The Mechanistic Significance of the Si-O-Pd Bond in the Palladium Catalyzed Cross-Coupling Reactions of Alkenylsilanolates

Steven A. Tymonko, Russell C. Smith, Andrea Ambrosi, and Scott E. Denmark*

Roger Adams Laboratory, Department of Chemistry, University of Illinois, Urbana, IL 61801

SUPPORTING INFORMATION: X-RAY DATA

Table of Contents Page

X-Ray Crystal Structure for Styryl Silanolate-Derived Complexes (Figure 2)

X-Ray data for 11p. Crystal data and structure refinement for ga64pas.

Identification code	ga64pas	
Empirical formula	C44 H46 O P2 Pd Si	
Formula weight	787.24	
Temperature	193(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	P b c a	
Unit cell dimensions	a = 16.0574(5) Å	α= 90°.
	b = 19.2846(5) Å	β= 90°.
	c = 25.5466(7) Å	γ = 90°.
Volume	7910.8(4) $Å^3$	
Z	8	
Density (calculated)	1.322 Mg/m^3	
Absorption coefficient	0.613 mm^{-1}	
F(000)	3264	
Crystal size	0.30 x 0.06 x 0.02 mm^3	
Theta range for data collection	1.83 to 25.71°.	
Index ranges	-19<=h<=19, -23<=k<=23, -31<=l<=31	
Reflections collected	100321	
Independent reflections	7526 [R(int) = 0.1659]	
Completeness to theta = 25.71°	99.7 %	
Absorption correction	Integration	
Max. and min. transmission	0.9879 and 0.8703	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	7526 / 0 / 445	
Goodness-of-fit on F^2	0.995	
Final R indices [I>2sigma(I)]	R1 = 0.0428, wR2 = 0.0683	
R indices (all data)	R1 = 0.1202, wR2 = 0.0903	
Largest diff. peak and hole	0.461 and -0.419 $e.Å^{-3}$	

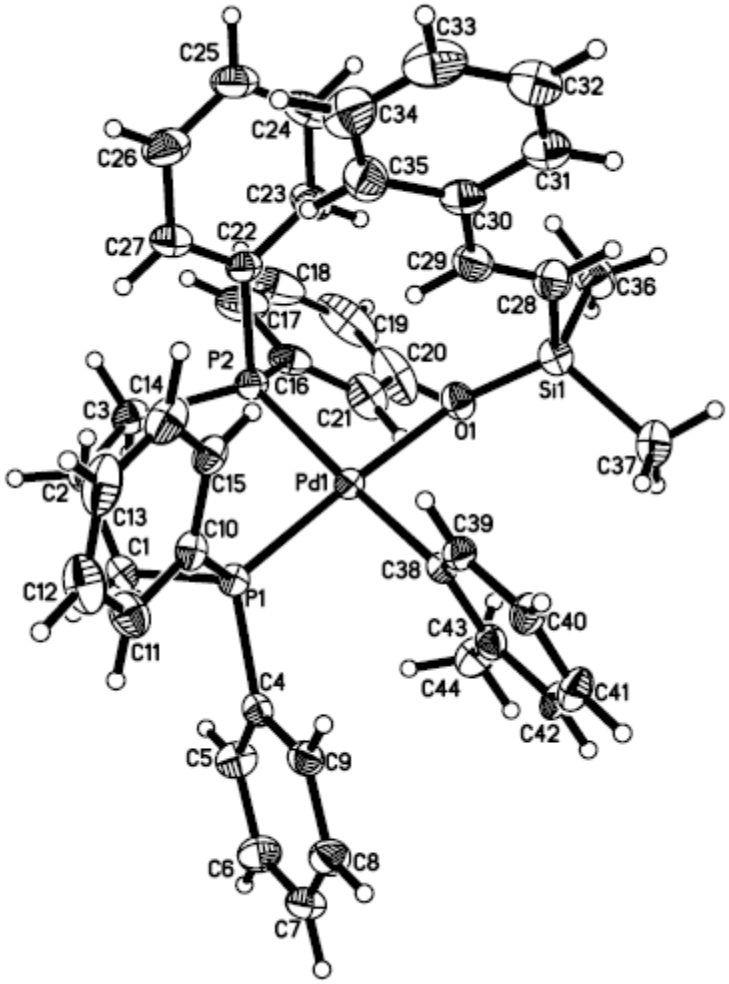

Figure 1. X-ray structure of complex **11p.**

The crystals were obtained directly from recrystallization as yellow needles 0.30 x 0.06 x 0.02 mm in size and mounted using oil (Parantone-N, Exxon) to a thin glass fiver with the (1 0 0) scattering planes roughly normal to the spindle axis. Systematic absences for **11p** were consistent with the space group P b c a. Unit cell dimensions were a = 16.0576() Å, b = 19.2846(5) Å, c = 25.5466(7) Å, α= 90°, β= 90°, γ = 90°. Integration absorption correction was applied and maximum and minimum transmission factors were 0.9879 and 0.8703. The 7526 data points were used in the full-matrix least-squares refinement. The structure was solved using direct

methods by using SHELXTL software package.[1] Hydrogen atoms were placed in "idealized" positions and their displacement parameters were fixed to be 20-50 % larger than those of the attached non-hydrogen atoms.

Table 1. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) for ga64pas. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

Atom	x	y	z	U(eq)
C(1)	1407(3)	2575(2)	7807(2)	33(1)
C(2)	1235(3)	3125(2)	7394(2)	37(1)
C(3)	926(3)	2845(2)	6874(2)	40(1)
C(4)	2395(3)	1533(2)	8297(2)	31(1)
C(5)	1659(3)	1218(2)	8453(2)	41(1)
C(6)	1646(3)	734(2)	8852(2)	46(1)
C(7)	2379(4)	559(2)	9100(2)	48(1)
C(8)	3107(3)	860(3)	8950(2)	45(1)
C(9)	3129(3)	1348(2)	8549(2)	37(1)
C(10)	3133(3)	2810(2)	7897(2)	31(1)
C(11)	3210(3)	3078(2)	8396(2)	47(1)
C(12)	3701(3)	3657(3)	8490(2)	57(2)
C(13)	4107(3)	3982(2)	8088(3)	55(2)
C(14)	4044(3)	3721(2)	7591(2)	46(1)
C(15)	3561(3)	3136(2)	7496(2)	35(1)
C(16)	1008(3)	1847(3)	6046(2)	42(1)
C(17)	420(3)	2188(3)	5746(2)	62(2)
C(18)	-56(4)	1826(5)	5391(2)	84(2)
C(19)	47(4)	1128(5)	5332(3)	86(3)
C(20)	617(4)	778(4)	5634(3)	77(2)
C(21)	1101(3)	1144(3)	5994(2)	54(2)
C(22)	2183(3)	2959(2)	6070(2)	36(1)
C(23)	2436(3)	2768(3)	5579(2)	50(1)
C(24)	2822(3)	3240(3)	5250(2)	63(2)
C(25)	2973(3)	3908(3)	5420(2)	55(2)
C(26)	2741(3)	4102(3)	5912(2)	57(2)

C(27)	2345(3)	3630(2)	6236(2)	49(1)
C(28)	4571(3)	1616(3)	5828(2)	47(1)
C(29)	4556(3)	2252(3)	6016(2)	45(1)
C(30)	5197(3)	2801(3)	5956(2)	40(1)
C(31)	5961(3)	2685(3)	5716(2)	46(1)
C(32)	6535(3)	3209(3)	5665(2)	54(2)
C(33)	6365(4)	3863(3)	5848(2)	66(2)
C(34)	5608(4)	3989(3)	6081(2)	63(2)
C(35)	5024(3)	3461(3)	6134(2)	52(1)
C(36)	3368(3)	728(3)	5243(2)	58(2)
C(37)	4263(3)	172(2)	6187(2)	50(1)
C(38)	3585(3)	1118(2)	7321(2)	26(1)
C(39)	4371(3)	1398(2)	7407(2)	33(1)
C(40)	5005(3)	1024(2)	7654(2)	37(1)
C(41)	4842(3)	360(2)	7821(2)	43(1)
C(42)	4068(3)	73(2)	7735(2)	39(1)
C(43)	3435(3)	435(2)	7489(2)	34(1)
C(44)	2598(3)	104(2)	7401(2)	44(1)
O(1)	2964(2)	1221(2)	6250(1)	38(1)
P(1)	2403(1)	2120(1)	7735(1)	28(1)
P(2)	1674(1)	2326(1)	6499(1)	33(1)
Pd(1)	2669(1)	1668(1)	6954(1)	26(1)
Si(1)	3726(1)	954(1)	5917(1)	37(1)

Table 2. Bond lengths [Å] and angles [°] for ga64pas.

C(1)-C(2)	1.522(6)
C(1)-P(1)	1.833(4)
C(1)-H(1A)	0.9900
C(1)-H(1B)	0.9900
C(2)-C(3)	1.517(6)
C(2)-H(2A)	0.9900
C(2)-H(2B)	0.9900
C(3)-P(2)	1.834(4)
C(3)-H(3A)	0.9900
C(3)-H(3B)	0.9900
C(4)-C(5)	1.388(6)
C(4)-C(9)	1.389(6)
C(4)-P(1)	1.830(4)
C(5)-C(6)	1.383(6)
C(5)-H(5)	0.9500
C(6)-C(7)	1.378(6)
C(6)-H(6)	0.9500
C(7)-C(8)	1.360(7)
C(7)-H(7)	0.9500
C(8)-C(9)	1.391(6)
C(8)-H(8)	0.9500
C(9)-H(9)	0.9500
C(10)-C(11)	1.383(6)
C(10)-C(15)	1.385(6)
C(10)-P(1)	1.820(4)
C(11)-C(12)	1.387(6)
C(11)-H(11)	0.9500
C(12)-C(13)	1.367(7)
C(12)-H(12)	0.9500
C(13)-C(14)	1.370(7)
C(13)-H(13)	0.9500
C(14)-C(15)	1.389(6)
C(14)-H(14)	0.9500
C(15)-H(15)	0.9500

C(16)-C(21)	1.371(7)
C(16)-C(17)	1.382(7)
C(16)-P(2)	1.825(5)
C(17)-C(18)	1.376(8)
C(17)-H(17)	0.9500
C(18)-C(19)	1.364(9)
C(18)-H(18)	0.9500
C(19)-C(20)	1.374(9)
C(19)-H(19)	0.9500
C(20)-C(21)	1.395(7)
C(20)-H(20)	0.9500
C(21)-H(21)	0.9500
C(22)-C(23)	1.371(6)
C(22)-C(27)	1.387(6)
C(22)-P(2)	1.832(4)
C(23)-C(24)	1.385(6)
C(23)-H(23)	0.9500
C(24)-C(25)	1.381(7)
C(24)-H(24)	0.9500
C(25)-C(26)	1.363(7)
C(25)-H(25)	0.9500
C(26)-C(27)	1.386(6)
C(26)-H(26)	0.9500
C(27)-H(27)	0.9500
C(28)-C(29)	1.317(6)
C(28)-Si(1)	1.877(5)
C(28)-H(28)	0.9500
C(29)-C(30)	1.485(6)
C(29)-H(29)	0.9500
C(30)-C(35)	1.381(7)
C(30)-C(31)	1.389(6)
C(31)-C(32)	1.373(6)
C(31)-H(31)	0.9500
C(32)-C(33)	1.374(7)
C(32)-H(32)	0.9500
C(33)-C(34)	1.374(8)

C(33)-H(33)	0.9500
C(34)-C(35)	1.390(7)
C(34)-H(34)	0.9500
C(35)-H(35)	0.9500
C(36)-Si(1)	1.868(5)
C(36)-H(36A)	0.9800
C(36)-H(36B)	0.9800
C(36)-H(36C)	0.9800
C(37)-Si(1)	1.868(5)
C(37)-H(37A)	0.9800
C(37)-H(37B)	0.9800
C(37)-H(37C)	0.9800
C(38)-C(39)	1.390(6)
C(38)-C(43)	1.407(6)
C(38)-Pd(1)	2.042(4)
C(39)-C(40)	1.400(6)
C(39)-H(39)	0.9500
C(40)-C(41)	1.373(6)
C(40)-H(40)	0.9500
C(41)-C(42)	1.378(6)
C(41)-H(41)	0.9500
C(42)-C(43)	1.384(6)
C(42)-H(42)	0.9500
C(43)-C(44)	1.504(6)
C(44)-H(44A)	0.9800
C(44)-H(44B)	0.9800
C(44)-H(44C)	0.9800
O(1)-Si(1)	1.577(3)
O(1)-Pd(1)	2.050(3)
P(1)-Pd(1)	2.2179(11)
P(2)-Pd(1)	2.3479(12)

C(2)-C(1)-P(1)	114.9(3)
C(2)-C(1)-H(1A)	108.5
P(1)-C(1)-H(1A)	108.5
C(2)-C(1)-H(1B)	108.5

P(1)-C(1)-H(1B)	108.5
H(1A)-C(1)-H(1B)	107.5
C(3)-C(2)-C(1)	114.8(4)
C(3)-C(2)-H(2A)	108.6
C(1)-C(2)-H(2A)	108.6
C(3)-C(2)-H(2B)	108.6
C(1)-C(2)-H(2B)	108.6
H(2A)-C(2)-H(2B)	107.6
C(2)-C(3)-P(2)	115.9(3)
C(2)-C(3)-H(3A)	108.3
P(2)-C(3)-H(3A)	108.3
C(2)-C(3)-H(3B)	108.3
P(2)-C(3)-H(3B)	108.3
H(3A)-C(3)-H(3B)	107.4
C(5)-C(4)-C(9)	118.6(4)
C(5)-C(4)-P(1)	120.1(4)
C(9)-C(4)-P(1)	121.2(3)
C(6)-C(5)-C(4)	121.2(5)
C(6)-C(5)-H(5)	119.4
C(4)-C(5)-H(5)	119.4
C(7)-C(6)-C(5)	119.5(5)
C(7)-C(6)-H(6)	120.3
C(5)-C(6)-H(6)	120.3
C(8)-C(7)-C(6)	120.0(5)
C(8)-C(7)-H(7)	120.0
C(6)-C(7)-H(7)	120.0
C(7)-C(8)-C(9)	121.2(5)
C(7)-C(8)-H(8)	119.4
C(9)-C(8)-H(8)	119.4
C(4)-C(9)-C(8)	119.5(5)
C(4)-C(9)-H(9)	120.2
C(8)-C(9)-H(9)	120.2
C(11)-C(10)-C(15)	117.8(4)
C(11)-C(10)-P(1)	122.8(4)
C(15)-C(10)-P(1)	118.9(4)
C(10)-C(11)-C(12)	120.8(5)

C(10)-C(11)-H(11)	119.6
C(12)-C(11)-H(11)	119.6
C(13)-C(12)-C(11)	120.7(5)
C(13)-C(12)-H(12)	119.7
C(11)-C(12)-H(12)	119.7
C(12)-C(13)-C(14)	119.4(5)
C(12)-C(13)-H(13)	120.3
C(14)-C(13)-H(13)	120.3
C(13)-C(14)-C(15)	120.2(5)
C(13)-C(14)-H(14)	119.9
C(15)-C(14)-H(14)	119.9
C(10)-C(15)-C(14)	121.1(5)
C(10)-C(15)-H(15)	119.4
C(14)-C(15)-H(15)	119.4
C(21)-C(16)-C(17)	119.4(5)
C(21)-C(16)-P(2)	119.8(4)
C(17)-C(16)-P(2)	120.7(4)
C(18)-C(17)-C(16)	120.3(6)
C(18)-C(17)-H(17)	119.9
C(16)-C(17)-H(17)	119.9
C(19)-C(18)-C(17)	120.4(7)
C(19)-C(18)-H(18)	119.8
C(17)-C(18)-H(18)	119.8
C(18)-C(19)-C(20)	120.2(6)
C(18)-C(19)-H(19)	119.9
C(20)-C(19)-H(19)	119.9
C(19)-C(20)-C(21)	119.6(7)
C(19)-C(20)-H(20)	120.2
C(21)-C(20)-H(20)	120.2
C(16)-C(21)-C(20)	120.2(6)
C(16)-C(21)-H(21)	119.9
C(20)-C(21)-H(21)	119.9
C(23)-C(22)-C(27)	118.4(4)
C(23)-C(22)-P(2)	120.0(4)
C(27)-C(22)-P(2)	121.5(4)
C(22)-C(23)-C(24)	120.7(5)

C(22)-C(23)-H(23)	119.6
C(24)-C(23)-H(23)	119.6
C(25)-C(24)-C(23)	120.1(5)
C(25)-C(24)-H(24)	120.0
C(23)-C(24)-H(24)	120.0
C(26)-C(25)-C(24)	119.9(5)
C(26)-C(25)-H(25)	120.1
C(24)-C(25)-H(25)	120.1
C(25)-C(26)-C(27)	119.8(5)
C(25)-C(26)-H(26)	120.1
C(27)-C(26)-H(26)	120.1
C(26)-C(27)-C(22)	121.0(5)
C(26)-C(27)-H(27)	119.5
C(22)-C(27)-H(27)	119.5
C(29)-C(28)-Si(1)	125.3(4)
C(29)-C(28)-H(28)	117.4
Si(1)-C(28)-H(28)	117.4
C(28)-C(29)-C(30)	127.9(5)
C(28)-C(29)-H(29)	116.0
C(30)-C(29)-H(29)	116.0
C(35)-C(30)-C(31)	118.1(5)
C(35)-C(30)-C(29)	118.9(5)
C(31)-C(30)-C(29)	122.9(5)
C(32)-C(31)-C(30)	121.1(5)
C(32)-C(31)-H(31)	119.5
C(30)-C(31)-H(31)	119.5
C(31)-C(32)-C(33)	120.7(5)
C(31)-C(32)-H(32)	119.7
C(33)-C(32)-H(32)	119.7
C(32)-C(33)-C(34)	119.0(5)
C(32)-C(33)-H(33)	120.5
C(34)-C(33)-H(33)	120.5
C(33)-C(34)-C(35)	120.7(5)
C(33)-C(34)-H(34)	119.6
C(35)-C(34)-H(34)	119.6
C(30)-C(35)-C(34)	120.4(5)

C(30)-C(35)-H(35)	119.8
C(34)-C(35)-H(35)	119.8
Si(1)-C(36)-H(36A)	109.5
Si(1)-C(36)-H(36B)	109.5
H(36A)-C(36)-H(36B)	109.5
Si(1)-C(36)-H(36C)	109.5
H(36A)-C(36)-H(36C)	109.5
H(36B)-C(36)-H(36C)	109.5
Si(1)-C(37)-H(37A)	109.5
Si(1)-C(37)-H(37B)	109.5
H(37A)-C(37)-H(37B)	109.5
Si(1)-C(37)-H(37C)	109.5
H(37A)-C(37)-H(37C)	109.5
H(37B)-C(37)-H(37C)	109.5
C(39)-C(38)-C(43)	118.1(4)
C(39)-C(38)-Pd(1)	121.6(3)
C(43)-C(38)-Pd(1)	120.3(3)
C(38)-C(39)-C(40)	122.1(4)
C(38)-C(39)-H(39)	118.9
C(40)-C(39)-H(39)	118.9
C(41)-C(40)-C(39)	118.8(4)
C(41)-C(40)-H(40)	120.6
C(39)-C(40)-H(40)	120.6
C(40)-C(41)-C(42)	119.9(4)
C(40)-C(41)-H(41)	120.1
C(42)-C(41)-H(41)	120.1
C(41)-C(42)-C(43)	122.1(4)
C(41)-C(42)-H(42)	118.9
C(43)-C(42)-H(42)	118.9
C(42)-C(43)-C(38)	119.0(4)
C(42)-C(43)-C(44)	120.7(4)
C(38)-C(43)-C(44)	120.3(4)
C(43)-C(44)-H(44A)	109.5
C(43)-C(44)-H(44B)	109.5
H(44A)-C(44)-H(44B)	109.5
C(43)-C(44)-H(44C)	109.5

H(44A)-C(44)-H(44C)	109.5
H(44B)-C(44)-H(44C)	109.5
Si(1)-O(1)-Pd(1)	142.16(18)
C(10)-P(1)-C(4)	106.1(2)
C(10)-P(1)-C(1)	100.9(2)
C(4)-P(1)-C(1)	102.2(2)
C(10)-P(1)-Pd(1)	111.56(15)
C(4)-P(1)-Pd(1)	117.72(13)
C(1)-P(1)-Pd(1)	116.54(15)
C(16)-P(2)-C(22)	102.7(2)
C(16)-P(2)-C(3)	102.9(2)
C(22)-P(2)-C(3)	103.9(2)
C(16)-P(2)-Pd(1)	116.05(17)
C(22)-P(2)-Pd(1)	110.60(14)
C(3)-P(2)-Pd(1)	118.82(15)
C(38)-Pd(1)-O(1)	91.02(14)
C(38)-Pd(1)-P(1)	85.97(12)
O(1)-Pd(1)-P(1)	176.99(9)
C(38)-Pd(1)-P(2)	176.74(12)
O(1)-Pd(1)-P(2)	87.15(9)
P(1)-Pd(1)-P(2)	95.86(4)
O(1)-Si(1)-C(36)	109.6(2)
O(1)-Si(1)-C(37)	115.0(2)
C(36)-Si(1)-C(37)	107.1(2)
O(1)-Si(1)-C(28)	113.8(2)
C(36)-Si(1)-C(28)	105.6(2)
C(37)-Si(1)-C(28)	105.1(2)

Table 3. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for ga64pas. 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)	31(3)	37(3)	30(3)	-5(2)	4(2)	-1(2)
C(2)	31(3)	35(3)	44(3)	-1(2)	8(2)	6(2)
C(3)	27(3)	44(3)	48(3)	10(3)	-1(2)	4(2)
C(4)	33(3)	31(2)	29(2)	-4(2)	3(2)	1(2)
C(5)	34(3)	44(3)	45(3)	6(3)	-4(3)	-8(2)
C(6)	46(4)	43(3)	48(3)	9(3)	1(3)	-11(3)
C(7)	65(4)	45(3)	33(3)	7(2)	9(3)	2(3)
C(8)	41(4)	59(3)	35(3)	4(3)	-6(3)	8(3)
C(9)	38(3)	42(3)	30(3)	0(2)	0(2)	2(2)
C(10)	23(3)	29(2)	42(3)	-4(2)	-1(2)	-1(2)
C(11)	41(3)	50(3)	50(4)	-9(3)	7(3)	-6(3)
C(12)	51(4)	56(4)	64(4)	-32(3)	-7(3)	-9(3)
C(13)	38(3)	35(3)	90(5)	-19(3)	-9(4)	-5(2)
C(14)	29(3)	34(3)	76(4)	7(3)	3(3)	-6(2)
C(15)	25(3)	29(3)	49(3)	3(2)	-2(2)	1(2)
C(16)	32(3)	62(4)	32(3)	9(3)	-1(2)	-10(2)
C(17)	48(4)	92(5)	44(4)	17(3)	-13(3)	-14(3)
C(18)	48(4)	159(8)	44(4)	24(5)	-15(3)	-30(5)
C(19)	43(4)	162(8)	51(4)	-37(5)	2(3)	-49(5)
C(20)	41(4)	113(6)	76(5)	-47(4)	6(4)	-18(4)
C(21)	35(3)	74(4)	54(4)	-16(3)	-3(3)	-5(3)
C(22)	25(3)	41(3)	40(3)	13(2)	3(2)	5(2)
C(23)	44(3)	59(3)	46(3)	5(3)	14(3)	-3(3)
C(24)	57(4)	82(5)	49(4)	10(3)	21(3)	-10(3)
C(25)	45(4)	67(4)	53(4)	28(3)	9(3)	4(3)
C(26)	60(4)	47(3)	63(4)	17(3)	5(3)	-7(3)
C(27)	57(4)	46(3)	44(3)	10(3)	13(3)	-4(3)
C(28)	41(3)	50(3)	48(3)	3(3)	1(2)	6(3)
C(29)	44(3)	53(3)	38(3)	4(3)	3(3)	4(3)
C(30)	47(3)	46(3)	26(3)	2(2)	-10(2)	-8(3)
C(31)	49(4)	52(3)	37(3)	3(3)	-10(3)	-6(3)

C(32)	49(4)	64(4)	49(4)	1(3)	-3(3)	-17(3)
C(33)	73(5)	59(4)	65(4)	9(3)	-13(4)	-29(4)
C(34)	91(5)	46(4)	54(4)	-8(3)	-13(4)	-9(4)
C(35)	59(4)	55(4)	43(3)	-5(3)	-4(3)	3(3)
C(36)	61(4)	69(4)	44(3)	-9(3)	-1(3)	1(3)
C(37)	42(3)	46(3)	63(4)	-7(3)	1(3)	6(3)
C(38)	26(3)	28(2)	24(3)	-2(2)	1(2)	-1(2)
C(39)	31(3)	32(2)	35(3)	3(2)	3(2)	2(2)
C(40)	27(3)	38(3)	47(3)	0(2)	-1(2)	3(2)
C(41)	39(3)	39(3)	52(3)	0(2)	-10(3)	12(2)
C(42)	51(3)	21(2)	45(3)	0(2)	0(3)	8(2)
C(43)	38(3)	30(3)	34(3)	-6(2)	4(2)	0(2)
C(44)	46(3)	31(2)	56(3)	-1(2)	-5(3)	-10(2)
O(1)	35(2)	47(2)	33(2)	-7(2)	-3(2)	5(2)
P(1)	24(1)	28(1)	32(1)	0(1)	0(1)	-2(1)
P(2)	27(1)	37(1)	35(1)	6(1)	1(1)	2(1)
Pd(1)	24(1)	26(1)	29(1)	1(1)	-1(1)	-1(1)
Si(1)	33(1)	41(1)	37(1)	-5(1)	-1(1)	-1(1)

Table 4. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for ga64pas.

Atom	x	y	z	U(eq)
H(1A)	952	2228	7797	39
H(1B)	1394	2798	8156	39
H(2A)	815	3452	7533	44
H(2B)	1754	3390	7331	44
H(3A)	749	3242	6654	48
H(3B)	426	2558	6940	48
H(5)	1154	1337	8281	49
H(6)	1136	524	8955	55
H(7)	2376	229	9376	57
H(8)	3609	735	9122	54

H(9)	3643	1553	8448	44
H(11)	2924	2864	8678	56
H(12)	3756	3829	8836	68
H(13)	4431	4385	8153	65
H(14)	4330	3940	7311	55
H(15)	3524	2958	7150	41
H(17)	344	2673	5785	74
H(18)	-459	2063	5186	100
H(19)	-276	883	5082	103
H(20)	681	291	5598	92
H(21)	1496	904	6204	65
H(23)	2345	2306	5462	60
H(24)	2983	3104	4907	75
H(25)	3238	4232	5195	66
H(26)	2851	4559	6032	68
H(27)	2181	3769	6578	59
H(28)	5047	1482	5632	56
H(29)	4078	2374	6214	54
H(31)	6089	2237	5585	55
H(32)	7054	3118	5500	65
H(33)	6765	4224	5815	79
H(34)	5483	4440	6207	76
H(35)	4502	3556	6294	63
H(36A)	2891	413	5264	87
H(36B)	3823	501	5052	87
H(36C)	3204	1151	5058	87
H(37A)	4546	295	6514	75
H(37B)	4672	3	5933	75
H(37C)	3851	-192	6256	75
H(39)	4481	1859	7294	39
H(40)	5539	1225	7706	45
H(41)	5262	100	7994	52
H(42)	3966	-388	7849	47
H(44A)	2594	-361	7555	67
H(44B)	2489	71	7025	67
H(44C)	2165	388	7567	67

X-Ray Crystal Structure of 11t (ga45xasd)

Crystal Data and Structure Refinement for ga45xasd:

Identification code	ga45xasd	
Empirical formula	C56 H53 O P2 Pd Si	
Formula weight	938.41	
Temperature	193(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 21/n	
Unit cell dimensions	a = 19.9632(11) Å	a= 90°.
	b = 11.8061(6) Å	b= 111.315(3)°.
	c = 21.5367(12) Å	g = 90°.
Volume	4728.7(5) $Å^3$	
Z	4	
Density (calculated)	1.318 Mg/m^3	
Absorption coefficient	0.524 mm^{-1}	
F(000)	1948	
Crystal size	0.56 x 0.18 x 0.12 mm^3	
Theta range for data collection	1.74 to 26.78°.	
Index ranges	-25<=h<=25, -14<=k<=14, -27<=l<=27	
Reflections collected	61435	
Independent reflections	10045 [R(int) = 0.0591]	
Completeness to theta = 26.78°	99.5 %	
Absorption correction	Integration	
Max. and min. transmission	0.9460 and 0.7940	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	10045 / 595 / 668	
Goodness-of-fit on F^2	1.009	
Final R indices [I>2sigma(I)]	R1 = 0.0370, wR2 = 0.0861	
R indices (all data)	R1 = 0.0557, wR2 = 0.0954	
Largest diff. peak and hole	2.124 and -0.654 $e.Å^{-3}$	

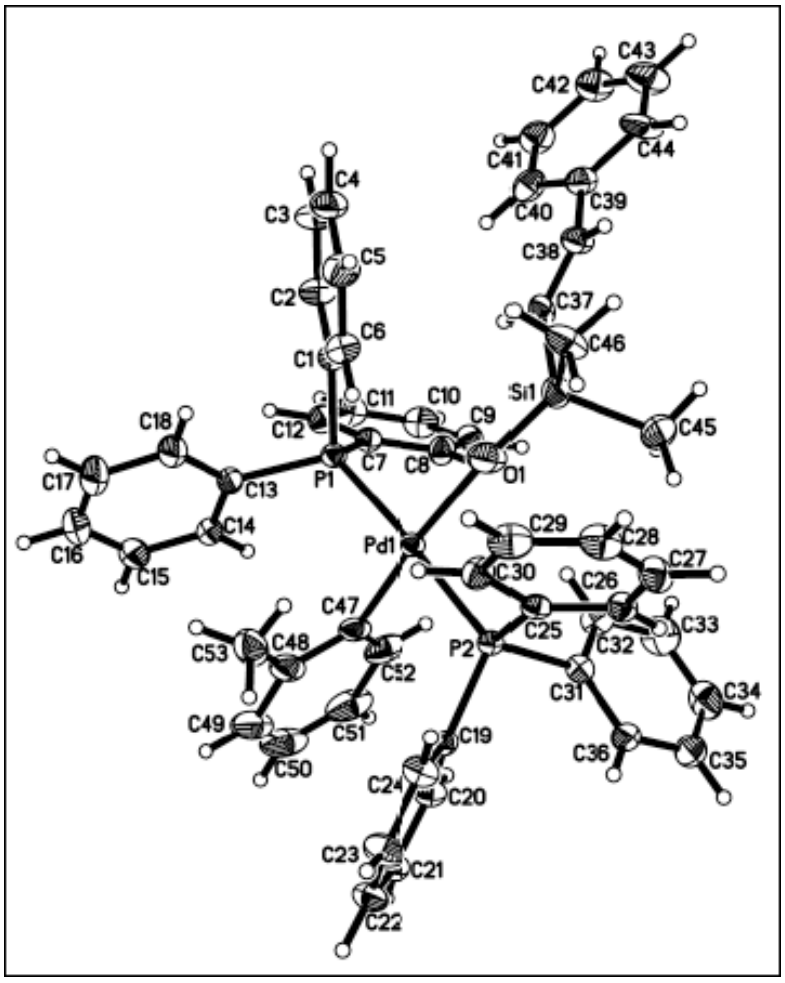

Figure 2. X-ray crystal structure of **11t.**

The crystals were obtained directly from recrystallization from hexane/benzene as yellow needles 0.56 x 0.18 x 0.12 mm in size and using epoxy to a 0.3 mm cryo-loop (Hampton Research) with the (-4 -2 3) scattering planes roughly normal to the spindle axis.. Systematic absences for **11t** were consistent with the space group P 21/n . Unit cell dimensions were a = 19.9632(11) Å, b = 11.8061(6) Å, c = 21.5367(12) Å, α= 90°, β= 111.315(3)°, γ = 90°. Integration absorption correction was applied and maximum and minimum transmission factors were 0.9460 and 0.7940. The 10045 data points were used in the full-matrix least-squares

refinement. The structure was solved using direct methods by using SHELXTL software package.[1] Hydrogen atoms were placed in "idealized" positions and their displacement parameters were fixed to be 20-50 % larger than those of the attached non-hydrogen atoms.

Table 5. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for ga45xasd. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

Atom	x	y	z	U(eq)
C(1)	8828(2)	3529(2)	362(1)	30(1)
C(2)	8860(2)	2386(3)	508(2)	45(1)
C(3)	9516(2)	1836(3)	762(2)	56(1)
C(4)	10141(2)	2428(3)	869(2)	52(1)
C(5)	10115(2)	3551(3)	715(2)	48(1)
C(6)	9463(2)	4112(3)	464(2)	39(1)
C(7)	7377(1)	3561(2)	373(1)	28(1)
C(8)	7314(2)	4011(2)	945(2)	36(1)
C(9)	6862(2)	3509(3)	1225(2)	44(1)
C(10)	6462(2)	2568(3)	929(2)	46(1)
C(11)	6528(2)	2105(3)	367(2)	42(1)
C(12)	6985(2)	2594(2)	89(2)	36(1)
C(13)	7628(2)	3923(2)	-856(1)	32(1)
C(14)	6893(2)	3969(2)	-1221(2)	38(1)
C(15)	6632(2)	3757(3)	-1899(2)	51(1)
C(16)	7099(2)	3525(4)	-2218(2)	63(1)
C(17)	7830(2)	3486(4)	-1865(2)	61(1)
C(18)	8098(2)	3676(3)	-1182(2)	44(1)
C(19)	7764(1)	9115(2)	-155(1)	26(1)
C(20)	7020(2)	9210(2)	-439(2)	34(1)
C(21)	6697(2)	9905(3)	-982(2)	40(1)
C(22)	7107(2)	10523(3)	-1250(2)	44(1)
C(23)	7841(2)	10452(3)	-971(2)	49(1)
C(24)	8172(2)	9749(3)	-426(2)	38(1)
C(25)	9077(1)	8554(2)	941(1)	28(1)

C(26)	9324(2)	9122(2)	1546(2)	34(1)
C(27)	10045(2)	9402(3)	1841(2)	45(1)
C(28)	10515(2)	9143(3)	1534(2)	48(1)
C(29)	10281(2)	8579(3)	935(2)	46(1)
C(30)	9566(2)	8263(3)	642(2)	38(1)
C(31)	7702(1)	8509(2)	1106(1)	31(1)
C(32)	7517(2)	7660(3)	1456(2)	46(1)
C(33)	7190(2)	7929(4)	1905(2)	63(1)
C(34)	7047(2)	9027(4)	2004(2)	58(1)
C(35)	7227(2)	9881(3)	1660(2)	50(1)
C(36)	7550(2)	9628(3)	1205(2)	38(1)
O(1)	8958(2)	5951(3)	1166(2)	57(1)
Si(1)	9417(1)	5634(1)	1890(1)	40(1)
C(37)	9331(2)	4132(3)	2128(2)	35(1)
C(38)	9781(2)	3572(3)	2648(2)	39(1)
C(39)	9716(2)	2487(2)	2950(1)	40(1)
C(40)	9184(2)	1730(3)	2588(1)	45(1)
C(41)	9071(2)	741(3)	2887(2)	52(1)
C(42)	9491(3)	509(3)	3547(2)	57(1)
C(43)	10022(2)	1266(3)	3909(1)	63(1)
C(44)	10135(2)	2255(2)	3611(2)	56(1)
C(45)	9180(3)	6454(4)	2533(2)	57(1)
C(46)	10398(2)	5881(5)	2067(3)	53(1)
C(47)	7144(1)	6444(3)	-446(1)	39(1)
C(48)	7088(1)	6710(3)	-1092(1)	53(1)
C(49)	6415(2)	6883(3)	-1584(1)	76(1)
C(50)	5799(1)	6790(3)	-1430(2)	86(2)
C(51)	5855(1)	6524(3)	-784(2)	74(1)
C(52)	6528(1)	6351(3)	-292(1)	54(1)
C(53)	7736(3)	6816(4)	-1269(2)	62(1)
P(1)	7974(1)	4287(1)	31(1)	27(1)
P(2)	8144(1)	8117(1)	533(1)	25(1)
Pd(1)	8073(1)	6188(1)	313(1)	26(1)
C(54)	4553(2)	10902(3)	-263(2)	57(1)
C(55)	4729(2)	10163(3)	-679(2)	55(1)
C(56)	5177(2)	9264(3)	-412(2)	53(1)

C(57)	7312(5)	6467(15)	-583(4)	39(3)
C(58)	6581(6)	6500(14)	-695(5)	52(2)
C(59)	6087(5)	6720(16)	-1330(6)	70(3)
C(60)	6324(7)	6906(16)	-1854(4)	74(3)
C(61)	7054(8)	6873(14)	-1742(4)	61(3)
C(62)	7548(6)	6653(15)	-1107(5)	51(3)
C(63)	6321(9)	6270(20)	-144(8)	54(3)
O(2)	8723(6)	5763(12)	1277(4)	40(3)
Si(2)	9356(5)	5755(8)	1952(4)	40(1)
C(64)	9556(9)	4416(10)	2438(6)	53(3)
C(65)	9357(10)	3356(10)	2321(7)	49(3)
C(66)	9530(10)	2359(10)	2758(7)	48(3)
C(67)	10009(10)	2467(12)	3411(8)	57(3)
C(68)	10055(14)	1618(17)	3873(8)	62(3)
C(69)	9622(15)	662(17)	3680(10)	58(3)
C(70)	9143(14)	554(14)	3027(11)	53(3)
C(71)	9097(12)	1403(11)	2566(8)	50(3)
C(72)	9224(15)	6811(15)	2555(8)	64(5)
C(73)	10243(6)	6120(20)	1876(11)	51(4)

Table 6. Bond lengths [Å] and angles [°] for ga45xasd.

C(1)-C(2)	1.381(4)
C(1)-C(6)	1.387(4)
C(1)-P(1)	1.825(3)
C(2)-C(3)	1.385(4)
C(2)-H(2)	0.9500
C(3)-C(4)	1.374(5)
C(3)-H(3)	0.9500
C(4)-C(5)	1.363(5)
C(4)-H(4)	0.9500
C(5)-C(6)	1.383(4)
C(5)-H(5)	0.9500
C(6)-H(6)	0.9500
C(7)-C(8)	1.388(4)

C(7)-C(12)	1.392(4)
C(7)-P(1)	1.827(3)
C(8)-C(9)	1.387(4)
C(8)-H(8)	0.9500
C(9)-C(10)	1.381(5)
C(9)-H(9)	0.9500
C(10)-C(11)	1.377(5)
C(10)-H(10)	0.9500
C(11)-C(12)	1.386(4)
C(11)-H(11)	0.9500
C(12)-H(12)	0.9500
C(13)-C(14)	1.391(4)
C(13)-C(18)	1.394(4)
C(13)-P(1)	1.830(3)
C(14)-C(15)	1.384(4)
C(14)-H(14)	0.9500
C(15)-C(16)	1.372(5)
C(15)-H(15)	0.9500
C(16)-C(17)	1.379(5)
C(16)-H(16)	0.9500
C(17)-C(18)	1.387(5)
C(17)-H(17)	0.9500
C(18)-H(18)	0.9500
C(19)-C(24)	1.382(4)
C(19)-C(20)	1.391(4)
C(19)-P(2)	1.828(3)
C(20)-C(21)	1.382(4)
C(20)-H(20)	0.9500
C(21)-C(22)	1.371(4)
C(21)-H(21)	0.9500
C(22)-C(23)	1.370(5)
C(22)-H(22)	0.9500
C(23)-C(24)	1.392(4)
C(23)-H(23)	0.9500
C(24)-H(24)	0.9500
C(25)-C(26)	1.387(4)

C(25)-C(30)	1.394(4)
C(25)-P(2)	1.821(3)
C(26)-C(27)	1.387(4)
C(26)-H(26)	0.9500
C(27)-C(28)	1.364(5)
C(27)-H(27)	0.9500
C(28)-C(29)	1.375(5)
C(28)-H(28)	0.9500
C(29)-C(30)	1.386(4)
C(29)-H(29)	0.9500
C(30)-H(30)	0.9500
C(31)-C(32)	1.383(4)
C(31)-C(36)	1.388(4)
C(31)-P(2)	1.820(3)
C(32)-C(33)	1.387(5)
C(32)-H(32)	0.9500
C(33)-C(34)	1.360(5)
C(33)-H(33)	0.9500
C(34)-C(35)	1.374(5)
C(34)-H(34)	0.9500
C(35)-C(36)	1.387(4)
C(35)-H(35)	0.9500
C(36)-H(36)	0.9500
O(1)-Si(1)	1.541(3)
O(1)-Pd(1)	2.053(3)
Si(1)-C(37)	1.871(4)
Si(1)-C(46)	1.878(3)
Si(1)-C(45)	1.885(4)
C(37)-C(38)	1.328(5)
C(37)-H(37)	0.9500
C(38)-C(39)	1.464(4)
C(38)-H(38)	0.9500
C(39)-C(40)	1.3900
C(39)-C(44)	1.3900
C(40)-C(41)	1.3900
C(40)-H(40)	0.9500

C(41)-C(42)	1.3900
C(41)-H(41)	0.9500
C(42)-C(43)	1.3900
C(42)-H(42)	0.9500
C(43)-C(44)	1.3900
C(43)-H(43)	0.9500
C(44)-H(44)	0.9500
C(45)-H(45A)	0.9800
C(45)-H(45B)	0.9800
C(45)-H(45C)	0.9800
C(46)-H(46A)	0.9800
C(46)-H(46B)	0.9800
C(46)-H(46C)	0.9800
C(47)-C(48)	1.3900
C(47)-C(52)	1.3900
C(47)-Pd(1)	1.9997(17)
C(48)-C(49)	1.3900
C(48)-C(53)	1.481(6)
C(49)-C(50)	1.3900
C(49)-H(49)	0.9500
C(50)-C(51)	1.3900
C(50)-H(50)	0.9500
C(51)-C(52)	1.3900
C(51)-H(51)	0.9500
C(52)-H(52)	0.9500
C(53)-H(53A)	0.9800
C(53)-H(531i)	0.9800
C(53)-H(53C)	0.9800
P(1)-Pd(1)	2.3154(7)
P(2)-Pd(1)	2.3195(7)
Pd(1)-C(57)	2.002(5)
Pd(1)-O(2)	2.072(5)
C(54)-C(56)#1	1.369(5)
C(54)-C(55)	1.384(5)
C(54)-H(54)	0.9500
C(55)-C(56)	1.371(5)

C(55)-H(55)	0.9500
C(56)-C(54)#1	1.369(5)
C(56)-H(56)	0.9500
C(57)-C(58)	1.3900
C(57)-C(62)	1.3900
C(58)-C(59)	1.3900
C(58)-C(63)	1.481(8)
C(59)-C(60)	1.3900
C(59)-H(59)	0.9500
C(60)-C(61)	1.3900
C(60)-H(60)	0.9500
C(61)-C(62)	1.3900
C(61)-H(61)	0.9500
C(62)-H(62)	0.9500
C(63)-H(63A)	0.9800
C(63)-H(631i)	0.9800
C(63)-H(63C)	0.9800
O(2)-Si(2)	1.540(5)
Si(2)-C(64)	1.858(6)
Si(2)-C(73)	1.886(5)
Si(2)-C(72)	1.888(5)
C(64)-C(65)	1.309(6)
C(64)-H(64)	0.9500
C(65)-C(66)	1.467(6)
C(65)-H(65)	0.9500
C(66)-C(67)	1.3900
C(66)-C(71)	1.3900
C(67)-C(68)	1.3900
C(67)-H(67)	0.9500
C(68)-C(69)	1.3900
C(68)-H(68)	0.9500
C(69)-C(70)	1.3900
C(69)-H(69)	0.9500
C(70)-C(71)	1.3900
C(70)-H(70)	0.9500
C(71)-H(71)	0.9500

C(72)-H(72A)	0.9800
C(72)-H(730i)	0.9800
C(72)-H(72C)	0.9800
C(73)-H(73A)	0.9800
C(73)-H(731i)	0.9800
C(73)-H(73C)	0.9800

C(2)-C(1)-C(6)	119.0(3)
C(2)-C(1)-P(1)	121.8(2)
C(6)-C(1)-P(1)	119.2(2)
C(1)-C(2)-C(3)	120.4(3)
C(1)-C(2)-H(2)	119.8
C(3)-C(2)-H(2)	119.8
C(4)-C(3)-C(2)	119.9(3)
C(4)-C(3)-H(3)	120.0
C(2)-C(3)-H(3)	120.0
C(5)-C(4)-C(3)	120.1(3)
C(5)-C(4)-H(4)	120.0
C(3)-C(4)-H(4)	120.0
C(4)-C(5)-C(6)	120.5(3)
C(4)-C(5)-H(5)	119.7
C(6)-C(5)-H(5)	119.7
C(5)-C(6)-C(1)	120.0(3)
C(5)-C(6)-H(6)	120.0
C(1)-C(6)-H(6)	120.0
C(8)-C(7)-C(12)	119.1(3)
C(8)-C(7)-P(1)	117.4(2)
C(12)-C(7)-P(1)	123.5(2)
C(9)-C(8)-C(7)	120.3(3)
C(9)-C(8)-H(8)	119.8
C(7)-C(8)-H(8)	119.8
C(10)-C(9)-C(8)	120.1(3)
C(10)-C(9)-H(9)	120.0
C(8)-C(9)-H(9)	120.0
C(11)-C(10)-C(9)	120.1(3)
C(11)-C(10)-H(10)	120.0

C(9)-C(10)-H(10)	120.0
C(10)-C(11)-C(12)	120.1(3)
C(10)-C(11)-H(11)	119.9
C(12)-C(11)-H(11)	119.9
C(11)-C(12)-C(7)	120.3(3)
C(11)-C(12)-H(12)	119.8
C(7)-C(12)-H(12)	119.8
C(14)-C(13)-C(18)	119.3(3)
C(14)-C(13)-P(1)	120.1(2)
C(18)-C(13)-P(1)	120.5(2)
C(15)-C(14)-C(13)	120.2(3)
C(15)-C(14)-H(14)	119.9
C(13)-C(14)-H(14)	119.9
C(16)-C(15)-C(14)	120.2(3)
C(16)-C(15)-H(15)	119.9
C(14)-C(15)-H(15)	119.9
C(15)-C(16)-C(17)	120.3(3)
C(15)-C(16)-H(16)	119.9
C(17)-C(16)-H(16)	119.9
C(16)-C(17)-C(18)	120.2(3)
C(16)-C(17)-H(17)	119.9
C(18)-C(17)-H(17)	119.9
C(17)-C(18)-C(13)	119.8(3)
C(17)-C(18)-H(18)	120.1
C(13)-C(18)-H(18)	120.1
C(24)-C(19)-C(20)	118.0(3)
C(24)-C(19)-P(2)	123.8(2)
C(20)-C(19)-P(2)	118.1(2)
C(21)-C(20)-C(19)	121.0(3)
C(21)-C(20)-H(20)	119.5
C(19)-C(20)-H(20)	119.5
C(22)-C(21)-C(20)	120.4(3)
C(22)-C(21)-H(21)	119.8
C(20)-C(21)-H(21)	119.8
C(21)-C(22)-C(23)	119.4(3)
C(21)-C(22)-H(22)	120.3

C(23)-C(22)-H(22)	120.3
C(22)-C(23)-C(24)	120.7(3)
C(22)-C(23)-H(23)	119.7
C(24)-C(23)-H(23)	119.7
C(19)-C(24)-C(23)	120.5(3)
C(19)-C(24)-H(24)	119.8
C(23)-C(24)-H(24)	119.8
C(26)-C(25)-C(30)	119.0(3)
C(26)-C(25)-P(2)	122.8(2)
C(30)-C(25)-P(2)	118.1(2)
C(25)-C(26)-C(27)	120.0(3)
C(25)-C(26)-H(26)	120.0
C(27)-C(26)-H(26)	120.0
C(28)-C(27)-C(26)	120.5(3)
C(28)-C(27)-H(27)	119.8
C(26)-C(27)-H(27)	119.8
C(27)-C(28)-C(29)	120.3(3)
C(27)-C(28)-H(28)	119.8
C(29)-C(28)-H(28)	119.9
C(28)-C(29)-C(30)	120.0(3)
C(28)-C(29)-H(29)	120.0
C(30)-C(29)-H(29)	120.0
C(29)-C(30)-C(25)	120.1(3)
C(29)-C(30)-H(30)	119.9
C(25)-C(30)-H(30)	119.9
C(32)-C(31)-C(36)	119.4(3)
C(32)-C(31)-P(2)	118.4(2)
C(36)-C(31)-P(2)	122.2(2)
C(31)-C(32)-C(33)	120.0(3)
C(31)-C(32)-H(32)	120.0
C(33)-C(32)-H(32)	120.0
C(34)-C(33)-C(32)	120.5(3)
C(34)-C(33)-H(33)	119.8
C(32)-C(33)-H(33)	119.8
C(33)-C(34)-C(35)	120.2(3)
C(33)-C(34)-H(34)	119.9

C(35)-C(34)-H(34)	119.9
C(34)-C(35)-C(36)	120.2(3)
C(34)-C(35)-H(35)	119.9
C(36)-C(35)-H(35)	119.9
C(35)-C(36)-C(31)	119.8(3)
C(35)-C(36)-H(36)	120.1
C(31)-C(36)-H(36)	120.1
Si(1)-O(1)-Pd(1)	160.2(3)
O(1)-Si(1)-C(37)	115.32(18)
O(1)-Si(1)-C(46)	111.1(2)
C(37)-Si(1)-C(46)	106.49(18)
O(1)-Si(1)-C(45)	113.78(19)
C(37)-Si(1)-C(45)	102.34(19)
C(46)-Si(1)-C(45)	107.0(2)
C(38)-C(37)-Si(1)	127.0(3)
C(38)-C(37)-H(37)	116.5
Si(1)-C(37)-H(37)	116.5
C(37)-C(38)-C(39)	131.9(3)
C(37)-C(38)-H(38)	114.0
C(39)-C(38)-H(38)	114.0
C(40)-C(39)-C(44)	120.0
C(40)-C(39)-C(38)	119.1(2)
C(44)-C(39)-C(38)	120.7(2)
C(41)-C(40)-C(39)	120.0
C(41)-C(40)-H(40)	120.0
C(39)-C(40)-H(40)	120.0
C(40)-C(41)-C(42)	120.0
C(40)-C(41)-H(41)	120.0
C(42)-C(41)-H(41)	120.0
C(41)-C(42)-C(43)	120.0
C(41)-C(42)-H(42)	120.0
C(43)-C(42)-H(42)	120.0
C(44)-C(43)-C(42)	120.0
C(44)-C(43)-H(43)	120.0
C(42)-C(43)-H(43)	120.0
C(43)-C(44)-C(39)	120.0

C(43)-C(44)-H(44)	120.0
C(39)-C(44)-H(44)	120.0
Si(1)-C(45)-H(45A)	109.5
Si(1)-C(45)-H(45B)	109.5
H(45A)-C(45)-H(45B)	109.5
Si(1)-C(45)-H(45C)	109.5
H(45A)-C(45)-H(45C)	109.5
H(45B)-C(45)-H(45C)	109.5
Si(1)-C(46)-H(46A)	109.5
Si(1)-C(46)-H(46B)	109.5
H(46A)-C(46)-H(46B)	109.5
Si(1)-C(46)-H(46C)	109.5
H(46A)-C(46)-H(46C)	109.5
H(46B)-C(46)-H(46C)	109.5
C(48)-C(47)-C(52)	120.0
C(48)-C(47)-Pd(1)	124.46(14)
C(52)-C(47)-Pd(1)	115.54(14)
C(47)-C(48)-C(49)	120.0
C(47)-C(48)-C(53)	121.0(2)
C(49)-C(48)-C(53)	119.0(2)
C(48)-C(49)-C(50)	120.0
C(48)-C(49)-H(49)	120.0
C(50)-C(49)-H(49)	120.0
C(51)-C(50)-C(49)	120.0
C(51)-C(50)-H(50)	120.0
C(49)-C(50)-H(50)	120.0
C(52)-C(51)-C(50)	120.0
C(52)-C(51)-H(51)	120.0
C(50)-C(51)-H(51)	120.0
C(51)-C(52)-C(47)	120.0
C(51)-C(52)-H(52)	120.0
C(47)-C(52)-H(52)	120.0
C(48)-C(53)-H(53A)	109.5
C(48)-C(53)-H(531i)	109.5
H(53A)-C(53)-H(531i)	109.5
C(48)-C(53)-H(53C)	109.5

H(53A)-C(53)-H(53C)	109.5
H(531i)-C(53)-H(53C)	109.5
C(1)-P(1)-C(7)	105.46(12)
C(1)-P(1)-C(13)	103.80(13)
C(7)-P(1)-C(13)	104.82(13)
C(1)-P(1)-Pd(1)	113.23(9)
C(7)-P(1)-Pd(1)	110.79(9)
C(13)-P(1)-Pd(1)	117.68(9)
C(31)-P(2)-C(25)	105.26(13)
C(31)-P(2)-C(19)	103.00(12)
C(25)-P(2)-C(19)	105.02(12)
C(31)-P(2)-Pd(1)	112.32(9)
C(25)-P(2)-Pd(1)	110.67(9)
C(19)-P(2)-Pd(1)	119.36(9)
C(47)-Pd(1)-O(1)	173.09(14)
C(57)-Pd(1)-O(2)	170.2(5)
C(47)-Pd(1)-P(1)	88.11(10)
C(57)-Pd(1)-P(1)	86.8(5)
O(1)-Pd(1)-P(1)	93.75(9)
O(2)-Pd(1)-P(1)	89.4(4)
C(47)-Pd(1)-P(2)	89.36(10)
C(57)-Pd(1)-P(2)	90.3(5)
O(1)-Pd(1)-P(2)	88.98(9)
O(2)-Pd(1)-P(2)	93.6(4)
P(1)-Pd(1)-P(2)	176.86(3)
C(56)#1-C(54)-C(55)	120.1(4)
C(56)#1-C(54)-H(54)	119.9
C(55)-C(54)-H(54)	119.9
C(56)-C(55)-C(54)	119.8(4)
C(56)-C(55)-H(55)	120.1
C(54)-C(55)-H(55)	120.1
C(54)#1-C(56)-C(55)	120.1(4)
C(54)#1-C(56)-H(56)	119.9
C(55)-C(56)-H(56)	119.9
C(58)-C(57)-C(62)	120.0
C(58)-C(57)-Pd(1)	123.6(6)

C(62)-C(57)-Pd(1)	116.4(6)
C(57)-C(58)-C(59)	120.0
C(57)-C(58)-C(63)	120.5(4)
C(59)-C(58)-C(63)	119.5(4)
C(58)-C(59)-C(60)	120.0
C(58)-C(59)-H(59)	120.0
C(60)-C(59)-H(59)	120.0
C(61)-C(60)-C(59)	120.0
C(61)-C(60)-H(60)	120.0
C(59)-C(60)-H(60)	120.0
C(60)-C(61)-C(62)	120.0
C(60)-C(61)-H(61)	120.0
C(62)-C(61)-H(61)	120.0
C(61)-C(62)-C(57)	120.0
C(61)-C(62)-H(62)	120.0
C(57)-C(62)-H(62)	120.0
C(58)-C(63)-H(63A)	109.5
C(58)-C(63)-H(631i)	109.5
H(63A)-C(63)-H(631i)	109.5
C(58)-C(63)-H(63C)	109.5
H(63A)-C(63)-H(63C)	109.5
H(631i)-C(63)-H(63C)	109.5
Si(2)-O(2)-Pd(1)	161.4(7)
O(2)-Si(2)-C(64)	118.1(5)
O(2)-Si(2)-C(73)	113.0(5)
C(64)-Si(2)-C(73)	103.2(4)
O(2)-Si(2)-C(72)	111.9(5)
C(64)-Si(2)-C(72)	103.2(4)
C(73)-Si(2)-C(72)	106.2(5)
C(65)-C(64)-Si(2)	135.8(8)
C(65)-C(64)-H(64)	112.1
Si(2)-C(64)-H(64)	112.1
C(64)-C(65)-C(66)	131.2(8)
C(64)-C(65)-H(65)	114.4
C(66)-C(65)-H(65)	114.4
C(67)-C(66)-C(71)	120.0

C(67)-C(66)-C(65)	119.4(4)
C(71)-C(66)-C(65)	119.0(5)
C(68)-C(67)-C(66)	120.0
C(68)-C(67)-H(67)	120.0
C(66)-C(67)-H(67)	120.0
C(67)-C(68)-C(69)	120.0
C(67)-C(68)-H(68)	120.0
C(69)-C(68)-H(68)	120.0
C(68)-C(69)-C(70)	120.0
C(68)-C(69)-H(69)	120.0
C(70)-C(69)-H(69)	120.0
C(71)-C(70)-C(69)	120.0
C(71)-C(70)-H(70)	120.0
C(69)-C(70)-H(70)	120.0
C(70)-C(71)-C(66)	120.0
C(70)-C(71)-H(71)	120.0
C(66)-C(71)-H(71)	120.0
Si(2)-C(72)-H(72A)	109.5
Si(2)-C(72)-H(730i)	109.5
H(72A)-C(72)-H(730i)	109.5
Si(2)-C(72)-H(72C)	109.5
H(72A)-C(72)-H(72C)	109.5
H(730i)-C(72)-H(72C)	109.5
Si(2)-C(73)-H(73A)	109.5
Si(2)-C(73)-H(731i)	109.5
H(73A)-C(73)-H(731i)	109.5
Si(2)-C(73)-H(73C)	109.5
H(73A)-C(73)-H(73C)	109.5
H(731i)-C(73)-H(73C)	109.5

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,-y+2,-z

Table 7. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for ga45xasd. The anisotropic displacement factor exponent takes the form: $-2p^2[\ h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

Atom	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	32(1)	29(1)	29(2)	2(1)	10(1)	3(1)
C(2)	41(2)	34(2)	56(2)	9(2)	15(2)	5(1)
C(3)	55(2)	40(2)	70(3)	21(2)	20(2)	17(2)
C(4)	42(2)	61(2)	50(2)	10(2)	14(2)	21(2)
C(5)	34(2)	55(2)	57(2)	-2(2)	18(2)	2(2)
C(6)	36(2)	36(2)	47(2)	2(1)	17(1)	0(1)
C(7)	27(1)	26(1)	31(2)	2(1)	9(1)	-1(1)
C(8)	40(2)	32(2)	36(2)	-4(1)	13(1)	-4(1)
C(9)	50(2)	47(2)	43(2)	0(2)	25(2)	1(2)
C(10)	38(2)	49(2)	57(2)	9(2)	24(2)	-3(2)
C(11)	38(2)	35(2)	50(2)	2(1)	14(2)	-10(1)
C(12)	40(2)	30(2)	37(2)	-2(1)	13(1)	-5(1)
C(13)	41(2)	25(1)	29(2)	0(1)	11(1)	1(1)
C(14)	42(2)	35(2)	35(2)	-2(1)	10(1)	5(1)
C(15)	51(2)	51(2)	39(2)	-3(2)	2(2)	9(2)
C(16)	75(3)	75(3)	32(2)	-5(2)	12(2)	13(2)
C(17)	72(3)	76(3)	43(2)	-5(2)	30(2)	9(2)
C(18)	45(2)	49(2)	38(2)	0(2)	18(2)	5(2)
C(19)	28(1)	22(1)	29(1)	-3(1)	9(1)	-2(1)
C(20)	31(2)	30(1)	40(2)	4(1)	11(1)	-2(1)
C(21)	34(2)	36(2)	43(2)	4(1)	5(1)	3(1)
C(22)	51(2)	39(2)	38(2)	13(1)	12(2)	6(2)
C(23)	48(2)	50(2)	51(2)	20(2)	21(2)	-4(2)
C(24)	31(2)	41(2)	42(2)	8(1)	12(1)	-2(1)
C(25)	26(1)	24(1)	33(2)	4(1)	8(1)	-2(1)
C(26)	33(2)	33(2)	34(2)	-1(1)	8(1)	-4(1)
C(27)	38(2)	44(2)	42(2)	-4(2)	0(1)	-8(1)
C(28)	25(2)	48(2)	61(2)	6(2)	3(2)	-7(1)
C(29)	27(2)	50(2)	63(2)	5(2)	18(2)	1(1)
C(30)	31(2)	40(2)	42(2)	-4(1)	13(1)	1(1)
C(31)	26(1)	35(2)	31(2)	1(1)	11(1)	-2(1)

C(32)	51(2)	43(2)	55(2)	4(2)	29(2)	-3(2)
C(33)	71(3)	72(3)	65(3)	14(2)	45(2)	0(2)
C(34)	51(2)	87(3)	44(2)	3(2)	28(2)	14(2)
C(35)	51(2)	58(2)	44(2)	-2(2)	19(2)	18(2)
C(36)	42(2)	37(2)	37(2)	1(1)	17(1)	6(1)
O(1)	54(2)	35(2)	60(2)	-4(1)	-7(2)	1(2)
Si(1)	51(1)	31(1)	34(1)	-3(1)	10(1)	-5(1)
C(37)	34(2)	32(2)	29(2)	-7(1)	2(2)	-10(1)
C(38)	34(2)	31(2)	43(2)	2(2)	3(2)	0(1)
C(39)	33(2)	34(2)	49(2)	0(2)	11(2)	2(1)
C(40)	52(2)	30(2)	56(2)	-5(2)	25(2)	-6(2)
C(41)	62(2)	39(2)	60(3)	3(2)	26(2)	-4(2)
C(42)	57(3)	40(2)	70(3)	9(2)	20(2)	-4(2)
C(43)	60(2)	39(3)	78(3)	19(2)	9(2)	-5(2)
C(44)	48(2)	40(2)	63(3)	23(2)	0(2)	5(2)
C(45)	77(3)	33(3)	57(3)	-3(2)	20(2)	0(2)
C(46)	47(2)	51(3)	48(3)	18(2)	2(2)	-5(2)
C(47)	39(2)	20(2)	43(2)	-2(2)	-2(2)	2(2)
C(48)	65(2)	25(2)	46(2)	-2(2)	-6(2)	2(2)
C(49)	80(3)	38(2)	66(3)	-9(2)	-25(2)	10(2)
C(50)	64(3)	44(2)	96(3)	-17(2)	-34(3)	12(2)
C(51)	38(2)	44(2)	111(3)	-20(2)	-6(2)	4(2)
C(52)	33(2)	30(2)	83(3)	-13(2)	2(2)	-1(2)
C(53)	94(3)	42(2)	43(2)	4(2)	18(2)	-5(2)
P(1)	29(1)	23(1)	27(1)	1(1)	9(1)	0(1)
P(2)	23(1)	23(1)	28(1)	1(1)	8(1)	-2(1)
Pd(1)	25(1)	22(1)	27(1)	1(1)	6(1)	-1(1)
C(54)	38(2)	53(2)	78(3)	-1(2)	20(2)	1(2)
C(55)	41(2)	65(2)	59(2)	-5(2)	18(2)	-9(2)
C(56)	40(2)	51(2)	74(3)	-14(2)	27(2)	-7(2)
C(57)	45(4)	15(5)	41(5)	-5(5)	-4(4)	-3(5)
C(58)	41(4)	25(4)	68(4)	-8(4)	-9(4)	3(4)
C(59)	54(5)	36(4)	79(4)	-10(5)	-24(4)	6(5)
C(60)	72(5)	37(5)	69(5)	-8(5)	-28(5)	3(5)
C(61)	79(4)	32(4)	46(4)	2(4)	-10(4)	-3(5)
C(62)	67(5)	27(5)	40(5)	2(5)	-1(4)	-9(5)

C(63)	28(5)	30(5)	88(5)	-15(5)	2(5)	4(5)
O(2)	42(5)	24(5)	63(5)	5(4)	29(4)	-13(4)
Si(2)	51(1)	31(1)	34(1)	-3(1)	10(1)	-5(1)
C(64)	52(6)	43(5)	51(6)	-4(5)	5(5)	-7(5)
C(65)	46(5)	41(4)	51(5)	-2(4)	7(4)	-3(4)
C(66)	48(4)	37(4)	54(4)	1(4)	11(4)	1(4)
C(67)	52(5)	43(5)	63(5)	9(4)	4(5)	-2(5)
C(68)	58(5)	44(5)	71(5)	12(4)	7(4)	-1(4)
C(69)	60(5)	42(4)	67(5)	9(4)	17(4)	-2(4)
C(70)	59(5)	38(4)	61(5)	6(4)	23(4)	-4(4)
C(71)	58(5)	33(5)	59(5)	-1(4)	22(5)	-5(5)
C(72)	85(9)	38(8)	62(8)	-11(7)	19(7)	-1(8)
C(73)	43(6)	51(9)	42(9)	26(7)	-7(6)	9(7)

Table 8. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for ga45xasd.

Atom	x	y	z	U(eq)
H(2)	8428	1975	432	53
H(3)	9534	1050	862	67
H(4)	10592	2054	1052	62
H(5)	10548	3951	780	58
H(6)	9449	4896	361	47
H(8)	7582	4665	1146	44
H(9)	6827	3813	1620	53
H(10)	6141	2240	1113	55
H(11)	6259	1449	169	50
H(12)	7032	2269	-296	43
H(14)	6568	4147	-1004	46
H(15)	6129	3772	-2144	61
H(16)	6919	3390	-2685	75
H(17)	8151	3329	-2089	73
H(18)	8601	3639	-938	52

H(20)	6729	8790	-257	41
H(21)	6187	9955	-1171	48
H(22)	6884	10995	-1626	53
H(23)	8128	10888	-1150	59
H(24)	8682	9704	-240	46
H(26)	8998	9319	1759	41
H(27)	10214	9778	2260	54
H(28)	11006	9354	1735	58
H(29)	10609	8405	721	55
H(30)	9408	7847	236	45
H(32)	7615	6891	1389	56
H(33)	7065	7343	2146	76
H(34)	6822	9203	2312	70
H(35)	7130	10646	1734	61
H(36)	7666	10218	962	46
H(37)	8922	3726	1848	41
H(38)	10227	3945	2862	47
H(40)	8898	1889	2137	54
H(41)	8708	224	2639	63
H(42)	9413	-167	3751	68
H(43)	10309	1107	4360	76
H(44)	10499	2772	3858	67
H(45A)	9201	7268	2452	85
H(45B)	9523	6269	2979	85
H(45C)	8693	6252	2503	85
H(46A)	10471	6667	1960	79
H(46B)	10562	5368	1794	79
H(46C)	10673	5737	2540	79
H(49)	6377	7065	-2025	91
H(50)	5339	6908	-1766	103
H(51)	5434	6460	-679	88
H(52)	6566	6169	149	64
H(53A)	8167	6684	-871	92
H(531i)	7756	7579	-1441	92
H(53C)	7715	6255	-1611	92
H(54)	4243	11526	-447	85

H(55)	4541	10278	-1148	66
H(56)	5299	8757	-696	80
H(59)	5588	6743	-1407	84
H(60)	5986	7057	-2288	89
H(61)	7216	7000	-2100	74
H(62)	8048	6630	-1030	61
H(63A)	5795	6312	-313	81
H(631i)	6521	6838	208	81
H(63C)	6476	5514	37	81
H(64)	9883	4528	2882	63
H(65)	9046	3206	1876	59
H(67)	10304	3120	3543	69
H(68)	10382	1691	4319	75
H(69)	9654	81	3995	70
H(70)	8847	-99	2896	63
H(71)	8769	1329	2119	60
H(72A)	9248	7581	2395	96
H(730i)	9602	6710	2995	96
H(72C)	8752	6691	2589	96
H(73A)	10248	6928	1770	77
H(731i)	10305	5668	1520	77
H(73C)	10635	5959	2298	77

(1) Sheldrick, G. M. SHELX-97, University of Gottingen, Gottingen, Germany, 1997.