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Supporting Information

for

Novel Constrained-Geometry Niobocene Complex with a Phosphanidoalkylcyclopentadienyl Ligand: [Nb(N^{t}Bu){(η^5-C_5H_4)CMe_2PPh-κ*P*}{(η^5-C_5H_4)CMe_2PHPh}]

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Crystal structure determination of 1 (c1612)

Table 1. Crystal data and structure refinement for c1612.

Identification code	c1612	
Empirical formula	C64 H80 N2 Nb2 P4	
Formula weight	1187.00	
Temperature	220(2) K	
Wavelength	71.073 pm	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 868.03(17) pm	α= 96.213(3)°.
	b = 1436.5(3) pm	β= 92.010(3)°.
	c = 2387.9(5) pm	γ = 93.761(3)°.
Volume	2.9511(10) nm^3	
Z	2	
Density (calculated)	1.336 Mg/m^3	
Absorption coefficient	0.537 mm^{-1}	
F(000)	1240	
Crystal size	0.30 x 0.20 x 0.10 mm^3	
Theta range for data collection	1.75 to 29.33°.	
Index ranges	-11<=h<=11, -18<=k<=19, -31<=l<=32	
Reflections collected	24351	
Independent reflections	14076 [R(int) = 0.0258]	
Completeness to theta = 29.33°	87.2 %	
Absorption correction	SADABS	
Max. and min. transmission	0.9482 and 0.8555	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	14076 / 0 / 658	
Goodness-of-fit on F^2	1.211	
Final R indices [I>2sigma(I)]	R1 = 0.0498, wR2 = 0.0972	
R indices (all data)	R1 = 0.0726, wR2 = 0.1041	
Extinction coefficient	0.0022(2)	
Largest diff. peak and hole	0.500 and -0.475 e.$Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (pm^2x 10^{-1}) for c1612. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	2909(3)	1450(2)	3641(1)	32(1)
C(2)	3338(4)	642(2)	3864(2)	38(1)
C(3)	3856(4)	890(2)	4431(2)	36(1)
C(4)	3669(3)	1853(2)	4566(1)	30(1)
C(5)	3140(3)	2222(2)	4076(1)	26(1)
C(6)	3089(3)	3249(2)	3981(1)	27(1)
C(7)	3319(4)	3892(2)	4533(1)	38(1)
C(8)	1613(4)	3444(3)	3661(2)	39(1)
C(9)	5993(3)	4337(2)	3744(1)	25(1)
C(10)	5346(4)	5180(2)	3661(1)	37(1)
C(11)	6221(5)	6023(2)	3754(2)	44(1)
C(12)	7745(5)	6052(2)	3922(2)	48(1)
C(13)	8415(4)	5225(3)	4006(2)	47(1)
C(14)	7538(4)	4370(2)	3920(1)	34(1)
C(15)	7340(4)	464(2)	3451(1)	29(1)
C(16)	6107(4)	507(2)	3047(1)	34(1)
C(17)	6204(4)	1386(2)	2853(1)	34(1)
C(18)	7529(4)	1904(2)	3122(1)	32(1)
C(19)	8253(4)	1320(2)	3469(1)	30(1)
C(20)	7801(4)	-404(2)	3709(2)	40(1)
C(21)	6396(5)	-1086(3)	3770(2)	62(1)
C(22)	8673(6)	-161(3)	4281(2)	62(1)
C(23)	8267(4)	-1266(2)	2554(2)	44(1)
C(24)	8374(5)	-613(3)	2162(2)	53(1)
C(25)	7706(5)	-812(3)	1629(2)	64(1)
C(26)	6913(6)	-1656(4)	1470(2)	72(1)
C(27)	6779(7)	-2312(3)	1849(2)	79(2)
C(28)	7458(6)	-2118(3)	2385(2)	62(1)
C(29)	7788(3)	2454(2)	5060(1)	29(1)
C(30)	7278(5)	1763(3)	5479(2)	47(1)
C(31)	9513(4)	2409(3)	4976(2)	50(1)

C(32)	7427(5)	3442(3)	5292(2)	50(1)
C(33)	-1862(3)	3445(2)	1381(1)	31(1)
C(34)	-2031(4)	2457(2)	1449(1)	35(1)
C(35)	-1627(4)	1953(3)	952(2)	42(1)
C(36)	-1185(4)	2595(3)	566(1)	41(1)
C(37)	-1398(4)	3505(2)	825(1)	34(1)
C(38)	-1887(3)	4236(2)	1853(1)	32(1)
C(39)	-1775(4)	5197(2)	1637(2)	40(1)
C(40)	-3308(4)	4139(3)	2211(2)	44(1)
C(41)	1129(4)	5018(2)	2426(1)	32(1)
C(42)	553(5)	5729(3)	2788(2)	45(1)
C(43)	1465(6)	6538(3)	2978(2)	59(1)
C(44)	2960(5)	6651(3)	2817(2)	58(1)
C(45)	3562(5)	5953(3)	2469(2)	52(1)
C(46)	2648(4)	5147(2)	2270(2)	40(1)
C(47)	2500(4)	1588(2)	1235(1)	31(1)
C(48)	1255(4)	1250(2)	1553(1)	34(1)
C(49)	1259(4)	1800(2)	2068(1)	36(1)
C(50)	2528(4)	2483(2)	2089(1)	34(1)
C(51)	3310(3)	2326(2)	1588(1)	31(1)
C(52)	3079(4)	1110(2)	694(1)	40(1)
C(53)	1756(5)	631(3)	303(2)	60(1)
C(54)	4055(5)	1802(3)	379(2)	59(1)
C(55)	3310(4)	-623(2)	1228(2)	43(1)
C(56)	3195(5)	-552(3)	1806(2)	52(1)
C(57)	2348(6)	-1237(4)	2057(2)	71(1)
C(58)	1585(6)	-1982(4)	1735(3)	77(2)
C(59)	1681(7)	-2063(3)	1164(3)	82(2)
C(60)	2549(6)	-1396(3)	913(2)	64(1)
C(61)	2609(4)	4437(3)	630(2)	41(1)
C(62)	2164(5)	4100(3)	11(2)	54(1)
C(63)	4368(4)	4478(3)	733(2)	59(1)
C(64)	2036(5)	5414(3)	776(2)	59(1)
N(1)	6949(3)	2183(2)	4520(1)	25(1)
N(2)	1886(3)	3781(2)	987(1)	30(1)
P(1)	4827(1)	3244(1)	3518(1)	23(1)

P(2)	9248(1)	-1003(1)	3245(1)	51(1)
P(3)	-71(1)	3920(1)	2240(1)	28(1)
P(4)	4479(1)	234(1)	890(1)	49(1)
Nb(1)	5775(1)	1735(1)	3912(1)	21(1)
Nb(2)	791(1)	2934(1)	1329(1)	24(1)

Table 3. Bond lengths [pm] and angles [°] for c1612.

C(1)-C(2)	139.6(4)
C(1)-C(5)	143.5(4)
C(1)-Nb(1)	254.4(3)
C(2)-C(3)	141.1(5)
C(2)-Nb(1)	254.2(3)
C(3)-C(4)	140.8(4)
C(3)-Nb(1)	244.6(3)
C(4)-C(5)	141.0(4)
C(4)-Nb(1)	244.8(3)
C(5)-C(6)	151.9(4)
C(5)-Nb(1)	246.7(3)
C(6)-C(7)	152.4(4)
C(6)-C(8)	152.6(4)
C(6)-P(1)	190.2(3)
C(9)-C(14)	138.8(4)
C(9)-C(10)	139.8(4)
C(9)-P(1)	183.0(3)
C(10)-C(11)	137.9(5)
C(11)-C(12)	136.5(5)
C(12)-C(13)	138.6(5)
C(13)-C(14)	139.4(5)
C(15)-C(19)	141.4(4)
C(15)-C(16)	142.4(4)
C(15)-C(20)	152.1(4)
C(15)-Nb(1)	252.7(3)
C(16)-C(17)	138.9(4)
C(16)-Nb(1)	260.4(3)
C(17)-C(18)	142.1(5)
C(17)-Nb(1)	256.9(3)
C(18)-C(19)	140.4(4)
C(18)-Nb(1)	248.8(3)
C(19)-Nb(1)	250.9(3)
C(20)-C(21)	153.4(5)
C(20)-C(22)	153.3(5)

C(20)-P(2)	189.2(4)
C(23)-C(28)	138.4(5)
C(23)-C(24)	139.6(5)
C(23)-P(2)	182.1(4)
C(24)-C(25)	137.4(6)
C(25)-C(26)	136.5(7)
C(26)-C(27)	137.7(7)
C(27)-C(28)	138.2(6)
C(29)-N(1)	146.1(4)
C(29)-C(31)	152.3(5)
C(29)-C(32)	152.3(5)
C(29)-C(30)	153.9(4)
C(33)-C(37)	141.0(4)
C(33)-C(34)	144.5(4)
C(33)-C(38)	151.3(4)
C(33)-Nb(2)	246.5(3)
C(34)-C(35)	139.0(5)
C(34)-Nb(2)	253.4(3)
C(35)-C(36)	141.7(5)
C(35)-Nb(2)	253.2(3)
C(36)-C(37)	141.1(5)
C(36)-Nb(2)	244.4(3)
C(37)-Nb(2)	244.6(3)
C(38)-C(39)	152.4(4)
C(38)-C(40)	153.2(4)
C(38)-P(3)	190.4(3)
C(41)-C(46)	138.8(5)
C(41)-C(42)	139.5(5)
C(41)-P(3)	183.6(3)
C(42)-C(43)	138.7(5)
C(43)-C(44)	137.1(6)
C(44)-C(45)	137.3(6)
C(45)-C(46)	139.0(5)
C(47)-C(51)	141.4(4)
C(47)-C(48)	143.2(4)
C(47)-C(52)	151.3(4)

C(47)-Nb(2)	250.9(3)
C(48)-C(49)	138.7(5)
C(48)-Nb(2)	258.7(3)
C(49)-C(50)	142.2(5)
C(49)-Nb(2)	256.9(3)
C(50)-C(51)	140.0(4)
C(50)-Nb(2)	248.6(3)
C(51)-Nb(2)	249.1(3)
C(52)-C(53)	153.2(5)
C(52)-C(54)	153.8(5)
C(52)-P(4)	188.9(4)
C(55)-C(56)	138.1(5)
C(55)-C(60)	138.6(5)
C(55)-P(4)	181.9(4)
C(56)-C(57)	139.1(6)
C(57)-C(58)	136.7(7)
C(58)-C(59)	136.2(7)
C(59)-C(60)	138.2(7)
C(61)-N(2)	146.4(4)
C(61)-C(64)	152.8(5)
C(61)-C(62)	153.2(5)
C(61)-C(63)	153.4(5)
N(1)-Nb(1)	177.9(2)
N(2)-Nb(2)	178.0(2)
P(1)-Nb(1)	262.42(9)
P(3)-Nb(2)	262.40(9)

C(2)-C(1)-C(5)	108.1(3)
C(2)-C(1)-Nb(1)	73.99(18)
C(5)-C(1)-Nb(1)	70.44(16)
C(1)-C(2)-C(3)	108.5(3)
C(1)-C(2)-Nb(1)	74.15(17)
C(3)-C(2)-Nb(1)	69.88(17)
C(4)-C(3)-C(2)	107.8(3)
C(4)-C(3)-Nb(1)	73.34(17)
C(2)-C(3)-Nb(1)	77.32(18)

C(3)-C(4)-C(5)	108.6(3)
C(3)-C(4)-Nb(1)	73.23(18)
C(5)-C(4)-Nb(1)	74.08(17)
C(4)-C(5)-C(1)	106.9(3)
C(4)-C(5)-C(6)	127.6(3)
C(1)-C(5)-C(6)	124.7(3)
C(4)-C(5)-Nb(1)	72.58(17)
C(1)-C(5)-Nb(1)	76.33(17)
C(6)-C(5)-Nb(1)	108.80(17)
C(5)-C(6)-C(7)	111.7(2)
C(5)-C(6)-C(8)	112.5(3)
C(7)-C(6)-C(8)	110.9(3)
C(5)-C(6)-P(1)	94.22(18)
C(7)-C(6)-P(1)	114.5(2)
C(8)-C(6)-P(1)	112.1(2)
C(14)-C(9)-C(10)	118.3(3)
C(14)-C(9)-P(1)	123.5(2)
C(10)-C(9)-P(1)	117.6(2)
C(11)-C(10)-C(9)	120.7(3)
C(12)-C(11)-C(10)	120.8(3)
C(11)-C(12)-C(13)	119.6(3)
C(12)-C(13)-C(14)	120.2(3)
C(9)-C(14)-C(13)	120.3(3)
C(19)-C(15)-C(16)	106.6(3)
C(19)-C(15)-C(20)	125.6(3)
C(16)-C(15)-C(20)	126.5(3)
C(19)-C(15)-Nb(1)	73.01(16)
C(16)-C(15)-Nb(1)	76.89(17)
C(20)-C(15)-Nb(1)	126.0(2)
C(17)-C(16)-C(15)	109.0(3)
C(17)-C(16)-Nb(1)	73.04(18)
C(15)-C(16)-Nb(1)	70.93(17)
C(16)-C(17)-C(18)	107.9(3)
C(16)-C(17)-Nb(1)	75.81(18)
C(18)-C(17)-Nb(1)	70.60(17)
C(19)-C(18)-C(17)	107.7(3)

C(19)-C(18)-Nb(1)	74.49(17)
C(17)-C(18)-Nb(1)	76.81(18)
C(18)-C(19)-C(15)	108.6(3)
C(18)-C(19)-Nb(1)	72.88(17)
C(15)-C(19)-Nb(1)	74.38(17)
C(15)-C(20)-C(21)	111.6(3)
C(15)-C(20)-C(22)	112.4(3)
C(21)-C(20)-C(22)	109.8(3)
C(15)-C(20)-P(2)	108.5(2)
C(21)-C(20)-P(2)	110.1(2)
C(22)-C(20)-P(2)	104.2(3)
C(28)-C(23)-C(24)	117.4(4)
C(28)-C(23)-P(2)	122.5(3)
C(24)-C(23)-P(2)	120.0(3)
C(25)-C(24)-C(23)	121.2(4)
C(26)-C(25)-C(24)	120.5(4)
C(25)-C(26)-C(27)	119.7(5)
C(26)-C(27)-C(28)	120.0(5)
C(27)-C(28)-C(23)	121.2(4)
N(1)-C(29)-C(31)	109.0(3)
N(1)-C(29)-C(32)	109.9(3)
C(31)-C(29)-C(32)	110.4(3)
N(1)-C(29)-C(30)	109.0(2)
C(31)-C(29)-C(30)	109.3(3)
C(32)-C(29)-C(30)	109.1(3)
C(37)-C(33)-C(34)	106.4(3)
C(37)-C(33)-C(38)	127.6(3)
C(34)-C(33)-C(38)	125.1(3)
C(37)-C(33)-Nb(2)	72.58(17)
C(34)-C(33)-Nb(2)	75.84(18)
C(38)-C(33)-Nb(2)	108.50(18)
C(35)-C(34)-C(33)	108.3(3)
C(35)-C(34)-Nb(2)	73.96(18)
C(33)-C(34)-Nb(2)	70.60(17)
C(34)-C(35)-C(36)	108.7(3)
C(34)-C(35)-Nb(2)	74.18(18)

C(36)-C(35)-Nb(2)	70.09(18)
C(37)-C(36)-C(35)	107.4(3)
C(37)-C(36)-Nb(2)	73.32(18)
C(35)-C(36)-Nb(2)	76.88(19)
C(33)-C(37)-C(36)	109.1(3)
C(33)-C(37)-Nb(2)	74.06(17)
C(36)-C(37)-Nb(2)	73.15(18)
C(33)-C(38)-C(39)	112.1(3)
C(33)-C(38)-C(40)	112.5(3)
C(39)-C(38)-C(40)	110.1(3)
C(33)-C(38)-P(3)	95.05(19)
C(39)-C(38)-P(3)	115.0(2)
C(40)-C(38)-P(3)	111.4(2)
C(46)-C(41)-C(42)	117.5(3)
C(46)-C(41)-P(3)	123.3(3)
C(42)-C(41)-P(3)	118.8(3)
C(43)-C(42)-C(41)	120.9(4)
C(44)-C(43)-C(42)	120.4(4)
C(43)-C(44)-C(45)	119.7(4)
C(44)-C(45)-C(46)	120.1(4)
C(41)-C(46)-C(45)	121.2(4)
C(51)-C(47)-C(48)	106.2(3)
C(51)-C(47)-C(52)	125.4(3)
C(48)-C(47)-C(52)	126.8(3)
C(51)-C(47)-Nb(2)	72.85(17)
C(48)-C(47)-Nb(2)	76.70(18)
C(52)-C(47)-Nb(2)	126.9(2)
C(49)-C(48)-C(47)	109.1(3)
C(49)-C(48)-Nb(2)	73.66(18)
C(47)-C(48)-Nb(2)	70.71(17)
C(48)-C(49)-C(50)	107.7(3)
C(48)-C(49)-Nb(2)	75.13(18)
C(50)-C(49)-Nb(2)	70.48(17)
C(51)-C(50)-C(49)	107.9(3)
C(51)-C(50)-Nb(2)	73.84(17)
C(49)-C(50)-Nb(2)	76.89(18)

C(50)-C(51)-C(47)	108.9(3)
C(50)-C(51)-Nb(2)	73.48(17)
C(47)-C(51)-Nb(2)	74.30(17)
C(47)-C(52)-C(53)	112.0(3)
C(47)-C(52)-C(54)	111.5(3)
C(53)-C(52)-C(54)	109.9(3)
C(47)-C(52)-P(4)	107.8(2)
C(53)-C(52)-P(4)	111.1(3)
C(54)-C(52)-P(4)	104.3(3)
C(56)-C(55)-C(60)	117.6(4)
C(56)-C(55)-P(4)	121.5(3)
C(60)-C(55)-P(4)	120.8(3)
C(55)-C(56)-C(57)	120.6(4)
C(58)-C(57)-C(56)	120.5(5)
C(57)-C(58)-C(59)	119.8(5)
C(58)-C(59)-C(60)	120.0(5)
C(59)-C(60)-C(55)	121.5(4)
N(2)-C(61)-C(64)	109.8(3)
N(2)-C(61)-C(62)	109.0(3)
C(64)-C(61)-C(62)	109.0(3)
N(2)-C(61)-C(63)	108.9(3)
C(64)-C(61)-C(63)	109.5(3)
C(62)-C(61)-C(63)	110.6(3)
C(29)-N(1)-Nb(1)	171.9(2)
C(61)-N(2)-Nb(2)	170.9(2)
C(9)-P(1)-C(6)	106.07(13)
C(9)-P(1)-Nb(1)	115.75(10)
C(6)-P(1)-Nb(1)	91.75(9)
C(23)-P(2)-C(20)	105.25(16)
C(41)-P(3)-C(38)	106.81(14)
C(41)-P(3)-Nb(2)	113.15(11)
C(38)-P(3)-Nb(2)	91.27(10)
C(55)-P(4)-C(52)	104.57(17)
N(1)-Nb(1)-C(3)	95.09(11)
N(1)-Nb(1)-C(4)	83.70(11)
C(3)-Nb(1)-C(4)	33.43(10)

N(1)-Nb(1)-C(5)	107.19(10)
C(3)-Nb(1)-C(5)	55.52(10)
C(4)-Nb(1)-C(5)	33.34(10)
N(1)-Nb(1)-C(18)	103.41(11)
C(3)-Nb(1)-C(18)	154.12(11)
C(4)-Nb(1)-C(18)	165.14(10)
C(5)-Nb(1)-C(18)	132.19(10)
N(1)-Nb(1)-C(19)	85.89(11)
C(3)-Nb(1)-C(19)	134.18(10)
C(4)-Nb(1)-C(19)	162.19(10)
C(5)-Nb(1)-C(19)	163.96(10)
C(18)-Nb(1)-C(19)	32.63(10)
N(1)-Nb(1)-C(15)	102.71(11)
C(3)-Nb(1)-C(15)	104.29(11)
C(4)-Nb(1)-C(15)	137.54(10)
C(5)-Nb(1)-C(15)	144.88(10)
C(18)-Nb(1)-C(15)	54.30(10)
C(19)-Nb(1)-C(15)	32.61(9)
N(1)-Nb(1)-C(2)	127.82(11)
C(3)-Nb(1)-C(2)	32.81(11)
C(4)-Nb(1)-C(2)	54.28(11)
C(5)-Nb(1)-C(2)	54.42(10)
C(18)-Nb(1)-C(2)	125.21(11)
C(19)-Nb(1)-C(2)	124.50(11)
C(15)-Nb(1)-C(2)	92.51(11)
N(1)-Nb(1)-C(1)	137.71(11)
C(3)-Nb(1)-C(1)	54.29(11)
C(4)-Nb(1)-C(1)	54.45(10)
C(5)-Nb(1)-C(1)	33.24(10)
C(18)-Nb(1)-C(1)	116.04(11)
C(19)-Nb(1)-C(1)	136.04(10)
C(15)-Nb(1)-C(1)	112.14(10)
C(2)-Nb(1)-C(1)	31.86(10)
N(1)-Nb(1)-C(17)	135.61(11)
C(3)-Nb(1)-C(17)	124.93(11)
C(4)-Nb(1)-C(17)	140.17(11)

C(5)-Nb(1)-C(17)	111.08(10)
C(18)-Nb(1)-C(17)	32.59(10)
C(19)-Nb(1)-C(17)	53.39(10)
C(15)-Nb(1)-C(17)	53.42(10)
C(2)-Nb(1)-C(17)	93.21(11)
C(1)-Nb(1)-C(17)	85.73(11)
N(1)-Nb(1)-C(16)	134.57(11)
C(3)-Nb(1)-C(16)	101.21(11)
C(4)-Nb(1)-C(16)	129.80(10)
C(5)-Nb(1)-C(16)	117.04(10)
C(18)-Nb(1)-C(16)	52.93(10)
C(19)-Nb(1)-C(16)	52.81(10)
C(15)-Nb(1)-C(16)	32.19(10)
C(2)-Nb(1)-C(16)	75.53(11)
C(1)-Nb(1)-C(16)	84.17(11)
C(17)-Nb(1)-C(16)	31.15(10)
N(1)-Nb(1)-P(1)	103.85(8)
C(3)-Nb(1)-P(1)	114.77(8)
C(4)-Nb(1)-P(1)	87.26(7)
C(5)-Nb(1)-P(1)	59.25(7)
C(18)-Nb(1)-P(1)	78.41(7)
C(19)-Nb(1)-P(1)	109.30(7)
C(15)-Nb(1)-P(1)	129.80(7)
C(2)-Nb(1)-P(1)	103.41(8)
C(1)-Nb(1)-P(1)	71.56(7)
C(17)-Nb(1)-P(1)	78.10(7)
C(16)-Nb(1)-P(1)	106.99(8)
N(2)-Nb(2)-C(36)	94.74(12)
N(2)-Nb(2)-C(37)	83.52(11)
C(36)-Nb(2)-C(37)	33.53(11)
N(2)-Nb(2)-C(33)	106.98(11)
C(36)-Nb(2)-C(33)	55.81(11)
C(37)-Nb(2)-C(33)	33.36(10)
N(2)-Nb(2)-C(50)	106.16(11)
C(36)-Nb(2)-C(50)	153.28(12)
C(37)-Nb(2)-C(50)	162.56(11)

C(33)-Nb(2)-C(50)	129.38(11)
N(2)-Nb(2)-C(51)	86.47(11)
C(36)-Nb(2)-C(51)	136.90(11)
C(37)-Nb(2)-C(51)	164.73(11)
C(33)-Nb(2)-C(51)	161.83(10)
C(50)-Nb(2)-C(51)	32.68(10)
N(2)-Nb(2)-C(47)	100.93(11)
C(36)-Nb(2)-C(47)	105.85(11)
C(37)-Nb(2)-C(47)	139.08(11)
C(33)-Nb(2)-C(47)	147.33(10)
C(50)-Nb(2)-C(47)	54.54(10)
C(51)-Nb(2)-C(47)	32.85(10)
N(2)-Nb(2)-C(35)	127.69(12)
C(36)-Nb(2)-C(35)	33.03(12)
C(37)-Nb(2)-C(35)	54.46(12)
C(33)-Nb(2)-C(35)	54.75(11)
C(50)-Nb(2)-C(35)	123.15(12)
C(51)-Nb(2)-C(35)	126.06(11)
C(47)-Nb(2)-C(35)	94.58(11)
N(2)-Nb(2)-C(34)	137.70(11)
C(36)-Nb(2)-C(34)	54.50(11)
C(37)-Nb(2)-C(34)	54.59(11)
C(33)-Nb(2)-C(34)	33.56(10)
C(50)-Nb(2)-C(34)	113.07(11)
C(51)-Nb(2)-C(34)	135.70(11)
C(47)-Nb(2)-C(34)	114.20(11)
C(35)-Nb(2)-C(34)	31.86(11)
N(2)-Nb(2)-C(49)	137.90(11)
C(36)-Nb(2)-C(49)	122.63(12)
C(37)-Nb(2)-C(49)	138.29(11)
C(33)-Nb(2)-C(49)	109.90(10)
C(50)-Nb(2)-C(49)	32.63(11)
C(51)-Nb(2)-C(49)	53.60(11)
C(47)-Nb(2)-C(49)	53.78(10)
C(35)-Nb(2)-C(49)	90.71(12)
C(34)-Nb(2)-C(49)	83.70(11)

N(2)-Nb(2)-C(48)	133.48(11)
C(36)-Nb(2)-C(48)	100.38(12)
C(37)-Nb(2)-C(48)	129.51(11)
C(33)-Nb(2)-C(48)	117.95(11)
C(50)-Nb(2)-C(48)	53.07(10)
C(51)-Nb(2)-C(48)	53.20(10)
C(47)-Nb(2)-C(48)	32.59(10)
C(35)-Nb(2)-C(48)	75.11(11)
C(34)-Nb(2)-C(48)	84.65(11)
C(49)-Nb(2)-C(48)	31.21(10)
N(2)-Nb(2)-P(3)	102.99(9)
C(36)-Nb(2)-P(3)	115.45(9)
C(37)-Nb(2)-P(3)	87.43(8)
C(33)-Nb(2)-P(3)	59.64(8)
C(50)-Nb(2)-P(3)	76.37(8)
C(51)-Nb(2)-P(3)	106.10(8)
C(47)-Nb(2)-P(3)	129.64(7)
C(35)-Nb(2)-P(3)	104.41(9)
C(34)-Nb(2)-P(3)	72.58(8)
C(49)-Nb(2)-P(3)	79.41(8)
C(48)-Nb(2)-P(3)	109.33(8)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($pm^2 x 10^{-1}$)for c1612. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	22(2)	36(2)	36(2)	8(1)	-2(1)	-4(1)
C(2)	31(2)	30(2)	52(2)	5(2)	1(2)	-7(1)
C(3)	29(2)	36(2)	48(2)	21(2)	6(1)	0(1)
C(4)	26(2)	35(2)	29(2)	10(1)	5(1)	2(1)
C(5)	16(1)	31(2)	31(2)	6(1)	3(1)	-1(1)
C(6)	26(2)	30(2)	28(2)	9(1)	4(1)	6(1)
C(7)	45(2)	34(2)	36(2)	2(1)	12(2)	7(2)
C(8)	28(2)	50(2)	44(2)	16(2)	3(1)	13(2)
C(9)	28(2)	24(1)	23(1)	3(1)	2(1)	2(1)
C(10)	40(2)	29(2)	41(2)	7(1)	4(2)	5(1)
C(11)	60(2)	22(2)	49(2)	1(2)	5(2)	1(2)
C(12)	64(3)	31(2)	44(2)	-1(2)	3(2)	-19(2)
C(13)	39(2)	49(2)	49(2)	2(2)	-3(2)	-9(2)
C(14)	33(2)	33(2)	36(2)	2(1)	2(1)	2(1)
C(15)	34(2)	21(1)	33(2)	1(1)	8(1)	7(1)
C(16)	40(2)	26(2)	34(2)	-6(1)	4(1)	2(1)
C(17)	43(2)	37(2)	24(2)	3(1)	4(1)	13(2)
C(18)	39(2)	24(2)	34(2)	6(1)	12(1)	6(1)
C(19)	28(2)	30(2)	31(2)	1(1)	8(1)	7(1)
C(20)	47(2)	28(2)	49(2)	9(2)	9(2)	13(2)
C(21)	70(3)	32(2)	91(3)	23(2)	30(2)	15(2)
C(22)	99(4)	48(2)	43(2)	14(2)	1(2)	34(2)
C(23)	45(2)	36(2)	51(2)	1(2)	10(2)	16(2)
C(24)	52(2)	46(2)	65(3)	11(2)	6(2)	9(2)
C(25)	66(3)	68(3)	64(3)	22(2)	4(2)	18(2)
C(26)	71(3)	82(4)	63(3)	1(3)	-10(2)	24(3)
C(27)	97(4)	52(3)	82(4)	-8(3)	-12(3)	-1(3)
C(28)	84(3)	37(2)	64(3)	5(2)	1(2)	6(2)
C(29)	30(2)	31(2)	26(2)	2(1)	-5(1)	-2(1)
C(30)	60(2)	50(2)	32(2)	13(2)	-7(2)	-11(2)
C(31)	31(2)	68(3)	48(2)	5(2)	-10(2)	-5(2)

C(32)	71(3)	41(2)	36(2)	-5(2)	-12(2)	7(2)
C(33)	18(1)	44(2)	32(2)	8(1)	-1(1)	4(1)
C(34)	25(2)	42(2)	39(2)	9(2)	0(1)	-3(1)
C(35)	29(2)	42(2)	49(2)	-6(2)	-8(2)	-6(2)
C(36)	32(2)	59(2)	30(2)	-2(2)	-7(1)	1(2)
C(37)	28(2)	45(2)	30(2)	8(1)	-4(1)	5(1)
C(38)	26(2)	39(2)	31(2)	9(1)	4(1)	7(1)
C(39)	41(2)	39(2)	41(2)	9(2)	-2(2)	13(2)
C(40)	33(2)	60(2)	41(2)	10(2)	9(2)	15(2)
C(41)	37(2)	30(2)	27(2)	3(1)	-4(1)	7(1)
C(42)	51(2)	46(2)	37(2)	-5(2)	-3(2)	13(2)
C(43)	80(3)	42(2)	52(2)	-13(2)	-17(2)	22(2)
C(44)	71(3)	30(2)	69(3)	2(2)	-28(2)	-1(2)
C(45)	44(2)	45(2)	66(3)	10(2)	-12(2)	-4(2)
C(46)	38(2)	38(2)	42(2)	2(2)	-5(2)	4(2)
C(47)	30(2)	33(2)	30(2)	4(1)	0(1)	8(1)
C(48)	35(2)	27(2)	41(2)	5(1)	0(1)	3(1)
C(49)	40(2)	39(2)	32(2)	15(1)	7(1)	11(2)
C(50)	39(2)	34(2)	29(2)	2(1)	-7(1)	12(1)
C(51)	24(2)	34(2)	37(2)	5(1)	-2(1)	8(1)
C(52)	50(2)	40(2)	32(2)	-2(2)	4(2)	13(2)
C(53)	72(3)	64(3)	41(2)	-16(2)	-13(2)	23(2)
C(54)	81(3)	57(3)	44(2)	11(2)	26(2)	25(2)
C(55)	47(2)	38(2)	43(2)	-2(2)	1(2)	17(2)
C(56)	56(2)	60(3)	42(2)	3(2)	-1(2)	20(2)
C(57)	76(3)	92(4)	53(3)	24(3)	11(2)	33(3)
C(58)	73(3)	65(3)	102(4)	37(3)	14(3)	12(3)
C(59)	100(4)	52(3)	92(4)	2(3)	-3(3)	-4(3)
C(60)	92(3)	44(2)	53(3)	-3(2)	-4(2)	7(2)
C(61)	31(2)	53(2)	41(2)	24(2)	3(1)	-2(2)
C(62)	49(2)	81(3)	37(2)	27(2)	3(2)	4(2)
C(63)	33(2)	85(3)	64(3)	38(2)	1(2)	-11(2)
C(64)	70(3)	48(2)	65(3)	31(2)	9(2)	-1(2)
N(1)	25(1)	24(1)	25(1)	3(1)	-1(1)	2(1)
N(2)	26(1)	37(1)	29(1)	11(1)	2(1)	2(1)
P(1)	24(1)	23(1)	24(1)	4(1)	2(1)	3(1)

P(2)	50(1)	48(1)	55(1)	-1(1)	4(1)	23(1)
P(3)	28(1)	33(1)	25(1)	6(1)	2(1)	6(1)
P(4)	47(1)	48(1)	56(1)	7(1)	8(1)	16(1)
Nb(1)	22(1)	19(1)	24(1)	3(1)	0(1)	1(1)
Nb(2)	22(1)	29(1)	22(1)	4(1)	1(1)	2(1)