Supporting information for

Construction of a Planar Tetrapalladium Cluster by the Reaction of Palladium(0) Bis(isocyanide) with Cyclic Tetrasilane

Yusuke Sunada*, Nobuhiro Taniyama, Kento Shimamoto, Soichiro Kyushin and Hideo Nagashima

Contents

Figure S1-1. ^{1}H NMR spectrum of solution of **4** in C_6D_6 at room temperature.

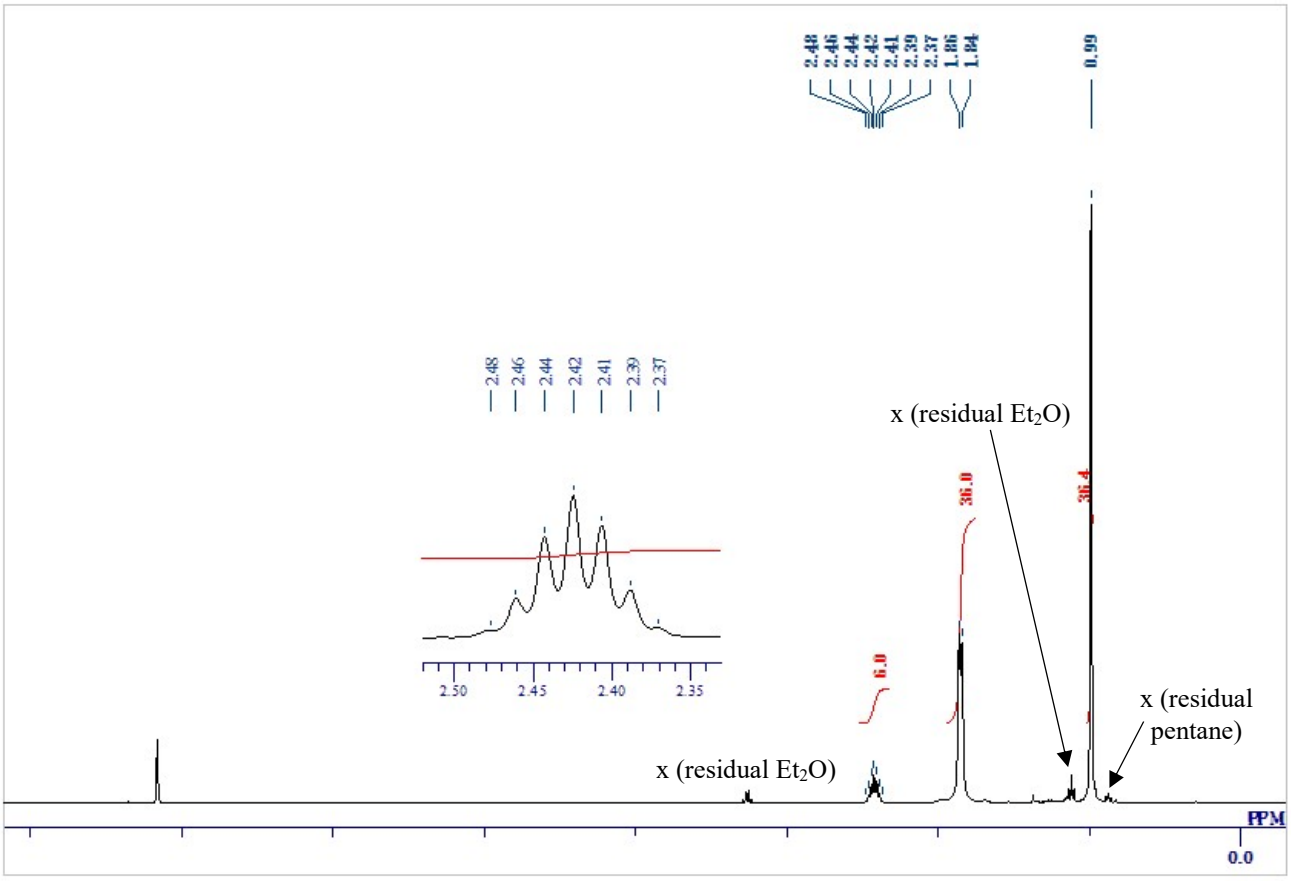


Figure S1-2. $^{13}C\{^{1}H\}$ NMR spectrum of solution of **4** in C_6D_6 at room temperature.

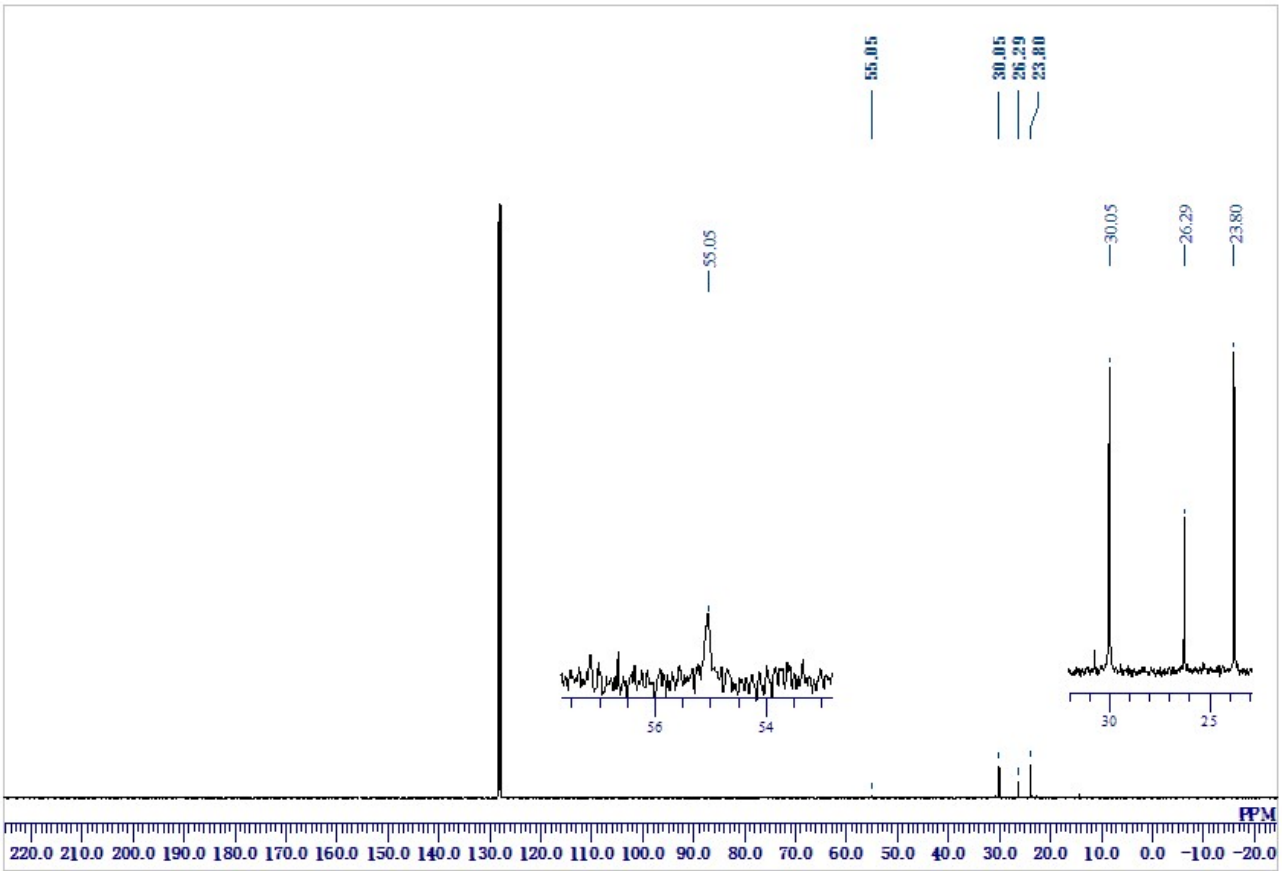


Figure S2-1. ^{1}H NMR spectrum of solution of **4** in toluene-d_8 at various temperatures.

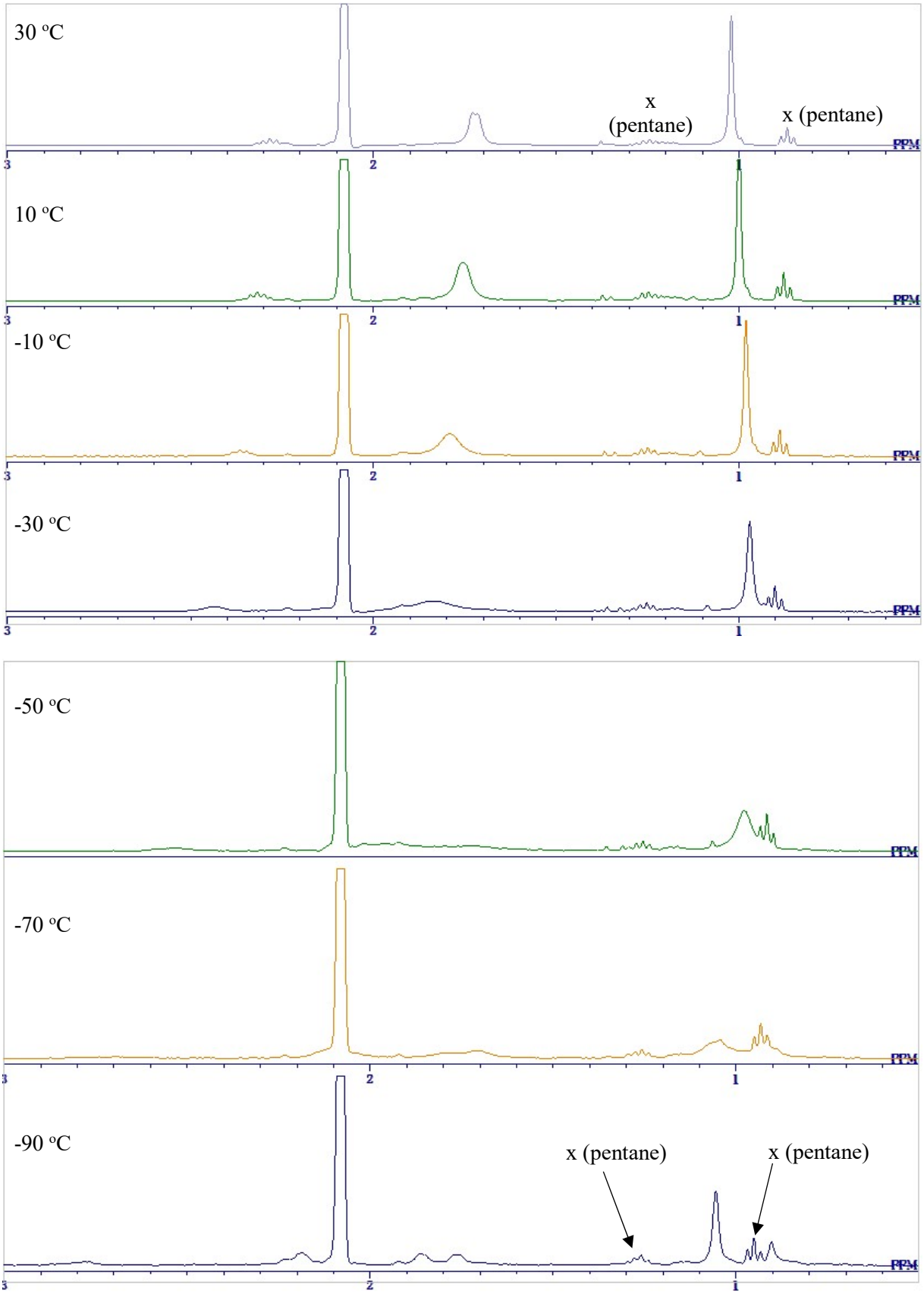


Figure S2-2. ^{1}H NMR spectrum of solution of **4** in toluene-d_8 at -90 °C.

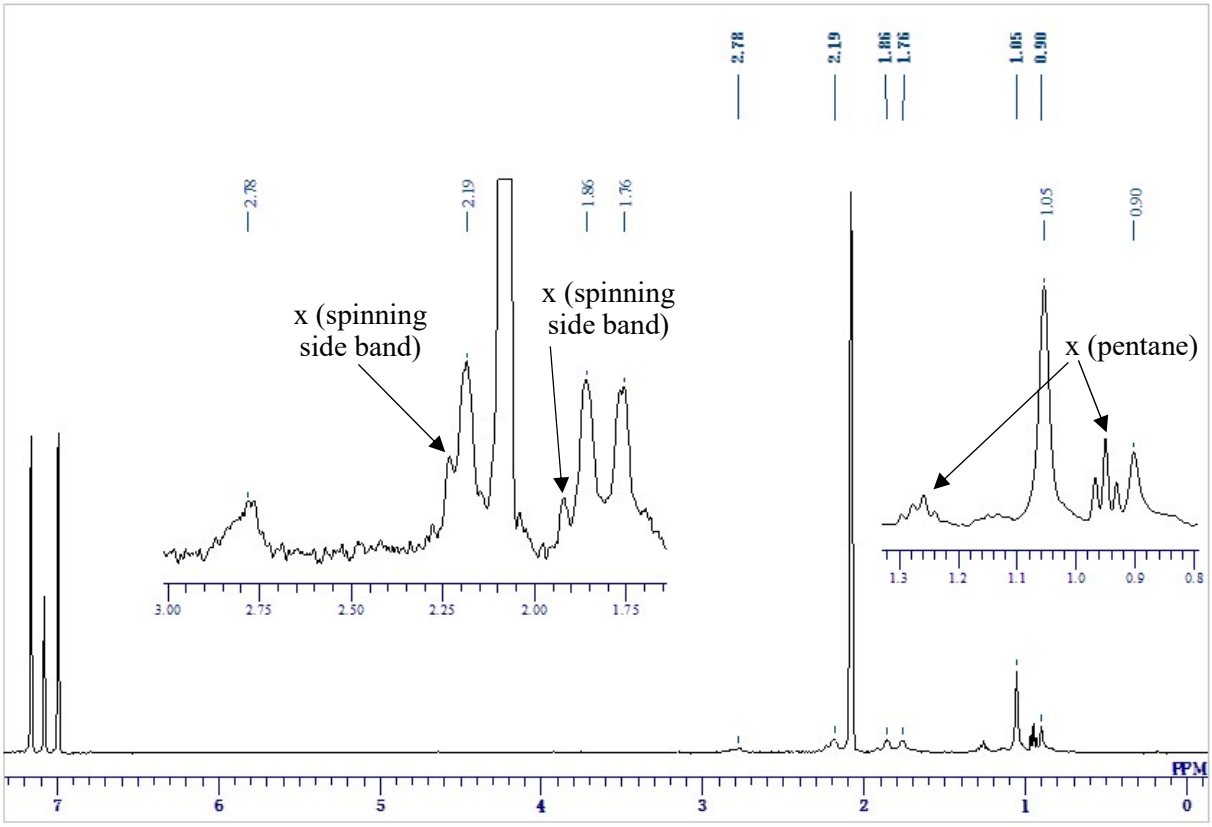


Figure S3-1. ^{1}H NMR spectrum of solution of **5** in C_6D_6 at room temperature.

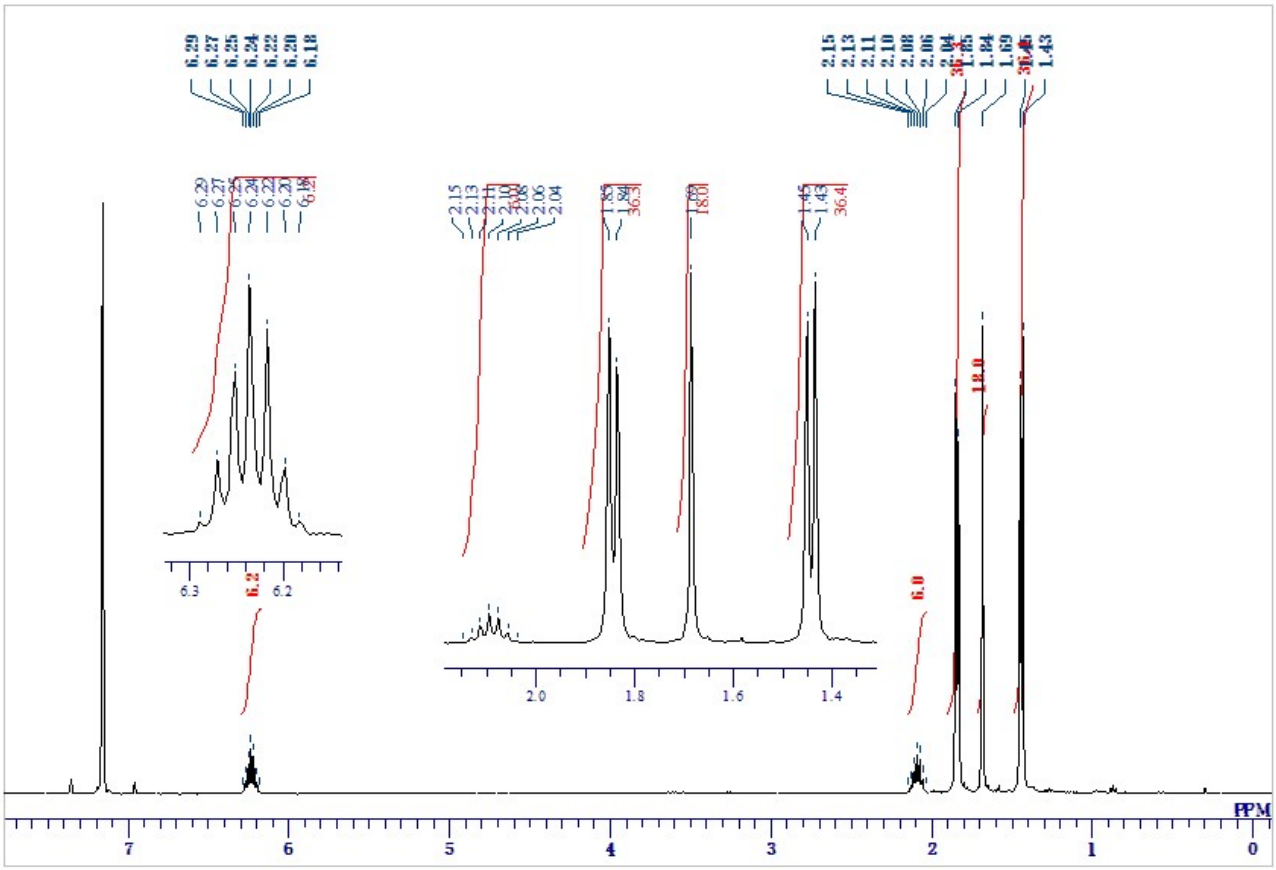


Figure S3-2. $^{13}C\{^{1}H\}$ NMR spectrum of solution of **5** in C_6D_6 at room temperature.

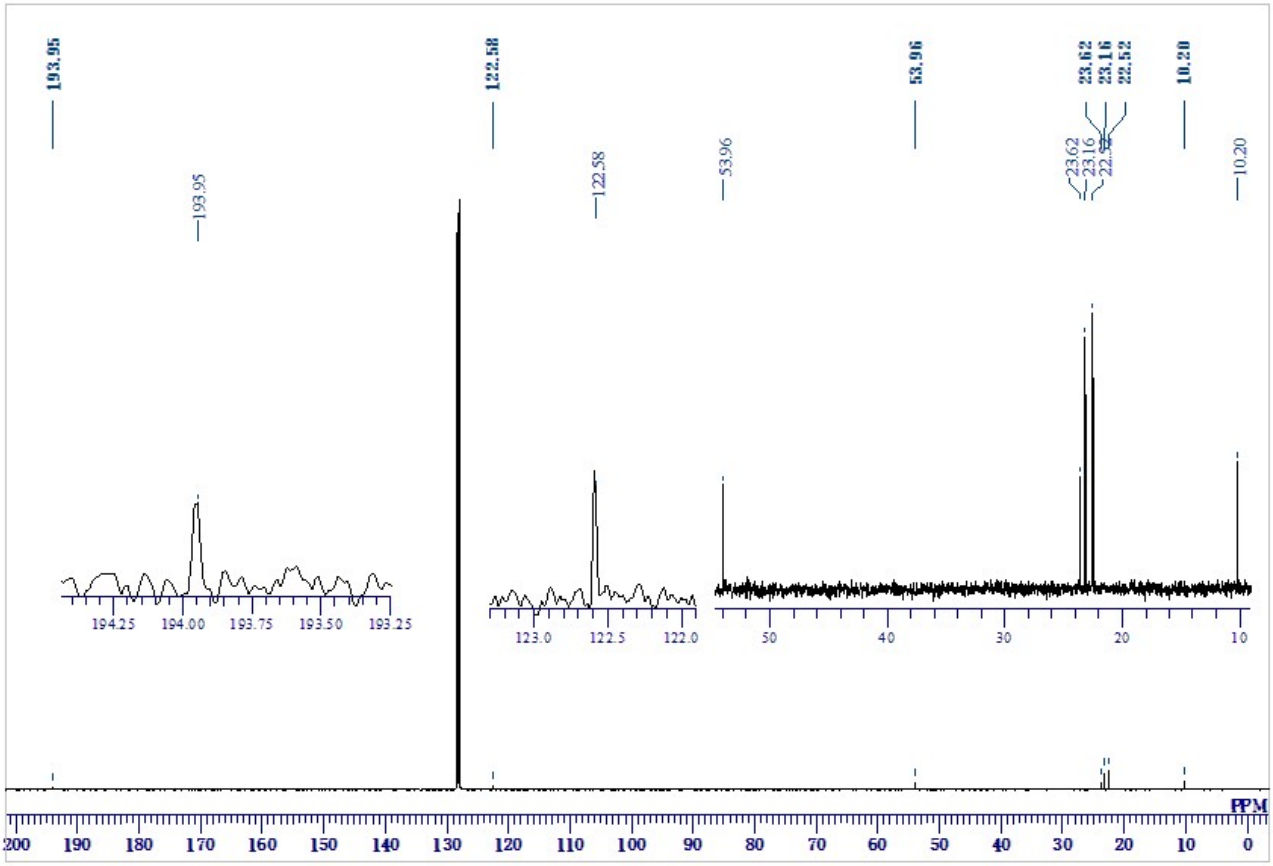


Figure S3-3. $^{29}Si\{^{1}H\}$ NMR spectrum of solution of **5** in C_6D_6 at room temperature.

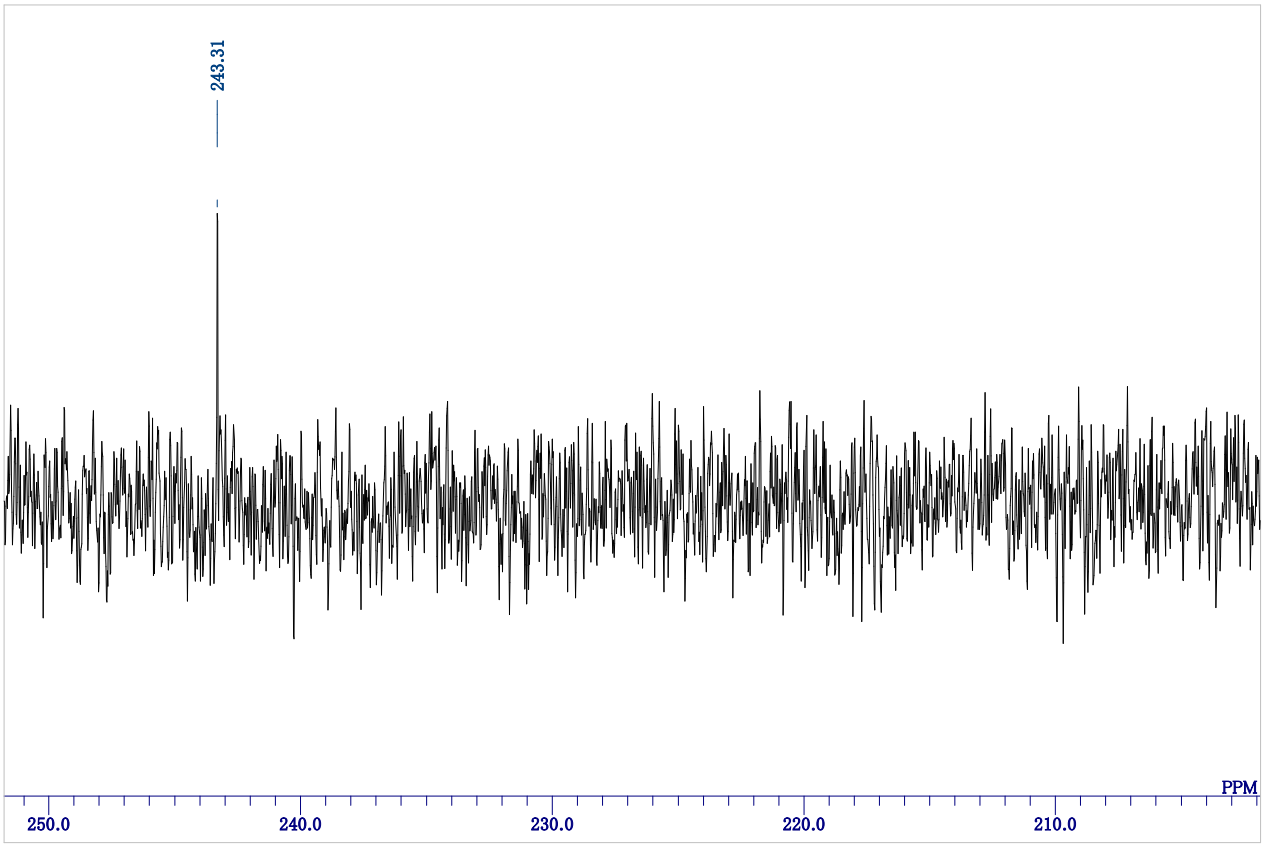


Figure S4-1. ^{1}H NMR spectrum of solution of **6** in C_6D_6 at room temperature.

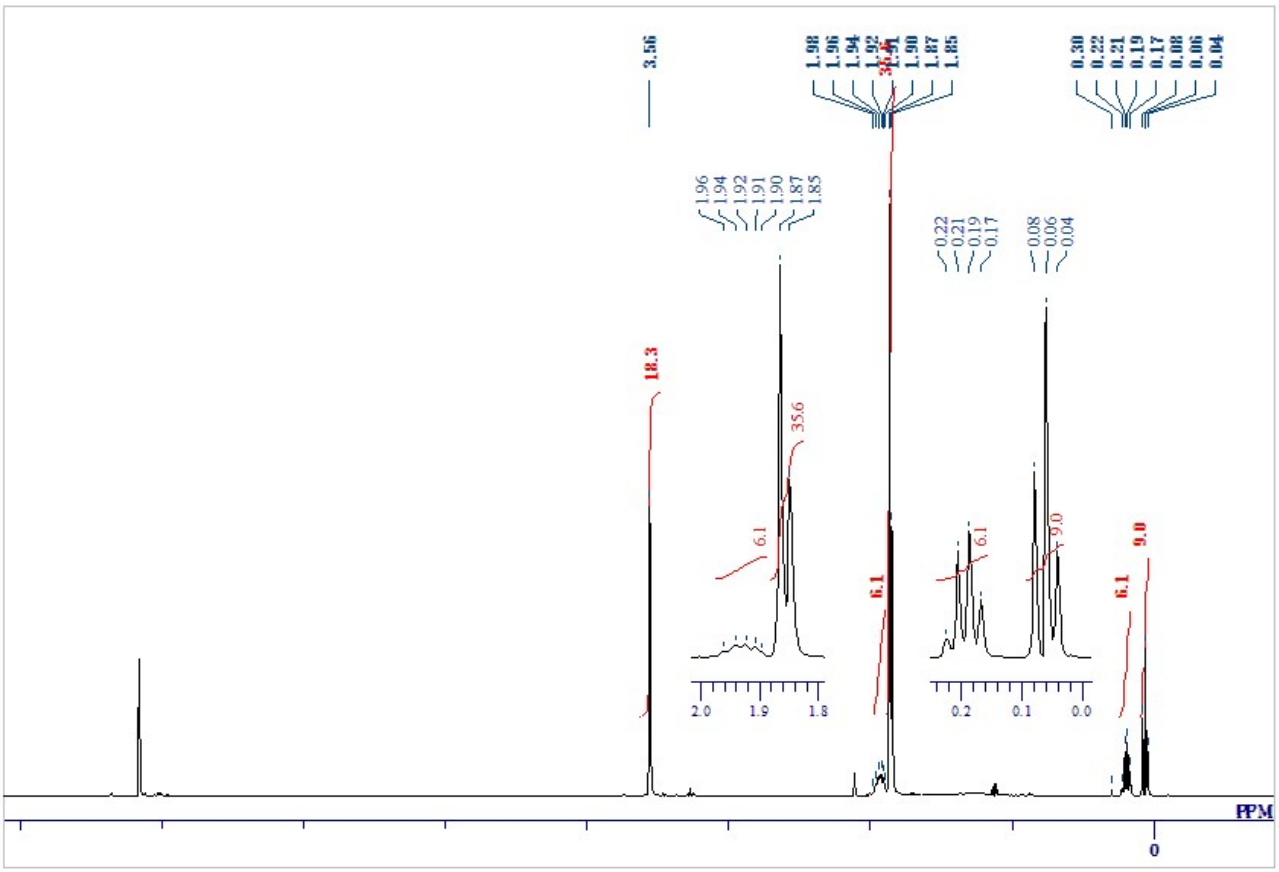


Figure S4-2. $^{13}C\{^{1}H\}$ NMR spectrum of solution of **6** in C_6D_6 at room temperature.

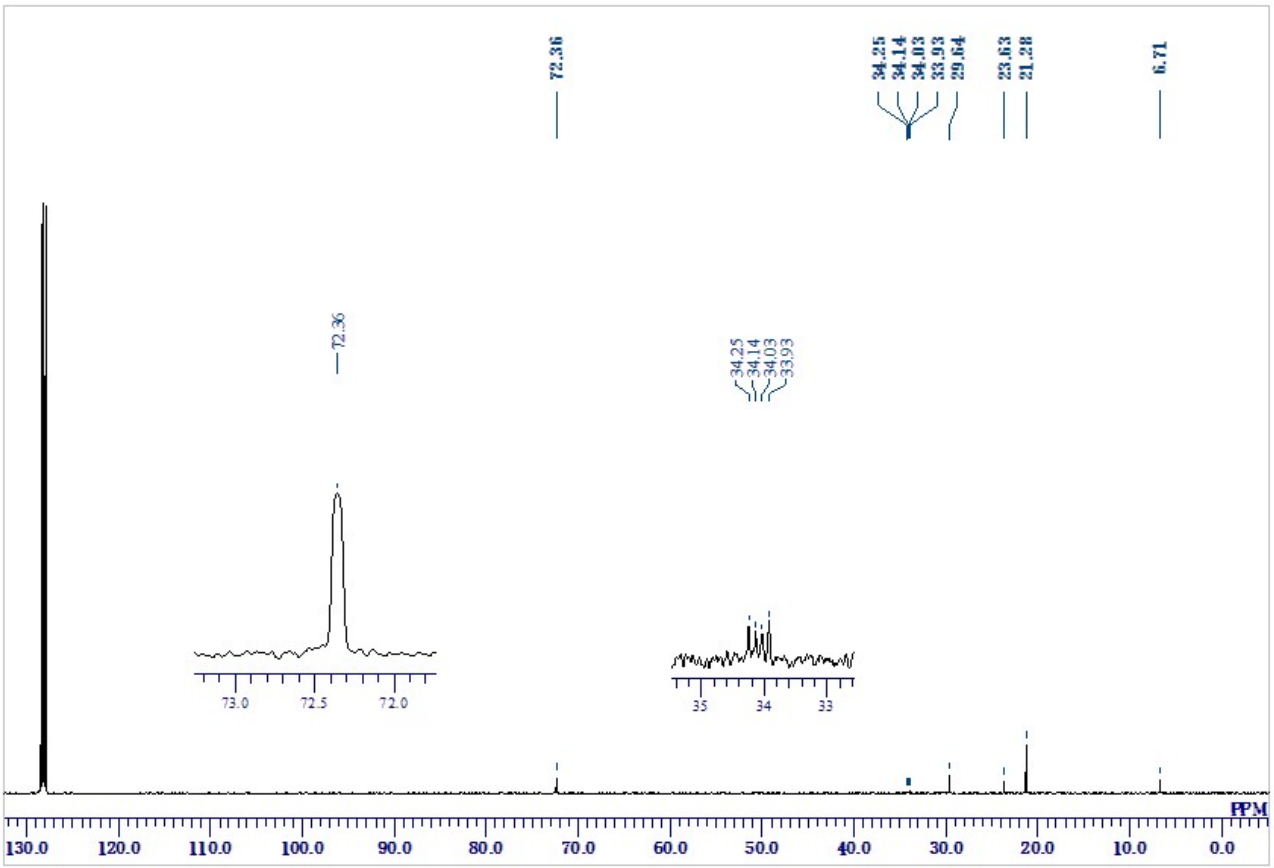


Figure S4-3. $^{31}P\{^{1}H\}$ NMR spectrum of solution of **6** in C_6D_6 at room temperature.

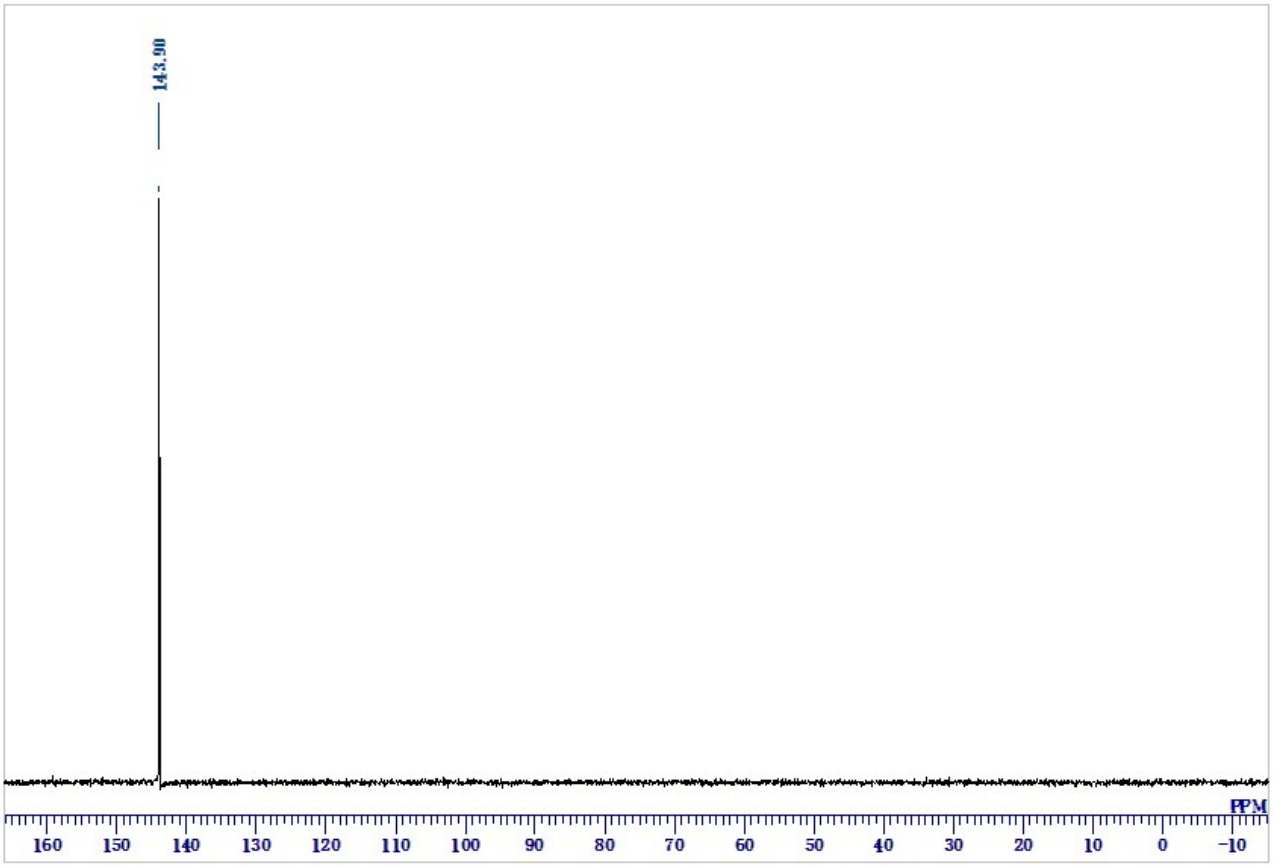


Figure S5-1. ^{1}H NMR spectrum of *in situ* generated Pd(trimethylolpropanephosphite)$_4$ in C_6D_6 at room temperature.

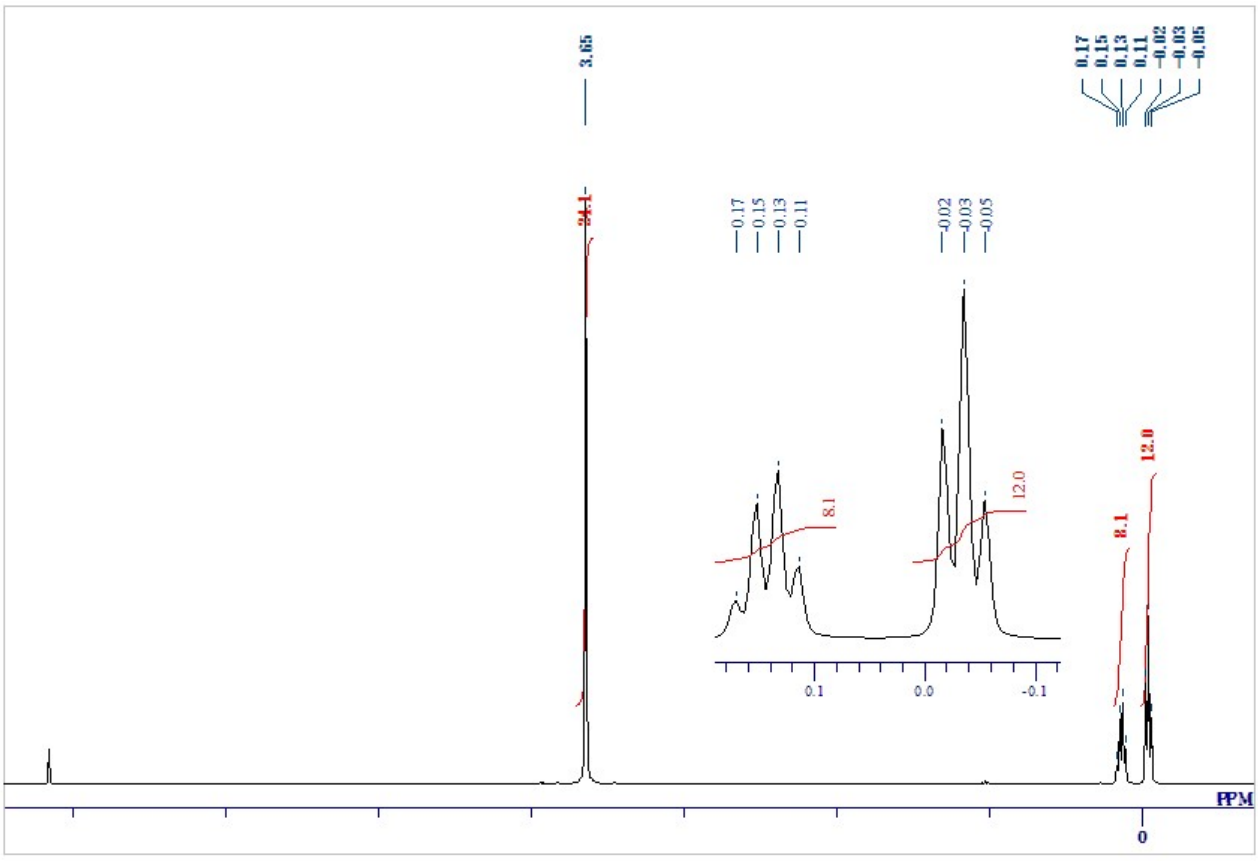


Figure S5-2. $^{31}P\{^{1}H\}$ NMR spectrum of *in situ* generated Pd(trimethylolpropanephosphite)$_4$ in C_6D_6 at room temperature.

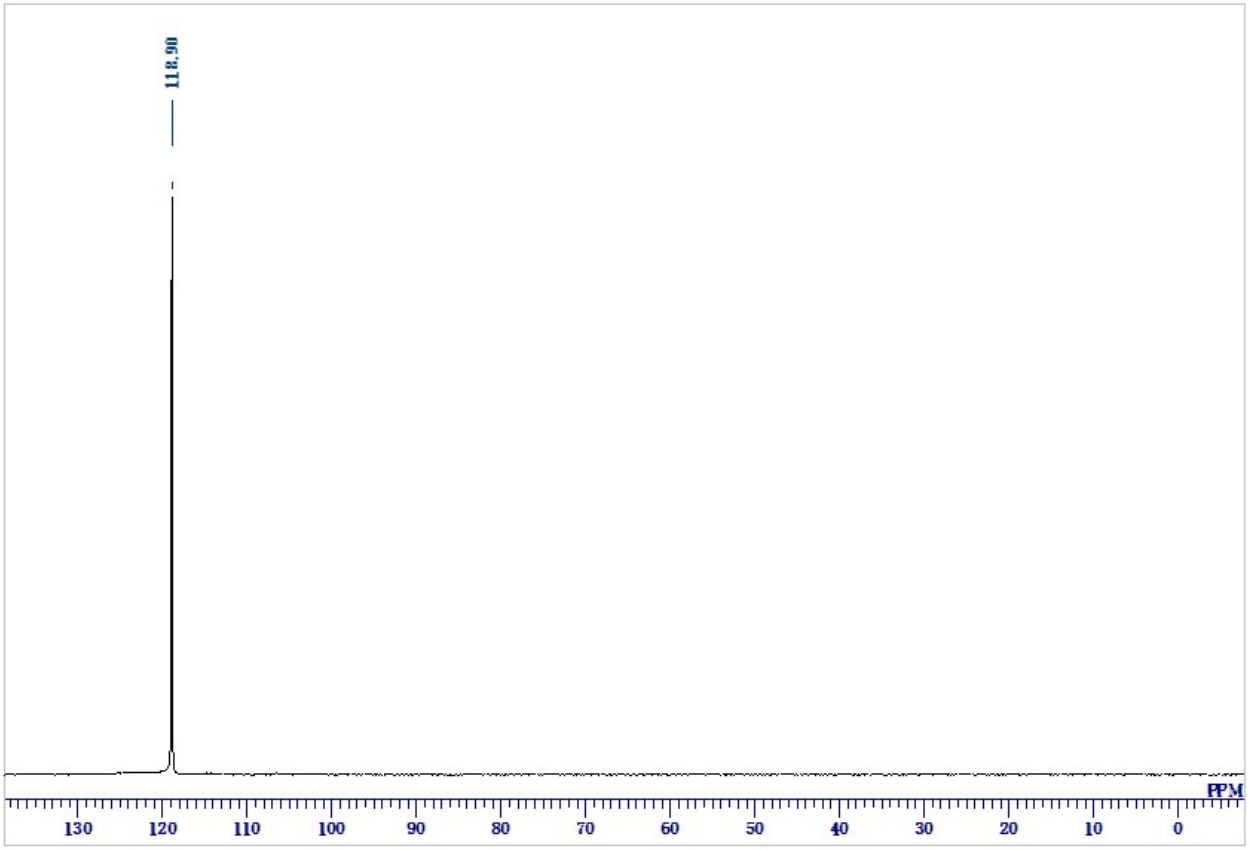
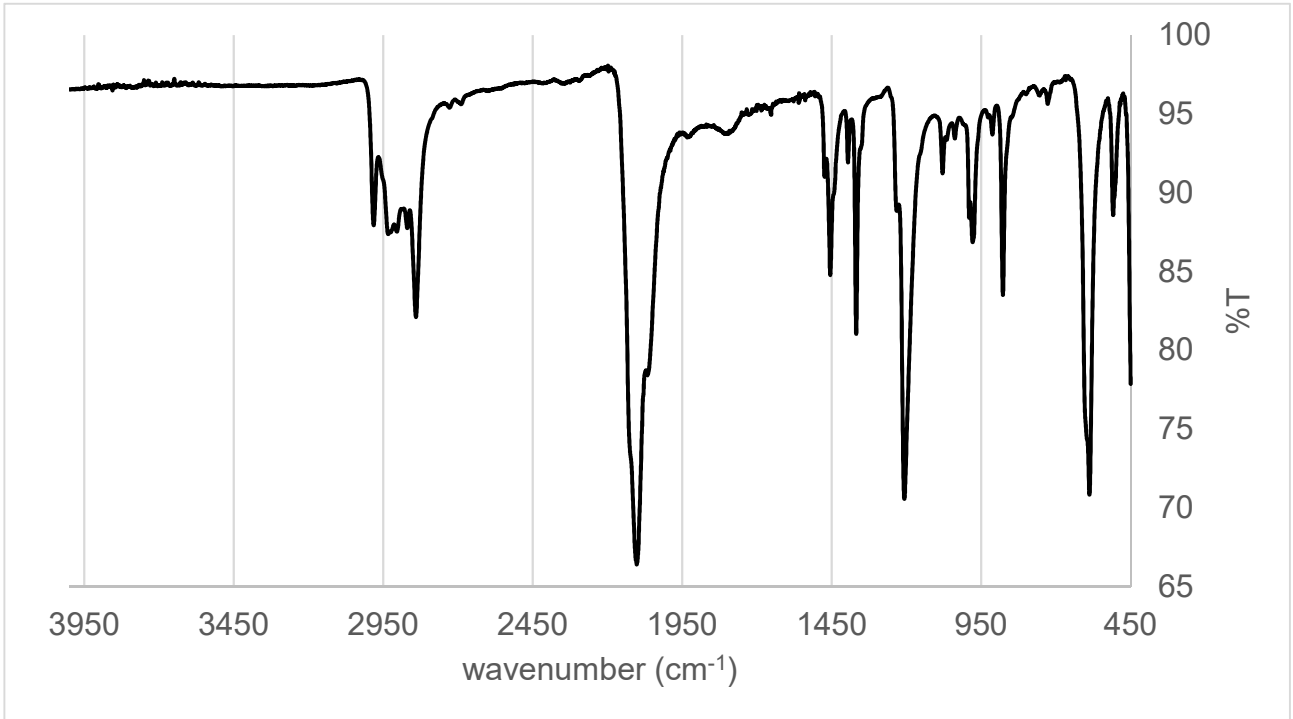


Figure S6. ATR-IR spectrum of **4** in the solid state.



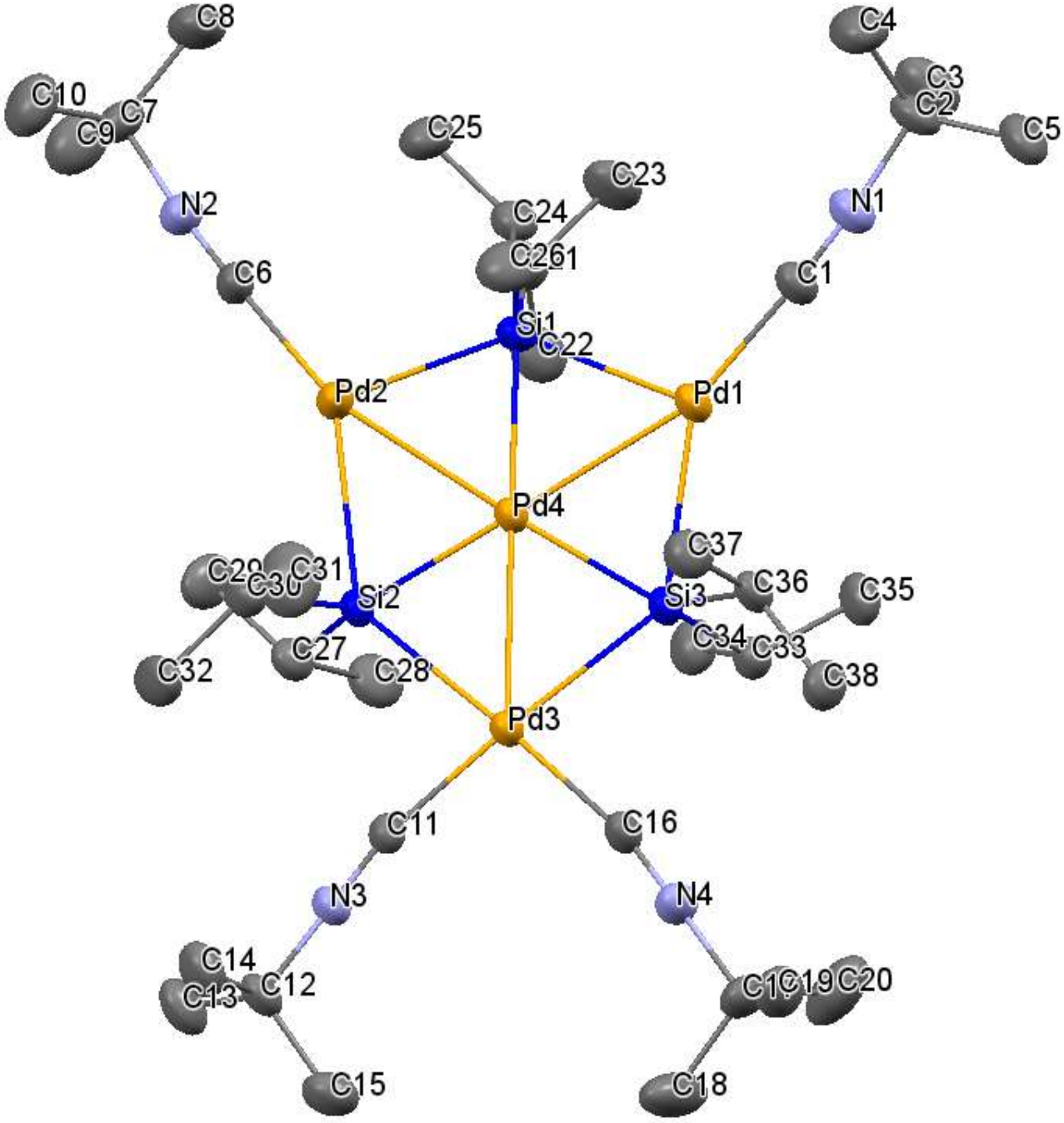


Figure S7. ORTEP drawing of **4** (50% probability of the thermal ellipsoids)

Table S1-1. Crystal data and structure refinement for **4**

Empirical Formula	$C_{38}H_{78}N_4Pd_4Si_3$
Formula Weight	1100.92
Crystal Color, Habit	yellow, block
Crystal Dimensions	0.150 X 0.100 X 0.080 mm
Crystal System	monoclinic
Lattice Type	Primitive
Lattice Parameters	a = 10.8179(6) Å b = 22.0783(12) Å c = 22.8654(12) Å β = 92.1391(12) ° V = 5457.4(5) Å^3
Space Group	$P2_1/n$ (#14)
Z value	4
D_{calc}	1.340 g/cm^3
F_{000}	2240.00
μ(MoKα)	13.888 cm^{-1}
Diffractometer	Saturn724
Radiation	MoKα (λ = 0.71075 Å) multi-layer mirror monochromated
Voltage, Current	50kV, 40mA
Temperature	-80.0°C
Detector Aperture	72.8 x 72.8 mm
Data Images	1080 exposures
ω oscillation Range (χ=45.0, ϕ=270.0)	-105.0 - 75.0°
Exposure Rate	20.0 sec./°
Detector Swing Angle	-14.65°
ω oscillation Range (χ=45.0, ϕ=0.0)	-105.0 - 75.0°
Exposure Rate	20.0 sec./°
Detector Swing Angle	-14.65°
ω oscillation Range (χ=45.0, ϕ=90.0)	-105.0 - 75.0°
Exposure Rate	20.0 sec./°
Detector Swing Angle	-14.65°
Detector Position	39.95 mm
Pixel Size	0.070 mm
$2\theta_{max}$	55.0°
No. of Reflections Measured	Total: 77678 Unique: 12489 (R_{int} = 0.0336)
Corrections	Lorentz-polarization Absorption (trans. factors: 0.784 - 0.895)
Structure Solution	Direct Methods (SIR2011)
Refinement	Full-matrix least-squares on F^2
Function Minimized	Σ w (Fo^2 - Fc^2)^2
Least Squares Weights	w = 1/ [$\sigma^2(Fo^2)$ + (0.0898 · P)^2 + 12.9959 · P] where P = (Max(Fo^2,0) + 2Fc^2)/3
$2\theta_{max}$ cutoff	55.0°
Anomalous Dispersion	All non-hydrogen atoms
No. Observations (All reflections)	12489
No. Variables	470
Reflection/Parameter Ratio	26.57
Residuals: R1 (I>2.00σ(I))	0.0516
Residuals: R (All reflections)	0.0537
Residuals: wR2 (All reflections)	0.1518
Goodness of Fit Indicator	1.101
Max Shift/Error in Final Cycle	0.001
Maximum peak in Final Diff. Map	2.30 e$^-$/Å^3
Minimum peak in Final Diff. Map	-0.81 e$^-$/Å^3

Table S1-2. Atomic coordinates and B_{iso}/B_{eq}

atom	x	y	z	B_{eq}	occ
Pd1	1.08441(3)	0.34714(2)	0.48005(2)	2.517(8)	1
Pd2	1.07048(3)	0.37266(2)	0.28340(2)	3.175(9)	1
Pd3	0.75754(3)	0.25373(2)	0.36938(2)	1.971(7)	1
Pd4	0.97266(3)	0.32031(2)	0.37665(2)	1.969(7)	1
Si1	1.14663(10)	0.38090(5)	0.38460(5)	2.210(18)	1
Si2	0.87993(10)	0.29843(5)	0.28888(4)	1.982(17)	1
Si3	0.89677(10)	0.27737(5)	0.45803(5)	2.054(17)	1
N1	1.2643(4)	0.40595(18)	0.57413(17)	2.90(6)	1
N2	1.2513(4)	0.4418(2)	0.20325(17)	3.24(7)	1
N3	0.5613(3)	0.21551(17)	0.27061(15)	2.47(6)	1
N4	0.5904(4)	0.1868(2)	0.45846(17)	3.06(7)	1
C1	1.1964(4)	0.3839(2)	0.54121(19)	2.93(8)	1
C2	1.3567(4)	0.4352(2)	0.6120(2)	2.99(8)	1
C3	1.4753(5)	0.4003(3)	0.6076(3)	4.77(12)	1
C4	1.3670(6)	0.5002(3)	0.5925(3)	4.80(12)	1
C5	1.3108(5)	0.4322(3)	0.6742(2)	3.77(9)	1
C6	1.1821(5)	0.4173(3)	0.2315(2)	3.57(10)	1
C7	1.3455(4)	0.4732(2)	0.1715(2)	2.96(8)	1
C8	1.4327(6)	0.5030(3)	0.2170(3)	5.12(14)	1
C9	1.4126(6)	0.4268(3)	0.1353(3)	4.79(12)	1
C10	1.2828(6)	0.5201(3)	0.1327(3)	4.53(11)	1
C11	0.6409(4)	0.23184(19)	0.30199(17)	2.23(6)	1
C12	0.4588(4)	0.1966(2)	0.23119(19)	2.69(7)	1
C13	0.5142(5)	0.1652(3)	0.1790(2)	3.83(10)	1
C14	0.3880(5)	0.2531(3)	0.2112(2)	3.68(9)	1
C15	0.3769(5)	0.1541(3)	0.2650(3)	3.86(10)	1
C16	0.6572(4)	0.2139(2)	0.43111(18)	2.61(7)	1
C17	0.5060(5)	0.1500(3)	0.4923(2)	3.54(9)	1
C18	0.4323(7)	0.1109(4)	0.4480(3)	6.22(19)	1
C19	0.4202(5)	0.1927(3)	0.5240(2)	4.14(11)	1
C20	0.5843(7)	0.1134(4)	0.5353(4)	6.10(18)	1
C21	1.3134(4)	0.3531(2)	0.3779(2)	2.83(7)	1
C22	1.3147(5)	0.2841(2)	0.3721(3)	3.66(9)	1
C23	1.4036(5)	0.3724(3)	0.4273(3)	4.04(10)	1
C24	1.1519(4)	0.4673(2)	0.3996(2)	2.93(7)	1
C25	1.2219(5)	0.5038(2)	0.3549(3)	3.82(10)	1
C26	1.0224(5)	0.4930(2)	0.4070(3)	4.31(11)	1
C27	0.9335(4)	0.2356(2)	0.23814(19)	2.66(7)	1
C28	0.9978(5)	0.1844(2)	0.2728(2)	3.53(9)	1
C29	1.0200(6)	0.2602(3)	0.1919(2)	4.12(11)	1
C30	0.7910(4)	0.3554(2)	0.2407(2)	2.90(8)	1
C31	0.7205(7)	0.3989(3)	0.2763(3)	5.36(14)	1
C32	0.7120(6)	0.3297(3)	0.1892(3)	4.67(13)	1
C33	0.9588(4)	0.2028(2)	0.49051(18)	2.59(7)	1
C34	1.0469(5)	0.1728(2)	0.4481(2)	3.44(9)	1
C35	1.0273(5)	0.2115(2)	0.5501(2)	3.40(9)	1
C36	0.8187(4)	0.3210(2)	0.51913(18)	2.50(7)	1
C37	0.7628(4)	0.3800(2)	0.4959(2)	3.10(8)	1
C38	0.7269(5)	0.2874(3)	0.5561(2)	3.33(8)	1
C39	0.7199(10)	0.5209(5)	0.0845(5)	3.72(18)	1/2
C40	0.7284(10)	0.5698(5)	0.1230(5)	3.73(18)	1/2
C41	0.8062(11)	0.5670(5)	0.1715(5)	3.98(19)	1/2
C42	0.8842(12)	0.5173(6)	0.1833(6)	4.4(2)	1/2
C43	0.8749(13)	0.4710(7)	0.1412(6)	5.2(3)	1/2
C44	0.8008(9)	0.4701(4)	0.1045(4)	3.04(15)	1/2
C45	0.6436(13)	0.5247(7)	0.0382(6)	5.1(3)	1/2

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

Table S1-3. Anisotropic displacement parameters

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Pd1	0.02821(18)	0.0446(2)	0.02250(16)	-0.01021(13)	-0.00339(12)	-0.00255(12)
Pd2	0.0398(2)	0.0565(2)	0.02411(17)	-0.02397(16)	-0.00301(14)	0.00626(14)
Pd3	0.02163(16)	0.03306(17)	0.02005(15)	-0.00557(11)	-0.00122(11)	-0.00019(10)
Pd4	0.02231(16)	0.03282(17)	0.01951(15)	-0.00602(11)	-0.00139(11)	-0.00014(10)
Si1	0.0223(5)	0.0329(6)	0.0286(5)	-0.0056(4)	-0.0013(4)	-0.0007(4)
Si2	0.0239(5)	0.0316(5)	0.0196(5)	-0.0030(4)	-0.0017(4)	0.0001(4)
Si3	0.0239(5)	0.0348(6)	0.0193(5)	-0.0026(4)	-0.0011(4)	0.0005(4)
N1	0.0303(18)	0.043(2)	0.036(2)	-0.0028(16)	-0.0073(15)	-0.0041(16)
N2	0.039(2)	0.050(2)	0.0336(19)	-0.0159(18)	0.0002(16)	0.0070(17)
N3	0.0290(17)	0.0389(19)	0.0256(16)	-0.0068(14)	-0.0032(14)	-0.0007(14)
N4	0.0321(19)	0.055(2)	0.0292(19)	-0.0143(17)	0.0041(15)	0.0011(17)
C1	0.033(2)	0.050(3)	0.028(2)	-0.0095(19)	-0.0033(17)	-0.0049(18)
C2	0.032(2)	0.036(2)	0.044(3)	-0.0033(18)	-0.0133(19)	-0.0079(19)
C3	0.034(3)	0.080(4)	0.066(4)	0.008(3)	-0.011(2)	-0.016(3)
C4	0.067(4)	0.048(3)	0.067(4)	-0.018(3)	-0.007(3)	0.009(3)
C5	0.056(3)	0.048(3)	0.039(3)	-0.006(2)	-0.014(2)	-0.006(2)
C6	0.048(3)	0.063(3)	0.025(2)	-0.026(2)	-0.0035(19)	0.007(2)
C7	0.033(2)	0.039(2)	0.040(2)	-0.0065(18)	0.0076(18)	0.0093(19)
C8	0.052(3)	0.081(4)	0.061(4)	-0.033(3)	-0.005(3)	0.008(3)
C9	0.059(4)	0.056(3)	0.069(4)	0.009(3)	0.021(3)	0.006(3)
C10	0.062(4)	0.055(3)	0.056(3)	0.007(3)	0.007(3)	0.020(3)
C11	0.0280(19)	0.033(2)	0.0236(18)	-0.0029(16)	0.0003(15)	0.0017(15)
C12	0.027(2)	0.046(2)	0.028(2)	-0.0048(18)	-0.0069(16)	-0.0065(18)
C13	0.045(3)	0.067(3)	0.033(2)	0.001(2)	-0.004(2)	-0.015(2)
C14	0.039(3)	0.062(3)	0.038(3)	0.003(2)	-0.010(2)	0.001(2)
C15	0.035(3)	0.056(3)	0.055(3)	-0.012(2)	-0.005(2)	-0.004(2)
C16	0.027(2)	0.048(2)	0.0230(18)	-0.0075(18)	-0.0019(15)	0.0005(17)
C17	0.041(3)	0.057(3)	0.037(2)	-0.019(2)	0.011(2)	0.005(2)
C18	0.080(5)	0.094(5)	0.065(4)	-0.054(4)	0.030(4)	-0.022(4)
C19	0.044(3)	0.077(4)	0.037(3)	-0.016(3)	0.012(2)	0.001(2)
C20	0.059(4)	0.092(5)	0.082(5)	0.002(4)	0.018(4)	0.046(4)
C21	0.024(2)	0.047(2)	0.036(2)	-0.0037(17)	0.0027(17)	0.0022(18)
C22	0.036(2)	0.053(3)	0.051(3)	0.009(2)	0.004(2)	-0.008(2)
C23	0.025(2)	0.071(4)	0.056(3)	-0.005(2)	-0.006(2)	-0.005(3)
C24	0.038(2)	0.035(2)	0.038(2)	-0.0070(18)	-0.0035(18)	-0.0026(18)
C25	0.049(3)	0.043(3)	0.054(3)	-0.015(2)	0.005(2)	0.006(2)
C26	0.050(3)	0.037(3)	0.077(4)	0.002(2)	0.011(3)	-0.001(3)
C27	0.034(2)	0.041(2)	0.027(2)	-0.0056(18)	0.0033(16)	-0.0089(17)
C28	0.045(3)	0.043(3)	0.047(3)	0.006(2)	0.002(2)	-0.013(2)
C29	0.062(3)	0.058(3)	0.039(3)	-0.009(3)	0.027(3)	-0.012(2)
C30	0.033(2)	0.041(2)	0.036(2)	-0.0053(18)	-0.0077(18)	0.0086(18)
C31	0.066(4)	0.064(4)	0.074(4)	0.032(3)	-0.004(3)	0.011(3)
C32	0.055(3)	0.068(4)	0.052(3)	-0.018(3)	-0.026(3)	0.024(3)
C33	0.030(2)	0.041(2)	0.027(2)	-0.0043(17)	-0.0020(16)	0.0048(17)
C34	0.046(3)	0.042(3)	0.042(3)	0.009(2)	-0.001(2)	0.008(2)
C35	0.048(3)	0.049(3)	0.032(2)	0.000(2)	-0.011(2)	0.0070(19)
C36	0.026(2)	0.046(2)	0.0221(18)	-0.0063(17)	-0.0012(15)	-0.0044(16)
C37	0.034(2)	0.042(2)	0.042(3)	0.0039(19)	0.0027(19)	-0.0027(19)
C38	0.042(3)	0.056(3)	0.030(2)	-0.005(2)	0.0110(19)	-0.002(2)

The general temperature factor expression: $\exp(-2p^2(a^{*2}U_{11}h^2 + b^{*2}U_{22}k^2 + c^{*2}U_{33}l^2 + 2a^*b^*U_{12}hk + 2a^*c^*U_{13}hl + 2b^*c^*U_{23}kl))$

Table S1-4. Bond lengths (Å)

atom	atom	distance	atom	atom	distance
Pd1	Pd4	2.6812(6)	Pd1	Si1	2.4252(12)

Pd1	Si3	2.5827(12)	Pd1	C1	1.988(4)
Pd2	Pd4	2.6778(6)	Pd2	Si1	2.4339(12)
Pd2	Si2	2.6401(12)	Pd2	C6	1.986(5)
Pd3	Pd4	2.7523(5)	Pd3	Si2	2.5094(11)
Pd3	Si3	2.5341(12)	Pd3	C11	2.014(4)
Pd3	C16	2.015(4)	Pd4	Si1	2.3106(12)
Pd4	Si2	2.2621(10)	Pd4	Si3	2.2692(12)
Si1	C21	1.917(4)	Si1	C24	1.938(5)
Si2	C27	1.913(5)	Si2	C30	1.910(5)
Si3	C33	1.916(5)	Si3	C36	1.919(4)
N1	C1	1.142(6)	N1	C2	1.449(6)
N2	C6	1.143(7)	N2	C7	1.449(6)
N3	C11	1.158(5)	N3	C12	1.464(5)
N4	C16	1.141(6)	N4	C17	1.465(7)
C2	C3	1.503(8)	C2	C4	1.509(8)
C2	C5	1.525(7)	C7	C8	1.527(8)
C7	C9	1.520(8)	C7	C10	1.507(8)
C12	C13	1.523(7)	C12	C14	1.525(7)
C12	C15	1.520(7)	C17	C18	1.533(9)
C17	C19	1.524(8)	C17	C20	1.509(9)
C21	C22	1.531(7)	C21	C23	1.524(7)
C24	C25	1.527(7)	C24	C26	1.527(7)
C27	C28	1.532(7)	C27	C29	1.538(8)
C30	C31	1.487(9)	C30	C32	1.537(8)
C33	C34	1.535(7)	C33	C35	1.538(6)
C36	C37	1.523(7)	C36	C38	1.521(7)
C39	C40	1.394(16)	C39	C44	1.484(15)
C39	C45	1.319(18)	C40	C41	1.369(16)
C41	C42	1.405(17)	C42	C43	1.406(19)
C43	C44	1.138(17)			

Table S1-5. Bond angles (°)

atom	atom	atom	angle	atom	atom	atom	angle
Pd4	Pd1	Si1	53.52(3)	Pd4	Pd1	Si3	51.03(3)
Pd4	Pd1	C1	162.37(14)	Si1	Pd1	Si3	104.50(4)
Si1	Pd1	C1	108.99(14)	Si3	Pd1	C1	146.51(14)
Pd4	Pd2	Si1	53.49(3)	Pd4	Pd2	Si2	50.34(2)
Pd4	Pd2	C6	163.14(14)	Si1	Pd2	Si2	103.79(4)
Si1	Pd2	C6	109.81(14)	Si2	Pd2	C6	146.08(14)
Pd4	Pd3	Si2	50.67(3)	Pd4	Pd3	Si3	50.63(3)
Pd4	Pd3	C11	132.73(12)	Pd4	Pd3	C16	131.87(12)
Si2	Pd3	Si3	101.05(4)	Si2	Pd3	C11	82.28(12)
Si2	Pd3	C16	176.83(13)	Si3	Pd3	C11	176.62(12)
Si3	Pd3	C16	81.33(12)	C11	Pd3	C16	95.32(17)
Pd1	Pd4	Pd2	115.354(18)	Pd1	Pd4	Pd3	121.58(2)
Pd1	Pd4	Si1	57.56(3)	Pd1	Pd4	Si2	179.32(3)
Pd1	Pd4	Si3	62.24(3)	Pd2	Pd4	Pd3	122.74(2)
Pd2	Pd4	Si1	57.85(3)	Pd2	Pd4	Si2	63.97(3)
Pd2	Pd4	Si3	177.56(3)	Pd3	Pd4	Si1	176.68(3)
Pd3	Pd4	Si2	59.10(3)	Pd3	Pd4	Si3	59.70(3)
Si1	Pd4	Si2	121.76(4)	Si1	Pd4	Si3	119.73(4)
Si2	Pd4	Si3	118.44(4)	Pd1	Si1	Pd2	137.49(5)
Pd1	Si1	Pd4	68.92(3)	Pd1	Si1	C21	105.49(15)
Pd1	Si1	C24	98.64(15)	Pd2	Si1	Pd4	68.66(3)
Pd2	Si1	C21	100.76(15)	Pd2	Si1	C24	104.40(15)
Pd4	Si1	C21	125.09(15)	Pd4	Si1	C24	127.02(15)
C21	Si1	C24	107.9(2)	Pd2	Si2	Pd3	135.50(4)
Pd2	Si2	Pd4	65.69(3)	Pd2	Si2	C27	99.62(14)
Pd2	Si2	C30	86.62(14)	Pd3	Si2	Pd4	70.24(3)
Pd3	Si2	C27	109.84(15)	Pd3	Si2	C30	114.49(15)

Pd4	Si2	C27	123.97(14)	Pd4	Si2	C30	124.66(15)
C27	Si2	C30	106.6(2)	Pd1	Si3	Pd3	135.90(5)
Pd1	Si3	Pd4	66.73(3)	Pd1	Si3	C33	100.10(14)
Pd1	Si3	C36	85.57(14)	Pd3	Si3	Pd4	69.67(3)
Pd3	Si3	C33	108.80(14)	Pd3	Si3	C36	114.91(13)
Pd4	Si3	C33	122.98(14)	Pd4	Si3	C36	124.75(15)
C33	Si3	C36	107.83(19)	C1	N1	C2	175.4(5)
C6	N2	C7	175.4(5)	C11	N3	C12	178.3(4)
C16	N4	C17	177.8(5)	Pd1	C1	N1	176.6(4)
N1	C2	C3	107.7(4)	N1	C2	C4	107.7(4)
N1	C2	C5	107.3(4)	C3	C2	C4	113.3(5)
C3	C2	C5	110.4(4)	C4	C2	C5	110.2(4)
Pd2	C6	N2	176.6(5)	N2	C7	C8	107.1(4)
N2	C7	C9	108.0(4)	N2	C7	C10	108.3(4)
C8	C7	C9	111.5(5)	C8	C7	C10	111.0(5)
C9	C7	C10	110.8(5)	Pd3	C11	N3	168.3(4)
N3	C12	C13	107.5(4)	N3	C12	C14	108.1(4)
N3	C12	C15	107.8(4)	C13	C12	C14	110.2(4)
C13	C12	C15	111.8(4)	C14	C12	C15	111.2(4)
Pd3	C16	N4	168.7(4)	N4	C17	C18	106.4(5)
N4	C17	C19	108.1(4)	N4	C17	C20	107.2(5)
C18	C17	C19	110.6(5)	C18	C17	C20	113.2(6)
C19	C17	C20	111.1(5)	Si1	C21	C22	109.7(3)
Si1	C21	C23	115.5(3)	C22	C21	C23	109.5(4)
Si1	C24	C25	114.4(3)	Si1	C24	C26	111.4(3)
C25	C24	C26	110.9(4)	Si2	C27	C28	111.3(3)
Si2	C27	C29	111.5(3)	C28	C27	C29	109.9(4)
Si2	C30	C31	111.5(4)	Si2	C30	C32	116.8(4)
C31	C30	C32	112.1(5)	Si3	C33	C34	110.0(3)
Si3	C33	C35	112.7(3)	C34	C33	C35	108.9(4)
Si3	C36	C37	110.8(3)	Si3	C36	C38	118.3(3)
C37	C36	C38	110.6(4)	C40	C39	C44	111.5(9)
C40	C39	C45	118.7(11)	C44	C39	C45	129.8(11)
C39	C40	C41	120.1(10)	C40	C41	C42	122.6(11)
C41	C42	C43	114.1(11)	C42	C43	C44	123.2(13)
C39	C44	C43	127.2(11)				

Table S1-6. Torsion Angles(°)

(Those having bond angles > 160 or < 20 degrees are excluded.)

atom1	atom2	atom3	atom4	angle	atom1	atom2	atom3	atom4	angle
Pd4	Pd1	Si1	Pd2	3.90(5)	Pd4	Pd1	Si1	Pd4	0.000(11)
Pd4	Pd1	Si1	C21	-122.18(6)	Pd4	Pd1	Si1	C24	126.44(5)
Si1	Pd1	Pd4	Pd2	-2.65(3)	Si1	Pd1	Pd4	Pd3	-176.22(4)
Si1	Pd1	Pd4	Si1	0.00(3)	Si1	Pd1	Pd4	Si3	176.91(4)
Pd4	Pd1	Si3	Pd3	-9.15(5)	Pd4	Pd1	Si3	Pd4	0.000(11)
Pd4	Pd1	Si3	C33	121.69(5)	Pd4	Pd1	Si3	C36	-130.96(5)
Si3	Pd1	Pd4	Pd2	-179.55(4)	Si3	Pd1	Pd4	Pd3	6.87(3)
Si3	Pd1	Pd4	Si1	-176.91(4)	Si3	Pd1	Pd4	Si3	-0.00(3)
Si1	Pd1	Si3	Pd3	-11.72(8)	Si1	Pd1	Si3	Pd4	-2.57(4)
Si1	Pd1	Si3	C33	119.12(5)	Si1	Pd1	Si3	C36	-133.53(4)
Si3	Pd1	Si1	Pd2	6.38(8)	Si3	Pd1	Si1	Pd4	2.48(4)
Si3	Pd1	Si1	C21	-119.69(5)	Si3	Pd1	Si1	C24	128.93(4)
C1	Pd1	Si1	Pd2	-173.57(16)	C1	Pd1	Si1	Pd4	-177.47(15)
C1	Pd1	Si1	C21	60.35(16)	C1	Pd1	Si1	C24	-51.03(16)
C1	Pd1	Si3	Pd3	168.2(3)	C1	Pd1	Si3	Pd4	177.4(3)
C1	Pd1	Si3	C33	-61.0(3)	C1	Pd1	Si3	C36	46.4(3)
Pd4	Pd2	Si1	Pd1	-3.90(5)	Pd4	Pd2	Si1	Pd4	-0.000(11)
Pd4	Pd2	Si1	C21	123.64(5)	Pd4	Pd2	Si1	C24	-124.54(5)
Si1	Pd2	Pd4	Pd1	2.64(3)	Si1	Pd2	Pd4	Pd3	176.13(4)
Si1	Pd2	Pd4	Si1	0.00(3)	Si1	Pd2	Pd4	Si2	-177.40(4)

Pd4	Pd2	Si2	Pd3	8.53(4)	Pd4	Pd2	Si2	Pd4	-0.000(11)
Pd4	Pd2	Si2	C27	-123.05(5)	Pd4	Pd2	Si2	C30	130.68(5)
Si2	Pd2	Pd4	Pd1	-179.96(4)	Si2	Pd2	Pd4	Pd3	-6.47(3)
Si2	Pd2	Pd4	Si1	177.40(4)	Si2	Pd2	Pd4	Si2	-0.00(3)
Si1	Pd2	Si2	Pd3	10.69(7)	Si1	Pd2	Si2	Pd4	2.15(4)
Si1	Pd2	Si2	C27	-120.89(4)	Si1	Pd2	Si2	C30	132.84(4)
Si2	Pd2	Si1	Pd1	-5.97(8)	Si2	Pd2	Si1	Pd4	-2.06(4)
Si2	Pd2	Si1	C21	121.58(4)	Si2	Pd2	Si1	C24	-126.60(5)
C6	Pd2	Si1	Pd1	178.75(18)	C6	Pd2	Si1	Pd4	-177.35(17)
C6	Pd2	Si1	C21	-53.71(18)	C6	Pd2	Si1	C24	58.11(18)
C6	Pd2	Si2	Pd3	-177.3(3)	C6	Pd2	Si2	Pd4	174.2(3)
C6	Pd2	Si2	C27	51.1(3)	C6	Pd2	Si2	C30	-55.1(3)
Pd4	Pd3	Si2	Pd2	-8.26(4)	Pd4	Pd3	Si2	Pd4	-0.000(11)
Pd4	Pd3	Si2	C27	120.11(6)	Pd4	Pd3	Si2	C30	-120.03(6)
Si2	Pd3	Pd4	Pd1	179.87(4)	Si2	Pd3	Pd4	Pd2	6.78(4)
Si2	Pd3	Pd4	Si2	-0.00(3)	Si2	Pd3	Pd4	Si3	-173.08(4)
Pd4	Pd3	Si3	Pd1	8.97(4)	Pd4	Pd3	Si3	Pd4	0.000(11)
Pd4	Pd3	Si3	C33	-119.15(6)	Pd4	Pd3	Si3	C36	119.87(6)
Si3	Pd3	Pd4	Pd1	-7.04(3)	Si3	Pd3	Pd4	Pd2	179.86(4)
Si3	Pd3	Pd4	Si2	173.08(4)	Si3	Pd3	Pd4	Si3	0.00(3)
C11	Pd3	Pd4	Pd1	173.31(16)	C11	Pd3	Pd4	Pd2	0.21(17)
C11	Pd3	Pd4	Si2	-6.57(16)	C11	Pd3	Pd4	Si3	-179.65(16)
C16	Pd3	Pd4	Pd1	-2.64(18)	C16	Pd3	Pd4	Pd2	-175.73(17)
C16	Pd3	Pd4	Si2	177.49(18)	C16	Pd3	Pd4	Si3	4.40(17)
Si2	Pd3	Si3	Pd1	14.41(7)	Si2	Pd3	Si3	Pd4	5.45(4)
Si2	Pd3	Si3	C33	-113.70(5)	Si2	Pd3	Si3	C36	125.32(5)
Si3	Pd3	Si2	Pd2	-13.70(7)	Si3	Pd3	Si2	Pd4	-5.44(4)
Si3	Pd3	Si2	C27	114.66(5)	Si3	Pd3	Si2	C30	-125.48(5)
C11	Pd3	Si2	Pd2	166.88(14)	C11	Pd3	Si2	Pd4	175.14(12)
C11	Pd3	Si2	C27	-64.76(13)	C11	Pd3	Si2	C30	55.11(13)
C16	Pd3	Si3	Pd1	-167.72(15)	C16	Pd3	Si3	Pd4	-176.68(13)
C16	Pd3	Si3	C33	64.16(14)	C16	Pd3	Si3	C36	-56.81(14)
Pd1	Pd4	Si1	Pd1	-0.000(10)	Pd1	Pd4	Si1	Pd2	-177.17(4)
Pd1	Pd4	Si1	C21	94.52(7)	Pd1	Pd4	Si1	C24	-84.89(7)
Pd1	Pd4	Si3	Pd1	-0.0	Pd1	Pd4	Si3	Pd3	173.22(3)
Pd1	Pd4	Si3	C33	-87.04(6)	Pd1	Pd4	Si3	C36	66.39(6)
Pd2	Pd4	Si1	Pd1	177.17(4)	Pd2	Pd4	Si1	Pd2	-0.000(10)
Pd2	Pd4	Si1	C21	-88.30(7)	Pd2	Pd4	Si1	C24	92.28(7)
Pd2	Pd4	Si2	Pd2	-0.0	Pd2	Pd4	Si2	Pd3	-173.66(3)
Pd2	Pd4	Si2	C27	85.23(6)	Pd2	Pd4	Si2	C30	-66.98(6)
Pd3	Pd4	Si2	Pd2	173.66(3)	Pd3	Pd4	Si2	Pd3	0.000(10)
Pd3	Pd4	Si2	C27	-101.12(6)	Pd3	Pd4	Si2	C30	106.68(7)
Pd3	Pd4	Si3	Pd1	-173.22(3)	Pd3	Pd4	Si3	Pd3	-0.000(10)
Pd3	Pd4	Si3	C33	99.74(6)	Pd3	Pd4	Si3	C36	-106.83(7)
Si1	Pd4	Si2	Pd2	-2.59(5)	Si1	Pd4	Si2	Pd3	-176.25(4)
Si1	Pd4	Si2	C27	82.63(7)	Si1	Pd4	Si2	C30	-69.57(8)
Si2	Pd4	Si1	Pd1	179.92(4)	Si2	Pd4	Si1	Pd2	2.75(5)
Si2	Pd4	Si1	C21	-85.55(8)	Si2	Pd4	Si1	C24	95.03(8)
Si1	Pd4	Si3	Pd1	3.01(5)	Si1	Pd4	Si3	Pd3	176.23(4)
Si1	Pd4	Si3	C33	-84.03(7)	Si1	Pd4	Si3	C36	69.39(7)
Si3	Pd4	Si1	Pd1	-3.15(5)	Si3	Pd4	Si1	Pd2	179.67(4)
Si3	Pd4	Si1	C21	91.37(7)	Si3	Pd4	Si1	C24	-88.05(8)
Si2	Pd4	Si3	Pd1	-179.97(4)	Si2	Pd4	Si3	Pd3	-6.75(5)
Si2	Pd4	Si3	C33	92.99(7)	Si2	Pd4	Si3	C36	-113.58(7)
Si3	Pd4	Si2	Pd2	-179.55(4)	Si3	Pd4	Si2	Pd3	6.79(5)
Si3	Pd4	Si2	C27	-94.33(7)	Si3	Pd4	Si2	C30	113.47(6)
Pd1	Si1	C21	C22	69.7(3)	Pd1	Si1	C21	C23	-54.6(3)
Pd1	Si1	C24	C25	163.9(2)	Pd1	Si1	C24	C26	-69.2(3)
Pd2	Si1	C21	C22	-76.5(3)	Pd2	Si1	C21	C23	159.2(2)
Pd2	Si1	C24	C25	-52.1(3)	Pd2	Si1	C24	C26	74.7(3)

Pd4	Si1	C21	C22	-5.1(3)	Pd4	Si1	C21	C23	-129.4(2)
Pd4	Si1	C24	C25	-126.0(2)	Pd4	Si1	C24	C26	0.8(4)
C21	Si1	C24	C25	54.5(3)	C21	Si1	C24	C26	-178.7(3)
C24	Si1	C21	C22	174.4(2)	C24	Si1	C21	C23	50.1(3)
Pd2	Si2	C27	C28	95.1(2)	Pd2	Si2	C27	C29	-28.0(3)
Pd2	Si2	C30	C31	-94.0(2)	Pd2	Si2	C30	C32	135.3(3)
Pd3	Si2	C27	C28	-51.0(3)	Pd3	Si2	C27	C29	-174.16(18)
Pd3	Si2	C30	C31	45.3(3)	Pd3	Si2	C30	C32	-85.4(3)
Pd4	Si2	C27	C28	28.0(3)	Pd4	Si2	C27	C29	-95.1(2)
Pd4	Si2	C30	C31	-36.8(3)	Pd4	Si2	C30	C32	-167.57(18)
C27	Si2	C30	C31	167.0(3)	C27	Si2	C30	C32	36.2(3)
C30	Si2	C27	C28	-175.6(2)	C30	Si2	C27	C29	61.3(3)
Pd1	Si3	C33	C34	-78.7(2)	Pd1	Si3	C33	C35	43.0(3)
Pd1	Si3	C36	C37	82.9(2)	Pd1	Si3	C36	C38	-147.9(3)
Pd3	Si3	C33	C34	67.5(2)	Pd3	Si3	C33	C35	-170.77(19)
Pd3	Si3	C36	C37	-56.4(3)	Pd3	Si3	C36	C38	72.8(3)
Pd4	Si3	C33	C34	-10.0(3)	Pd4	Si3	C33	C35	111.7(2)
Pd4	Si3	C36	C37	25.3(3)	Pd4	Si3	C36	C38	154.47(18)
C33	Si3	C36	C37	-178.0(2)	C33	Si3	C36	C38	-48.7(3)
C36	Si3	C33	C34	-167.3(2)	C36	Si3	C33	C35	-45.5(3)
C40	C39	C44	C43	-10.7(15)	C44	C39	C40	C41	1.0(14)
C45	C39	C40	C41	179.7(11)	C45	C39	C44	C43	170.8(12)
C39	C40	C41	C42	3.1(17)	C40	C41	C42	C43	-0.0(17)
C41	C42	C43	C44	-9(2)	C42	C43	C44	C39	15(2)

Table S1-7. Least Squares Planes

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

Atoms Defining Plane		Distance	esd
Pd1	[1; 0; 0; 0]	0.0280	0.0006
Pd2	[1; 0; 0; 0]	0.0276	0.0006
Pd3	[1; 0; 0; 0]	0.0456	0.0006
Pd4	[1; 0; 0; 0]	-0.0560	0.0005
Si1	[1; 0; 0; 0]	-0.0109	0.0012
Si2	[1; 0; 0; 0]	-0.1243	0.0012
Si3	[1; 0; 0; 0]	-0.1378	0.0012

Least-squares plane

$-6.14739x + 18.03153y + 2.77755z = 0.89857$

(0.00113) (0.00162) (0.00306) (0.00196)

Mean deviation from plane is 0.0615 angstrom

Weight scheem: Sigma Weights

Chi-squared: 61941.881

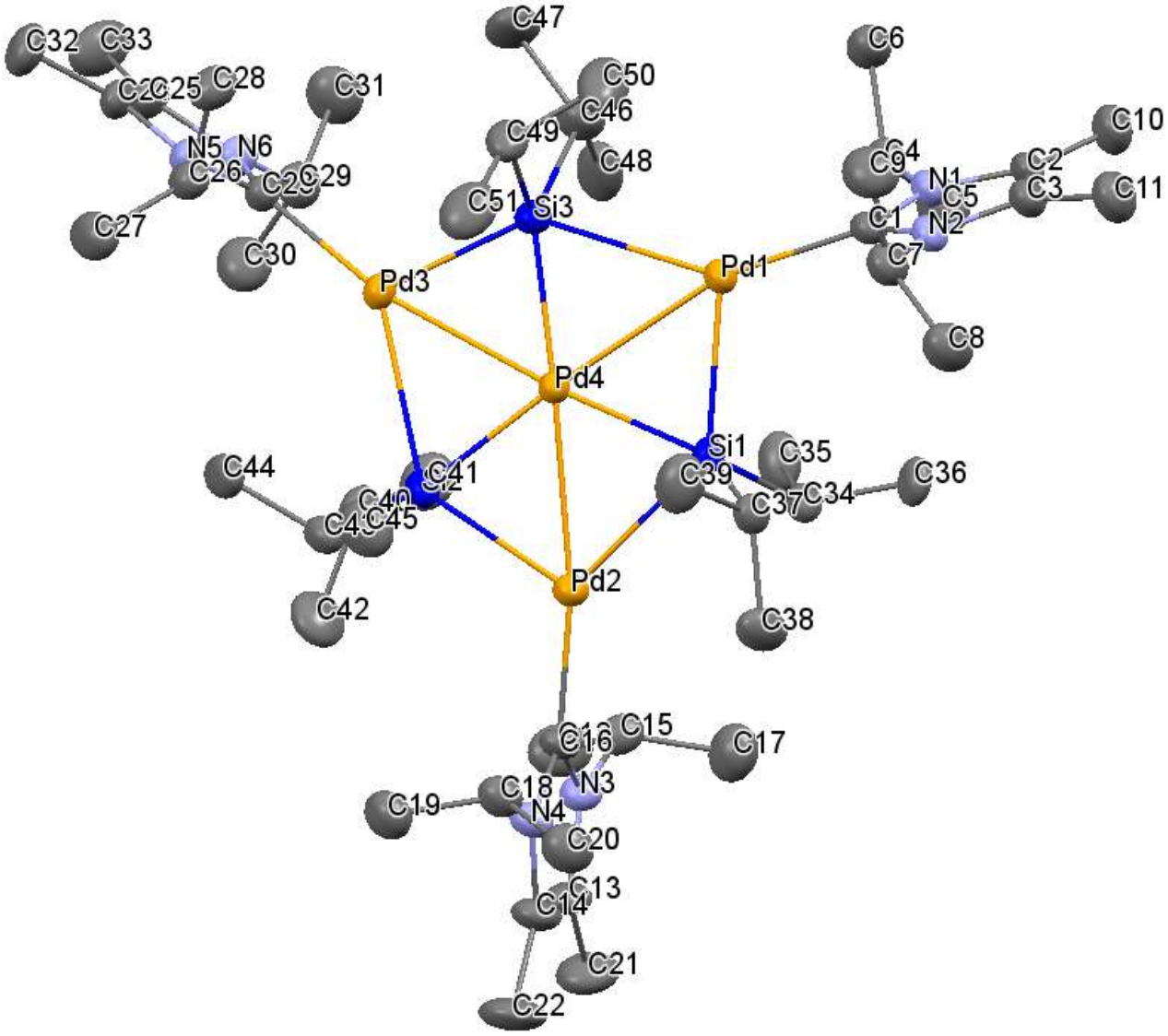


Figure S8. ORTEP drawing of **5** (50% probability of the thermal ellipsoids)

Table S2-1. Crystal data and structure refinement for **5**

Empirical Formula	$C_{51}H_{100}N_6Pd_4Si_3$
Formula Weight	1307.25
Crystal Color, Habit	red, block
Crystal Dimensions	0.100 X 0.050 X 0.050 mm
Crystal System	triclinic
Lattice Type	Primitive
Lattice Parameters	a = 14.505(3) Å b = 15.339(4) Å c = 15.655(4) Å α = 89.593(12) ° β = 63.724(6) ° γ = 81.301(11) ° V = 3080.2(13) Å^3
Space Group	P-1 (#2)
Z value	2
D_{calc}	1.409 g/cm^3
F_{000}	1348.00
μ(MoKα)	12.434 cm^{-1}
Diffractometer	Saturn724
Radiation	MoKα (λ = 0.71075 Å) multi-layer mirror monochromated
Voltage, Current	50kV, 24mA
Temperature	-79.8°C
Detector Aperture	72.8 x 72.8 mm
Data Images	1080 exposures
ω oscillation Range (χ=45.0, ϕ=0.0)	-70.0 - 110.0°
Exposure Rate	10.0 sec./°
Detector Swing Angle	19.98°
ω oscillation Range (χ=45.0, ϕ=90.0)	-70.0 - 110.0°
Exposure Rate	10.0 sec./°
Detector Swing Angle	19.98°
ω oscillation Range (χ=45.0, ϕ=180.0)	-70.0 - 110.0°
Exposure Rate	10.0 sec./°
Detector Swing Angle	19.98°
Detector Position	44.77 mm
Pixel Size	0.141 mm
$2\theta_{max}$	55.0°
No. of Reflections Measured	Total: 38434 Unique: 14053 (R_{int} = 0.0393)
Corrections	Lorentz-polarization Absorption (trans. factors: 0.863 - 0.940)
Structure Solution	Direct Methods (SIR2011)
Refinement	Full-matrix least-squares on F^2
Function Minimized	Σ w (Fo^2 - Fc^2)^2
Least Squares Weights	w = 1/ [$\sigma^2(Fo^2)$ + (0.0453 · P)^2 + 1.3612 · P] where P = (Max(Fo^2,0) + 2Fc^2)/3
$2\theta_{max}$ cutoff	55.0°
Anomalous Dispersion	All non-hydrogen atoms
No. Observations (All reflections)	14053
No. Variables	577
Reflection/Parameter Ratio	24.36
Residuals: R1 (I>2.00σ(I))	0.0439
Residuals: R (All reflections)	0.0585
Residuals: wR2 (All reflections)	0.1016
Goodness of Fit Indicator	1.076
Max Shift/Error in Final Cycle	0.002
Maximum peak in Final Diff. Map	1.05 e$^-$/Å^3
Minimum peak in Final Diff. Map	-0.67 e$^-$/Å^3

Table S2-2. Atomic coordinates and B_{iso}/B_{eq}

atom	x	y	z	B_{eq}
Pd1	0.38085(2)	0.88810(2)	0.27741(2)	1.924(6)
Pd2	0.23736(2)	0.75487(2)	0.56677(2)	1.862(6)
Pd3	0.15184(2)	0.68954(2)	0.32153(2)	1.875(6)
Pd4	0.24908(2)	0.78344(2)	0.39219(2)	1.753(6)
Si1	0.34369(8)	0.86013(7)	0.43732(7)	1.767(17)
Si2	0.14246(8)	0.69797(7)	0.49529(7)	1.933(17)
Si3	0.26036(8)	0.79491(7)	0.24397(7)	2.095(18)
N1	0.6012(2)	0.9271(2)	0.1542(2)	2.31(6)
N2	0.5021(3)	1.0479(2)	0.2301(2)	2.30(6)
N3	0.2763(3)	0.6487(2)	0.7205(2)	2.29(6)
N4	0.1412(3)	0.7496(2)	0.7870(2)	2.40(6)
N5	0.0057(3)	0.6498(2)	0.2350(2)	2.25(6)
N6	0.1373(3)	0.5456(2)	0.1918(2)	2.23(6)
C1	0.5009(3)	0.9609(3)	0.2157(3)	2.09(6)
C2	0.6646(3)	0.9931(3)	0.1304(3)	2.80(8)
C3	0.6024(3)	1.0683(3)	0.1785(3)	2.80(8)
C4	0.6279(3)	0.8357(3)	0.1139(3)	2.71(7)
C5	0.7190(4)	0.7818(3)	0.1253(4)	4.08(10)
C6	0.6421(4)	0.8312(3)	0.0117(3)	3.56(9)
C7	0.4041(3)	1.1082(3)	0.2866(3)	2.86(8)
C8	0.4072(4)	1.1650(3)	0.3637(3)	3.95(10)
C9	0.3689(4)	1.1623(3)	0.2215(4)	4.11(10)
C10	0.7794(4)	0.9764(3)	0.0673(3)	3.93(10)
C11	0.6323(4)	1.1566(3)	0.1805(4)	4.03(10)
C12	0.2153(3)	0.7153(2)	0.7004(2)	2.04(6)
C13	0.2392(4)	0.6451(3)	0.8196(3)	2.73(8)
C14	0.1543(4)	0.7067(3)	0.8606(3)	3.02(8)
C15	0.3707(3)	0.5984(3)	0.6424(3)	2.60(7)
C16	0.3734(5)	0.4996(3)	0.6445(4)	4.30(11)
C17	0.4680(4)	0.6268(4)	0.6387(4)	4.32(10)
C18	0.0591(3)	0.8227(3)	0.7944(3)	2.72(7)
C19	-0.0468(4)	0.7946(3)	0.8319(3)	3.67(9)
C20	0.0590(4)	0.9050(3)	0.8482(3)	3.55(9)
C21	0.2887(4)	0.5801(3)	0.8656(4)	4.33(11)
C22	0.0864(4)	0.7298(4)	0.9654(3)	4.80(12)
C23	0.0959(3)	0.6253(2)	0.2426(3)	1.98(6)
C24	-0.0090(3)	0.5859(3)	0.1812(3)	2.72(8)
C25	0.0734(4)	0.5212(3)	0.1541(3)	2.74(8)
C26	-0.0615(3)	0.7356(3)	0.2809(3)	2.48(7)
C27	-0.1707(3)	0.7254(3)	0.3529(3)	3.79(9)
C28	-0.0607(4)	0.8012(3)	0.2081(3)	3.33(8)
C29	0.2338(3)	0.4947(3)	0.1885(3)	2.76(7)
C30	0.2105(4)	0.4185(3)	0.2535(4)	4.16(10)
C31	0.3175(4)	0.4649(3)	0.0878(3)	4.31(11)
C32	-0.1015(4)	0.5925(3)	0.1613(4)	3.98(10)
C33	0.0947(5)	0.4359(3)	0.0962(4)	4.80(12)
C34	0.4703(3)	0.8126(2)	0.4435(3)	2.17(6)
C35	0.5196(3)	0.7243(3)	0.3860(4)	3.31(9)
C36	0.5497(3)	0.8762(3)	0.4137(3)	2.71(7)
C37	0.2948(3)	0.9705(2)	0.5120(3)	2.19(6)
C38	0.2839(4)	0.9608(3)	0.6133(3)	3.51(9)
C39	0.1916(4)	1.0156(3)	0.5149(4)	3.71(9)
C40	0.1606(3)	0.5722(3)	0.4953(3)	2.87(8)
C41	0.2744(4)	0.5299(3)	0.4389(4)	3.80(10)
C42	0.1135(4)	0.5384(3)	0.5962(4)	4.28(11)
C43	-0.0042(3)	0.7366(3)	0.5735(3)	2.41(7)
C44	-0.0698(3)	0.6982(4)	0.5339(3)	3.79(10)
C45	-0.0313(4)	0.8375(3)	0.5860(4)	4.08(10)

C46	0.3752(4)	0.7422(3)	0.1273(3)	3.38(9)
C47	0.3435(5)	0.7161(4)	0.0518(3)	5.10(13)
C48	0.4411(4)	0.6636(3)	0.1470(4)	4.30(11)
C49	0.1833(4)	0.8874(3)	0.2065(3)	3.06(8)
C50	0.2527(5)	0.9541(4)	0.1500(4)	5.08(13)
C51	0.0896(4)	0.9335(3)	0.2941(4)	4.18(10)

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

Table 2-3. Anisotropic displacement parameters

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Pd1	0.02255(15)	0.02815(16)	0.02228(15)	-0.00810(12)	-0.00871(12)	0.00373(11)
Pd2	0.02381(15)	0.02657(16)	0.02012(15)	-0.00437(12)	-0.00955(12)	0.00252(11)
Pd3	0.02231(15)	0.02508(16)	0.02494(15)	-0.00496(12)	-0.01116(12)	-0.00119(11)
Pd4	0.02209(14)	0.02603(15)	0.01997(14)	-0.00775(12)	-0.00957(11)	0.00278(11)
Si1	0.0200(5)	0.0220(5)	0.0248(5)	-0.0023(4)	-0.0100(4)	-0.0017(4)
Si2	0.0199(5)	0.0261(5)	0.0268(5)	-0.0046(4)	-0.0096(4)	0.0050(4)
Si3	0.0290(6)	0.0292(6)	0.0228(5)	-0.0068(5)	-0.0122(4)	0.0024(4)
N1	0.0245(17)	0.0384(19)	0.0241(17)	-0.0104(15)	-0.0085(14)	0.0059(14)
N2	0.0294(18)	0.0328(19)	0.0262(17)	-0.0119(15)	-0.0115(14)	0.0082(14)
N3	0.0326(18)	0.0272(17)	0.0272(17)	-0.0010(14)	-0.0147(15)	0.0021(14)
N4	0.0347(19)	0.0300(18)	0.0235(17)	-0.0053(15)	-0.0103(14)	0.0051(14)
N5	0.0285(17)	0.0344(19)	0.0251(17)	-0.0091(15)	-0.0130(14)	0.0001(14)
N6	0.0323(18)	0.0222(16)	0.0295(18)	-0.0042(14)	-0.0131(15)	-0.0023(13)
C1	0.0263(19)	0.032(2)	0.0213(19)	-0.0072(16)	-0.0099(16)	0.0047(15)
C2	0.033(2)	0.056(3)	0.023(2)	-0.025(2)	-0.0116(17)	0.0093(19)
C3	0.035(2)	0.046(3)	0.027(2)	-0.019(2)	-0.0111(18)	0.0070(19)
C4	0.028(2)	0.036(2)	0.037(2)	-0.0046(18)	-0.0121(18)	-0.0008(18)
C5	0.037(3)	0.053(3)	0.054(3)	0.002(2)	-0.014(2)	0.002(2)
C6	0.044(3)	0.058(3)	0.032(2)	-0.017(2)	-0.013(2)	-0.004(2)
C7	0.039(2)	0.035(2)	0.034(2)	-0.0129(19)	-0.0139(19)	0.0047(18)
C8	0.058(3)	0.048(3)	0.040(3)	-0.018(2)	-0.015(2)	-0.002(2)
C9	0.055(3)	0.048(3)	0.053(3)	-0.002(2)	-0.026(3)	0.009(2)
C10	0.038(3)	0.068(3)	0.042(3)	-0.024(2)	-0.012(2)	0.003(2)
C11	0.053(3)	0.054(3)	0.046(3)	-0.027(3)	-0.016(2)	0.006(2)
C12	0.029(2)	0.030(2)	0.0150(18)	-0.0068(17)	-0.0057(15)	0.0029(15)
C13	0.045(3)	0.039(2)	0.025(2)	-0.011(2)	-0.0198(19)	0.0122(18)
C14	0.047(3)	0.045(3)	0.021(2)	-0.010(2)	-0.0131(19)	0.0082(18)
C15	0.038(2)	0.028(2)	0.034(2)	0.0026(18)	-0.0193(19)	-0.0027(17)
C16	0.078(4)	0.029(2)	0.056(3)	0.003(2)	-0.033(3)	0.000(2)
C17	0.038(3)	0.065(3)	0.059(3)	-0.004(2)	-0.020(2)	-0.007(3)
C18	0.032(2)	0.035(2)	0.028(2)	-0.0020(18)	-0.0079(18)	-0.0016(17)
C19	0.034(2)	0.058(3)	0.039(3)	-0.008(2)	-0.009(2)	0.002(2)
C20	0.047(3)	0.036(3)	0.041(3)	-0.002(2)	-0.013(2)	-0.003(2)
C21	0.074(4)	0.055(3)	0.046(3)	-0.003(3)	-0.038(3)	0.014(2)
C22	0.071(4)	0.082(4)	0.022(2)	-0.005(3)	-0.017(2)	0.009(2)
C23	0.0234(18)	0.028(2)	0.0229(19)	-0.0059(16)	-0.0087(15)	-0.0022(15)
C24	0.040(2)	0.041(2)	0.032(2)	-0.021(2)	-0.0203(19)	0.0042(18)
C25	0.047(3)	0.031(2)	0.033(2)	-0.015(2)	-0.022(2)	-0.0029(18)
C26	0.028(2)	0.037(2)	0.028(2)	-0.0031(18)	-0.0133(17)	-0.0001(17)
C27	0.029(2)	0.066(3)	0.043(3)	-0.002(2)	-0.014(2)	0.004(2)
C28	0.045(3)	0.045(3)	0.042(3)	-0.004(2)	-0.026(2)	0.001(2)
C29	0.034(2)	0.028(2)	0.037(2)	-0.0020(18)	-0.0122(19)	-0.0046(18)
C30	0.055(3)	0.044(3)	0.062(3)	-0.004(2)	-0.030(3)	0.010(2)
C31	0.047(3)	0.049(3)	0.051(3)	0.002(2)	-0.009(2)	-0.014(2)
C32	0.047(3)	0.063(3)	0.057(3)	-0.021(2)	-0.034(3)	0.003(3)
C33	0.095(5)	0.036(3)	0.067(4)	-0.012(3)	-0.049(3)	-0.006(2)
C34	0.0247(19)	0.029(2)	0.030(2)	-0.0051(16)	-0.0126(16)	0.0058(16)
C35	0.028(2)	0.029(2)	0.065(3)	0.0032(18)	-0.019(2)	-0.000(2)
C36	0.0199(19)	0.041(2)	0.044(2)	-0.0045(17)	-0.0157(18)	-0.0014(19)

C37	0.027(2)	0.025(2)	0.028(2)	-0.0061(16)	-0.0094(16)	-0.0021(16)
C38	0.058(3)	0.039(3)	0.030(2)	-0.013(2)	-0.013(2)	-0.0060(19)
C39	0.035(2)	0.037(3)	0.060(3)	0.009(2)	-0.018(2)	-0.018(2)
C40	0.042(2)	0.025(2)	0.053(3)	-0.0080(19)	-0.030(2)	0.0039(19)
C41	0.051(3)	0.029(2)	0.065(3)	0.010(2)	-0.032(3)	-0.005(2)
C42	0.063(3)	0.037(3)	0.063(3)	-0.016(2)	-0.027(3)	0.023(2)
C43	0.0233(19)	0.039(2)	0.026(2)	-0.0040(17)	-0.0085(16)	0.0064(17)
C44	0.026(2)	0.083(4)	0.037(3)	-0.019(2)	-0.013(2)	0.012(2)
C45	0.033(3)	0.052(3)	0.056(3)	0.007(2)	-0.011(2)	0.005(2)
C46	0.042(3)	0.055(3)	0.025(2)	-0.012(2)	-0.0082(19)	-0.004(2)
C47	0.075(4)	0.092(4)	0.028(3)	-0.033(3)	-0.018(3)	-0.010(3)
C48	0.031(2)	0.063(3)	0.048(3)	-0.007(2)	0.001(2)	-0.023(2)
C49	0.046(3)	0.040(2)	0.042(3)	-0.016(2)	-0.028(2)	0.018(2)
C50	0.082(4)	0.060(3)	0.081(4)	-0.034(3)	-0.058(4)	0.041(3)
C51	0.061(3)	0.037(3)	0.071(4)	0.007(2)	-0.043(3)	0.002(2)

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 2-4. Bond lengths (Å)

atom	atom	distance	atom	atom	distance
Pd1	Pd4	2.7029(6)	Pd1	Si1	2.3668(13)
Pd1	Si3	2.6359(14)	Pd1	C1	2.073(4)
Pd2	Pd4	2.6991(8)	Pd2	Si1	2.6518(12)
Pd2	Si2	2.3769(15)	Pd2	C12	2.073(4)
Pd3	Pd4	2.7030(7)	Pd3	Si2	2.6659(14)
Pd3	Si3	2.3693(12)	Pd3	C23	2.073(5)
Pd4	Si1	2.2638(14)	Pd4	Si2	2.2558(11)
Pd4	Si3	2.2603(13)	Si1	C34	1.915(5)
Si1	C37	1.915(4)	Si2	C40	1.908(4)
Si2	C43	1.924(4)	Si3	C46	1.919(4)
Si3	C49	1.922(5)	N1	C1	1.360(4)
N1	C2	1.409(6)	N1	C4	1.464(5)
N2	C1	1.358(5)	N2	C3	1.400(5)
N2	C7	1.470(5)	N3	C12	1.375(5)
N3	C13	1.402(5)	N3	C15	1.475(4)
N4	C12	1.348(4)	N4	C14	1.394(6)
N4	C18	1.471(5)	N5	C23	1.363(6)
N5	C24	1.396(6)	N5	C26	1.484(5)
N6	C23	1.363(5)	N6	C25	1.393(7)
N6	C29	1.475(6)	C2	C3	1.345(6)
C2	C10	1.494(6)	C3	C11	1.488(7)
C4	C5	1.529(7)	C4	C6	1.521(7)
C7	C8	1.514(8)	C7	C9	1.519(8)
C13	C14	1.333(6)	C13	C21	1.504(8)
C14	C22	1.503(5)	C15	C16	1.511(6)
C15	C17	1.514(8)	C18	C19	1.512(7)
C18	C20	1.522(7)	C24	C25	1.339(6)
C24	C32	1.495(8)	C25	C33	1.509(7)
C26	C27	1.515(5)	C26	C28	1.512(6)
C29	C30	1.521(6)	C29	C31	1.521(5)
C34	C35	1.522(5)	C34	C36	1.534(6)
C37	C38	1.530(7)	C37	C39	1.533(7)
C40	C41	1.522(6)	C40	C42	1.539(7)
C43	C44	1.528(8)	C43	C45	1.529(6)
C46	C47	1.522(9)	C46	C48	1.539(7)
C49	C50	1.534(7)	C49	C51	1.516(6)

Table 2-5. Bond angles (°)

atom	atom	atom	angle	atom	atom	atom	angle

Pd4	Pd1	Si1	52.53(3)	Pd4	Pd1	Si3	50.08(3)
Pd4	Pd1	C1	163.61(13)	Si1	Pd1	Si3	102.60(4)
Si1	Pd1	C1	112.24(13)	Si3	Pd1	C1	144.65(13)
Pd4	Pd2	Si1	50.05(3)	Pd4	Pd2	Si2	52.30(3)
Pd4	Pd2	C12	170.18(12)	Si1	Pd2	Si2	102.21(4)
Si1	Pd2	C12	139.60(13)	Si2	Pd2	C12	118.18(13)
Pd4	Pd3	Si2	49.68(3)	Pd4	Pd3	Si3	52.42(4)
Pd4	Pd3	C23	169.15(9)	Si2	Pd3	Si3	101.99(4)
Si2	Pd3	C23	140.98(10)	Si3	Pd3	C23	117.02(10)
Pd1	Pd4	Pd2	119.78(2)	Pd1	Pd4	Pd3	119.41(2)
Pd1	Pd4	Si1	56.08(3)	Pd1	Pd4	Si2	176.26(4)
Pd1	Pd4	Si3	63.42(3)	Pd2	Pd4	Pd3	120.198(19)
Pd2	Pd4	Si1	63.89(3)	Pd2	Pd4	Si2	56.48(4)
Pd2	Pd4	Si3	175.17(3)	Pd3	Pd4	Si1	174.52(2)
Pd3	Pd4	Si2	64.30(4)	Pd3	Pd4	Si3	56.18(3)
Si1	Pd4	Si2	120.18(5)	Si1	Pd4	Si3	119.50(4)
Si2	Pd4	Si3	120.31(5)	Pd1	Si1	Pd2	137.15(6)
Pd1	Si1	Pd4	71.38(4)	Pd1	Si1	C34	109.40(12)
Pd1	Si1	C37	108.70(13)	Pd2	Si1	Pd4	66.06(3)
Pd2	Si1	C34	91.90(12)	Pd2	Si1	C37	100.38(11)
Pd4	Si1	C34	125.85(13)	Pd4	Si1	C37	126.47(15)
C34	Si1	C37	105.1(2)	Pd2	Si2	Pd3	136.37(4)
Pd2	Si2	Pd4	71.21(4)	Pd2	Si2	C40	110.29(19)
Pd2	Si2	C43	109.06(16)	Pd3	Si2	Pd4	66.01(3)
Pd3	Si2	C40	90.46(17)	Pd3	Si2	C43	101.49(16)
Pd4	Si2	C40	128.66(12)	Pd4	Si2	C43	123.74(13)
C40	Si2	C43	104.74(18)	Pd1	Si3	Pd3	137.60(5)
Pd1	Si3	Pd4	66.50(4)	Pd1	Si3	C46	91.15(18)
Pd1	Si3	C49	99.23(17)	Pd3	Si3	Pd4	71.40(3)
Pd3	Si3	C46	110.14(16)	Pd3	Si3	C49	109.01(16)
Pd4	Si3	C46	126.16(18)	Pd4	Si3	C49	125.36(14)
C46	Si3	C49	105.5(2)	C1	N1	C2	110.9(3)
C1	N1	C4	120.2(3)	C2	N1	C4	128.5(3)
C1	N2	C3	111.2(3)	C1	N2	C7	120.1(3)
C3	N2	C7	128.5(3)	C12	N3	C13	110.2(3)
C12	N3	C15	120.1(3)	C13	N3	C15	129.5(4)
C12	N4	C14	111.7(3)	C12	N4	C18	120.1(4)
C14	N4	C18	128.2(3)	C23	N5	C24	111.3(3)
C23	N5	C26	119.7(4)	C24	N5	C26	129.0(4)
C23	N6	C25	111.1(3)	C23	N6	C29	120.0(4)
C25	N6	C29	128.7(3)	Pd1	C1	N1	125.1(3)
Pd1	C1	N2	130.2(2)	N1	C1	N2	104.6(3)
N1	C2	C3	106.5(3)	N1	C2	C10	124.0(4)
C3	C2	C10	129.5(5)	N2	C3	C2	106.8(4)
N2	C3	C11	125.4(3)	C2	C3	C11	127.7(4)
N1	C4	C5	113.5(4)	N1	C4	C6	111.7(4)
C5	C4	C6	112.9(3)	N2	C7	C8	113.9(4)
N2	C7	C9	110.4(3)	C8	C7	C9	112.6(4)
Pd2	C12	N3	127.2(2)	Pd2	C12	N4	128.7(3)
N3	C12	N4	104.2(3)	N3	C13	C14	107.1(4)
N3	C13	C21	123.8(3)	C14	C13	C21	129.1(4)
N4	C14	C13	106.8(3)	N4	C14	C22	125.3(4)
C13	C14	C22	127.9(5)	N3	C15	C16	113.1(3)
N3	C15	C17	110.8(4)	C16	C15	C17	113.4(4)
N4	C18	C19	112.4(4)	N4	C18	C20	112.3(4)
C19	C18	C20	113.3(3)	Pd3	C23	N5	128.1(2)
Pd3	C23	N6	127.9(3)	N5	C23	N6	103.9(4)
N5	C24	C25	106.6(5)	N5	C24	C32	124.3(4)
C25	C24	C32	129.1(5)	N6	C25	C24	107.1(4)
N6	C25	C33	124.9(4)	C24	C25	C33	128.0(6)

N5	C26	C27	112.9(3)	N5	C26	C28	111.9(3)
C27	C26	C28	112.8(4)	N6	C29	C30	111.2(4)
N6	C29	C31	113.7(4)	C30	C29	C31	112.3(3)
Si1	C34	C35	111.3(4)	Si1	C34	C36	113.6(3)
C35	C34	C36	110.5(3)	Si1	C37	C38	112.7(3)
Si1	C37	C39	110.9(3)	C38	C37	C39	110.5(3)
Si2	C40	C41	112.0(3)	Si2	C40	C42	113.3(3)
C41	C40	C42	110.8(4)	Si2	C43	C44	111.6(3)
Si2	C43	C45	111.5(3)	C44	C43	C45	110.7(4)
Si3	C46	C47	113.9(4)	Si3	C46	C48	110.9(3)
C47	C46	C48	111.2(4)	Si3	C49	C50	110.9(4)
Si3	C49	C51	109.9(4)	C50	C49	C51	110.4(4)

Table 2-6. Torsion Angles(°)
(Those having bond angles > 160 or < 20 degrees are excluded.)

atom1	atom2	atom3	atom4	angle	atom1	atom2	atom3	atom4	angle
Pd4	Pd1	Si1	Pd2	6.90(4)	Pd4	Pd1	Si1	Pd4	-0.0
Pd4	Pd1	Si1	C34	122.45(6)	Pd4	Pd1	Si1	C37	-123.24(6)
Si1	Pd1	Pd4	Pd2	-5.31(3)	Si1	Pd1	Pd4	Pd3	-176.33(3)
Si1	Pd1	Pd4	Si1	-0.00(3)	Si1	Pd1	Pd4	Si3	178.79(3)
Pd4	Pd1	Si3	Pd3	-7.20(4)	Pd4	Pd1	Si3	Pd4	-0.0
Pd4	Pd1	Si3	C46	-129.40(5)	Pd4	Pd1	Si3	C49	124.66(4)
Si3	Pd1	Pd4	Pd2	175.90(3)	Si3	Pd1	Pd4	Pd3	4.88(3)
Si3	Pd1	Pd4	Si1	-178.79(3)	Si3	Pd1	Pd4	Si3	-0.00(3)
Si1	Pd1	Si3	Pd3	-8.19(7)	Si1	Pd1	Si3	Pd4	-0.98(3)
Si1	Pd1	Si3	C46	-130.39(4)	Si1	Pd1	Si3	C49	123.68(4)
Si3	Pd1	Si1	Pd2	7.85(7)	Si3	Pd1	Si1	Pd4	0.95(3)
Si3	Pd1	Si1	C34	123.40(5)	Si3	Pd1	Si1	C37	-122.29(5)
Si1	Pd1	C1	N1	101.5(3)	Si1	Pd1	C1	N2	-73.6(4)
C1	Pd1	Si1	Pd2	-166.07(11)	C1	Pd1	Si1	Pd4	-172.97(10)
C1	Pd1	Si1	C34	-50.52(12)	C1	Pd1	Si1	C37	63.79(12)
Si3	Pd1	C1	N1	-68.2(4)	Si3	Pd1	C1	N2	116.7(3)
C1	Pd1	Si3	Pd3	162.05(18)	C1	Pd1	Si3	Pd4	169.25(18)
C1	Pd1	Si3	C46	39.85(19)	C1	Pd1	Si3	C49	-66.08(18)
Pd4	Pd2	Si1	Pd1	-7.16(4)	Pd4	Pd2	Si1	Pd4	0.0
Pd4	Pd2	Si1	C34	-128.78(4)	Pd4	Pd2	Si1	C37	125.44(6)
Si1	Pd2	Pd4	Pd1	4.90(3)	Si1	Pd2	Pd4	Pd3	175.85(3)
Si1	Pd2	Pd4	Si1	0.00(3)	Si1	Pd2	Pd4	Si2	-174.96(3)
Pd4	Pd2	Si2	Pd3	11.69(4)	Pd4	Pd2	Si2	Pd4	-0.0
Pd4	Pd2	Si2	C40	125.29(5)	Pd4	Pd2	Si2	C43	-120.21(6)
Si2	Pd2	Pd4	Pd1	179.87(3)	Si2	Pd2	Pd4	Pd3	-9.18(3)
Si2	Pd2	Pd4	Si1	174.96(3)	Si2	Pd2	Pd4	Si2	-0.00(3)
Si1	Pd2	Si2	Pd3	15.64(7)	Si1	Pd2	Si2	Pd4	3.95(3)
Si1	Pd2	Si2	C40	129.24(4)	Si1	Pd2	Si2	C43	-116.26(5)
Si2	Pd2	Si1	Pd1	-11.23(7)	Si2	Pd2	Si1	Pd4	-4.07(3)
Si2	Pd2	Si1	C34	-132.86(4)	Si2	Pd2	Si1	C37	121.36(5)
Si1	Pd2	C12	N3	-84.7(3)	Si1	Pd2	C12	N4	92.9(4)
C12	Pd2	Si1	Pd1	170.19(14)	C12	Pd2	Si1	Pd4	177.35(14)
C12	Pd2	Si1	C34	48.56(15)	C12	Pd2	Si1	C37	-57.21(15)
Si2	Pd2	C12	N3	96.8(3)	Si2	Pd2	C12	N4	-85.5(3)
C12	Pd2	Si2	Pd3	-165.41(11)	C12	Pd2	Si2	Pd4	-177.10(10)
C12	Pd2	Si2	C40	-51.81(11)	C12	Pd2	Si2	C43	62.69(12)
Pd4	Pd3	Si2	Pd2	-12.12(4)	Pd4	Pd3	Si2	Pd4	0.000(12)
Pd4	Pd3	Si2	C40	-132.85(5)	Pd4	Pd3	Si2	C43	122.00(5)
Si2	Pd3	Pd4	Pd1	179.47(3)	Si2	Pd3	Pd4	Pd2	8.49(3)
Si2	Pd3	Pd4	Si2	0.00(3)	Si2	Pd3	Pd4	Si3	-175.27(3)
Pd4	Pd3	Si3	Pd1	6.97(4)	Pd4	Pd3	Si3	Pd4	0.000(14)
Pd4	Pd3	Si3	C46	122.66(7)	Pd4	Pd3	Si3	C49	-122.00(5)
Si3	Pd3	Pd4	Pd1	-5.25(3)	Si3	Pd3	Pd4	Pd2	-176.24(3)
Si3	Pd3	Pd4	Si2	175.27(3)	Si3	Pd3	Pd4	Si3	0.00(3)

Si2	Pd3	Si3	Pd1	10.65(6)	Si2	Pd3	Si3	Pd4	3.68(3)
Si2	Pd3	Si3	C46	126.34(6)	Si2	Pd3	Si3	C49	-118.32(5)
Si3	Pd3	Si2	Pd2	-15.95(7)	Si3	Pd3	Si2	Pd4	-3.83(3)
Si3	Pd3	Si2	C40	-136.68(4)	Si3	Pd3	Si2	C43	118.17(5)
Si2	Pd3	C23	N5	88.5(3)	Si2	Pd3	C23	N6	-86.4(3)
C23	Pd3	Si2	Pd2	165.05(15)	C23	Pd3	Si2	Pd4	177.17(15)
C23	Pd3	Si2	C40	44.32(16)	C23	Pd3	Si2	C43	-60.83(16)
Si3	Pd3	C23	N5	-90.4(3)	Si3	Pd3	C23	N6	94.7(3)
C23	Pd3	Si3	Pd1	-170.05(11)	C23	Pd3	Si3	Pd4	-177.02(11)
C23	Pd3	Si3	C46	-54.36(12)	C23	Pd3	Si3	C49	60.98(12)
Pd1	Pd4	Si1	Pd1	-0.0	Pd1	Pd4	Si1	Pd2	-174.87(3)
Pd1	Pd4	Si1	C34	-100.89(6)	Pd1	Pd4	Si1	C37	99.89(7)
Pd1	Pd4	Si3	Pd1	0.0	Pd1	Pd4	Si3	Pd3	174.88(3)
Pd1	Pd4	Si3	C46	73.11(7)	Pd1	Pd4	Si3	C49	-84.59(7)
Pd2	Pd4	Si1	Pd1	174.87(3)	Pd2	Pd4	Si1	Pd2	0.000(13)
Pd2	Pd4	Si1	C34	73.98(6)	Pd2	Pd4	Si1	C37	-85.24(6)
Pd2	Pd4	Si2	Pd2	-0.000(11)	Pd2	Pd4	Si2	Pd3	-171.20(3)
Pd2	Pd4	Si2	C40	-101.35(9)	Pd2	Pd4	Si2	C43	100.81(7)
Pd3	Pd4	Si2	Pd2	171.20(3)	Pd3	Pd4	Si2	Pd3	-0.000(12)
Pd3	Pd4	Si2	C40	69.84(8)	Pd3	Pd4	Si2	C43	-87.99(7)
Pd3	Pd4	Si3	Pd1	-174.88(3)	Pd3	Pd4	Si3	Pd3	-0.0
Pd3	Pd4	Si3	C46	-101.78(7)	Pd3	Pd4	Si3	C49	100.52(7)
Si1	Pd4	Si2	Pd2	-5.23(4)	Si1	Pd4	Si2	Pd3	-176.43(3)
Si1	Pd4	Si2	C40	-106.58(8)	Si1	Pd4	Si2	C43	95.58(8)
Si2	Pd4	Si1	Pd1	179.73(3)	Si2	Pd4	Si1	Pd2	4.86(4)
Si2	Pd4	Si1	C34	78.84(6)	Si2	Pd4	Si1	C37	-80.39(7)
Si1	Pd4	Si3	Pd1	1.15(4)	Si1	Pd4	Si3	Pd3	176.04(3)
Si1	Pd4	Si3	C46	74.26(8)	Si1	Pd4	Si3	C49	-83.44(8)
Si3	Pd4	Si1	Pd1	-1.24(4)	Si3	Pd4	Si1	Pd2	-176.11(3)
Si3	Pd4	Si1	C34	-102.13(6)	Si3	Pd4	Si1	C37	98.64(6)
Si2	Pd4	Si3	Pd1	-179.82(3)	Si2	Pd4	Si3	Pd3	-4.94(4)
Si2	Pd4	Si3	C46	-106.71(7)	Si2	Pd4	Si3	C49	95.59(7)
Si3	Pd4	Si2	Pd2	175.75(3)	Si3	Pd4	Si2	Pd3	4.55(4)
Si3	Pd4	Si2	C40	74.39(9)	Si3	Pd4	Si2	C43	-83.44(8)
Pd1	Si1	C34	C35	-62.8(2)	Pd1	Si1	C34	C36	62.7(2)
Pd1	Si1	C37	C38	-171.55(18)	Pd1	Si1	C37	C39	64.0(2)
Pd2	Si1	C34	C35	79.30(19)	Pd2	Si1	C34	C36	-155.2(2)
Pd2	Si1	C37	C38	40.4(3)	Pd2	Si1	C37	C39	-84.1(2)
Pd4	Si1	C34	C35	17.8(3)	Pd4	Si1	C34	C36	143.29(16)
Pd4	Si1	C37	C38	108.2(3)	Pd4	Si1	C37	C39	-16.3(3)
C34	Si1	C37	C38	-54.5(3)	C34	Si1	C37	C39	-178.94(19)
C37	Si1	C34	C35	-179.4(2)	C37	Si1	C34	C36	-53.9(3)
Pd2	Si2	C40	C41	-60.7(3)	Pd2	Si2	C40	C42	65.5(3)
Pd2	Si2	C43	C44	-177.13(18)	Pd2	Si2	C43	C45	58.5(3)
Pd3	Si2	C40	C41	80.0(3)	Pd3	Si2	C40	C42	-153.7(3)
Pd3	Si2	C43	C44	34.5(2)	Pd3	Si2	C43	C45	-89.9(3)
Pd4	Si2	C40	C41	21.0(4)	Pd4	Si2	C40	C42	147.25(18)
Pd4	Si2	C43	C44	103.2(2)	Pd4	Si2	C43	C45	-21.2(4)
C40	Si2	C43	C44	-59.1(3)	C40	Si2	C43	C45	176.6(3)
C43	Si2	C40	C41	-177.9(3)	C43	Si2	C40	C42	-51.7(4)
Pd1	Si3	C46	C47	-150.9(3)	Pd1	Si3	C46	C48	82.7(3)
Pd1	Si3	C49	C50	35.8(3)	Pd1	Si3	C49	C51	-86.5(3)
Pd3	Si3	C46	C47	66.5(3)	Pd3	Si3	C46	C48	-59.9(3)
Pd3	Si3	C49	C50	-176.3(2)	Pd3	Si3	C49	C51	61.5(3)
Pd4	Si3	C46	C47	147.70(19)	Pd4	Si3	C46	C48	21.3(4)
Pd4	Si3	C49	C50	103.5(2)	Pd4	Si3	C49	C51	-18.8(4)
C46	Si3	C49	C50	-58.0(3)	C46	Si3	C49	C51	179.7(3)
C49	Si3	C46	C47	-51.0(3)	C49	Si3	C46	C48	-177.4(3)
C1	N1	C2	C3	0.4(5)	C1	N1	C2	C10	177.6(4)
C2	N1	C1	Pd1	-176.1(3)	C2	N1	C1	N2	0.0(5)

C1	N1	C4	C5	-128.8(4)	C1	N1	C4	C6	102.1(4)
C4	N1	C1	Pd1	10.5(6)	C4	N1	C1	N2	-173.3(4)
C2	N1	C4	C5	59.1(6)	C2	N1	C4	C6	-69.9(6)
C4	N1	C2	C3	173.1(4)	C4	N1	C2	C10	-9.8(7)
C1	N2	C3	C2	0.7(5)	C1	N2	C3	C11	-177.7(4)
C3	N2	C1	Pd1	175.4(4)	C3	N2	C1	N1	-0.4(5)
C1	N2	C7	C8	130.4(4)	C1	N2	C7	C9	-101.7(4)
C7	N2	C1	Pd1	-9.8(7)	C7	N2	C1	N1	174.4(4)
C3	N2	C7	C8	-55.8(6)	C3	N2	C7	C9	72.1(6)
C7	N2	C3	C2	-173.6(4)	C7	N2	C3	C11	8.0(8)
C12	N3	C13	C14	1.9(5)	C12	N3	C13	C21	-179.5(4)
C13	N3	C12	Pd2	176.9(3)	C13	N3	C12	N4	-1.3(5)
C12	N3	C15	C16	-126.7(4)	C12	N3	C15	C17	104.8(4)
C15	N3	C12	Pd2	1.8(6)	C15	N3	C12	N4	-176.3(3)
C13	N3	C15	C16	59.4(6)	C13	N3	C15	C17	-69.2(5)
C15	N3	C13	C14	176.4(4)	C15	N3	C13	C21	-5.1(7)
C12	N4	C14	C13	1.0(5)	C12	N4	C14	C22	178.8(4)
C14	N4	C12	Pd2	-177.9(3)	C14	N4	C12	N3	0.2(5)
C12	N4	C18	C19	110.6(4)	C12	N4	C18	C20	-120.2(4)
C18	N4	C12	Pd2	3.0(6)	C18	N4	C12	N3	-178.9(3)
C14	N4	C18	C19	-68.3(6)	C14	N4	C18	C20	60.9(5)
C18	N4	C14	C13	180.0(4)	C18	N4	C14	C22	-2.2(8)
C23	N5	C24	C25	-0.6(4)	C23	N5	C24	C32	178.9(3)
C24	N5	C23	Pd3	-175.2(3)	C24	N5	C23	N6	0.6(4)
C23	N5	C26	C27	-121.2(4)	C23	N5	C26	C28	110.3(4)
C26	N5	C23	Pd3	5.0(5)	C26	N5	C23	N6	-179.1(3)
C24	N5	C26	C27	59.2(5)	C24	N5	C26	C28	-69.4(5)
C26	N5	C24	C25	179.0(3)	C26	N5	C24	C32	-1.4(6)
C23	N6	C25	C24	-0.1(4)	C23	N6	C25	C33	-178.4(3)
C25	N6	C23	Pd3	175.5(3)	C25	N6	C23	N5	-0.3(4)
C23	N6	C29	C30	103.3(4)	C23	N6	C29	C31	-128.7(3)
C29	N6	C23	Pd3	-0.3(5)	C29	N6	C23	N5	-176.2(3)
C25	N6	C29	C30	-71.7(5)	C25	N6	C29	C31	56.2(5)
C29	N6	C25	C24	175.4(3)	C29	N6	C25	C33	-3.0(6)
N1	C2	C3	N2	-0.6(5)	N1	C2	C3	C11	177.7(4)
C10	C2	C3	N2	-177.6(5)	C10	C2	C3	C11	0.8(9)
N3	C13	C14	N4	-1.8(5)	N3	C13	C14	C22	-179.5(4)
C21	C13	C14	N4	179.8(5)	C21	C13	C14	C22	2.1(9)
N5	C24	C25	N6	0.4(4)	N5	C24	C25	C33	178.7(3)
C32	C24	C25	N6	-179.1(4)	C32	C24	C25	C33	-0.8(7)

Table 2-7. Least Squares Planes

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

Atoms Defining Plane		Distance	esd
Pd1	[1; 0; 0; 0]	-0.0310	0.0004
Pd2	[1; 0; 0; 0]	-0.0390	0.0004
Pd4	[1; 0; 0; 0]	0.0869	0.0003
Pd3	[1; 0; 0; 0]	-0.0382	0.0004
Si1	[1; 0; 0; 0]	0.0576	0.0012
Si2	[1; 0; 0; 0]	0.1778	0.0012
Si3	[1; 0; 0; 0]	0.0575	0.0012

Least-squares plane
-8.38405x + 9.77603y + 0.31631z = 5.60783
(0.00109) (0.00109) (0.00144) (0.00130)

Mean deviation from plane is 0.0697 angstrom
Weight scheem: Sigma Weights

Chi-squared: 78571.687

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

Atoms Defining Plane		Distance	esd
N1	[1; 0; 0; 0]	0.0006	0.0045
N2	[1; 0; 0; 0]	-0.0022	0.0047
C1	[1; 0; 0; 0]	0.0013	0.0052
C2	[1; 0; 0; 0]	-0.0031	0.0058
C3	[1; 0; 0; 0]	0.0044	0.0059

Least-squares plane
8.35265x - 2.64123y + 15.08449z = 4.89848
(0.02731) (0.03331) (0.00888) (0.04217)

Mean deviation from plane is 0.0023 angstrom
Weight scheem: Sigma Weights
Chi-squared: 2.031

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

Atoms Defining Plane		Distance	esd
N3	[1; 0; 0; 0]	-0.0064	0.0049
N4	[1; 0; 0; 0]	0.0006	0.0049
C12	[1; 0; 0; 0]	0.0045	0.0053
C14	[1; 0; 0; 0]	-0.0087	0.0064
C13	[1; 0; 0; 0]	0.0123	0.0063

Least-squares plane
10.98669x + 11.65599y + 4.72860z = 14.01011
(0.02168) (0.02285) (0.03687) (0.02599)

Mean deviation from plane is 0.0065 angstrom
Weight scheem: Sigma Weights
Chi-squared: 14.606

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

Atoms Defining Plane		Distance	esd
N5	[1; 0; 0; 0]	0.0026	0.0047
N6	[1; 0; 0; 0]	0.0010	0.0047
C24	[1; 0; 0; 0]	-0.0037	0.0061
C23	[1; 0; 0; 0]	-0.0028	0.0051
C25	[1; 0; 0; 0]	0.0012	0.0062

Least-squares plane
3.10271x + 8.32522y - 10.62092z = 2.92936
(0.03247) (0.02954) (0.02747) (0.02251)

Mean deviation from plane is 0.0023 angstrom
Weight scheem: Sigma Weights
Chi-squared: 1.669

Dihedral angles between least-squares planes
---

plane	plane	angle	esd
1	2	104.347	0.122
1	3	87.518	0.130
1	4	92.416	0.125
2	3	74.314	0.193
2	4	130.870	0.189
3	4	60.441	0.197

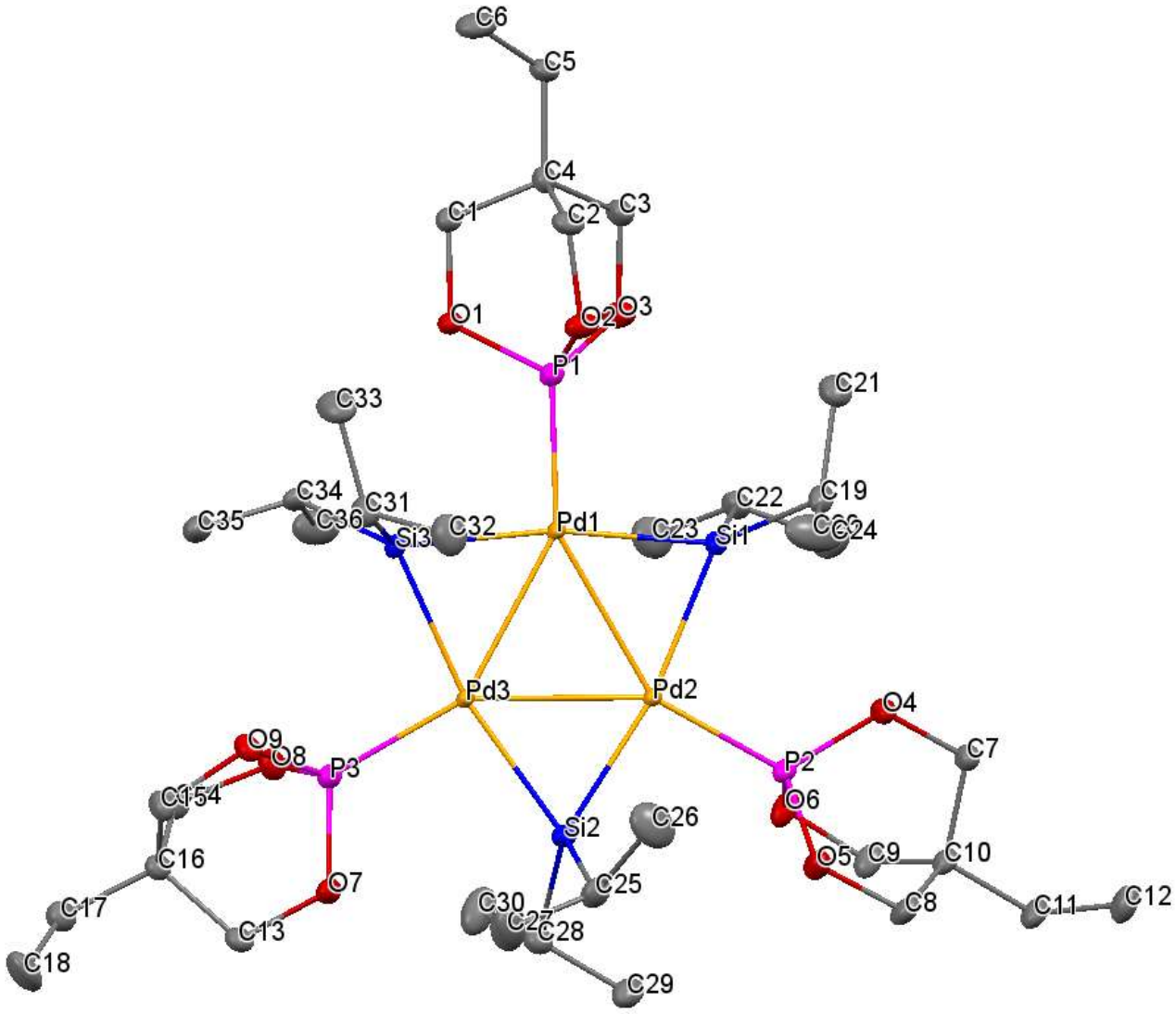


Figure S9. ORTEP drawing of **6** (50% probability of the thermal ellipsoids)

Table S3-1. Crystal data and structure refinement for **6**

Empirical Formula	$C_{36}H_{75}O_9P_3Pd_3Si_3$
Formula Weight	1148.36
Crystal Color, Habit	yellow, block
Crystal Dimensions	0.120 X 0.120 X 0.080 mm
Crystal System	triclinic
Lattice Type	Primitive
Lattice Parameters	a = 11.2891(18) Å b = 12.711(2) Å c = 19.549(3) Å α = 81.516(6) ° β = 85.854(6) ° γ = 64.096(5) ° V = 2495.6(7) Å^3
Space Group	P-1 (#2)
Z value	2
D_{calc}	1.528 g/cm^3
F_{000}	1176.00
Diffractometer	R-AXIS IV
Radiation	synchrotron (λ = 0.71075Å)
Voltage, Current	8kV, 100mA
Temperature	-170.0°C
Detector Aperture	300.0 x 300.0 mm
Data Images	360 exposures
ω oscillation Range (χ=45.0, ϕ=0.0)	0.0 - 180.0°
Exposure Rate	60.0 sec./°
Detector Swing Angle	0.00°
ω oscillation Range (χ=45.0, ϕ=90.0)	0.0 - 180.0°
Exposure Rate	60.0 sec./°
Detector Swing Angle	0.00°
Detector Position	60.00 mm
Pixel Size	0.068 mm
$2\theta_{max}$	55.0°
No. of Reflections Measured	Total: 44577 Unique: 11457 (R_{int} = 0.0682)
Corrections	Lorentz-polarization Absorption (trans. factors: 0.834 - 1.000)
Structure Solution	Direct Methods (SIR2011)
Refinement	Full-matrix least-squares on F^2
Function Minimized	Σ w (Fo^2 - Fc^2)^2
Least Squares Weights	w = 1/ [σ^2(Fo^2) + (0.0264 · P)^2 + 4.7817 · P] where P = (Max(Fo^2,0) + 2Fc^2)/3
$2\theta_{max}$ cutoff	55.0°
Anomalous Dispersion	All non-hydrogen atoms
No. Observations (All reflections)	11457
No. Variables	507
Reflection/Parameter Ratio	22.60
Residuals: R1 (I>2.00σ(I))	0.0370
Residuals: R (All reflections)	0.0523
Residuals: wR2 (All reflections)	0.0830
Goodness of Fit Indicator	1.023
Max Shift/Error in Final Cycle	0.002
Maximum peak in Final Diff. Map	2.32 e$^-$/Å^3
Minimum peak in Final Diff. Map	-0.94 e$^-$/Å^3

Table 3-2. Atomic coordinates and B_{iso}/B_{eq} and occupancy

atom	x	y	z	B_{eq}	occ
Pd1	0.40545(2)	0.64688(2)	0.69084(2)	0.756(5)	1
Pd2	0.15895(2)	0.69365(2)	0.73988(2)	0.743(5)	1
Pd3	0.36775(2)	0.50009(2)	0.79582(2)	0.751(5)	1
P1	0.54080(9)	0.68852(8)	0.61862(5)	1.108(14)	1
P2	-0.05105(8)	0.81329(8)	0.73782(5)	1.044(14)	1
P3	0.45177(9)	0.36352(8)	0.88396(5)	1.101(14)	1
Si1	0.21440(9)	0.81733(9)	0.65383(5)	1.053(16)	1
Si2	0.14509(9)	0.54421(9)	0.82409(5)	1.104(16)	1
Si3	0.57365(9)	0.46996(9)	0.74286(5)	1.036(15)	1
O1	0.6915(2)	0.6411(2)	0.64241(13)	1.33(4)	1
O2	0.5605(3)	0.6379(3)	0.54612(14)	1.50(4)	1
O3	0.5085(3)	0.8257(2)	0.59212(15)	1.76(5)	1
O4	-0.1091(3)	0.9077(2)	0.66961(14)	1.69(5)	1
O5	-0.1583(2)	0.7601(2)	0.74748(14)	1.48(4)	1
O6	-0.0964(2)	0.8994(3)	0.79694(14)	1.64(5)	1
O7	0.3583(2)	0.3185(2)	0.93423(14)	1.44(4)	1
O8	0.5123(3)	0.4095(2)	0.93893(14)	1.36(4)	1
O9	0.5739(3)	0.2381(2)	0.87387(13)	1.32(4)	1
C1	0.7797(4)	0.6711(4)	0.59428(19)	1.38(6)	1
C2	0.6621(4)	0.6495(4)	0.49974(19)	1.45(6)	1
C3	0.5939(4)	0.8441(3)	0.5380(2)	1.55(6)	1
C4	0.7123(4)	0.7306(3)	0.52554(19)	1.27(6)	1
C5	0.8041(4)	0.7601(4)	0.4727(2)	1.55(6)	1
C6	0.9242(4)	0.6549(4)	0.4510(2)	2.10(7)	1
C7	-0.2436(3)	0.9953(3)	0.6731(2)	1.48(6)	1
C8	-0.2963(3)	0.8453(3)	0.7471(2)	1.53(6)	1
C9	-0.2350(4)	0.9783(4)	0.8002(2)	1.54(6)	1
C10	-0.3095(3)	0.9705(3)	0.74075(19)	1.12(6)	1
C11	-0.4549(3)	1.0611(4)	0.7450(2)	1.57(6)	1
C12	-0.5381(4)	1.0818(4)	0.6817(2)	1.95(7)	1
C13	0.4129(4)	0.2527(4)	1.00084(19)	1.41(6)	1
C14	0.5859(4)	0.3230(3)	0.99585(19)	1.38(6)	1
C15	0.6194(4)	0.1545(3)	0.93636(19)	1.33(6)	1
C16	0.5612(3)	0.2135(3)	1.00067(18)	1.11(6)	1
C17	0.6244(4)	0.1330(4)	1.0669(2)	1.66(6)	1
C18	0.6292(5)	0.0098(4)	1.0746(2)	2.59(8)	1
C19	0.1456(4)	0.8493(4)	0.5636(2)	1.69(7)	1
C20	0.1380(6)	0.7407(5)	0.5436(3)	3.59(11)	1
C21	0.2196(4)	0.8953(4)	0.5081(2)	2.24(8)	1
C22	0.2087(4)	0.9598(3)	0.6767(2)	1.40(6)	1
C23	0.2660(5)	0.9378(4)	0.7486(2)	2.50(8)	1
C24	0.0722(4)	1.0643(4)	0.6716(3)	2.42(8)	1
C25	0.0777(4)	0.4464(4)	0.7933(2)	1.56(6)	1
C26	0.0796(5)	0.4546(5)	0.7148(2)	2.94(9)	1
C27	0.1496(5)	0.3177(4)	0.8248(3)	2.50(8)	1
C28	0.0763(4)	0.5662(4)	0.9153(2)	1.53(6)	1
C29	-0.0695(4)	0.6516(4)	0.9170(2)	2.06(7)	1
C30	0.1554(4)	0.6037(5)	0.9575(3)	2.74(9)	1
C31	0.6505(4)	0.3420(3)	0.6899(2)	1.48(6)	1
C32	0.5484(4)	0.3421(4)	0.6428(2)	2.09(7)	1
C33	0.7707(4)	0.3393(4)	0.6474(2)	2.14(7)	1
C34	0.7111(4)	0.4759(4)	0.7900(2)	1.50(6)	1
C35	0.7984(4)	0.3591(4)	0.8312(2)	2.33(8)	1
C36	0.6540(5)	0.5749(5)	0.8351(2)	2.60(8)	1
C37	0.0086(8)	1.0611(8)	0.8851(5)	1.93(14)	1/2
C38	0.0010(11)	0.9498(11)	0.9343(6)	3.7(2)	1/2
C39	-0.0002(11)	1.0246(10)	0.9459(6)	3.29(19)	1/2
C40	-0.0105(8)	0.9183(7)	0.9846(4)	1.64(13)	1/2

C41	-0.0206(11)	0.8874(11)	1.0397(6)	3.9(2)	1/2

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

Table 3-3. Anisotropic displacement parameters

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Pd1	0.00651(11)	0.00985(13)	0.01099(13)	-0.00282(10)	0.00090(9)	0.00000(10)
Pd2	0.00667(11)	0.01099(13)	0.00944(13)	-0.00339(10)	0.00021(9)	0.00049(10)
Pd3	0.00642(11)	0.01122(13)	0.01048(13)	-0.00403(10)	-0.00063(9)	0.00084(10)
P1	0.0113(4)	0.0145(5)	0.0154(5)	-0.0052(4)	0.0009(3)	-0.0007(4)
P2	0.0103(4)	0.0158(5)	0.0129(4)	-0.0052(4)	0.0008(3)	-0.0020(4)
P3	0.0119(4)	0.0158(5)	0.0145(5)	-0.0066(4)	-0.0005(3)	-0.0012(4)
Si1	0.0118(4)	0.0156(5)	0.0105(5)	-0.0046(4)	-0.0005(4)	0.0004(4)
Si2	0.0118(4)	0.0190(5)	0.0124(5)	-0.0082(4)	0.0000(4)	-0.0005(4)
Si3	0.0090(4)	0.0149(5)	0.0142(5)	-0.0041(4)	-0.0009(4)	-0.0008(4)
O1	0.0125(12)	0.0240(14)	0.0134(13)	-0.0087(11)	0.0000(10)	0.0022(11)
O2	0.0188(13)	0.0281(15)	0.0164(14)	-0.0154(12)	0.0031(10)	-0.0061(11)
O3	0.0182(13)	0.0142(13)	0.0299(16)	-0.0050(11)	0.0075(11)	-0.0002(12)
O4	0.0134(12)	0.0234(15)	0.0184(14)	-0.0026(11)	0.0027(10)	0.0046(11)
O5	0.0137(12)	0.0149(13)	0.0266(15)	-0.0059(11)	-0.0017(11)	0.0000(11)
O6	0.0129(12)	0.0262(15)	0.0214(14)	-0.0039(11)	-0.0027(10)	-0.0111(12)
O7	0.0130(12)	0.0256(15)	0.0164(14)	-0.0100(11)	-0.0028(10)	0.0025(11)
O8	0.0212(13)	0.0155(13)	0.0166(13)	-0.0090(11)	-0.0043(10)	-0.0012(10)
O9	0.0190(13)	0.0164(13)	0.0117(13)	-0.0052(11)	0.0013(10)	-0.0009(10)
C1	0.0139(16)	0.025(2)	0.0137(18)	-0.0088(15)	-0.0005(14)	0.0004(15)
C2	0.0212(18)	0.024(2)	0.0124(18)	-0.0129(16)	0.0038(14)	-0.0017(15)
C3	0.0179(18)	0.0178(19)	0.020(2)	-0.0066(15)	0.0007(15)	0.0034(15)
C4	0.0151(16)	0.0167(18)	0.0145(18)	-0.0057(14)	-0.0013(14)	0.0005(14)
C5	0.0185(18)	0.024(2)	0.0160(19)	-0.0108(16)	0.0018(14)	0.0030(15)
C6	0.026(2)	0.035(2)	0.023(2)	-0.0177(19)	0.0110(17)	-0.0090(18)
C7	0.0135(17)	0.0189(19)	0.0187(19)	-0.0038(15)	0.0010(14)	0.0020(15)
C8	0.0105(16)	0.0185(19)	0.028(2)	-0.0053(15)	0.0019(14)	-0.0023(16)
C9	0.0145(17)	0.022(2)	0.020(2)	-0.0040(15)	0.0002(14)	-0.0098(16)
C10	0.0101(15)	0.0141(17)	0.0163(18)	-0.0029(14)	0.0017(13)	-0.0042(14)
C11	0.0111(16)	0.024(2)	0.021(2)	-0.0033(15)	0.0009(14)	-0.0033(16)
C12	0.0151(18)	0.020(2)	0.035(2)	-0.0035(16)	-0.0051(16)	-0.0033(18)
C13	0.0189(18)	0.024(2)	0.0110(17)	-0.0103(16)	0.0007(14)	0.0006(15)
C14	0.0213(18)	0.0187(19)	0.0153(18)	-0.0101(16)	-0.0046(14)	-0.0035(15)
C15	0.0180(17)	0.0124(17)	0.0149(18)	-0.0021(14)	-0.0007(14)	-0.0009(14)
C16	0.0158(16)	0.0170(18)	0.0110(17)	-0.0082(14)	-0.0008(13)	-0.0021(14)
C17	0.0215(19)	0.025(2)	0.0173(19)	-0.0112(17)	-0.0025(15)	-0.0010(16)
C18	0.045(3)	0.028(2)	0.028(2)	-0.021(2)	-0.011(2)	0.0118(19)
C19	0.0143(17)	0.034(2)	0.0122(18)	-0.0076(16)	-0.0019(14)	0.0010(16)
C20	0.067(4)	0.081(4)	0.019(2)	-0.059(3)	0.001(2)	-0.011(2)
C21	0.026(2)	0.038(3)	0.017(2)	-0.012(2)	0.0010(17)	0.0016(18)
C22	0.0197(18)	0.0131(18)	0.020(2)	-0.0077(15)	0.0000(15)	0.0008(15)
C23	0.042(3)	0.031(2)	0.027(2)	-0.020(2)	-0.004(2)	-0.0074(19)
C24	0.025(2)	0.018(2)	0.045(3)	-0.0059(18)	0.0025(19)	-0.0066(19)
C25	0.0158(17)	0.023(2)	0.024(2)	-0.0107(16)	-0.0027(15)	-0.0028(16)
C26	0.056(3)	0.045(3)	0.024(2)	-0.032(3)	-0.010(2)	-0.006(2)
C27	0.035(2)	0.023(2)	0.043(3)	-0.018(2)	-0.014(2)	0.002(2)
C28	0.0207(18)	0.023(2)	0.0143(18)	-0.0105(16)	0.0001(14)	-0.0004(15)
C29	0.0177(18)	0.041(3)	0.017(2)	-0.0112(18)	0.0016(15)	-0.0027(18)
C30	0.024(2)	0.045(3)	0.031(3)	-0.006(2)	-0.0050(18)	-0.018(2)
C31	0.0191(18)	0.0150(18)	0.0185(19)	-0.0041(15)	0.0008(15)	-0.0022(15)
C32	0.034(2)	0.021(2)	0.027(2)	-0.0115(18)	-0.0053(18)	-0.0073(17)
C33	0.029(2)	0.021(2)	0.026(2)	-0.0064(18)	0.0120(18)	-0.0090(17)
C34	0.0146(17)	0.031(2)	0.0157(19)	-0.0144(16)	-0.0015(14)	0.0010(16)
C35	0.0166(18)	0.047(3)	0.023(2)	-0.0158(19)	-0.0039(16)	0.009(2)
C36	0.042(3)	0.046(3)	0.027(2)	-0.033(2)	0.003(2)	-0.012(2)

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 3-4. Bond lengths (Å)

atom	atom	distance	atom	atom	distance
Pd1	Pd2	2.7117(5)	Pd1	Pd3	2.7041(6)
Pd1	P1	2.1869(11)	Pd1	Si1	2.3557(9)
Pd1	Si3	2.3602(9)	Pd2	Pd3	2.7050(4)
Pd2	P2	2.1864(8)	Pd2	Si1	2.3707(12)
Pd2	Si2	2.3754(11)	Pd3	P3	2.1902(10)
Pd3	Si2	2.3658(11)	Pd3	Si3	2.3691(11)
P1	O1	1.615(3)	P1	O2	1.604(3)
P1	O3	1.627(3)	P2	O4	1.617(3)
P2	O5	1.613(3)	P2	O6	1.610(3)
P3	O7	1.618(3)	P3	O8	1.614(4)
P3	O9	1.617(2)	Si1	C19	1.895(4)
Si1	C22	1.902(5)	Si2	C25	1.898(5)
Si2	C28	1.903(4)	Si3	C31	1.899(4)
Si3	C34	1.895(5)	O1	C1	1.454(5)
O2	C2	1.455(5)	O3	C3	1.442(5)
O4	C7	1.442(4)	O5	C8	1.458(4)
O6	C9	1.446(4)	O7	C13	1.456(4)
O8	C14	1.453(4)	O9	C15	1.455(4)
C1	C4	1.517(5)	C2	C4	1.530(7)
C3	C4	1.516(5)	C4	C5	1.535(6)
C5	C6	1.518(5)	C7	C10	1.530(5)
C8	C10	1.519(6)	C9	C10	1.522(6)
C10	C11	1.544(4)	C11	C12	1.528(6)
C13	C16	1.523(5)	C14	C16	1.522(7)
C15	C16	1.518(5)	C16	C17	1.530(5)
C17	C18	1.527(7)	C19	C20	1.528(9)
C19	C21	1.525(7)	C22	C23	1.525(6)
C22	C24	1.531(5)	C25	C26	1.521(6)
C25	C27	1.525(5)	C28	C29	1.527(5)
C28	C30	1.517(8)	C31	C32	1.526(7)
C31	C33	1.529(6)	C34	C35	1.519(5)
C34	C36	1.522(7)	C37	C38	1.620(16)
C37	C39	1.224(14)	C37	C41[1]	1.731(17)
C38	C39	1.00(2)	C38	C40	1.026(15)
C39	C40	1.495(16)	C39	C40[1]	1.668(16)
C39	C41[1]	1.31(2)	C40	C41	1.108(15)

Symmetry Operators:

(1) -X,-Y+2,-Z+2

Table 3-5. Bond angles (°)

atom	atom	atom	angle	atom	atom	atom	angle
Pd2	Pd1	Pd3	59.929(11)	Pd2	Pd1	P1	151.20(2)
Pd2	Pd1	Si1	55.25(3)	Pd2	Pd1	Si3	115.16(3)
Pd3	Pd1	P1	148.84(2)	Pd3	Pd1	Si1	115.05(3)
Pd3	Pd1	Si3	55.28(3)	P1	Pd1	Si1	96.10(4)
P1	Pd1	Si3	93.56(4)	Si1	Pd1	Si3	170.27(4)
Pd1	Pd2	Pd3	59.895(13)	Pd1	Pd2	P2	148.47(3)
Pd1	Pd2	Si1	54.73(2)	Pd1	Pd2	Si2	114.65(2)
Pd3	Pd2	P2	151.43(3)	Pd3	Pd2	Si1	114.49(3)
Pd3	Pd2	Si2	55.05(2)	P2	Pd2	Si1	93.74(4)
P2	Pd2	Si2	96.88(4)	Si1	Pd2	Si2	169.31(3)

Pd1	Pd3	Pd2	60.175(14)	Pd1	Pd3	P3	147.75(3)
Pd1	Pd3	Si2	115.26(3)	Pd1	Pd3	Si3	54.97(2)
Pd2	Pd3	P3	148.42(3)	Pd2	Pd3	Si2	55.38(3)
Pd2	Pd3	Si3	115.09(3)	P3	Pd3	Si2	95.99(4)
P3	Pd3	Si3	94.97(4)	Si2	Pd3	Si3	167.66(4)
Pd1	P1	O1	117.91(10)	Pd1	P1	O2	114.72(14)
Pd1	P1	O3	119.53(10)	O1	P1	O2	101.45(14)
O1	P1	O3	99.44(16)	O2	P1	O3	100.69(16)
Pd2	P2	O4	118.35(10)	Pd2	P2	O5	119.70(9)
Pd2	P2	O6	113.69(11)	O4	P2	O5	99.63(16)
O4	P2	O6	100.84(14)	O5	P2	O6	101.58(16)
Pd3	P3	O7	120.31(10)	Pd3	P3	O8	110.55(11)
Pd3	P3	O9	121.17(10)	O7	P3	O8	100.59(16)
O7	P3	O9	99.83(15)	O8	P3	O9	101.01(15)
Pd1	Si1	Pd2	70.02(3)	Pd1	Si1	C19	122.87(12)
Pd1	Si1	C22	114.45(12)	Pd2	Si1	C19	119.37(17)
Pd2	Si1	C22	119.00(13)	C19	Si1	C22	107.62(19)
Pd2	Si2	Pd3	69.57(3)	Pd2	Si2	C25	116.17(13)
Pd2	Si2	C28	125.24(15)	Pd3	Si2	C25	116.29(11)
Pd3	Si2	C28	122.41(14)	C25	Si2	C28	104.7(2)
Pd1	Si3	Pd3	69.75(3)	Pd1	Si3	C31	117.54(12)
Pd1	Si3	C34	119.44(14)	Pd3	Si3	C31	116.16(15)
Pd3	Si3	C34	122.57(12)	C31	Si3	C34	107.71(17)
P1	O1	C1	117.3(2)	P1	O2	C2	117.0(3)
P1	O3	C3	115.3(2)	P2	O4	C7	117.1(2)
P2	O5	C8	116.6(3)	P2	O6	C9	116.8(3)
P3	O7	C13	116.5(3)	P3	O8	C14	116.4(3)
P3	O9	C15	115.7(2)	O1	C1	C4	110.4(3)
O2	C2	C4	110.4(3)	O3	C3	C4	112.5(3)
C1	C4	C2	108.0(3)	C1	C4	C3	108.2(3)
C1	C4	C5	111.9(3)	C2	C4	C3	107.9(3)
C2	C4	C5	112.0(3)	C3	C4	C5	108.8(3)
C4	C5	C6	115.5(4)	O4	C7	C10	110.7(3)
O5	C8	C10	111.0(3)	O6	C9	C10	111.2(3)
C7	C10	C8	108.6(3)	C7	C10	C9	107.9(4)
C7	C10	C11	111.8(3)	C8	C10	C9	108.1(3)
C8	C10	C11	111.6(4)	C9	C10	C11	108.7(3)
C10	C11	C12	115.5(3)	O7	C13	C16	110.1(3)
O8	C14	C16	110.4(3)	O9	C15	C16	111.3(3)
C13	C16	C14	108.2(3)	C13	C16	C15	108.3(3)
C13	C16	C17	111.6(3)	C14	C16	C15	108.0(3)
C14	C16	C17	108.5(4)	C15	C16	C17	112.1(3)
C16	C17	C18	115.7(4)	Si1	C19	C20	110.6(3)
Si1	C19	C21	114.3(3)	C20	C19	C21	110.3(4)
Si1	C22	C23	109.6(3)	Si1	C22	C24	114.7(3)
C23	C22	C24	110.8(3)	Si2	C25	C26	112.1(4)
Si2	C25	C27	112.5(3)	C26	C25	C27	109.8(4)
Si2	C28	C29	113.2(3)	Si2	C28	C30	112.1(3)
C29	C28	C30	110.4(4)	Si3	C31	C32	110.6(2)
Si3	C31	C33	113.7(3)	C32	C31	C33	110.0(3)
Si3	C34	C35	113.5(4)	Si3	C34	C36	109.8(3)
C35	C34	C36	111.6(4)	C38	C37	C39	38.2(9)
C38	C37	C41[1]	86.8(8)	C39	C37	C41[1]	49.1(9)
C37	C38	C39	49.0(9)	C37	C38	C40	143.8(14)
C39	C38	C40	94.9(14)	C37	C39	C38	92.9(12)
C37	C39	C40	136.0(12)	C37	C39	C40[1]	127.6(12)
C37	C39	C41[1]	86.1(11)	C38	C39	C40	43.2(9)
C38	C39	C40[1]	138.7(12)	C38	C39	C41[1]	170.0(13)
C40	C39	C40[1]	96.2(8)	C40	C39	C41[1]	137.4(11)
C40[1]	C39	C41[1]	41.5(7)	C38	C40	C39	41.9(10)

C38	C40	C39[1]	125.2(13)	C38	C40	C41	176.8(17)
C39	C40	C39[1]	83.8(8)	C39	C40	C41	135.1(12)
C39[1]	C40	C41	51.7(10)	C37[1]	C41	C39[1]	44.8(7)
C37[1]	C41	C40	131.6(13)	C39[1]	C41	C40	86.8(12)

Symmetry Operators:

(1) -X,-Y+2,-Z+2

Table 3-6. Torsion Angles(°)
(Those having bond angles > 160 or < 20 degrees are excluded.)

atom1	atom2	atom3	atom4	angle	atom1	atom2	atom3	atom4	angle
Pd2	Pd1	Pd3	Pd2	0.0	Pd2	Pd1	Pd3	P3	-158.68(3)
Pd2	Pd1	Pd3	Si2	5.942(15)	Pd2	Pd1	Pd3	Si3	177.205(17)
Pd3	Pd1	Pd2	Pd3	0.0	Pd3	Pd1	Pd2	P2	174.99(4)
Pd3	Pd1	Pd2	Si1	175.596(17)	Pd3	Pd1	Pd2	Si2	-5.888(15)
Pd2	Pd1	P1	O1	155.35(4)	Pd2	Pd1	P1	O2	-85.24(8)
Pd2	Pd1	P1	O3	34.46(12)	P1	Pd1	Pd2	Pd3	177.84(7)
P1	Pd1	Pd2	P2	-7.17(9)	P1	Pd1	Pd2	Si1	-6.57(7)
P1	Pd1	Pd2	Si2	171.95(7)	Pd2	Pd1	Si1	Pd2	0.0
Pd2	Pd1	Si1	C19	-112.73(8)	Pd2	Pd1	Si1	C22	113.67(5)
Si1	Pd1	Pd2	Pd3	-175.60(4)	Si1	Pd1	Pd2	P2	-0.60(5)
Si1	Pd1	Pd2	Si1	-0.00(4)	Si1	Pd1	Pd2	Si2	178.52(4)
Pd2	Pd1	Si3	Pd3	-2.67(4)	Pd2	Pd1	Si3	C31	107.06(5)
Pd2	Pd1	Si3	C34	-119.46(5)	Si3	Pd1	Pd2	Pd3	2.54(3)
Si3	Pd1	Pd2	P2	177.53(4)	Si3	Pd1	Pd2	Si1	178.13(4)
Si3	Pd1	Pd2	Si2	-3.35(4)	Pd3	Pd1	P1	O1	-28.27(11)
Pd3	Pd1	P1	O2	91.14(7)	Pd3	Pd1	P1	O3	-149.16(4)
P1	Pd1	Pd3	Pd2	-177.99(7)	P1	Pd1	Pd3	P3	23.33(8)
P1	Pd1	Pd3	Si2	-172.04(6)	P1	Pd1	Pd3	Si3	-0.78(7)
Pd3	Pd1	Si1	Pd2	-4.21(4)	Pd3	Pd1	Si1	C19	-116.94(6)
Pd3	Pd1	Si1	C22	109.46(5)	Si1	Pd1	Pd3	Pd2	3.99(3)
Si1	Pd1	Pd3	P3	-154.69(4)	Si1	Pd1	Pd3	Si2	9.94(4)
Si1	Pd1	Pd3	Si3	-178.80(4)	Pd3	Pd1	Si3	Pd3	0.0
Pd3	Pd1	Si3	C31	109.73(7)	Pd3	Pd1	Si3	C34	-116.78(6)
Si3	Pd1	Pd3	Pd2	-177.21(4)	Si3	Pd1	Pd3	P3	24.11(5)
Si3	Pd1	Pd3	Si2	-171.26(4)	Si3	Pd1	Pd3	Si3	0.00(4)
P1	Pd1	Si1	Pd2	176.82(4)	P1	Pd1	Si1	C19	64.10(7)
P1	Pd1	Si1	C22	-69.51(6)	Si1	Pd1	P1	O1	149.93(6)
Si1	Pd1	P1	O2	-90.66(5)	Si1	Pd1	P1	O3	29.04(7)
P1	Pd1	Si3	Pd3	179.59(4)	P1	Pd1	Si3	C31	-70.67(7)
P1	Pd1	Si3	C34	62.81(6)	Si3	Pd1	P1	O1	-28.91(7)
Si3	Pd1	P1	O2	90.50(5)	Si3	Pd1	P1	O3	-149.80(7)
Pd1	Pd2	Pd3	Pd1	0.0	Pd1	Pd2	Pd3	P3	158.26(3)
Pd1	Pd2	Pd3	Si2	-173.468(17)	Pd1	Pd2	Pd3	Si3	-2.527(15)
Pd1	Pd2	P2	O4	22.19(12)	Pd1	Pd2	P2	O5	143.96(4)
Pd1	Pd2	P2	O6	-95.86(7)	Pd1	Pd2	Si1	Pd1	-0.000(14)
Pd1	Pd2	Si1	C19	117.26(6)	Pd1	Pd2	Si1	C22	-107.57(6)
Pd1	Pd2	Si2	Pd3	6.22(4)	Pd1	Pd2	Si2	C25	-103.88(4)
Pd1	Pd2	Si2	C28	122.14(5)	Pd3	Pd2	P2	O4	-166.90(4)
Pd3	Pd2	P2	O5	-45.13(11)	Pd3	Pd2	P2	O6	75.05(10)
P2	Pd2	Pd3	Pd1	-174.52(7)	P2	Pd2	Pd3	P3	-16.26(9)
P2	Pd2	Pd3	Si2	12.01(7)	P2	Pd2	Pd3	Si3	-177.05(7)
Pd3	Pd2	Si1	Pd1	4.19(4)	Pd3	Pd2	Si1	C19	121.45(4)
Pd3	Pd2	Si1	C22	-103.39(4)	Si1	Pd2	Pd3	Pd1	-3.95(3)
Si1	Pd2	Pd3	P3	154.31(4)	Si1	Pd2	Pd3	Si2	-177.42(4)
Si1	Pd2	Pd3	Si3	-6.48(4)	Pd3	Pd2	Si2	Pd3	0.0
Pd3	Pd2	Si2	C25	-110.10(5)	Pd3	Pd2	Si2	C28	115.93(7)
Si2	Pd2	Pd3	Pd1	173.47(4)	Si2	Pd2	Pd3	P3	-28.27(4)
Si2	Pd2	Pd3	Si2	0.00(3)	Si2	Pd2	Pd3	Si3	170.94(4)

P2	Pd2	Si1	Pd1	179.68(4)	P2	Pd2	Si1	C19	-63.05(5)
P2	Pd2	Si1	C22	72.11(6)	Si1	Pd2	P2	O4	21.69(7)
Si1	Pd2	P2	O5	143.47(6)	Si1	Pd2	P2	O6	-96.35(6)
P2	Pd2	Si2	Pd3	-174.25(4)	P2	Pd2	Si2	C25	75.65(5)
P2	Pd2	Si2	C28	-58.32(7)	Si2	Pd2	P2	O4	-157.01(7)
Si2	Pd2	P2	O5	-35.23(7)	Si2	Pd2	P2	O6	84.95(6)
Pd1	Pd3	P3	O7	173.47(3)	Pd1	Pd3	P3	O8	56.96(8)
Pd1	Pd3	P3	O9	-60.76(11)	Pd1	Pd3	Si2	Pd2	-6.27(4)
Pd1	Pd3	Si2	C25	103.67(5)	Pd1	Pd3	Si2	C28	-125.79(5)
Pd1	Pd3	Si3	Pd1	0.0	Pd1	Pd3	Si3	C31	-111.58(5)
Pd1	Pd3	Si3	C34	112.71(7)	Pd2	Pd3	P3	O7	30.50(12)
Pd2	Pd3	P3	O8	-86.02(8)	Pd2	Pd3	P3	O9	156.27(4)
Pd2	Pd3	Si2	Pd2	0.0	Pd2	Pd3	Si2	C25	109.93(5)
Pd2	Pd3	Si2	C28	-119.53(7)	Pd2	Pd3	Si3	Pd1	2.68(4)
Pd2	Pd3	Si3	C31	-108.90(4)	Pd2	Pd3	Si3	C34	115.39(5)
P3	Pd3	Si2	Pd2	165.56(4)	P3	Pd3	Si2	C25	-84.51(5)
P3	Pd3	Si2	C28	46.03(7)	Si2	Pd3	P3	O7	7.43(7)
Si2	Pd3	P3	O8	-109.09(5)	Si2	Pd3	P3	O9	133.20(7)
P3	Pd3	Si3	Pd1	-167.36(4)	P3	Pd3	Si3	C31	81.06(5)
P3	Pd3	Si3	C34	-54.65(6)	Si3	Pd3	P3	O7	-166.90(7)
Si3	Pd3	P3	O8	76.58(5)	Si3	Pd3	P3	O9	-41.14(8)
Pd1	P1	O1	C1	-179.03(13)	Pd1	P1	O2	C2	-172.22(11)
Pd1	P1	O3	C3	-172.29(13)	O1	P1	O2	C2	-44.0(2)
O2	P1	O1	C1	54.8(2)	O1	P1	O3	C3	58.0(2)
O3	P1	O1	C1	-48.2(2)	O2	P1	O3	C3	-45.7(2)
O3	P1	O2	C2	58.06(19)	Pd2	P2	O4	C7	-172.18(16)
Pd2	P2	O5	C8	178.64(12)	Pd2	P2	O6	C9	-177.97(15)
O4	P2	O5	C8	-50.7(2)	O5	P2	O4	C7	56.3(3)
O4	P2	O6	C9	54.3(2)	O6	P2	O4	C7	-47.6(3)
O5	P2	O6	C9	-48.0(2)	O6	P2	O5	C8	52.5(2)
Pd3	P3	O7	C13	-163.96(12)	Pd3	P3	O8	C14	-172.62(13)
Pd3	P3	O9	C15	-179.22(14)	O7	P3	O8	C14	59.19(19)
O8	P3	O7	C13	-42.4(2)	O7	P3	O9	C15	-44.5(3)
O9	P3	O7	C13	60.8(2)	O8	P3	O9	C15	58.4(3)
O9	P3	O8	C14	-43.1(2)	Pd1	Si1	C19	C20	47.8(3)
Pd1	Si1	C19	C21	-77.5(3)	Pd1	Si1	C22	C23	-38.4(2)
Pd1	Si1	C22	C24	-163.67(16)	Pd2	Si1	C19	C20	-36.3(2)
Pd2	Si1	C19	C21	-161.53(17)	Pd2	Si1	C22	C23	41.4(2)
Pd2	Si1	C22	C24	-83.9(2)	C19	Si1	C22	C23	-178.8(2)
C19	Si1	C22	C24	56.0(3)	C22	Si1	C19	C20	-176.0(2)
C22	Si1	C19	C21	58.8(3)	Pd2	Si2	C25	C26	16.7(2)
Pd2	Si2	C25	C27	141.11(17)	Pd2	Si2	C28	C29	63.3(4)
Pd2	Si2	C28	C30	-62.4(2)	Pd3	Si2	C25	C26	-62.3(2)
Pd3	Si2	C25	C27	62.1(3)	Pd3	Si2	C28	C29	150.0(2)
Pd3	Si2	C28	C30	24.3(3)	C25	Si2	C28	C29	-74.8(3)
C25	Si2	C28	C30	159.5(2)	C28	Si2	C25	C26	159.31(18)
C28	Si2	C25	C27	-76.3(2)	Pd1	Si3	C31	C32	-33.7(3)
Pd1	Si3	C31	C33	90.6(2)	Pd1	Si3	C34	C35	169.96(14)
Pd1	Si3	C34	C36	44.3(3)	Pd3	Si3	C31	C32	46.0(3)
Pd3	Si3	C31	C33	170.34(14)	Pd3	Si3	C34	C35	86.3(2)
Pd3	Si3	C34	C36	-39.3(3)	C31	Si3	C34	C35	-52.5(3)
C31	Si3	C34	C36	-178.2(2)	C34	Si3	C31	C32	-172.2(2)
C34	Si3	C31	C33	-47.8(3)	P1	O1	C1	C4	-7.2(4)
P1	O2	C2	C4	-10.8(3)	P1	O3	C3	C4	-10.3(4)
P2	O4	C7	C10	-6.4(5)	P2	O5	C8	C10	-2.7(4)
P2	O6	C9	C10	-5.2(4)	P3	O7	C13	C16	-14.8(4)
P3	O8	C14	C16	-13.9(3)	P3	O9	C15	C16	-12.6(4)
O1	C1	C4	C2	-54.6(3)	O1	C1	C4	C3	62.0(4)
O1	C1	C4	C5	-178.2(3)	O2	C2	C4	C1	65.0(3)
O2	C2	C4	C3	-51.7(3)	O2	C2	C4	C5	-171.4(2)

O3	C3	C4	C1	-52.7(5)	O3	C3	C4	C2	63.9(4)
O3	C3	C4	C5	-174.4(3)	C1	C4	C5	C6	64.1(5)
C2	C4	C5	C6	-57.3(4)	C3	C4	C5	C6	-176.5(3)
O4	C7	C10	C8	-54.9(4)	O4	C7	C10	C9	62.1(4)
O4	C7	C10	C11	-178.5(3)	O5	C8	C10	C7	59.9(4)
O5	C8	C10	C9	-56.9(4)	O5	C8	C10	C11	-176.4(3)
O6	C9	C10	C7	-55.7(4)	O6	C9	C10	C8	61.7(4)
O6	C9	C10	C11	-177.1(3)	C7	C10	C11	C12	49.9(5)
C8	C10	C11	C12	-72.1(4)	C9	C10	C11	C12	168.9(3)
O7	C13	C16	C14	66.9(4)	O7	C13	C16	C15	-49.9(4)
O7	C13	C16	C17	-173.9(3)	O8	C14	C16	C13	-50.9(3)
O8	C14	C16	C15	66.2(3)	O8	C14	C16	C17	-172.1(2)
O9	C15	C16	C13	65.7(4)	O9	C15	C16	C14	-51.3(4)
O9	C15	C16	C17	-170.7(3)	C13	C16	C17	C18	70.5(4)
C14	C16	C17	C18	-170.3(3)	C15	C16	C17	C18	-51.2(5)
C38	C37	C39	C38	-0.0(7)	C38	C37	C39	C40	-2.4(9)
C38	C37	C39	C40[1]	171.1(16)	C38	C37	C39	C41[1]	170.0(12)
C39	C37	C38	C39	-0.0(8)	C39	C37	C38	C40	4.1(16)
C38	C37	C41[1]	C39	-6.2(5)	C38	C37	C41[1]	C40[1]	-7.8(12)
C41[1]	C37	C38	C39	7.5(6)	C41[1]	C37	C38	C40	11.6(18)
C39	C37	C41[1]	C39	0.0(6)	C39	C37	C41[1]	C40[1]	-1.7(11)
C41[1]	C37	C39	C38	-170.0(11)	C41[1]	C37	C39	C40	-172.4(16)
C41[1]	C37	C39	C40[1]	1.1(7)	C41[1]	C37	C39	C41[1]	0.0(5)
C37	C38	C39	C37	0.0(4)	C37	C38	C39	C40	177.6(9)
C37	C38	C39	C40[1]	-169(2)	C37	C38	C40	C39	-3.1(12)
C37	C38	C40	C39[1]	-14(2)	C39	C38	C40	C39	0.0(6)
C39	C38	C40	C39[1]	-10.6(14)	C40	C38	C39	C37	-177.6(9)
C40	C38	C39	C40	-0.0(4)	C40	C38	C39	C40[1]	13(2)
C37	C39	C40	C38	3.5(10)	C37	C39	C40	C39[1]	174.8(13)
C37	C39	C40	C41	-178.4(10)	C37	C39	C40[1]	C38[1]	177.5(9)
C37	C39	C40[1]	C39[1]	-175.5(10)	C37	C39	C40[1]	C41[1]	-1.6(9)
C37	C39	C41[1]	C37	0.0(4)	C37	C39	C41[1]	C40[1]	178.7(8)
C38	C39	C40	C38	-0.0(10)	C38	C39	C40	C39[1]	171.3(12)
C38	C39	C40	C41	178.2(15)	C38	C39	C40[1]	C38[1]	-16(2)
C38	C39	C40[1]	C39[1]	-9.0(18)	C38	C39	C40[1]	C41[1]	164.9(19)
C40	C39	C40[1]	C38[1]	-7.1(10)	C40	C39	C40[1]	C39[1]	0.0(6)
C40	C39	C40[1]	C41[1]	173.9(8)	C40[1]	C39	C40	C38	-171.3(9)
C40[1]	C39	C40	C39[1]	0.0(5)	C40[1]	C39	C40	C41	6.8(12)
C40	C39	C41[1]	C37	172.2(16)	C40	C39	C41[1]	C40[1]	-9.0(15)
C41[1]	C39	C40	C38	-165.3(17)	C41[1]	C39	C40	C39[1]	6.0(13)
C41[1]	C39	C40	C41	13(2)	C40[1]	C39	C41[1]	C37	-178.7(8)
C40[1]	C39	C41[1]	C40[1]	-0.0(4)	C41[1]	C39	C40[1]	C38[1]	179.1(12)
C41[1]	C39	C40[1]	C39[1]	-173.9(9)	C41[1]	C39	C40[1]	C41[1]	0.0(7)
C39	C40	C41	C37[1]	-10(2)	C39	C40	C41	C39[1]	-8.7(14)
C39[1]	C40	C41	C37[1]	-1.2(8)	C39[1]	C40	C41	C39[1]	0.0(4)

Symmetry Operators:

(1) -X,-Y+2,-Z+2

Table 3-7. Least Squares Planes

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

Atoms Defining Plane		Distance	esd
Pd1	[1; 0; 0; 0]	-0.0191	0.0005
Pd2	[1; 0; 0; 0]	-0.0000	0.0005
Pd3	[1; 0; 0; 0]	0.0366	0.0005
Si1	[1; 0; 0; 0]	0.1009	0.0013
Si2	[1; 0; 0; 0]	-0.1722	0.0013

Si3	[1; 0; 0; 0]	-0.0786	0.0013

Least-squares plane
4.70206x + 9.27045y + 15.18138z = 18.41028
(0.00180) (0.00153) (0.00216) (0.00057)

Additional Atoms		Distance	esd
P1	[1; 0; 0; 0]	-0.0930	0.0012
P2	[1; 0; 0; 0]	0.0904	0.0012
P3	[1; 0; 0; 0]	0.5037	0.0012

Mean deviation from plane is 0.0679 angstrom
Weight scheem: Sigma Weights
Chi-squared: 65270.436