Hydrogen Oxidation Catalysis by a Nickel Diphosphine Complex with Pendant *t*-Butyl Amines

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Supplementary Material (ESI) for Chemical Communications

Experimental

General Experimental Procedures. ^{1}H and ^{31}P NMR spectra were recorded on a Varian Inova spectrometer (500 MHz for ^{1}H) at 20 °C unless otherwise noted. All ^{1}H chemical shifts have been internally calibrated to the monoprotio impurity of the deuterated solvent. The ^{31}P NMR spectra were proton decoupled and referenced to external phosphoric acid.

All electrochemical experiments were carried out under an atmosphere of nitrogen, or hydrogen when indicated, in 0.2 M Et_4NBF_4 acetonitrile solutions or 0.2 M Bu_4NPF_6 benzonitrile solutions. Cyclic voltammetry experiments were performed with a CH Instruments model 660C potentiostat. Ferrocene was used as an internal standard, and all potentials are referenced to the ferrocenium/ferrocene couple.

Synthesis and Materials. All reactions and manipulations were performed under an N_2 atmosphere using standard Schlenk techniques or a glovebox unless otherwise indicated. Solvents were dried using an activated alumnia column. $[Ni(CH_3CN)_6](BF_4)_2$ was prepared as described using literature methods.[1]

Bishydroxymethylcyclohexylphosphine·$(H_2O)_{0.2}$. Cyclohexyl phosphine (10.03 g, 86.36 mmol) was added to 20 mL of absolute ethanol with paraformaldehyde (5.31 g, 177 mmol). After heating the solution to 70 °C for 2 hours, the solvent was removed under reduced pressure. The residue was dissolved in 20 mL of THF. Hexane (80 mL) was added and the mixture was cooled in a −35 °C freezer overnight, precipitating the product as colorless crystals. The product was isolated by filtration and washed with 2 x 20 mL of hexane (14.9 g, 98% yield). ^{1}H NMR (d^6-acetone): δ 4.13 (m, 4H), 2.23 (m, 2H), 2.06 (s, 1H), 1.87-1.70 (m, 4H), 1.33-1.22 (m, 4H). ^{31}P NMR (CD_3CN): δ −11.83. ^{13}C NMR (CD_3CN): δ 58.85 (d, J = 18.7 Hz), 44.99 (d, J = 0.8 Hz), 29.00 (d, J = 14.0 Hz), 26.97 (d, J = 6.7 Hz), 26.34 (dd, J = 22.1, 5.9 Hz). Anal. Calcd. for $C_8H_{17.4}O_{2.2}P$: C, 53.44; H, 9.75; N, 0.00. Found: C, 53.23; H, 9.76; N, 0.00.

$P^{Cy}{}_2N^{t\text{-}Bu}{}_2$. Bishydroxymethylcyclohexylphosphine (4.00 g, 0.023 mol) was dissolved in 100 mL of degassed ethanol and heated to 70 °C. *t*-Butylamine (2.40 mL, 0.023 mol) was added dropwise over 30 minutes, and the reaction was stirred for 12 hours at 70 °C. The solvent was

removed under reduced pressure to give an oil. This was redissolved in 15 mL of diethyl ether, followed by addition of 30 mL of acetonitrile and cooled in a −35 °C freezer overnight. The product precipitated as a colorless microcrystalline solid, and was isolated by filtration and washed with 2 × 6 mL acetonitrile (3.44 g, 70% yield). ^{1}H NMR (CD_2Cl_2) δ 3.42 (d, J = 9.5 Hz, 2H), 3.37-3.15 (m, 4H), 3.03 (d, J = 13 Hz, 2H), 1.99 (m, 12H), 1.49 (bs, 10H), 1.40 (s, 9H), 1.36 (s, 9H). ^{31}P NMR (CD_2Cl_2): δ −21.37, −26.06 (ratio 3:4). ^{13}C NMR (CD_2Cl_2): δ 56.30 (d, *J* = 5.6 Hz), 55.96 (s), 48.95 (s), 47.65 (dd, *J* = 12.0, 7.5 Hz), 45.09 – 44.91 (m), 37.02 (s), 35.46 (d, *J* = 13.0 Hz), 29.90 (dd, *J* = 13.5, 9.6 Hz), 27.33 (s), 27.26 – 26.92 (m), 26.68 (d, *J* = 19.1 Hz). Anal. Calcd for $C_{24}H_{48}N_2P_2$: C, 67.57; H, 11.34; N, 6.57. Found: C, 67.76; H, 11.55; N, 6.53.

[Ni($P^{Cy}_2N^{t\text{-}Bu}_2$)]$(BF_4)_2$·$(CH_3CN)_{1.4}(Et_2O)_{0.6}$ (1). $P^{Cy}_2N^{t\text{-}Bu}_2$ (1.00 g, 2.30 mmol) and $[Ni(CH_3CN)_6](BF_4)_2$ (0.576 g, 1.15 mmol) was added to 6 mL of acetonitrile. After stirring for one hour at room temperature, 10 mL of diethyl ether was added and the solution was left to stand overnight. The product precipitated as dark red crystals, which were isolated by filtration, and washed with a 6 mL of a 1:3 acetonitrile: diethyl ether solution (0.80 g, 61% yield). ^{1}H NMR (CD_3CN) δ 3.61 (d, *J* = 13.6 Hz, 4H), 3.21 (d, *J* = 13.7 Hz, 4H), 3.14 (d, *J* = 13.3 Hz, 4H), 3.06 (d, *J* = 13.7 Hz, 4H), 1.99 (m, 12H), 1.84 (s, 4H), 1.76 (d, *J* = 13.2 Hz, 4H), 1.54 (s, 8H), 1.44 (d, *J* = 8.5 Hz, 12H), 1.19 (s, 36H). ^{31}P NMR (CD_3CN): δ 9.38. Anal. Calcd. for $C_{53.1}H_{106}B_2F_8N_{5.42}NiP_4O_{0.6}$: C, 53.79; H, 9.00; N, 6.40. Found: C, 53.20; H, 9.08; N, 6.05.

[Ni($P^{Cy}_2N^{t\text{-}Bu}_2$)] (2). $[Ni(P^{Cy}_2N^{t\text{-}Bu}_2)](BF_4)_2$ (0.488 g, 0.432 mmol) was dissolved in 6 mL of acetonitrile. After the solution was purged with hydrogen for 10 minutes, 1,8-diazabicyclo[5.4.0]undec-7-ene (DBU, 0.16 mL, 1.1 mmol) was added. The resulting very pale yellow precipitate was collected by filtration and washed with 2 × 6 mL of acetonitrile to give 0.350 g product (88% yield). ^{1}H NMR (C_6D_6): δ 3.67 (s, 4H), 3.14 (s, 4H), 2.93 (d, *J* = 6.4 Hz, 8H), 2.85 (s, 4H), 2.65 (s, 4H), 2.09 (s, 8H), 1.98 (s, 8H), 1.74 (d, *J* = 4.9 Hz, 12H), 1.59 (s, 4H), 1.53 – 1.27 (m, 36H). ^{31}P NMR (C_6D_6): δ 7.41. Anal. Calcd. for $C_{48}H_{96}N_4NiP_4$: C, 63.22; H, 10.61; N, 6.14. Found: C, 63.15; H, 10.71; N, 5.96.

Electrocatalytic Oxidation of Hydrogen with 2. A benzonitrile solution (3.0 mL) containing 0.2 M Bu_4NPF_6 and **2** (0.57 mM) was added to an electrochemical cell under nitrogen. After the solution was purged with hydrogen for 10 min, successive cyclic voltammograms were recorded upon addition of increasing amounts of triethylamine. The initial amount of triethylamine added was 1.0 µL (4 equiv) and the final amount was 30 µL (124 equiv). The catalytic current was taken at −0.65 V. A plot of the catalytic current/peak current (i_c/i_p) versus the concentration of triethylamine showed no dependence on base after addition of 20 µL (83 equiv) of treithylamine. The plot is shown below.

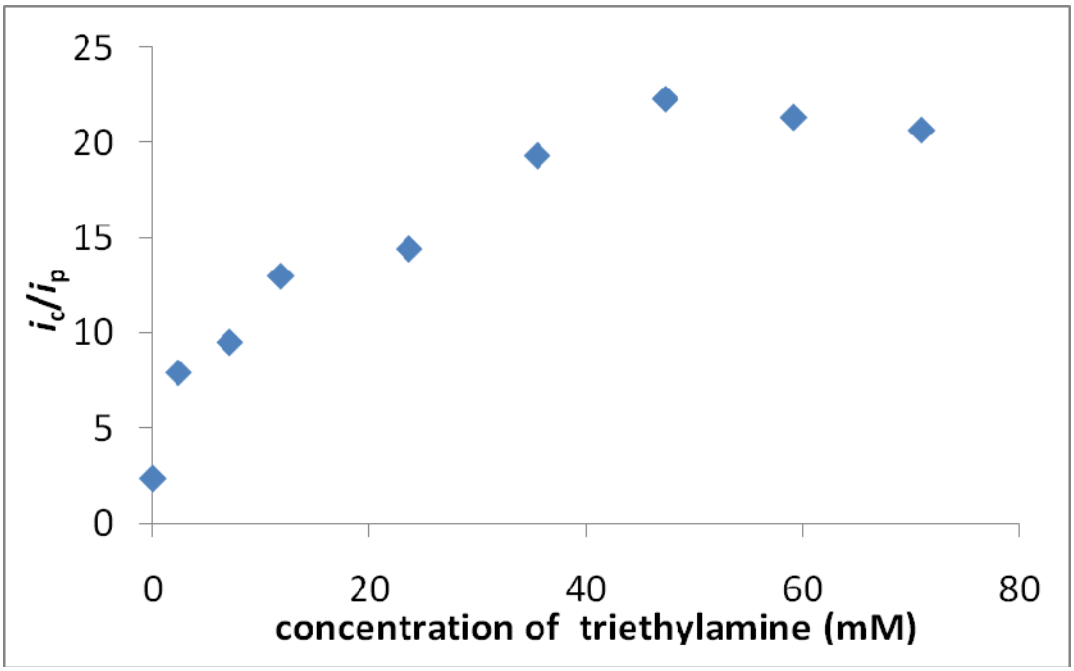

Table S1. Crystal data and structure refinement for [Ni($P^{Cy}_2N^{t\text{-}Bu}_2$)]$(BF_4)_2$ (**1**).

Identification code	pnl086	
Empirical formula	C26.57 H53 B F4 N2.71 Ni0.50 O0.29 P2	
Formula weight	593.25	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	C2/c	
Unit cell dimensions	a = 20.9513(10) Å	□= 90°.
	b = 13.9953(6) Å	□= 101.782(2)°.
	c = 22.0669(10) Å	□ = 90°.
Volume	6334.1(5) $Å^3$	
Z	8	
Density (calculated)	1.244 Mg/m^3	
Absorption coefficient	0.470 mm^{-1}	
F(000)	2550	
Crystal size	0.16 x 0.16 x 0.08 mm^3	
Theta range for data collection	1.89 to 33.27°.	
Index ranges	-31<=h<=32, -13<=k<=21, -32<=l<=33	
Reflections collected	40666	
Independent reflections	12025 [R(int) = 0.0428]	
Completeness to theta = 25.00°	100.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9634 and 0.9286	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	12025 / 2 / 359	
Goodness-of-fit on F^2	1.018	
Final R indices [I>2sigma(I)]	R1 = 0.0472, wR2 = 0.1150	
R indices (all data)	R1 = 0.0791, wR2 = 0.1296	
Largest diff. peak and hole	0.990 and -0.533 $e.Å^{-3}$	

Table S2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for [Ni($P^{Cy}_2N^{t\text{-}Bu}_2$)]($BF_4$)$_2$ (**1**). U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Ni(1)	10000	1122(1)	7500	12(1)
B(1)	9401(1)	2560(2)	4517(1)	24(1)
F(1)	9422(1)	1655(1)	4780(1)	41(1)
F(2)	9304(1)	2468(1)	3880(1)	35(1)
F(3)	9990(1)	3016(1)	4744(1)	41(1)
F(4)	8901(1)	3073(1)	4683(1)	57(1)
N(1)	9217(1)	766(1)	8614(1)	16(1)
N(2)	8703(1)	1472(1)	6422(1)	17(1)
P(1)	9950(1)	2130(1)	6710(1)	14(1)
P(2)	10317(1)	110(1)	8282(1)	13(1)
C(1)	10922(1)	3485(1)	7170(1)	23(1)
C(2)	11088(1)	4542(1)	7298(1)	32(1)
C(3)	10984(1)	5111(1)	6698(1)	35(1)
C(4)	10299(1)	4982(1)	6315(1)	34(1)
C(5)	10139(1)	3925(1)	6181(1)	25(1)
C(6)	10221(1)	3383(1)	6799(1)	18(1)
C(7)	10451(1)	1660(1)	6172(1)	18(1)
C(8)	8604(1)	612(1)	8856(1)	22(1)
C(9)	8290(1)	-330(1)	8599(1)	31(1)
C(10)	8732(1)	599(2)	9564(1)	31(1)
C(11)	8122(1)	1409(2)	8602(1)	32(1)
C(12)	9691(1)	-10(1)	8756(1)	16(1)
C(13)	11060(1)	-1224(1)	7776(1)	19(1)
C(14)	11180(1)	-2278(1)	7644(1)	25(1)
C(15)	11389(1)	-2830(1)	8246(1)	29(1)
C(16)	10896(1)	-2720(1)	8664(1)	27(1)
C(17)	10781(1)	-1671(1)	8800(1)	20(1)
C(18)	10553(1)	-1139(1)	8183(1)	15(1)
C(19)	11061(1)	582(1)	8800(1)	18(1)
C(20)	7978(1)	1603(1)	6179(1)	24(1)

C(21)	7623(1)	871(2)	6507(1)	36(1)
C(22)	7785(1)	1465(2)	5475(1)	36(1)
C(23)	7773(1)	2589(2)	6352(1)	44(1)
C(24)	9106(1)	2256(1)	6271(1)	18(1)
N(3)	11633(2)	-5122(2)	9025(2)	54(1)
C(25)	11178(2)	-4721(3)	9999(2)	43(1)
C(26)	11433(2)	-4950(2)	9471(2)	35(1)
C(27)	12841(5)	-1935(7)	9751(5)	50(1)
C(28)	12428(6)	-2727(6)	9984(6)	50(1)
C(29)	11596(5)	-4525(7)	9910(5)	50(1)
C(30)	11603(6)	-5260(9)	9380(6)	50(1)
O(1)	12084(3)	-3776(4)	9778(3)	50(1)

Table S3. Bond lengths [Å] and angles [°] for $[Ni(P^{Cy}{}_2N^{t\text{-}Bu}{}_2)](BF_4)_2$ (**1**).

Ni(1)-P(2)	2.2272(4)
Ni(1)-P(2)#1	2.2272(4)
Ni(1)-P(1)	2.2281(4)
Ni(1)-P(1)#1	2.2282(4)
B(1)-F(4)	1.381(2)
B(1)-F(2)	1.385(2)
B(1)-F(1)	1.390(2)
B(1)-F(3)	1.389(2)
N(1)-C(12)	1.4608(19)
N(1)-C(7)#1	1.462(2)
N(1)-C(8)	1.505(2)
N(2)-C(19)#1	1.460(2)
N(2)-C(24)	1.465(2)
N(2)-C(20)	1.515(2)
P(1)-C(6)	1.8413(16)
P(1)-C(24)	1.8439(16)
P(1)-C(7)	1.8591(16)
P(2)-C(18)	1.8413(15)
P(2)-C(12)	1.8428(16)
P(2)-C(19)	1.8568(16)
C(1)-C(2)	1.533(3)
C(1)-C(6)	1.534(2)
C(2)-C(3)	1.523(3)
C(3)-C(4)	1.520(3)
C(4)-C(5)	1.533(3)
C(5)-C(6)	1.539(2)
C(7)-N(1)#1	1.462(2)
C(8)-C(10)	1.531(3)
C(8)-C(11)	1.531(2)
C(8)-C(9)	1.529(3)
C(13)-C(18)	1.529(2)
C(13)-C(14)	1.533(2)
C(14)-C(15)	1.522(3)
C(15)-C(16)	1.527(3)

C(16)-C(17)	1.527(2)
C(17)-C(18)	1.540(2)
C(19)-N(2)#1	1.460(2)
C(20)-C(23)	1.517(3)
C(20)-C(21)	1.532(3)
C(20)-C(22)	1.536(3)
N(3)-C(26)	1.170(5)
C(25)-C(26)	1.415(5)
C(27)-C(28)	1.557(14)
C(28)-O(1)	1.657(9)
C(29)-O(1)	1.534(11)
C(29)-C(30)	1.560(13)

P(2)-Ni(1)-P(2)#1	100.99(2)
P(2)-Ni(1)-P(1)	165.477(14)
P(2)#1-Ni(1)-P(1)	80.643(15)
P(2)-Ni(1)-P(1)#1	80.642(15)
P(2)#1-Ni(1)-P(1)#1	165.475(14)
P(1)-Ni(1)-P(1)#1	101.45(2)
F(4)-B(1)-F(2)	110.83(17)
F(4)-B(1)-F(1)	108.99(17)
F(2)-B(1)-F(1)	108.95(16)
F(4)-B(1)-F(3)	109.36(17)
F(2)-B(1)-F(3)	110.18(16)
F(1)-B(1)-F(3)	108.49(16)
C(12)-N(1)-C(7)#1	108.06(12)
C(12)-N(1)-C(8)	114.21(12)
C(7)#1-N(1)-C(8)	113.03(13)
C(19)#1-N(2)-C(24)	108.15(12)
C(19)#1-N(2)-C(20)	111.64(13)
C(24)-N(2)-C(20)	114.31(12)
C(6)-P(1)-C(24)	101.95(7)
C(6)-P(1)-C(7)	101.74(7)
C(24)-P(1)-C(7)	107.69(8)
C(6)-P(1)-Ni(1)	123.73(6)
C(24)-P(1)-Ni(1)	110.97(5)

C(7)-P(1)-Ni(1)	109.51(5)
C(18)-P(2)-C(12)	102.77(7)
C(18)-P(2)-C(19)	101.46(7)
C(12)-P(2)-C(19)	106.84(8)
C(18)-P(2)-Ni(1)	123.78(5)
C(12)-P(2)-Ni(1)	111.30(5)
C(19)-P(2)-Ni(1)	109.25(5)
C(2)-C(1)-C(6)	110.14(15)
C(3)-C(2)-C(1)	110.96(16)
C(4)-C(3)-C(2)	111.86(16)
C(3)-C(4)-C(5)	111.53(16)
C(4)-C(5)-C(6)	108.97(16)
C(1)-C(6)-C(5)	110.45(14)
C(1)-C(6)-P(1)	112.68(11)
C(5)-C(6)-P(1)	113.47(12)
N(1)#1-C(7)-P(1)	112.85(11)
N(1)-C(8)-C(10)	112.26(14)
N(1)-C(8)-C(11)	108.30(14)
C(10)-C(8)-C(11)	110.29(16)
N(1)-C(8)-C(9)	108.99(14)
C(10)-C(8)-C(9)	109.86(16)
C(11)-C(8)-C(9)	106.98(16)
N(1)-C(12)-P(2)	109.99(11)
C(18)-C(13)-C(14)	110.33(14)
C(15)-C(14)-C(13)	110.63(15)
C(14)-C(15)-C(16)	111.51(15)
C(15)-C(16)-C(17)	111.67(15)
C(16)-C(17)-C(18)	109.00(14)
C(13)-C(18)-C(17)	110.72(13)
C(13)-C(18)-P(2)	112.36(11)
C(17)-C(18)-P(2)	113.35(11)
N(2)#1-C(19)-P(2)	113.41(11)
N(2)-C(20)-C(23)	109.65(15)
N(2)-C(20)-C(21)	107.45(14)
C(23)-C(20)-C(21)	107.44(17)
N(2)-C(20)-C(22)	112.36(15)

C(23)-C(20)-C(22)	109.86(18)
C(21)-C(20)-C(22)	109.94(17)
N(2)-C(24)-P(1)	110.20(11)
N(3)-C(26)-C(25)	178.2(4)
C(27)-C(28)-O(1)	141.2(9)
O(1)-C(29)-C(30)	101.5(8)
C(29)-O(1)-C(28)	145.3(7)

Symmetry transformations used to generate equivalent atoms:
#1 -x+2,y,-z+3/2

Table S4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for $[Ni(P^{Cy}_2N^{t\text{-}Bu}_2)](BF_4)_2$ (**1**). 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}
Ni(1)	13(1)	8(1)	17(1)	0	4(1)	0
B(1)	26(1)	20(1)	25(1)	-1(1)	5(1)	0(1)
F(1)	66(1)	23(1)	30(1)	2(1)	2(1)	-8(1)
F(2)	43(1)	36(1)	23(1)	2(1)	2(1)	0(1)
F(3)	42(1)	45(1)	36(1)	-7(1)	7(1)	-20(1)
F(4)	47(1)	64(1)	62(1)	-11(1)	17(1)	26(1)
N(1)	12(1)	13(1)	23(1)	2(1)	6(1)	1(1)
N(2)	12(1)	11(1)	28(1)	3(1)	6(1)	1(1)
P(1)	14(1)	10(1)	20(1)	1(1)	6(1)	0(1)
P(2)	12(1)	10(1)	17(1)	0(1)	3(1)	0(1)
C(1)	19(1)	20(1)	31(1)	-3(1)	8(1)	-5(1)
C(2)	29(1)	22(1)	47(1)	-11(1)	16(1)	-12(1)
C(3)	36(1)	16(1)	59(1)	-4(1)	23(1)	-11(1)
C(4)	38(1)	14(1)	55(1)	9(1)	20(1)	-3(1)
C(5)	26(1)	15(1)	35(1)	7(1)	10(1)	0(1)
C(6)	19(1)	10(1)	28(1)	1(1)	10(1)	-2(1)
C(7)	18(1)	14(1)	22(1)	0(1)	9(1)	-1(1)
C(8)	16(1)	22(1)	30(1)	7(1)	10(1)	2(1)
C(9)	18(1)	27(1)	50(1)	3(1)	13(1)	-5(1)
C(10)	30(1)	35(1)	33(1)	9(1)	20(1)	5(1)
C(11)	18(1)	30(1)	49(1)	12(1)	12(1)	6(1)
C(12)	15(1)	14(1)	21(1)	2(1)	6(1)	2(1)
C(13)	17(1)	17(1)	22(1)	0(1)	3(1)	4(1)
C(14)	25(1)	21(1)	28(1)	-5(1)	4(1)	9(1)
C(15)	29(1)	18(1)	36(1)	-1(1)	0(1)	10(1)
C(16)	32(1)	14(1)	35(1)	4(1)	2(1)	5(1)
C(17)	22(1)	15(1)	22(1)	3(1)	2(1)	3(1)
C(18)	15(1)	10(1)	19(1)	0(1)	1(1)	2(1)
C(19)	14(1)	14(1)	24(1)	0(1)	1(1)	0(1)
C(20)	12(1)	18(1)	43(1)	6(1)	5(1)	3(1)

C(21)	16(1)	35(1)	57(1)	9(1)	12(1)	-3(1)
C(22)	21(1)	39(1)	42(1)	9(1)	-7(1)	4(1)
C(23)	18(1)	27(1)	87(2)	-8(1)	10(1)	8(1)
C(24)	16(1)	14(1)	24(1)	4(1)	4(1)	1(1)
N(3)	66(2)	46(2)	57(2)	12(2)	31(2)	16(2)
C(25)	52(2)	44(2)	34(2)	4(1)	11(2)	19(2)
C(26)	37(2)	22(1)	45(2)	2(1)	9(1)	5(1)
C(27)	54(3)	45(2)	54(2)	-16(2)	14(2)	6(2)
C(28)	54(3)	45(2)	54(2)	-16(2)	14(2)	6(2)
C(29)	54(3)	45(2)	54(2)	-16(2)	14(2)	6(2)
C(30)	54(3)	45(2)	54(2)	-16(2)	14(2)	6(2)
O(1)	54(3)	45(2)	54(2)	-16(2)	14(2)	6(2)

Table 6. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for $[Ni(P^{Cy}_2N^{t\text{-}Bu}_2)](BF_4)_2$ (**1**).

	x	y	z	U(eq)
H(1A)	10968	3135	7567	27
H(1B)	11229	3202	6934	27
H(2A)	10808	4806	7569	38
H(2B)	11548	4601	7518	38
H(3A)	11061	5797	6796	42
H(3B)	11305	4902	6453	42
H(4A)	10261	5331	5918	41
H(4B)	9980	5260	6540	41
H(5A)	10434	3654	5928	30
H(5B)	9685	3859	5946	30
H(6A)	9933	3709	7045	22
H(7A)	10167	1554	5760	21
H(7B)	10781	2144	6122	21
H(9A)	8250	-343	8149	46
H(9B)	7857	-387	8699	46
H(9C)	8564	-865	8785	46
H(10A)	9030	74	9719	46
H(10B)	8319	508	9700	46
H(10C)	8929	1207	9725	46
H(11A)	8094	1473	8155	47
H(11B)	8273	2013	8807	47
H(11C)	7691	1251	8682	47
H(12A)	9466	-632	8669	19
H(12B)	9900	9	9200	19
H(13A)	11474	-925	7988	23
H(13B)	10904	-882	7381	23
H(14A)	10776	-2561	7399	30
H(14B)	11524	-2325	7397	30
H(15A)	11820	-2596	8466	34
H(15B)	11434	-3515	8151	34

H(16A)	11059	-3060	9059	33
H(16B)	10478	-3017	8462	33
H(17A)	11189	-1382	9033	24
H(17B)	10445	-1620	9055	24
H(18A)	10152	-1475	7959	18
H(19A)	10967	693	9216	21
H(19B)	11410	95	8841	21
H(21A)	7778	925	6956	53
H(21B)	7711	226	6372	53
H(21C)	7153	994	6403	53
H(22A)	8054	1879	5271	54
H(22B)	7324	1632	5333	54
H(22C)	7853	796	5372	54
H(23A)	7931	2694	6797	66
H(23B)	7296	2636	6254	66
H(23C)	7959	3073	6118	66
H(24A)	8924	2874	6374	21
H(24B)	9103	2250	5822	21
H(25A)	11513	-4393	10304	65
H(25B)	11047	-5308	10182	65
H(25C)	10799	-4302	9879	65
H(27A)	12929	-1420	10058	76
H(27B)	12601	-1679	9357	76
H(27C)	13255	-2208	9692	76
H(28A)	12054	-2354	10069	61
H(28B)	12695	-2872	10398	61
H(29A)	11157	-4246	9884	61
H(29B)	11744	-4820	10323	61
H(30A)	11301	-5783	9413	76
H(30B)	12044	-5515	9415	76
H(30C)	11467	-4942	8979	76

Theoretical Methods

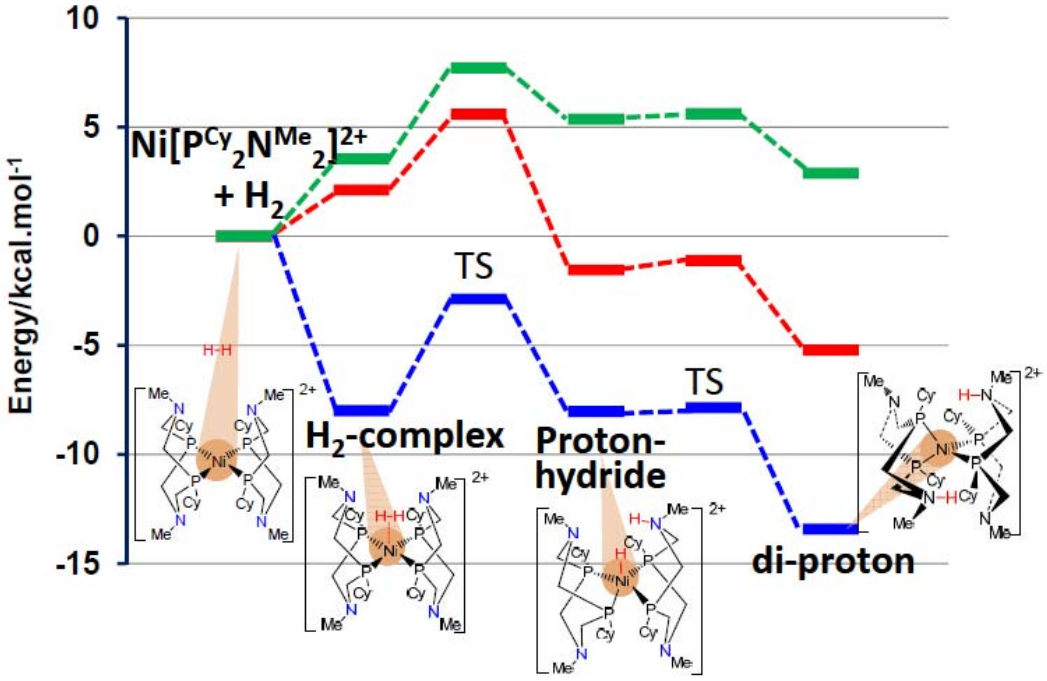

Figure S1. Reaction profile for all boat confomer. Blue is the gas phase energy included vdw correction; Green is gas phase free energy (gas phase energy plus ZPE, thermal correction and entropy term); Red is the free energy in acetonitrile solution (gas phase free energy plus solvation free energy).

All structures were fully optimized without symmetry constraints using PBE[2] functional as implemented in Gaussian 09[3]. Stugart basis set with effective core potential (ECP)[4] was used for the Ni atom and a 6-31G* basis set[5] was used for other non-metal atoms with a p-polarization function added onto H atoms. Each stationary point was confirmed by frequency calculation at the same level of theory to be real minimium without imaginary frequency, or trasition state with only one imaginary frequency. The empirical long-rane contribution calculated using Grimme scheme[6] as implemented in NWchem[7] was added to energy, gas phase free energy and free energy in solution. The gas phase free energy was corrected with ZPE, thermal corrections and entorpy terms at 1 atm and 298K. The solvation free energy contribution to total free energy in acetonitrile was calculated by using the C-PCM model[8] in Gaussian 09 at the same level of theory as that for optimization. Bondi redii was used with a scale factor (α) of 1.0.

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The Cartesian coordinates and energies of optimized structures of minima and transition states.

The reported energies (in Hartree) include vdw dispersion correction calculated using Grimme scheme.

H_2

E = -1.16466

H	0.000000	0.000000	0.374888
H	0.000000	0.000000	-0.374888

$[Ni(P_2{}^{Cy}N_2{}^{Me})_2]^{2+}$

E = -3167.41305

Ni	-0.000002	0.000000	0.000003
P	1.381691	-0.502187	1.679557
P	-1.381806	0.502140	1.679479
N	-0.828754	-2.066200	2.475426
N	0.828586	2.066130	2.475542
C	0.499496	-1.646080	2.913092
H	1.131994	-2.544872	2.992488
H	0.503341	-1.161854	3.918873
C	-1.828957	-1.018004	2.666400
H	-1.969415	-0.737897	3.738712
H	-2.802007	-1.382336	2.290746
C	1.828777	1.017929	2.666552
H	1.969164	0.737790	3.738865
H	2.801852	1.382273	2.290973
C	-0.499693	1.645998	2.913106
H	-1.132197	2.544787	2.992484
H	-0.503606	1.161744	3.918872
C	2.998091	-1.400296	1.358394
H	3.542932	-0.733654	0.660311
C	3.870941	-1.575600	2.623330
H	4.067462	-0.604010	3.111212
H	3.340138	-2.206466	3.362657
C	5.207855	-2.252408	2.252618
H	5.792614	-1.566646	1.608371

H	5.802093	-2.400525	3.170994
C	4.993136	-3.587826	1.525020
H	5.965616	-4.022848	1.237564
H	4.519250	-4.312228	2.216002
C	4.101720	-3.413353	0.285276
H	3.911809	-4.389351	-0.195501
H	4.629722	-2.788555	-0.463780
C	2.757725	-2.749917	0.646184
H	2.200529	-3.429904	1.320419
H	2.122527	-2.612216	-0.248528
C	-2.998183	1.400263	1.358243
H	-3.542982	0.733644	0.660104
C	-2.757768	2.749906	0.646091
H	-2.200614	3.429870	1.320385
H	-2.122511	2.612233	-0.248583
C	-4.101737	3.413359	0.285119
H	-3.911791	4.389371	-0.195615
H	-4.629693	2.788586	-0.463992
C	-4.993232	3.587795	1.524811
H	-5.965692	4.022829	1.237307
H	-4.519387	4.312174	2.215846
C	-5.208001	2.252354	2.252352
H	-5.792721	1.566614	1.608045
H	-5.802297	2.400444	3.170695
C	-3.871113	1.575531	2.623129
H	-3.340353	2.206372	3.362508
H	-4.067668	0.603927	3.110968
C	-1.247828	-3.310996	3.143873
H	-2.227995	-3.622134	2.746661
H	-1.333880	-3.204949	4.247007
C	1.247615	3.310906	3.144054
H	2.227809	3.622056	2.746917
H	1.333593	3.204826	4.247190
P	1.381801	0.502190	-1.679458
P	-1.381695	-0.502139	-1.679564
N	-0.828595	2.066203	-2.475468
N	0.828750	-2.066127	-2.475480
C	0.499685	1.646085	-2.913048
H	1.132186	2.544879	-2.992398
H	0.503597	1.161864	-3.918831
C	-1.828785	1.018007	-2.666510
H	-1.969174	0.737902	-3.738832
H	-2.801860	1.382338	-2.290918
C	1.828953	-1.017926	-2.666423
H	1.969413	-0.737788	-3.738727

H	2.802003	-1.382270	-2.290778
C	-0.499499	-1.645992	-2.913135
H	-1.131996	-2.544782	-2.992560
H	-0.503342	-1.161735	-3.918901
C	2.998179	1.400302	-1.358198
H	3.542964	0.733679	-0.660052
C	3.871129	1.575565	-2.623071
H	4.067686	0.603959	-3.110907
H	3.340386	2.206409	-3.362460
C	5.208015	2.252381	-2.252274
H	5.792721	1.566638	-1.607958
H	5.802326	2.400467	-3.170607
C	4.993242	3.587823	-1.524736
H	5.965700	4.022851	-1.237216
H	4.519413	4.312205	-2.215779
C	4.101726	3.413393	-0.285058
H	3.911778	4.389406	0.195672
H	4.629666	2.788617	0.464061
C	2.757759	2.749948	-0.646053
H	2.200619	3.429912	-1.320357
H	2.122485	2.612280	0.248610
C	-2.998090	-1.400267	-1.358434
H	-3.542940	-0.733649	-0.660336
C	-2.757717	-2.749909	-0.646264
H	-2.200514	-3.429870	-1.320519
H	-2.122521	-2.612232	0.248452
C	-4.101708	-3.413367	-0.285382
H	-3.911791	-4.389378	0.195365
H	-4.629717	-2.788596	0.463693
C	-4.993119	-3.587807	-1.525134
H	-5.965598	-4.022843	-1.237695
H	-4.519226	-4.312185	-2.216137
C	-5.207844	-2.252368	-2.252692
H	-5.792609	-1.566629	-1.608426
H	-5.802077	-2.400461	-3.171075
C	-3.870933	-1.575541	-2.623379
H	-3.340122	-2.206382	-3.362721
H	-4.067457	-0.603938	-3.111234
C	-1.247626	3.311000	-3.143940
H	-2.227819	3.622136	-2.746791
H	-1.333605	3.204955	-4.247079
C	1.247824	-3.310902	-3.143964
H	2.227991	-3.622053	-2.746761
H	1.333877	-3.204822	-4.247095
H	0.520573	-4.108077	-2.921118

H	-0.520391	4.108168	-2.921018
H	0.520380	4.108081	2.921157
H	-0.520578	-4.108164	2.921002

$[H_2Ni(P_2^{Cy}N_2^{Me})_2]^{2+}$ dihydrogen adduct

E = -3168.59044

Ni	-0.000145	0.000821	-0.281670
P	1.320461	1.662588	0.498689
P	-1.452965	1.706948	-0.476452
N	-0.870416	2.288609	2.166653
N	0.680788	2.653727	-2.029497
C	0.547031	2.551982	1.970693
H	1.087155	2.188367	2.860902
H	0.774292	3.641833	1.865890
C	-1.671900	2.776883	1.056591
H	-1.468712	3.842728	0.788239
H	-2.737977	2.712675	1.335820
C	1.486266	2.976874	-0.857358
H	1.267694	3.986073	-0.434880
H	2.546579	2.975883	-1.162668
C	-0.741328	2.852280	-1.796884
H	-1.279854	2.625710	-2.733286
H	-0.996763	3.900554	-1.510421
C	3.108717	1.505696	1.085208
H	3.641168	1.125092	0.190204
C	3.749854	2.861750	1.472208
H	3.650347	3.607210	0.663503
H	3.235170	3.277598	2.359240
C	5.243738	2.660547	1.805733
H	5.778135	2.339566	0.889720
H	5.680734	3.631205	2.098170
C	5.447205	1.619974	2.916500
H	6.524398	1.462434	3.097001
H	5.024935	2.006774	3.864459
C	4.766453	0.287529	2.566777
H	4.863916	-0.427881	3.402775
H	5.278388	-0.172248	1.696554
C	3.275049	0.490581	2.233317
H	2.759543	0.869294	3.137634
H	2.781292	-0.465629	1.988495
C	-3.209277	1.430814	-1.084418
H	-3.711772	0.949492	-0.222343
C	-3.273886	0.473578	-2.292123

H	-2.751834	0.929992	-3.156693
H	-2.739323	-0.469098	-2.070601
C	-4.738465	0.193030	-2.685286
H	-4.760711	-0.465580	-3.571379
H	-5.234922	-0.363994	-1.864858
C	-5.508807	1.493849	-2.959490
H	-6.564772	1.268746	-3.187255
H	-5.092330	1.983071	-3.861637
C	-5.419142	2.458370	-1.768155
H	-5.942740	2.023988	-0.893710
H	-5.929920	3.409585	-1.997917
C	-3.954409	2.755615	-1.383507
H	-3.462785	3.282019	-2.223545
H	-3.927249	3.437815	-0.514657
C	-1.334179	2.838223	3.451794
H	-2.390632	2.563095	3.605987
H	-1.245076	3.944832	3.511678
C	1.133663	3.378238	-3.229964
H	2.192840	3.140094	-3.419742
H	1.030179	4.480398	-3.137474
P	1.452328	-1.705568	-0.476828
P	-1.320471	-1.660789	0.499800
N	-0.682280	-2.652585	-2.028511
N	0.871274	-2.286515	2.166730
C	0.739991	-2.851036	-1.796741
H	1.277941	-2.624495	-2.733482
H	0.995668	-3.899273	-1.510355
C	-1.486990	-2.975475	-0.855780
H	-1.268051	-3.984533	-0.433155
H	-2.547505	-2.974675	-1.160402
C	1.671976	-2.775220	1.056302
H	1.468383	-3.841079	0.788315
H	2.738238	-2.711176	1.334858
C	-0.546323	-2.549731	1.971696
H	-1.085880	-2.185682	2.862076
H	-0.773821	-3.639583	1.867432
C	3.208382	-1.429660	-1.085632
H	3.708444	-0.938544	-0.227675
C	3.958071	-2.754833	-1.371350
H	3.932081	-3.428888	-0.496131
H	3.469095	-3.290708	-2.206937
C	5.422294	-2.456540	-1.757147
H	5.943510	-2.012308	-0.886234
H	5.936352	-3.408238	-1.977397
C	5.510281	-1.502961	-2.957394

H	6.565787	-1.276567	-3.186003
H	5.096505	-2.001999	-3.855396
C	4.735379	-0.202135	-2.696369
H	4.756570	0.448190	-3.588586
H	5.229008	0.364189	-1.880614
C	3.271249	-0.483786	-2.302340
H	2.751824	-0.950209	-3.163141
H	2.733248	0.459160	-2.090500
C	-3.108448	-1.503978	1.087214
H	-3.640968	-1.121275	0.193140
C	-3.273887	-0.491187	2.237486
H	-2.758492	-0.872195	3.140904
H	-2.779517	0.465191	1.994644
C	-4.765105	-0.287861	2.571597
H	-4.861993	0.425929	3.409046
H	-5.276893	0.173975	1.702377
C	-5.446611	-1.620595	2.918749
H	-6.523676	-1.462764	3.099752
H	-5.024415	-2.009555	3.865856
C	-5.243962	-2.659069	1.805864
H	-5.778376	-2.335975	0.890606
H	-5.681437	-3.630061	2.096467
C	-3.750259	-2.860450	1.471616
H	-3.235638	-3.278385	2.357699
H	-3.651332	-3.604324	0.661372
C	-1.135884	-3.377397	-3.228520
H	-2.195188	-3.139336	-3.417692
H	-1.032301	-4.479531	-3.135832
C	1.335738	-2.835836	3.451742
H	2.392326	-2.560823	3.605215
H	1.246504	-3.942414	3.511993
H	0.744679	-2.392757	4.269492
H	-0.548452	-3.042425	-4.098893
H	0.545675	3.043080	-4.099889
H	-0.742556	2.395465	4.269309
H	0.245797	0.330469	-2.010225
H	-0.247151	-0.329262	-2.009995

$[H_2Ni(P_2^{Cy}N_2^{Me})_2]^{2+}$ Transition state between H_2-adduct and first proton-hydride

E = -3168.58229

Ni	0.004452	-0.292240	-0.089761
P	1.190775	1.041249	-1.501652
P	-1.556049	-0.127742	-1.645392
N	-1.106514	2.625813	-1.814236
N	0.652186	-1.279438	-2.929346
C	0.217999	2.408426	-2.384645
H	0.798546	3.335398	-2.245933
H	0.199365	2.207368	-3.483872
C	-2.064786	1.594302	-2.181741
H	-2.273625	1.560322	-3.280305
H	-3.024804	1.810842	-1.678315
C	1.605657	-0.150436	-2.918956
H	1.628274	0.362144	-3.900950
H	2.610949	-0.562766	-2.725555
C	-0.730390	-0.860700	-3.204887
H	-1.309959	-1.748306	-3.503727
H	-0.780569	-0.125377	-4.030079
C	2.855410	1.851367	-1.159848
H	3.447798	1.035707	-0.693724
C	3.611285	2.340530	-2.415103
H	3.750601	1.523656	-3.146431
H	3.020179	3.128262	-2.922175
C	4.986317	2.920391	-2.020486
H	5.619613	2.104475	-1.619415
H	5.495182	3.293959	-2.926058
C	4.858057	4.035681	-0.972329
H	5.858769	4.397070	-0.679462
H	4.331645	4.901841	-1.418957
C	4.082153	3.554674	0.263767
H	3.950178	4.381746	0.983807
H	4.668940	2.771365	0.785810
C	2.702842	2.985272	-0.122455
H	2.096596	3.803679	-0.559544
H	2.148162	2.625481	0.763013
C	-3.170933	-1.074975	-1.514070
H	-3.691845	-0.590542	-0.662624
C	-2.919052	-2.552348	-1.143295
H	-2.371387	-3.052160	-1.968457
H	-2.271097	-2.622682	-0.249933
C	-4.254443	-3.290467	-0.923896
H	-4.052843	-4.351130	-0.692174
H	-4.763533	-2.863959	-0.036260
C	-5.173898	-3.169818	-2.149013

H	-6.138931	-3.666991	-1.951311
H	-4.716778	-3.705049	-3.004431
C	-5.406689	-1.700663	-2.530096
H	-5.973724	-1.192189	-1.725842
H	-6.024172	-1.627273	-3.442092
C	-4.078722	-0.948462	-2.760872
H	-3.568180	-1.384280	-3.642255
H	-4.286154	0.109963	-2.999528
C	-1.632484	3.960173	-2.149048
H	-2.596496	4.110989	-1.635522
H	-1.789994	4.105822	-3.239986
C	1.102046	-2.417640	-3.760724
H	2.109765	-2.722443	-3.437857
H	1.135142	-2.154505	-4.834025
P	1.472463	-1.001073	1.401764
P	-1.182792	0.123051	1.762368
N	-0.726248	-2.595610	2.107165
N	1.110177	1.428488	2.722277
C	0.655121	-2.328382	2.484715
H	1.236623	-3.253162	2.331889
H	0.781241	-2.040000	3.556099
C	-1.641564	-1.535681	2.520196
H	-1.704773	-1.424045	3.629785
H	-2.653689	-1.791403	2.157866
C	2.048898	0.324087	2.596429
H	2.263174	-0.174235	3.574286
H	3.007628	0.714108	2.208750
C	-0.207232	0.975534	3.147316
H	-0.794619	1.859722	3.442868
H	-0.176497	0.298900	4.035404
C	3.098935	-1.782748	0.854469
H	3.601519	-0.972567	0.286011
C	3.999331	-2.159447	2.059280
H	4.176637	-1.288750	2.713896
H	3.492846	-2.928081	2.674929
C	5.351794	-2.720638	1.573057
H	5.910873	-1.918853	1.051901
H	5.956914	-3.003552	2.451865
C	5.167129	-3.918050	0.631988
H	6.147017	-4.273469	0.269987
H	4.714660	-4.761337	1.189459
C	4.266307	-3.549323	-0.555384
H	4.094724	-4.428278	-1.201589
H	4.775902	-2.789348	-1.181445
C	2.907873	-2.989899	-0.086064

H	2.352616	-3.790312	0.441716
H	2.292982	-2.706287	-0.958149
C	-2.801446	1.086704	1.764433
H	-3.400704	0.605271	0.964860
C	-2.577612	2.564342	1.377241
H	-1.981884	3.064479	2.166141
H	-1.986075	2.640039	0.446684
C	-3.926930	3.299896	1.253733
H	-3.746289	4.359579	0.999305
H	-4.507201	2.866852	0.412774
C	-4.747086	3.189945	2.548515
H	-5.727150	3.681971	2.424889
H	-4.223548	3.735554	3.357806
C	-4.940975	1.724086	2.962904
H	-5.575044	1.207080	2.215618
H	-5.478297	1.659646	3.925068
C	-3.597359	0.973558	3.085424
H	-3.010747	1.416063	3.914106
H	-3.787412	-0.080727	3.353468
C	-1.181831	-3.905209	2.601250
H	-2.202230	-4.096200	2.229897
H	-1.195356	-3.974550	3.710804
C	1.646364	2.462219	3.623659
H	2.616910	2.815204	3.237078
H	1.795907	2.098061	4.663590
H	0.954782	3.319877	3.646321
H	-0.521605	-4.695300	2.207661
H	0.413153	-3.265186	-3.617019
H	-0.929784	4.728781	-1.788966
H	0.472774	-1.573355	-1.465550
H	0.150080	-1.824724	-0.592714

$[H_2Ni(P_2^{Cy}N_2^{Me})_2]^{2+}$ first proton-dydride

E = -3168.58958

Ni	0.024869	-0.277618	-0.068099
P	-1.469336	-0.457178	-1.632138
P	1.153854	0.984146	-1.558921
N	0.854184	-1.530513	-2.783691
N	-1.251775	2.303432	-2.126827
C	-0.599100	-1.298201	-3.106218
H	-1.057490	-2.285341	-3.274220
H	-0.665651	-0.712884	-4.037027
C	1.689378	-0.278235	-2.883214

H	1.623614	0.095604	-3.918378
H	2.730160	-0.579633	-2.680604
C	-2.086998	1.146564	-2.405014
H	-2.240159	0.969416	-3.499392
H	-3.085951	1.328978	-1.968181
C	0.113784	2.172843	-2.613522
H	0.595162	3.161328	-2.526826
H	0.174209	1.885339	-3.692583
C	-3.035771	-1.469493	-1.433543
H	-3.592896	-0.894628	-0.662890
C	-3.911374	-1.548871	-2.705817
H	-4.153718	-0.542505	-3.091138
H	-3.356228	-2.075702	-3.508008
C	-5.214441	-2.321958	-2.414506
H	-5.826235	-1.738923	-1.698606
H	-5.805956	-2.395334	-3.343553
C	-4.933327	-3.716782	-1.837558
H	-5.882624	-4.227329	-1.601286
H	-4.427582	-4.337808	-2.603170
C	-4.049269	-3.633665	-0.583907
H	-3.811853	-4.644209	-0.207362
H	-4.603820	-3.117782	0.225471
C	-2.738089	-2.870334	-0.858788
H	-2.140177	-3.451082	-1.592491
H	-2.124660	-2.785248	0.057079
C	2.771968	1.924063	-1.327539
H	3.417192	1.190435	-0.797333
C	2.543419	3.126307	-0.384957
H	1.871956	3.857146	-0.879005
H	2.031300	2.794353	0.536385
C	3.878126	3.828515	-0.067556
H	3.688024	4.700913	0.582409
H	4.525285	3.138301	0.511063
C	4.608137	4.259946	-1.348684
H	5.580132	4.719589	-1.100092
H	4.014784	5.042047	-1.861715
C	4.815661	3.071178	-2.298732
H	5.509922	2.342557	-1.835436
H	5.290940	3.401795	-3.238668
C	3.485671	2.359427	-2.626113
H	2.835346	3.055381	-3.191571
H	3.684511	1.497368	-3.289785
C	1.441618	-2.679681	-3.546799
H	2.478725	-2.834457	-3.214847
H	1.423498	-2.451410	-4.622722

C	-1.891557	3.533663	-2.621743
H	-2.888238	3.637998	-2.162040
H	-2.012017	3.547001	-3.727141
P	-1.142616	0.471918	1.726929
P	1.405018	-0.953746	1.477210
N	1.262322	1.646015	2.549547
N	-0.910877	-2.243760	2.393064
C	-0.096890	1.385464	3.013873
H	-0.585432	2.358253	3.188995
H	-0.131951	0.830242	3.982054
C	2.091549	0.449677	2.529307
H	2.274101	0.035301	3.551923
H	3.076823	0.715740	2.104383
C	-1.717205	-1.057065	2.670538
H	-1.760480	-0.815762	3.760246
H	-2.752306	-1.264240	2.343203
C	0.496924	-2.064369	2.716028
H	0.986872	-3.052056	2.672508
H	0.673412	-1.661971	3.742343
C	-2.722841	1.501128	1.657571
H	-3.359504	0.947441	0.933792
C	-3.484365	1.590638	2.999704
H	-3.713231	0.588270	3.402080
H	-2.850149	2.100550	3.751332
C	-4.794986	2.386583	2.826495
H	-5.476584	1.818656	2.162563
H	-5.303660	2.463318	3.803295
C	-4.545137	3.781172	2.234749
H	-5.503402	4.306959	2.081673
H	-3.966372	4.389518	2.957149
C	-3.767401	3.691234	0.913019
H	-3.547134	4.701335	0.523696
H	-4.397893	3.188814	0.150479
C	-2.451236	2.906423	1.081216
H	-1.796610	3.467935	1.777371
H	-1.906448	2.827447	0.123417
C	2.973596	-1.908624	1.049312
H	3.518087	-1.218371	0.369391
C	2.685706	-3.217013	0.286633
H	2.107519	-3.905415	0.933823
H	2.043851	-3.020177	-0.593400
C	3.991229	-3.913689	-0.143659
H	3.751524	-4.855785	-0.668030
H	4.527303	-3.269736	-0.870623
C	4.902279	-4.185081	1.063058

H	5.850072	-4.640736	0.728846
H	4.416390	-4.925430	1.728064
C	5.179449	-2.895053	1.846483
H	5.776387	-2.201170	1.222315
H	5.786271	-3.108123	2.743528
C	3.876062	-2.190844	2.276918
H	3.333397	-2.840100	2.991635
H	4.122312	-1.259134	2.814242
C	1.909239	2.698724	3.350141
H	2.908305	2.913690	2.935188
H	2.029006	2.420031	4.420176
C	-1.474398	-3.423541	3.067463
H	-2.515631	-3.568471	2.734383
H	-1.473501	-3.336782	4.176302
H	-0.896784	-4.319407	2.785706
H	1.308379	3.621068	3.293290
H	-1.285262	4.404501	-2.324035
H	0.847715	-3.583245	-3.344168
H	0.040289	-1.785656	-0.208530
H	0.831235	-1.734890	-1.728848

$[H_2Ni(P_2^{Cy}N_2^{Me})_2]^{2+}$ Transition state between 1st proton-hydride and 2nd proton-hydride

E = -3168.58820

Ni	0.004567	-0.264204	-0.068766
P	1.054359	0.925673	-1.642355
P	-1.454232	-0.719183	-1.607720
N	-1.444678	1.999491	-2.316995
N	0.952354	-1.715006	-2.601408
C	-0.064535	1.959745	-2.774284
H	0.332657	2.987865	-2.736051
H	0.042605	1.616482	-3.833245
C	-2.164960	0.757627	-2.541560
H	-2.248041	0.486923	-3.624394
H	-3.195323	0.884047	-2.163015
C	1.670379	-0.412419	-2.853847
H	1.548155	-0.152214	-3.917854
H	2.737969	-0.598573	-2.653142
C	-0.509775	-1.659445	-2.970331
H	-0.875339	-2.697316	-3.012809
H	-0.604887	-1.205810	-3.969693
C	2.610709	1.981209	-1.503771
H	3.304077	1.338050	-0.920265
C	3.280203	2.339422	-2.849781

H	3.524314	1.435487	-3.438204
H	2.580880	2.941152	-3.462781
C	4.568136	3.156579	-2.612740
H	5.311405	2.516704	-2.097378
H	5.009959	3.426265	-3.587801
C	4.299501	4.413126	-1.771890
H	5.244451	4.951019	-1.583153
H	3.653227	5.107868	-2.343371
C	3.613567	4.056650	-0.444767
H	3.378178	4.970835	0.128241
H	4.309486	3.462348	0.181605
C	2.320153	3.248918	-0.670697
H	1.597528	3.889912	-1.214704
H	1.850438	2.967989	0.288886
C	-2.966336	-1.796145	-1.324922
H	-3.564667	-1.181993	-0.617997
C	-2.613428	-3.123414	-0.622981
H	-1.973560	-3.737673	-1.290762
H	-2.027901	-2.927957	0.293670
C	-3.888998	-3.924413	-0.293720
H	-3.607218	-4.881616	0.179150
H	-4.482066	-3.364019	0.456346
C	-4.745337	-4.169111	-1.545012
H	-5.672688	-4.702109	-1.273779
H	-4.196650	-4.832686	-2.242272
C	-5.082923	-2.849461	-2.252664
H	-5.735921	-2.234560	-1.602939
H	-5.652199	-3.037470	-3.179466
C	-3.813936	-2.041603	-2.596372
H	-3.216925	-2.613024	-3.335637
H	-4.099485	-1.091272	-3.080972
C	-2.177388	3.138314	-2.895032
H	-3.188097	3.182281	-2.456928
H	-2.275846	3.077094	-4.000971
C	1.659622	-2.892086	-3.203924
H	2.694185	-2.915953	-2.831227
H	1.657906	-2.796762	-4.299723
P	1.437828	-0.854706	1.481476
P	-1.085185	0.718315	1.700114
N	-0.901666	-1.947609	2.569750
N	1.404492	1.832703	2.353376
C	0.514392	-1.779007	2.861159
H	0.971966	-2.779438	2.939592
H	0.709764	-1.258330	3.826373
C	-1.678706	-0.722469	2.767027

H	-1.698898	-0.408310	3.836853
H	-2.722563	-0.930918	2.469808
C	2.203261	0.614295	2.378478
H	2.434436	0.275090	3.418652
H	3.170596	0.823186	1.885164
C	0.054108	1.659645	2.885752
H	-0.382047	2.664269	3.015341
H	0.036559	1.174287	3.890911
C	2.950268	-1.932866	1.147219
H	3.501385	-1.368775	0.363784
C	3.891456	-2.113564	2.362862
H	4.213532	-1.138002	2.765681
H	3.347681	-2.633125	3.176235
C	5.132262	-2.943952	1.973946
H	5.737970	-2.368649	1.246234
H	5.767283	-3.084144	2.865789
C	4.749134	-4.300670	1.366721
H	5.654344	-4.849126	1.054645
H	4.255269	-4.924960	2.136706
C	3.797685	-4.126381	0.172654
H	3.484730	-5.110026	-0.220327
H	4.332773	-3.608196	-0.649778
C	2.554612	-3.307098	0.568653
H	1.980300	-3.876475	1.325535
H	1.871575	-3.186388	-0.295151
C	-2.631271	1.797603	1.644182
H	-3.328075	1.208619	1.009135
C	-2.346914	3.133025	0.924520
H	-1.617461	3.722122	1.516040
H	-1.884306	2.936150	-0.059234
C	-3.638191	3.961563	0.774529
H	-3.404487	4.924201	0.285577
H	-4.337312	3.426206	0.099863
C	-4.322031	4.197098	2.129962
H	-5.264946	4.753961	1.991868
H	-3.671997	4.834348	2.761275
C	-4.591479	2.869317	2.852374
H	-5.335417	2.280324	2.280113
H	-5.035100	3.050096	3.847054
C	-3.305206	2.033328	3.014183
H	-2.606812	2.575419	3.681895
H	-3.547088	1.078258	3.513142
C	-1.493832	-3.074816	3.306589
H	-2.537432	-3.213871	2.978630
H	-1.493800	-2.923986	4.407692

C	2.118380	2.911754	3.056380
H	3.106471	3.063624	2.590405
H	2.272362	2.699199	4.137275
H	1.547020	3.849846	2.962607
H	-0.935447	-3.997833	3.079046
H	1.136403	-3.812860	-2.906554
H	-1.654819	4.074757	-2.640670
H	0.930482	-1.770494	-1.526788
H	-0.373926	-1.643964	0.348509

$[H_2Ni(P_2^{Cy}N_2^{Me})_2]^{2+}$ Second proton-hydride

E = -3168.59050

Ni	-0.204700	0.120971	0.018376
P	0.982340	-0.640391	-1.718235
P	-0.983546	1.611241	-1.352793
N	1.662391	2.050911	-2.146171
N	-1.688633	-0.800157	-2.572182
C	1.757778	0.741239	-2.772412
H	2.826986	0.487876	-2.865335
H	1.336525	0.711776	-3.807985
C	0.331855	2.632817	-2.233792
H	0.006045	2.820647	-3.287699
H	0.347638	3.612152	-1.722202
C	-0.321508	-1.336678	-2.914001
H	-0.125323	-1.118309	-3.976457
H	-0.368597	-2.429403	-2.777083
C	-1.806563	0.687272	-2.809344
H	-2.880278	0.928861	-2.838128
H	-1.363773	0.920471	-3.790709
C	2.268820	-2.019592	-1.820833
H	1.795371	-2.851998	-1.260235
C	2.585769	-2.484832	-3.261110
H	1.674169	-2.819436	-3.789542
H	3.000009	-1.638181	-3.843318
C	3.616090	-3.633326	-3.253642
H	3.163530	-4.522172	-2.771734
H	3.842624	-3.922139	-4.294799
C	4.897724	-3.239658	-2.506684
H	5.600869	-4.089892	-2.484662
H	5.409495	-2.424449	-3.054986
C	4.579151	-2.775537	-1.078202
H	5.499259	-2.451177	-0.560376
H	4.172461	-3.626629	-0.497376

C	3.555882	-1.622459	-1.067362
H	4.017657	-0.737738	-1.549007
H	3.299564	-1.338627	-0.033163
C	-2.280861	2.896901	-0.916409
H	-1.765811	3.493584	-0.133608
C	-3.527113	2.251280	-0.275085
H	-4.038902	1.607485	-1.020898
H	-3.226660	1.595877	0.562223
C	-4.520331	3.328681	0.202932
H	-5.414986	2.841450	0.629443
H	-4.054177	3.908578	1.023987
C	-4.913876	4.279447	-0.937793
H	-5.588698	5.066896	-0.560816
H	-5.486094	3.718248	-1.702898
C	-3.674393	4.911454	-1.587096
H	-3.167661	5.571840	-0.856580
H	-3.963888	5.551474	-2.438488
C	-2.674378	3.842488	-2.074265
H	-3.146672	3.257363	-2.889389
H	-1.786699	4.335314	-2.508427
C	2.673616	2.983589	-2.670076
H	2.613906	3.933767	-2.114408
H	2.547044	3.202727	-3.753030
C	-2.788458	-1.584254	-3.223793
H	-2.685926	-2.643172	-2.944506
H	-2.713029	-1.475718	-4.315697
P	-1.028537	-1.516981	1.287473
P	1.109819	0.621078	1.783102
N	-1.476310	0.796706	2.789971
N	1.675399	-2.145721	1.826083
C	-1.690759	-0.648504	2.850394
H	-2.776069	-0.833828	2.895558
H	-1.239168	-1.109978	3.753270
C	-0.105137	1.196040	3.113847
H	0.209883	0.837870	4.116918
H	-0.067245	2.299272	3.124727
C	0.314717	-2.656795	1.960770
H	0.055940	-2.913804	3.017554
H	0.247080	-3.594985	1.379928
C	1.913689	-0.907082	2.567688
H	3.001821	-0.722874	2.564416
H	1.608224	-0.976020	3.639487
C	-2.399439	-2.768611	0.911630
H	-1.992875	-3.341272	0.048961
C	-2.703260	-3.772927	2.048520

H	-1.789874	-4.307102	2.362521
H	-3.073258	-3.222718	2.936081
C	-3.771604	-4.794351	1.607168
H	-3.356464	-5.422806	0.794641
H	-3.991023	-5.476532	2.446738
C	-5.056178	-4.107545	1.121942
H	-5.781368	-4.859605	0.766745
H	-5.538954	-3.584249	1.970329
C	-4.757898	-3.092723	0.006964
H	-5.680690	-2.565761	-0.294670
H	-4.390241	-3.631736	-0.890099
C	-3.697901	-2.069359	0.456994
H	-4.113228	-1.477967	1.296905
H	-3.491576	-1.334498	-0.347450
C	2.447213	1.942213	1.914028
H	1.918636	2.859422	1.577805
C	3.601377	1.676621	0.926499
H	4.111912	0.730553	1.197782
H	3.191758	1.551670	-0.091762
C	4.632605	2.821610	0.962483
H	5.464585	2.591091	0.273022
H	4.156444	3.748346	0.584227
C	5.161992	3.063395	2.384129
H	5.865015	3.914204	2.390646
H	5.739112	2.178025	2.716529
C	4.010632	3.320443	3.366820
H	3.503777	4.269854	3.104135
H	4.395587	3.445086	4.394032
C	2.976829	2.175541	3.347561
H	3.459736	1.250623	3.719802
H	2.153180	2.408685	4.046170
C	-2.486408	1.572080	3.529540
H	-2.327870	2.646265	3.340789
H	-2.443343	1.398111	4.623908
C	2.634031	-3.184544	2.241451
H	2.478678	-4.091963	1.634244
H	2.535680	-3.463879	3.313879
H	3.662636	-2.827580	2.068645
H	-3.492339	1.299922	3.170534
H	-3.757788	-1.199993	-2.874447
H	3.679118	2.559894	-2.513236
H	-1.170098	0.807546	0.964930
H	-1.723012	-0.884197	-1.504699

$[H_2Ni(P_2^{Cy}N_2^{Me})_2]^{2+}$ Transition state between second proton-hydride and di-proton

E = -3168.59023

Ni	-0.206608	-0.097954	-0.044877
P	0.966390	0.577864	1.739815
P	-1.016661	-1.645313	1.247507
N	1.632297	-2.132678	2.032782
N	-1.699586	0.707346	2.590380
C	1.728395	-0.857663	2.729339
H	2.798463	-0.616023	2.843969
H	1.300140	-0.882088	3.762106
C	0.298742	-2.715077	2.073873
H	-0.032407	-2.967713	3.112259
H	0.319729	-3.661808	1.503900
C	-0.334506	1.226434	2.963789
H	-0.145349	0.961159	4.016828
H	-0.377926	2.324263	2.874052
C	-1.814689	-0.789176	2.761555
H	-2.887473	-1.032200	2.800747
H	-1.353739	-1.066872	3.722648
C	2.255857	1.947199	1.918992
H	1.779386	2.810287	1.409028
C	2.581121	2.332200	3.380637
H	1.671991	2.634273	3.932562
H	3.000042	1.454883	3.911911
C	3.609272	3.481368	3.432060
H	3.152454	4.395007	3.003417
H	3.842049	3.711981	4.486313
C	4.887043	3.132937	2.656447
H	5.588796	3.984387	2.677726
H	5.403283	2.289246	3.155287
C	4.560815	2.748027	1.206191
H	5.478763	2.455109	0.666104
H	4.149075	3.629152	0.675496
C	3.539029	1.595833	1.137278
H	4.003685	0.685493	1.565676
H	3.277205	1.371268	0.089769
C	-2.336571	-2.911425	0.800944
H	-1.863798	-3.459278	-0.042113
C	-3.613156	-2.228950	0.265736
H	-4.094913	-1.649108	1.080387
H	-3.356194	-1.503183	-0.527154
C	-4.624964	-3.272833	-0.246030
H	-5.537778	-2.761386	-0.599779
H	-4.193973	-3.795311	-1.123179

C	-4.968748	-4.299516	0.844198
H	-5.657497	-5.063007	0.443833
H	-5.509979	-3.792103	1.667124
C	-3.702591	-4.967448	1.399551
H	-3.227334	-5.579065	0.607840
H	-3.956880	-5.661465	2.219306
C	-2.681693	-3.929881	1.910959
H	-3.116479	-3.398219	2.781650
H	-1.777415	-4.448853	2.273693
C	2.630746	-3.096854	2.522432
H	2.574500	-4.017442	1.918455
H	2.486972	-3.370827	3.590875
C	-2.803739	1.462139	3.267170
H	-2.700288	2.532193	3.034169
H	-2.735458	1.307539	4.354002
P	-1.016141	1.575672	-1.254684
P	1.154319	-0.556009	-1.768333
N	-1.431460	-0.746743	-2.700799
N	1.688239	2.211997	-1.791563
C	-1.691811	0.699492	-2.810532
H	-2.781724	0.853334	-2.845768
H	-1.258402	1.127753	-3.733218
C	-0.064681	-1.123461	-3.103875
H	0.187250	-0.729943	-4.106749
H	-0.016587	-2.224844	-3.144125
C	0.325766	2.711197	-1.944311
H	0.073569	2.953573	-3.006415
H	0.248242	3.656363	-1.376529
C	1.949833	0.983011	-2.539306
H	3.039675	0.810033	-2.523559
H	1.657832	1.056550	-3.615042
C	-2.380815	2.837921	-0.889133
H	-1.965437	3.417385	-0.035545
C	-2.686145	3.830362	-2.035885
H	-1.771830	4.353925	-2.364559
H	-3.067784	3.271687	-2.913550
C	-3.743257	4.865454	-1.599252
H	-3.316821	5.500295	-0.797715
H	-3.964045	5.539121	-2.445338
C	-5.029143	4.194527	-1.095630
H	-5.745309	4.956460	-0.743164
H	-5.523163	3.665690	-1.934167
C	-4.729879	3.190218	0.028499
H	-5.654271	2.673758	0.343139
H	-4.350800	3.735555	0.916700

C	-3.680646	2.153826	-0.417197
H	-4.107186	1.555136	-1.246801
H	-3.473037	1.429771	0.396074
C	2.496152	-1.869891	-1.929267
H	1.974442	-2.793610	-1.600322
C	3.659039	-1.615215	-0.948867
H	4.163944	-0.663230	-1.209323
H	3.258564	-1.508036	0.074614
C	4.693441	-2.756110	-1.012605
H	5.530905	-2.533413	-0.327346
H	4.223946	-3.690220	-0.644389
C	5.210516	-2.973794	-2.442607
H	5.916141	-3.822041	-2.468959
H	5.781681	-2.081457	-2.766466
C	4.051031	-3.219424	-3.418745
H	3.549810	-4.174628	-3.166415
H	4.426825	-3.326233	-4.451354
C	3.013976	-2.078484	-3.370886
H	3.490418	-1.145936	-3.732189
H	2.185157	-2.302896	-4.066774
C	-2.474261	-1.594324	-3.313415
H	-2.277318	-2.648105	-3.059271
H	-2.495745	-1.491569	-4.414611
C	2.647498	3.262568	-2.174028
H	2.474095	4.160262	-1.557467
H	2.569325	3.555896	-3.244419
H	3.674739	2.909988	-1.984636
H	-3.459429	-1.310687	-2.911313
H	-3.770785	1.092492	2.896108
H	3.640962	-2.671945	2.403060
H	-1.725934	0.836805	1.526144
H	-1.165436	-0.764416	-1.179311

$[H_2Ni(P_2^{Cy}N_2^{Me})_2]^{2+}$ di-proton

E = -3168.59908

Ni	0.139754	-0.000001	0.000009
P	1.025004	-1.576921	-1.224096
P	-1.075405	0.554899	-1.763689
N	1.553765	0.759469	-2.675709
N	-1.637987	-2.191102	-1.924462
C	1.774955	-0.730567	-2.772757
H	2.863107	-0.895421	-2.790187
H	1.348820	-1.085641	-3.724419

C	0.158463	1.163883	-3.078196
H	-0.026130	0.792687	-4.099473
H	0.138492	2.266010	-3.089011
C	-0.275976	-2.698437	-2.019656
H	0.026070	-2.926470	-3.072520
H	-0.231018	-3.651777	-1.461902
C	-1.848430	-0.941473	-2.645985
H	-2.935336	-0.753074	-2.678142
H	-1.504830	-0.984516	-3.709277
C	2.389299	-2.844619	-0.861235
H	1.944875	-3.437060	-0.031656
C	2.738526	-3.819229	-2.009136
H	1.838008	-4.338942	-2.379401
H	3.153353	-3.250026	-2.865574
C	3.781314	-4.859033	-1.549195
H	3.326436	-5.505832	-0.773426
H	4.035476	-5.520308	-2.395714
C	5.045730	-4.193137	-0.987506
H	5.750439	-4.959056	-0.620858
H	5.569312	-3.650478	-1.799133
C	4.702573	-3.206997	0.140192
H	5.613544	-2.694164	0.497310
H	4.291422	-3.766055	1.004891
C	3.667479	-2.165923	-0.327366
H	4.126979	-1.552836	-1.129873
H	3.422189	-1.456875	0.488022
C	-2.393219	1.893192	-1.968239
H	-1.881517	2.803377	-1.589391
C	-3.595385	1.617306	-1.041850
H	-4.090845	0.672906	-1.344458
H	-3.232980	1.484477	-0.007731
C	-4.624188	2.762303	-1.116654
H	-5.488903	2.523222	-0.471987
H	-4.168508	3.684726	-0.704538
C	-5.083216	3.020254	-2.559545
H	-5.785822	3.870818	-2.591384
H	-5.642006	2.138650	-2.930859
C	-3.884733	3.289754	-3.480780
H	-3.392301	4.235818	-3.180995
H	-4.218055	3.426733	-4.524388
C	-2.853404	2.144012	-3.421777
H	-3.317854	1.224254	-3.828414
H	-1.998735	2.385737	-4.080794
C	2.609321	1.557742	-3.376360
H	2.430470	2.627253	-3.190605

H	2.562599	1.354412	-4.456355
C	-2.597340	-3.221031	-2.353998
H	-2.460483	-4.127218	-1.740815
H	-2.485209	-3.504616	-3.424159
P	-1.075299	-0.554886	1.763781
P	1.025121	1.576891	1.224066
N	-1.637803	2.191131	1.924647
N	1.553930	-0.759526	2.675611
C	-1.848212	0.941495	2.646168
H	-2.935119	0.753121	2.678425
H	-1.504511	0.984514	3.709428
C	-0.275772	2.698437	2.019726
H	0.026362	2.926464	3.072565
H	-0.230837	3.651775	1.461968
C	0.158649	-1.163926	3.078186
H	-0.025866	-0.792756	4.099486
H	0.138663	-2.266053	3.088970
C	1.775149	0.730505	2.772672
H	2.863305	0.895341	2.790041
H	1.349075	1.085571	3.724364
C	-2.393138	-1.893150	1.968383
H	-1.881370	-2.803403	1.589792
C	-2.853567	-2.143685	3.421893
H	-1.999012	-2.385280	4.081102
H	-3.318087	-1.223846	3.828270
C	-3.884904	-3.289417	3.480950
H	-3.392417	-4.235541	3.181439
H	-4.218403	-3.426188	4.524529
C	-5.083230	-3.020107	2.559456
H	-5.785839	-3.870667	2.591348
H	-5.642086	-2.138430	2.930497
C	-4.623958	-2.762450	1.116592
H	-5.488564	-2.523505	0.471728
H	-4.168200	-3.684954	0.704742
C	-3.595150	-1.617461	1.041732
H	-4.090671	-0.673004	1.344058
H	-3.232574	-1.484842	0.007645
C	2.389429	2.844553	0.861135
H	1.945041	3.436910	0.031476
C	3.667636	2.165802	0.327399
H	4.127095	1.552800	1.129994
H	3.422386	1.456667	-0.487924
C	4.702752	3.206827	-0.140218
H	5.613740	2.693958	-0.497238
H	4.291642	3.765794	-1.004996

C	5.045853	4.193087	0.987392
H	5.750579	4.958969	0.620697
H	5.569398	3.650515	1.799101
C	3.781410	4.859040	1.548951
H	3.326567	5.505757	0.773093
H	4.035530	5.520404	2.395413
C	2.738602	3.819282	2.008952
H	3.153391	3.250169	2.865468
H	1.838065	4.339031	2.379121
C	-2.597094	3.221076	2.354283
H	-2.460271	4.127268	1.741100
H	-2.484861	3.504643	3.424438
C	2.609522	-1.557829	3.376172
H	2.430640	-2.627334	3.190410
H	2.562881	-1.354519	4.456174
H	3.596723	-1.271880	2.984476
H	-3.625053	2.854446	2.197598
H	-3.625276	-2.854375	-2.197227
H	3.596545	1.271783	-2.984729
H	1.554006	0.934122	-1.613107
H	1.554095	-0.934159	1.613006