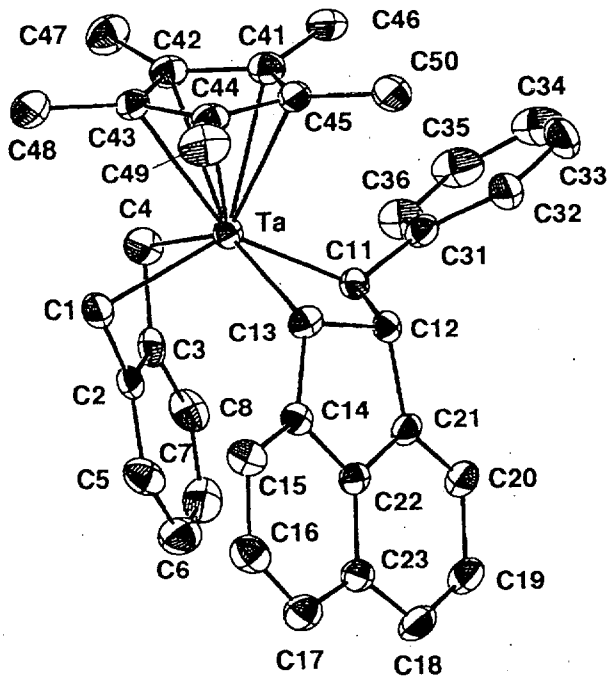

Figure S4. *ORTEP* drawing of **15** with numbering scheme. Hydrogen atoms are omitted for clarity.