Supporting Information: Understanding the Solution and Solid State Structures of Pd and Pt PSiP Pincer Supported Hydrides

Hee-Won Suh,[a] David Balcells,[b,*] Alison J. Edwards,[c,*] Louise M. Guard,[a] Nilay Hazari,[a,*] Elizabeth A. Mader,[a,*] Brandon Q. Mercado[a] and Michal Repisky[d]

[a]The Department of Chemistry, Yale University, P. O. Box 208107, New Haven, Connecticut, 06520, USA, [b]Centre for Theoretical and Computational Chemistry (CTCC), Department of Chemistry, University of Oslo, P. O. Box 1033 Blindern, 0315 Oslo, Norway, [c]Bragg Institute, Australian Nuclear Science and Technology Organization, New Illawarra Road, Lucas Heights, NSW 2234, Australia, and [d]Centre for Theoretical and Computational Chemistry (CTCC), University of Tromsø-The Arctic University of Norway, N-9037 Tromsø, Norway. E-mail: david.balcells@kjemi.uio.no, aed@ansto.gov.au, nilay.hazari@yale.edu, elizabeth.mader@yale.edu.

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X-Ray Crystallography

X-ray Data for (^{Cy}PSiP)PdH

The compound (^{Cy}PSiP)PdH crystallized in the space group $P2_1/n$ with two molecules in the asymmetric unit along with three molecules of pentane.

Table S1: Crystal data and structure refinement for (^{Cy}PSiP)PdH.

Empirical formula	$C_{89}H_{148}P_4Pd_2Si_2$
Formula weight	1610.93
Temperature/K	93
Crystal system	monoclinic
Space group	$P2_1/n$
a/Å	16.7478(3)
b/Å	22.2540(4)
c/Å	23.8470(17)
α/°	90
β/°	94.911(7)
γ/°	90
Volume/Å^3	8855.3(7)
Z	4
ρ_{calc}g/cm^3	1.208
μ/mm^{-1}	4.515
F(000)	3448.0
Crystal size/mm^3	0.2 × 0.2 × 0.2
Radiation	CuKα (λ = 1.54187)
2Θ range for data collection/°	5.442 to 127.368
Index ranges	$-19 \le h \le 19$, $-25 \le k \le 25$, $-26 \le l \le 27$
Reflections collected	204543
Independent reflections	14479 [R_{int} = 0.0855, R_{sigma} = 0.0360]
Data/restraints/parameters	14479/81/890
Goodness-of-fit on F^2	1.092
Final R indexes [I>=2σ (I)]	R_1 = 0.0388, wR_2 = 0.1027
Final R indexes [all data]	R_1 = 0.0490, wR_2 = 0.1098
Largest diff. peak/hole / e Å^{-3}	1.36/-0.79

Table S2: Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for (^{Cy}PSiP)PdH. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	***x***	***y***	***z***	**U(eq)**
Pd2	756.6(2)	446.5(2)	2358.7(2)	15.87(8)
Pd1	5757.3(2)	-542.6(2)	2327.9(2)	15.14(8)
P2	5396.8(4)	-184.8(3)	1454.7(3)	15.76(16)
Si1	6672.1(5)	248.7(3)	2388.5(3)	16.76(18)
P3	1524.9(5)	797.2(3)	3118.5(3)	19.06(17)
Si2	1675.8(5)	-343.5(3)	2394.6(3)	17.44(18)
P1	6528.1(5)	-915.5(3)	3073.8(3)	18.19(17)
P4	405.2(5)	124.3(3)	1472.0(3)	16.34(17)
C13	7539.2(19)	-586.0(13)	3093.1(13)	18.2(6)
C50	2538.6(19)	479.8(12)	3117.6(13)	18.8(7)
C58	2390.7(19)	-939.1(13)	1454.7(14)	22.5(7)

C32	4436.6(18)	224.3(13)	1372.4(13)	18.6(6)
C55	2634.3(18)	-27.8(13)	2776.3(12)	18.6(6)
C7	6165(2)	-797.2(15)	3772.9(13)	25.3(7)
C44	1181(2)	638.1(15)	3819.8(13)	25.4(7)
C46	1276(2)	803.4(18)	4873.3(15)	38.3(9)
C57	1795.7(19)	-558.3(12)	1634.5(13)	18.8(7)
C17	8396.6(19)	180.3(13)	2760.5(13)	21.2(7)
C37	4489.4(19)	788.0(13)	1743.6(14)	21.5(7)
C33	4098(2)	387.2(14)	773.8(14)	24.1(7)
C24	6170(2)	528.8(13)	672.8(14)	22.6(7)
C21	7375.8(19)	887.1(13)	1468.4(14)	21.9(7)
C15	8960(2)	-583.2(14)	3388.8(14)	24.0(7)
C42	1033(2)	2641.4(14)	3076.6(16)	33.9(9)
C51	3209.8(19)	730.6(14)	3424.4(13)	23.6(7)
C54	3397.8(19)	-268.6(13)	2756.4(13)	22.3(7)
C8	6114(2)	-121.3(16)	3898.4(14)	30.3(8)
C48	827(2)	-194.0(18)	4483.2(15)	36.9(9)
C12	6632(2)	-1118.4(17)	4266.5(14)	33.9(8)
C20	6785.2(19)	499.8(12)	1636.1(13)	17.6(7)
C68	-852(2)	-469.4(14)	773.1(14)	25.0(7)
C14	8205.3(19)	-835.5(13)	3404.2(13)	22.3(7)
C52	3968(2)	490.7(14)	3388.7(14)	25.4(7)
C63	-536.1(18)	-307.0(13)	1374.6(13)	18.5(6)
C10	6208(2)	-334(2)	4935.4(16)	46.2(11)
C40	2149(2)	2448.6(14)	2465.0(17)	36.1(9)
C19	6491(2)	976.3(14)	2758.7(14)	26.9(7)
C49	1169(2)	-39.3(15)	3923.1(14)	27.7(8)
C11	6255(2)	-998(2)	4820.2(15)	44.5(10)
C53	4063(2)	-10.1(14)	3054.2(14)	25.6(7)
C35	3322(2)	1239.8(14)	1150.2(15)	28.4(8)
C39	2036(2)	1770.6(14)	2536.7(15)	29.1(8)
C61	1214(2)	-523.1(14)	661.3(14)	23.2(7)
C18	7628.2(18)	-68.5(13)	2764.5(12)	17.9(6)
C16	9055.2(19)	-73.7(14)	3065.1(14)	24.0(7)
C36	3673(2)	1096.2(14)	1741.3(15)	28.7(8)
C59	2407(2)	-1098.9(14)	895.9(14)	26.4(7)
C56	1518(2)	-1090.3(14)	2741.3(14)	27.4(7)
C69	310.0(18)	727.8(13)	935.1(12)	17.5(6)
C38	1694.8(19)	1616.1(13)	3095.8(14)	23.2(7)
C25	6172.3(18)	321.0(12)	1228.9(13)	17.6(6)
C43	920(2)	1967.6(14)	3164.5(15)	29.1(8)
C9	5739(2)	-9.9(19)	4452.1(15)	40.9(10)
C70	1083.5(19)	1104.8(14)	982.8(14)	24.8(7)
C45	1638(2)	959.1(16)	4319.2(14)	31.4(8)
C62	1195.8(18)	-355.4(13)	1226.2(13)	17.4(6)
C34	3274.5(19)	678.4(14)	779.8(15)	26.6(7)
C41	1360(2)	2777.2(14)	2516.0(16)	36.0(9)
C71	1023(2)	1651.1(14)	594.3(15)	27.6(8)
C30	4623.6(19)	-1186.6(14)	957.4(14)	23.3(7)

C74	-428.6(19)	1115.6(13)	1001.1(14)	22.8(7)
C73	-463(2)	1666.5(14)	617.7(15)	26.9(7)
C67	-1671.2(19)	-771.4(14)	767.1(15)	27.8(8)
C23	6770.9(19)	910.3(15)	522.5(14)	25.9(7)
C31	5335.8(18)	-769.7(13)	899.2(12)	18.3(6)
C65	-1287(2)	-1189.9(14)	1731.8(15)	28.5(8)
C66	-1619(2)	-1334.3(15)	1133.0(16)	31.5(8)
C1	6713.4(19)	-1730.2(13)	3027.9(13)	22.0(7)
C22	7372(2)	1088.4(14)	921.1(14)	25.4(7)
C72	304(2)	2038.6(14)	701.6(15)	29.7(8)
C2	7057(2)	-1862.7(14)	2464.4(14)	26.2(7)
C64	-477.4(19)	-871.3(13)	1741.5(14)	23.3(7)
C26	6124.0(19)	-1117.4(14)	927.1(14)	24.2(7)
C29	4613(2)	-1721.9(14)	555.3(14)	25.1(7)
C28	5401(2)	-2067.0(14)	625.8(15)	29.6(8)
C5	6078(2)	-2763.3(14)	2983.3(15)	33.3(8)
C3	7192(2)	-2536.0(14)	2378.6(16)	33.0(8)
C4	6415(2)	-2880.9(14)	2419.3(16)	34.8(9)
C60	1818.9(19)	-889.5(15)	499.2(14)	27.2(8)
C27	6091(2)	-1649.5(14)	522.0(15)	28.7(8)
C47	1286(2)	133.0(18)	4972.7(15)	38.9(9)
C6	5949(2)	-2098.3(14)	3080.9(15)	28.4(8)
C85	6522(4)	-2403(2)	5590(2)	78.7(16)
C87	5712(3)	-2389(2)	6438(2)	63.3(12)
C86	5715(3)	-2288(3)	5820(2)	77.6(15)
C88	4910(3)	-2265(2)	6663(2)	64.1(13)
C89	4918(4)	-2388(2)	7304(2)	77.7(16)
C83	1650(6)	3368(4)	208(4)	165(4)
C82	2285(5)	3676(3)	-127(3)	128(3)
C80	3203(7)	3665(4)	-924(4)	166(4)
C81	2513(7)	3323(4)	-641(4)	165(4)
C84	1481(6)	3709(5)	823(5)	177(4)
C79	6598(4)	2590(2)	736(2)	84.1(18)
C78	6090(3)	2437(2)	1210(2)	78.1(16)
C75	3877(3)	2937(2)	936(2)	71.5(14)
C76	4761(4)	2944(3)	1062(3)	117(3)
C77	5183(4)	2416(3)	1092(3)	108(2)

Table S3: Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for (^{Cy}PSiP)PdH. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	$\mathbf{U_{11}}$	$\mathbf{U_{22}}$	$\mathbf{U_{33}}$	$\mathbf{U_{23}}$	$\mathbf{U_{13}}$	$\mathbf{U_{12}}$
Pd2	16.72(14)	12.79(12)	18.04(14)	-2.71(8)	1.17(9)	1.01(8)
Pd1	16.37(14)	13.02(12)	15.87(13)	1.79(8)	0.45(9)	-0.87(8)
P2	16.2(4)	13.9(4)	17.1(4)	1.1(3)	1.1(3)	-0.8(3)
Si1	18.7(4)	13.0(4)	18.4(4)	0.1(3)	0.3(3)	-1.2(3)
P3	18.8(4)	17.2(4)	21.0(4)	-5.3(3)	0.7(3)	1.0(3)
Si2	20.6(5)	13.0(4)	18.7(4)	-1.1(3)	1.5(3)	1.3(3)
P1	18.3(4)	18.1(4)	18.1(4)	3.9(3)	0.9(3)	-0.6(3)
P4	16.1(4)	14.4(4)	18.5(4)	-1.3(3)	1.6(3)	-0.2(3)

C13	19.4(17)	17.3(15)	17.8(16)	-2.3(12)	0.3(13)	-1.3(12)
C50	19.5(17)	16.6(15)	20.3(17)	1.5(12)	2.0(13)	0.6(12)
C58	21.5(18)	19.9(16)	25.8(18)	-3.5(13)	0.3(14)	0.6(13)
C32	17.1(17)	18.4(15)	20.3(16)	2.1(12)	2.3(13)	2.5(12)
C55	18.9(17)	19.4(15)	17.3(16)	2.2(12)	0.2(12)	2.0(12)
C7	20.2(18)	36.5(19)	19.1(17)	4.9(14)	0.0(13)	-0.2(14)
C44	25.0(19)	31.3(18)	19.9(18)	-8.6(14)	2.1(14)	1.2(14)
C46	32(2)	61(3)	21.7(19)	-13.6(17)	-2.0(15)	3.4(18)
C57	19.7(17)	13.1(14)	23.7(17)	-2.3(12)	2.8(13)	-0.7(12)
C17	23.9(18)	16.5(15)	23.1(17)	2.2(12)	1.0(13)	-3.4(13)
C37	20.8(17)	18.1(15)	25.5(18)	-2.7(13)	1.2(13)	0.1(13)
C33	22.6(18)	25.9(17)	23.5(18)	3.2(13)	0.5(14)	2.4(13)
C24	20.3(18)	26.4(17)	20.8(18)	4.1(13)	0.9(14)	2.7(13)
C21	19.5(17)	18.5(15)	27.4(18)	4.2(13)	-0.3(13)	-0.7(13)
C15	20.0(18)	22.7(16)	28.7(19)	-2.2(13)	-1.8(14)	2.1(13)
C42	37(2)	19.3(17)	45(2)	-12.9(15)	-4.1(17)	7.6(15)
C51	23.1(18)	22.6(16)	24.2(18)	-3.7(13)	-2.1(14)	1.0(13)
C54	26.4(18)	18.5(15)	22.0(17)	-1.8(13)	1.8(14)	5.8(13)
C8	23.7(19)	40(2)	27.5(19)	-3.8(15)	2.4(15)	5.1(15)
C48	33(2)	48(2)	31(2)	1.5(17)	7.8(16)	-6.3(17)
C12	34(2)	43(2)	24.3(19)	8.4(16)	2.8(15)	2.0(17)
C20	17.6(17)	12.5(14)	22.6(17)	1.4(11)	1.9(13)	1.8(11)
C68	23.5(19)	26.0(17)	25.4(19)	-2.6(13)	1.1(14)	-2.5(13)
C14	25.3(18)	19.0(15)	22.3(17)	3.6(13)	-0.8(13)	1.0(13)
C52	24.4(19)	23.8(17)	27.2(19)	-0.6(13)	-1.9(15)	-2.6(13)
C63	17.1(17)	18.8(15)	20.0(16)	-2.6(12)	3.7(13)	-2.8(12)
C10	32(2)	83(3)	24(2)	-5(2)	3.6(17)	12(2)
C40	42(2)	18.5(17)	48(2)	-1.2(15)	4.7(18)	-5.4(15)
C19	30(2)	20.6(16)	30.0(19)	-4.1(14)	0.2(15)	1.4(14)
C49	27.1(19)	30.2(18)	26.0(19)	-1.1(14)	4.5(15)	-3.0(14)
C11	34(2)	79(3)	20(2)	13.5(19)	1.1(16)	3(2)
C53	22.5(18)	24.6(17)	29.1(19)	2.0(14)	-0.6(14)	6.4(14)
C35	19.3(18)	19.6(16)	46(2)	4.6(15)	1.7(15)	1.9(13)
C39	31(2)	19.2(16)	37(2)	-1.7(14)	4.4(16)	2.9(14)
C61	20.5(18)	27.2(17)	21.8(18)	-1.3(13)	0.4(14)	-1.3(13)
C18	21.0(17)	18.0(15)	14.3(15)	-4.3(12)	-0.2(12)	-0.2(12)
C16	19.2(17)	22.0(16)	30.6(19)	-1.5(14)	1.1(14)	-3.6(13)
C36	24.1(19)	18.6(16)	44(2)	-5.8(14)	5.3(16)	2.0(13)
C59	20.4(18)	26.6(17)	33(2)	-9.3(14)	6.2(15)	2.5(14)
C56	33(2)	20.1(16)	29.0(19)	-1.1(14)	3.0(15)	-0.6(14)
C69	19.0(17)	16.8(15)	16.4(16)	-0.6(12)	-1.1(12)	-1.9(12)
C38	21.5(18)	16.2(15)	31.4(19)	-8.0(13)	0.0(14)	-0.7(13)
C25	20.5(17)	11.7(14)	20.9(17)	1.9(12)	3.5(13)	1.4(12)
C43	28(2)	23.3(17)	36(2)	-9.6(14)	0.8(15)	6.9(14)
C9	31(2)	65(3)	28(2)	-6.7(18)	4.5(16)	9.7(19)
C70	18.6(17)	23.1(16)	32.5(19)	1.7(14)	1.2(14)	-4.8(13)
C45	32(2)	34.3(19)	27.6(19)	-9.4(15)	-1.7(15)	-1.1(15)
C62	18.9(17)	13.9(14)	19.5(16)	-1.5(12)	3.1(13)	-1.5(12)
C34	22.2(18)	23.5(16)	34(2)	6.7(14)	-0.1(15)	2.0(14)

C41	42(2)	15.9(16)	48(2)	-3.4(15)	-3.5(18)	2.2(15)
C71	27.6(19)	22.4(17)	33(2)	4.0(14)	2.3(15)	-5.8(14)
C30	21.3(18)	22.2(16)	26.2(18)	-1.9(13)	1.1(14)	-1.7(13)
C74	18.9(17)	20.6(16)	28.9(18)	3.3(13)	1.2(14)	0.3(13)
C73	26.6(19)	21.2(16)	32(2)	4.4(14)	-1.3(15)	2.1(14)
C67	19.7(18)	27.9(17)	35(2)	-8.0(15)	-2.1(14)	-4.3(14)
C23	23.1(18)	31.5(18)	23.8(18)	11.6(14)	5.6(14)	0.6(14)
C31	21.3(17)	17.4(15)	15.8(16)	-0.4(12)	-0.9(12)	1.0(12)
C65	26.6(19)	18.2(16)	42(2)	3.0(14)	8.2(16)	-2.6(14)
C66	23.1(19)	23.0(17)	48(2)	-5.3(15)	3.1(16)	-4.1(14)
C1	23.9(18)	15.7(15)	26.0(18)	7.6(13)	0.7(14)	-1.1(13)
C22	22.0(18)	23.0(16)	32(2)	7.2(14)	4.4(14)	-1.8(13)
C72	35(2)	19.2(16)	34(2)	4.6(14)	-1.4(16)	-0.2(14)
C2	25.9(19)	19.6(16)	34(2)	2.1(14)	6.5(15)	-2.9(13)
C64	24.1(18)	20.4(16)	25.9(18)	-0.7(13)	6.0(14)	-1.2(13)
C26	22.6(18)	22.6(16)	27.1(18)	-2.5(13)	0.2(14)	2.6(13)
C29	28.1(19)	19.8(16)	26.8(18)	-4.8(13)	-1.5(14)	-6.0(13)
C28	41(2)	17.5(16)	29.8(19)	-4.4(14)	-0.9(16)	1.3(14)
C5	38(2)	19.2(17)	42(2)	12.4(15)	-4.4(17)	-8.3(15)
C3	36(2)	19.5(17)	43(2)	-1.6(15)	4.6(17)	0.8(15)
C4	41(2)	16.5(16)	45(2)	5.3(15)	-7.5(17)	-4.3(15)
C60	23.9(19)	33.8(18)	24.4(18)	-12.0(14)	5.1(14)	-2.3(14)
C27	28(2)	25.1(17)	32(2)	-5.4(14)	-0.7(15)	7.8(14)
C47	33(2)	60(3)	24(2)	0.9(17)	5.7(16)	-1.4(18)
C6	26.0(19)	25.4(17)	34(2)	9.8(14)	0.8(15)	-6.6(14)
C85	108(4)	41(3)	86(4)	-16(3)	5(3)	7(3)
C87	78(3)	38(2)	70(3)	4(2)	-11(2)	-2(2)
C86	93(4)	76(4)	61(3)	3(3)	-9(3)	-1(3)
C88	76(3)	40(2)	74(3)	-2(2)	-3(3)	-6(2)
C89	110(5)	48(3)	74(3)	-6(2)	-4(3)	-7(3)
C83	172(8)	99(6)	219(9)	65(6)	-6(7)	-34(6)
C82	146(6)	61(4)	172(7)	6(4)	-20(5)	1(4)
C80	264(11)	142(8)	86(6)	-30(5)	-26(6)	29(7)
C81	292(12)	96(6)	102(6)	12(4)	-11(6)	44(6)
C84	141(8)	139(8)	251(11)	-10(7)	16(8)	8(7)
C79	134(5)	34(2)	77(4)	-10(2)	-36(3)	-17(3)
C78	91(4)	58(3)	78(4)	-19(3)	-38(3)	0(3)
C75	91(4)	46(3)	77(4)	-9(2)	6(3)	5(3)
C76	90(4)	105(5)	150(7)	-77(4)	-19(4)	4(3)
C77	100(4)	105(5)	110(5)	-54(4)	-45(4)	22(3)

Table S4: Bond lengths for (^{Cy}PSiP)PdH.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Pd2	P3	2.2689(8)	C8	C9	1.530(5)
Pd2	Si2	2.3335(8)	C48	C49	1.536(5)
Pd2	P4	2.2626(8)	C48	C47	1.526(5)
Pd1	P2	2.2626(8)	C12	C11	1.534(5)
Pd1	Si1	2.3303(8)	C20	C25	1.409(4)
Pd1	P1	2.2641(8)	C68	C63	1.529(4)

P2	C32	1.844(3)	C68	C67	1.527(4)
P2	C25	1.834(3)	C52	C53	1.387(4)
P2	C31	1.854(3)	C63	C64	1.529(4)
Si1	C20	1.904(3)	C10	C11	1.507(6)
Si1	C19	1.881(3)	C10	C9	1.520(5)
Si1	C18	1.903(3)	C40	C39	1.532(4)
P3	C50	1.839(3)	C40	C41	1.525(5)
P3	C44	1.849(3)	C35	C36	1.514(5)
P3	C38	1.846(3)	C35	C34	1.528(5)
Si2	C55	1.910(3)	C39	C38	1.533(5)
Si2	C57	1.902(3)	C61	C62	1.401(4)
Si2	C56	1.885(3)	C61	C60	1.381(5)
P1	C13	1.842(3)	C59	C60	1.386(5)
P1	C7	1.842(3)	C69	C70	1.539(4)
P1	C1	1.844(3)	C69	C74	1.527(4)
P4	C63	1.843(3)	C38	C43	1.535(4)
P4	C69	1.853(3)	C70	C71	1.527(4)
P4	C62	1.835(3)	C71	C72	1.520(5)
C13	C14	1.401(4)	C30	C31	1.527(4)
C13	C18	1.408(4)	C30	C29	1.528(4)
C50	C55	1.410(4)	C74	C73	1.528(4)
C50	C51	1.404(4)	C73	C72	1.527(5)
C58	C57	1.403(4)	C67	C66	1.525(5)
C58	C59	1.382(5)	C23	C22	1.382(5)
C32	C37	1.533(4)	C31	C26	1.527(4)
C32	C33	1.534(4)	C65	C66	1.522(5)
C55	C54	1.391(4)	C65	C64	1.528(4)
C7	C8	1.538(5)	C1	C2	1.535(4)
C7	C12	1.533(5)	C1	C6	1.534(4)
C44	C49	1.528(4)	C2	C3	1.532(4)
C44	C45	1.535(5)	C26	C27	1.526(4)
C46	C45	1.539(5)	C29	C28	1.524(5)
C46	C47	1.511(6)	C28	C27	1.520(5)
C57	C62	1.412(4)	C5	C4	1.525(5)
C17	C18	1.402(4)	C5	C6	1.516(5)
C17	C16	1.388(4)	C3	C4	1.522(5)
C37	C36	1.529(4)	C85	C86	1.524(7)
C33	C34	1.525(4)	C87	C86	1.491(6)
C24	C25	1.404(4)	C87	C88	1.514(6)
C24	C23	1.387(4)	C88	C89	1.551(6)
C21	C20	1.396(4)	C83	C82	1.545(9)
C21	C22	1.379(5)	C83	C84	1.696(10)
C15	C14	1.386(5)	C82	C81	1.531(9)
C15	C16	1.388(4)	C80	C81	1.581(10)
C42	C43	1.528(4)	C79	C78	1.512(7)
C42	C41	1.517(5)	C78	C77	1.522(7)
C51	C52	1.387(5)	C75	C76	1.484(7)
C54	C53	1.393(5)	C76	C77	1.369(7)

Table S5: Bond angles for (^{Cy}PSiP)PdH.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
P3	Pd2	Si2	84.41(3)	C21	C20	C25	118.0(3)
P4	Pd2	P3	160.00(3)	C25	C20	Si1	116.2(2)
P4	Pd2	Si2	85.04(3)	C67	C68	C63	110.6(3)
P2	Pd1	Si1	85.03(3)	C15	C14	C13	120.8(3)
P2	Pd1	P1	160.28(3)	C51	C52	C53	119.7(3)
P1	Pd1	Si1	84.30(3)	C68	C63	P4	117.7(2)
C32	P2	Pd1	115.67(10)	C64	C63	P4	110.1(2)
C32	P2	C31	106.05(14)	C64	C63	C68	110.0(2)
C25	P2	Pd1	110.26(10)	C11	C10	C9	111.1(3)
C25	P2	C32	107.39(13)	C41	C40	C39	110.3(3)
C25	P2	C31	102.61(13)	C44	C49	C48	111.9(3)
C31	P2	Pd1	113.86(10)	C10	C11	C12	111.1(3)
C20	Si1	Pd1	106.33(10)	C52	C53	C54	119.9(3)
C19	Si1	Pd1	123.23(11)	C36	C35	C34	111.2(3)
C19	Si1	C20	102.86(14)	C40	C39	C38	112.1(3)
C19	Si1	C18	105.13(14)	C60	C61	C62	120.2(3)
C18	Si1	Pd1	105.74(9)	C13	C18	Si1	116.1(2)
C18	Si1	C20	113.91(13)	C17	C18	Si1	125.9(2)
C50	P3	Pd2	109.11(10)	C17	C18	C13	117.9(3)
C50	P3	C44	106.64(15)	C17	C16	C15	120.0(3)
C50	P3	C38	103.56(14)	C35	C36	C37	111.9(3)
C44	P3	Pd2	117.22(11)	C58	C59	C60	120.0(3)
C38	P3	Pd2	113.23(11)	C70	C69	P4	108.8(2)
C38	P3	C44	106.04(15)	C74	C69	P4	111.2(2)
C55	Si2	Pd2	105.39(9)	C74	C69	C70	111.6(2)
C57	Si2	Pd2	106.12(10)	C39	C38	P3	108.5(2)
C57	Si2	C55	113.18(14)	C39	C38	C43	111.1(3)
C56	Si2	Pd2	124.30(11)	C43	C38	P3	111.5(2)
C56	Si2	C55	105.01(14)	C24	C25	P2	122.3(2)
C56	Si2	C57	103.09(14)	C24	C25	C20	120.1(3)
C13	P1	Pd1	109.56(10)	C20	C25	P2	117.6(2)
C13	P1	C1	103.52(14)	C42	C43	C38	111.7(3)
C7	P1	Pd1	116.65(11)	C10	C9	C8	110.7(3)
C7	P1	C13	107.13(15)	C71	C70	C69	112.2(3)
C7	P1	C1	105.34(15)	C44	C45	C46	110.8(3)
C1	P1	Pd1	113.65(11)	C57	C62	P4	117.1(2)
C63	P4	Pd2	115.72(10)	C61	C62	P4	122.5(2)
C63	P4	C69	105.56(14)	C61	C62	C57	120.3(3)
C69	P4	Pd2	114.59(10)	C33	C34	C35	110.5(3)
C62	P4	Pd2	110.22(10)	C42	C41	C40	110.8(3)
C62	P4	C63	106.83(13)	C72	C71	C70	111.2(3)
C62	P4	C69	102.87(13)	C31	C30	C29	112.6(3)
C14	C13	P1	123.0(2)	C69	C74	C73	112.4(3)
C14	C13	C18	120.1(3)	C72	C73	C74	111.6(3)
C18	C13	P1	116.9(2)	C66	C67	C68	110.4(3)
C55	C50	P3	117.3(2)	C22	C23	C24	120.0(3)
C51	C50	P3	123.0(2)	C30	C31	P2	110.9(2)

C51	C50	C55	119.6(3)	C26	C31	P2	109.3(2)
C59	C58	C57	121.5(3)	C26	C31	C30	111.6(2)
C37	C32	P2	109.6(2)	C66	C65	C64	111.4(3)
C37	C32	C33	110.0(2)	C65	C66	C67	111.2(3)
C33	C32	P2	117.7(2)	C2	C1	P1	108.6(2)
C50	C55	Si2	115.9(2)	C6	C1	P1	112.0(2)
C54	C55	Si2	125.4(2)	C6	C1	C2	110.3(3)
C54	C55	C50	118.6(3)	C21	C22	C23	120.1(3)
C8	C7	P1	110.1(2)	C71	C72	C73	109.9(3)
C12	C7	P1	116.3(2)	C3	C2	C1	112.1(3)
C12	C7	C8	109.9(3)	C65	C64	C63	111.0(3)
C49	C44	P3	110.2(2)	C27	C26	C31	112.4(3)
C49	C44	C45	110.3(3)	C28	C29	C30	111.1(3)
C45	C44	P3	116.1(2)	C27	C28	C29	109.7(3)
C47	C46	C45	110.9(3)	C6	C5	C4	111.8(3)
C58	C57	Si2	125.4(2)	C4	C3	C2	110.3(3)
C58	C57	C62	117.7(3)	C3	C4	C5	110.7(3)
C62	C57	Si2	116.7(2)	C61	C60	C59	120.1(3)
C16	C17	C18	121.6(3)	C28	C27	C26	111.0(3)
C36	C37	C32	110.9(3)	C46	C47	C48	110.7(3)
C34	C33	C32	110.8(3)	C5	C6	C1	112.2(3)
C23	C24	C25	120.2(3)	C86	C87	C88	113.6(4)
C22	C21	C20	121.7(3)	C87	C86	C85	114.1(5)
C14	C15	C16	119.6(3)	C87	C88	C89	112.6(4)
C41	C42	C43	112.0(3)	C82	C83	C84	115.0(7)
C52	C51	C50	120.8(3)	C81	C82	C83	114.7(8)
C55	C54	C53	121.4(3)	C82	C81	C80	109.6(8)
C9	C8	C7	111.1(3)	C79	C78	C77	119.0(5)
C47	C48	C49	111.0(3)	C77	C76	C75	120.3(6)
C7	C12	C11	111.1(3)	C76	C77	C78	119.2(6)
C21	C20	Si1	125.5(2)				

X-ray Data for (^{Cy}PSiP)PtH

Polymorph 1

The compound (^{Cy}PSiP)PtH crystallized in the space group *C2/c* with two molecules in the asymmetric unit along with three molecules of pentane which were disordered.

Table S6: Crystal data and structure refinement for (^{Cy}PSiP)PtH.

Empirical formula	$C_{173}H_{284}P_8Pt_4Si_4$
Formula weight	1752.23
Temperature/K	93
Crystal system	monoclinic
Space group	C2/c
a/Å	29.5946(5)
b/Å	17.3883(3)
c/Å	33.970(2)
α/°	90

β/°	99.690(7)
γ/°	90
Volume/Å^3	17231.5(12)
Z	4
ρ_{calc}mg/mm^3	1.351
m/mm^{-1}	7.249
F(000)	7240.0
Crystal size/mm^3	0.05 × 0.01 × 0.01
Radiation	CuKα (λ = 1.54187)
2Θ range for data collection	5.278 to 136.706°
Index ranges	-35 ≤ h ≤ 35, -19 ≤ k ≤ 20, -40 ≤ l ≤ 40
Reflections collected	297570
Independent reflections	15754[R(int) = 0.0661]
Data/restraints/parameters	15754/204/902
Goodness-of-fit on F^2	1.047
Final R indexes [I>=2σ (I)]	R_1 = 0.0271, wR_2 = 0.0669
Final R indexes [all data]	R_1 = 0.0283, wR_2 = 0.0676
Largest diff. peak/hole / e Å^{-3}	1.08/-0.88

Table S7: Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for (^{Cy}PSiP)PtH. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	***x***	***y***	***z***	**U(eq)**
Pt1	3251.0(2)	5895.8(2)	3484.0(2)	23.59(4)
Pt2	5699.6(2)	8805.4(2)	4067.4(2)	24.10(4)
P3	5926.4(2)	7589.4(4)	4231.0(2)	24.47(15)
P1	3409.5(2)	5042.3(4)	3991.6(2)	24.74(15)
Si2	6210.2(3)	8748.8(5)	3616.5(2)	25.74(17)
P2	3332.2(2)	6806.6(4)	3026.1(2)	24.88(15)
P4	5705.4(3)	10083.5(5)	3970.9(2)	29.51(16)
Si1	3606.4(3)	6791.3(5)	3948.2(2)	27.36(17)
C50	6485.7(10)	7418.9(18)	4079.5(8)	26.4(6)
C13	3871.7(10)	5420.9(18)	4371.5(8)	27.9(6)
C45	5565.9(11)	7416(2)	4927.2(9)	34.0(7)
C62	6223.3(10)	10349.0(19)	3770.0(9)	31.3(7)
C54	7061.6(10)	7824.9(19)	3699.2(9)	30.4(6)
C44	6028.8(10)	7414.7(19)	4777.2(9)	29.2(6)
C55	6630.9(10)	7948.9(17)	3812.0(8)	26.2(6)
C57	6469.5(10)	9750.3(19)	3622.3(9)	29.3(6)
C51	6768.0(11)	6799.8(19)	4228.0(9)	32.4(7)
C23	4407.8(11)	8349(2)	3165.2(10)	36.4(7)
C17	4319.5(12)	6507(2)	4652.1(9)	38.1(8)
C38	5529.1(10)	6829.8(18)	4011.6(9)	28.8(6)
C25	3809.7(10)	7439.4(17)	3236.0(9)	26.5(6)
C21	4330.3(10)	7888.0(18)	3813.7(9)	30.2(6)
C31	3917.0(11)	5908(2)	2665.1(9)	33.8(7)
C56	6040.8(12)	8526(2)	3067.5(9)	37.4(7)
C20	3953(1)	7422.7(17)	3654.3(9)	26.8(6)
C12	2775.5(11)	5497(2)	4463.2(10)	35.3(7)
C26	3505.4(10)	6451.7(18)	2562.3(8)	27.8(6)
C18	3975.3(11)	6208.2(19)	4353.0(9)	30.0(7)

C39	5439.6(10)	6881.0(19)	3553.4(9)	30.3(7)
C1	3638(1)	4123.6(18)	3844.4(9)	28.7(6)
C8	3027.2(11)	4121(2)	4563.7(10)	35.3(7)
C22	4554.4(11)	8342.3(19)	3576.3(10)	35.6(7)
C41	5147.0(12)	5514(2)	3515(1)	40.3(8)
C47	5916.0(13)	8138(2)	5545.9(9)	42.1(8)
C24	4037.9(11)	7904.8(19)	2996.9(9)	32.7(7)
C53	7339.5(11)	7220(2)	3852.6(10)	34.7(7)
C7	2938.7(10)	4786.3(19)	4261.5(9)	29.3(6)
C2	4045.0(11)	4276(2)	3630.2(10)	34.1(7)
C11	2345.6(12)	5311(2)	4637.1(10)	42.5(8)
C3	4228.5(12)	3532(2)	3475.6(11)	42.6(8)
C5	3459.5(13)	2911(2)	3435.7(10)	41.4(8)
C60	6781.0(13)	11284(2)	3627.0(12)	44.5(9)
C69	5755.9(11)	10647(2)	4434.5(10)	36.5(7)
C6	3263.0(11)	3649.0(19)	3585.9(10)	33.7(7)
C63	5211.3(11)	10494.9(19)	3637.1(10)	37.1(7)
C27	3118.4(11)	6062(2)	2275.5(9)	34.6(7)
C14	4112.3(10)	4956(2)	4676.1(9)	32.8(7)
C9	2590.1(12)	3933(2)	4731.2(10)	41.6(8)
C46	5614.0(12)	7468(2)	5382.3(9)	39.1(8)
C52	7194.6(11)	6708(2)	4117(1)	35.0(7)
C10	2420.1(12)	4632(2)	4926.8(10)	46.7(9)
C58	6870.9(11)	9955(2)	3473.7(10)	35.1(7)
C43	5650.4(12)	5997.8(19)	4138.7(10)	36.2(7)
C49	6359.3(11)	8035(2)	4978.3(9)	35.0(7)
C70	5316.1(12)	10671(2)	4615.8(12)	43.4(8)
C32	2833.6(10)	7424.8(19)	2851.3(10)	32.3(7)
C74	6147.4(12)	10315(2)	4734.9(11)	46.0(9)
C40	5054.7(11)	6338(2)	3374.5(10)	36.5(7)
C16	4552.6(12)	6047(2)	4949.1(10)	42.6(9)
C33	2917.5(11)	8071(2)	2564.2(10)	37.1(7)
C15	4449.9(11)	5270(2)	4963.1(10)	39.0(8)
C19	3293.5(13)	7481(2)	4235.8(11)	43.0(8)
C59	7027.5(12)	10709(2)	3479.8(11)	40.0(8)
C67	4703.7(13)	10399(2)	2967.3(12)	51(1)
C30	4088.2(12)	5649(2)	2285.4(10)	41.6(8)
C61	6379.2(12)	11108(2)	3768.7(11)	39.1(8)
C34	2475.8(13)	8510(2)	2412.1(12)	50.7(10)
C4	3848.3(13)	3089(2)	3211.1(10)	44.4(9)
C48	6389.7(12)	8060(2)	5433.0(9)	40.4(8)
C37	2629.2(12)	7762(2)	3199.1(11)	41.8(8)
C68	5151.1(12)	10138(2)	3219.9(11)	40.7(8)
C28	3291.5(13)	5784(2)	1899.9(10)	43.0(8)
C42	5251.0(13)	5464(2)	3971.2(11)	43.5(8)
C64	5195.7(13)	11373(2)	3604.5(13)	46.8(9)
C66	4678.8(16)	11273(3)	2943.4(14)	60.8(12)
C71	5391.4(16)	11106(2)	5010.5(13)	56.0(11)
C65	4749.5(15)	11638(2)	3354.6(14)	58.0(11)

C72	5780.8(17)	10770(3)	5304.2(13)	61.5(12)
C35	2251.4(14)	8816(2)	2750.1(14)	56.0(11)
C29	3708.3(13)	5264(2)	1995.7(11)	45.2(9)
C73	6221.8(16)	10762(3)	5126.7(13)	61.7(12)
C36	2180.9(14)	8180(3)	3045.2(15)	59.0(11)
C77	6535(4)	3469(7)	4203(3)	130(4)
C79	5714(4)	3196(6)	4107(4)	145(5)
C78	6079(4)	3788(6)	4127(4)	130(4)
C76	6574(5)	2974(7)	4559(3)	160(5)
C75	7085(6)	2699(12)	4661(4)	256(11)
C79A	6905(10)	3680(13)	4338(6)	147(7)
C77A	7399(8)	4322(15)	4098(7)	179(10)
C75A	7949(7)	4866(16)	3863(6)	138(8)
C76A	7504(11)	4530(30)	3709(7)	245(14)
C78A	6900(8)	4350(13)	4079(6)	147(7)
C80	5000	3279(7)	2500	170(6)
C81	5389(4)	3511(8)	2731(5)	230(7)
C82	5769(5)	3204(7)	2952(3)	209(7)
C83	8266(5)	5692(6)	3188(4)	257(7)
C85	8337(6)	6155(10)	2573(6)	318(9)
C84	8328(5)	5492(9)	2780(5)	264(7)
C86	8423(4)	4918(6)	3370(5)	211(5)
C87	8334(9)	4954(11)	3773(5)	367(13)

Table S8: Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for (^{Cy}PSiP)PtH. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	$\mathbf{U_{11}}$	$\mathbf{U_{22}}$	$\mathbf{U_{33}}$	$\mathbf{U_{23}}$	$\mathbf{U_{13}}$	$\mathbf{U_{12}}$
Pt1	21.65(7)	27.07(7)	22.09(7)	0.33(4)	3.83(5)	-1.50(4)
Pt2	20.87(7)	28.59(8)	23.62(7)	-1.62(4)	6.01(5)	-0.55(5)
P3	22.4(3)	29.2(4)	22.1(3)	-0.7(3)	4.6(3)	-0.9(3)
P1	22.1(3)	28.5(4)	23.5(3)	1.5(3)	3.7(3)	-2.4(3)
Si2	24.3(4)	31.1(4)	22.9(4)	-1.9(3)	7.0(3)	0.4(3)
P2	23.3(3)	27.2(4)	23.4(3)	1.8(3)	1.9(3)	-0.4(3)
P4	24.9(4)	30.0(4)	36.0(4)	-0.8(3)	12.2(3)	-0.2(3)
Si1	29.4(4)	29.0(4)	23.9(4)	-3.3(3)	5.4(3)	-3.2(3)
C50	23.8(14)	32.5(16)	22.8(14)	-4.4(12)	3.7(11)	0.3(12)
C13	24.4(14)	36.3(17)	23.6(14)	0.6(12)	5.9(11)	-2.8(12)
C45	34.1(17)	40.6(19)	29.3(16)	3.4(13)	10.7(13)	0.1(14)
C62	26.2(15)	35.9(17)	34.1(16)	0.0(13)	11.3(12)	-3.0(13)
C54	27.9(15)	34.4(17)	30.3(15)	-2.9(13)	9.2(12)	-3.7(13)
C44	28.4(15)	34.2(17)	25.0(14)	0.2(12)	4.5(12)	1.6(13)
C55	25.4(14)	29.6(16)	23.9(14)	-6.8(12)	5.2(11)	-2.7(12)
C57	26.8(15)	37.6(18)	24.6(14)	1.8(12)	7.5(12)	-1.3(13)
C51	31.3(16)	35.4(18)	30.4(16)	0.0(13)	4.7(13)	0.0(13)
C23	34.2(17)	34.9(18)	39.3(18)	7.7(14)	3.9(14)	-8.7(14)
C17	44.0(19)	44(2)	26.0(15)	-2.0(14)	4.6(14)	-15.2(16)
C38	26.3(15)	35.2(17)	25.9(15)	-3.3(12)	7.0(12)	-3.8(13)
C25	23.4(14)	28.8(16)	26.4(14)	2.0(12)	1.8(11)	0.3(12)
C21	31.0(16)	30.8(16)	27.5(15)	-2.6(12)	1.1(12)	-1.0(13)
C31	29.9(16)	42.6(19)	29.0(16)	2.1(13)	5.1(13)	4.0(14)

C56	38.8(18)	46(2)	28.5(16)	0.3(14)	7.3(13)	2.3(15)
C20	28.2(15)	23.4(15)	28.4(15)	-2.9(11)	3.5(12)	-0.4(12)
C12	28.5(16)	45(2)	33.3(16)	-2.2(14)	9.3(13)	-2.9(14)
C26	27.4(15)	30.9(16)	24.3(14)	3.1(12)	1.9(11)	-2.3(12)
C18	31.2(16)	39.3(18)	20.9(14)	-2.9(12)	8.6(12)	-6.1(13)
C39	27.6(15)	35.8(18)	27.2(15)	-3.8(13)	4.0(12)	-2.6(13)
C1	26.6(15)	29.8(16)	29.0(15)	2.0(12)	3.0(12)	-0.4(12)
C8	33.4(17)	43(2)	31.1(16)	7.9(14)	8.6(13)	-4.6(14)
C22	32.2(17)	31.6(18)	41.2(18)	0.7(14)	1.0(14)	-6.8(13)
C41	37.4(18)	44(2)	41.5(19)	-14.1(15)	13.6(15)	-13.8(15)
C47	54(2)	49(2)	22.5(15)	-2.0(14)	5.7(14)	14.5(17)
C24	33.1(16)	33.5(17)	29.7(16)	3.2(13)	0.0(13)	-3.7(13)
C53	26.2(15)	40.5(19)	38.7(17)	-5.8(14)	9.3(13)	1.7(14)
C7	23.0(14)	38.6(18)	26.2(14)	1.3(13)	3.4(11)	-3.9(13)
C2	29.8(16)	38.6(18)	34.4(17)	0.2(14)	6.8(13)	0.0(14)
C11	35.0(18)	59(2)	36.8(18)	-3.2(16)	15.4(14)	-2.1(16)
C3	38.6(19)	49(2)	40.6(19)	-0.5(16)	8.0(15)	11.8(16)
C5	50(2)	33.7(19)	36.3(18)	-3.6(14)	-3.9(15)	3.7(16)
C60	44(2)	35(2)	59(2)	1.8(16)	23.9(18)	-8.2(15)
C69	34.8(17)	33.2(18)	46.0(19)	-8.0(14)	19.8(15)	-2.9(14)
C6	34.6(17)	30.0(17)	34.6(17)	0.3(13)	0.7(13)	-2.1(13)
C63	32.1(17)	34.8(19)	46.6(19)	8.1(15)	13.5(14)	3.6(14)
C27	31.9(17)	41.8(19)	28.4(16)	-2.5(14)	0.7(13)	-1.9(14)
C14	27.1(15)	39.8(19)	30.9(16)	5.0(13)	3.7(12)	-5.6(13)
C9	35.4(18)	56(2)	34.5(18)	9.8(16)	8.0(14)	-12.2(16)
C46	47(2)	46(2)	26.8(16)	6.1(14)	12.7(14)	11.1(16)
C52	30.5(16)	36.0(18)	38.5(17)	0.7(14)	5.2(13)	5.6(14)
C10	35.0(18)	75(3)	32.6(17)	1.1(17)	12.2(14)	-11.2(18)
C58	31.4(16)	40.8(19)	35.9(17)	2.2(14)	14.0(13)	3.9(14)
C43	40.8(19)	33.3(18)	34.6(17)	-0.2(14)	6.9(14)	-6.0(14)
C49	33.6(17)	39.6(19)	30.9(16)	-4.3(14)	2.5(13)	-2.4(14)
C70	41.0(19)	38(2)	58(2)	-3.0(17)	29.4(17)	2.8(16)
C32	25.5(15)	31.9(17)	37.3(17)	0.5(13)	-0.8(13)	-1.3(13)
C74	34.5(18)	63(2)	43(2)	-23.3(18)	13.5(15)	-6.9(17)
C40	28.7(16)	50(2)	31.3(16)	-11.4(14)	6.2(13)	-5.1(14)
C16	35.8(18)	62(2)	28.4(17)	1.2(16)	0.1(14)	-20.3(17)
C33	36.9(18)	36.7(19)	35.3(17)	5.7(14)	-0.7(14)	4.0(14)
C15	30.8(17)	56(2)	28.9(16)	10.7(15)	0.0(13)	-8.1(15)
C19	46(2)	45(2)	41.9(19)	-7.7(16)	17.6(16)	-2.9(16)
C59	32.2(17)	43(2)	49(2)	5.9(16)	19.4(15)	-2.7(15)
C67	41(2)	61(3)	50(2)	15.4(19)	5.8(17)	8.5(18)
C30	40.6(19)	51(2)	36.2(18)	-1.0(16)	15.9(15)	2.6(16)
C61	34.3(18)	33.8(18)	53(2)	-2.6(15)	19.2(16)	-0.7(14)
C34	47(2)	44(2)	55(2)	5.3(18)	-11.9(18)	7.8(17)
C4	54(2)	43(2)	34.5(18)	-5.1(15)	2.8(16)	13.9(17)
C48	45(2)	45(2)	27.2(16)	-4.7(14)	-3.8(14)	5.7(16)
C37	38.1(19)	38(2)	52(2)	5.1(16)	16.4(16)	4.6(15)
C68	32.8(17)	43(2)	47(2)	5.7(16)	7.3(15)	1.2(15)
C28	47(2)	53(2)	28.7(17)	-7.2(15)	3.4(15)	-8.7(17)

C42	52(2)	38(2)	42.4(19)	-5.7(15)	13.8(16)	-16.5(16)
C64	47(2)	36(2)	61(2)	8.3(17)	20.2(18)	5.6(16)
C66	55(3)	63(3)	64(3)	27(2)	10(2)	15(2)
C71	70(3)	44(2)	67(3)	-9.2(19)	47(2)	3(2)
C65	58(3)	46(2)	75(3)	22(2)	24(2)	19(2)
C72	78(3)	61(3)	53(2)	-23(2)	33(2)	-5(2)
C35	43(2)	43(2)	79(3)	6(2)	0(2)	14.9(17)
C29	53(2)	50(2)	37.2(18)	-9.5(16)	18.4(16)	-3.2(18)
C73	62(3)	76(3)	50(2)	-33(2)	18(2)	-15(2)
C36	43(2)	49(2)	88(3)	3(2)	18(2)	14.1(18)
C77	182(9)	124(9)	95(6)	-37(6)	53(7)	17(7)
C79	208(11)	83(7)	172(11)	-76(7)	110(10)	-48(7)
C78	171(9)	90(7)	148(9)	-34(6)	80(8)	-10(6)
C76	274(14)	106(9)	118(8)	-36(6)	84(9)	19(9)
C75	320(20)	310(20)	146(12)	-57(13)	52(13)	140(20)
C79A	206(15)	119(13)	86(11)	-66(9)	-60(10)	30(12)
C77A	214(17)	170(20)	146(19)	-101(16)	13(16)	54(17)
C75A	155(15)	180(20)	58(11)	-17(12)	-42(10)	128(14)
C76A	250(20)	270(30)	200(30)	-10(30)	1(18)	0(30)
C78A	206(15)	119(13)	86(11)	-66(9)	-60(10)	30(12)
C80	380(20)	71(7)	59(5)	0	34(9)	0
C81	178(12)	128(9)	420(20)	-86(12)	143(11)	-38(8)
C82	349(18)	187(13)	87(6)	-15(6)	24(8)	-149(12)
C83	235(12)	137(7)	329(12)	-139(8)	-153(11)	71(8)
C85	163(13)	270(20)	470(20)	13(16)	-93(16)	-57(14)
C84	115(9)	278(19)	409(16)	-5(12)	73(13)	-28(12)
C86	125(8)	120(7)	378(15)	-83(8)	11(11)	-21(6)
C87	510(30)	284(18)	251(13)	-139(11)	-91(18)	70(20)

Table S9: Bond lengths for (^{Cy}PSiP)PtH.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Pt1	P1	2.2636(7)	C8	C9	1.534(4)
Pt1	P2	2.2609(7)	C41	C40	1.520(5)
Pt1	Si1	2.3366(8)	C41	C42	1.531(5)
Pt2	P3	2.2594(8)	C47	C46	1.516(5)
Pt2	Si2	2.3278(8)	C47	C48	1.520(5)
Pt2	P4	2.2469(8)	C53	C52	1.384(5)
P3	C50	1.838(3)	C2	C3	1.531(5)
P3	C44	1.854(3)	C11	C10	1.529(5)
P3	C38	1.841(3)	C3	C4	1.525(5)
P1	C13	1.837(3)	C5	C6	1.531(5)
P1	C1	1.837(3)	C5	C4	1.515(5)
P1	C7	1.847(3)	C60	C59	1.381(5)
Si2	C55	1.910(3)	C60	C61	1.390(5)
Si2	C57	1.902(3)	C69	C70	1.531(4)
Si2	C56	1.888(3)	C69	C74	1.523(5)
P2	C25	1.838(3)	C63	C68	1.530(5)
P2	C26	1.843(3)	C63	C64	1.531(5)
P2	C32	1.841(3)	C27	C28	1.531(5)

P4	C62	1.838(3)	C14	C15	1.386(4)
P4	C69	1.840(3)	C9	C10	1.511(6)
P4	C63	1.838(3)	C58	C59	1.389(5)
Si1	C20	1.897(3)	C43	C42	1.535(5)
Si1	C18	1.899(3)	C49	C48	1.533(4)
Si1	C19	1.886(3)	C70	C71	1.523(5)
C50	C55	1.411(4)	C32	C33	1.535(5)
C50	C51	1.403(4)	C32	C37	1.532(5)
C13	C18	1.406(5)	C74	C73	1.524(5)
C13	C14	1.408(4)	C16	C15	1.387(5)
C45	C44	1.540(4)	C33	C34	1.527(5)
C45	C46	1.531(4)	C67	C68	1.521(5)
C62	C57	1.411(4)	C67	C66	1.523(6)
C62	C61	1.398(5)	C30	C29	1.519(5)
C54	C55	1.408(4)	C34	C35	1.516(6)
C54	C53	1.382(5)	C37	C36	1.526(5)
C44	C49	1.536(4)	C28	C29	1.520(5)
C57	C58	1.412(4)	C64	C65	1.517(6)
C51	C52	1.386(4)	C66	C65	1.516(7)
C23	C22	1.391(5)	C71	C72	1.510(7)
C23	C24	1.382(4)	C72	C73	1.527(6)
C17	C18	1.411(4)	C35	C36	1.530(6)
C17	C16	1.378(5)	C77	C78	1.441(11)
C38	C39	1.537(4)	C77	C76	1.473(11)
C38	C43	1.535(5)	C79	C78	1.485(10)
C25	C20	1.413(4)	C76	C75	1.567(13)
C25	C24	1.399(4)	C79A	C78A	1.457(15)
C21	C20	1.411(4)	C77A	C76A	1.452(15)
C21	C22	1.376(5)	C77A	C78A	1.466(15)
C31	C26	1.535(4)	C75A	C76A	1.453(16)
C31	C30	1.531(4)	C80	C81[1]	1.340(11)
C12	C7	1.530(5)	C80	C81	1.341(11)
C12	C11	1.525(4)	C81	C82	1.352(12)
C26	C27	1.531(4)	C83	C84	1.470(12)
C39	C40	1.525(4)	C83	C86	1.521(11)
C1	C2	1.532(4)	C85	C84	1.353(13)
C1	C6	1.535(4)	C86	C87	1.437(13)
C8	C7	1.539(4)			

[1]1-X,+Y,1/2-Z

Table S10: Bond angles for (^{Cy}PSiP)PtH.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
P1	Pt1	Si1	84.88(3)	C27	C26	C31	110.6(3)
P2	Pt1	P1	161.99(3)	C13	C18	Si1	116.7(2)
P2	Pt1	Si1	84.81(3)	C13	C18	C17	117.5(3)
P3	Pt2	Si2	85.60(3)	C17	C18	Si1	125.6(3)
P4	Pt2	P3	162.23(3)	C40	C39	C38	111.0(3)
P4	Pt2	Si2	85.64(3)	C2	C1	P1	109.5(2)

C50	P3	Pt2	109.05(10)	C2	C1	C6	111.9(3)
C50	P3	C44	104.51(13)	C6	C1	P1	111.1(2)
C50	P3	C38	108.36(14)	C9	C8	C7	110.4(3)
C44	P3	Pt2	113.03(11)	C21	C22	C23	119.5(3)
C38	P3	Pt2	115.40(10)	C40	C41	C42	111.5(3)
C38	P3	C44	105.86(14)	C46	C47	C48	110.5(3)
C13	P1	Pt1	109.54(10)	C23	C24	C25	120.6(3)
C13	P1	C7	105.82(13)	C54	C53	C52	120.3(3)
C1	P1	Pt1	113.66(10)	C12	C7	P1	110.4(2)
C1	P1	C13	103.78(14)	C12	C7	C8	109.8(3)
C1	P1	C7	105.59(14)	C8	C7	P1	117.0(2)
C7	P1	Pt1	117.34(10)	C3	C2	C1	111.7(3)
C55	Si2	Pt2	105.04(9)	C12	C11	C10	112.0(3)
C57	Si2	Pt2	105.07(9)	C4	C3	C2	111.1(3)
C57	Si2	C55	115.14(13)	C4	C5	C6	111.1(3)
C56	Si2	Pt2	124.40(11)	C59	C60	C61	120.0(3)
C56	Si2	C55	104.06(14)	C70	C69	P4	114.0(2)
C56	Si2	C57	103.76(15)	C74	C69	P4	108.4(2)
C25	P2	Pt1	108.43(10)	C74	C69	C70	110.1(3)
C25	P2	C26	103.06(14)	C5	C6	C1	111.2(3)
C25	P2	C32	107.33(14)	C68	C63	P4	111.7(2)
C26	P2	Pt1	115.50(10)	C68	C63	C64	109.9(3)
C32	P2	Pt1	117.30(11)	C64	C63	P4	116.4(3)
C32	P2	C26	104.06(14)	C28	C27	C26	110.5(3)
C62	P4	Pt2	109.27(11)	C15	C14	C13	120.4(3)
C62	P4	C69	103.36(15)	C10	C9	C8	110.8(3)
C69	P4	Pt2	113.80(12)	C47	C46	C45	111.4(3)
C63	P4	Pt2	116.76(12)	C53	C52	C51	119.9(3)
C63	P4	C62	107.44(15)	C9	C10	C11	111.1(3)
C63	P4	C69	105.20(16)	C59	C58	C57	122.1(3)
C20	Si1	Pt1	104.62(9)	C38	C43	C42	109.7(3)
C20	Si1	C18	113.23(13)	C48	C49	C44	113.2(3)
C18	Si1	Pt1	105.75(10)	C71	C70	C69	111.0(3)
C19	Si1	Pt1	124.68(12)	C33	C32	P2	115.2(2)
C19	Si1	C20	105.12(15)	C37	C32	P2	112.0(2)
C19	Si1	C18	103.71(15)	C37	C32	C33	109.7(3)
C55	C50	P3	117.5(2)	C69	C74	C73	112.0(3)
C51	C50	P3	122.2(2)	C41	C40	C39	112.1(3)
C51	C50	C55	120.3(3)	C17	C16	C15	120.3(3)
C18	C13	P1	117.3(2)	C34	C33	C32	111.1(3)
C18	C13	C14	120.3(3)	C14	C15	C16	119.8(3)
C14	C13	P1	122.3(2)	C60	C59	C58	119.6(3)
C46	C45	C44	113.4(3)	C68	C67	C66	111.0(4)
C57	C62	P4	117.4(2)	C29	C30	C31	111.2(3)
C61	C62	P4	122.3(2)	C60	C61	C62	120.8(3)
C61	C62	C57	120.3(3)	C35	C34	C33	112.2(3)
C53	C54	C55	121.5(3)	C5	C4	C3	110.7(3)
C45	C44	P3	109.0(2)	C47	C48	C49	110.9(3)
C49	C44	P3	108.3(2)	C36	C37	C32	110.6(3)

C49	C44	C45	112.8(3)	C67	C68	C63	110.9(3)
C50	C55	Si2	116.6(2)	C29	C28	C27	112.5(3)
C54	C55	Si2	125.7(2)	C41	C42	C43	110.6(3)
C54	C55	C50	117.6(3)	C65	C64	C63	110.9(3)
C62	C57	Si2	116.6(2)	C65	C66	C67	111.8(3)
C62	C57	C58	117.2(3)	C72	C71	C70	111.8(3)
C58	C57	Si2	126.1(2)	C66	C65	C64	111.1(3)
C52	C51	C50	120.3(3)	C71	C72	C73	110.5(4)
C24	C23	C22	120.2(3)	C34	C35	C36	111.6(3)
C16	C17	C18	121.7(3)	C30	C29	C28	111.2(3)
C39	C38	P3	111.0(2)	C74	C73	C72	110.0(3)
C43	C38	P3	117.3(2)	C37	C36	C35	111.2(3)
C43	C38	C39	109.4(3)	C78	C77	C76	108.4(10)
C20	C25	P2	117.3(2)	C77	C78	C79	113.1(10)
C24	C25	P2	122.4(2)	C77	C76	C75	107.4(11)
C24	C25	C20	120.2(3)	C76A	C77A	C78A	108.8(19)
C22	C21	C20	122.2(3)	C77A	C76A	C75A	95.5(13)
C30	C31	C26	110.6(3)	C79A	C78A	C77A	92.4(12)
C25	C20	Si1	116.3(2)	C81[1]	C80	C81	145.0(17)
C21	C20	Si1	126.4(2)	C80	C81	C82	139.3(14)
C21	C20	C25	117.3(3)	C84	C83	C86	95.6(11)
C11	C12	C7	110.4(3)	C85	C84	C83	107.7(14)
C31	C26	P2	109.6(2)	C87	C86	C83	104.9(10)
C27	C26	P2	114.0(2)				

[1]1-X,+Y,1/2-Z

Polymorph 2

The compound (^{Cy}PSiP)PtH crystallized in the space group *C2/c* with two molecules in the asymmetric unit along with one molecule of pentane.

Table S11: Crystal data and structure refinement for (^{Cy}PSiP)PtH.

Empirical formula	$C_{79}H_{124}P_4Pt_2Si_2$	
Formula weight	1644.01	
Temperature	150(2) K	
Wavelength	0.71075 Å	
Crystal system	Monoclinic	
Space group	C 2/c	
Unit cell dimensions	a = 24.4262(5) Å	α = 90°.
	b = 16.3000(3) Å	β = 105.394(7)°.
	c = 39.968(3) Å	γ = 90°.
Volume	15342.3(13) Å^3	
Z	8	
Density (calculated)	1.423 Mg/m^3	
Absorption coefficient	3.798 mm^{-1}	
F(000)	6736	
Crystal size	0.150 x 0.150 x 0.080 mm^3	
Crystal color and habit	Colorless Block	
Diffractometer	Rigaku R-AXIS RAPID imaging plate	
θ range for data collection	3.006 to 25.350°.	

Index ranges	$-29 \le h \le 29$, $-19 \le k \le 19$, $-48 \le l \le 48$
Reflections collected	132065
Independent reflections	14010 [R(int) = 0.1719]
Observed reflections ($I > 2\sigma(I)$)	9740
Completeness to $\theta = 25.242°$	99.7 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.751 and 0.491
Solution method	SHELXS-2013 (Sheldrick, 2013)
Refinement method	SHELXL-2014/7 (Sheldrick, 2014)
Data / restraints / parameters	14010 / 0 / 795
Goodness-of-fit on F^2	1.038
Final R indices [$I>2\sigma(I)$]	R1 = 0.0767, wR2 = 0.1998
R indices (all data)	R1 = 0.1087, wR2 = 0.2157
Extinction coefficient	0.00028(3)
Largest diff. peak and hole	2.784 and -1.719 e.Å^{-3}

Table S12: Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters (Å$^2 \times 10^3$) for (^{Cy}PSiP)PtH. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	***x***	***y***	***z***	***U(eq)***
Pt(1)	3166(1)	6133(1)	4656(1)	32(1)
P(1)	3486(2)	7437(2)	4736(1)	32(1)
P(2)	3165(2)	4772(2)	4561(1)	35(1)
Si(1)	3314(2)	6254(2)	4106(1)	35(1)
C(1)	2723(6)	6549(9)	3709(4)	42(4)
C(2)	2990(6)	8327(8)	4635(4)	34(3)
C(3)	2591(6)	8275(9)	4269(4)	36(3)
C(4)	2179(6)	8946(8)	4186(4)	40(3)
C(5)	2479(6)	9783(9)	4246(4)	41(3)
C(6)	2855(6)	9846(8)	4611(4)	38(3)
C(7)	3288(6)	9167(8)	4691(3)	31(3)
C(8)	3919(6)	7629(8)	5182(3)	30(3)
C(9)	3550(6)	7754(10)	5433(4)	41(4)
C(10)	3909(8)	7861(12)	5805(4)	61(5)
C(11)	4315(7)	7143(11)	5916(4)	54(4)
C(12)	4687(7)	6995(12)	5675(4)	63(5)
C(13)	4330(7)	6906(10)	5296(4)	46(4)
C(14)	3973(6)	7566(8)	4461(3)	33(3)
C(15)	4413(6)	8159(9)	4531(4)	36(3)
C(16)	4768(6)	8229(9)	4314(4)	38(3)
C(17)	4691(6)	7725(10)	4022(4)	43(4)
C(18)	4273(6)	7169(9)	3957(3)	34(3)
C(19)	3903(6)	7059(8)	4168(3)	29(3)
C(20)	3550(6)	5219(8)	3993(3)	33(3)
C(21)	3793(6)	5046(10)	3719(4)	44(4)
C(22)	3933(6)	4268(9)	3636(3)	39(3)
C(23)	3826(6)	3605(10)	3838(4)	42(4)
C(24)	3589(6)	3744(9)	4109(4)	42(4)
C(25)	3453(5)	4551(9)	4189(4)	34(3)
C(26)	2472(6)	4255(10)	4498(4)	41(4)
C(27)	2413(8)	3397(11)	4338(5)	65(5)
C(28)	1818(10)	3058(13)	4325(6)	85(7)
C(29)	1352(9)	3616(15)	4132(5)	79(7)
C(30)	1405(8)	4447(12)	4282(5)	65(5)
C(31)	1993(7)	4819(12)	4296(5)	62(5)
C(32)	3661(7)	4168(9)	4909(4)	43(4)

C(33)	3476(6)	4232(10)	5251(4)	43(4)
C(34)	3917(7)	3827(11)	5560(4)	54(4)
C(35)	4502(7)	4194(10)	5601(4)	52(4)
C(36)	4682(7)	4065(11)	5265(4)	53(4)
C(37)	4265(6)	4484(10)	4957(4)	43(4)
Pt(2)	3500(1)	2012(1)	3219(1)	32(1)
P(3)	2960(2)	2790(2)	2786(1)	34(1)
P(4)	3906(2)	930(2)	3536(1)	32(1)
Si(2)	2641(2)	1414(2)	3237(1)	34(1)
C(38)	2199(7)	1677(10)	3543(4)	46(4)
C(39)	2717(7)	3796(8)	2901(3)	38(3)
C(40)	2342(7)	3667(9)	3158(4)	42(4)
C(41)	2147(7)	4488(9)	3265(4)	45(4)
C(42)	1843(7)	4997(10)	2952(4)	51(4)
C(43)	2199(6)	5127(9)	2702(4)	39(3)
C(44)	2383(6)	4308(9)	2582(3)	38(3)
C(45)	3288(6)	2998(9)	2427(4)	40(3)
C(46)	3788(7)	3600(10)	2546(4)	45(4)
C(47)	4096(7)	3742(12)	2267(5)	60(5)
C(48)	4269(8)	2928(14)	2135(5)	74(6)
C(49)	3774(8)	2375(11)	2003(4)	54(4)
C(50)	3476(7)	2222(9)	2288(4)	48(4)
C(51)	2322(6)	2203(8)	2584(3)	33(3)
C(52)	1979(7)	2351(9)	2247(4)	46(4)
C(53)	1509(6)	1896(10)	2107(4)	44(4)
C(54)	1341(7)	1269(9)	2297(4)	41(4)
C(55)	1668(7)	1114(9)	2627(4)	44(4)
C(56)	2174(5)	1557(8)	2782(3)	33(3)
C(57)	2819(6)	286(8)	3349(3)	34(3)
C(58)	2416(7)	-345(9)	3312(4)	41(4)
C(59)	2587(7)	-1139(9)	3404(3)	38(3)
C(60)	3158(6)	-1324(9)	3537(3)	40(3)
C(61)	3553(6)	-719(9)	3583(3)	36(3)
C(62)	3384(6)	95(8)	3486(3)	32(3)
C(63)	4490(6)	429(9)	3402(3)	36(3)
C(64)	4303(6)	189(10)	3022(3)	41(4)
C(65)	4772(8)	-279(13)	2920(5)	65(5)
C(66)	5314(7)	206(14)	3001(5)	71(6)
C(67)	5503(6)	485(12)	3377(4)	57(5)
C(68)	5039(6)	948(10)	3475(4)	46(4)
C(69)	4178(6)	1119(9)	4011(3)	36(3)
C(70)	4513(7)	400(9)	4213(4)	43(4)
C(71)	4769(6)	666(10)	4595(4)	43(4)
C(72)	4310(7)	963(10)	4759(4)	47(4)
C(73)	3967(7)	1659(9)	4547(4)	45(4)
C(74)	3713(7)	1397(9)	4166(3)	40(4)
C(75)	5420(20)	5000(30)	3423(14)	220(30)
C(76)	5267(17)	5940(40)	3365(9)	200(30)
C(77)	5447(17)	6380(30)	3133(13)	175(19)
C(78)	5420(20)	7320(40)	3136(12)	190(20)
C(79)	5705(16)	7700(30)	2935(18)	230(30)

Table S13: Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for (^{Cy}PSiP)PtH. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	**U_{11}**	**U_{22}**	**U_{33}**	**U_{23}**	**U_{13}**	**U_{12}**
Pt(1)	37(1)	28(1)	31(1)	-1(1)	9(1)	-3(1)

P(1)	35(2)	29(2)	31(2)	-2(2)	6(2)	-2(2)
P(2)	40(2)	30(2)	36(2)	0(2)	12(2)	-1(2)
Si(1)	42(2)	30(2)	30(2)	0(2)	8(2)	-4(2)
C(1)	51(9)	33(8)	39(8)	-6(6)	10(7)	-2(7)
C(2)	29(7)	33(8)	38(8)	6(6)	9(6)	-3(6)
C(3)	32(8)	36(8)	43(8)	5(6)	13(6)	-2(6)
C(4)	41(8)	35(8)	43(8)	7(6)	10(7)	-5(7)
C(5)	40(8)	34(8)	45(8)	8(7)	2(7)	-3(7)
C(6)	42(9)	27(7)	46(8)	6(6)	13(7)	-7(6)
C(7)	35(8)	19(7)	37(7)	2(5)	3(6)	3(6)
C(8)	31(7)	28(7)	33(7)	-3(6)	10(6)	-10(6)
C(9)	44(9)	42(9)	36(8)	-4(6)	10(6)	-13(7)
C(10)	71(12)	76(13)	30(8)	-8(8)	5(8)	-16(10)
C(11)	60(11)	71(12)	25(7)	10(7)	3(7)	-15(9)
C(12)	52(11)	76(13)	43(9)	9(9)	-19(8)	-13(10)
C(13)	44(9)	52(10)	42(8)	3(7)	11(7)	-11(8)
C(14)	37(8)	30(7)	32(7)	1(6)	8(6)	-3(6)
C(15)	36(8)	33(8)	37(8)	2(6)	8(6)	-5(6)
C(16)	37(8)	38(8)	35(8)	3(6)	4(6)	-4(7)
C(17)	37(8)	53(10)	42(8)	6(7)	17(7)	8(7)
C(18)	34(8)	42(8)	23(6)	-1(6)	1(5)	2(7)
C(19)	35(7)	31(7)	24(6)	4(5)	14(5)	-10(6)
C(20)	40(8)	30(7)	32(7)	-7(6)	12(6)	-3(6)
C(21)	46(9)	51(10)	30(7)	-3(7)	6(6)	-8(8)
C(22)	55(9)	31(8)	30(7)	-18(6)	11(6)	-8(7)
C(23)	41(9)	39(9)	43(8)	-18(7)	7(7)	3(7)
C(24)	52(9)	34(8)	38(8)	-1(6)	9(7)	7(7)
C(25)	23(7)	38(8)	39(8)	-8(6)	6(6)	1(6)
C(26)	37(8)	54(10)	30(7)	-11(7)	6(6)	-14(7)
C(27)	58(11)	52(11)	90(14)	-32(10)	26(10)	-17(9)
C(28)	107(18)	71(15)	94(16)	-43(13)	58(15)	-44(14)
C(29)	58(13)	116(19)	63(12)	-23(13)	13(10)	-42(13)
C(30)	54(11)	75(14)	61(11)	-10(10)	3(9)	-25(10)
C(31)	41(10)	76(13)	59(11)	-5(10)	-2(8)	-10(9)
C(32)	62(10)	32(8)	39(8)	-2(6)	24(7)	-3(7)
C(33)	44(9)	48(9)	41(8)	9(7)	19(7)	5(7)
C(34)	66(11)	52(10)	43(9)	16(8)	15(8)	20(9)
C(35)	54(10)	40(9)	57(10)	8(8)	4(8)	-3(8)
C(36)	51(10)	49(10)	64(11)	8(8)	21(8)	7(8)
C(37)	43(9)	49(10)	37(8)	8(7)	12(7)	-2(7)
Pt(2)	37(1)	30(1)	27(1)	2(1)	3(1)	-1(1)
P(3)	39(2)	31(2)	30(2)	3(2)	6(2)	1(2)
P(4)	36(2)	28(2)	29(2)	1(1)	3(1)	1(2)
Si(2)	38(2)	33(2)	28(2)	3(2)	6(2)	1(2)
C(38)	53(10)	45(9)	39(8)	8(7)	10(7)	5(8)
C(39)	58(9)	32(8)	17(6)	6(5)	-3(6)	1(7)
C(40)	52(9)	38(8)	38(8)	0(6)	18(7)	-3(7)
C(41)	56(10)	42(9)	42(9)	6(7)	22(7)	0(8)
C(42)	49(10)	43(10)	65(11)	7(8)	22(8)	10(8)
C(43)	48(9)	28(8)	42(8)	8(6)	14(7)	7(7)
C(44)	43(8)	44(9)	23(7)	1(6)	-1(6)	6(7)
C(45)	40(8)	37(8)	41(8)	2(6)	8(6)	-2(7)
C(46)	49(9)	54(10)	32(8)	8(7)	11(7)	2(8)
C(47)	43(10)	79(14)	62(11)	20(10)	22(8)	2(9)
C(48)	60(12)	100(17)	65(12)	10(12)	25(10)	17(12)
C(49)	69(12)	53(11)	46(9)	0(8)	25(8)	13(9)

C(50)	63(11)	38(9)	46(9)	5(7)	16(8)	13(8)
C(51)	41(8)	35(8)	22(6)	-10(6)	5(6)	-1(6)
C(52)	49(10)	37(9)	47(9)	6(7)	4(7)	-1(7)
C(53)	41(9)	57(10)	26(7)	3(7)	-7(6)	2(8)
C(54)	47(9)	32(8)	44(8)	0(6)	11(7)	1(7)
C(55)	52(10)	42(9)	35(8)	-1(7)	8(7)	2(7)
C(56)	28(7)	32(8)	38(8)	-3(6)	7(6)	0(6)
C(57)	46(8)	31(7)	24(7)	0(6)	7(6)	-5(7)
C(58)	44(9)	43(9)	36(8)	2(7)	9(6)	8(7)
C(59)	52(9)	40(8)	23(7)	-3(6)	12(6)	-14(7)
C(60)	44(9)	41(9)	32(7)	-9(6)	7(6)	2(7)
C(61)	33(8)	45(9)	30(7)	4(6)	9(6)	-6(7)
C(62)	42(8)	29(7)	25(7)	2(5)	9(6)	3(6)
C(63)	44(8)	35(8)	30(7)	8(6)	10(6)	6(7)
C(64)	48(9)	44(9)	29(7)	-5(6)	7(6)	-5(7)
C(65)	62(12)	77(14)	61(11)	-10(10)	28(9)	6(10)
C(66)	35(10)	111(17)	72(13)	6(12)	23(9)	10(10)
C(67)	27(8)	80(13)	62(11)	19(9)	9(7)	-1(8)
C(68)	33(8)	54(10)	48(9)	10(7)	8(7)	-4(7)
C(69)	41(8)	35(8)	22(6)	4(6)	-5(6)	5(6)
C(70)	49(9)	40(9)	34(8)	3(6)	3(7)	-8(7)
C(71)	38(8)	55(10)	34(8)	9(7)	5(6)	-5(7)
C(72)	54(10)	45(9)	35(8)	-5(7)	-1(7)	-13(8)
C(73)	57(10)	42(9)	34(8)	-6(7)	8(7)	-24(8)
C(74)	54(9)	39(8)	24(7)	4(6)	5(6)	-4(7)
C(75)	270(60)	180(40)	280(60)	-100(40)	210(50)	-60(40)
C(76)	100(30)	410(90)	90(20)	20(40)	30(20)	70(40)
C(77)	150(30)	180(40)	240(50)	-80(40)	120(40)	-40(30)
C(78)	170(50)	240(70)	150(40)	-20(40)	40(30)	60(50)
C(79)	90(30)	140(40)	440(100)	-70(50)	50(40)	10(20)

Table S14: Bond lengths for (^{Cy}PSiP)PtH.

Pt(1)-P(2)	2.251(4)
Pt(1)-P(1)	2.258(4)
Pt(1)-Si(1)	2.326(4)
Pt(1)-H(1PT)	1.49(14)
P(1)-C(14)	1.830(14)
P(1)-C(8)	1.842(13)
P(1)-C(2)	1.863(14)
P(2)-C(25)	1.840(14)
P(2)-C(26)	1.848(14)
P(2)-C(32)	1.865(16)
Si(1)-C(20)	1.877(14)
Si(1)-C(1)	1.903(15)
Si(1)-C(19)	1.915(13)
C(2)-C(3)	1.529(19)
C(2)-C(7)	1.539(18)
C(3)-C(4)	1.464(19)
C(4)-C(5)	1.537(19)
C(5)-C(6)	1.507(19)
C(6)-C(7)	1.505(19)
C(8)-C(9)	1.528(19)
C(8)-C(13)	1.54(2)
C(9)-C(10)	1.52(2)
C(10)-C(11)	1.52(2)
C(11)-C(12)	1.51(2)

C(12)-C(13)	1.54(2)
C(14)-C(19)	1.408(18)
C(14)-C(15)	1.418(19)
C(15)-C(16)	1.38(2)
C(16)-C(17)	1.40(2)
C(17)-C(18)	1.34(2)
C(18)-C(19)	1.400(18)
C(20)-C(25)	1.397(19)
C(20)-C(21)	1.407(19)
C(21)-C(22)	1.38(2)
C(22)-C(23)	1.42(2)
C(23)-C(24)	1.37(2)
C(24)-C(25)	1.415(19)
C(26)-C(27)	1.53(2)
C(26)-C(31)	1.54(2)
C(27)-C(28)	1.54(3)
C(28)-C(29)	1.50(3)
C(29)-C(30)	1.47(3)
C(30)-C(31)	1.55(2)
C(32)-C(37)	1.53(2)
C(32)-C(33)	1.553(19)
C(33)-C(34)	1.55(2)
C(34)-C(35)	1.52(2)
C(35)-C(36)	1.53(2)
C(36)-C(37)	1.53(2)
Pt(2)-P(4)	2.244(4)
Pt(2)-P(3)	2.266(4)
Pt(2)-Si(2)	2.332(4)
Pt(2)-H(2PT)	1.56(14)
P(3)-C(51)	1.825(14)
P(3)-C(39)	1.843(15)
P(3)-C(45)	1.849(15)
P(4)-C(62)	1.838(14)
P(4)-C(63)	1.843(15)
P(4)-C(69)	1.862(13)
Si(2)-C(38)	1.884(16)
Si(2)-C(56)	1.888(14)
Si(2)-C(57)	1.915(14)
C(39)-C(44)	1.559(17)
C(39)-C(40)	1.56(2)
C(40)-C(41)	1.52(2)
C(41)-C(42)	1.52(2)
C(42)-C(43)	1.50(2)
C(43)-C(44)	1.526(19)
C(45)-C(50)	1.50(2)
C(45)-C(46)	1.54(2)
C(46)-C(47)	1.52(2)
C(47)-C(48)	1.53(3)
C(48)-C(49)	1.49(3)
C(49)-C(50)	1.53(2)
C(51)-C(52)	1.405(19)
C(51)-C(56)	1.419(19)
C(52)-C(53)	1.36(2)
C(53)-C(54)	1.40(2)
C(54)-C(55)	1.37(2)
C(55)-C(56)	1.42(2)

C(57)-C(62)	1.379(19)
C(57)-C(58)	1.40(2)
C(58)-C(59)	1.38(2)
C(59)-C(60)	1.39(2)
C(60)-C(61)	1.36(2)
C(61)-C(62)	1.414(19)
C(63)-C(64)	1.517(18)
C(63)-C(68)	1.55(2)
C(64)-C(65)	1.52(2)
C(65)-C(66)	1.50(3)
C(66)-C(67)	1.52(3)
C(67)-C(68)	1.50(2)
C(69)-C(74)	1.50(2)
C(69)-C(70)	1.531(19)
C(70)-C(71)	1.547(19)
C(71)-C(72)	1.52(2)
C(72)-C(73)	1.53(2)
C(73)-C(74)	1.542(18)
C(75)-C(76)	1.57(6)
C(76)-C(77)	1.34(5)
C(77)-C(78)	1.54(6)
C(78)-C(79)	1.34(6)

Table S15: Bond angles for (^{Cy}PSiP)PtH.

P(2)-Pt(1)-P(1)	159.46(14)
P(2)-Pt(1)-Si(1)	85.28(13)
P(1)-Pt(1)-Si(1)	85.36(13)
P(2)-Pt(1)-H(1PT)	100(5)
P(1)-Pt(1)-H(1PT)	90(5)
Si(1)-Pt(1)-H(1PT)	175(6)
C(14)-P(1)-C(8)	105.3(6)
C(14)-P(1)-C(2)	105.6(6)
C(8)-P(1)-C(2)	104.5(6)
C(14)-P(1)-Pt(1)	106.2(5)
C(8)-P(1)-Pt(1)	112.6(4)
C(2)-P(1)-Pt(1)	121.4(4)
C(25)-P(2)-C(26)	109.5(6)
C(25)-P(2)-C(32)	100.8(6)
C(26)-P(2)-C(32)	104.5(7)
C(25)-P(2)-Pt(1)	110.2(5)
C(26)-P(2)-Pt(1)	115.6(5)
C(32)-P(2)-Pt(1)	115.0(5)
C(20)-Si(1)-C(1)	103.9(6)
C(20)-Si(1)-C(19)	112.3(6)
C(1)-Si(1)-C(19)	108.1(6)
C(20)-Si(1)-Pt(1)	106.6(4)
C(1)-Si(1)-Pt(1)	122.5(5)
C(19)-Si(1)-Pt(1)	103.7(4)
C(3)-C(2)-C(7)	110.2(11)
C(3)-C(2)-P(1)	112.1(10)
C(7)-C(2)-P(1)	114.0(9)
C(4)-C(3)-C(2)	113.7(12)
C(3)-C(4)-C(5)	110.9(12)
C(6)-C(5)-C(4)	110.8(12)
C(7)-C(6)-C(5)	111.6(12)
C(6)-C(7)-C(2)	110.2(11)

C(9)-C(8)-C(13)	111.1(12)
C(9)-C(8)-P(1)	111.8(9)
C(13)-C(8)-P(1)	108.6(9)
C(10)-C(9)-C(8)	111.6(13)
C(11)-C(10)-C(9)	111.0(14)
C(12)-C(11)-C(10)	113.2(14)
C(11)-C(12)-C(13)	111.2(14)
C(8)-C(13)-C(12)	111.9(14)
C(19)-C(14)-C(15)	118.8(12)
C(19)-C(14)-P(1)	118.5(10)
C(15)-C(14)-P(1)	122.7(10)
C(16)-C(15)-C(14)	120.2(13)
C(15)-C(16)-C(17)	120.4(14)
C(18)-C(17)-C(16)	119.1(14)
C(17)-C(18)-C(19)	123.4(13)
C(18)-C(19)-C(14)	118.1(12)
C(18)-C(19)-Si(1)	126.4(10)
C(14)-C(19)-Si(1)	115.5(9)
C(25)-C(20)-C(21)	116.8(13)
C(25)-C(20)-Si(1)	117.2(10)
C(21)-C(20)-Si(1)	126.0(11)
C(22)-C(21)-C(20)	123.7(14)
C(21)-C(22)-C(23)	118.1(13)
C(24)-C(23)-C(22)	120.2(14)
C(23)-C(24)-C(25)	120.4(14)
C(20)-C(25)-C(24)	120.8(13)
C(20)-C(25)-P(2)	117.3(10)
C(24)-C(25)-P(2)	122.0(11)
C(27)-C(26)-C(31)	110.7(13)
C(27)-C(26)-P(2)	117.0(11)
C(31)-C(26)-P(2)	110.0(11)
C(26)-C(27)-C(28)	109.0(15)
C(29)-C(28)-C(27)	112.2(18)
C(30)-C(29)-C(28)	112.2(16)
C(29)-C(30)-C(31)	110.8(17)
C(26)-C(31)-C(30)	110.8(15)
C(37)-C(32)-C(33)	111.4(12)
C(37)-C(32)-P(2)	109.2(10)
C(33)-C(32)-P(2)	109.8(10)
C(34)-C(33)-C(32)	111.6(13)
C(35)-C(34)-C(33)	110.7(13)
C(34)-C(35)-C(36)	109.4(14)
C(35)-C(36)-C(37)	110.9(13)
C(32)-C(37)-C(36)	111.4(12)
P(4)-Pt(2)-P(3)	162.23(13)
P(4)-Pt(2)-Si(2)	85.42(13)
P(3)-Pt(2)-Si(2)	84.95(13)
P(4)-Pt(2)-H(2PT)	78(5)
P(3)-Pt(2)-H(2PT)	109(5)
Si(2)-Pt(2)-H(2PT)	163(5)
C(51)-P(3)-C(39)	106.4(7)
C(51)-P(3)-C(45)	104.4(6)
C(39)-P(3)-C(45)	105.4(7)
C(51)-P(3)-Pt(2)	107.4(5)
C(39)-P(3)-Pt(2)	117.9(4)
C(45)-P(3)-Pt(2)	114.3(5)

C(62)-P(4)-C(63)	102.0(6)
C(62)-P(4)-C(69)	106.5(6)
C(63)-P(4)-C(69)	105.9(6)
C(62)-P(4)-Pt(2)	109.3(4)
C(63)-P(4)-Pt(2)	116.4(5)
C(69)-P(4)-Pt(2)	115.5(5)
C(38)-Si(2)-C(56)	107.2(6)
C(38)-Si(2)-C(57)	101.5(7)
C(56)-Si(2)-C(57)	112.6(6)
C(38)-Si(2)-Pt(2)	126.9(5)
C(56)-Si(2)-Pt(2)	103.7(4)
C(57)-Si(2)-Pt(2)	105.0(5)
C(44)-C(39)-C(40)	109.8(12)
C(44)-C(39)-P(3)	113.9(9)
C(40)-C(39)-P(3)	109.2(9)
C(41)-C(40)-C(39)	110.5(12)
C(40)-C(41)-C(42)	111.6(13)
C(43)-C(42)-C(41)	112.5(13)
C(42)-C(43)-C(44)	110.8(12)
C(43)-C(44)-C(39)	110.3(11)
C(50)-C(45)-C(46)	110.8(13)
C(50)-C(45)-P(3)	111.7(10)
C(46)-C(45)-P(3)	110.5(10)
C(47)-C(46)-C(45)	112.2(13)
C(46)-C(47)-C(48)	110.9(15)
C(49)-C(48)-C(47)	112.0(15)
C(48)-C(49)-C(50)	109.8(15)
C(45)-C(50)-C(49)	113.0(13)
C(52)-C(51)-C(56)	119.1(13)
C(52)-C(51)-P(3)	123.7(11)
C(56)-C(51)-P(3)	117.2(9)
C(53)-C(52)-C(51)	121.8(14)
C(52)-C(53)-C(54)	120.7(13)
C(55)-C(54)-C(53)	118.6(14)
C(54)-C(55)-C(56)	122.8(15)
C(51)-C(56)-C(55)	117.0(12)
C(51)-C(56)-Si(2)	116.8(10)
C(55)-C(56)-Si(2)	126.1(11)
C(62)-C(57)-C(58)	118.5(13)
C(62)-C(57)-Si(2)	116.8(10)
C(58)-C(57)-Si(2)	124.7(11)
C(59)-C(58)-C(57)	120.3(14)
C(58)-C(59)-C(60)	120.6(14)
C(61)-C(60)-C(59)	120.0(14)
C(60)-C(61)-C(62)	120.0(14)
C(57)-C(62)-C(61)	120.6(13)
C(57)-C(62)-P(4)	117.9(10)
C(61)-C(62)-P(4)	121.4(10)
C(64)-C(63)-C(68)	110.1(12)
C(64)-C(63)-P(4)	110.8(10)
C(68)-C(63)-P(4)	113.8(10)
C(63)-C(64)-C(65)	110.6(13)
C(66)-C(65)-C(64)	111.2(16)
C(65)-C(66)-C(67)	112.9(15)
C(68)-C(67)-C(66)	111.0(13)
C(67)-C(68)-C(63)	110.8(14)

C(74)-C(69)-C(70)	111.7(12)
C(74)-C(69)-P(4)	111.5(9)
C(70)-C(69)-P(4)	114.1(10)
C(69)-C(70)-C(71)	109.0(12)
C(72)-C(71)-C(70)	111.3(12)
C(71)-C(72)-C(73)	110.8(13)
C(72)-C(73)-C(74)	111.1(13)
C(69)-C(74)-C(73)	110.0(12)
C(77)-C(76)-C(75)	121(4)
C(76)-C(77)-C(78)	121(4)
C(79)-C(78)-C(77)	115(5)

X-ray Data for (^{iPr}PSiP)PdCl

The compound (^{iPr}PSiP)PdCl crystallized in the space group *P21/n* with one molecule in the asymmetric unit.

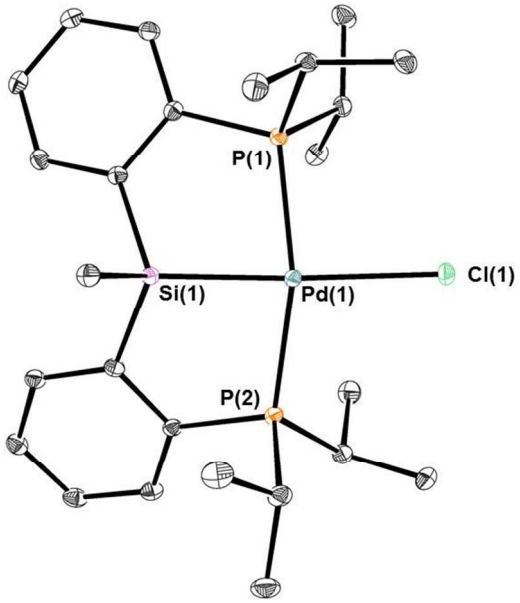

Figure S1: Ortep[1] of (^{Cy}PSiP)PdCl at 30% probability. Hydrogen atoms and solvent of crystallization are omitted for clarity.

Table S16: Crystal data and structure refinement for (^{iPr}PSiP)PdCl.

Empirical formula	$C_{25}H_{39}ClP_2PdSi$	
Formula weight	571.44	
Temperature	93(2) K	
Wavelength	0.71075 Å	
Crystal system	Monoclinic	
Space group	P 2_1/n	
Unit cell dimensions	a = 12.2218(3) Å	a= 90°.
	b = 13.9074(4) Å	b= 102.870(7)°.
	c = 16.2380(11) Å	g = 90°.
Volume	2690.7(2) Å^3	
Z	4	
Density (calculated)	1.411 Mg/m^3	
Absorption coefficient	0.963 mm^{-1}	
F(000)	1184	

Crystal size	0.320 x 0.220 x 0.210 mm^3
Crystal color and habit	Colorless Prism
Diffractometer	Rigaku Mercury275R CCD
Θ range for data collection	3.120 to 27.486°.
Index ranges	$-15 \leq h \leq 15$, $-18 \leq k \leq 18$, $-21 \leq l \leq 21$
Reflections collected	50623
Independent reflections	6153 [R(int) = 0.0336]
Observed reflections (I > 2σ(I))	5910
Completeness to θ = 25.242°	99.8 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	1.000 and 0.866
Solution method	SHELXT-2014/5 (Sheldrick, 2014)
Refinement method	SHELXL-2014/7 (Sheldrick, 2014)
Data / restraints / parameters	6153 / 0 / 280
Goodness-of-fit on F^2	1.262
Final R indices [I>2σ(I)]	R1 = 0.0382, wR2 = 0.0675
R indices (all data)	R1 = 0.0417, wR2 = 0.0686
Largest diff. peak and hole	0.576 and -0.310 e.$Å^{-3}$

Table S17: Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for (^{iPr}PSiP)PdCl. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	*U(eq)*
Pd(1)	5357(1)	3247(1)	7382(1)	15(1)
Cl(1)	6731(1)	3840(1)	8620(1)	20(1)
P(1)	3902(1)	4298(1)	7418(1)	16(1)
P(2)	6304(1)	1820(1)	7312(1)	15(1)
Si(1)	4134(1)	2640(1)	6224(1)	15(1)
C(1)	2579(2)	3755(2)	6865(2)	16(1)
C(2)	1523(2)	4050(2)	6969(2)	21(1)
C(3)	559(2)	3653(2)	6466(2)	23(1)
C(4)	639(2)	2981(2)	5851(2)	21(1)
C(5)	1687(2)	2675(2)	5754(2)	19(1)
C(6)	2670(2)	3036(2)	6272(2)	16(1)
C(7)	4322(2)	2973(2)	5142(2)	21(1)
C(8)	4330(2)	1290(2)	6226(1)	16(1)
C(9)	3591(2)	645(2)	5728(2)	19(1)
C(10)	3901(2)	-307(2)	5648(2)	21(1)
C(11)	4968(2)	-621(2)	6037(2)	22(1)
C(12)	5723(2)	9(2)	6524(2)	20(1)
C(13)	5400(2)	956(2)	6638(2)	17(1)
C(14)	3937(2)	5487(2)	6912(2)	23(1)
C(15)	4060(3)	5373(2)	6005(2)	31(1)
C(16)	2943(2)	6152(2)	6949(2)	31(1)
C(17)	3692(2)	4588(2)	8480(2)	21(1)
C(18)	4502(2)	5366(2)	8917(2)	28(1)
C(19)	3783(2)	3671(2)	9013(2)	26(1)
C(20)	7637(2)	1808(2)	6960(2)	21(1)
C(21)	7457(2)	2291(2)	6093(2)	28(1)
C(22)	8575(2)	2316(2)	7597(2)	24(1)
C(23)	6626(2)	1291(2)	8385(2)	20(1)
C(24)	7292(2)	350(2)	8489(2)	27(1)
C(25)	5532(2)	1179(2)	8686(2)	24(1)

Table S18: Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for (^{iPr}PSiP)PdCl. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Pd(1)	14(1)	13(1)	16(1)	-1(1)	3(1)	0(1)
Cl(1)	16(1)	22(1)	21(1)	-5(1)	1(1)	-3(1)
P(1)	17(1)	14(1)	18(1)	-1(1)	4(1)	1(1)
P(2)	13(1)	14(1)	18(1)	-1(1)	2(1)	0(1)
Si(1)	14(1)	14(1)	15(1)	0(1)	4(1)	0(1)
C(1)	17(1)	13(1)	19(1)	0(1)	4(1)	0(1)
C(2)	21(1)	19(1)	24(1)	-1(1)	9(1)	2(1)
C(3)	16(1)	20(1)	32(1)	3(1)	8(1)	2(1)
C(4)	17(1)	20(1)	26(1)	3(1)	2(1)	-2(1)
C(5)	19(1)	17(1)	21(1)	2(1)	4(1)	2(1)
C(6)	16(1)	15(1)	18(1)	4(1)	5(1)	1(1)
C(7)	24(1)	22(1)	20(1)	2(1)	6(1)	2(1)
C(8)	17(1)	17(1)	15(1)	1(1)	6(1)	1(1)
C(9)	17(1)	23(1)	18(1)	-1(1)	4(1)	-1(1)
C(10)	24(1)	20(1)	20(1)	-5(1)	5(1)	-5(1)
C(11)	25(1)	17(1)	24(1)	-2(1)	8(1)	2(1)
C(12)	19(1)	19(1)	22(1)	0(1)	5(1)	3(1)
C(13)	17(1)	17(1)	17(1)	-1(1)	6(1)	-1(1)
C(14)	24(1)	14(1)	31(1)	1(1)	5(1)	-2(1)
C(15)	37(2)	25(1)	35(2)	8(1)	15(1)	-1(1)
C(16)	35(2)	18(1)	39(2)	4(1)	7(1)	6(1)
C(17)	20(1)	24(1)	19(1)	-4(1)	4(1)	4(1)
C(18)	34(2)	23(1)	25(1)	-8(1)	0(1)	3(1)
C(19)	29(1)	29(1)	20(1)	0(1)	8(1)	0(1)
C(20)	15(1)	20(1)	27(1)	-3(1)	7(1)	1(1)
C(21)	24(1)	34(2)	27(1)	-4(1)	11(1)	-3(1)
C(22)	16(1)	26(1)	30(1)	-1(1)	4(1)	-1(1)
C(23)	20(1)	19(1)	19(1)	0(1)	-1(1)	-1(1)
C(24)	26(1)	23(1)	30(1)	7(1)	1(1)	3(1)
C(25)	32(1)	21(1)	22(1)	0(1)	9(1)	-3(1)

Table S19: Bond lengths for (^{iPr}PSiP)PdCl.

Pd(1)-Si(1)	2.2867(7)
Pd(1)-P(1)	2.3126(6)
Pd(1)-P(2)	2.3137(6)
Pd(1)-Cl(1)	2.4572(6)
P(1)-C(1)	1.829(2)
P(1)-C(17)	1.843(2)
P(1)-C(14)	1.851(3)
P(2)-C(13)	1.823(2)
P(2)-C(20)	1.844(2)
P(2)-C(23)	1.851(3)
Si(1)-C(7)	1.880(2)
Si(1)-C(6)	1.891(2)
Si(1)-C(8)	1.893(2)
C(1)-C(2)	1.400(3)
C(1)-C(6)	1.408(3)
C(2)-C(3)	1.390(4)
C(3)-C(4)	1.387(4)
C(4)-C(5)	1.391(3)
C(5)-C(6)	1.398(3)
C(8)-C(9)	1.396(3)
C(8)-C(13)	1.410(3)

C(9)-C(10)	1.392(3)
C(10)-C(11)	1.387(4)
C(11)-C(12)	1.385(3)
C(12)-C(13)	1.399(3)
C(14)-C(15)	1.523(4)
C(14)-C(16)	1.537(4)
C(17)-C(19)	1.531(4)
C(17)-C(18)	1.532(4)
C(20)-C(21)	1.531(4)
C(20)-C(22)	1.534(3)
C(23)-C(24)	1.530(3)
C(23)-C(25)	1.530(4)

Table S20: Bond angles for (^{iPr}PSiP)PdCl.

Si(1)-Pd(1)-P(1)	83.61(2)
Si(1)-Pd(1)-P(2)	83.41(2)
P(1)-Pd(1)-P(2)	159.94(2)
Si(1)-Pd(1)-Cl(1)	177.38(2)
P(1)-Pd(1)-Cl(1)	99.00(2)
P(2)-Pd(1)-Cl(1)	94.00(2)
C(1)-P(1)-C(17)	104.94(11)
C(1)-P(1)-C(14)	104.83(11)
C(17)-P(1)-C(14)	103.98(12)
C(1)-P(1)-Pd(1)	109.10(8)
C(17)-P(1)-Pd(1)	115.48(8)
C(14)-P(1)-Pd(1)	117.34(9)
C(13)-P(2)-C(20)	105.50(11)
C(13)-P(2)-C(23)	106.04(11)
C(20)-P(2)-C(23)	105.76(11)
C(13)-P(2)-Pd(1)	110.63(8)
C(20)-P(2)-Pd(1)	120.59(8)
C(23)-P(2)-Pd(1)	107.39(8)
C(7)-Si(1)-C(6)	106.27(11)
C(7)-Si(1)-C(8)	101.79(11)
C(6)-Si(1)-C(8)	114.17(10)
C(7)-Si(1)-Pd(1)	118.94(8)
C(6)-Si(1)-Pd(1)	108.05(8)
C(8)-Si(1)-Pd(1)	107.82(8)
C(2)-C(1)-C(6)	120.4(2)
C(2)-C(1)-P(1)	123.85(18)
C(6)-C(1)-P(1)	115.66(17)
C(3)-C(2)-C(1)	119.7(2)
C(4)-C(3)-C(2)	120.3(2)
C(3)-C(4)-C(5)	120.1(2)
C(4)-C(5)-C(6)	120.8(2)
C(5)-C(6)-C(1)	118.6(2)
C(5)-C(6)-Si(1)	124.40(18)
C(1)-C(6)-Si(1)	117.03(17)
C(9)-C(8)-C(13)	118.4(2)
C(9)-C(8)-Si(1)	124.84(18)
C(13)-C(8)-Si(1)	115.56(17)
C(10)-C(9)-C(8)	120.8(2)
C(11)-C(10)-C(9)	120.3(2)
C(12)-C(11)-C(10)	120.0(2)
C(11)-C(12)-C(13)	120.0(2)
C(12)-C(13)-C(8)	120.4(2)

C(12)-C(13)-P(2)	123.34(19)
C(8)-C(13)-P(2)	116.23(17)
C(15)-C(14)-C(16)	110.5(2)
C(15)-C(14)-P(1)	110.68(18)
C(16)-C(14)-P(1)	115.08(18)
C(19)-C(17)-C(18)	111.6(2)
C(19)-C(17)-P(1)	109.84(17)
C(18)-C(17)-P(1)	112.18(18)
C(21)-C(20)-C(22)	110.5(2)
C(21)-C(20)-P(2)	109.02(17)
C(22)-C(20)-P(2)	111.44(17)
C(24)-C(23)-C(25)	111.1(2)
C(24)-C(23)-P(2)	116.10(18)
C(25)-C(23)-P(2)	108.83(17)

X-ray Data for (^{iPr}PSiP)PdH

The compound (^{Cy}PSiP)PtH crystallized in the space group $P\,2_1/c$ with one molecule in the asymmetric unit.

Table S21: Crystal data and structure refinement for (^{iPr}PSiP)PdH.

Empirical formula	$C_{25}H_{40}P_2PdSi$	
Formula weight	537.00	
Temperature	93(2) K	
Wavelength	0.71075 Å	
Crystal system	Monoclinic	
Space group	$P\,2_1/c$	
Unit cell dimensions	a = 19.3892(13) Å	α = 90°.
	b = 9.00120(10) Å	β = 94.714(7)°.
	c = 14.9432(2) Å	γ = 90°.
Volume	2599.16(18) Å^3	
Z	4	
Density (calculated)	1.372 Mg/m^3	
Absorption coefficient	0.893 mm^{-1}	
F(000)	1120	
Crystal size	0.400 x 0.320 x 0.310 mm^3	
Crystal color and habit	Colorless Block	
Diffractometer	Rigaku R-AXIS RAPID imaging plate	
Θ range for data collection	3.012 to 27.483°.	
Index ranges	$-25 \le h \le 25$, $-11 \le k \le 11$, $-19 \le l \le 19$	
Reflections collected	120045	
Independent reflections	5971 [R(int) = 0.0343]	
Observed reflections (I > 2σ(I))	5745	
Completeness to θ = 25.242°	99.8 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.769 and 0.576	
Solution method	SHELXT-2014/5 (Sheldrick, 2014)	
Refinement method	SHELXL-2014/7 (Sheldrick, 2014)	
Data / restraints / parameters	5971 / 0 / 275	
Goodness-of-fit on F^2	1.217	
Final R indices [I>2σ(I)]	R1 = 0.0259, wR2 = 0.0574	
R indices (all data)	R1 = 0.0270, wR2 = 0.0578	
Largest diff. peak and hole	0.666 and -0.459 e.Å^{-3}	

Table S22: Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for (^{iPr}PSiP)PdH. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	*U(eq)*
Pd(1)	7270(1)	6345(1)	5570(1)	12(1)
P(1)	8375(1)	6410(1)	5175(1)	13(1)
P(2)	6322(1)	6588(1)	6355(1)	13(1)
Si(1)	7457(1)	8868(1)	5929(1)	13(1)
C(1)	8844(1)	7907(2)	5806(1)	15(1)
C(2)	9570(1)	7976(2)	5924(1)	18(1)
C(3)	9898(1)	9128(2)	6408(1)	20(1)
C(4)	9503(1)	10233(2)	6771(1)	21(1)
C(5)	8786(1)	10175(2)	6648(1)	19(1)
C(6)	8440(1)	9015(2)	6175(1)	15(1)
C(7)	7224(1)	10584(2)	5231(1)	19(1)
C(8)	6995(1)	9138(2)	6996(1)	15(1)
C(9)	7119(1)	10316(2)	7604(1)	18(1)
C(10)	6789(1)	10405(2)	8391(1)	19(1)
C(11)	6303(1)	9334(2)	8574(1)	20(1)
C(12)	6141(1)	8197(2)	7968(1)	19(1)
C(13)	6490(1)	8081(2)	7184(1)	15(1)
C(14)	8502(1)	6741(2)	3971(1)	16(1)
C(15)	9256(1)	6863(3)	3757(1)	22(1)
C(16)	8090(1)	8091(3)	3628(2)	24(1)
C(17)	8906(1)	4744(2)	5469(1)	18(1)
C(18)	8859(1)	4380(2)	6466(2)	24(1)
C(19)	8683(1)	3420(2)	4871(2)	23(1)
C(20)	5495(1)	7114(2)	5712(1)	17(1)
C(21)	5612(1)	8430(2)	5096(2)	22(1)
C(22)	4892(1)	7431(3)	6282(2)	28(1)
C(23)	6080(1)	4955(2)	7016(1)	18(1)
C(24)	5815(1)	3679(2)	6402(2)	22(1)
C(25)	6703(1)	4453(3)	7636(2)	26(1)

Table S23: Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for (^{iPr}PSiP)PdH. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	**U_{11}**	**U_{22}**	**U_{33}**	**U_{23}**	**U_{13}**	**U_{12}**
Pd(1)	10(1)	11(1)	14(1)	1(1)	2(1)	0(1)
P(1)	11(1)	12(1)	17(1)	1(1)	3(1)	0(1)
P(2)	11(1)	14(1)	14(1)	0(1)	2(1)	-1(1)
Si(1)	13(1)	11(1)	17(1)	1(1)	3(1)	0(1)
C(1)	14(1)	16(1)	16(1)	3(1)	2(1)	-2(1)
C(2)	15(1)	20(1)	21(1)	1(1)	3(1)	0(1)
C(3)	14(1)	25(1)	22(1)	3(1)	-1(1)	-5(1)
C(4)	22(1)	19(1)	21(1)	1(1)	0(1)	-7(1)
C(5)	20(1)	15(1)	23(1)	1(1)	4(1)	-2(1)
C(6)	15(1)	13(1)	16(1)	4(1)	3(1)	-2(1)
C(7)	21(1)	16(1)	22(1)	4(1)	4(1)	1(1)
C(8)	14(1)	15(1)	17(1)	2(1)	1(1)	2(1)
C(9)	17(1)	14(1)	23(1)	0(1)	2(1)	0(1)
C(10)	23(1)	17(1)	18(1)	-4(1)	-1(1)	3(1)
C(11)	22(1)	22(1)	16(1)	0(1)	4(1)	3(1)
C(12)	18(1)	20(1)	18(1)	1(1)	4(1)	-3(1)
C(13)	14(1)	16(1)	14(1)	-1(1)	1(1)	0(1)
C(14)	13(1)	17(1)	19(1)	0(1)	4(1)	-1(1)
C(15)	17(1)	29(1)	22(1)	1(1)	7(1)	-3(1)
C(16)	25(1)	26(1)	21(1)	7(1)	5(1)	5(1)

C(17)	13(1)	15(1)	26(1)	3(1)	4(1)	2(1)
C(18)	23(1)	21(1)	27(1)	7(1)	1(1)	4(1)
C(19)	21(1)	15(1)	34(1)	0(1)	7(1)	3(1)
C(20)	11(1)	21(1)	18(1)	-4(1)	0(1)	1(1)
C(21)	20(1)	20(1)	25(1)	1(1)	-3(1)	5(1)
C(22)	15(1)	39(1)	29(1)	-6(1)	4(1)	3(1)
C(23)	20(1)	18(1)	17(1)	1(1)	4(1)	-5(1)
C(24)	24(1)	19(1)	24(1)	-1(1)	2(1)	-8(1)
C(25)	33(1)	21(1)	23(1)	7(1)	-6(1)	-8(1)

Table S24: Bond lengths for (^{iPr}PSiP)PdH.

Pd(1)-P(2)	2.2701(5)
Pd(1)-P(1)	2.2701(5)
Pd(1)-Si(1)	2.3541(5)
Pd(1)-H(1)	1.65(3)
P(1)-C(1)	1.842(2)
P(1)-C(17)	1.852(2)
P(1)-C(14)	1.859(2)
P(2)-C(13)	1.839(2)
P(2)-C(23)	1.853(2)
P(2)-C(20)	1.8606(19)
Si(1)-C(7)	1.898(2)
Si(1)-C(8)	1.908(2)
Si(1)-C(6)	1.9165(19)
C(1)-C(2)	1.406(3)
C(1)-C(6)	1.409(3)
C(2)-C(3)	1.388(3)
C(3)-C(4)	1.391(3)
C(4)-C(5)	1.388(3)
C(5)-C(6)	1.400(3)
C(8)-C(9)	1.404(3)
C(8)-C(13)	1.410(3)
C(9)-C(10)	1.388(3)
C(10)-C(11)	1.391(3)
C(11)-C(12)	1.385(3)
C(12)-C(13)	1.405(3)
C(14)-C(16)	1.520(3)
C(14)-C(15)	1.526(3)
C(17)-C(19)	1.530(3)
C(17)-C(18)	1.535(3)
C(20)-C(21)	1.528(3)
C(20)-C(22)	1.529(3)
C(23)-C(25)	1.529(3)
C(23)-C(24)	1.532(3)

Table S25: Bond angles for (^{iPr}PSiP)PdH.

P(2)-Pd(1)-P(1)	162.471(19)
P(2)-Pd(1)-Si(1)	84.585(18)
P(1)-Pd(1)-Si(1)	84.457(18)
P(2)-Pd(1)-H(1)	95.0(9)
P(1)-Pd(1)-H(1)	93.4(9)
Si(1)-Pd(1)-H(1)	169.9(9)
C(1)-P(1)-C(17)	103.26(9)
C(1)-P(1)-C(14)	106.19(9)
C(17)-P(1)-C(14)	104.13(9)

C(1)-P(1)-Pd(1)	108.83(6)
C(17)-P(1)-Pd(1)	115.84(6)
C(14)-P(1)-Pd(1)	117.32(6)
C(13)-P(2)-C(23)	105.01(9)
C(13)-P(2)-C(20)	105.03(9)
C(23)-P(2)-C(20)	103.44(9)
C(13)-P(2)-Pd(1)	108.20(6)
C(23)-P(2)-Pd(1)	116.72(7)
C(20)-P(2)-Pd(1)	117.23(6)
C(7)-Si(1)-C(8)	104.41(9)
C(7)-Si(1)-C(6)	103.73(9)
C(8)-Si(1)-C(6)	110.99(8)
C(7)-Si(1)-Pd(1)	129.41(7)
C(8)-Si(1)-Pd(1)	103.84(6)
C(6)-Si(1)-Pd(1)	104.05(6)
C(2)-C(1)-C(6)	120.21(18)
C(2)-C(1)-P(1)	122.97(15)
C(6)-C(1)-P(1)	116.82(14)
C(3)-C(2)-C(1)	120.57(19)
C(2)-C(3)-C(4)	119.67(18)
C(5)-C(4)-C(3)	119.84(19)
C(4)-C(5)-C(6)	121.92(19)
C(5)-C(6)-C(1)	117.78(17)
C(5)-C(6)-Si(1)	125.23(15)
C(1)-C(6)-Si(1)	116.89(14)
C(9)-C(8)-C(13)	117.75(18)
C(9)-C(8)-Si(1)	124.75(15)
C(13)-C(8)-Si(1)	117.50(14)
C(10)-C(9)-C(8)	121.73(19)
C(9)-C(10)-C(11)	119.55(19)
C(12)-C(11)-C(10)	120.38(19)
C(11)-C(12)-C(13)	120.04(19)
C(12)-C(13)-C(8)	120.42(18)
C(12)-C(13)-P(2)	123.07(15)
C(8)-C(13)-P(2)	116.51(14)
C(16)-C(14)-C(15)	110.99(17)
C(16)-C(14)-P(1)	110.28(14)
C(15)-C(14)-P(1)	114.82(14)
C(19)-C(17)-C(18)	111.36(17)
C(19)-C(17)-P(1)	111.52(14)
C(18)-C(17)-P(1)	109.06(14)
C(21)-C(20)-C(22)	110.38(18)
C(21)-C(20)-P(2)	110.15(13)
C(22)-C(20)-P(2)	115.20(14)
C(25)-C(23)-C(24)	110.57(18)
C(25)-C(23)-P(2)	109.64(14)
C(24)-C(23)-P(2)	111.23(14)

Neutron diffraction

Neutron Data for (^{Cy}PSiP)PtH

Table S26: Crystal data and structure refinement for (^{Cy}PSiP)PtH.

Chemical formula	$2(C_{37}H_{56}P_2PtSi)C_5H_{12}$	
*M*r	1644.10	
Crystal system	Monoclinic	
Space group	*C*2/*c*	
Temperature	150K	
Unit cell dimensions	a = 24.4262(5) Å	α = 90°.
	b = 16.3000(3) Å	β = 105.394(7)°.
	c = 39.968(3) Å	γ = 90°.
Volume	15342.2 (12)Å^3	
Z	8	
Radiation type Neutron,	λ = 0.85 Å	
μ (mm^{-1})	3.80	
Crystal size (mm)	1.50 × 1.0 × 0.8	
Diffractometer KOALA diffractometer		
No. of measured, independent and observed [$I > 2.0\sigma(I)$] reflections	48674, 8466, 4173	
*R*int	0.502	
(sin θ/λ)max (Å^{-1})	1.106	
$R[F2 > 2\sigma(F2)]$, $wR(F2)$, S	0.170, 0.115, 1.15	
No. of reflections	3158	
No. of parameters	803	
No. of restraints	7	
H-atom treatment H atoms treated by a mixture of independent and constrained refinement $\Delta\rho$max, $\Delta\rho$min (e Å^{-3})		
1.66, -1.80		

Table S27: Bond lengths for (^{Cy}PSiP)PtH.

Pt1-H1 1.62 (2)	C26-C31 1.50 (3)
Pt1-P1 2.248 (19)	C27-C28 1.48 (3)
Pt1-P2 2.265 (18)	C28-C29 1.56 (3)
Pt1-Si1 2.33 (2)	C29-C30 1.58 (3)
Pt2-H2 1.72 (3)	C30-C31 1.56 (3)
Pt2-P3 2.22 (2)	C32-C33 1.52 (2)
Pt2-P4 2.244 (19)	C32-C37 1.50 (2)
Pt2-Si2 2.35 (3)	C33-C34 1.54 (3)
P1-C2 1.86 (2)	C34-C35 1.52 (3)
P1-C8 1.85 (3)	C35-C36 1.53 (3)
P1-C14 1.85 (2)	C36-C37 1.54 (3)
P2-C25 1.81 (2)	C39-C40 1.51 (2)
P2-C26 1.83 (2)	C39-C44 1.50 (2)
P2-C32 1.88 (2)	C40-C41 1.53 (2)
P3-C39 1.86 (2)	C41-C42 1.57 (2)
P3-C45 1.83 (2)	C42-C43 1.50 (2)
P3-C51 1.86 (2)	C43-C44 1.54 (2)
P4-C62 1.825 (19)	C45-C46 1.52 (2)
P4-C63 1.82 (2)	C45-C50 1.53 (2)
P4-C69 1.85 (2)	C46-C47 1.53 (2)
Si1-C1 1.88 (3)	C47-C48 1.56 (3)
Si1-C19 1.85 (2)	C48-C49 1.50 (3)
Si1-C20 1.99 (2)	C49-C50 1.53 (2)
Si2-C38 1.91 (3)	C51-C52 1.43 (2)
Si2-C56 1.91 (3)	C51-C56 1.399 (19)
Si2-C57 1.87 (3)	C52-C53 1.36 (2)

C2-C3 1.55 (2)	C53-C54 1.44 (2)
C2-C7 1.508 (19)	C54-C55 1.38 (2)
C3-C4 1.52 (2)	C55-C56 1.40 (2)
C4-C5 1.49 (2)	C57-C58 1.40 (2)
C5-C6 1.53 (3)	C57-C62 1.393 (19)
C6-C7 1.54 (2)	C58-C59 1.39 (2)
C8-C9 1.50 (2)	C59-C60 1.38 (2)
C8-C13 1.60 (2)	C60-C61 1.33 (2)
C9-C10 1.50 (3)	C61-C62 1.461 (18)
C10-C11 1.56 (3)	C63-C64 1.53 (2)
C11-C12 1.52 (3)	C63-C68 1.49 (2)
C12-C13 1.55 (3)	C64-C65 1.53 (2)
C14-C15 1.35 (2)	C65-C66 1.45 (3)
C14-C19 1.418 (19)	C66-C67 1.54 (3)
C15-C16 1.395 (19)	C67-C68 1.56 (2)
C16-C17 1.41 (2)	C69-C70 1.50 (2)
C17-C18 1.38 (2)	C69-C74 1.54 (2)
C18-C19 1.40 (2)	C70-C71 1.52 (2)
C20-C21 1.36 (2)	C71-C72 1.56 (2)
C20-C25 1.38 (2)	C72-C73 1.53 (2)
C21-C22 1.42 (2)	C73-C74 1.56 (2)
C22-C23 1.41 (2)	C75-C76 1.541 (10)
C23-C24 1.35 (2)	C76-C77 1.536 (10)
C24-C25 1.39 (2)	C77-C78 1.537 (10)
C26-C27 1.50 (2)	C78-C79 1.535 (10)

Table S28: Bond angles for (^{Cy}PSiP)PtH.

H1-Pt1-P1 94.5 (10)	C21-C22-C23 117.8 (13)
H1-Pt1-P2 94.9 (10)	C22-C23-C24 120.9 (13)
P1-Pt1-P2 159.9 (7)	C23-C24-C25 122.2 (13)
H1-Pt1-Si1 178.2 (11)	P2-C25-C24 123.1 (12)
P1-Pt1-Si1 83.7 (7)	P2-C25-C20 120.3 (12)
P2-Pt1-Si1 86.7 (7)	C24-C25-C20 116.6 (12)
H2-Pt2-P3 96.4 (11)	P2-C26-C27 115.5 (12)
H2-Pt2-P4 91.0 (11)	P2-C26-C31 110.4 (12)
P3-Pt2-P4 162.0 (8)	C27-C26-C31 108.9 (14)
H2-Pt2-Si2 173.8 (12)	C26-C27-C28 114.2 (16)
P3-Pt2-Si2 86.0 (8)	C27-C28-C29 109.9 (19)
P4-Pt2-Si2 85.1 (8)	C28-C29-C30 111 (2)
Pt1-P1-C2 122.6 (11)	C29-C30-C31 108.4 (17)
Pt1-P1-C8 113.8 (10)	C30-C31-C26 111.4 (16)
C2-P1-C8 101.3 (10)	P2-C32-C33 111.3 (11)
Pt1-P1-C14 108.2 (9)	P2-C32-C37 110.6 (12)
C2-P1-C14 104.9 (10)	C33-C32-C37 113.9 (14)
C8-P1-C14 104.4 (12)	C32-C33-C34 111.1 (12)
Pt1-P2-C25 110.0 (9)	C33-C34-C35 114.2 (15)
Pt1-P2-C26 114.5 (9)	C34-C35-C36 107.8 (16)
C25-P2-C26 111.2 (11)	C35-C36-C37 112.5 (14)
Pt1-P2-C32 112.6 (9)	C36-C37-C32 112.9 (14)
C25-P2-C32 101.6 (10)	P3-C39-C40 110.0 (10)
C26-P2-C32 106.1 (10)	P3-C39-C44 117.2 (11)
Pt2-P3-C39 119.8 (10)	C40-C39-C44 113.2 (12)
Pt2-P3-C45 116.8 (10)	C39-C40-C41 113.3 (12)
C39-P3-C45 103.8 (11)	C40-C41-C42 113.3 (13)
Pt2-P3-C51 107.4 (9)	C41-C42-C43 111.2 (13)
C39-P3-C51 102.8 (10)	C42-C43-C44 111.7 (12)

C45-P3-C51 104.4 (11)
Pt2-P4-C62 108.7 (9)
Pt2-P4-C63 117.5 (9)
C62-P4-C63 103.1 (9)
Pt2-P4-C69 115.1 (9)
C62-P4-C69 106.0 (10)
C63-P4-C69 105.3 (10)
Pt1-Si1-C1 123.3 (11)
Pt1-Si1-C19 104.1 (10)
C1-Si1-C19 110.5 (12)
Pt1-Si1-C20 104.2 (9)
C1-Si1-C20 102.4 (12)
C19-Si1-C20 112.4 (11)
Pt2-Si2-C38 124.2 (13)
Pt2-Si2-C56 104.1 (11)
C38-Si2-C56 105.0 (13)
Pt2-Si2-C57 106.2 (11)
C38-Si2-C57 103.3 (13)
C56-Si2-C57 114.7 (14)
P1-C2-C3 108.7 (11)
P1-C2-C7 114.2 (11)
C3-C2-C7 110.1 (11)
C2-C3-C4 110.8 (12)
C3-C4-C5 110.4 (13)
C4-C5-C6 111.5 (14)
C5-C6-C7 109.3 (13)
C6-C7-C2 109.4 (12)
P1-C8-C9 113.7 (12)
P1-C8-C13 108.6 (11)
C9-C8-C13 108.0 (12)
C8-C9-C10 115.1 (13)
C9-C10-C11 112.3 (16)
C10-C11-C12 108.5 (17)
C11-C12-C13 113.6 (16)
C12-C13-C8 111.1 (13)
P1-C14-C15 124.2 (12)
P1-C14-C19 114.6 (11)
C15-C14-C19 121.0 (12)
C14-C15-C16 122.5 (13)
C15-C16-C17 118.6 (13)
C16-C17-C18 117.9 (14)
C17-C18-C19 124.3 (14)
C14-C19-C18 115.5 (12)
C14-C19-Si1 118.0 (11)
C18-C19-Si1 126.5 (12)
Si1-C20-C21 120.7 (12)
Si1-C20-C25 115.5 (11)
C21-C20-C25 123.8 (13)
C20-C21-C22 118.7 (13)
C43-C44-C39 113.3 (12)
P3-C45-C46 110.4 (12)
P3-C45-C50 109.2 (13)
C46-C45-C50 110.0 (13)
C45-C46-C47 112.1 (14)
C46-C47-C48 110.9 (15)
C47-C48-C49 108.1 (16)
C48-C49-C50 113.2 (15)
C49-C50-C45 111.9 (14)
P3-C51-C52 122.1 (11)
P3-C51-C56 118.7 (12)
C52-C51-C56 119.2 (12)
C51-C52-C53 120.6 (14)
C52-C53-C54 120.5 (17)
C53-C54-C55 118.3 (15)
C54-C55-C56 121.8 (14)
C55-C56-C51 119.4 (13)
C55-C56-Si2 124.9 (13)
C51-C56-Si2 115.7 (12)
Si2-C57-C58 126.0 (13)
Si2-C57-C62 115.4 (11)
C58-C57-C62 118.6 (12)
C57-C58-C59 122.6 (14)
C58-C59-C60 119.0 (15)
C59-C60-C61 120.3 (14)
C60-C61-C62 122.5 (13)
C61-C62-P4 123.2 (10)
C61-C62-C57 117.0 (11)
P4-C62-C57 119.8 (10)
P4-C63-C64 110.0 (11)
P4-C63-C68 112.4 (11)
C64-C63-C68 110.7 (11)
C63-C64-C65 108.8 (13)
C64-C65-C66 115.5 (17)
C65-C66-C67 110.5 (18)
C66-C67-C68 111.5 (15)
C67-C68-C63 109.7 (12)
P4-C69-C70 116.2 (11)
P4-C69-C74 111.0 (11)
C70-C69-C74 110.6 (11)
C69-C70-C71 113.5 (12)
C70-C71-C72 110.4 (14)
C71-C72-C73 109.9 (14)
C72-C73-C74 112.9 (14)
C69-C74-C73 108.5 (12)
C75-C76-C77 109.6 (5)
C76-C77-C78 109.5 (5)
C77-C78-C79 109.4 (5)

Information about XAS

The Fourier magnitude and imaginary parts of the Pt L_{III} EXAFS and Pd K-edge data and fits of the M-P/Si, M-Cl, and M-O first shell fits, are show below.

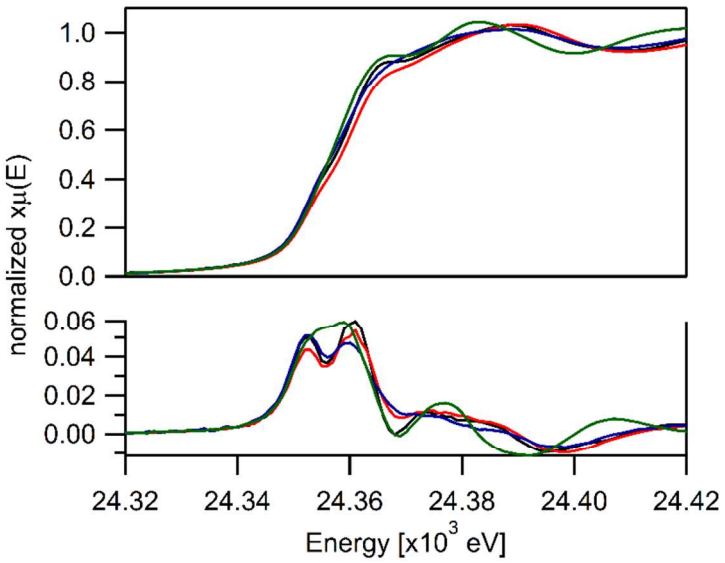

Figure S2: Pd K-Edge XANES (top) and 1st derivative spectra (bottom) for **$Pd(PPh_3)_4$** (green), **(^{Ph}PSiP)$_2$Pd$_2$** (blue), **(^{Cy}PSiP)PdCl** (black), and **(^{Cy}PSiP)PdH** (red) in room temperature benzene.

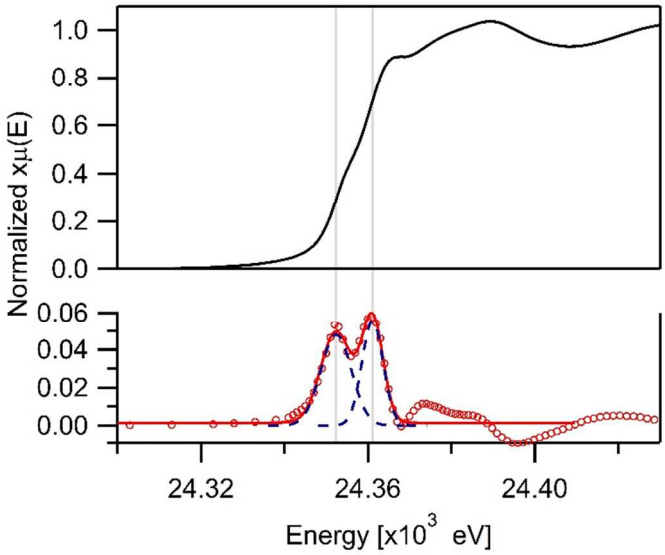

Figure S3: Top: Pd K-edge XANES experimental data for **(^{Cy}PSiP)PdCl**. First derivative of edge (○) with peak fit (─, red) and component peaks(---, blue). Peak maxima are identified by vertical lines.

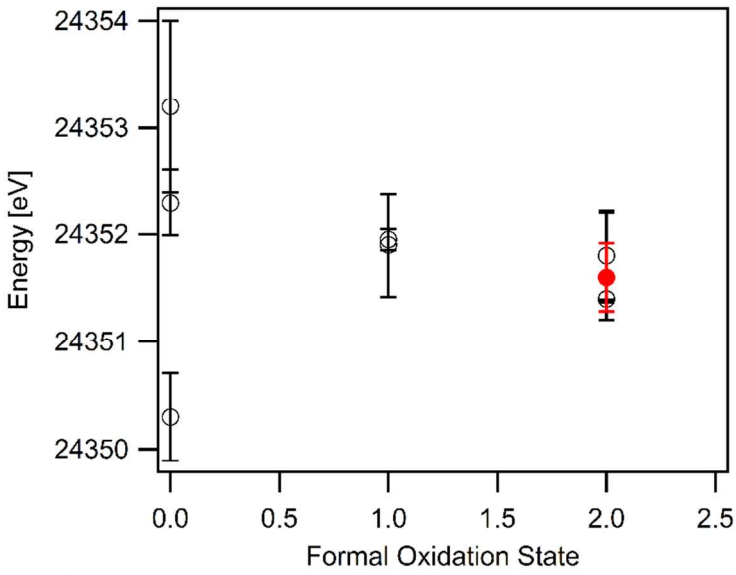

Figure S4: Energy of the 1st peak in the Pd K-edge XANES experimental data reference Pd pincer compounds (○) and PdH (●) listed in Table S29.

Table S29: Solution XANES Edge positions in molecular compounds dissolved in room temperature benzene at the Pd K edge.

Formal Ox. State	Compound	Edge Position	
		Peak 1, eV	Peak 2, eV
Pd(0)	Pd-Foil	24352.6 [a]	24362.2 ± 0.4
Pd(0)	$Pd(PPh_3)_4$ (solid)	24353.2 ± 0.8	24359.9 ± 0.2
Pd(0)	$Pd(PPh_3)_4$ (C_6H_6)	24350.3 ± 0.4	24359.2 ± 0.4
Pd(0)	$(^{Ph}PSi^{H}P)Pd\text{-}PPh_3$	24352.3 ± 0.3	24359.8 ± 0.3
Pd(I)	$(^{Ph}PSiP)_2Pd_2$ (solid)	24352.0 ± 0.1	24360.3 ± 0.2
Pd(I)	$(^{Ph}PSiP)_2Pd_2$ (C_6H_6)	24351.9 ± 0.4	24360.4 ± 0.4
Pd(II)	$(^{Cy}PSiP)PdOTf$	24351.4 ± 0.2	24361.0 ± 0.2
Pd(II)	$(^{Cy}PSiP)PdCl$	24351.8 ± 0.4	24360.5 ± 0.3
Pd(II)	$(^{iPr2}PSiP)PdCl$	24351.8 ± 0.4	24360.4 ± 0.3
	$(^{Cy}PSiP)PdH$	24351.6 ± 0.3	24360.7 ± 0.3
Pt(0)	Pt-foil	11562.76[a]	--
Pt(0)	$Pt(PPh_3)_4$	11565.4 ± 0.2	--
Pt(II)	$(^{Cy}PSiP)PtCl$	11565.2 ± 0.2	--
	$(^{Cy}PSiP)PtH$	11566.4 ± 0.2	--

[a]Pt foil edge energy defined in reference [2].

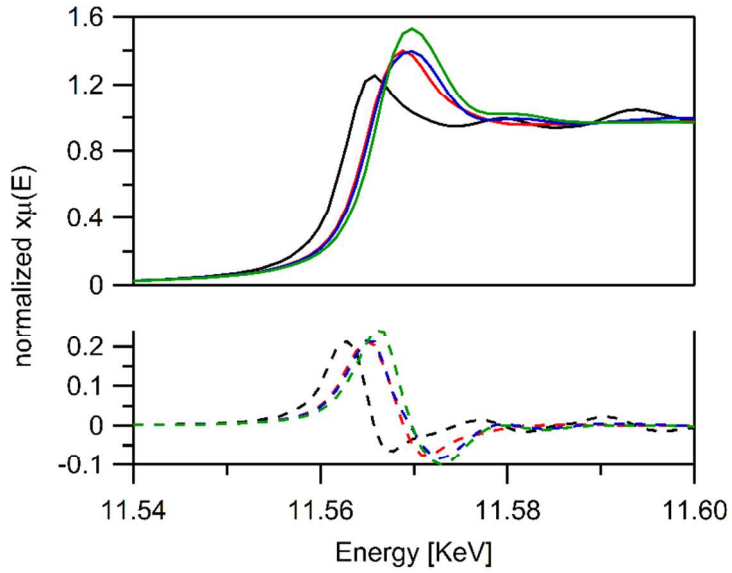

Figure S5: Pt L_{III}-edge XANES (solid) and 1st derivative (dashed) experimental data. Compounds include **Pt-foil** (black), **$Pt(PPh_3)_4$** (red), **(^{Cy}PSiP)PtCl** (blue), and **(^{Cy}PSiP)PtH** (green).

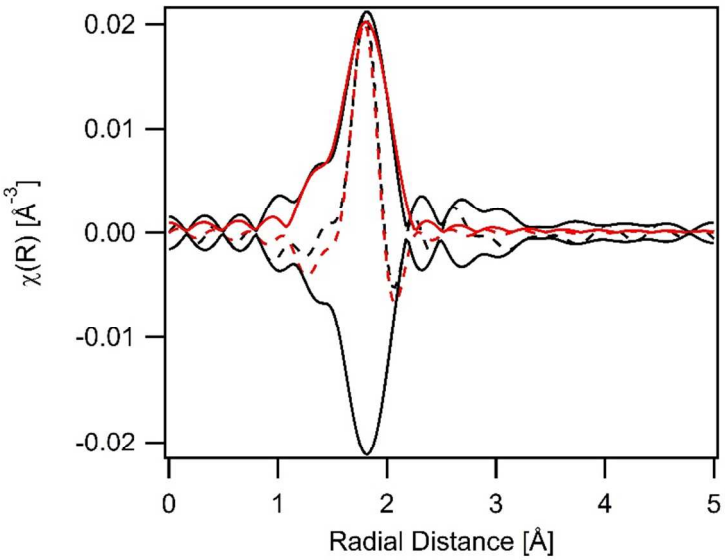

Figure S6: Pd K-edge EXAFS region of **$Pd(PPh_3)_4$** in room temperature benzene. Experimental data (black) and quantitative fits (red) of the first coordination shell are shown for both the fourier transform magnitude and inverse magnitude (─, solid lines) and imaginary components (---, dashed lines).

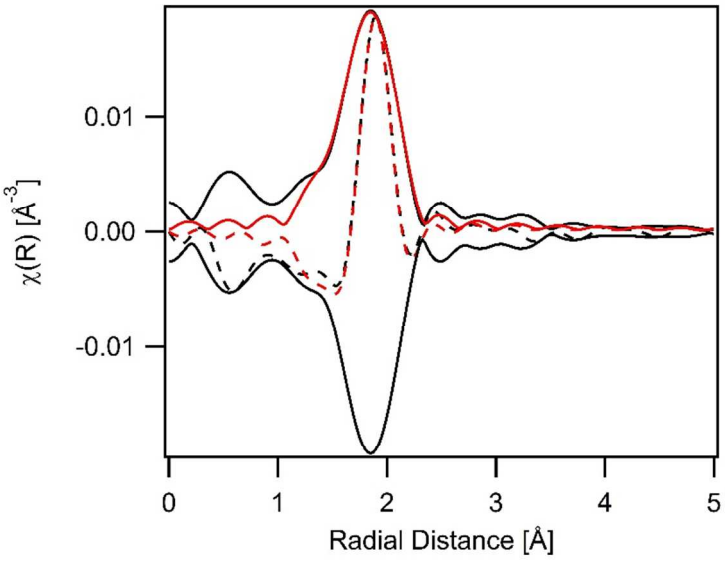

Figure S7: Pd K-edge EXAFS region of **(^{Ph}PSi^{H}P)Pd-PPh$_3$** in room temperature benzene. Experimental data (black) and quantitative fits (red) of the first coordination shell are shown for both the fourier transform magnitude and inverse magnitude (—, solid lines) and imaginary components (---, dashed lines).

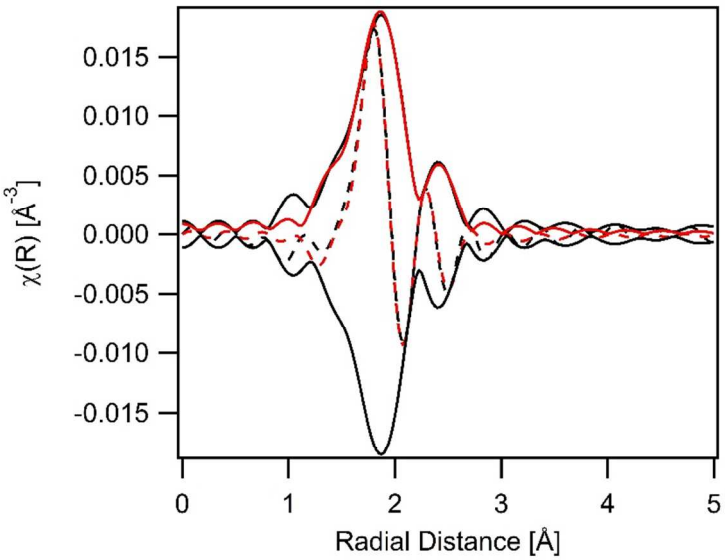

Figure S8: Pd K-edge EXAFS region of **(^{Ph}PSiP)$_2$Pd$_2$** in room temperature benzene. Experimental data (black) and quantitative fits (red) of the first coordination shell are shown for both the fourier transform magnitude and inverse magnitude (—, solid lines) and imaginary components (---, dashed lines).

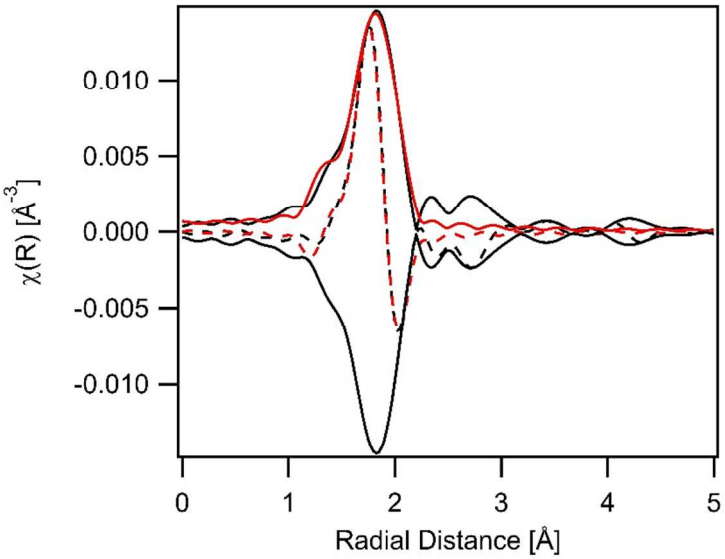

Figure S9: Pd K-edge EXAFS region of (**^{Cy}PSiP)PdOTf** in room temperature benzene. Experimental data (black) and quantitative fits (red) of the first coordination shell are shown for both the fourier transform magnitude and inverse magnitude (—, solid lines) and imaginary components (---, dashed lines).

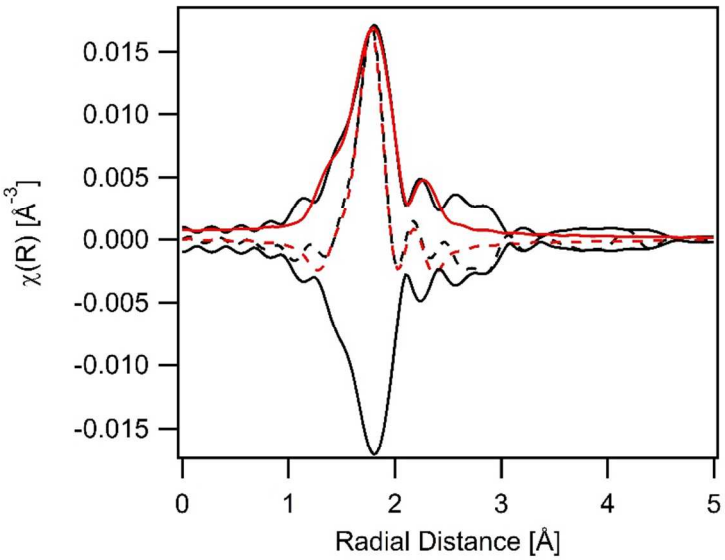

Figure S10: Pd K-edge EXAFS region of (**^{Cy}PSiP)PdCl** in room temperature benzene. Experimental data (black) and quantitative fits (red) of the first coordination shell are shown for both the fourier transform magnitude and inverse magnitude (—, solid lines) and imaginary components (---, dashed lines).

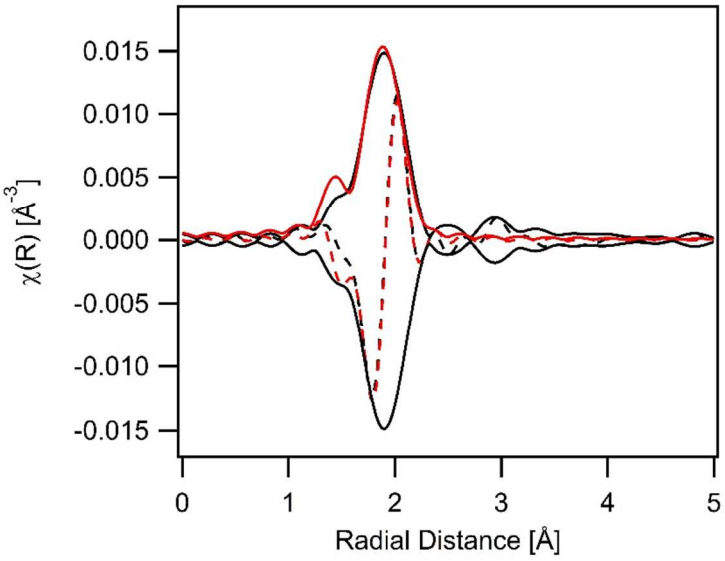

Figure S11: Pd K-edge EXAFS region of the difference spectrum for **(^{Pn}PSi^{H}P)Pd-PPh$_3$** - **(^{Cy}PSiP)PdH** in room temperature benzene. Experimental data (black) and quantitative fits (red) of the first coordination shell are shown for both the fourier transform magnitude and inverse magnitude (—, solid lines) and imaginary components (---, dashed lines).

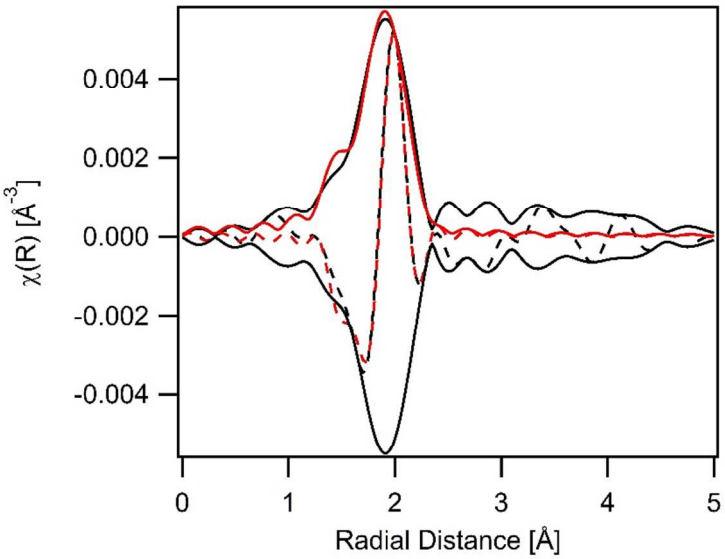

Figure S12: Pd K-edge EXAFS region of the difference spectrum for **(^{Cy}PSiP)PdCl** - **(^{Cy}PSiP)PdH** in room temperature benzene. Experimental data (black) and quantitative fits (red) of the first coordination shell are shown for both the fourier transform magnitude and inverse magnitude (—, solid lines) and imaginary components (---, dashed lines).

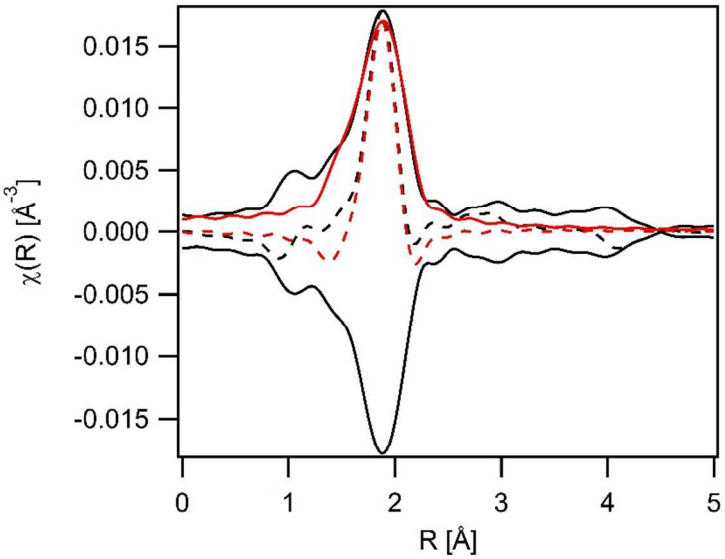

Figure S13: Pt L_{III} edge EXAFS region of **$Pt(PPh_3)_4$** in room temperature benzene. Experimental data (black) and quantitative fits (red) of the first coordination shell are shown for both the fourier transform magnitude and inverse magnitude (─, solid lines) and imaginary components (---, dashed lines).

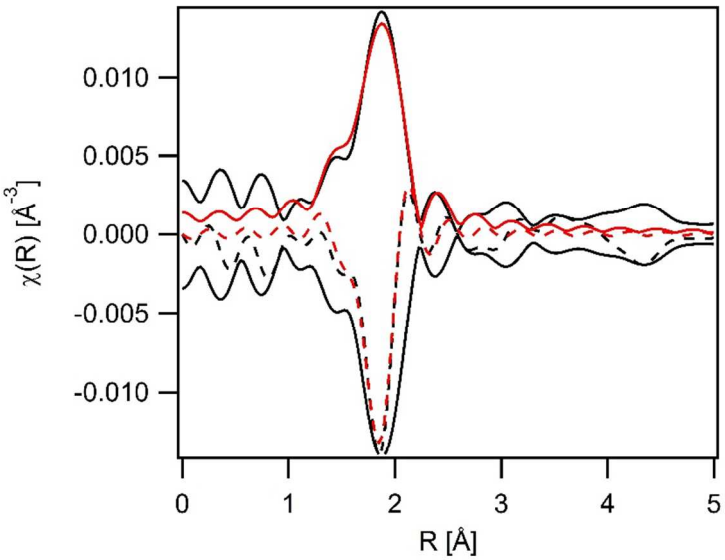

Figure S14: Pt L_{III} edge EXAFS region of **(^{Cy}PSiP)PtCl** in room temperature benzene. Experimental data (black) and quantitative fits (red) of the first coordination shell are shown for both the fourier transform magnitude and inverse magnitude (─, solid lines) and imaginary components (---, dashed lines).

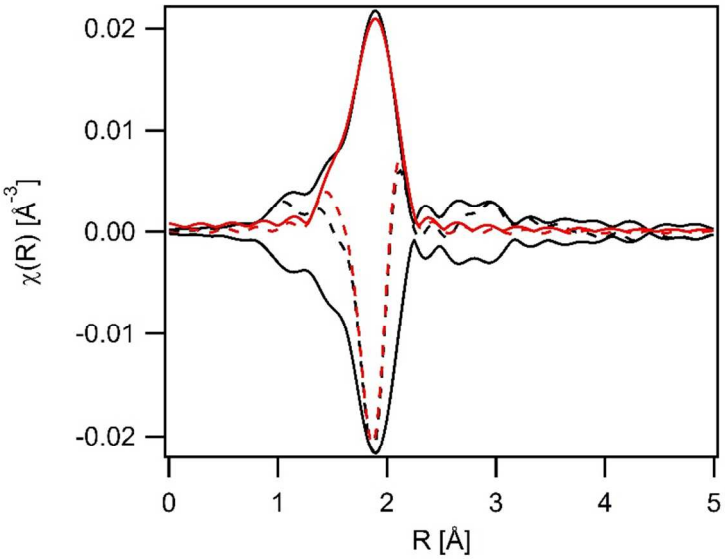

Figure S15: Pt L_{III} edge EXAFS region of **(^{Cy}PSiP)PtH** in room temperature benzene. Experimental data (black) and quantitative fits (red) of the first coordination shell are shown for both the fourier transform magnitude and inverse magnitude (─, solid lines) and imaginary components (---, dashed lines).

Information about DFT calculations, optimized coordinates and energies

Calculations were carried out at the DFT level with the B3LYP, TPSSh, ωB97xd and PBE0 functionals, as implemented in Gaussian09 (Rev. D.01). The lighter elements (P, Si, C and H) were described with the all-electron 6-311+G** basis set, which has a triple-ζ valence shell including both polarization and diffuse functions. The heavier elements (Pd and Pt) were described with the small-core electron core potential LANL08(f) basis set, which has a triple-ζ valence shell and accounts for the relativistic effects on the metal center. All geometries include the full real ligands and were optimized in the gas phase without any symmetry or geometry constraint. A pruned (99,590) grid was used for high accuracy in the calculation of the two-electron integrals and their derivatives. The DFT-optimized geometries were compared to the X-Ray structure by computing the root mean square deviation (RMSD) for each functional (Table S29). With the Pd complex (^{Cy}PSiP)PdH, accuracy can be significantly enhanced by using the PBE0 functional (RMSD = 0.02293 Å) instead of the classical B3LYP (RMSD = 0.04127 Å). All other functionals also outperform the B3LYP functional, yielding lower RMSD values. This includes the ωB97xd functional (RMSD = 0.02370 Å), which is very close to the best in the series, the PBE0 functional. The performance of the latter functional can be further improved by adding dispersion with the Grimme's GD3BJ method, including Becke-Johnson damping (RMSD = 0.01600 Å). The same trends were observed with the Pt complex, (^{Cy}PSiP)PtH. On the basis of these results, the DFT(PBE0+GD3BJ) level of theory was used to carry out the present study.

Table S30: Comparison of geometric parameters from X-Ray experiments and DFT calculations in Å for (^{Cy}PSiP)MH (M = Pd or Pt).

(^{Cy}PSiP)PdH						
	M-P	M-Si	Si-C	C-C	P-C	RMSD[a]
X-Ray[b]	2.263	2.331	1.903	1.408	1.838	0.00000
B3LYP[c]	2.321	2.392	1.929	1.413	1.865	0.04127
TPSSh[c]	2.298	2.375	1.926	1.415	1.855	0.02838
□b97xd[c]	2.294	2.371	1.915	1.406	1.848	0.02370
PBE0[c]	2.289	2.370	1.920	1.408	1.850	0.02293
PBE0+GD3BJ[c]	2.276	2.362	1.914	1.406	1.843	0.01600
(^{Cy}PSiP)PPtH						
	M-P	M-Si	Si-C	C-C	P-C	RMSD[a]
X-Ray[b]	2.262	2.336	1.898	1.410	1.838	0.00000
B3LYP[c]	2.304	2.384	1.927	1.414	1.866	0.03379
TPSSh[c]	2.285	2.370	1.924	1.415	1.856	0.02328
□b97xd[c]	2.283	2.365	1.914	1.406	1.848	0.01819
PBE0[c]	2.276	2.363	1.918	1.409	1.850	0.01715
PBE0+GD3BJ[c]	2.266	2.357	1.913	1.407	1.844	0.01206

[a]Root mean square deviation of the DFT geometries from the X-Ray structure; [b]Mean values from the two independent molecules in the unit cell; [c]From the gas phase DFT full geometry optimizations.

DFT-optimized geometries

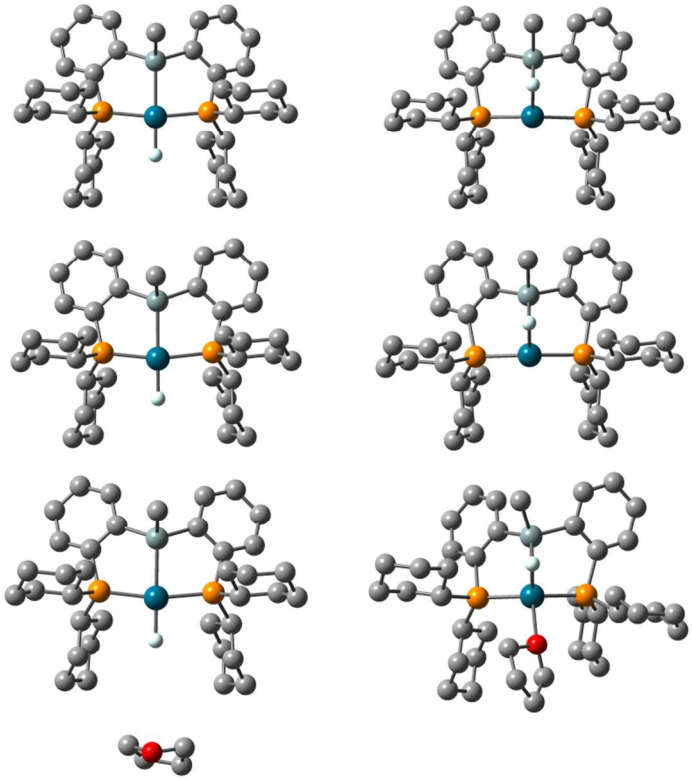

Figure S16: DFT(PBE0+GD3BJ/LANL08(f),6-311+G**) optimized geometries of the Pd(II) hydride isomer of (^{Cy}PSiP)PdH (gas phase, top-left; implicit THF, middle-left; explicit THF, bottom-left) and Pd(0) η^2-silane isomer (gas phase, top-right; implicit THF, middle-right; explicit THF, bottom-right). All hydrogens were removed for clarity, except the hydride/agostic one.

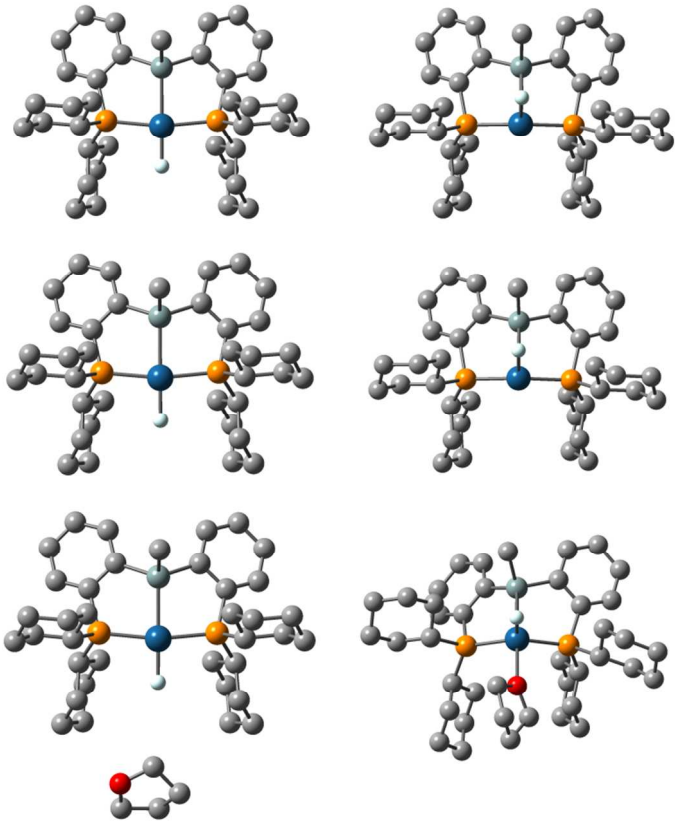

Figure S17: DFT(PBE0+GD3BJ/LANL08(f),6-311+G**) optimized geometries of the Pt(II) hydride isomer of (^{Cy}PSiP)PtH (gas phase, top-left; implicit THF, middle-left; explicit THF, bottom-left) and Pt(0) η^2-silane isomer (gas phase, top-right; implicit THF, middle-right; explicit THF, bottom-right). All hydrogens were removed for clarity, except the hydride/agostic one.

DFT-optimized coordinates (Cartesians, in Å) and energies (Gibbs, in hartrees)

Pd(II) hydride gas phase; G = -2540.365763

Pd	0.00000000	0.13110700	-0.60599700
P	-2.24268300	0.15900400	-0.21688900
Si	-0.00000900	-1.71418900	0.86876800
P	2.24268300	0.15900000	-0.21688600
C	2.59486300	-0.67689100	1.38762700
C	-3.31276700	-0.67433600	-1.47717500
H	-3.10090700	-0.10991000	-2.39623900
C	3.31277100	-0.67430500	-1.47719000
H	3.10091200	-0.10985600	-2.39624000
C	1.85106500	-2.16776300	3.12030200
H	1.10441000	-2.83296500	3.54421400
C	-2.83795200	-2.11219600	-1.68836700
H	-1.76498800	-2.11710200	-1.90730100
H	-2.97194800	-2.67010700	-0.75178100
C	-4.81424800	-0.63002700	-1.20388700
H	-5.02202300	-1.15123400	-0.26135100
H	-5.15666800	0.40329100	-1.08260300
C	-3.80052500	-0.50011300	2.07307200
H	-4.56912100	0.15449700	1.67546300
C	-1.85106500	-2.16771300	3.12032800
H	-1.10441500	-2.83292300	3.54424000
C	4.02435500	-1.14833700	3.27968700
H	4.95894400	-0.99847400	3.81074900
C	2.83796400	-2.11216200	-1.68842100
H	2.97196100	-2.67009600	-0.75184900
H	1.76500100	-2.11706800	-1.90735800
C	4.81425100	-0.62999700	-1.20389400
H	5.02202400	-1.15122700	-0.26137100
H	5.15666500	0.40331900	-1.08258300
C	-1.59051200	-1.50925700	1.91358300
C	3.80053900	-0.50018000	2.07304600
H	4.56914100	0.15442400	1.67543800
C	5.12340500	-2.74280500	-2.54201800
H	5.35385000	-3.33269000	-1.64446900
H	5.67211600	-3.20444800	-3.36976500
C	-0.00003100	-3.54762900	0.37443100
H	-0.88594200	-3.79846700	-0.21474000
H	-0.00005200	-4.18294900	1.26794900
H	0.88588900	-3.79849300	-0.21471600
C	5.59301500	-1.30798200	-2.32924200
H	5.45352900	-0.73856900	-3.25822400
H	6.66513100	-1.28504400	-2.10593100
C	-5.12338700	-2.74287100	-2.54195700
H	-5.35383300	-3.33273400	-1.64439300
H	-5.67209300	-3.20453800	-3.36969400
C	1.59051000	-1.50928900	1.91356600
C	3.04719400	-1.98882400	3.80290500
H	3.21876300	-2.50081300	4.74484900
C	-3.62214800	-2.79595700	-2.80311300
H	-3.40156200	-2.29574500	-3.75578900
H	-3.28861500	-3.83368600	-2.91024300
C	-2.59485900	-0.67685200	1.38764200
C	3.62216700	-2.79589100	-2.80318200

H	3.28863900	-3.83361800	-2.91034000
H	3.40158300	-2.29565400	-3.75584600
C	-5.59300500	-1.30804400	-2.32922000
H	-5.45351600	-0.73865500	-3.25821600
H	-6.66512100	-1.28510600	-2.10591400
C	-2.99350600	2.61696700	-1.31256800
H	-3.63883200	2.10812200	-2.03713500
H	-1.97926100	2.61744400	-1.73169800
C	-4.02433700	-1.14825100	3.27972400
H	-4.95891800	-0.99836800	3.81079400
C	-2.96224200	1.84746200	0.00713900
H	-3.99108700	1.72907100	0.37306000
C	2.96223700	1.84745500	0.00717800
H	3.99108700	1.72905800	0.37308500
C	-3.04718300	-1.98874700	3.80294100
H	-3.21875100	-2.50072200	4.74489300
C	2.14231700	2.59210200	1.06287600
H	1.09727800	2.60332100	0.72770000
H	2.16419700	2.04613700	2.01169500
C	-2.14231200	2.59214000	1.06280900
H	-2.16418200	2.04619900	2.01164200
H	-1.09727700	2.60335200	0.72762200
C	-3.47610400	4.05077100	-1.11058200
H	-3.44939000	4.58511800	-2.06635800
H	-4.52622400	4.04215000	-0.78619400
C	-2.63795300	4.78157500	-0.06802300
H	-1.60630500	4.87064500	-0.43421400
H	-3.01169200	5.80105200	0.07587200
C	3.47607900	4.05079400	-1.11049200
H	3.44935300	4.58516600	-2.06625400
H	4.52620300	4.04216700	-0.78611700
C	2.63343500	4.02212100	1.25355900
H	2.00314200	4.53391800	1.98889300
H	3.65093500	4.00902600	1.66861800
C	2.63793900	4.78156900	-0.06790400
H	3.01167900	5.80104200	0.07601300
H	1.60628700	4.87064700	-0.43408100
C	-2.63343100	4.02216200	1.25346000
H	-3.65092600	4.00907500	1.66853100
H	-2.00313100	4.53398000	1.98877400
C	2.99348300	2.61699400	-1.31250900
H	3.63880100	2.10817000	-2.03709900
H	1.97923200	2.61747900	-1.73162700
H	0.00000100	1.51689500	-1.49942300

Pd(II) hydride implicit THF; G = -2540.403401

Pd	-0.00181200	0.11643600	-0.59309600
P	-2.26140700	0.12690400	-0.21111500
Si	0.00417200	-1.62017500	0.99112300
P	2.25716400	0.14564300	-0.21111300
C	2.63148600	-0.64981800	1.41021800
C	-3.30373100	-0.73664700	-1.47003200
H	-3.08634900	-0.17427100	-2.38896700
C	3.29262000	-0.71062100	-1.48108100
H	3.06836200	-0.14504500	-2.39634300

C	1.89142500	-2.06725200	3.21051300
H	1.13888200	-2.69928000	3.67342000
C	-2.80928800	-2.16932000	-1.66925200
H	-1.73292300	-2.16507300	-1.87418300
H	-2.95374000	-2.73002900	-0.73607000
C	-4.80930900	-0.70518100	-1.21958700
H	-5.03033000	-1.23092600	-0.28279200
H	-5.16142200	0.32500400	-1.10265000
C	-3.84576100	-0.48775000	2.07466300
H	-4.63846800	0.09762200	1.62100900
C	-1.83202800	-1.97407900	3.27492800
H	-1.06010000	-2.56303500	3.76166200
C	4.10268000	-1.11627200	3.27155200
H	5.05847900	-0.98382800	3.76916000
C	2.79719300	-2.14305000	-1.68179500
H	2.94497800	-2.70669400	-0.75083500
H	1.71989900	-2.13748900	-1.88208700
C	4.79970100	-0.67831300	-1.24039000
H	5.02754800	-1.20536500	-0.30600900
H	5.15128800	0.35214300	-1.12391700
C	-1.58640000	-1.39421800	2.02434200
C	3.86439600	-0.49475900	2.05245700
H	4.64319900	0.11909400	1.61248600
C	5.05744100	-2.78887500	-2.59315300
H	5.30695200	-3.38424900	-1.70413900
H	5.58001600	-3.25088100	-3.43800000
C	-0.01711100	-3.45289800	0.50446100
H	-0.91892300	-3.71183900	-0.05746900
H	0.00445500	-4.07676500	1.40715900
H	0.85392500	-3.71601700	-0.10283600
C	5.54407700	-1.35876100	-2.38724700
H	5.38703000	-0.78427900	-3.31034500
H	6.62140300	-1.34685500	-2.18768600
C	-5.07381100	-2.81851900	-2.56699200
H	-5.31803300	-3.41272400	-1.67573200
H	-5.60079000	-3.28211700	-3.40821800
C	1.61738400	-1.42988600	1.99417300
C	3.11557700	-1.90960800	3.84947800
H	3.30134700	-2.40319100	4.79891800
C	-3.56734300	-2.85992400	-2.79818300
H	-3.33148800	-2.35786200	-3.74620100
H	-3.22369300	-3.89563300	-2.89614300
C	-2.61784400	-0.64880400	1.42446500
C	3.54975700	-2.83078700	-2.81615800
H	3.20622800	-3.86651100	-2.91440700
H	3.30853300	-2.32696700	-3.76189000
C	-5.56022900	-1.38840300	-2.36051900
H	-5.40922100	-0.81536900	-3.28552600
H	-6.63632400	-1.37696100	-2.15442000
C	-3.05341700	2.55444400	-1.37066700
H	-3.69046200	2.00987700	-2.07540800
H	-2.04664900	2.58383800	-1.80560400
C	-4.05979300	-1.06121600	3.32148700
H	-5.01193000	-0.92350100	3.82464400
C	-2.98817700	1.81789200	-0.03377100
H	-4.01075500	1.68886300	0.34427900

C	2.97948300	1.83699400	-0.02746700
H	4.00477300	1.70916000	0.34362600
C	-3.05008900	-1.80666600	3.92320000
H	-3.21289800	-2.25502500	4.89892600
C	2.16819900	2.61469900	1.01098500
H	1.12393700	2.64863200	0.67371400
H	2.17357700	2.08498000	1.96967300
C	-2.17377800	2.60528100	0.99482900
H	-2.17175000	2.08183200	1.95692600
H	-1.13162700	2.64055000	0.65123700
C	-3.57727300	3.97709600	-1.19185200
H	-3.57784300	4.49155400	-2.15926700
H	-4.62240800	3.94045400	-0.85395300
C	-2.74979000	4.75542800	-0.17555200
H	-1.72637200	4.87171600	-0.55756000
H	-3.15623200	5.76466300	-0.04632700
C	3.55406200	4.00547800	-1.17516500
H	3.54700100	4.52623400	-2.13917500
H	4.60132900	3.97027700	-0.84378400
C	2.69311400	4.03533600	1.18357800
H	2.06800500	4.57406300	1.90435200
H	3.70606500	4.00092800	1.60814200
C	2.72995700	4.77431300	-0.14888100
H	3.13373700	5.78405900	-0.01546000
H	1.70392500	4.88962200	-0.52413000
C	-2.70270200	4.02515500	1.16133600
H	-3.71307200	3.99000900	1.59196600
H	-2.07531900	4.57065100	1.87502200
C	3.03395700	2.58226700	-1.35998600
H	3.66815400	2.04409000	-2.07218000
H	2.02434300	2.61090100	-1.78829300
H	-0.00748200	1.37859000	-1.69177900

Pd(II) hydride explicit THF; G = -2772.558230

Pd	0.06119900	-0.26518400	0.37966900
P	2.31539600	-0.03022100	0.03069600
Si	0.45120500	-2.49549000	-0.25993900
P	-2.13917100	-0.80391300	0.01809200
C	-2.23754400	-2.25595300	-1.11589500
C	3.36661400	-0.04037400	1.55120900
H	2.99416000	0.83069500	2.10839100
C	-3.15396600	-1.21104100	1.50900900
H	-3.11863800	-0.27817500	2.08890900
C	-1.12182300	-4.11670800	-2.15935500
H	-0.24039900	-4.73260900	-2.31128500
C	3.07004300	-1.28885300	2.38232800
H	1.99162200	-1.36698200	2.55894700
H	3.36456500	-2.17883700	1.81023200
C	4.86681200	0.12671300	1.32237500
H	5.23871500	-0.71697900	0.72848400
H	5.07148700	1.03879100	0.75185600
C	4.17278800	-1.32298500	-1.69714100
H	4.81550500	-0.45813000	-1.57150400
C	2.54608000	-3.54376800	-2.05302000
H	1.93164500	-4.42758900	-2.19847500

C	-3.43562400	-3.67918900	-2.66131400
H	-4.34800000	-3.92684600	-3.19509600
C	-2.46910200	-2.30099700	2.33312000
H	-2.42715700	-3.22468300	1.74062200
H	-1.43425800	-2.01001100	2.54353200
C	-4.61351500	-1.56533700	1.23434300
H	-4.65490300	-2.47243400	0.61927500
H	-5.10492600	-0.76823300	0.66692000
C	2.08909400	-2.49737600	-1.24206200
C	-3.41218000	-2.59236600	-1.79690700
H	-4.31329600	-2.00213500	-1.66917700
C	-4.68761300	-2.90471300	3.36766500
H	-4.74427100	-3.85736800	2.82319000
H	-5.22106400	-3.05027600	4.31347200
C	0.67320700	-3.90085600	0.99406000
H	1.55383200	-3.73582900	1.62179100
H	0.81034200	-4.85346000	0.46684100
H	-0.19908300	-4.00267200	1.64571100
C	-5.36379000	-1.81725400	2.54024900
H	-5.39872700	-0.88584400	3.12163500
H	-6.40190400	-2.09232800	2.32302900
C	5.32645700	-1.08026200	3.48677600
H	5.72424900	-1.96185800	2.96552000
H	5.84680100	-1.02206300	4.44917700
C	-1.06655500	-3.01407100	-1.29794900
C	-2.28744300	-4.44474100	-2.84167000
H	-2.30153700	-5.29540700	-3.51674400
C	3.82849500	-1.26158300	3.70517000
H	3.44807800	-0.43320700	4.31795100
H	3.63192500	-2.18325200	4.26419900
C	2.92979900	-1.38522900	-1.05858100
C	-3.22477600	-2.56568300	3.63129900
H	-2.73768400	-3.37630300	4.18445800
H	-3.16794900	-1.67156100	4.26665900
C	5.61479600	0.16345100	2.65352200
H	5.30857200	1.05672900	3.21482100
H	6.69077500	0.25957600	2.47042200
C	2.65638400	2.74955100	-0.04595000
H	3.32799600	2.69517700	0.81714900
H	1.63342000	2.79752600	0.34726900
C	4.59380900	-2.36377600	-2.51462100
H	5.55572700	-2.30464400	-3.01445700
C	2.78758800	1.49304400	-0.90371000
H	3.83877800	1.37562600	-1.19738900
C	-3.08800300	0.49811200	-0.89115000
H	-4.03830000	0.04669300	-1.20359200
C	3.78010400	-3.47951400	-2.68932700
H	4.10796600	-4.29723500	-3.32439800
C	-2.29826300	0.90820200	-2.13596100
H	-1.30909300	1.25801900	-1.81292200
H	-2.13041800	0.03883800	-2.78071800
C	1.92644900	1.58739300	-2.16510200
H	2.06795500	0.69643000	-2.78626700
H	0.87192400	1.59570400	-1.85984800
C	2.95727600	4.00718000	-0.85637700
H	2.81827500	4.89243900	-0.22621300

H	4.01382700	4.00071700	-1.15870800
C	2.08130500	4.09598700	-2.10017100
H	1.03078000	4.19378500	-1.79437500
H	2.32785300	4.99455000	-2.67699700
C	-4.08876500	2.80943300	-0.79088200
H	-4.26147700	3.67097000	-0.13632000
H	-5.07835600	2.45838700	-1.11489700
C	-3.00015200	2.01848100	-2.90922800
H	-2.38674300	2.31300400	-3.76799600
H	-3.94903600	1.64004000	-3.31400900
C	-3.27720500	3.22015900	-2.01373200
H	-3.79936400	4.00386800	-2.57389200
H	-2.32099100	3.64753700	-1.68267000
C	2.23397800	2.84905700	-2.96322200
H	3.26168800	2.79660200	-3.34856900
H	1.57329800	2.90273300	-3.83566400
C	-3.39195600	1.70322300	-0.00340200
H	-4.01437800	1.40489800	0.84655400
H	-2.44812600	2.08173800	0.40818600
H	-0.21943100	1.33494000	0.78779500
C	0.05682500	5.65691800	1.09807600
O	-0.88083600	5.52634200	2.15826500
C	-2.11590100	5.24597100	1.52106900
C	-2.17183700	6.21370700	0.34600900
C	-0.69128400	6.33472600	-0.06189400
H	0.90701000	6.23050400	1.47317400
H	0.40999400	4.66060300	0.79961300
H	-2.12560100	4.20304600	1.17124600
H	-2.91614800	5.37691400	2.25268600
H	-2.80938500	5.85148500	-0.46330600
H	-2.56107900	7.17960400	0.67930300
H	-0.48480600	5.82380500	-1.00530400
H	-0.39458000	7.37950900	-0.17769100

Pd(0) η^2-silane gas phase; G = -2540.349800

Pd	0.00014200	-0.21023200	-0.80694900
P	-2.21026300	0.23035500	-0.30303100
Si	0.00023200	-2.19383100	0.61484700
P	2.21033900	0.23075700	-0.30276400
C	2.49492900	-0.72841300	1.24279300
C	-3.49641800	-0.44277000	-1.47891400
H	-3.31663600	0.12489400	-2.40369100
C	3.49600400	-0.43926300	-1.48095400
H	3.31514200	0.13014800	-2.40445100
C	1.83222800	-2.46625300	2.76831700
H	1.15651200	-3.26393600	3.06103800
C	-3.19913500	-1.91429300	-1.77405700
H	-2.15961800	-2.02261500	-2.09777300
H	-3.29847500	-2.48995700	-0.84354400
C	-4.95611000	-0.25750700	-1.07172800
H	-5.13292300	-0.78019200	-0.12356100
H	-5.18143200	0.80058400	-0.90251900
C	-3.59458600	-0.46576600	2.06442900
H	-4.29398000	0.31959700	1.79810600
C	-1.82858400	-2.46214000	2.77150600

H	-1.15262100	-3.25952400	3.06448400
C	3.81302200	-1.19126900	3.22755900
H	4.67060500	-0.96800800	3.85427600
C	3.19922600	-1.91035400	-1.77876000
H	3.29969400	-2.48780500	-0.84947800
H	2.15946600	-2.01858400	-2.10174600
C	4.95596000	-0.25405000	-1.07468900
H	5.13389900	-0.77853800	-0.12773500
H	5.18089100	0.80381600	-0.90359300
C	-1.57707100	-1.73626500	1.60054000
C	3.59777900	-0.46936000	2.06163700
H	4.29696200	0.31625800	1.79550300
C	5.60699100	-2.28003600	-2.42588500
H	5.81208400	-2.87251800	-1.52385600
H	6.27535100	-2.65686000	-3.20755300
C	-0.00123500	-4.09208900	0.60449900
H	-0.88717200	-4.45365700	0.07292700
H	-0.00144700	-4.54848200	1.59899600
H	0.88388700	-4.45511300	0.07256400
C	5.90139700	-0.81297700	-2.13643800
H	5.78834700	-0.23158500	-3.06183800
H	6.94042900	-0.68657700	-1.81285100
C	-5.60728500	-2.28652100	-2.41829300
H	-5.81126200	-2.87731000	-1.51490000
H	-6.27614200	-2.66525300	-3.19861100
C	1.57922100	-1.73855100	1.59879500
C	2.92596300	-2.19918800	3.58121300
H	3.08344800	-2.77500800	4.48779600
C	-4.15067500	-2.47920700	-2.82346300
H	-3.97175500	-1.97222100	-3.78156000
H	-3.93543500	-3.54070000	-2.98712700
C	-2.49296000	-0.72630900	1.24441400
C	4.15012100	-2.47268100	-2.83013900
H	3.93528800	-3.53395900	-2.99572200
H	3.97008000	-1.96388400	-3.78706300
C	-5.90220700	-0.81904300	-2.13151200
H	-5.79028500	-0.23943900	-3.05817000
H	-6.94101700	-0.69254100	-1.80725000
C	-2.74751100	2.80427300	-1.14844100
H	-3.38341100	2.40151300	-1.94457800
H	-1.71413700	2.76584400	-1.52060700
C	-3.80833600	-1.18588500	3.23173600
H	-4.66496500	-0.96147200	3.85934700
C	-2.83756900	1.92834200	0.10260100
H	-3.88877200	1.86740800	0.41280100
C	2.83664400	1.92841400	0.10581500
H	3.88868300	1.86791100	0.41325900
C	-2.92103500	-2.19351300	3.58561500
H	-3.07733500	-2.76789900	4.49331200
C	2.01862000	2.52106700	1.25106200
H	0.96115200	2.47109000	0.96740500
H	2.12551300	1.90836000	2.15131900
C	-2.01730100	2.52500500	1.24410300
H	-2.12071600	1.91435200	2.14617300
H	-0.96059800	2.47591000	0.95742300
C	-3.13530300	4.25063100	-0.85587900

H	-3.02588300	4.85446900	-1.76329400
H	-4.19750900	4.29309600	-0.57802600
C	-2.29785300	4.83237000	0.27684500
H	-1.24683400	4.87690800	-0.03971700
H	-2.60536000	5.86174600	0.49009400
C	3.12890400	4.25358800	-0.84745500
H	3.01638900	4.85957300	-1.75306000
H	4.19173300	4.29685400	-0.57211600
C	2.40471100	3.96731800	1.53953900
H	1.77040000	4.36667500	2.33855100
H	3.43742500	4.00340500	1.91332100
C	2.29344100	4.83125800	0.28880600
H	2.59999400	5.86054500	0.50386300
H	1.24155800	4.87505200	-0.02497400
C	-2.40467400	3.97141400	1.53002500
H	-3.43644900	4.00700300	1.90643700
H	-1.76881400	4.37364900	2.32636200
C	2.74239100	2.80744200	-1.14273800
H	3.37688900	2.40755100	-1.94144500
H	1.70817300	2.76852000	-1.51249200
H	-0.00016500	-2.02593300	-0.95681400

Pd(0) η^2-silane implicit THF; G = -2540.385755

Pd	0.00028000	-0.22771200	-0.78792800
P	-2.21750800	0.22362500	-0.30383300
Si	0.00035000	-2.18520600	0.67234500
P	2.21787600	0.22430300	-0.30366200
C	2.51007500	-0.72281900	1.25073300
C	-3.49068900	-0.45876700	-1.48690400
H	-3.31835200	0.12466300	-2.40289400
C	3.48936800	-0.44850900	-1.49400800
H	3.31462600	0.14135600	-2.40542400
C	1.84294100	-2.42425900	2.82068900
H	1.16126400	-3.20697900	3.14010100
C	-3.17307300	-1.92132000	-1.80319700
H	-2.13315000	-2.01101900	-2.13313700
H	-3.26331200	-2.51504000	-0.88310100
C	-4.95302000	-0.29802500	-1.07733000
H	-5.12651000	-0.83747300	-0.13804100
H	-5.19208800	0.75394100	-0.89198500
C	-3.61821800	-0.45082000	2.05989700
H	-4.32681100	0.31730600	1.76967100
C	-1.83292000	-2.41182200	2.83018000
H	-1.15093100	-3.19408700	3.15002600
C	3.84814500	-1.16578400	3.22833000
H	4.71773300	-0.94177900	3.83875400
C	3.17192400	-1.90895300	-1.82010300
H	3.26449100	-2.50922600	-0.90449700
H	2.13129400	-1.99686400	-2.14835900
C	4.95254000	-0.28972700	-1.08665500
H	5.12862900	-0.83580100	-0.15170100
H	5.19139400	0.76103400	-0.89437300
C	-1.58107800	-1.70880700	1.64343200
C	3.62793000	-0.46296300	2.05060700
H	4.33628900	0.30546600	1.76059300

C	5.57431000	-2.29539000	-2.48248800
H	5.77661800	-2.91002700	-1.59443700
H	6.23388400	-2.66242000	-3.27688000
C	-0.00362000	-4.08207800	0.70020800
H	-0.89034200	-4.45665100	0.17608700
H	-0.00336200	-4.51317200	1.70662600
H	0.88027200	-4.46034200	0.17395900
C	5.88745500	-0.83872400	-2.16289800
H	5.77984300	-0.23631800	-3.07532000
H	6.92857400	-0.73348600	-1.83687800
C	-5.57670700	-2.31405800	-2.45723900
H	-5.77651300	-2.92240700	-1.56430300
H	-6.23789000	-2.68724200	-3.24741600
C	1.58697200	-1.71585900	1.63800300
C	2.95120600	-2.15413200	3.61481100
H	3.11230900	-2.71296600	4.53187300
C	-4.11708800	-2.48302800	-2.86168800
H	-3.94255300	-1.95973000	-3.81184600
H	-3.88826200	-3.54009700	-3.03834300
C	-2.50419700	-0.71561700	1.25633000
C	4.11386700	-2.46244800	-2.88474800
H	3.88532300	-3.51837500	-3.06844200
H	3.93678400	-1.93247900	-3.83073200
C	-5.89008600	-0.85534000	-2.14740500
H	-5.78500700	-0.25944000	-3.06438900
H	-6.93051000	-0.74843800	-1.81971600
C	-2.74418800	2.79562700	-1.17524900
H	-3.36320100	2.38042400	-1.97784700
H	-1.70492200	2.77546000	-1.53292800
C	-3.83428700	-1.14840100	3.24150600
H	-4.70085700	-0.92057400	3.85479900
C	-2.84239400	1.92714900	0.08073600
H	-3.89557400	1.86239200	0.37983500
C	2.84024000	1.92654100	0.09064900
H	3.89605300	1.86259200	0.38049300
C	-2.93715500	-2.13651300	3.62814100
H	-3.09498800	-2.69119200	4.54829000
C	2.04546400	2.52452000	1.24933000
H	0.98123000	2.49079400	0.98782700
H	2.16385700	1.91200700	2.14881900
C	-2.03976000	2.53820200	1.22702200
H	-2.14771600	1.93321500	2.13292600
H	-0.97784400	2.50607200	0.95598600
C	-3.15590000	4.23821100	-0.89519900
H	-3.03831400	4.83792500	-1.80475800
H	-4.22293600	4.26694000	-0.63463600
C	-2.34315800	4.83794300	0.24594800
H	-1.28895300	4.89995000	-0.05757600
H	-2.67329200	5.86222900	0.45233600
C	3.13731700	4.24738300	-0.86720500
H	3.00972600	4.85474800	-1.77031000
H	4.20643000	4.27782100	-0.61549700
C	2.45363200	3.96611500	1.53325800
H	1.83470100	4.37100300	2.34204600
H	3.49252500	3.98779800	1.89087900
C	2.33222800	4.83393100	0.28616600

H	2.66043400	5.85755900	0.49881600
H	1.27519500	4.89472600	-0.00758400
C	-2.45057000	3.98084000	1.50173200
H	-3.48634700	4.00213400	1.86829800
H	-1.82598600	4.39507000	2.30140000
C	2.72851200	2.80580900	-1.15664600
H	3.34222900	2.39997500	-1.96808000
H	1.68634800	2.78498000	-1.50576200
H	-0.00097700	-2.04587400	-0.90145300

Pd(0) η^2-silane explicit THF; G = -2772.544232

Pd	-0.03750400	-0.13479600	-0.72297600
P	2.12720900	-0.04949600	0.17607600
Si	0.01331000	2.18929300	-1.11300100
P	-2.16829900	0.08009900	0.20619700
C	-2.60954000	1.87012100	0.11999600
C	3.56199400	-0.18828400	-1.02077400
H	3.52200300	-1.23924400	-1.34201800
C	-3.47402800	-0.79615200	-0.79800800
H	-3.16562800	-1.84770600	-0.70629300
C	-2.04692100	4.11247500	-0.55976100
H	-1.36832900	4.81649300	-1.03285900
C	3.30822700	0.67964900	-2.25235800
H	2.32434000	0.44820400	-2.67129700
H	3.27920900	1.73407400	-1.94588200
C	4.94894000	0.08923800	-0.44564700
H	4.98417100	1.12261700	-0.07790000
H	5.15338200	-0.56122600	0.41055700
C	3.16638200	2.10766000	1.71879000
H	3.85685900	1.39231000	2.15316400
C	1.42609400	3.96008100	0.62885400
H	0.74988300	4.70139900	0.21080200
C	-4.12978400	3.70711100	0.56869400
H	-5.06609100	4.06800900	0.98378200
C	-3.33708200	-0.41067400	-2.27196500
H	-3.59554900	0.65082300	-2.39000400
H	-2.29337600	-0.52028200	-2.58181000
C	-4.92753800	-0.69293800	-0.34484100
H	-5.26109500	0.34846900	-0.42322700
H	-5.03192300	-0.98759900	0.70452300
C	1.34590600	2.62973400	0.19949600
C	-3.80966600	2.35757800	0.64864000
H	-4.50375400	1.68398300	1.13922000
C	-5.70025800	-1.18999700	-2.69233100
H	-6.07434100	-0.16702600	-2.83611100
H	-6.32865400	-1.84357100	-3.30794600
C	0.43526500	3.40040100	-2.51575700
H	1.37691000	3.09310600	-2.98448400
H	0.56222300	4.43447100	-2.17665900
H	-0.34058500	3.38561200	-3.28944600
C	-5.82879700	-1.56297800	-1.21971300
H	-5.55068300	-2.61771100	-1.08625700
H	-6.87023900	-1.46883900	-0.89145000
C	5.78052500	0.76238100	-2.73063900
H	5.85241100	1.82132700	-2.44659700

H	6.55164900	0.58651400	-3.48913100
C	-1.69549200	2.75783300	-0.47656200
C	-3.24788100	4.58836600	-0.04721400
H	-3.49198700	5.64401400	-0.12174200
C	4.39519300	0.49308600	-3.30563400
H	4.35427200	-0.53758500	-3.68507500
H	4.20047000	1.15075200	-4.16058100
C	2.23925000	1.69556900	0.75651300
C	-4.24846100	-1.25948900	-3.15256300
H	-4.16300200	-0.93825600	-4.19683500
H	-3.90646600	-2.30340700	-3.11614100
C	6.03625700	-0.10179400	-1.50187000
H	6.06389900	-1.15847800	-1.80227100
H	7.01709400	0.12742300	-1.07001800
C	2.89652200	-2.51092400	1.21229900
H	3.62340500	-2.60588600	0.39878900
H	1.93527800	-2.87361100	0.82274300
C	3.21078700	3.42885000	2.14805000
H	3.92593000	3.72810300	2.90842100
C	2.73579100	-1.04564100	1.62223900
H	3.71844800	-0.66486600	1.92767200
C	-2.61486600	-0.33500700	1.95872600
H	-3.67718900	-0.10394000	2.11108900
C	2.33653600	4.36098700	1.60013500
H	2.36074800	5.39522400	1.93074200
C	-1.78880200	0.51490800	2.92326000
H	-0.72642500	0.37930100	2.69046600
H	-2.00623300	1.57627000	2.76667800
C	1.77639500	-0.92279500	2.80260700
H	1.68032900	0.12429700	3.10796000
H	0.78050800	-1.24335300	2.47243400
C	3.32583900	-3.38118900	2.39052200
H	3.39094100	-4.42804200	2.07250600
H	4.33577100	-3.08556100	2.70672700
C	2.37148600	-3.24077200	3.57073700
H	1.38507300	-3.63311000	3.28647300
H	2.71956900	-3.84495900	4.41595200
C	-2.67734600	-2.19511000	3.66608100
H	-2.48067000	-3.26181000	3.82345400
H	-3.74285100	-2.03607300	3.88272200
C	-2.05562000	0.13550100	4.37648200
H	-1.41221900	0.72800500	5.03692900
H	-3.09246000	0.39447700	4.63340900
C	-1.83811300	-1.35378400	4.62033200
H	-2.07321900	-1.60778500	5.66022900
H	-0.77763000	-1.59315300	4.46874400
C	2.22578200	-1.78026800	3.98050200
H	3.19018800	-1.40974100	4.35484400
H	1.51189000	-1.68247800	4.80596800
C	-2.39979300	-1.82715400	2.21165800
H	-3.03671800	-2.42225500	1.54765800
H	-1.35998100	-2.07840900	1.96027400
H	-0.04542400	0.90168300	-2.13920900
C	0.86366100	-2.61177300	-2.77514000
O	-0.23796900	-2.31193300	-1.92752900
C	-0.51949800	-3.50420700	-1.19818200

C	-0.14820400	-4.67491300	-2.12198500
C	0.55446200	-3.99840100	-3.31310100
H	0.92096000	-1.83030600	-3.53499700
H	1.79579700	-2.60659200	-2.19152300
H	0.07674400	-3.51654400	-0.27720100
H	-1.57529300	-3.47837200	-0.92267000
H	0.51629700	-5.37355300	-1.60820800
H	-1.03084600	-5.23167100	-2.44329800
H	1.45232400	-4.52986900	-3.63639000
H	-0.12276000	-3.92085700	-4.16775500

Pt(II) hydride gas phase; G = -2532.837531

Pt	0.00000000	0.12357200	-0.52264600
P	-2.23802400	0.14765300	-0.17006600
Si	-0.00002600	-1.71508900	0.95225200
P	2.23802100	0.14764000	-0.17005000
C	2.59936500	-0.68564500	1.43438300
C	-3.28494500	-0.69308500	-1.44254500
H	-3.06119100	-0.13038500	-2.35984500
C	3.28496200	-0.69300500	-1.44257300
H	3.06121000	-0.13025000	-2.35983900
C	1.87114900	-2.15277600	3.19334600
H	1.12538100	-2.80772500	3.63489700
C	-2.80117700	-2.12967100	-1.64225600
H	-1.72516000	-2.12922600	-1.84456000
H	-2.94742600	-2.68522500	-0.70608600
C	-4.79035200	-0.65280200	-1.19095500
H	-5.01060000	-1.17249600	-0.25043900
H	-5.13838400	0.37957000	-1.07755300
C	-3.81633700	-0.51081200	2.09953200
H	-4.58391700	0.13398600	1.68431800
C	-1.87115900	-2.15264100	3.19340900
H	-1.12540600	-2.80760600	3.63496200
C	4.05368500	-1.14785400	3.30979000
H	4.99731500	-0.99913300	3.82489100
C	2.80122100	-2.12958600	-1.64238100
H	2.94747100	-2.68519600	-0.70624500
H	1.72520700	-2.12914700	-1.84469600
C	4.79036500	-0.65271400	-1.19096200
H	5.01061000	-1.17246200	-0.25047500
H	5.13837800	0.37965700	-1.07749100
C	-1.59759900	-1.50729300	1.98302200
C	3.81636100	-0.51098100	2.09947900
H	4.58395300	0.13380400	1.68427000
C	5.07188400	-2.76983000	-2.52850300
H	5.31399400	-3.35832400	-1.63311300
H	5.60664800	-3.23516000	-3.36329000
C	-0.00008600	-3.55066700	0.46729700
H	-0.88571100	-3.80359300	-0.12153200
H	-0.00011700	-4.18367600	1.36227200
H	0.88553300	-3.80365200	-0.12151300
C	5.54959500	-1.33611400	-2.32629800
H	5.39775200	-0.76833600	-3.25435100
H	6.62504500	-1.31624800	-2.11939300
C	-5.07181900	-2.77000700	-2.52836500

H	-5.31393000	-3.35844700	-1.63294100
H	-5.60656500	-3.23539900	-3.36312900
C	1.59758600	-1.50738200	1.98298300
C	3.07806200	-1.97426800	3.85720500
H	3.25957400	-2.47632200	4.80263000
C	-3.56660800	-2.81872800	-2.76653600
H	-3.33316500	-2.32041400	-3.71716300
H	-3.22807100	-3.85559600	-2.86583100
C	-2.59936300	-0.68554400	1.43441400
C	3.56667700	-2.81855900	-2.76669600
H	3.22815700	-3.85542700	-2.86606100
H	3.33323800	-2.32018800	-3.71729400
C	-5.54955500	-1.33628600	-2.32625800
H	-5.39771000	-0.76856400	-3.25434500
H	-6.62500900	-1.31642400	-2.11936800
C	-2.98281300	2.60132400	-1.28067800
H	-3.61494700	2.08703400	-2.01290700
H	-1.96434000	2.61030400	-1.68803300
C	-4.05365500	-1.14763400	3.30987100
H	-4.99726800	-0.99886100	3.82499000
C	-2.96353700	1.83380800	0.04083800
H	-3.99665400	1.71121900	0.39284600
C	2.96352400	1.83378700	0.04094900
H	3.99664300	1.71118700	0.39294600
C	-3.07804900	-1.97406600	3.85729100
H	-3.25955900	-2.47608300	4.80273600
C	2.16239800	2.58418500	1.10732300
H	1.11233300	2.60002500	0.78888100
H	2.19468900	2.03854800	2.05592000
C	-2.16241200	2.58427100	1.10716500
H	-2.19469700	2.03868800	2.05579400
H	-1.11234800	2.60009900	0.78872000
C	-3.47853900	4.03161500	-1.08581700
H	-3.44414200	4.56569800	-2.04148300
H	-4.53248000	4.01479100	-0.77454300
C	-2.65918900	4.76911600	-0.03307800
H	-1.62352600	4.86557900	-0.38597800
H	-3.04207600	5.78599200	0.10492000
C	3.47850500	4.03166300	-1.08558300
H	3.44410000	4.56580000	-2.04121800
H	4.53244900	4.01482700	-0.77431600
C	2.66623200	4.01083000	1.28934100
H	2.04961200	4.52811100	2.03232800
H	3.68904900	3.99086800	1.69090300
C	2.65915700	4.76909900	-0.03279700
H	3.04203900	5.78596900	0.10525800
H	1.62349200	4.86557600	-0.38568600
C	-2.66625300	4.01092300	1.28910400
H	-3.68906900	3.99097800	1.69067100
H	-2.04963300	4.52825000	2.03205800
C	2.98278800	2.60138000	-1.28052200
H	3.61492000	2.08713600	-2.01278600
H	1.96431200	2.61037700	-1.68787000
H	-0.00000100	1.49443900	-1.44289500

Pt(II) hydride implicit THF; G = -2532.872068

Pt	-0.00000900	0.12890900	-0.50255300
P	-2.25253600	0.14237100	-0.16495900
Si	0.00002200	-1.66820400	1.01628100
P	2.25251200	0.14249500	-0.16494400
C	2.61734500	-0.67369300	1.44901300
C	-3.27100500	-0.71638200	-1.44569500
H	-3.04240800	-0.14961700	-2.35909700
C	3.27099000	-0.71613200	-1.44575900
H	3.04233700	-0.14932900	-2.35912400
C	1.88766300	-2.10005000	3.24491900
H	1.13853000	-2.73474200	3.70944700
C	-2.77095300	-2.14778900	-1.64239300
H	-1.69255500	-2.13971500	-1.83485300
H	-2.92396000	-2.71064100	-0.71188300
C	-4.77979100	-0.68776300	-1.21341000
H	-5.01153400	-1.21403300	-0.27951100
H	-5.13541200	0.34164800	-1.10074300
C	-3.85007900	-0.51520800	2.09024600
H	-4.62568600	0.10346400	1.65143900
C	-1.88729200	-2.09944100	3.24535100
H	-1.13803400	-2.73386000	3.71004700
C	4.09402300	-1.13885600	3.30715400
H	5.05005000	-1.00290600	3.80332200
C	2.77100100	-2.14755500	-1.64251500
H	2.92405100	-2.71044400	-0.71203400
H	1.69259800	-2.13951900	-1.83495200
C	4.77978200	-0.68744700	-1.21351700
H	5.01158000	-1.21374900	-0.27965000
H	5.13535200	0.34197700	-1.10081100
C	-1.60774500	-1.46493600	2.02916200
C	3.85020000	-0.51529600	2.09010000
H	4.62572200	0.10355000	1.65138700
C	5.02420300	-2.79999300	-2.56630400
H	5.27696200	-3.39557500	-1.67835300
H	5.54098400	-3.26376900	-3.41374300
C	-0.00011300	-3.50089000	0.52841700
H	-0.88668900	-3.76032800	-0.05766200
H	-0.00007800	-4.12930600	1.42805800
H	0.88636300	-3.76039900	-0.05778500
C	5.51571600	-1.37110000	-2.36384400
H	5.35516700	-0.79671700	-3.28642000
H	6.59410700	-1.36179100	-2.17010700
C	-5.02414400	-2.80038300	-2.56609600
H	-5.27685000	-3.39594100	-1.67811400
H	-5.54092400	-3.26422100	-3.41350200
C	1.60793400	-1.46517200	2.02896600
C	3.11076300	-1.93638400	3.88485500
H	3.29847300	-2.42925700	4.83430400
C	-3.51518100	-2.83799100	-2.78054000
H	-3.26993000	-2.33437700	-3.72537300
H	-3.16792500	-3.87273700	-2.87586500
C	-2.61726000	-0.67366200	1.44910400
C	3.51523600	-2.83766800	-2.78071000
H	3.16803100	-3.87242700	-2.87607300

H	3.26993700	-2.33402400	-3.72551400
C	-5.51572300	-1.37150600	-2.36368500
H	-5.35522900	-0.79715600	-3.28629000
H	-6.59411000	-1.36224500	-2.16991800
C	-3.03936300	2.57676700	-1.30456600
H	-3.65859800	2.03476500	-2.02688800
H	-2.02599000	2.62206100	-1.72174600
C	-4.09374700	-1.13845700	3.30749000
H	-5.04974600	-1.00246000	3.80369800
C	-2.99049400	1.82463500	0.02490900
H	-4.01846600	1.68517200	0.38331300
C	2.99038700	1.82477900	0.02503200
H	4.01837200	1.68534500	0.38341500
C	-3.11034700	-1.93569300	3.88535300
H	-3.29790900	-2.42827500	4.83498200
C	2.19982900	2.60574400	1.07723800
H	1.15183300	2.65468500	0.75351300
H	2.20964500	2.06977100	2.03233900
C	-2.19996900	2.60571900	1.07705100
H	-2.20974200	2.06981200	2.03218800
H	-1.15198000	2.65470200	0.75331000
C	-3.58010200	3.99184300	-1.11716500
H	-3.56888500	4.51870500	-2.07780000
H	-4.63057800	3.94042500	-0.79831900
C	-2.77826200	4.76481500	-0.07649900
H	-1.74964300	4.89639900	-0.43914500
H	-3.19712500	5.76817500	0.05848700
C	3.57985300	3.99210300	-1.11689800
H	3.56859500	4.51903000	-2.07749600
H	4.63033600	3.94072700	-0.79806500
C	2.74643600	4.01793500	1.25197900
H	2.13736700	4.56078100	1.98328200
H	3.76376200	3.96714600	1.66433100
C	2.77797600	4.76495400	-0.07617100
H	3.19677800	5.76833100	0.05887900
H	1.74934500	4.89649900	-0.43879700
C	-2.74666200	4.01788800	1.25170000
H	-3.76398100	3.96706400	1.66406600
H	-2.13761900	4.56082200	1.98296100
C	3.03919900	2.57700700	-1.30439100
H	3.65845900	2.03509000	-2.02675500
H	2.02582000	2.62226700	-1.72155800
H	-0.00004600	1.44966600	-1.51034800

Pt(II) hydride explicit THF; G = -2765.033577

Pt	-0.10518100	-0.25004600	0.33678700
P	2.02392100	-0.98610600	-0.00914400
Si	-0.73276600	-2.38936000	-0.41266100
P	-2.30222400	0.26951100	0.02744200
C	-3.03804500	-0.93193000	-1.16585200
C	2.93690200	-1.56167900	1.49020100
H	2.97407400	-0.65704400	2.11310800
C	-3.36666900	0.25081600	1.53743500
H	-2.91600000	1.03466400	2.16230900
C	-2.88996500	-3.03731800	-2.32312300

H	-2.37944800	-3.97322500	-2.53096500
C	2.11480600	-2.61283700	2.23630300
H	1.10792300	-2.22622500	2.42726400
H	1.99993700	-3.49810200	1.59655200
C	4.36232200	-2.05062100	1.24423000
H	4.33452200	-2.92817000	0.58709800
H	4.95197600	-1.28310500	0.73217500
C	3.14187200	-2.83988700	-1.84903700
H	4.09386900	-2.34841600	-1.67916800
C	0.72271900	-4.11535100	-2.31580900
H	-0.21095600	-4.63725300	-2.50544300
C	-4.77403500	-1.59098000	-2.71580300
H	-5.71141500	-1.37913900	-3.22093300
C	-3.21238000	-1.08175500	2.27037900
H	-3.59375100	-1.88776200	1.62932400
H	-2.15051300	-1.28834200	2.44219000
C	-4.83929300	0.58501800	1.31189100
H	-5.28530500	-0.17292800	0.65657500
H	-4.94510300	1.55070800	0.80671900
C	0.75078800	-3.03244400	-1.42878700
C	-4.25175600	-0.67498900	-1.81151000
H	-4.79375900	0.24580700	-1.62290800
C	-5.44841600	-0.72352100	3.37824800
H	-5.92948200	-1.51818700	2.79146200
H	-5.97116200	-0.68216900	4.34020500
C	-1.15343300	-3.83312000	0.74303100
H	-0.30269000	-4.09456800	1.37948400
H	-1.41971000	-4.72238400	0.15800000
H	-2.00261200	-3.59345400	1.38982200
C	-5.59682800	0.60106800	2.63804200
H	-5.20773300	1.41447500	3.26550000
H	-6.65472600	0.82115600	2.45684200
C	4.22291600	-3.48674400	3.31046400
H	4.20592100	-4.41512200	2.72305100
H	4.70334600	-3.72777000	4.26510100
C	-2.33184600	-2.12227900	-1.42257300
C	-4.09172200	-2.77663500	-2.97127100
H	-4.49711200	-3.49611100	-3.67664200
C	2.79203100	-3.01430200	3.54259300
H	2.80102900	-2.15014100	4.22058800
H	2.20645300	-3.79671300	4.03809700
C	1.98684100	-2.40199900	-1.19281900
C	-3.97977600	-1.07527400	3.58813300
H	-3.88572900	-2.05150100	4.07671900
H	-3.52327700	-0.33920700	4.26367200
C	5.03445400	-2.43678500	2.55996100
H	5.13967200	-1.54089100	3.18687200
H	6.04758700	-2.80505100	2.36363200
C	3.55675000	1.35984700	0.09779800
H	4.10979700	0.95799900	0.95310400
H	2.66126000	1.84768600	0.49892300
C	3.08278000	-3.90316200	-2.74072300
H	3.98209900	-4.23027500	-3.25345400
C	3.13465600	0.23185800	-0.84183500
H	4.03354800	-0.31759000	-1.14993300
C	-2.60055200	1.90112200	-0.78507400

H	-3.65194100	1.91081700	-1.10015600
C	1.86989600	-4.54488000	-2.97280400
H	1.81991500	-5.37829300	-3.66741600
C	-1.71198300	2.01408000	-2.02590500
H	-0.66618900	1.91301400	-1.70839000
H	-1.91398200	1.18460800	-2.71200200
C	2.43702900	0.77789000	-2.08948100
H	2.17771900	-0.04219700	-2.76780200
H	1.49167900	1.24127400	-1.77909400
C	4.41339100	2.39201000	-0.62972100
H	4.65568800	3.20512500	0.06089600
H	5.36224600	1.92874100	-0.93515800
C	3.70335600	2.93829000	-1.86249900
H	2.80286800	3.48098000	-1.54486500
H	4.34225200	3.66118400	-2.38255400
C	-2.58117100	4.40278300	-0.55756200
H	-2.40255300	5.23382400	0.13346200
H	-3.63046100	4.48095900	-0.87455800
C	-1.90521800	3.35028000	-2.73393400
H	-1.22328800	3.41581000	-3.58902200
H	-2.92516500	3.40442300	-3.13905300
C	-1.67971400	4.51848700	-1.78095600
H	-1.85321600	5.47073500	-2.29456700
H	-0.62997800	4.51925000	-1.45694200
C	3.29914200	1.81111200	-2.80551700
H	4.20250100	1.32383600	-3.19826600
H	2.75549200	2.20862000	-3.66996100
C	-2.37437800	3.07498000	0.16654600
H	-3.05306900	3.00983900	1.02304000
H	-1.35220800	3.02178800	0.56204100
H	0.34606700	1.27350700	0.82460300
C	3.07964500	5.85687400	0.65813100
O	2.80314900	4.65344900	1.37865600
C	1.40809000	4.37955600	1.30269000
C	0.75108100	5.73713000	1.14877200
C	1.73364000	6.42577800	0.20478100
H	3.60426800	6.54179900	1.33433300
H	3.74358300	5.63689600	-0.18591200
H	1.19009400	3.73765000	0.43682000
H	1.11955200	3.83713500	2.20626700
H	-0.26370400	5.67716700	0.75139800
H	0.71735700	6.24975700	2.11611500
H	1.52226200	6.13712200	-0.82982200
H	1.70433500	7.51601800	0.26357400

Pt(0) η^2-silane gas phase; G = -2532.793601

Pt	0.00096600	-0.21478000	-0.67481500
P	-2.19081200	0.22369800	-0.23155200
Si	-0.00100500	-2.11000300	0.70602200
P	2.19183200	0.22303300	-0.22880800
C	2.51898200	-0.74119000	1.30601100
C	-3.44858600	-0.44712600	-1.43705400
H	-3.19631900	0.06331500	-2.37801800
C	3.44324000	-0.41203500	-1.45983100
H	3.17785800	0.11690500	-2.38688000

C	1.87303600	-2.46787700	2.85152400
H	1.18836300	-3.24959500	3.16784200
C	-3.22207900	-1.94605800	-1.64470900
H	-2.17728400	-2.12682500	-1.91135500
H	-3.39856000	-2.46636000	-0.69345000
C	-4.91299100	-0.16387500	-1.10785300
H	-5.16130600	-0.62865300	-0.14549700
H	-5.08793400	0.91131000	-1.00120800
C	-3.62656900	-0.45568100	2.11189100
H	-4.32951000	0.31818200	1.82175400
C	-1.84382300	-2.41877700	2.88628500
H	-1.15986900	-3.20043800	3.20433800
C	3.90206400	-1.24067500	3.23286100
H	4.78875900	-1.04100600	3.82605600
C	3.22453600	-1.90771500	-1.69762500
H	3.41412100	-2.44705300	-0.75957300
H	2.17819500	-2.08982500	-1.95728100
C	4.90908300	-0.12550800	-1.14014700
H	5.17133900	-0.60937500	-0.19103300
H	5.07767100	0.94836000	-1.01212700
C	-1.57839200	-1.70213500	1.71449200
C	3.65844400	-0.50650900	2.07964000
H	4.36213900	0.26728200	1.79116000
C	5.61130000	-2.14851900	-2.47179000
H	5.90334500	-2.70043700	-1.56798500
H	6.25771800	-2.50607100	-3.28047300
C	-0.02007700	-4.00164700	0.57888000
H	-0.91193400	-4.33148200	0.03735100
H	-0.02197700	-4.49466100	1.55704000
H	0.86097200	-4.34950300	0.03098600
C	5.82785000	-0.65833700	-2.23808800
H	5.62759500	-0.11260700	-3.17038000
H	6.87280700	-0.45806900	-1.97704000
C	-5.61495100	-2.22000600	-2.38804600
H	-5.89334400	-2.75452100	-1.46959400
H	-6.26732500	-2.59928400	-3.18191200
C	1.59504700	-1.73119700	1.69505000
C	3.00628900	-2.22956400	3.61883800
H	3.18850300	-2.81212700	4.51651100
C	-4.15422700	-2.50965600	-2.71184200
H	-3.90281300	-2.06135600	-3.68281200
H	-3.99068500	-3.58787100	-2.81446000
C	-2.50065900	-0.71044700	1.32500700
C	4.14924700	-2.44176800	-2.78619500
H	3.99216800	-3.51870300	-2.91009200
H	3.88436500	-1.97473800	-3.74467900
C	-5.83978700	-0.72673700	-2.18383000
H	-5.65372900	-0.19973100	-3.12974400
H	-6.88326800	-0.52830200	-1.91557100
C	-2.67875200	2.79191500	-1.12287500
H	-3.29363200	2.38016000	-1.93106600
H	-1.63496600	2.74357900	-1.46375700
C	-3.85740400	-1.17007000	3.28011600
H	-4.73326900	-0.95464100	3.88379300
C	-2.80360800	1.93389900	0.13683800
H	-3.86158300	1.87741000	0.42396700

C	2.79711600	1.92709200	0.17770400
H	3.86242000	1.87242400	0.43683300
C	-2.96294000	-2.15957000	3.66754200
H	-3.13523200	-2.72654700	4.57707800
C	2.02630500	2.48781200	1.36992300
H	0.95802300	2.42463500	1.13491800
H	2.18607700	1.86292600	2.25385900
C	-2.00801800	2.54031100	1.28946200
H	-2.13487700	1.94113300	2.19632800
H	-0.94623500	2.48259900	1.02500700
C	-3.07014000	4.24267800	-0.85915300
H	-2.93526500	4.83441000	-1.77111000
H	-4.13913100	4.29180000	-0.60960600
C	-2.26018000	4.83667100	0.28700300
H	-1.20203400	4.87592600	-0.00482400
H	-2.57114500	5.86893600	0.48040800
C	3.01305300	4.26914200	-0.75156200
H	2.84790400	4.88730800	-1.64072900
H	4.08743500	4.32391500	-0.52765100
C	2.40698800	3.93478100	1.66254200
H	1.80578300	4.31302900	2.49662300
H	3.45558100	3.97957100	1.98828000
C	2.22593100	4.81696100	0.43287300
H	2.52966300	5.84658000	0.65043000
H	1.16008800	4.85188900	0.17002400
C	-2.39812800	3.99123200	1.54776200
H	-3.43807400	4.03463000	1.90028600
H	-1.77932400	4.40185100	2.35320400
C	2.63198600	2.82252300	-1.05088300
H	3.23133400	2.44341800	-1.88631700
H	1.58080700	2.77163300	-1.36776900
H	-0.00211400	-1.92744800	-0.98800000

Pt(0) η^2-silane implicit THF; G = -2532.827352

Pt	0.00880800	-0.21485000	-0.65157500
P	-2.19994100	0.20814100	-0.24046000
Si	0.00712000	-2.10784000	0.75561200
P	2.20924400	0.21137200	-0.22303000
C	2.56619600	-0.78343800	1.28635100
C	-3.44696100	-0.49377700	-1.43612000
H	-3.19006200	-0.00179700	-2.38530500
C	3.42964100	-0.36597700	-1.50688000
H	3.13388600	0.20188800	-2.40086900
C	1.92493800	-2.49383900	2.85556600
H	1.23000800	-3.25579600	3.19753700
C	-3.22166200	-1.99663500	-1.61144800
H	-2.17710000	-2.18745900	-1.87380000
H	-3.40391300	-2.49922100	-0.65172300
C	-4.91225100	-0.20009800	-1.11833200
H	-5.16706100	-0.64337400	-0.14761500
H	-5.08363700	0.87753900	-1.03627700
C	-3.62596000	-0.42788800	2.12165300
H	-4.34732400	0.31718000	1.80355500
C	-1.80426400	-2.33013700	2.96558200
H	-1.10502900	-3.08663700	3.31139100

C	3.99952500	-1.31978300	3.16667600
H	4.91111700	-1.14408300	3.72953500
C	3.21392500	-1.85162400	-1.80327700
H	3.43557000	-2.43238800	-0.89733300
H	2.16213900	-2.03262800	-2.04317400
C	4.90176600	-0.07861500	-1.21844700
H	5.20041800	-0.60098100	-0.30130100
H	5.06263800	0.99022900	-1.04773400
C	-1.55804000	-1.65476400	1.76400100
C	3.73702400	-0.57743200	2.02227100
H	4.44888500	0.18017600	1.71218000
C	5.57805400	-2.03267100	-2.66247000
H	5.90622300	-2.62201700	-1.79525600
H	6.19924400	-2.34530300	-3.50910900
C	-0.05260500	-4.00086000	0.67324500
H	-0.94977800	-4.33068500	0.13857600
H	-0.06664600	-4.46517500	1.66578000
H	0.82194300	-4.38299500	0.13562000
C	5.78818300	-0.55226300	-2.36876600
H	5.55252800	0.03302400	-3.26819500
H	6.83926000	-0.35379400	-2.13091500
C	-5.61252200	-2.28068700	-2.36015500
H	-5.89799100	-2.79710200	-1.43340700
H	-6.26029600	-2.67351800	-3.15168900
C	1.63115800	-1.75066600	1.70503500
C	3.08931500	-2.28363500	3.58489200
H	3.28495600	-2.86924300	4.47817700
C	-4.15111700	-2.58068700	-2.67070600
H	-3.89352700	-2.15362600	-3.64957400
H	-3.98969500	-3.66174600	-2.74715000
C	-2.49628200	-0.69090200	1.34143300
C	4.10955700	-2.32854100	-2.94226100
H	3.95892100	-3.40130300	-3.10628900
H	3.80911300	-1.82284600	-3.87010800
C	-5.83509000	-0.78338500	-2.18670900
H	-5.64527300	-0.27529700	-3.14229400
H	-6.87911600	-0.57867100	-1.92417600
C	-2.73094100	2.74894600	-1.19742100
H	-3.35463600	2.30295900	-1.97963700
H	-1.69432000	2.71949900	-1.56154100
C	-3.84036000	-1.10255600	3.31729800
H	-4.71996100	-0.88112500	3.91390300
C	-2.81315500	1.92482600	0.08827200
H	-3.86307700	1.86325600	0.40077900
C	2.78765600	1.91277800	0.22731200
H	3.86162100	1.86278000	0.44790900
C	-2.92490700	-2.05818700	3.74193400
H	-3.08275000	-2.59075600	4.67501400
C	2.05042400	2.41513400	1.46636200
H	0.97329400	2.33785300	1.27866300
H	2.26374000	1.76757500	2.32236100
C	-2.00147300	2.57680200	1.20413700
H	-2.09352100	2.00098800	2.13071100
H	-0.94466300	2.53913400	0.91633500
C	-3.14857400	4.19773700	-0.96269700
H	-3.04314200	4.76685000	-1.89313300

H	-4.21350700	4.22889400	-0.69391100
C	-2.32954600	4.84066300	0.15010300
H	-1.27896000	4.90041500	-0.16557500
H	-2.66508300	5.86890400	0.32511600
C	2.94131200	4.28943700	-0.62154500
H	2.73836300	4.93575300	-1.48271500
H	4.02111300	4.35213700	-0.42809800
C	2.41452300	3.85915400	1.79561200
H	1.83199400	4.19642800	2.66033100
H	3.47208500	3.90968500	2.09023500
C	2.18144500	4.78107600	0.60465400
H	2.47705300	5.80682400	0.85188700
H	1.10774100	4.80765400	0.37445400
C	-2.41790400	4.02554600	1.43515200
H	-3.44926300	4.05410500	1.81332700
H	-1.78653300	4.46989900	2.21294000
C	2.57081200	2.84928400	-0.96219300
H	3.14850400	2.50749800	-1.82828800
H	1.51082600	2.79957800	-1.24889600
H	0.00543200	-1.94780000	-0.92325400

Pt(0) η^2-silane explicit THF; G = -2764.993678

Pt	-0.02003800	0.04007500	-0.87302200
P	2.09429200	-0.01365700	0.15793600
Si	0.05063100	2.28858400	-0.65728300
P	-2.12952900	0.11614000	0.15391700
C	-2.59343400	1.88885100	0.34778500
C	3.54480600	-0.01723400	-1.03283700
H	3.39346400	-0.94487100	-1.60427600
C	-3.45252600	-0.63737600	-0.93360600
H	-3.00023300	-1.60020900	-1.21156200
C	-1.97627100	4.20872600	0.14245600
H	-1.25912100	4.97646400	-0.13630200
C	3.43012700	1.14930800	-2.01157500
H	2.43622400	1.14413100	-2.46670800
H	3.52440800	2.09263700	-1.45656900
C	4.93929200	-0.05383300	-0.41016700
H	5.08643800	0.84715200	0.19899800
H	5.04893700	-0.91363100	0.25693100
C	3.24373500	1.82422800	2.00569500
H	3.92348100	1.03037700	2.29762200
C	1.51878900	3.87456500	1.29052200
H	0.84808900	4.68785000	1.02419800
C	-4.14863600	3.62662300	0.99564400
H	-5.11877500	3.91968300	1.38558300
C	-3.60700100	0.18242200	-2.21641600
H	-4.05285600	1.15371900	-1.96449500
H	-2.62185800	0.38770400	-2.64569600
C	-4.82399400	-0.92610700	-0.32366100
H	-5.31278000	0.01565200	-0.04779200
H	-4.73508200	-1.52096500	0.58970600
C	1.38337200	2.62969000	0.66706600
C	-3.83557400	2.28028300	0.85689200
H	-4.56539400	1.53646200	1.15702600
C	-5.85812700	-0.87390900	-2.62603900

H	-6.39939300	0.05956400	-2.41835000
H	-6.46526900	-1.43538700	-3.34510200
C	0.43330500	3.44147200	-2.09915200
H	1.38189800	3.17966700	-2.57515600
H	0.50401800	4.48169800	-1.75836500
H	-0.35634000	3.38324600	-2.85504500
C	-5.71038200	-1.66071000	-1.32880300
H	-5.26631400	-2.64195500	-1.54693800
H	-6.69384000	-1.85305400	-0.88496500
C	5.90386100	1.04335100	-2.47120000
H	6.09514400	1.98768800	-1.94314200
H	6.66747600	0.95908900	-3.25289600
C	-1.63999900	2.85644700	-0.00006900
C	-3.21787700	4.59577300	0.63191300
H	-3.46032400	5.64955300	0.73323200
C	4.51043400	1.08948400	-3.08592900
H	4.35502600	0.19304100	-3.70212000
H	4.41510200	1.95127000	-3.75625800
C	2.26896900	1.59910900	1.02962700
C	-4.49684700	-0.53703600	-3.22432800
H	-4.61711200	0.08021400	-4.12192600
H	-3.99972600	-1.46345000	-3.54411400
C	6.02325300	-0.11245500	-1.48600600
H	5.93407000	-1.06258500	-2.03102600
H	7.01245800	-0.11345200	-1.01403000
C	2.71613700	-2.65027700	0.75921600
H	3.41837100	-2.64308700	-0.08084400
H	1.72968200	-2.88784200	0.34338800
C	3.34733700	3.06345500	2.62738500
H	4.10049000	3.22284100	3.39320100
C	2.64569700	-1.26890200	1.41243100
H	3.65309800	-0.99319000	1.74797500
C	-2.54727300	-0.50893400	1.85709700
H	-3.61702700	-0.31596700	2.01441200
C	2.48608600	4.09443100	2.26543300
H	2.56358900	5.06420600	2.74815800
C	-1.76019000	0.25683100	2.91955900
H	-0.68917400	0.15862700	2.70777100
H	-1.99033900	1.32495400	2.86138200
C	1.72399600	-1.29148200	2.62599200
H	1.69841900	-0.30644100	3.10313400
H	0.70398300	-1.49714300	2.28371800
C	3.12177100	-3.72705500	1.76128700
H	3.11936200	-4.70844800	1.27328800
H	4.15417400	-3.54241600	2.08855400
C	2.20578000	-3.73499200	2.97962000
H	1.19225200	-4.02594900	2.66956800
H	2.54099200	-4.48719300	3.70232800
C	-2.62044300	-2.52630600	3.36920900
H	-2.40430700	-3.59921700	3.42960100
H	-3.69685700	-2.41092400	3.55755800
C	-2.06617300	-0.26353300	4.32111200
H	-1.45228400	0.27041200	5.05540300
H	-3.11385900	-0.03999800	4.56662900
C	-1.83615800	-1.76658900	4.43283000
H	-2.10998100	-2.11999100	5.43337000

H	-0.76639600	-1.97683800	4.30606300
C	2.15137900	-2.35735100	3.62917700
H	3.14304900	-2.10473800	4.02920100
H	1.46322100	-2.36383500	4.48171200
C	-2.29666300	-2.00987200	1.97087800
H	-2.87733600	-2.55850700	1.22129100
H	-1.23980400	-2.20061800	1.74884500
H	-0.00496800	0.51240600	-2.44901600
C	0.71115900	-2.52526200	-2.76723300
O	-0.08039900	-2.17853700	-1.62027500
C	-0.59805000	-3.35912000	-0.99008600
C	0.12564500	-4.51987500	-1.64714800
C	0.38527200	-3.97854400	-3.05062400
H	0.44812300	-1.83868400	-3.57394000
H	1.76918200	-2.38302700	-2.51752400
H	-0.42270700	-3.28169700	0.08365600
H	-1.67903400	-3.40349200	-1.16849100
H	1.07321400	-4.71603800	-1.13510700
H	-0.46919300	-5.43545900	-1.63556900
H	1.19795400	-4.49096500	-3.56944700
H	-0.51936100	-4.05375000	-3.66235600

THF implicit THF; G = -232.166742

C	-1.12461300	-0.46505800	0.15932000
O	-0.00023600	-1.19752100	-0.29996400
C	1.12435900	-0.46552000	0.15948600
C	0.77182600	1.00876900	-0.05143500
C	-0.77134800	1.00915100	-0.05120700
H	-1.99964400	-0.79824100	-0.40237800
H	-1.29387500	-0.67655700	1.22652500
H	1.29322800	-0.67685000	1.22679400
H	1.99940400	-0.79923600	-0.40188000
H	1.19429300	1.63804500	0.73510800
H	1.15940900	1.36482100	-1.00882700
H	-1.19322800	1.63833700	0.73572200
H	-1.15904400	1.36579600	-1.00832900

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2. Kraft, S.; Stümpel, J.; Becker, P.; Kuetgens, U. *Rev. Sci. Instrum.* **1996**, *67*, 681.