Electronic Supplementary Material (ESI) for ChemComm.

Supporting Information

Efficient and Selective Catalysis for Hydrogenation and Hydrosilation of Alkenes and Alkynes with PNP Complexes of Scandium and Yttrium

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1. Spectroscopic Characterization

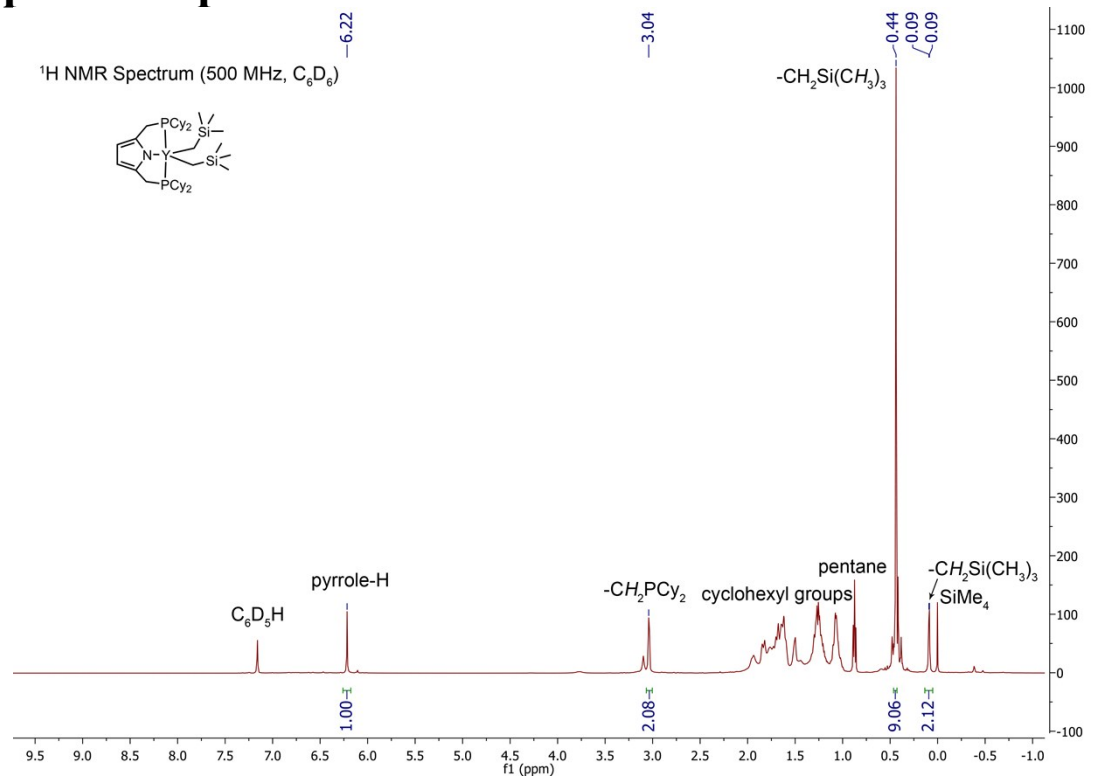

Figure S1. ^{1}H NMR Spectrum of (PNP-Cy)Y(CH_2SiMe_3)$_2$.

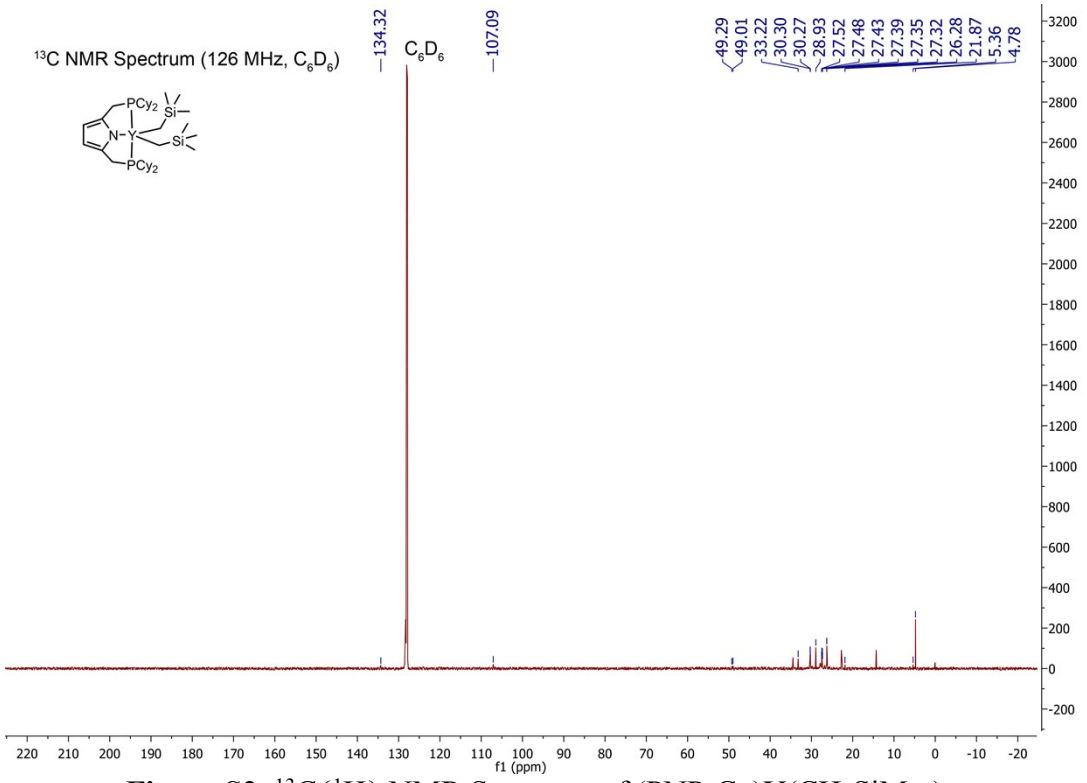

Figure S2. ^{13}C{^{1}H} NMR Spectrum of (PNP-Cy)Y(CH_2SiMe_3)$_2$.

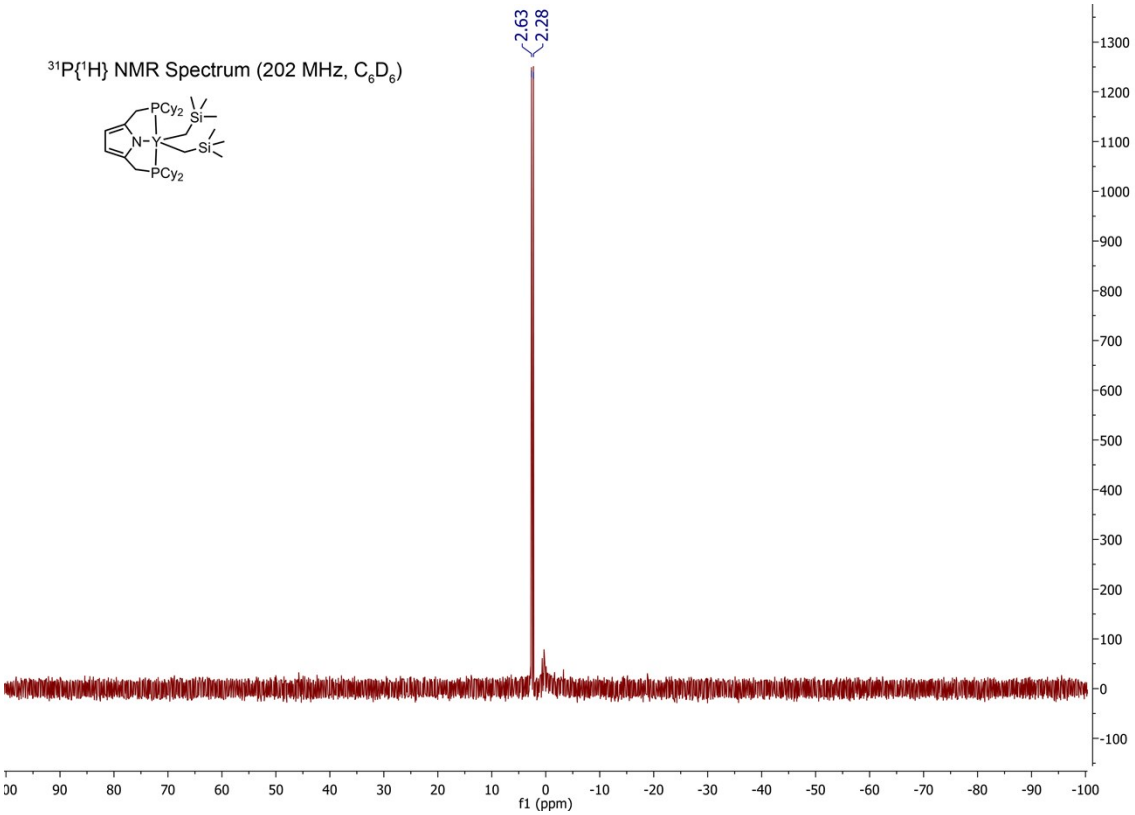

Figure S3. $^{31}P\{^{1}H\}$ NMR Spectrum of (PNP-Cy)Y(CH_2SiMe_3)$_2$.

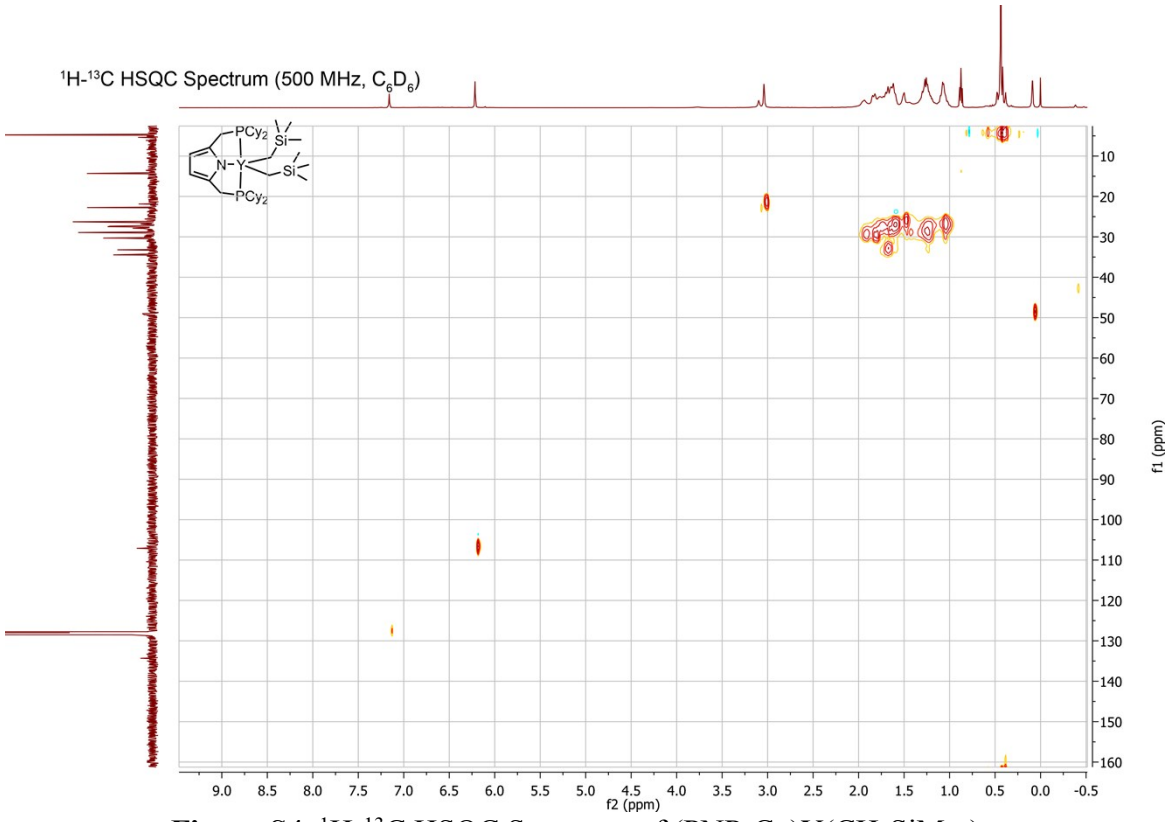

Figure S4. ^{1}H-^{13}C HSQC Spectrum of (PNP-Cy)Y(CH_2SiMe_3)$_2$.

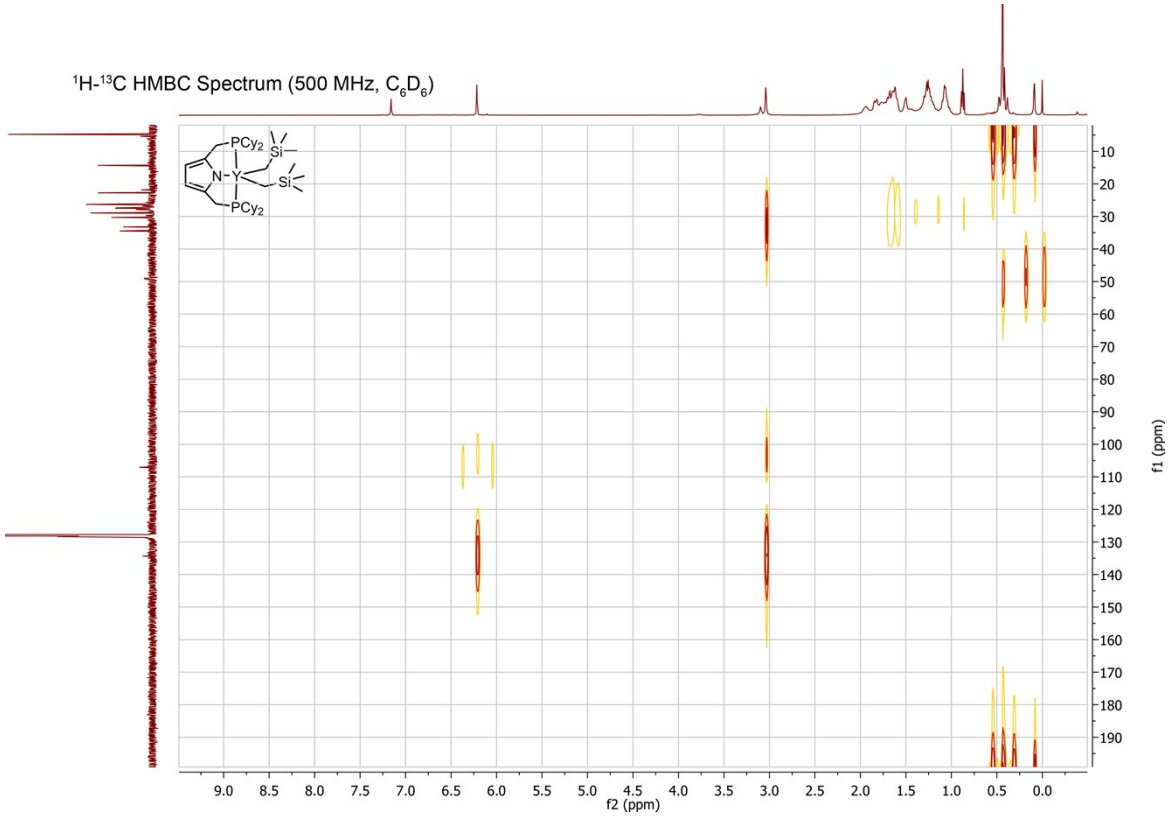

Figure S5. ^{1}H-^{13}C HMBC Spectrum of (PNP-Cy)Y(CH_2SiMe_3)$_2$.

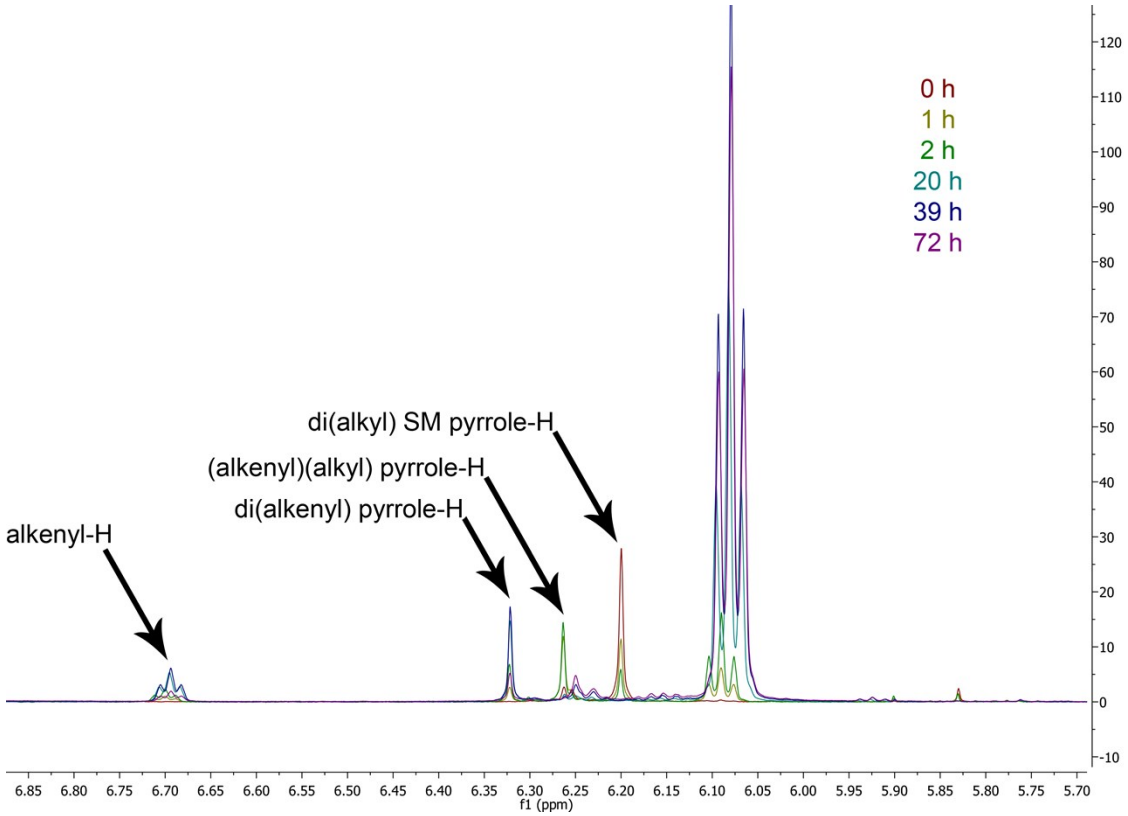

Figure S6. Conversion of Sc starting material to di(alkenyl) resting state.

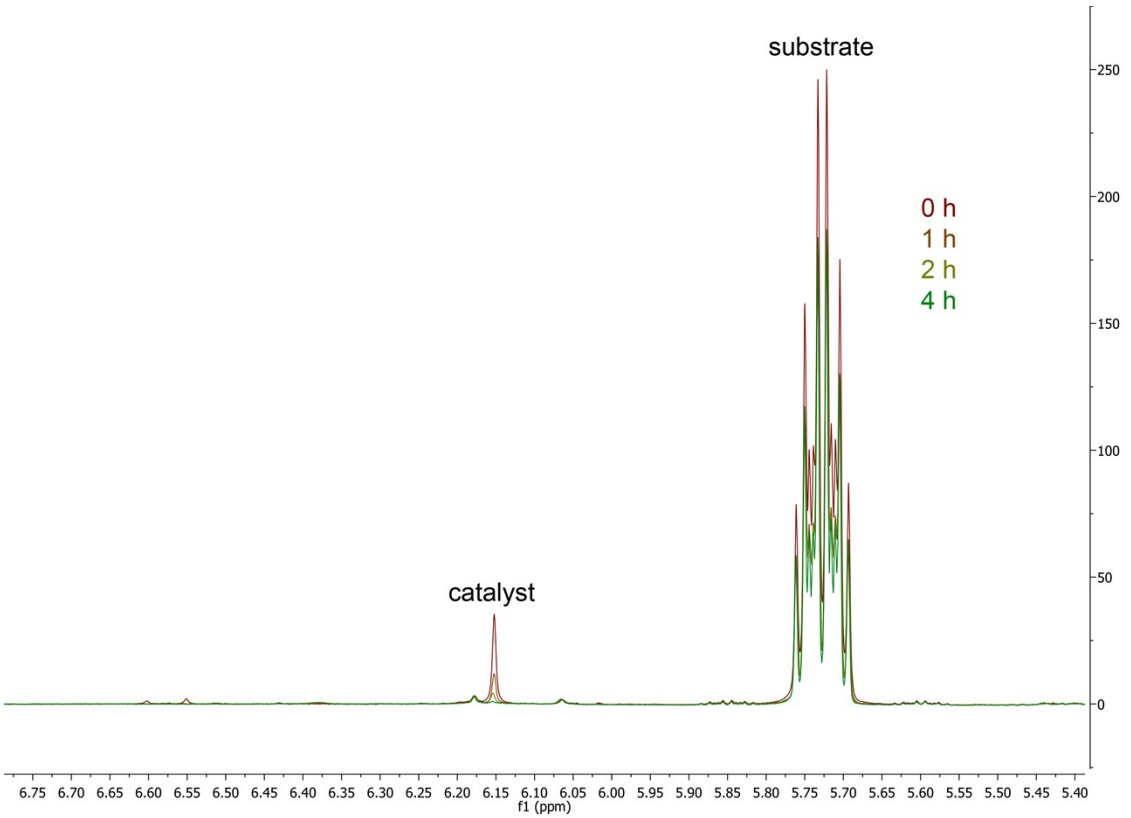

Figure S7. Decomposition of PNP-Y during catalysis.

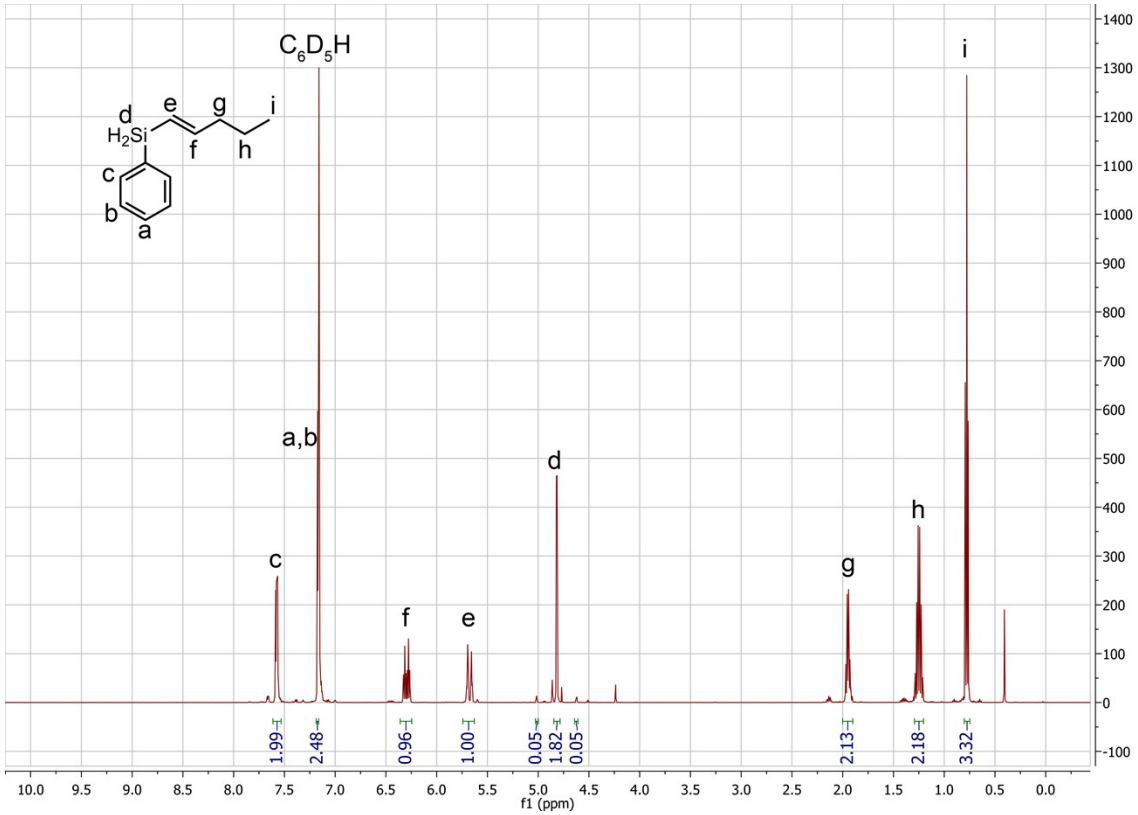

Figure S8. Phenyl(trans-1-pentenyl)silane.

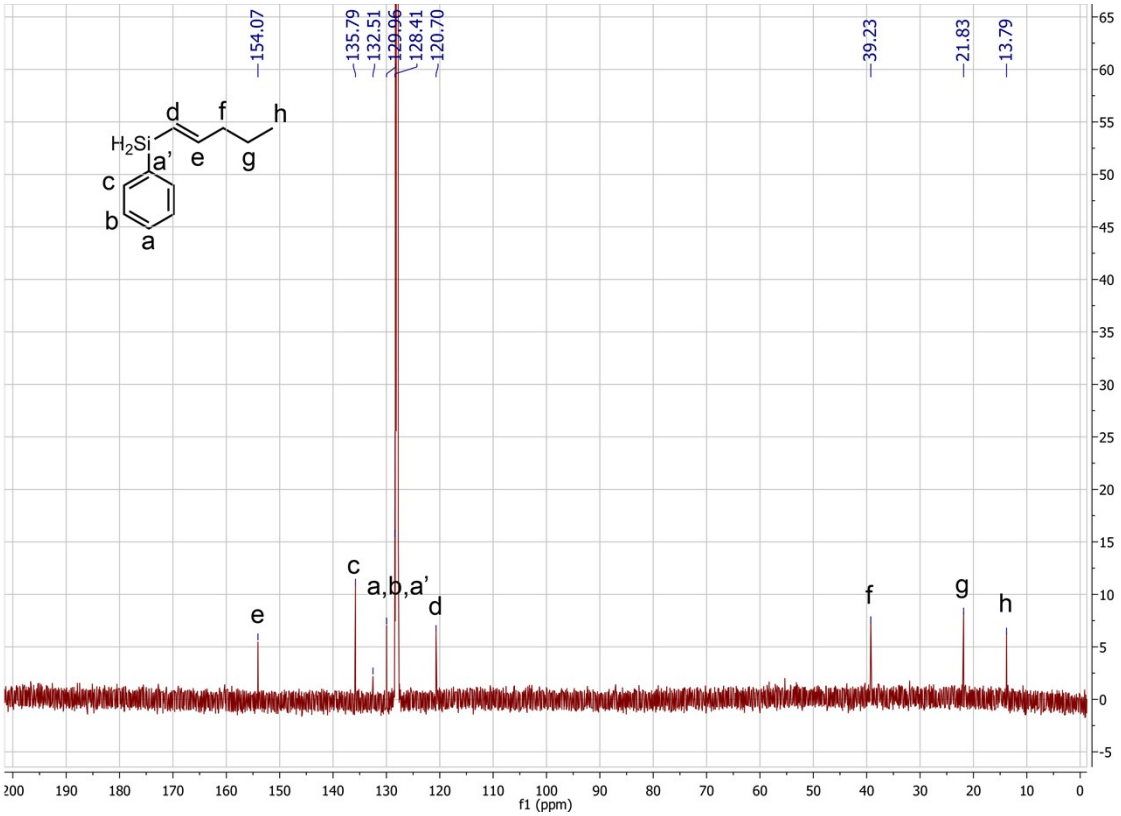

Figure S9. Phenyl(trans-1-pentenyl)silane.

2. Experimental Details

General

Unless otherwise noted, all experiments were conducted in dry, oxygen-free solvents using standard Schlenk techniques or in a N_2 atmosphere glovebox. Deuterated solvents were purchased from Cambridge Isotope Laboratories, Inc. Benzene-d_6 was dried by vacuum distillation from Na/K alloy. Toluene-d_8 was dried by refluxing over molten sodium metal followed by vacuum distillation. Unless otherwise noted, reagents were obtained from commercial suppliers and used as received. 4-phenylpyridine was obtained from Aldrich and sublimed. (PNP-Cy)H, (PNP-Cy)Sc(CH_2SiMe_3)$_2$, Y(CH_2SiMe_3)$_3$(THF)$_2$ were prepared according to literature procedures.[1,2] Characterizations were based on comparisons of NMR data with that previously published for these compounds, which was definitive.[3–8]

Analytical Methods

Solution NMR spectroscopy was performed using Bruker AV-300, AVB-400, AVQ-400, AV-500, or AV-600 MHz spectrometers at room temperature. ^{1}H, $^{13}C\{^{1}H\}$, and $^{31}P\{^{1}H\}$ NMR spectra were calibrated internally to either the resonance for the solvent or residual proteo solvent relative to tetramethylsilane. Elemental analyses were carried out by the College of Chemistry Microanalytical Laboratory at the University of California, Berkeley.

Computational Details

Calculations were carried out with Q-Chem 4.3,[9] employing the ωB97X-D range-separated hybrid functional and 6-31++G** basis set for non-metal atoms. Metal atoms were treated with the relativistic ECP and basis set of the Stuttgart group. Gibbs free energies were calculated at 298 K and 1 atm of pressure. To save computational time, some truncations were made to the system: the ligand cyclohexyl groups were replaced with methyl groups, the alkyl groups of the catalyst resting state were replaced with methyl groups, the alkene studied was propylene, and, for the initiation reactions that generate a hydride ligand from exchange of a $–CH_2SiMe_3$ group, one alkyl group was replaced with a methyl group.

X-ray Crystallography Details

X-ray diffraction data for crystals of (PNP-Cy)Y(CH_2SiMe_3)$_2$ were collected using a Bruker AXS modified four-circle diffractometer coupled CCD detector with Mo Kα (λ = 0.71073 Å) radiation monochromated by a system of QUAZAR multilayer mirrors. Crystals were kept at 100(2) K throughout collection. Data collection, refinement, and reduction were performed with Bruker APEX2 software (v. 2013.4). Structures were solved by direct methods using SHELXS-97. All structures were refined with SHELXL-97 with refinement of F^2 against all reflections by full-matrix least squares. In all models, non-hydrogen atoms were refined anisotropically, and hydrogen atoms were included at their geometrically-calculated positions and refined using a riding model. The 3D molecular structure figures were visualized with ORTEP 3.2, rendered with POV-Ray 3.6, and annotated with Adobe Photoshop CS6.

Synthesis of (PNP-Cy)Y(CH_2SiMe_3)$_2$

A solution of (PNP-Cy)H (341.7 mg, 0.70 mmol) in pentane (5 mL) was added to a solution of Y(CH_2SiMe_3)$_3$(THF)$_2$ (346.7 mg, 0.70 mmol) in pentane (5 mL) and the reaction mixture was then stirred for 1 h. The reaction mixture was concentrated to 3 mL and stored at -35 °C for 2 d to afford crystalline, colorless product (296.5 mg, 57% yield). ^{1}H NMR (500 MHz, C_6D_6) δ 6.22 (s, 2H, $^1J_{CH}$ = 163.5 Hz), 3.04 (d, $^2J_{HP}$ = 3.3 Hz, 4H), 2.03 – 1.44 (m, 24H), 1.38 – 1.17 (m, 12H), 1.12 – 0.99 (m, 8H), 0.44 (s, 18H, $^1J_{CH}$ = 116.2 Hz), 0.09 (d, $^2J_{YH}$ = 2.6 Hz, 4H, $^1J_{CH}$ = 100.6 Hz). ^{13}C{^{1}H} NMR (151 MHz, C_6D_6) δ 134.32, 107.09, 49.15 (d, $^1J_{YC}$ = 35.7 Hz), 33.22, 30.28 (d, J_{CP} = 3.3 Hz), 28.93 , 27.48 (t, J_{CP} = 5.9 Hz), 27.35 (t, J_{CP} = 4.4 Hz), 26.28, 21.87, 4.78. ^{31}P{^{1}H} NMR (202 MHz, C_6D_6) δ 2.46 (d, $^1J_{YP}$ = 70.5 Hz).Anal. Calcd. for $C_{38}H_{72}YNP_2Si_2$: C, 60.85; H, 9.68; N, 1.87, Found: C, 61.18; H, 9.94; N, 1.50.

Typical procedure for catalytic hydrogenation

A sample of (PNP-Cy)Y(CH_2SiMe_3)$_2$ (7.5 mg, 0.01 mmol) was dissolved in 1 mL benzene-d_6, along with hexamethylbenzene (2.1 mg, 0.013 mmol) as an internal standard in a 5mm NMR tube with a Teflon screw cap. To this was added 1-octene (21.3 mg, 0.19 mmol). The tube was degassed to remove nitrogen, cooled to 77 K, and placed under vacuum. The tube was exposed to hydrogen at 1 atm for 2 min and then sealed. The sealed tube was allowed to warm to room temperature to attain a hydrogen pressure of approximately 3.9 atm due to gas expansion.The tube was sealed and monitored by ^{1}H NMR spectroscopy.

Typical procedure for catalytic hydrosilation

A sample of (PNP-Cy)Y(CH_2SiMe_3)$_2$ (7.5 mg, 0.01 mmol) was dissolved in 1 mL benzene-d_6, along with hexamethylbenzene (2.1 mg, 0.013 mmol) as an internal standard in a 5mm NMR tube with a Teflon screw cap. To this was added, subsequently, 1-octene (21.3 mg, 0.19 mmol) and $PhSiH_3$ (21.6 mg, 0.20 mmol). The tube was sealed and monitored by ^{1}H NMR spectroscopy.

Preparative procedure for catalytic hydrosilation: Phenyl(trans-1-pentenyl)silane

A sample of (PNP-Cy)Sc(CH_2SiMe_3)$_2$ (100 mg, 0.15 mmol) was dissolved in 10 mL of toluene. To this was added, subsequently, 1-pentyne (204.4 mg, 3.0 mmol) and $PhSiH_3$ (324.7 mg, 3.0 mmol). After 2.5 hours, the volatile materials were removed by vacuum to afford 500 mg of crude product as yellow oil. Distillation of the crude under reduced pressure at 100 °C afforded the product as a colorless oil (355.1 mg 68% yield). ^{1}H NMR (500 MHz, C_6D_6) δ 7.57 (ddd, J = 5.5, 4.1, 2.3 Hz, 2H), 7.17 (m, J = 3.0 Hz, 3H), 6.30 (dt, $^3J_{HH}$ = 18.4, 6.3 Hz, 1H), 5.68 (dtt, $^3J_{HH}$ = 18.4, 3.2, 1.6 Hz, 1H), 4.82 (d, $^3J_{HH}$ = 3.1 Hz, $^1J_{SiH}$ = 195.5 Hz, 2H), 1.95 (td, $^3J_{HH}$ = 7.7, 6.3 Hz, 2H), 1.25 (qt ≈ h, $^3J_{HH}$ = 7.7, 7.4 Hz, 2H), 0.78 (t, $^3J_{HH}$ = 7.4 Hz, 3H). ^{13}C NMR (126 MHz, C_6D_6) δ 154.07, 135.79, 132.51, 129.96, 128.41, 120.70, 39.23, 21.83, 13.79.

3. Computational Data

$PhSiH_3$

0 1

Si	-1.90516	-1.31411	-0.00000
C	-0.38537	-0.26385	-0.00000
C	-0.49406	1.13383	-0.00000
C	0.65920	1.92547	0.00000
C	0.88121	-0.86414	0.00000
C	2.03249	-0.06970	0.00000
C	1.92160	1.32418	0.00000
H	-1.90974	-2.16317	1.20033
H	-1.90974	-2.16317	-1.20033
H	-1.46731	1.60873	-0.00000
H	0.57438	3.00449	-0.00000
H	0.97657	-1.94298	0.00000
H	3.01004	-0.53427	0.00000
H	2.81318	1.93783	0.00000
H	-3.10568	-0.46460	-0.00000

Final Energy: -522.855085121198

Translational Enthalpy:	0.889 kcal/mol
Rotational Enthalpy:	0.889 kcal/mol
Vibrational Enthalpy:	74.918 kcal/mol
gas constant (RT):	0.592 kcal/mol
Translational Entropy:	39.948 cal/mol.K
Rotational Entropy:	27.916 cal/mol.K

Vibrational Entropy: 10.535 cal/mol.K

Total Enthalpy: 77.288 kcal/mol
Total Entropy: 78.400 cal/mol.K

Propylene

0 1

C	-0.98095	-0.85818	0.00000
C	0.26628	-0.38928	0.00000
C	0.64166	1.06299	0.00000
H	-1.83877	-0.18926	0.00000
H	-1.18715	-1.92405	0.00000
H	-0.24405	1.70490	0.00000
H	1.24518	1.31013	-0.88068
H	1.24518	1.31013	0.88068
H	1.09390	-1.09838	0.00000

Final Energy: -117.8768218957

Translational Enthalpy: 0.889 kcal/mol
Rotational Enthalpy: 0.889 kcal/mol
Vibrational Enthalpy: 51.232 kcal/mol
gas constant (RT): 0.592 kcal/mol
Translational Entropy: 37.135 cal/mol.K
Rotational Entropy: 22.036 cal/mol.K
Vibrational Entropy: 3.885 cal/mol.K

Total Enthalpy: 53.602 kcal/mol
Total Entropy: 63.056 cal/mol.K

$MePhSiH_2$

0 1

Si	-1.49149	-1.30633	-0.00000
C	0.05509	-0.23339	-0.00000
C	-0.02111	1.16588	-0.00000
C	1.13047	1.95249	0.00000
C	1.32988	-0.82059	0.00000
C	2.48366	-0.04166	0.00000
C	2.38488	1.34909	0.00000
C	-3.04821	-0.25295	0.00000
H	-1.47448	-2.19253	1.19569
H	-1.47448	-2.19253	-1.19569
H	-0.99067	1.65717	-0.00000
H	1.04681	3.03488	0.00000
H	1.42754	-1.90392	0.00000
H	3.45927	-0.51768	0.00000

H	3.28289	1.95881	0.00000
H	-3.09337	0.38770	0.88633
H	-3.93933	-0.88798	0.00000
H	-3.09337	0.38770	-0.88633

Final Energy: -562.1765947309

Translational Enthalpy:	0.889 kcal/mol
Rotational Enthalpy:	0.889 kcal/mol
Vibrational Enthalpy:	95.030 kcal/mol
gas constant (RT):	0.592 kcal/mol
Translational Entropy:	40.312 cal/mol.K
Rotational Entropy:	28.851 cal/mol.K
Vibrational Entropy:	25.154 cal/mol.K
Total Enthalpy:	97.400 kcal/mol
Total Entropy:	94.317 cal/mol.K

(PNP-Me)Sc(H)(CH_3)(CH_2CMe_2) Insertion TS

0 1

C	2.21597	-1.76425	-0.83165
H	2.52872	-1.29985	-1.77600
H	2.89562	-2.59897	-0.62859
C	0.78669	-2.21962	-0.85522
C	0.23731	-3.48426	-0.81271
H	0.78014	-4.42016	-0.84725
C	-1.17344	-3.30985	-0.70202
H	-1.92505	-4.08606	-0.63600
C	-1.40150	-1.94928	-0.68598
C	-2.66822	-1.16938	-0.48858
H	-3.47355	-1.80879	-0.11129
H	-3.01822	-0.69557	-1.41422
C	-3.80637	1.19898	0.78279
H	-3.70599	1.97599	1.54570
C	-2.26644	-0.71258	2.31488
H	-3.23809	-1.17254	2.52104
C	2.26234	-1.53387	2.00774
H	1.32663	-2.10026	1.99431
C	4.06800	0.08224	0.45607
H	4.76446	-0.76160	0.49456
C	-1.30083	1.82391	-2.12096
N	-0.20616	-1.26708	-0.77592
P	-2.27843	0.18600	0.71335
P	2.31674	-0.47562	0.50218
Sc	0.03487	0.88502	-0.61664
H	-4.68484	0.58748	1.01149

H	-3.94870	1.68607	-0.18572
H	-2.00815	-0.03479	3.13259
H	-1.50994	-1.50027	2.25724
H	4.27210	0.74476	1.30233
H	4.23440	0.64558	-0.46604
H	2.28725	-0.91612	2.90955
H	3.09861	-2.24035	2.03373
H	-1.91600	2.63389	-1.69440
H	-1.99788	1.11711	-2.59659
C	0.30028	2.71827	1.02569
C	1.11594	4.22475	-0.82802
C	1.30039	3.11689	0.17493
H	0.09996	4.22532	-1.23096
H	1.28572	5.18517	-0.32603
H	1.81600	4.13327	-1.65943
H	-0.69909	3.13925	0.92643
H	0.52386	2.17051	1.93703
H	-0.71445	2.27618	-2.93531
H	2.32572	2.87306	0.43788
H	1.57995	1.78316	-1.16709

Final Energy: -1334.42640701893

Translational Enthalpy:	0.889 kcal/mol
Rotational Enthalpy:	0.889 kcal/mol
Vibrational Enthalpy:	256.118 kcal/mol
gas constant (RT):	0.592 kcal/mol
Translational Entropy:	43.158 cal/mol.K
Rotational Entropy:	34.015 cal/mol.K
Vibrational Entropy:	92.484 cal/mol.K

Total Enthalpy:	258.488 kcal/mol
Total Entropy:	169.657 cal/mol.K

(PNP-Me)ScMe$_2$(PhSiH$_3$) σ-bond metathesis TS

0 1

C	-3.16068	2.22930	-0.12353
H	-2.95585	2.65435	0.86920
H	-4.04634	2.73836	-0.51935
C	-3.37530	0.74518	-0.03911
C	-4.55984	0.05319	0.10311
H	-5.55407	0.48129	0.10186
C	-4.21147	-1.31270	0.28073
H	-4.88433	-2.14503	0.44292
C	-2.83443	-1.37581	0.23636
C	-1.94168	-2.55600	0.49337

H	-2.46523	-3.49981	0.30551
H	-1.60137	-2.57278	1.53842
C	0.75284	-3.61827	0.07458
H	1.64202	-3.62507	-0.56135
C	-0.98423	-3.06603	-2.17480
H	-1.26042	-4.12146	-2.08990
C	-2.35618	2.49655	-2.86952
H	-2.83295	1.52447	-3.01970
C	-1.26961	4.31240	-0.90580
H	-2.12976	4.95630	-1.11337
C	0.55789	0.66003	1.59268
H	-0.27650	1.38367	1.48742
H	0.12026	-0.24563	2.03801
C	0.15685	0.17925	-2.77107
H	-0.78112	-0.06290	-3.29690
H	0.53402	1.11768	-3.20384
N	-2.29690	-0.12019	0.01236
P	-0.44645	-2.38678	-0.56218
P	-1.68039	2.54457	-1.16802
Sc	-0.21293	0.32141	-0.58141
H	0.32201	-4.62380	0.09987
H	1.06375	-3.33554	1.08389
H	-0.18869	-2.94878	-2.91415
H	-1.85061	-2.49109	-2.51222
H	-0.44345	4.59696	-1.56252
H	-0.94968	4.46437	0.12836
H	-1.54903	2.59687	-3.59845
H	-3.09571	3.28885	-3.02149
H	1.18961	1.10374	2.36349
C	3.47499	0.22142	1.57553
C	4.74991	0.79138	1.67773
C	3.14172	-0.79525	2.48358
C	5.65069	0.38463	2.66286
H	5.05019	1.55912	0.96834
C	4.04387	-1.22795	3.45043
H	2.16228	-1.26215	2.43260
C	5.30042	-0.63003	3.54850
H	6.62808	0.85313	2.73031
H	3.76750	-2.02763	4.13145
H	6.00256	-0.95832	4.30895
H	0.88506	-0.59701	-3.04592
Si	2.35224	0.73996	0.12801
H	1.36745	1.78435	-0.48612
H	1.86725	-0.46831	-0.63937
H	3.47807	1.26662	-0.74080

Final Energy: -1778.70561003517

Translational Enthalpy:	0.889 kcal/mol
Rotational Enthalpy:	0.889 kcal/mol
Vibrational Enthalpy:	301.473 kcal/mol
gas constant (RT):	0.592 kcal/mol
Translational Entropy:	43.829 cal/mol.K
Rotational Entropy:	35.818 cal/mol.K
Vibrational Entropy:	110.629 cal/mol.K
Total Enthalpy:	303.843 kcal/mol
Total Entropy:	190.276 cal/mol.K

(PNP-Me)ScMe(CH_2SiMe_3)(SiH_3Ph) σ-bond metathesis hydride formation TS

0 1

C	-2.87557	2.13389	-0.50230
H	-2.49154	2.50335	0.45873
H	-3.74661	2.74545	-0.76237
C	-3.23263	0.67722	-0.42369
C	-4.44018	0.09839	-0.09620
H	-5.36395	0.62267	0.11180
C	-4.22283	-1.30533	-0.06936
H	-4.94652	-2.07561	0.16405
C	-2.89458	-1.50562	-0.37990
C	-2.11914	-2.79291	-0.38500
H	-2.77418	-3.64803	-0.58481
H	-1.64311	-2.96967	0.59064
C	0.30907	-4.11897	-1.28087
H	1.09507	-4.18366	-2.03772
C	-1.59328	-3.08853	-3.20543
H	-1.98991	-4.10834	-3.19405
C	-2.43480	2.30804	-3.33750
H	-3.01749	1.38540	-3.40201
C	-0.90704	4.01900	-1.58239
H	-1.71485	4.75026	-1.68242
C	0.77788	-0.57993	0.83302
H	-0.16699	-1.10205	0.59255
H	1.42146	-1.41126	1.13121
C	-1.49014	-0.01112	2.83848
H	-1.82046	0.57615	3.70314
H	-1.57870	-1.07065	3.10598
H	-2.18630	0.17292	2.01247
C	0.37897	2.26874	2.03257
H	1.40028	2.59680	1.80696
H	0.03590	2.83522	2.90544
H	-0.25544	2.55014	1.18429

C	1.40399	0.01561	3.84110
H	2.43928	0.32277	3.66461
H	1.40697	-1.06009	4.04975
H	1.04318	0.52924	4.73984
C	0.17127	-0.05974	-3.51404
H	-0.76822	-0.17718	-4.07793
H	0.62721	0.88724	-3.84478
N	-2.26722	-0.29493	-0.62254
P	-0.76458	-2.67349	-1.62655
P	-1.53084	2.30395	-1.74399
Sc	-0.19850	-0.02365	-1.32989
H	-0.26262	-5.05213	-1.27863
H	0.78425	-3.98746	-0.30485
H	-0.89149	-2.97329	-4.03481
H	-2.41658	-2.38448	-3.35272
H	-0.15789	4.20472	-2.35656
H	-0.42552	4.14500	-0.60922
H	-1.72574	2.32744	-4.16833
H	-3.11060	3.16607	-3.40633
Si	0.28946	0.40818	2.37433
C	3.54721	0.18185	1.01899
C	4.18810	1.28835	1.59054
C	3.89998	-1.08868	1.49514
C	5.10270	1.14235	2.63290
H	3.97594	2.28629	1.21191
C	4.83854	-1.24782	2.51094
H	3.44596	-1.97769	1.06369
C	5.43003	-0.12923	3.09611
H	5.56684	2.01942	3.07410
H	5.10357	-2.24433	2.85190
H	6.14891	-0.25012	3.90073
H	0.84720	-0.86012	-3.84816
Si	2.32306	0.51101	-0.40413
H	1.10119	1.41402	-0.80918
H	2.24208	-0.52509	-1.49369
H	3.19896	1.57744	-1.04737

Final Energy: -2187.3548220924

Translational Enthalpy:	0.889 kcal/mol
Rotational Enthalpy:	0.889 kcal/mol
Vibrational Enthalpy:	370.478 kcal/mol
gas constant (RT):	0.592 kcal/mol
Translational Entropy:	44.326 cal/mol.K
Rotational Entropy:	36.424 cal/mol.K
Vibrational Entropy:	141.088 cal/mol.K

Total Enthalpy: 372.848 kcal/mol
Total Entropy: 221.838 cal/mol.K

(PNP-Me)ScMe(CH_2SiMe_3)(SiH_3Ph) σ-bond metathesis silyl formation TS

0 1

C	-1.72290	2.32250	0.35179
H	-1.35016	2.69410	1.31587
H	-2.46157	3.04864	-0.00622
C	-2.32685	0.95451	0.49325
C	-3.61513	0.62341	0.85638
H	-4.42099	1.31838	1.05426
C	-3.66427	-0.79424	0.92956
H	-4.51433	-1.40814	1.19848
C	-2.40400	-1.24906	0.60596
C	-1.89481	-2.66078	0.60624
H	-2.72046	-3.37557	0.51906
H	-1.35840	-2.89044	1.53857
C	0.01506	-4.52374	-0.56484
H	0.67148	-4.75534	-1.40768
C	-1.75342	-2.98074	-2.25449
H	-2.39630	-3.86488	-2.20453
C	-1.04087	2.42794	-2.44940
H	-1.77319	1.62981	-2.59689
C	0.61634	3.79872	-0.53210
H	-0.06163	4.65517	-0.59850
C	1.70019	-1.12245	1.40020
H	1.05975	-2.01712	1.30406
H	2.71536	-1.52764	1.49414
C	1.28742	1.63492	2.79299
H	0.95939	2.13553	3.71083
H	0.60247	1.93615	1.99346
H	2.28652	2.00423	2.54032
C	2.55809	-0.67744	4.32741
H	2.58414	-1.75675	4.51405
H	2.33811	-0.17616	5.27681
H	3.55712	-0.36160	4.00796
C	-0.43458	-0.75899	3.62099
H	-0.48226	-1.84120	3.78997
H	-1.21648	-0.49269	2.90193
H	-0.66996	-0.26768	4.57205
C	0.84419	-0.50278	-2.67428
H	-0.13974	-0.61990	-3.16098
H	1.33354	0.34882	-3.16596
H	2.22736	-0.21024	0.33163
H	2.79992	1.89395	-1.78208

N	-1.56296	-0.18654	0.31619
P	-0.68856	-2.84184	-0.77134
P	-0.28529	2.22430	-0.79184
Sc	0.49195	-0.37455	-0.47565
H	-0.77336	-5.28057	-0.50845
H	0.61071	-4.56101	0.35145
H	-1.13401	-3.02506	-3.15365
H	-2.37909	-2.08566	-2.30891
H	1.39581	3.89878	-1.29179
H	1.09510	3.79067	0.45089
H	-0.27105	2.33140	-3.21861
H	-1.53918	3.39772	-2.54307
Si	1.27247	-0.23806	3.01857
Si	3.15089	0.80908	-0.81944
C	4.16245	1.65618	0.53541
C	4.18775	3.05251	0.66357
C	4.81183	0.90447	1.52739
C	4.81773	3.67390	1.74097
H	3.70404	3.66916	-0.09016
C	5.44612	1.51646	2.60571
H	4.82015	-0.18184	1.46400
C	5.44455	2.90577	2.71949
H	4.81926	4.75744	1.81648
H	5.93848	0.91016	3.36066
H	5.93286	3.38554	3.56218
H	4.03545	-0.15569	-1.53667
H	1.43056	-1.39596	-2.94366

Final Energy: -2187.3515855273

Translational Enthalpy:	0.889 kcal/mol
Rotational Enthalpy:	0.889 kcal/mol
Vibrational Enthalpy:	369.298 kcal/mol
gas constant (RT):	0.592 kcal/mol
Translational Entropy:	44.326 cal/mol.K
Rotational Entropy:	36.353 cal/mol.K
Vibrational Entropy:	144.080 cal/mol.K

Total Enthalpy:	371.668 kcal/mol
Total Entropy:	224.758 cal/mol.K

(PNP-Me)ScMe$_2$

0 1

C	2.08752	-1.88351	-0.83871
H	2.25878	-1.69345	-1.90716
H	2.79321	-2.66135	-0.52674

C	0.66909	-2.30721	-0.58235
C	0.16330	-3.58379	-0.45396
H	0.73630	-4.50213	-0.46760
C	-1.24619	-3.45008	-0.32936
H	-1.97383	-4.24500	-0.22696
C	-1.51926	-2.09965	-0.38901
C	-2.85520	-1.41251	-0.39493
H	-3.63074	-2.05649	0.03415
H	-3.16681	-1.15781	-1.41714
C	-4.27862	1.05901	0.24458
H	-4.30363	1.96892	0.84983
C	-2.81201	-0.36557	2.28644
H	-3.78183	-0.82448	2.50241
C	2.72339	-0.84620	1.77093
H	1.85965	-1.41970	2.11818
C	4.03233	0.27770	-0.54512
H	4.79530	-0.49714	-0.42157
C	-0.21574	2.21324	-1.82237
N	-0.34933	-1.37150	-0.52131
P	-2.70226	0.16818	0.53610
P	2.39733	-0.30202	0.05094
Sc	-0.11599	0.79835	-0.13836
H	-5.13992	0.43515	0.50284
H	-4.34676	1.34750	-0.80734
H	-2.65140	0.48861	2.94846
H	-2.02175	-1.09832	2.47138
H	4.33356	1.16641	0.01553
H	3.96381	0.54779	-1.60193
H	2.84282	0.02327	2.42159
H	3.61647	-1.47644	1.82642
H	-0.57341	3.20378	-1.49896
H	-0.88595	1.87961	-2.63020
C	0.16228	1.72233	1.85961
H	0.76946	2.37886	-2.28895
H	1.10868	2.28277	1.93122
H	-0.63835	2.44030	2.10020
H	0.17490	0.98278	2.67714

Final Energy: -1255.86691680606

Translational Enthalpy:	0.889 kcal/mol
Rotational Enthalpy:	0.889 kcal/mol
Vibrational Enthalpy:	221.133 kcal/mol
gas constant (RT):	0.592 kcal/mol
Translational Entropy:	42.882 cal/mol.K
Rotational Entropy:	33.461 cal/mol.K

Vibrational Entropy: 87.417 cal/mol.K

Total Enthalpy: 223.503 kcal/mol
Total Entropy: 163.760 cal/mol.K

(PNP-Me)ScMeH

0 1

C	2.09411	-1.85171	-0.83921
H	2.29498	-1.54632	-1.87517
H	2.79554	-2.65643	-0.59267
C	0.67174	-2.30563	-0.66970
C	0.16453	-3.58736	-0.68723
H	0.73781	-4.49977	-0.79002
C	-1.24713	-3.46710	-0.56532
H	-1.97435	-4.26881	-0.55554
C	-1.52155	-2.11878	-0.48075
C	-2.85452	-1.42916	-0.40753
H	-3.63159	-2.11299	-0.04862
H	-3.16879	-1.06161	-1.39392
C	-4.26275	0.96185	0.51367
H	-4.27452	1.80616	1.20758
C	-2.78396	-0.68320	2.37456
H	-3.74851	-1.17290	2.54137
C	2.60729	-1.09893	1.89294
H	1.71970	-1.68582	2.14438
C	4.02759	0.25258	-0.23033
H	4.78348	-0.53347	-0.13846
C	-0.26974	2.21784	-1.57308
N	-0.34949	-1.38266	-0.52137
P	-2.68858	0.03921	0.69360
P	2.36603	-0.37394	0.22735
Sc	-0.13079	0.72958	0.03203
H	-5.12375	0.31846	0.71952
H	-4.34314	1.35453	-0.50312
H	-2.62819	0.09731	3.12255
H	-1.98492	-1.42245	2.47714
H	4.29916	1.08591	0.42262
H	4.01291	0.61611	-1.26093
H	2.71238	-0.30203	2.63231
H	3.48637	-1.75061	1.91749
H	-0.42042	3.22968	-1.16329
H	-1.10297	2.02612	-2.26747
H	0.09055	1.35504	1.77409
H	0.64057	2.26316	-2.19294

Final Energy: -1216.54636431064

Translational Enthalpy:	0.889 kcal/mol
Rotational Enthalpy:	0.889 kcal/mol
Vibrational Enthalpy:	201.562 kcal/mol
gas constant (RT):	0.592 kcal/mol
Translational Entropy:	42.734 cal/mol.K
Rotational Entropy:	33.235 cal/mol.K
Vibrational Entropy:	77.851 cal/mol.K
Total Enthalpy:	203.932 kcal/mol
Total Entropy:	153.821 cal/mol.K

(PNP-Me)ScMe(CH_2CMe_2)

0 1

C	2.06407	-1.95732	-0.81476
H	2.24712	-1.79420	-1.88564
H	2.76789	-2.72457	-0.47383
C	0.64404	-2.37568	-0.55791
C	0.14066	-3.64671	-0.37579
H	0.71532	-4.56380	-0.35184
C	-1.26863	-3.50990	-0.25322
H	-1.99494	-4.30077	-0.11594
C	-1.54354	-2.16322	-0.36692
C	-2.88051	-1.47822	-0.38674
H	-3.64838	-2.10012	0.08649
H	-3.21000	-1.27283	-1.41443
C	-4.30483	1.00955	0.18975
H	-4.31891	1.94301	0.75842
C	-2.75174	-0.30574	2.24073
H	-3.71281	-0.74969	2.51807
C	2.60252	-0.85283	1.78565
H	1.72885	-1.42717	2.10574
C	4.01010	0.20884	-0.50336
H	4.76669	-0.56251	-0.32928
C	-0.17835	2.08362	-2.03941
N	-0.37534	-1.43962	-0.53282
P	-2.71087	0.14491	0.46390
P	2.35120	-0.35243	0.03976
Sc	-0.13884	0.75573	-0.28482
H	-5.15004	0.38878	0.50278
H	-4.41264	1.25390	-0.87000
H	-2.56199	0.57873	2.85367
H	-1.95637	-1.03244	2.42806
H	4.28777	1.11199	0.04668
H	3.98515	0.45267	-1.56849
H	2.68757	0.03222	2.42087

H	3.49710	-1.47339	1.89616
H	-0.51849	3.09482	-1.76332
H	-0.83933	1.73385	-2.84752
C	0.13002	1.86003	1.62781
H	0.82030	2.20868	-2.48975
C	1.33113	2.81749	1.66341
H	-0.78826	2.45448	1.79523
H	0.18429	1.17367	2.49286
C	1.42423	3.67553	2.93025
H	1.30220	3.48462	0.78949
H	2.26907	2.25009	1.56222
H	0.53001	4.29987	3.03590
H	2.29956	4.33635	2.91984
H	1.48734	3.03948	3.82092

Final Energy: -1334.47445524817

Translational Enthalpy:	0.889 kcal/mol
Rotational Enthalpy:	0.889 kcal/mol
Vibrational Enthalpy:	259.196 kcal/mol
gas constant (RT):	0.592 kcal/mol
Translational Entropy:	43.158 cal/mol.K
Rotational Entropy:	34.167 cal/mol.K
Vibrational Entropy:	101.561 cal/mol.K

Total Enthalpy:	261.566 kcal/mol
Total Entropy:	178.887 cal/mol.K

(PNP-Me)ScMe(CH_2SiMe_3)

0 1

C	-2.51096	2.09657	0.10318
H	-2.58736	2.27655	1.18433
H	-3.08567	2.88262	-0.39917
C	-3.02709	0.73384	-0.26188
C	-4.28623	0.38271	-0.70073
H	-5.10614	1.06165	-0.89722
C	-4.29509	-1.03381	-0.81604
H	-5.12300	-1.66166	-1.11968
C	-3.04030	-1.46594	-0.44222
C	-2.53005	-2.87300	-0.31428
H	-3.13926	-3.56776	-0.90282
H	-2.55415	-3.21526	0.72942
C	-0.14312	-4.56052	-0.42397
H	0.87119	-4.68324	-0.81257
C	-0.88985	-2.91476	-2.68251
H	-1.38329	-3.82392	-3.03970

C	-0.76569	2.48950	-2.15148
H	-1.31729	1.67463	-2.62819
C	-0.12992	3.77205	0.35206
H	-0.77091	4.60283	0.04133
C	0.83890	-0.90500	2.06608
H	0.13729	-1.54201	2.63081
H	1.73894	-1.51340	1.86893
C	-0.25496	1.52559	3.56903
H	-0.01739	2.45951	4.09137
H	-0.89296	0.92790	4.22999
H	-0.85664	1.77394	2.68703
C	2.46754	1.69031	2.12341
H	3.40358	1.16928	1.89160
H	2.72117	2.59655	2.68555
H	2.02654	1.99856	1.16839
C	2.19145	0.12135	4.72232
H	3.12066	-0.42391	4.52213
H	1.56089	-0.51850	5.34998
H	2.44513	1.01731	5.30137
C	1.47377	-0.26727	-1.52479
H	1.02668	-0.15635	-2.52615
H	2.13602	0.60161	-1.37873
N	-2.23152	-0.39008	-0.11679
P	-0.77061	-2.89245	-0.85379
P	-0.72812	2.18446	-0.34415
Sc	-0.02821	-0.44311	0.09545
H	-0.78230	-5.34468	-0.84126
H	-0.10665	-4.66680	0.66321
H	0.10800	-2.83927	-3.12124
H	-1.47328	-2.04523	-2.99781
H	0.89056	3.96191	0.00907
H	-0.11563	3.71505	1.44335
H	0.25283	2.49391	-2.54688
H	-1.25797	3.43877	-2.38406
Si	1.30877	0.55897	3.10747
H	2.13095	-1.15069	-1.57025

Final Energy: -1664.51961963274

Translational Enthalpy:	0.889 kcal/mol
Rotational Enthalpy:	0.889 kcal/mol
Vibrational Enthalpy:	290.705 kcal/mol
gas constant (RT):	0.592 kcal/mol
Translational Entropy:	43.545 cal/mol.K
Rotational Entropy:	34.935 cal/mol.K
Vibrational Entropy:	115.157 cal/mol.K

Total Enthalpy: 293.075 kcal/mol
Total Entropy: 193.638 cal/mol.K

$PhSiH_2(CH_2SiMe_3)$

0 1

C	2.20112	1.37986	-0.05579
C	3.47603	1.89581	-0.28385
C	4.57551	1.04207	-0.32187
C	4.39411	-0.32739	-0.13491
C	3.11735	-0.83590	0.09107
C	1.99661	0.00702	0.13914
Si	0.28300	-0.69157	0.48444
C	-1.07203	0.49285	-0.04155
Si	-2.82938	-0.20278	-0.02624
C	-3.01837	-1.45495	-1.42014
C	-4.04569	1.21313	-0.28554
H	1.35487	2.06241	-0.03488
H	3.61004	2.96302	-0.43281
H	5.56966	1.44087	-0.49935
H	5.24716	-0.99848	-0.16814
H	2.99451	-1.90800	0.22808
H	0.14637	-0.98201	1.93875
H	0.16255	-1.99537	-0.22711
H	-0.85454	0.85786	-1.05453
H	-1.04171	1.36905	0.62057
H	-2.31816	-2.28905	-1.30637
H	-2.82997	-0.99101	-2.39462
H	-4.03248	-1.86870	-1.43851
H	-3.95723	1.96058	0.51063
H	-5.07996	0.85171	-0.29110
H	-3.86331	1.71879	-1.24019
C	-3.17755	-1.03509	1.62758
H	-2.53240	-1.90653	1.78348
H	-4.21718	-1.37654	1.67960
H	-3.00982	-0.34577	2.46235

Final Energy: -970.819646723606

Translational Enthalpy: 0.889 kcal/mol
Rotational Enthalpy: 0.889 kcal/mol
Vibrational Enthalpy: 164.356 kcal/mol
gas constant (RT): 0.592 kcal/mol
Translational Entropy: 41.695 cal/mol.K
Rotational Entropy: 32.208 cal/mol.K
Vibrational Entropy: 53.747 cal/mol.K

Total Enthalpy: 166.726 kcal/mol
Total Entropy: 127.649 cal/mol.K

(PNP-Me)YMe(CH_2SiMe_3)

0 1

C	-2.01360	2.59445	0.02793
H	-1.77033	2.84189	1.07054
H	-2.69406	3.37234	-0.33658
C	-2.65822	1.24142	-0.07481
C	-4.00594	0.95528	-0.16699
H	-4.80864	1.67793	-0.24090
C	-4.12202	-0.45816	-0.11535
H	-5.03180	-1.04428	-0.14370
C	-2.83843	-0.95271	0.00445
C	-2.41667	-2.38393	0.17923
H	-3.23422	-3.06014	-0.09462
H	-2.14991	-2.59934	1.22306
C	-0.41414	-4.42566	-0.37542
H	0.42110	-4.74939	-1.00169
C	-1.60932	-2.90824	-2.53114
H	-2.29694	-3.75789	-2.58827
C	-0.99119	2.87508	-2.64759
H	-1.66070	2.05205	-2.91264
C	0.33529	4.23083	-0.45965
H	-0.35760	5.06120	-0.62732
C	2.10293	-0.40047	1.12760
H	2.51579	-1.42194	1.05891
H	2.94324	0.28619	0.93019
C	-0.05107	-1.28093	3.09737
H	-0.42323	-1.23434	4.12685
H	0.23277	-2.32125	2.89448
H	-0.88813	-1.01687	2.43790
C	0.72173	1.66154	2.88861
H	1.48701	2.39572	2.60971
H	0.35465	1.92156	3.88755
H	-0.12402	1.77019	2.19705
C	2.62177	-0.31375	4.26062
H	3.46851	0.37455	4.16033
H	3.02622	-1.33190	4.28525
H	2.13938	-0.11866	5.22577
C	1.11009	-0.22982	-2.81846
H	0.25779	-0.18423	-3.51753
H	1.77945	0.59945	-3.10151
N	-1.91545	0.07780	0.00937
P	-0.92108	-2.72530	-0.84107

P	-0.43228	2.62960	-0.91792
Y	0.40662	-0.14494	-0.53927
H	-1.24303	-5.13041	-0.49381
H	-0.08418	-4.43490	0.66672
H	-0.80220	-3.03669	-3.25617
H	-2.15423	-1.99320	-2.77991
H	1.23890	4.39527	-1.05200
H	0.61551	4.20715	0.59688
H	-0.13553	2.85146	-3.32647
H	-1.52801	3.82213	-2.76067
Si	1.41250	-0.10575	2.82093
H	1.65838	-1.15368	-3.06666

Final Energy: -1656.10228334252

Translational Enthalpy:	0.889 kcal/mol
Rotational Enthalpy:	0.889 kcal/mol
Vibrational Enthalpy:	290.138 kcal/mol
gas constant (RT):	0.592 kcal/mol
Translational Entropy:	43.888 cal/mol.K
Rotational Entropy:	35.034 cal/mol.K
Vibrational Entropy:	124.883 cal/mol.K
Total Enthalpy:	292.508 kcal/mol
Total Entropy:	203.805 cal/mol.K

(PNP-Me)YMe(CH_2CMe_2)

0 1

C	2.06927	-1.91579	-0.77796
H	2.23367	-1.80078	-1.85813
H	2.78264	-2.66465	-0.41607
C	0.66066	-2.34256	-0.47561
C	0.21382	-3.59821	-0.11505
H	0.82826	-4.47732	0.03192
C	-1.19840	-3.50554	-0.00144
H	-1.89048	-4.29908	0.25032
C	-1.52941	-2.19863	-0.29934
C	-2.90021	-1.58943	-0.38127
H	-3.63853	-2.24285	0.09688
H	-3.21624	-1.44545	-1.42357
C	-4.58381	0.72255	0.19105
H	-4.69126	1.67287	0.72022
C	-2.79940	-0.33304	2.20448
H	-3.68237	-0.89410	2.52634
C	2.56045	-0.68730	1.77789
H	1.65130	-1.20195	2.10097

C	4.08808	0.18211	-0.51415
H	4.80095	-0.61062	-0.26691
C	-0.24046	2.34741	-2.38548
N	-0.39603	-1.45617	-0.57443
P	-2.88281	0.07238	0.41774
P	2.38719	-0.27439	-0.00042
Y	-0.22991	0.93746	-0.46001
H	-5.32722	0.01616	0.57354
H	-4.77309	0.89943	-0.87086
H	-2.70752	0.58317	2.79269
H	-1.90895	-0.94414	2.37661
H	4.38912	1.10278	-0.00727
H	4.11292	0.36239	-1.59191
H	2.66768	0.22787	2.36571
H	3.42045	-1.34150	1.95165
H	-0.11776	3.41173	-2.12520
H	-1.17260	2.28503	-2.97184
C	0.05106	2.04080	1.65037
H	0.56945	2.11570	-3.09746
C	1.25840	2.99055	1.71608
H	-0.85521	2.61115	1.92699
H	0.15412	1.27888	2.44716
C	1.49627	3.63875	3.08503
H	1.14469	3.78801	0.96723
H	2.17772	2.45497	1.42695
H	0.62048	4.22397	3.38727
H	2.36746	4.30545	3.08431
H	1.65574	2.86994	3.85054

Final Energy: -1326.05533190397

Translational Enthalpy:	0.889 kcal/mol
Rotational Enthalpy:	0.889 kcal/mol
Vibrational Enthalpy:	258.810 kcal/mol
gas constant (RT):	0.592 kcal/mol
Translational Entropy:	43.545 cal/mol.K
Rotational Entropy:	34.391 cal/mol.K
Vibrational Entropy:	103.530 cal/mol.K
Total Enthalpy:	261.180 kcal/mol
Total Entropy:	181.466 cal/mol.K

(PNP-Me)Y(H)(Me)

0 1

C	2.09620	-1.83682	-0.83647
H	2.26361	-1.53281	-1.87886

H	2.79441	-2.65273	-0.61864
C	0.67905	-2.28320	-0.61521
C	0.19930	-3.57290	-0.50845
H	0.79119	-4.47892	-0.53506
C	-1.21172	-3.46900	-0.38318
H	-1.92435	-4.27895	-0.29350
C	-1.51021	-2.12205	-0.42073
C	-2.86403	-1.47170	-0.39282
H	-3.62338	-2.18067	-0.04433
H	-3.16756	-1.13185	-1.39252
C	-4.47294	0.77613	0.54173
H	-4.56555	1.60723	1.24552
C	-2.80661	-0.70756	2.37930
H	-3.72392	-1.27442	2.56704
C	2.63987	-1.10626	1.89151
H	1.72108	-1.64753	2.13396
C	4.15712	0.13745	-0.23076
H	4.85423	-0.70094	-0.13620
C	-0.23074	2.48931	-1.83556
N	-0.35630	-1.36915	-0.54080
P	-2.80956	0.01699	0.69531
P	2.45298	-0.36943	0.22295
Y	-0.14154	0.95213	-0.03145
H	-5.25904	0.04369	0.75011
H	-4.60874	1.16795	-0.46957
H	-2.69795	0.08155	3.12661
H	-1.94980	-1.38208	2.46163
H	4.48714	0.94981	0.42173
H	4.17258	0.49961	-1.26196
H	2.78416	-0.31949	2.63525
H	3.48168	-1.80523	1.92113
H	-0.28338	3.53588	-1.49299
H	-1.10021	2.33804	-2.49642
H	0.07605	1.70944	1.85284
H	0.65201	2.43039	-2.49465

Final Energy: -1208.12984786332

Translational Enthalpy:	0.889 kcal/mol
Rotational Enthalpy:	0.889 kcal/mol
Vibrational Enthalpy:	200.444 kcal/mol
gas constant (RT):	0.592 kcal/mol
Translational Entropy:	43.176 cal/mol.K
Rotational Entropy:	33.533 cal/mol.K
Vibrational Entropy:	78.687 cal/mol.K

Total Enthalpy: 202.814 kcal/mol
Total Entropy: 155.395 cal/mol.K

(PNP-Me)YMe$_2$

0 1

C	2.09186	-1.89182	-0.85121
H	2.24415	-1.70955	-1.92392
H	2.79115	-2.68020	-0.55107
C	0.67729	-2.30440	-0.55822
C	0.20187	-3.57297	-0.29178
H	0.79505	-4.47585	-0.22159
C	-1.20677	-3.45471	-0.15814
H	-1.91722	-4.24815	0.03604
C	-1.50715	-2.12103	-0.35095
C	-2.86346	-1.47577	-0.37997
H	-3.61480	-2.14392	0.05571
H	-3.18059	-1.25166	-1.40771
C	-4.48263	0.84028	0.34151
H	-4.56352	1.75691	0.93137
C	-2.74487	-0.40293	2.28627
H	-3.64630	-0.95870	2.56316
C	2.66338	-0.85194	1.76926
H	1.74571	-1.36105	2.07675
C	4.17117	0.12343	-0.49427
H	4.86322	-0.70491	-0.31325
C	-0.19047	2.47336	-2.15861
N	-0.35738	-1.38734	-0.57742
P	-2.80292	0.12599	0.53106
P	2.46709	-0.31472	0.02693
Y	-0.13231	0.98621	-0.29585
H	-5.24905	0.13364	0.67484
H	-4.66076	1.09212	-0.70706
H	-2.63180	0.46763	2.93659
H	-1.87398	-1.05043	2.42107
H	4.51321	1.00039	0.06133
H	4.17991	0.36961	-1.55921
H	2.80943	0.01690	2.41529
H	3.50579	-1.54207	1.87911
H	-0.23375	3.53291	-1.85796
H	-1.05505	2.30891	-2.82310
C	0.15508	1.97552	1.86383
H	0.69789	2.38075	-2.80643
H	1.09692	2.54142	1.95825
H	-0.64715	2.68506	2.12641
H	0.17101	1.22329	2.67084

Final Energy: -1247.44822708414

Translational Enthalpy:	0.889 kcal/mol
Rotational Enthalpy:	0.889 kcal/mol
Vibrational Enthalpy:	219.969 kcal/mol
gas constant (RT):	0.592 kcal/mol
Translational Entropy:	43.304 cal/mol.K
Rotational Entropy:	33.733 cal/mol.K
Vibrational Entropy:	91.093 cal/mol.K

Total Enthalpy:	222.338 kcal/mol
Total Entropy:	168.131 cal/mol.K

(PNP-Me)Y(Me)(H)(CH_2CMe_2) Insertion TS

0 1

C	2.24493	-2.00849	-0.83484
H	2.52138	-1.70486	-1.85391
H	2.88498	-2.85473	-0.56044
C	0.79469	-2.37753	-0.72141
C	0.21212	-3.61149	-0.51135
H	0.72852	-4.56062	-0.44288
C	-1.18932	-3.38298	-0.40763
H	-1.96413	-4.12198	-0.24661
C	-1.37694	-2.02373	-0.56132
C	-2.64517	-1.22295	-0.50323
H	-3.48025	-1.84180	-0.15655
H	-2.91815	-0.81118	-1.48338
C	-3.95112	1.16107	0.53334
H	-3.94103	1.98386	1.25362
C	-2.45601	-0.58399	2.28821
H	-3.42657	-1.06268	2.45429
C	2.47067	-1.38990	1.93488
H	1.48703	-1.85547	2.04737
C	4.32543	-0.19552	0.08942
H	4.94058	-1.09177	0.22078
C	-1.40368	1.86725	-2.37126
N	-0.16489	-1.38728	-0.74393
P	-2.38265	0.21393	0.63585
P	2.53580	-0.56435	0.29109
Y	0.09622	0.96226	-0.73727
H	-4.81826	0.52370	0.73401
H	-4.03967	1.58592	-0.47050
H	-2.27887	0.15208	3.07691
H	-1.67539	-1.34883	2.33624
H	4.63417	0.55617	0.82144
H	4.49738	0.21771	-0.90807

H	2.60954	-0.65835	2.73573
H	3.23747	-2.16695	2.02287
H	-1.97652	2.71359	-1.95145
H	-2.15283	1.15637	-2.75683
C	0.32715	2.70986	1.21005
C	1.02398	4.50492	-0.41538
C	1.29557	3.28565	0.42687
H	0.02238	4.46809	-0.85393
H	1.08082	5.39580	0.22244
H	1.74809	4.60133	-1.22507
H	-0.69500	3.08614	1.18105
H	0.58901	2.05022	2.03469
H	-0.88455	2.27007	-3.25521
H	2.33679	3.07425	0.64922
H	1.69262	2.17896	-1.13911

Final Energy: -1325.99991569754

Translational Enthalpy:	0.889 kcal/mol
Rotational Enthalpy:	0.889 kcal/mol
Vibrational Enthalpy:	255.523 kcal/mol
gas constant (RT):	0.592 kcal/mol
Translational Entropy:	43.545 cal/mol.K
Rotational Entropy:	34.289 cal/mol.K
Vibrational Entropy:	101.250 cal/mol.K

Total Enthalpy:	257.893 kcal/mol
Total Entropy:	179.084 cal/mol.K

(PNP-Me)YMe(CH_2SiMe_3)(SiH_3Ph) σ-bond metathesis hydride formation TS

0 1

C	-0.84672	2.87451	0.37763
H	-0.01614	3.14481	1.04401
H	-1.52435	3.73517	0.34126
C	-1.56930	1.65172	0.86854
C	-2.69567	1.61033	1.66605
H	-3.25970	2.46480	2.01825
C	-2.95370	0.24013	1.92802
H	-3.75637	-0.17575	2.52389
C	-1.96973	-0.47540	1.27480
C	-1.75504	-1.96178	1.30309
H	-2.69699	-2.48626	1.50052
H	-1.05121	-2.24455	2.09682
C	-0.56660	-4.27782	0.01794
H	-0.19099	-4.72604	-0.90570
C	-2.45406	-2.61835	-1.40801

H	-3.19062	-3.34428	-1.04963
C	-1.52958	2.76154	-2.41543
H	-2.31805	2.06797	-2.11119
C	0.95206	4.00600	-1.60921
H	0.39670	4.94144	-1.48962
C	2.72729	-1.79858	-1.18982
H	1.79718	-2.18981	-1.64908
H	3.43331	-1.79628	-2.02808
C	-0.17788	-0.49769	-3.13778
H	-1.25114	-0.26408	-3.22736
H	0.34127	0.16754	-3.84793
N	-1.11217	0.37353	0.60132
P	-1.01083	-2.52256	-0.28160
P	-0.10946	2.54857	-1.27672
Y	0.63800	-0.20955	-0.91869
H	-1.42849	-4.85390	0.36892
H	0.22740	-4.33080	0.76794
H	-2.12747	-2.88669	-2.41546
H	-2.91721	-1.62913	-1.45249
H	1.34151	3.94967	-2.62901
H	1.80361	4.00090	-0.92356
H	-1.23139	2.51480	-3.43711
H	-1.91769	3.78426	-2.37904
H	3.06171	-2.58637	-0.50563
C	2.42494	0.03205	1.29109
C	2.02433	1.26336	1.83746
C	1.97678	-1.13573	1.93324
C	1.18686	1.32959	2.94790
H	2.37757	2.18351	1.37571
C	1.16992	-1.07398	3.06805
H	2.27414	-2.10791	1.54871
C	0.75496	0.15866	3.56400
H	0.85972	2.29245	3.32801
H	0.85662	-1.99008	3.56047
H	0.09134	0.20711	4.42088
H	-0.05081	-1.51831	-3.53264
Si	3.51633	0.01733	-0.27839
H	2.57984	0.78148	-1.30794
H	4.74776	-0.84264	-0.21497
H	4.23175	1.35014	-0.07084

Final Energy: -1770.30883449745

Translational Enthalpy:	0.889 kcal/mol
Rotational Enthalpy:	0.889 kcal/mol
Vibrational Enthalpy:	300.244 kcal/mol

gas constant (RT): 0.592 kcal/mol
Translational Entropy: 44.142 cal/mol.K
Rotational Entropy: 35.125 cal/mol.K
Vibrational Entropy: 115.364 cal/mol.K

Total Enthalpy: 302.614 kcal/mol
Total Entropy: 194.630 cal/mol.K

(PNP-Me)YMe(CH_2SiMe_3)(SiH_3Ph) σ-bond metathesis silyl formation TS

0 1

C	-1.73073	2.40411	0.32178
H	-1.34798	2.70431	1.30729
H	-2.43587	3.18009	0.00323
C	-2.40799	1.06466	0.38324
C	-3.75450	0.80636	0.53975
H	-4.54422	1.54481	0.59347
C	-3.88625	-0.60358	0.63701
H	-4.79813	-1.16991	0.77785
C	-2.61301	-1.12544	0.53314
C	-2.20110	-2.56643	0.63738
H	-3.06910	-3.22216	0.50624
H	-1.76844	-2.79175	1.62210
C	-0.41506	-4.67095	-0.26818
H	0.28557	-5.02072	-1.03084
C	-1.86236	-3.05429	-2.17596
H	-2.59037	-3.87045	-2.13411
C	-1.03424	2.52738	-2.47665
H	-1.77498	1.73570	-2.61874
C	0.60786	3.90165	-0.53251
H	-0.06573	4.76005	-0.61664
C	2.10558	-1.29099	1.35072
H	1.61043	-2.26831	1.20143
H	3.16860	-1.54193	1.44380
C	1.28634	1.35826	2.73486
H	0.92504	1.81324	3.66404
H	0.52189	1.56119	1.97279
H	2.20834	1.86968	2.44047
C	2.84459	-0.74624	4.32052
H	3.01281	-1.81026	4.51894
H	2.53183	-0.27100	5.25706
H	3.79848	-0.29906	4.02171
C	-0.10198	-1.22859	3.52072
H	-0.05544	-2.32068	3.60261
H	-0.89876	-0.96388	2.81562
H	-0.39186	-0.83391	4.50100
C	0.81412	-0.64305	-2.78368

H	-0.17317	-0.72460	-3.26952
H	1.32652	0.20240	-3.26748
H	2.54014	-0.28749	0.27288
H	2.91317	1.94141	-1.73692
N	-1.68312	-0.11398	0.35672
P	-0.90448	-2.93651	-0.61799
P	-0.28443	2.32660	-0.81595
Y	0.55524	-0.41196	-0.42705
H	-1.28728	-5.33205	-0.25597
H	0.08360	-4.72338	0.70354
H	-1.18593	-3.20349	-3.02090
H	-2.39363	-2.10993	-2.32271
H	1.41048	4.00112	-1.26813
H	1.05720	3.88903	0.46457
H	-0.26534	2.41796	-3.24527
H	-1.52442	3.50066	-2.57786
Si	1.55009	-0.50011	2.97396
Si	3.38002	0.90038	-0.77031
C	4.25412	1.83860	0.61731
C	4.13532	3.22886	0.75817
C	4.94475	1.14375	1.62302
C	4.66662	3.89672	1.86068
H	3.61818	3.80311	-0.00637
C	5.48254	1.80331	2.72541
H	5.06294	0.06449	1.55057
C	5.33799	3.18404	2.85153
H	4.55794	4.97411	1.94515
H	6.01092	1.24035	3.48954
H	5.75087	3.70027	3.71271
H	4.38386	0.06249	-1.48914
H	1.37476	-1.54607	-3.07571

Final Energy: -2178.9373516727

Translational Enthalpy:	0.889 kcal/mol
Rotational Enthalpy:	0.889 kcal/mol
Vibrational Enthalpy:	368.445 kcal/mol
gas constant (RT):	0.592 kcal/mol
Translational Entropy:	44.593 cal/mol.K
Rotational Entropy:	36.524 cal/mol.K
Vibrational Entropy:	153.185 cal/mol.K
Total Enthalpy:	370.814 kcal/mol
Total Entropy:	234.301 cal/mol.K

(PNP-Me)Y(Me)(CH_2SiMe_3)(SiH_3Ph) σ-bond metathesis hydride formation TS

0 1

Y	-0.19303	0.23628	-1.09678
P	-0.58523	-2.60415	-1.52674
P	-1.87189	2.54246	-1.67759
N	-2.47237	-0.30209	-0.71183
C	-1.68396	4.31919	-1.25969
C	-2.38429	2.55722	-3.43792
C	-3.41145	2.03369	-0.80195
C	-3.56352	0.53928	-0.84192
C	-4.73131	-0.19124	-0.92989
C	-4.36175	-1.55882	-0.83198
C	-2.98930	-1.58539	-0.68969
C	-2.10067	-2.77972	-0.48777
C	0.47971	-4.01280	-1.02755
C	-1.17809	-3.05254	-3.20018
H	-0.84175	4.74317	-1.81238
H	-2.59108	4.88032	-1.50488
H	-1.47917	4.42340	-0.19077
H	-3.17653	3.29233	-3.61118
H	-2.75562	1.56204	-3.69614
H	-1.52763	2.77741	-4.07891
H	-4.28563	2.52243	-1.24661
H	-3.32462	2.40020	0.22993
H	-5.72997	0.21257	-1.03751
H	-5.01840	-2.41934	-0.84991
H	-2.63846	-3.70315	-0.72972
H	-1.76767	-2.86206	0.55689
H	-0.05238	-4.96590	-1.10743
H	1.36851	-4.04669	-1.66323
H	0.80444	-3.86955	0.00690
H	-0.38117	-2.90268	-3.93235
H	-1.52615	-4.08955	-3.23644
H	-2.00732	-2.38702	-3.45535
C	0.29757	0.24185	-3.42660
H	0.66249	1.22503	-3.76763
H	1.05922	-0.48785	-3.73893
H	-0.60559	0.02373	-4.02064
C	0.85947	-0.48328	1.13987
Si	0.25567	0.52412	2.60783
C	-1.14464	1.64729	2.00886
C	-0.42662	-0.59573	3.96345
C	1.60252	1.61918	3.34393
H	-0.02332	-1.10919	0.88196
H	1.56024	-1.23711	1.50143
H	-1.55179	2.24469	2.83200
H	-1.96437	1.05501	1.58587

H	-0.79011	2.35368	1.24525
H	-1.25310	-1.20629	3.58293
H	-0.80238	-0.01432	4.81308
H	0.34846	-1.27440	4.33633
H	1.19787	2.17846	4.19536
H	2.45673	1.03242	3.69537
H	1.97914	2.35260	2.62111
Si	2.46701	0.76344	-0.07251
H	2.25958	-0.06835	-1.31090
H	3.36481	1.88554	-0.55628
H	1.24065	1.73320	-0.21679
C	3.76480	0.01947	1.10348
C	3.98676	-1.35855	1.23482
H	3.34897	-2.06294	0.70535
C	5.02488	-1.85371	2.01977
H	5.18452	-2.92546	2.09342
C	5.85602	-0.97423	2.71196
H	6.65762	-1.35768	3.33594
C	5.66033	0.39870	2.58700
H	6.30984	1.09207	3.11294
C	4.63849	0.88452	1.77277
H	4.52256	1.95981	1.65799

Final Energy: -2178.94261493912

Translational Enthalpy:	0.889 kcal/mol
Rotational Enthalpy:	0.889 kcal/mol
Vibrational Enthalpy:	370.138 kcal/mol
gas constant (RT):	0.592 kcal/mol
Translational Entropy:	44.593 cal/mol.K
Rotational Entropy:	36.670 cal/mol.K
Vibrational Entropy:	148.226 cal/mol.K
Total Enthalpy:	372.508 kcal/mol
Total Entropy:	229.489 cal/mol.K

4. ORTEP diagram

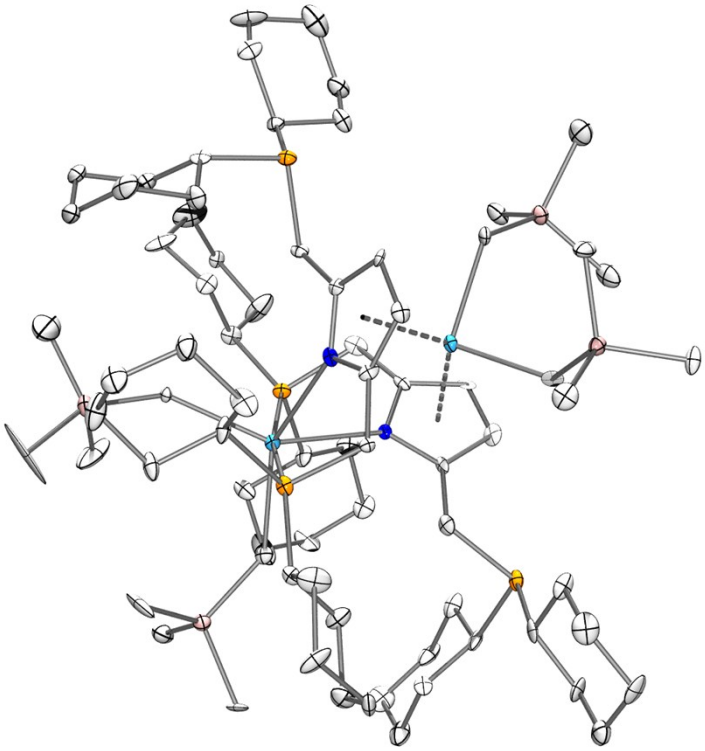

Figure S6. ORTEP diagram of (PNP-Cy)Y(CH_2SiMe_3)$_2$. H atoms omitted for clarity.

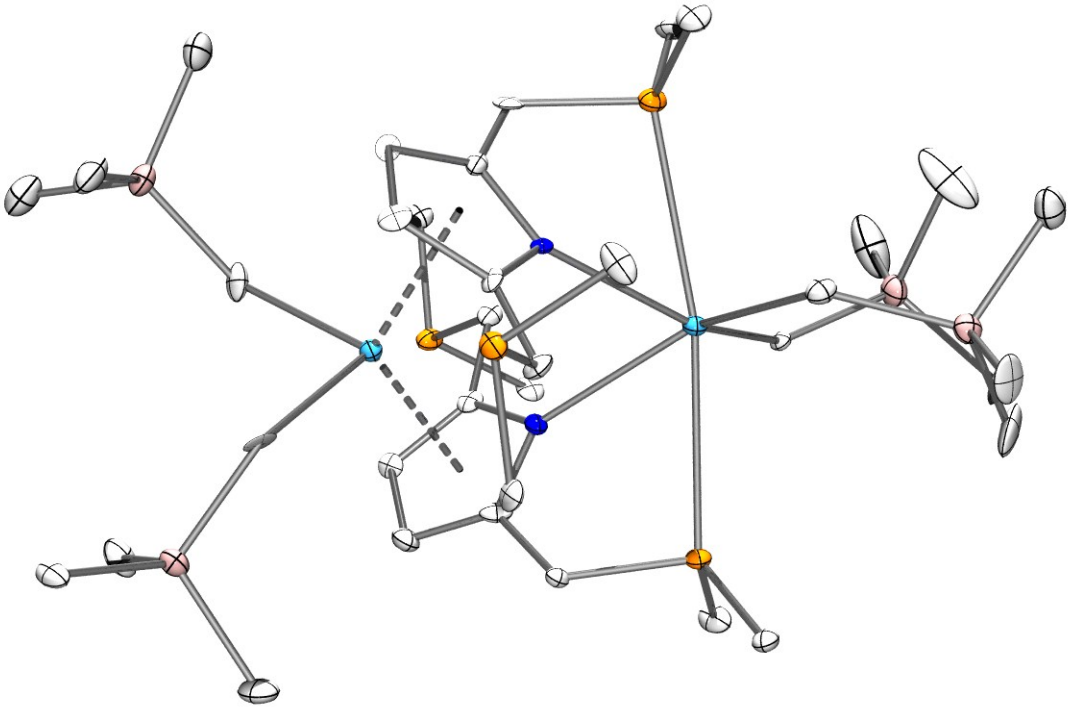

Figure S7. ORTEP diagram of (PNP-Cy)Y(CH_2SiMe_3)$_2$. H atoms and cyclohexyl groups omitted for clarity.

5. X-ray Data Tables

Table 1. Crystal data and structure refinement for (PNP-Cy)Y(CH2SiMe3)2.

Identification code	shelx	
Empirical formula	C76 H144 N2 P4 Si4 Y2	
Formula weight	1499.98	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P -1	
Unit cell dimensions	a = 14.5955(8) Å	α= 79.645(3)°.
	b = 16.2010(10) Å	β= 76.624(3)°.
	c = 20.8185(12) Å	γ = 80.373(3)°.
Volume	4670.5(5) $Å^3$	
Z	2	
Density (calculated)	1.067 Mg/m^3	
Absorption coefficient	1.391 mm^{-1}	
F(000)	1616	
Crystal size	0.08 x 0.08 x 0.02 mm^3	
Theta range for data collection	1.016 to 25.417°.	
Index ranges	-16<=h<=17, -19<=k<=19, 0<=l<=25	
Reflections collected	15860	
Independent reflections	15860 [R(int) = 0.087]	
Completeness to theta = 25.000°	95.9 %	
Absorption correction	Semi-empirical from equivalents	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	15860 / 42 / 806	
Goodness-of-fit on F^2	1.042	
Final R indices [I>2sigma(I)]	R1 = 0.0625, wR2 = 0.1416	
R indices (all data)	R1 = 0.1161, wR2 = 0.1692	
Extinction coefficient	n/a	
Largest diff. peak and hole	1.076 and -0.843 e.$Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for (PNP-Cy)Y(CH2SiMe3)2. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	5778(7)	5930(7)	7489(5)	19(3)
C(2)	5504(8)	5208(7)	7910(5)	24(3)
C(3)	5844(7)	5179(7)	8498(5)	17(2)
C(4)	6277(7)	5884(7)	8403(5)	18(3)
C(5)	5476(7)	6316(6)	6828(4)	14(2)
C(6)	5013(6)	7817(6)	5920(4)	20(2)
C(7)	5876(7)	7645(8)	5372(5)	33(3)
C(8)	5664(8)	7986(7)	4665(5)	38(3)
C(9)	4861(7)	7602(6)	4561(5)	28(2)
C(10)	3962(7)	7817(8)	5130(5)	39(3)
C(11)	4169(8)	7454(8)	5818(6)	42(3)
C(12)	4292(7)	7702(6)	7424(5)	28(3)
C(13)	3462(8)	7193(7)	7574(6)	39(3)
C(14)	2785(8)	7435(7)	8214(6)	39(3)
C(15)	2426(8)	8340(7)	8161(6)	46(3)
C(16)	3235(8)	8872(7)	7982(6)	48(3)
C(17)	3922(7)	8657(6)	7333(5)	31(3)
C(18)	6725(7)	6162(7)	8904(4)	18(3)
C(19)	5265(7)	6619(6)	10045(5)	22(3)
C(20)	4494(8)	6785(7)	9625(5)	31(3)
C(21)	3663(8)	7416(8)	9903(6)	46(4)
C(22)	4065(9)	8264(7)	9904(5)	45(3)
C(23)	4816(8)	8109(7)	10323(5)	38(3)
C(24)	5664(8)	7454(7)	10059(5)	32(3)
C(25)	7107(7)	5752(7)	10245(5)	22(3)
C(26)	7937(7)	5010(7)	10085(6)	28(3)
C(27)	8691(9)	4922(8)	10499(6)	39(3)
C(28)	8252(10)	4769(8)	11211(7)	56(4)
C(29)	7437(9)	5486(9)	11422(6)	54(4)
C(30)	6653(7)	5586(8)	11016(5)	32(3)
C(31)	7362(7)	4021(6)	6830(5)	21(3)

C(32)	6094(8)	2871(7)	7862(4)	32(3)
C(33)	5398(7)	3855(8)	6612(6)	34(3)
C(34)	6928(7)	2341(6)	6521(5)	29(3)
C(35)	7915(8)	4004(6)	8422(5)	27(3)
C(36)	9576(8)	2872(8)	7648(5)	43(3)
C(37)	9912(9)	3834(8)	8687(6)	40(3)
C(38)	8849(9)	2309(8)	9102(6)	47(3)
C(39)	8940(7)	5948(6)	7349(5)	19(3)
C(40)	9402(7)	5217(6)	7105(5)	16(2)
C(41)	9097(7)	5177(7)	6527(5)	25(3)
C(42)	8425(7)	5893(6)	6406(5)	17(2)
C(43)	9120(7)	6312(7)	7891(5)	24(3)
C(44)	9868(7)	7739(7)	7004(5)	29(3)
C(45)	9915(7)	8715(6)	6889(5)	32(3)
C(46)	10595(9)	8945(7)	6222(7)	66(4)
C(47)	11522(7)	8463(6)	6144(6)	43(3)
C(48)	11472(7)	7490(7)	6277(6)	35(3)
C(49)	10813(7)	7228(7)	6949(5)	34(3)
C(50)	9096(7)	7821(7)	8471(5)	24(2)
C(51)	10028(9)	7419(10)	8688(6)	59(4)
C(52)	10118(7)	7688(7)	9366(5)	19(2)
C(53)	9258(10)	7637(10)	9878(6)	68(4)
C(54)	8352(8)	8055(9)	9638(5)	44(3)
C(55)	8252(7)	7698(8)	9033(5)	28(3)
C(56)	7931(7)	6131(7)	5832(5)	23(3)
C(57)	9268(8)	6615(7)	4616(5)	28(3)
C(58)	9987(8)	6772(7)	4998(5)	33(3)
C(59)	10569(8)	7446(8)	4579(5)	37(3)
C(60)	10025(8)	8236(8)	4329(6)	49(3)
C(61)	9307(8)	8090(7)	3972(5)	39(3)
C(62)	8693(7)	7439(6)	4382(5)	24(2)
C(63)	7707(7)	5706(7)	4587(5)	24(3)
C(64)	8171(8)	5563(7)	3886(5)	32(3)
C(65)	7481(8)	5472(7)	3472(6)	36(3)
C(66)	6877(8)	4797(8)	3794(5)	38(4)
C(67)	6354(8)	4967(9)	4504(6)	42(3)

C(68)	7070(7)	5046(8)	4918(5)	31(3)
C(69)	7698(7)	8477(6)	6171(4)	22(2)
C(70)	6063(7)	9974(6)	6130(6)	57(4)
C(71)	8094(7)	10276(6)	5762(4)	39(2)
C(72)	7333(7)	9611(6)	4833(4)	34(2)
C(73)	6265(6)	8523(5)	8013(4)	13(2)
C(74)	5359(10)	10401(7)	7932(9)	106(5)
C(75)	7465(10)	9988(9)	7761(6)	82(5)
C(76)	6269(11)	9609(8)	9103(6)	82(5)
N(1)	6282(6)	6348(5)	7778(4)	18(2)
N(2)	8313(5)	6376(5)	6926(4)	13(2)
Si(1)	6471(2)	3281(2)	6966(1)	23(1)
Si(2)	9016(2)	3292(2)	8469(2)	26(1)
Si(3)	7275(2)	9555(2)	5751(1)	23(1)
Si(4)	6315(2)	9584(2)	8204(1)	29(1)
P(1)	5340(2)	7465(2)	6738(1)	19(1)
P(2)	6159(2)	5717(2)	9787(1)	20(1)
P(3)	8896(2)	7484(2)	7712(1)	21(1)
P(4)	8639(2)	5705(2)	5068(1)	21(1)
Y(1)	7492(1)	4999(1)	7513(1)	17(1)
Y(2)	7097(1)	7636(1)	7204(1)	16(1)

Table 3. Bond lengths [Å] and angles [°] for (PNP-Cy)Y(CH2SiMe3)2.

C(1)-N(1)	1.371(12)
C(1)-C(2)	1.386(14)
C(1)-C(5)	1.535(13)
C(1)-Y(1)	2.702(10)
C(2)-C(3)	1.414(14)
C(2)-Y(1)	2.807(11)
C(2)-H(2)	0.9500
C(3)-C(4)	1.358(14)
C(3)-Y(1)	2.788(10)
C(3)-H(3)	0.9500
C(4)-N(1)	1.381(12)
C(4)-C(18)	1.517(13)
C(4)-Y(1)	2.687(10)
C(5)-P(1)	1.819(10)
C(5)-H(5A)	0.9900
C(5)-H(5B)	0.9900
C(6)-C(7)	1.516(13)
C(6)-C(11)	1.522(13)
C(6)-P(1)	1.840(9)
C(6)-H(6)	1.0000
C(7)-C(8)	1.560(13)
C(7)-H(7A)	0.9900
C(7)-H(7B)	0.9900
C(8)-C(9)	1.488(14)
C(8)-H(8A)	0.9900
C(8)-H(8B)	0.9900
C(9)-C(10)	1.588(13)
C(9)-H(9A)	0.9900
C(9)-H(9B)	0.9900
C(10)-C(11)	1.525(13)
C(10)-H(10A)	0.9900
C(10)-H(10B)	0.9900
C(11)-H(11A)	0.9900
C(11)-H(11B)	0.9900

C(12)-C(13)	1.520(13)
C(12)-C(17)	1.544(13)
C(12)-P(1)	1.877(9)
C(12)-H(12)	1.0000
C(13)-C(14)	1.535(15)
C(13)-H(13A)	0.9900
C(13)-H(13B)	0.9900
C(14)-C(15)	1.466(15)
C(14)-H(14A)	0.9900
C(14)-H(14B)	0.9900
C(15)-C(16)	1.514(15)
C(15)-H(15A)	0.9900
C(15)-H(15B)	0.9900
C(16)-C(17)	1.541(14)
C(16)-H(16A)	0.9900
C(16)-H(16B)	0.9900
C(17)-H(17A)	0.9900
C(17)-H(17B)	0.9900
C(18)-P(2)	1.897(9)
C(18)-H(18A)	0.9900
C(18)-H(18B)	0.9900
C(19)-C(20)	1.541(13)
C(19)-C(24)	1.567(15)
C(19)-P(2)	1.856(11)
C(19)-H(19)	1.0000
C(20)-C(21)	1.525(14)
C(20)-H(20A)	0.9900
C(20)-H(20B)	0.9900
C(21)-C(22)	1.580(17)
C(21)-H(21A)	0.9900
C(21)-H(21B)	0.9900
C(22)-C(23)	1.516(15)
C(22)-H(22A)	0.9900
C(22)-H(22B)	0.9900
C(23)-C(24)	1.554(14)
C(23)-H(23A)	0.9900

C(23)-H(23B)	0.9900
C(24)-H(24A)	0.9900
C(24)-H(24B)	0.9900
C(25)-C(26)	1.579(14)
C(25)-C(30)	1.583(13)
C(25)-P(2)	1.867(11)
C(25)-H(25)	1.0000
C(26)-C(27)	1.523(14)
C(26)-H(26A)	0.9900
C(26)-H(26B)	0.9900
C(27)-C(28)	1.466(16)
C(27)-H(27A)	0.9900
C(27)-H(27B)	0.9900
C(28)-C(29)	1.562(18)
C(28)-H(28A)	0.9900
C(28)-H(28B)	0.9900
C(29)-C(30)	1.544(15)
C(29)-H(29A)	0.9900
C(29)-H(29B)	0.9900
C(30)-H(30A)	0.9900
C(30)-H(30B)	0.9900
C(31)-Si(1)	1.853(10)
C(31)-Y(1)	2.367(10)
C(31)-H(31A)	0.9900
C(31)-H(31B)	0.9900
C(32)-Si(1)	1.853(9)
C(32)-H(32A)	0.9800
C(32)-H(32B)	0.9800
C(32)-H(32C)	0.9800
C(33)-Si(1)	1.913(11)
C(33)-H(33A)	0.9800
C(33)-H(33B)	0.9800
C(33)-H(33C)	0.9800
C(34)-Si(1)	1.872(9)
C(34)-H(34A)	0.9800
C(34)-H(34B)	0.9800

C(34)-H(34C)	0.9800
C(35)-Si(2)	1.826(11)
C(35)-Y(1)	2.382(10)
C(35)-H(35A)	0.9900
C(35)-H(35B)	0.9900
C(36)-Si(2)	1.907(11)
C(36)-H(36A)	0.9800
C(36)-H(36B)	0.9800
C(36)-H(36C)	0.9800
C(37)-Si(2)	1.868(12)
C(37)-H(37A)	0.9800
C(37)-H(37B)	0.9800
C(37)-H(37C)	0.9800
C(38)-Si(2)	1.888(12)
C(38)-H(38A)	0.9800
C(38)-H(38B)	0.9800
C(38)-H(38C)	0.9800
C(39)-C(40)	1.381(14)
C(39)-N(2)	1.428(12)
C(39)-C(43)	1.455(14)
C(39)-Y(1)	2.741(10)
C(40)-C(41)	1.391(14)
C(40)-Y(1)	2.783(10)
C(40)-H(40)	0.9500
C(41)-C(42)	1.414(14)
C(41)-Y(1)	2.752(10)
C(41)-H(41)	0.9500
C(42)-N(2)	1.412(12)
C(42)-C(56)	1.495(13)
C(42)-Y(1)	2.697(10)
C(43)-P(3)	1.856(11)
C(43)-H(43A)	0.9900
C(43)-H(43B)	0.9900
C(44)-C(49)	1.476(14)
C(44)-C(45)	1.567(14)
C(44)-P(3)	1.834(10)

C(44)-H(44)	1.0000
C(45)-C(46)	1.534(14)
C(45)-H(45A)	0.9900
C(45)-H(45B)	0.9900
C(46)-C(47)	1.434(15)
C(46)-H(46A)	0.9900
C(46)-H(46B)	0.9900
C(47)-C(48)	1.561(15)
C(47)-H(47A)	0.9900
C(47)-H(47B)	0.9900
C(48)-C(49)	1.538(14)
C(48)-H(48A)	0.9900
C(48)-H(48B)	0.9900
C(49)-H(49A)	0.9900
C(49)-H(49B)	0.9900
C(50)-C(55)	1.502(13)
C(50)-C(51)	1.537(14)
C(50)-P(3)	1.860(9)
C(50)-H(50)	1.0000
C(51)-C(52)	1.589(13)
C(51)-H(51A)	0.9900
C(51)-H(51B)	0.9900
C(52)-C(53)	1.449(15)
C(52)-H(52A)	0.9900
C(52)-H(52B)	0.9900
C(53)-C(54)	1.529(16)
C(53)-H(53A)	0.9900
C(53)-H(53B)	0.9900
C(54)-C(55)	1.522(14)
C(54)-H(54A)	0.9900
C(54)-H(54B)	0.9900
C(55)-H(55A)	0.9900
C(55)-H(55B)	0.9900
C(56)-P(4)	1.863(10)
C(56)-H(56A)	0.9900
C(56)-H(56B)	0.9900

C(57)-C(62)	1.518(15)
C(57)-C(58)	1.533(14)
C(57)-P(4)	1.859(11)
C(57)-H(57)	1.0000
C(58)-C(59)	1.516(15)
C(58)-H(58A)	0.9900
C(58)-H(58B)	0.9900
C(59)-C(60)	1.467(16)
C(59)-H(59A)	0.9900
C(59)-H(59B)	0.9900
C(60)-C(61)	1.486(15)
C(60)-H(60A)	0.9900
C(60)-H(60B)	0.9900
C(61)-C(62)	1.511(14)
C(61)-H(61A)	0.9900
C(61)-H(61B)	0.9900
C(62)-H(62A)	0.9900
C(62)-H(62B)	0.9900
C(63)-C(68)	1.502(15)
C(63)-C(64)	1.501(14)
C(63)-P(4)	1.867(11)
C(63)-H(63)	1.0000
C(64)-C(65)	1.508(14)
C(64)-H(64A)	0.9900
C(64)-H(64B)	0.9900
C(65)-C(66)	1.485(16)
C(65)-H(65A)	0.9900
C(65)-H(65B)	0.9900
C(66)-C(67)	1.549(14)
C(66)-H(66A)	0.9900
C(66)-H(66B)	0.9900
C(67)-C(68)	1.532(14)
C(67)-H(67A)	0.9900
C(67)-H(67B)	0.9900
C(68)-H(68A)	0.9900
C(68)-H(68B)	0.9900

C(69)-Si(3)	1.880(9)
C(69)-Y(2)	2.393(9)
C(69)-H(69A)	0.9900
C(69)-H(69B)	0.9900
C(70)-Si(3)	1.832(10)
C(70)-H(70A)	0.9800
C(70)-H(70B)	0.9800
C(70)-H(70C)	0.9800
C(71)-Si(3)	1.812(9)
C(71)-H(71A)	0.9800
C(71)-H(71B)	0.9800
C(71)-H(71C)	0.9800
C(72)-Si(3)	1.879(8)
C(72)-H(72A)	0.9800
C(72)-H(72B)	0.9800
C(72)-H(72C)	0.9800
C(73)-Si(4)	1.850(8)
C(73)-Y(2)	2.389(8)
C(73)-H(73A)	0.9900
C(73)-H(73B)	0.9900
C(74)-Si(4)	1.869(11)
C(74)-H(74A)	0.9800
C(74)-H(74B)	0.9800
C(74)-H(74C)	0.9800
C(75)-Si(4)	1.878(11)
C(75)-H(75A)	0.9800
C(75)-H(75B)	0.9800
C(75)-H(75C)	0.9800
C(76)-Si(4)	1.866(13)
C(76)-H(76A)	0.9800
C(76)-H(76B)	0.9800
C(76)-H(76C)	0.9800
N(1)-Y(2)	2.544(8)
N(1)-Y(1)	2.625(8)
N(2)-Y(2)	2.528(8)
N(2)-Y(1)	2.673(8)

P(1)-Y(2)	3.014(3)
P(3)-Y(2)	3.008(3)

N(1)-C(1)-C(2)	110.8(9)
N(1)-C(1)-C(5)	121.4(9)
C(2)-C(1)-C(5)	127.4(10)
N(1)-C(1)-Y(1)	72.0(6)
C(2)-C(1)-Y(1)	79.7(7)
C(5)-C(1)-Y(1)	121.5(6)
C(1)-C(2)-C(3)	106.6(10)
C(1)-C(2)-Y(1)	71.3(6)
C(3)-C(2)-Y(1)	74.6(6)
C(1)-C(2)-H(2)	126.7
C(3)-C(2)-H(2)	126.7
Y(1)-C(2)-H(2)	119.4
C(4)-C(3)-C(2)	105.6(10)
C(4)-C(3)-Y(1)	71.5(6)
C(2)-C(3)-Y(1)	76.1(6)
C(4)-C(3)-H(3)	127.2
C(2)-C(3)-H(3)	127.2
Y(1)-C(3)-H(3)	117.4
C(3)-C(4)-N(1)	112.5(9)
C(3)-C(4)-C(18)	126.1(9)
N(1)-C(4)-C(18)	121.4(9)
C(3)-C(4)-Y(1)	79.8(6)
N(1)-C(4)-Y(1)	72.5(5)
C(18)-C(4)-Y(1)	114.9(6)
C(1)-C(5)-P(1)	110.0(7)
C(1)-C(5)-H(5A)	109.7
P(1)-C(5)-H(5A)	109.7
C(1)-C(5)-H(5B)	109.7
P(1)-C(5)-H(5B)	109.7
H(5A)-C(5)-H(5B)	108.2
C(7)-C(6)-C(11)	110.7(9)
C(7)-C(6)-P(1)	109.3(7)
C(11)-C(6)-P(1)	115.6(7)

C(7)-C(6)-H(6)	106.9
C(11)-C(6)-H(6)	106.9
P(1)-C(6)-H(6)	106.9
C(6)-C(7)-C(8)	111.8(9)
C(6)-C(7)-H(7A)	109.3
C(8)-C(7)-H(7A)	109.3
C(6)-C(7)-H(7B)	109.3
C(8)-C(7)-H(7B)	109.3
H(7A)-C(7)-H(7B)	107.9
C(9)-C(8)-C(7)	110.7(9)
C(9)-C(8)-H(8A)	109.5
C(7)-C(8)-H(8A)	109.5
C(9)-C(8)-H(8B)	109.5
C(7)-C(8)-H(8B)	109.5
H(8A)-C(8)-H(8B)	108.1
C(8)-C(9)-C(10)	108.0(8)
C(8)-C(9)-H(9A)	110.1
C(10)-C(9)-H(9A)	110.1
C(8)-C(9)-H(9B)	110.1
C(10)-C(9)-H(9B)	110.1
H(9A)-C(9)-H(9B)	108.4
C(11)-C(10)-C(9)	110.6(9)
C(11)-C(10)-H(10A)	109.5
C(9)-C(10)-H(10A)	109.5
C(11)-C(10)-H(10B)	109.5
C(9)-C(10)-H(10B)	109.5
H(10A)-C(10)-H(10B)	108.1
C(6)-C(11)-C(10)	110.0(9)
C(6)-C(11)-H(11A)	109.7
C(10)-C(11)-H(11A)	109.7
C(6)-C(11)-H(11B)	109.7
C(10)-C(11)-H(11B)	109.7
H(11A)-C(11)-H(11B)	108.2
C(13)-C(12)-C(17)	109.8(9)
C(13)-C(12)-P(1)	119.7(7)
C(17)-C(12)-P(1)	110.0(7)

C(13)-C(12)-H(12)	105.4
C(17)-C(12)-H(12)	105.4
P(1)-C(12)-H(12)	105.4
C(12)-C(13)-C(14)	108.1(9)
C(12)-C(13)-H(13A)	110.1
C(14)-C(13)-H(13A)	110.1
C(12)-C(13)-H(13B)	110.1
C(14)-C(13)-H(13B)	110.1
H(13A)-C(13)-H(13B)	108.4
C(15)-C(14)-C(13)	112.9(10)
C(15)-C(14)-H(14A)	109.0
C(13)-C(14)-H(14A)	109.0
C(15)-C(14)-H(14B)	109.0
C(13)-C(14)-H(14B)	109.0
H(14A)-C(14)-H(14B)	107.8
C(14)-C(15)-C(16)	111.1(10)
C(14)-C(15)-H(15A)	109.4
C(16)-C(15)-H(15A)	109.4
C(14)-C(15)-H(15B)	109.4
C(16)-C(15)-H(15B)	109.4
H(15A)-C(15)-H(15B)	108.0
C(15)-C(16)-C(17)	110.6(8)
C(15)-C(16)-H(16A)	109.5
C(17)-C(16)-H(16A)	109.5
C(15)-C(16)-H(16B)	109.5
C(17)-C(16)-H(16B)	109.5
H(16A)-C(16)-H(16B)	108.1
C(16)-C(17)-C(12)	108.9(8)
C(16)-C(17)-H(17A)	109.9
C(12)-C(17)-H(17A)	109.9
C(16)-C(17)-H(17B)	109.9
C(12)-C(17)-H(17B)	109.9
H(17A)-C(17)-H(17B)	108.3
C(4)-C(18)-P(2)	110.4(7)
C(4)-C(18)-H(18A)	109.6
P(2)-C(18)-H(18A)	109.6

C(4)-C(18)-H(18B)	109.6
P(2)-C(18)-H(18B)	109.6
H(18A)-C(18)-H(18B)	108.1
C(20)-C(19)-C(24)	111.4(9)
C(20)-C(19)-P(2)	110.0(7)
C(24)-C(19)-P(2)	116.2(7)
C(20)-C(19)-H(19)	106.2
C(24)-C(19)-H(19)	106.2
P(2)-C(19)-H(19)	106.2
C(21)-C(20)-C(19)	111.1(9)
C(21)-C(20)-H(20A)	109.4
C(19)-C(20)-H(20A)	109.4
C(21)-C(20)-H(20B)	109.4
C(19)-C(20)-H(20B)	109.4
H(20A)-C(20)-H(20B)	108.0
C(20)-C(21)-C(22)	107.8(10)
C(20)-C(21)-H(21A)	110.1
C(22)-C(21)-H(21A)	110.1
C(20)-C(21)-H(21B)	110.1
C(22)-C(21)-H(21B)	110.1
H(21A)-C(21)-H(21B)	108.5
C(23)-C(22)-C(21)	111.1(9)
C(23)-C(22)-H(22A)	109.4
C(21)-C(22)-H(22A)	109.4
C(23)-C(22)-H(22B)	109.4
C(21)-C(22)-H(22B)	109.4
H(22A)-C(22)-H(22B)	108.0
C(22)-C(23)-C(24)	111.6(9)
C(22)-C(23)-H(23A)	109.3
C(24)-C(23)-H(23A)	109.3
C(22)-C(23)-H(23B)	109.3
C(24)-C(23)-H(23B)	109.3
H(23A)-C(23)-H(23B)	108.0
C(23)-C(24)-C(19)	108.2(9)
C(23)-C(24)-H(24A)	110.1
C(19)-C(24)-H(24A)	110.1

C(23)-C(24)-H(24B)	110.1
C(19)-C(24)-H(24B)	110.1
H(24A)-C(24)-H(24B)	108.4
C(26)-C(25)-C(30)	107.8(9)
C(26)-C(25)-P(2)	109.3(7)
C(30)-C(25)-P(2)	107.1(7)
C(26)-C(25)-H(25)	110.8
C(30)-C(25)-H(25)	110.8
P(2)-C(25)-H(25)	110.8
C(27)-C(26)-C(25)	113.2(9)
C(27)-C(26)-H(26A)	108.9
C(25)-C(26)-H(26A)	108.9
C(27)-C(26)-H(26B)	108.9
C(25)-C(26)-H(26B)	108.9
H(26A)-C(26)-H(26B)	107.8
C(28)-C(27)-C(26)	109.6(11)
C(28)-C(27)-H(27A)	109.8
C(26)-C(27)-H(27A)	109.8
C(28)-C(27)-H(27B)	109.8
C(26)-C(27)-H(27B)	109.8
H(27A)-C(27)-H(27B)	108.2
C(27)-C(28)-C(29)	112.2(11)
C(27)-C(28)-H(28A)	109.2
C(29)-C(28)-H(28A)	109.2
C(27)-C(28)-H(28B)	109.2
C(29)-C(28)-H(28B)	109.2
H(28A)-C(28)-H(28B)	107.9
C(30)-C(29)-C(28)	111.3(11)
C(30)-C(29)-H(29A)	109.4
C(28)-C(29)-H(29A)	109.4
C(30)-C(29)-H(29B)	109.4
C(28)-C(29)-H(29B)	109.4
H(29A)-C(29)-H(29B)	108.0
C(29)-C(30)-C(25)	109.5(9)
C(29)-C(30)-H(30A)	109.8
C(25)-C(30)-H(30A)	109.8

C(29)-C(30)-H(30B)	109.8
C(25)-C(30)-H(30B)	109.8
H(30A)-C(30)-H(30B)	108.2
Si(1)-C(31)-Y(1)	129.1(5)
Si(1)-C(31)-H(31A)	105.0
Y(1)-C(31)-H(31A)	105.0
Si(1)-C(31)-H(31B)	105.0
Y(1)-C(31)-H(31B)	105.0
H(31A)-C(31)-H(31B)	105.9
Si(1)-C(32)-H(32A)	109.5
Si(1)-C(32)-H(32B)	109.5
H(32A)-C(32)-H(32B)	109.5
Si(1)-C(32)-H(32C)	109.5
H(32A)-C(32)-H(32C)	109.5
H(32B)-C(32)-H(32C)	109.5
Si(1)-C(33)-H(33A)	109.5
Si(1)-C(33)-H(33B)	109.5
H(33A)-C(33)-H(33B)	109.5
Si(1)-C(33)-H(33C)	109.5
H(33A)-C(33)-H(33C)	109.5
H(33B)-C(33)-H(33C)	109.5
Si(1)-C(34)-H(34A)	109.5
Si(1)-C(34)-H(34B)	109.5
H(34A)-C(34)-H(34B)	109.5
Si(1)-C(34)-H(34C)	109.5
H(34A)-C(34)-H(34C)	109.5
H(34B)-C(34)-H(34C)	109.5
Si(2)-C(35)-Y(1)	129.7(5)
Si(2)-C(35)-H(35A)	104.8
Y(1)-C(35)-H(35A)	104.8
Si(2)-C(35)-H(35B)	104.8
Y(1)-C(35)-H(35B)	104.8
H(35A)-C(35)-H(35B)	105.8
Si(2)-C(36)-H(36A)	109.5
Si(2)-C(36)-H(36B)	109.5
H(36A)-C(36)-H(36B)	109.5

Si(2)-C(36)-H(36C)	109.5
H(36A)-C(36)-H(36C)	109.5
H(36B)-C(36)-H(36C)	109.5
Si(2)-C(37)-H(37A)	109.5
Si(2)-C(37)-H(37B)	109.5
H(37A)-C(37)-H(37B)	109.5
Si(2)-C(37)-H(37C)	109.5
H(37A)-C(37)-H(37C)	109.5
H(37B)-C(37)-H(37C)	109.5
Si(2)-C(38)-H(38A)	109.5
Si(2)-C(38)-H(38B)	109.5
H(38A)-C(38)-H(38B)	109.5
Si(2)-C(38)-H(38C)	109.5
H(38A)-C(38)-H(38C)	109.5
H(38B)-C(38)-H(38C)	109.5
C(40)-C(39)-N(2)	108.9(9)
C(40)-C(39)-C(43)	127.8(10)
N(2)-C(39)-C(43)	122.9(9)
C(40)-C(39)-Y(1)	77.2(6)
N(2)-C(39)-Y(1)	72.1(5)
C(43)-C(39)-Y(1)	122.8(7)
C(39)-C(40)-C(41)	108.0(10)
C(39)-C(40)-Y(1)	73.8(6)
C(41)-C(40)-Y(1)	74.2(6)
C(39)-C(40)-H(40)	126.0
C(41)-C(40)-H(40)	126.0
Y(1)-C(40)-H(40)	118.0
C(40)-C(41)-C(42)	109.0(10)
C(40)-C(41)-Y(1)	76.7(6)
C(42)-C(41)-Y(1)	72.8(6)
C(40)-C(41)-H(41)	125.5
C(42)-C(41)-H(41)	125.5
Y(1)-C(41)-H(41)	116.9
N(2)-C(42)-C(41)	107.2(9)
N(2)-C(42)-C(56)	124.9(9)
C(41)-C(42)-C(56)	127.9(9)

N(2)-C(42)-Y(1)	73.8(5)
C(41)-C(42)-Y(1)	77.1(6)
C(56)-C(42)-Y(1)	116.1(7)
C(39)-C(43)-P(3)	109.5(7)
C(39)-C(43)-H(43A)	109.8
P(3)-C(43)-H(43A)	109.8
C(39)-C(43)-H(43B)	109.8
P(3)-C(43)-H(43B)	109.8
H(43A)-C(43)-H(43B)	108.2
C(49)-C(44)-C(45)	113.1(9)
C(49)-C(44)-P(3)	120.7(8)
C(45)-C(44)-P(3)	109.2(6)
C(49)-C(44)-H(44)	104.0
C(45)-C(44)-H(44)	104.0
P(3)-C(44)-H(44)	104.0
C(46)-C(45)-C(44)	108.7(8)
C(46)-C(45)-H(45A)	110.0
C(44)-C(45)-H(45A)	110.0
C(46)-C(45)-H(45B)	110.0
C(44)-C(45)-H(45B)	110.0
H(45A)-C(45)-H(45B)	108.3
C(47)-C(46)-C(45)	115.4(10)
C(47)-C(46)-H(46A)	108.4
C(45)-C(46)-H(46A)	108.4
C(47)-C(46)-H(46B)	108.4
C(45)-C(46)-H(46B)	108.4
H(46A)-C(46)-H(46B)	107.5
C(46)-C(47)-C(48)	111.9(9)
C(46)-C(47)-H(47A)	109.2
C(48)-C(47)-H(47A)	109.2
C(46)-C(47)-H(47B)	109.2
C(48)-C(47)-H(47B)	109.2
H(47A)-C(47)-H(47B)	107.9
C(49)-C(48)-C(47)	111.5(9)
C(49)-C(48)-H(48A)	109.3
C(47)-C(48)-H(48A)	109.3

C(49)-C(48)-H(48B)	109.3
C(47)-C(48)-H(48B)	109.3
H(48A)-C(48)-H(48B)	108.0
C(44)-C(49)-C(48)	111.4(9)
C(44)-C(49)-H(49A)	109.4
C(48)-C(49)-H(49A)	109.4
C(44)-C(49)-H(49B)	109.4
C(48)-C(49)-H(49B)	109.4
H(49A)-C(49)-H(49B)	108.0
C(55)-C(50)-C(51)	111.4(9)
C(55)-C(50)-P(3)	109.8(7)
C(51)-C(50)-P(3)	115.6(8)
C(55)-C(50)-H(50)	106.5
C(51)-C(50)-H(50)	106.5
P(3)-C(50)-H(50)	106.5
C(50)-C(51)-C(52)	112.7(9)
C(50)-C(51)-H(51A)	109.0
C(52)-C(51)-H(51A)	109.0
C(50)-C(51)-H(51B)	109.0
C(52)-C(51)-H(51B)	109.0
H(51A)-C(51)-H(51B)	107.8
C(53)-C(52)-C(51)	112.9(9)
C(53)-C(52)-H(52A)	109.0
C(51)-C(52)-H(52A)	109.0
C(53)-C(52)-H(52B)	109.0
C(51)-C(52)-H(52B)	109.0
H(52A)-C(52)-H(52B)	107.8
C(52)-C(53)-C(54)	114.1(10)
C(52)-C(53)-H(53A)	108.7
C(54)-C(53)-H(53A)	108.7
C(52)-C(53)-H(53B)	108.7
C(54)-C(53)-H(53B)	108.7
H(53A)-C(53)-H(53B)	107.6
C(55)-C(54)-C(53)	111.2(10)
C(55)-C(54)-H(54A)	109.4
C(53)-C(54)-H(54A)	109.4

C(55)-C(54)-H(54B)	109.4
C(53)-C(54)-H(54B)	109.4
H(54A)-C(54)-H(54B)	108.0
C(50)-C(55)-C(54)	110.8(8)
C(50)-C(55)-H(55A)	109.5
C(54)-C(55)-H(55A)	109.5
C(50)-C(55)-H(55B)	109.5
C(54)-C(55)-H(55B)	109.5
H(55A)-C(55)-H(55B)	108.1
C(42)-C(56)-P(4)	112.3(7)
C(42)-C(56)-H(56A)	109.2
P(4)-C(56)-H(56A)	109.2
C(42)-C(56)-H(56B)	109.2
P(4)-C(56)-H(56B)	109.2
H(56A)-C(56)-H(56B)	107.9
C(62)-C(57)-C(58)	111.0(9)
C(62)-C(57)-P(4)	119.3(8)
C(58)-C(57)-P(4)	110.4(8)
C(62)-C(57)-H(57)	105.0
C(58)-C(57)-H(57)	105.0
P(4)-C(57)-H(57)	105.0
C(59)-C(58)-C(57)	109.2(9)
C(59)-C(58)-H(58A)	109.8
C(57)-C(58)-H(58A)	109.8
C(59)-C(58)-H(58B)	109.8
C(57)-C(58)-H(58B)	109.8
H(58A)-C(58)-H(58B)	108.3
C(60)-C(59)-C(58)	115.9(10)
C(60)-C(59)-H(59A)	108.3
C(58)-C(59)-H(59A)	108.3
C(60)-C(59)-H(59B)	108.3
C(58)-C(59)-H(59B)	108.3
H(59A)-C(59)-H(59B)	107.4
C(59)-C(60)-C(61)	112.6(10)
C(59)-C(60)-H(60A)	109.1
C(61)-C(60)-H(60A)	109.1

C(59)-C(60)-H(60B)	109.1
C(61)-C(60)-H(60B)	109.1
H(60A)-C(60)-H(60B)	107.8
C(60)-C(61)-C(62)	111.6(9)
C(60)-C(61)-H(61A)	109.3
C(62)-C(61)-H(61A)	109.3
C(60)-C(61)-H(61B)	109.3
C(62)-C(61)-H(61B)	109.3
H(61A)-C(61)-H(61B)	108.0
C(61)-C(62)-C(57)	112.9(9)
C(61)-C(62)-H(62A)	109.0
C(57)-C(62)-H(62A)	109.0
C(61)-C(62)-H(62B)	109.0
C(57)-C(62)-H(62B)	109.0
H(62A)-C(62)-H(62B)	107.8
C(68)-C(63)-C(64)	110.7(9)
C(68)-C(63)-P(4)	111.1(8)
C(64)-C(63)-P(4)	109.5(8)
C(68)-C(63)-H(63)	108.5
C(64)-C(63)-H(63)	108.5
P(4)-C(63)-H(63)	108.5
C(63)-C(64)-C(65)	113.7(10)
C(63)-C(64)-H(64A)	108.8
C(65)-C(64)-H(64A)	108.8
C(63)-C(64)-H(64B)	108.8
C(65)-C(64)-H(64B)	108.8
H(64A)-C(64)-H(64B)	107.7
C(66)-C(65)-C(64)	112.3(10)
C(66)-C(65)-H(65A)	109.2
C(64)-C(65)-H(65A)	109.2
C(66)-C(65)-H(65B)	109.2
C(64)-C(65)-H(65B)	109.2
H(65A)-C(65)-H(65B)	107.9
C(65)-C(66)-C(67)	110.0(10)
C(65)-C(66)-H(66A)	109.7
C(67)-C(66)-H(66A)	109.7

C(65)-C(66)-H(66B)	109.7
C(67)-C(66)-H(66B)	109.7
H(66A)-C(66)-H(66B)	108.2
C(68)-C(67)-C(66)	110.3(9)
C(68)-C(67)-H(67A)	109.6
C(66)-C(67)-H(67A)	109.6
C(68)-C(67)-H(67B)	109.6
C(66)-C(67)-H(67B)	109.6
H(67A)-C(67)-H(67B)	108.1
C(63)-C(68)-C(67)	112.7(10)
C(63)-C(68)-H(68A)	109.1
C(67)-C(68)-H(68A)	109.1
C(63)-C(68)-H(68B)	109.1
C(67)-C(68)-H(68B)	109.1
H(68A)-C(68)-H(68B)	107.8
Si(3)-C(69)-Y(2)	133.1(5)
Si(3)-C(69)-H(69A)	104.0
Y(2)-C(69)-H(69A)	104.0
Si(3)-C(69)-H(69B)	104.0
Y(2)-C(69)-H(69B)	104.0
H(69A)-C(69)-H(69B)	105.4
Si(3)-C(70)-H(70A)	109.5
Si(3)-C(70)-H(70B)	109.5
H(70A)-C(70)-H(70B)	109.5
Si(3)-C(70)-H(70C)	109.5
H(70A)-C(70)-H(70C)	109.5
H(70B)-C(70)-H(70C)	109.5
Si(3)-C(71)-H(71A)	109.5
Si(3)-C(71)-H(71B)	109.5
H(71A)-C(71)-H(71B)	109.5
Si(3)-C(71)-H(71C)	109.5
H(71A)-C(71)-H(71C)	109.5
H(71B)-C(71)-H(71C)	109.5
Si(3)-C(72)-H(72A)	109.5
Si(3)-C(72)-H(72B)	109.5
H(72A)-C(72)-H(72B)	109.5

Si(3)-C(72)-H(72C)	109.5
H(72A)-C(72)-H(72C)	109.5
H(72B)-C(72)-H(72C)	109.5
Si(4)-C(73)-Y(2)	137.5(4)
Si(4)-C(73)-H(73A)	102.7
Y(2)-C(73)-H(73A)	102.7
Si(4)-C(73)-H(73B)	102.7
Y(2)-C(73)-H(73B)	102.7
H(73A)-C(73)-H(73B)	105.0
Si(4)-C(74)-H(74A)	109.5
Si(4)-C(74)-H(74B)	109.5
H(74A)-C(74)-H(74B)	109.5
Si(4)-C(74)-H(74C)	109.5
H(74A)-C(74)-H(74C)	109.5
H(74B)-C(74)-H(74C)	109.5
Si(4)-C(75)-H(75A)	109.5
Si(4)-C(75)-H(75B)	109.5
H(75A)-C(75)-H(75B)	109.5
Si(4)-C(75)-H(75C)	109.5
H(75A)-C(75)-H(75C)	109.5
H(75B)-C(75)-H(75C)	109.5
Si(4)-C(76)-H(76A)	109.5
Si(4)-C(76)-H(76B)	109.5
H(76A)-C(76)-H(76B)	109.5
Si(4)-C(76)-H(76C)	109.5
H(76A)-C(76)-H(76C)	109.5
H(76B)-C(76)-H(76C)	109.5
C(1)-N(1)-C(4)	104.5(8)
C(1)-N(1)-Y(2)	125.1(6)
C(4)-N(1)-Y(2)	130.3(6)
C(1)-N(1)-Y(1)	78.2(6)
C(4)-N(1)-Y(1)	77.4(5)
Y(2)-N(1)-Y(1)	107.4(3)
C(42)-N(2)-C(39)	106.9(8)
C(42)-N(2)-Y(2)	128.9(6)
C(39)-N(2)-Y(2)	123.7(6)

C(42)-N(2)-Y(1)	75.7(5)
C(39)-N(2)-Y(1)	77.4(5)
Y(2)-N(2)-Y(1)	106.5(3)
C(31)-Si(1)-C(32)	111.5(5)
C(31)-Si(1)-C(34)	112.7(5)
C(32)-Si(1)-C(34)	106.9(5)
C(31)-Si(1)-C(33)	109.0(5)
C(32)-Si(1)-C(33)	110.2(5)
C(34)-Si(1)-C(33)	106.3(5)
C(35)-Si(2)-C(37)	111.3(5)
C(35)-Si(2)-C(38)	113.5(5)
C(37)-Si(2)-C(38)	107.4(5)
C(35)-Si(2)-C(36)	112.2(5)
C(37)-Si(2)-C(36)	107.8(6)
C(38)-Si(2)-C(36)	104.2(5)
C(71)-Si(3)-C(70)	110.1(5)
C(71)-Si(3)-C(72)	102.4(4)
C(70)-Si(3)-C(72)	107.5(5)
C(71)-Si(3)-C(69)	108.7(4)
C(70)-Si(3)-C(69)	113.7(4)
C(72)-Si(3)-C(69)	113.9(4)
C(73)-Si(4)-C(76)	113.9(5)
C(73)-Si(4)-C(74)	112.9(5)
C(76)-Si(4)-C(74)	108.2(7)
C(73)-Si(4)-C(75)	111.5(5)
C(76)-Si(4)-C(75)	104.1(6)
C(74)-Si(4)-C(75)	105.6(7)
C(5)-P(1)-C(6)	104.2(4)
C(5)-P(1)-C(12)	102.3(4)
C(6)-P(1)-C(12)	110.1(5)
C(5)-P(1)-Y(2)	98.1(3)
C(6)-P(1)-Y(2)	130.5(3)
C(12)-P(1)-Y(2)	107.4(3)
C(19)-P(2)-C(25)	102.4(5)
C(19)-P(2)-C(18)	101.8(5)
C(25)-P(2)-C(18)	101.3(5)

C(44)-P(3)-C(43)	102.9(5)
C(44)-P(3)-C(50)	109.7(5)
C(43)-P(3)-C(50)	102.9(5)
C(44)-P(3)-Y(2)	108.9(4)
C(43)-P(3)-Y(2)	98.3(3)
C(50)-P(3)-Y(2)	130.0(3)
C(57)-P(4)-C(56)	101.9(5)
C(57)-P(4)-C(63)	103.7(5)
C(56)-P(4)-C(63)	102.1(5)
C(31)-Y(1)-C(35)	97.91(19)
C(31)-Y(1)-N(1)	126.2(3)
C(35)-Y(1)-N(1)	118.5(3)
C(31)-Y(1)-N(2)	118.1(3)
C(35)-Y(1)-N(2)	126.6(3)
N(1)-Y(1)-N(2)	71.20(13)
C(31)-Y(1)-C(4)	135.5(3)
C(35)-Y(1)-C(4)	88.5(3)
N(1)-Y(1)-C(4)	30.1(3)
N(2)-Y(1)-C(4)	90.9(3)
C(31)-Y(1)-C(42)	87.7(3)
C(35)-Y(1)-C(42)	136.3(4)
N(1)-Y(1)-C(42)	90.7(3)
N(2)-Y(1)-C(42)	30.5(2)
C(4)-Y(1)-C(42)	117.04(16)
C(31)-Y(1)-C(1)	97.0(3)
C(35)-Y(1)-C(1)	126.3(3)
N(1)-Y(1)-C(1)	29.8(3)
N(2)-Y(1)-C(1)	88.9(3)
C(4)-Y(1)-C(1)	47.6(3)
C(42)-Y(1)-C(1)	95.4(3)
C(31)-Y(1)-C(39)	127.4(3)
C(35)-Y(1)-C(39)	96.4(4)
N(1)-Y(1)-C(39)	88.5(3)
N(2)-Y(1)-C(39)	30.5(3)
C(4)-Y(1)-C(39)	95.1(3)
C(42)-Y(1)-C(39)	49.6(3)

C(1)-Y(1)-C(39)	113.87(17)
C(31)-Y(1)-C(41)	79.3(3)
C(35)-Y(1)-C(41)	108.5(3)
N(1)-Y(1)-C(41)	119.0(3)
N(2)-Y(1)-C(41)	49.6(3)
C(4)-Y(1)-C(41)	139.9(3)
C(42)-Y(1)-C(41)	30.1(3)
C(1)-Y(1)-C(41)	124.9(3)
C(39)-Y(1)-C(41)	48.2(3)
C(31)-Y(1)-C(40)	101.9(3)
C(35)-Y(1)-C(40)	87.4(3)
N(1)-Y(1)-C(40)	116.9(3)
N(2)-Y(1)-C(40)	49.5(3)
C(4)-Y(1)-C(40)	122.4(3)
C(42)-Y(1)-C(40)	49.2(3)
C(1)-Y(1)-C(40)	138.3(3)
C(39)-Y(1)-C(40)	28.9(3)
C(41)-Y(1)-C(40)	29.1(3)
C(31)-Y(1)-C(3)	109.9(3)
C(35)-Y(1)-C(3)	78.3(3)
N(1)-Y(1)-C(3)	49.6(3)
N(2)-Y(1)-C(3)	118.6(3)
C(4)-Y(1)-C(3)	28.7(3)
C(42)-Y(1)-C(3)	139.9(3)
C(1)-Y(1)-C(3)	48.2(3)
C(39)-Y(1)-C(3)	122.5(3)
C(41)-Y(1)-C(3)	168.15(18)
C(40)-Y(1)-C(3)	146.5(3)
C(31)-Y(1)-C(2)	88.4(3)
C(35)-Y(1)-C(2)	100.6(3)
N(1)-Y(1)-C(2)	49.2(3)
N(2)-Y(1)-C(2)	117.3(3)
C(4)-Y(1)-C(2)	47.3(3)
C(42)-Y(1)-C(2)	122.9(3)
C(1)-Y(1)-C(2)	29.1(3)
C(39)-Y(1)-C(2)	137.6(3)

C(41)-Y(1)-C(2)	149.6(3)
C(40)-Y(1)-C(2)	166.05(16)
C(3)-Y(1)-C(2)	29.3(3)
C(73)-Y(2)-C(69)	110.42(19)
C(73)-Y(2)-N(2)	148.2(3)
C(69)-Y(2)-N(2)	92.2(3)
C(73)-Y(2)-N(1)	95.0(3)
C(69)-Y(2)-N(1)	146.8(3)
N(2)-Y(2)-N(1)	74.90(13)
C(73)-Y(2)-P(3)	91.3(2)
C(69)-Y(2)-P(3)	93.9(2)
N(2)-Y(2)-P(3)	64.25(18)
N(1)-Y(2)-P(3)	106.9(2)
C(73)-Y(2)-P(1)	94.3(2)
C(69)-Y(2)-P(1)	91.7(2)
N(2)-Y(2)-P(1)	107.56(18)
N(1)-Y(2)-P(1)	64.65(19)
P(3)-Y(2)-P(1)	170.25(5)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for (PNP-Cy)Y(CH2SiMe3)2. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	9(6)	31(7)	16(6)	-5(5)	-1(4)	-3(5)
C(2)	17(5)	23(6)	32(6)	-6(5)	0(4)	-7(4)
C(3)	15(6)	19(6)	16(5)	-11(5)	3(4)	1(5)
C(4)	8(6)	21(6)	21(6)	-4(5)	2(5)	2(5)
C(5)	13(6)	16(6)	13(5)	-1(4)	-2(4)	-6(4)
C(6)	12(5)	21(5)	26(5)	0(4)	-4(4)	-1(4)
C(7)	21(6)	54(8)	25(6)	-11(6)	-7(5)	-1(5)
C(8)	38(7)	38(6)	38(7)	-1(5)	-17(5)	5(5)
C(9)	35(6)	18(5)	37(6)	-13(5)	-19(5)	7(4)
C(10)	24(5)	80(8)	22(5)	-21(5)	-4(4)	-18(5)
C(11)	27(7)	59(8)	47(7)	3(6)	-25(5)	-18(6)
C(12)	18(6)	27(6)	39(6)	-19(5)	4(4)	-1(5)
C(13)	17(6)	36(7)	59(8)	2(6)	4(5)	-14(5)
C(14)	33(7)	35(7)	45(7)	-13(6)	5(5)	-1(5)
C(15)	31(7)	47(7)	49(7)	-7(5)	13(5)	-6(5)
C(16)	23(6)	59(7)	69(8)	-39(6)	-8(5)	3(5)
C(17)	16(5)	20(5)	52(7)	-10(5)	3(5)	1(4)
C(18)	14(6)	21(6)	16(6)	2(5)	2(4)	-1(5)
C(19)	16(6)	27(7)	19(6)	2(5)	5(4)	-10(5)
C(20)	20(7)	30(7)	40(7)	-4(6)	-9(5)	8(5)
C(21)	27(7)	68(10)	34(7)	-7(7)	0(5)	16(6)
C(22)	58(9)	34(7)	27(7)	-1(5)	9(6)	16(6)
C(23)	45(8)	35(7)	21(6)	-4(5)	10(5)	9(6)
C(24)	38(7)	31(7)	22(6)	-4(5)	0(5)	-1(5)
C(25)	19(7)	25(6)	19(6)	-2(5)	0(5)	-4(5)
C(26)	24(7)	19(6)	45(7)	-3(6)	-14(5)	-5(5)
C(27)	43(9)	30(7)	43(8)	5(7)	-17(6)	-2(6)
C(28)	51(10)	38(9)	85(12)	0(8)	-31(8)	-8(7)
C(29)	49(9)	96(12)	19(7)	15(7)	-18(6)	-25(8)
C(30)	18(7)	46(8)	32(7)	-5(6)	3(5)	-15(6)
C(31)	15(5)	29(6)	19(5)	3(4)	-15(4)	1(4)

C(32)	45(8)	30(7)	21(6)	2(5)	-1(5)	-18(6)
C(33)	15(6)	45(8)	43(8)	-8(6)	-6(5)	-6(5)
C(34)	13(6)	29(6)	46(7)	-21(6)	3(5)	-4(5)
C(35)	35(7)	15(5)	24(6)	-7(5)	3(5)	4(5)
C(36)	29(8)	37(7)	53(8)	4(6)	-8(6)	10(6)
C(37)	46(9)	26(7)	44(8)	6(6)	-16(6)	-2(6)
C(38)	42(8)	43(8)	53(8)	-5(7)	-15(6)	10(6)
C(39)	10(6)	17(6)	26(6)	5(5)	0(5)	-2(4)
C(40)	13(4)	17(4)	14(4)	5(3)	3(3)	-3(3)
C(41)	7(6)	31(7)	32(6)	-10(5)	9(4)	1(5)
C(42)	9(6)	14(6)	22(6)	-2(5)	2(5)	4(4)
C(43)	7(6)	31(7)	34(7)	4(6)	-6(5)	-10(5)
C(44)	15(6)	36(6)	32(6)	-12(5)	6(4)	0(5)
C(45)	16(6)	29(6)	42(6)	9(5)	2(4)	-2(4)
C(46)	40(8)	34(6)	96(10)	8(6)	26(6)	2(5)
C(47)	20(6)	39(6)	56(7)	16(5)	9(5)	-12(5)
C(48)	13(6)	48(7)	41(7)	-12(6)	5(5)	-8(5)
C(49)	28(7)	41(7)	33(7)	1(5)	-6(5)	-14(5)
C(50)	19(4)	32(4)	28(4)	-3(3)	-15(3)	-9(3)
C(51)	33(8)	107(12)	43(7)	-37(8)	-18(6)	14(7)
C(52)	18(3)	23(3)	21(3)	-6(2)	-9(2)	-2(2)
C(53)	70(11)	104(11)	43(8)	-11(8)	-29(7)	-27(9)
C(54)	24(6)	90(10)	17(6)	-4(6)	5(5)	-18(6)
C(55)	16(6)	36(7)	32(7)	-5(5)	2(5)	-16(5)
C(56)	11(6)	23(7)	32(7)	-6(5)	-4(5)	7(5)
C(57)	34(7)	28(7)	21(6)	-15(5)	15(5)	-13(5)
C(58)	17(7)	46(8)	32(7)	-19(6)	9(5)	-3(6)
C(59)	35(7)	54(8)	24(6)	-16(6)	11(5)	-24(6)
C(60)	55(9)	48(8)	48(8)	-3(6)	4(6)	-41(7)
C(61)	37(8)	41(7)	37(7)	-13(6)	8(6)	-10(6)
C(62)	21(6)	23(6)	23(6)	-1(5)	9(4)	-9(4)
C(63)	17(6)	13(6)	39(7)	-11(5)	-4(5)	6(5)
C(64)	42(8)	33(7)	27(7)	-21(6)	-8(6)	-6(6)
C(65)	33(8)	33(7)	40(8)	-11(6)	-5(6)	5(6)
C(66)	30(7)	59(10)	39(7)	-33(7)	-18(6)	0(6)
C(67)	20(7)	53(8)	59(9)	-13(8)	-13(6)	-9(7)

C(68)	18(7)	43(7)	37(7)	-22(7)	1(5)	-14(6)
C(69)	17(6)	27(6)	22(6)	-3(4)	-3(4)	-1(4)
C(70)	45(7)	29(6)	68(8)	32(5)	9(6)	11(5)
C(71)	57(7)	28(5)	38(5)	0(4)	-19(5)	-11(5)
C(72)	60(7)	28(5)	10(5)	10(4)	-12(4)	-5(5)
C(73)	10(5)	13(5)	16(5)	-4(4)	-2(4)	1(4)
C(74)	99(10)	23(6)	213(14)	15(8)	-98(10)	1(6)
C(75)	103(12)	97(11)	47(8)	-33(7)	43(7)	-70(9)
C(76)	130(14)	48(8)	61(9)	-4(7)	11(8)	-37(9)
N(1)	13(5)	15(4)	26(5)	-3(4)	-1(4)	-3(4)
N(2)	3(4)	16(4)	19(4)	-2(4)	-1(3)	-3(3)
Si(1)	24(2)	23(2)	23(2)	-5(1)	-4(1)	-7(1)
Si(2)	25(2)	23(2)	28(2)	-3(1)	-5(1)	4(1)
Si(3)	21(2)	23(1)	22(1)	-2(1)	-1(1)	-4(1)
Si(4)	31(2)	21(1)	34(2)	-8(1)	-5(1)	0(1)
P(1)	11(2)	20(2)	28(2)	-3(1)	-4(1)	-2(1)
P(2)	14(2)	26(2)	19(2)	1(1)	-2(1)	-4(1)
P(3)	17(2)	25(2)	20(2)	0(1)	-2(1)	-6(1)
P(4)	14(2)	19(2)	29(2)	-8(1)	2(1)	0(1)
Y(1)	12(1)	15(1)	22(1)	-4(1)	-2(1)	-1(1)
Y(2)	12(1)	18(1)	19(1)	-2(1)	-2(1)	-3(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for (PNP-Cy)Y(CH2SiMe3)2.

	x	y	z	U(eq)
H(2)	5155	4811	7822	29
H(3)	5783	4755	8880	20
H(5A)	4867	6129	6821	17
H(5B)	5961	6118	6451	17
H(6)	4838	8446	5878	24
H(7A)	6082	7028	5407	39
H(7B)	6403	7917	5434	39
H(8A)	5502	8609	4616	46
H(8B)	6237	7850	4321	46
H(9A)	5030	6981	4584	34
H(9B)	4718	7836	4117	34
H(10A)	3793	8438	5099	47
H(10B)	3414	7577	5066	47
H(11A)	3604	7597	6166	50
H(11B)	4311	6830	5857	50
H(12)	4549	7590	7842	34
H(13A)	3695	6580	7636	47
H(13B)	3127	7319	7198	47
H(14A)	2240	7108	8318	47
H(14B)	3121	7277	8589	47
H(15A)	2013	8463	8591	55
H(15B)	2038	8491	7814	55
H(16A)	3583	8765	8350	58
H(16B)	2976	9479	7923	58
H(17A)	4462	8991	7232	37
H(17B)	3589	8802	6956	37
H(18A)	6639	6788	8854	22
H(18B)	7415	5962	8817	22
H(19)	4941	6429	10514	26
H(20A)	4772	7008	9158	37

H(20B)	4261	6245	9623	37
H(21A)	3360	7187	10363	56
H(21B)	3181	7526	9622	56
H(22A)	4343	8499	9440	55
H(22B)	3538	8685	10084	55
H(23A)	4530	7900	10791	46
H(23B)	5052	8650	10316	46
H(24A)	6127	7340	10355	38
H(24B)	5991	7678	9604	38
H(25)	7351	6313	10122	26
H(26A)	7665	4472	10168	34
H(26B)	8241	5113	9606	34
H(27A)	9188	4446	10383	46
H(27B)	8995	5446	10401	46
H(28A)	8743	4725	11477	68
H(28B)	7992	4222	11311	68
H(29A)	7157	5353	11903	65
H(29B)	7702	6027	11350	65
H(30A)	6164	6065	11140	39
H(30B)	6343	5065	11119	39
H(31A)	7331	4362	6389	25
H(31B)	7984	3659	6770	25
H(32A)	6639	2539	8029	48
H(32B)	5596	2510	7919	48
H(32C)	5847	3346	8114	48
H(33A)	5056	4285	6888	51
H(33B)	4973	3446	6613	51
H(33C)	5614	4127	6154	51
H(34A)	7089	2530	6039	43
H(34B)	6438	1964	6618	43
H(34C)	7496	2036	6674	43
H(35A)	7821	4338	8792	32
H(35B)	7410	3630	8553	32
H(36A)	9137	2549	7538	64
H(36B)	10170	2503	7693	64
H(36C)	9711	3347	7291	64

H(37A)	9896	4413	8446	60
H(37B)	10547	3524	8560	60
H(37C)	9763	3851	9169	60
H(38A)	8559	2471	9543	71
H(38B)	9467	1968	9118	71
H(38C)	8434	1977	8975	71
H(40)	9851	4812	7297	20
H(41)	9306	4740	6257	30
H(43A)	9787	6132	7938	29
H(43B)	8699	6109	8316	29
H(44)	9640	7645	6609	35
H(45A)	9274	9030	6879	39
H(45B)	10144	8871	7257	39
H(46A)	10300	8871	5856	80
H(46B)	10668	9552	6170	80
H(47A)	11867	8606	6458	51
H(47B)	11883	8619	5685	51
H(48A)	11236	7330	5913	42
H(48B)	12118	7182	6276	42
H(49A)	10741	6622	6994	41
H(49B)	11103	7301	7317	41
H(50)	9124	8445	8364	29
H(51A)	10571	7588	8332	71
H(51B)	10065	6795	8745	71
H(52A)	10649	7316	9534	23
H(52B)	10271	8276	9276	23
H(53A)	9317	7910	10253	81
H(53B)	9198	7034	10050	81
H(54A)	7794	7959	10004	53
H(54B)	8368	8673	9521	53
H(55A)	8195	7087	9157	33
H(55B)	7667	7986	8884	33
H(56A)	7808	6756	5733	28
H(56B)	7310	5912	5960	28
H(57)	9662	6416	4197	34
H(58A)	9648	6961	5428	39

H(58B)	10410	6242	5095	39
H(59A)	10983	7583	4850	44
H(59B)	10986	7204	4192	44
H(60A)	10469	8601	4021	59
H(60B)	9700	8539	4709	59
H(61A)	9635	7896	3543	47
H(61B)	8900	8630	3872	47
H(62A)	8268	7321	4111	29
H(62B)	8290	7675	4776	29
H(63)	7312	6274	4569	28
H(64A)	8638	5044	3903	38
H(64B)	8523	6044	3664	38
H(65A)	7069	6017	3401	43
H(65B)	7840	5338	3030	43
H(66A)	7278	4240	3822	46
H(66B)	6408	4784	3522	46
H(67A)	5906	5497	4474	50
H(67B)	5984	4498	4727	50
H(68A)	6720	5190	5359	37
H(68B)	7464	4492	4993	37
H(69A)	8358	8516	6194	27
H(69B)	7754	8103	5832	27
H(70A)	5953	10584	5980	86
H(70B)	5979	9868	6617	86
H(70C)	5608	9693	5995	86
H(71A)	8157	10265	6222	59
H(71B)	7852	10851	5581	59
H(71C)	8716	10102	5489	59
H(72A)	7190	10202	4636	50
H(72B)	6868	9278	4768	50
H(72C)	7973	9382	4617	50
H(73A)	5596	8555	7976	16
H(73B)	6312	8153	8441	16
H(74A)	5426	10452	7448	159
H(74B)	5414	10947	8050	159
H(74C)	4737	10231	8157	159

H(75A)	7987	9649	7951	123
H(75B)	7431	10581	7816	123
H(75C)	7576	9944	7285	123
H(76A)	5606	9677	9343	123
H(76B)	6576	10086	9145	123
H(76C)	6602	9079	9295	123

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