Supplementary Material (ESI) for Dalton Transactions

Nickel(II) hydride and fluoride pincer complexes and their reactivity with Lewis acids $BX_3 \bullet L$ (X = H, L = thf; X = F, L = Et_2O)

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Supporting Information

Table S1. Crystal data and structure refinement for **2**.

CCDC number	786190
Empirical formula	C_{24} H_{43} F Ni P_2
Formula weight	471.23
Temperature	150(2) K
Wavelength	0.71069 Å
Crystal system	Tetragonal
Space group	*I* 4_1 *c d*
Unit cell dimensions	a = b = 16.044(7) Å; c = 19.529(10) Å
Volume	5027(3) $Å^3$
Z	8
Density (calculated)	1.245 Mg/m^3
Absorption coefficient	0.914 mm^{-1}
F(000)	2032
Crystal size	0.05 x 0.05 x 0.2 mm^3
Theta range for data collection	4.23 to 29.00°.
Index ranges	-21<=h<=20, -20<=k<=21, -26<=l<=26
Reflections collected	15468
Independent reflections	3014 [R(int) = 0.0524]
Completeness to theta = 25.00°	99.4 %
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3014 / 1 / 135
Goodness-of-fit on F^2	0.860
Final R indices [I>2sigma(I)]	R1 = 0.0304, wR2 = 0.0648
R indices (all data)	R1 = 0.0595, wR2 = 0.0702
Absolute structure parameter	-0.003(15)
Largest diff. peak and hole	0.314 and -0.236 $e.Å^{-3}$
Absorption correction	Semiempirical from equivalents

Table S2. Selected bond lengths [Å] and angles [°] for **2**.

C(1)-Ni(1)	1.917(4)
F(1)-Ni(1)	1.867(3)
P(2)-Ni(1)	2.1702(8)
Ni(1)-P(2)#1	2.1702(8)
F(1)-Ni(1)-C(1)	180.0
F(1)-Ni(1)-P(2)#1	93.95(2)
C(1)-Ni(1)-P(2)#1	86.05(2)
F(1)-Ni(1)-P(2)	93.95(2)
C(1)-Ni(1)-P(2)	86.05(2)
P(2)#1-Ni(1)-P(2)	172.09(5)

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,-y,z

Table S3. Crystal data and structure refinement for **5**.

CCDC number	786191
Empirical formula	C_{24} H_{45} B F_4 Ni O P_2
Formula weight	557.06
Temperature	123(2) K
Wavelength	0.71069 Å
Crystal system	Orthorhombic
Space group	*P b c a*
Unit cell dimensions	a = 17.280(8) Å
	b =15.826(11) Å
	c = 20.966(13) Å
Volume	5734(6) $Å^3$
Z	8
Density (calculated)	1.291 Mg/m^3
Absorption coefficient	0.829 mm^{-1}
F(000)	2368
Crystal size	0.05 x 0.05 x 0.1 mm^3
Theta range for data collection	4.15 to 22.99°.
Index ranges	-18<=h<=14, -13<=k<=16, -22<=l<=17
Reflections collected	10876
Independent reflections	2958 [R(int) = 0.0723]
Completeness to theta = 20.00°	95.8 %
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2958 / 0 / 304
Goodness-of-fit on F^2	0.755
Final R indices [I>2sigma(I)]	R1 = 0.0326, wR2 = 0.0465
R indices (all data)	R1 = 0.0806, wR2 = 0.0525
Largest diff. peak and hole	0.261 and -0.222 $e.Å^{-3}$
Absorption correction	Semiempirical from equivalents

Table S4. Selected bond lengths [Å] and angles [°] for **5**.

C(1)-Ni(1)	1.905(4)
B(1)-F(2)	1.378(5)
B(1)-F(3)	1.385(5)
B(1)-F(4)	1.394(5)
B(1)-F(1)	1.407(5)
O(1)-Ni(1)	1.964(3)
O(1)-H(1A)	0.79(4)
O(1)-H(1B)	0.73(3)
P(1)-Ni(1)	2.2078(12)
P(2)-Ni(1)	2.2099(13)
F(2)-B(1)-F(3)	110.8(4)
F(2)-B(1)-F(4)	109.9(4)
F(3)-B(1)-F(4)	109.1(4)
F(2)-B(1)-F(1)	109.8(4)
F(3)-B(1)-F(1)	108.7(4)
F(4)-B(1)-F(1)	108.5(4)
Ni(1)-O(1)-H(1A)	117(3)
Ni(1)-O(1)-H(1B)	127(4)
H(1A)-O(1)-H(1B)	116(5)
C(1)-Ni(1)-P(1)	85.19(15)
O(1)-Ni(1)-P(1)	94.18(10)
C(1)-Ni(1)-P(2)	85.66(15)
O(1)-Ni(1)-P(2)	95.01(10)
P(1)-Ni(1)-P(2)	170.72(4)

Table S5. Hydrogen bonds for **5** [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(1)-H(1A)...F(1)#1	0.79(4)	1.91(4)	2.683(4)	166(4)
O(1)-H(1B)...F(3)	0.73(3)	2.58(4)	3.111(4)	132(4)
O(1)-H(1B)...F(4)	0.73(3)	2.04(3)	2.761(3)	171(5)

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

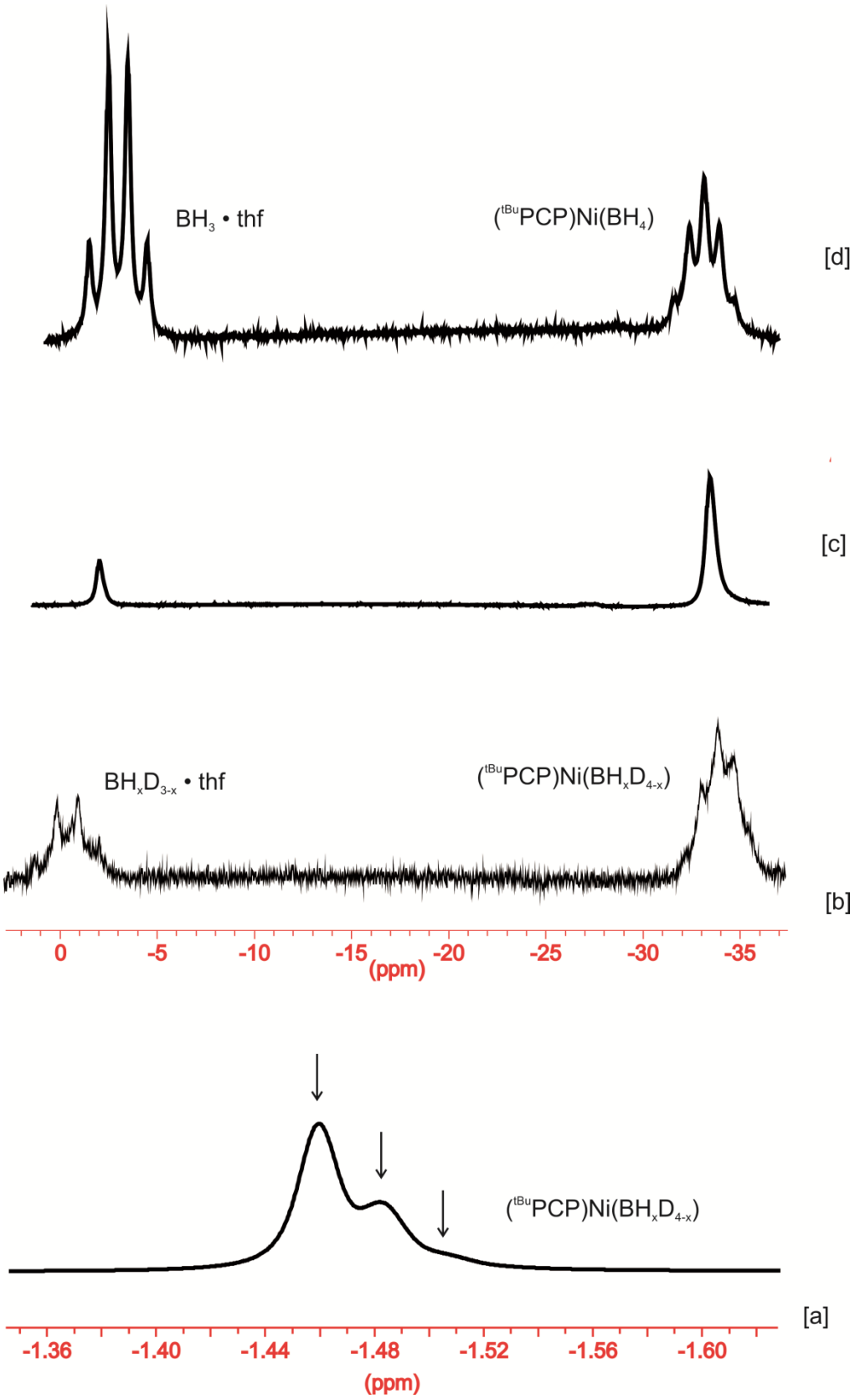
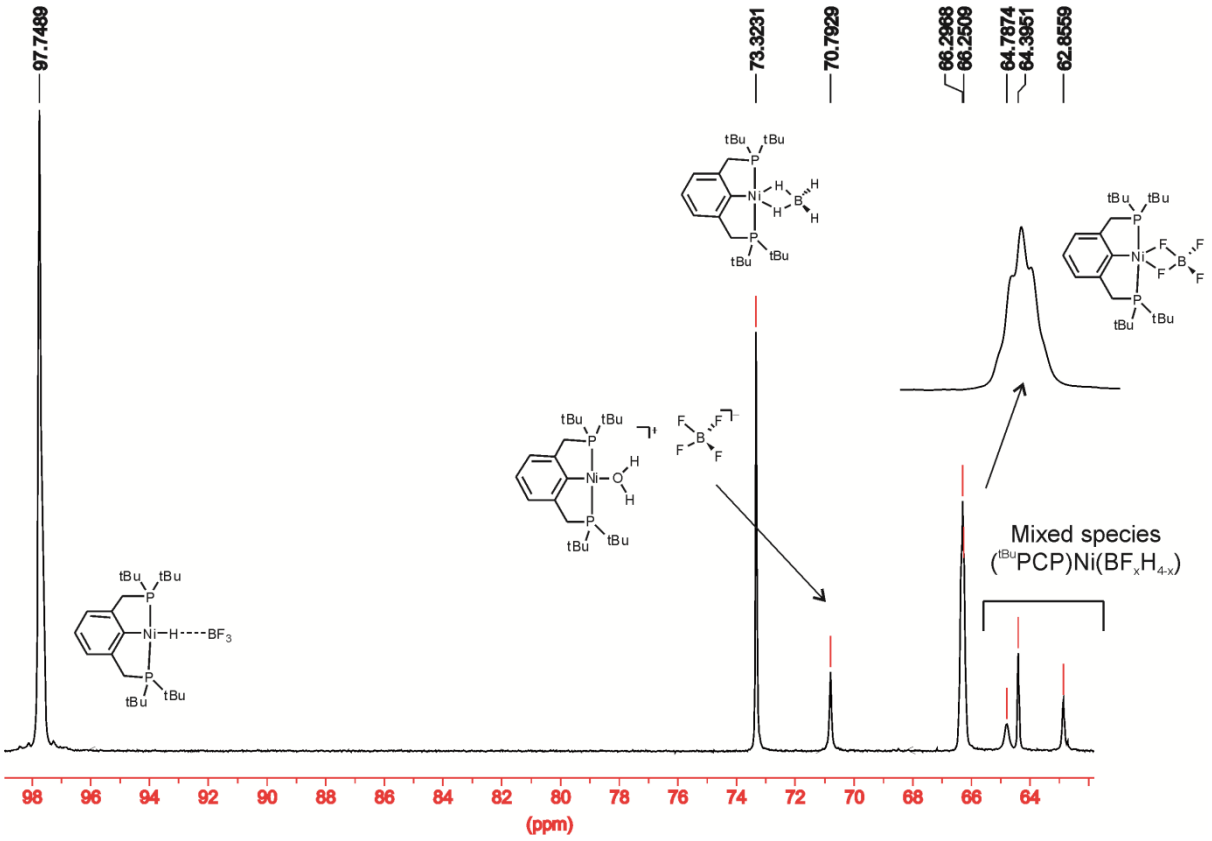
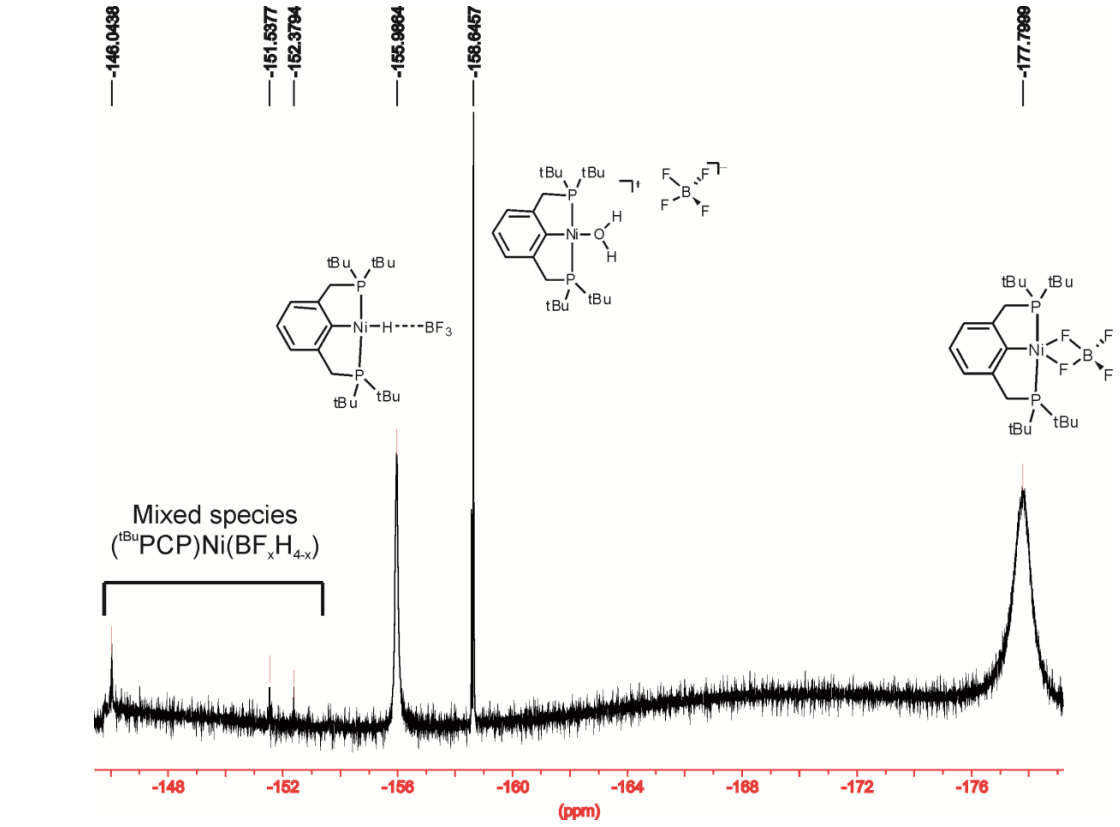


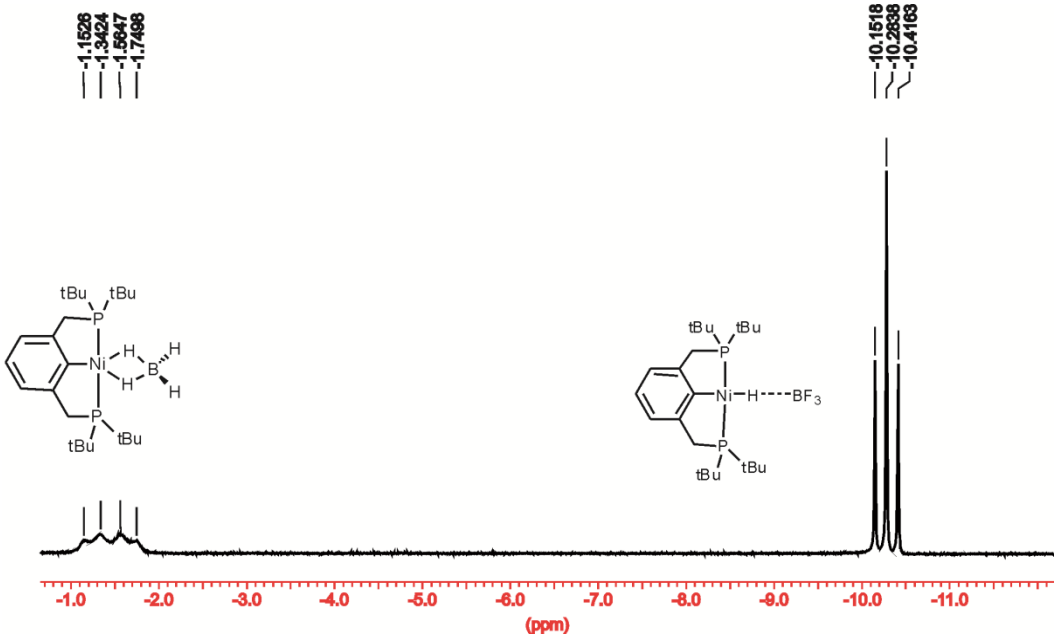
Figure S1. (a) $^{1}H\{^{11}B\}$ NMR spectrum of the **1-*d*$_1$** + BH_3 • thf mixture, at 298 K . (b) ^{11}B and (c) $^{11}B\{^{1}H\}$ NMR spectra of the same mixture, and comparison with the deuterium-free system (d).


97.7489
73.3231
70.7929
66.2968
66.2509
64.7874
64.3951
62.8559
Mixed species
(tBuPCP)Ni(BFxH4-x)
98
96
94
92
90
88
86
84
82
80
78
76
74
72
70
68
66
64
(ppm)

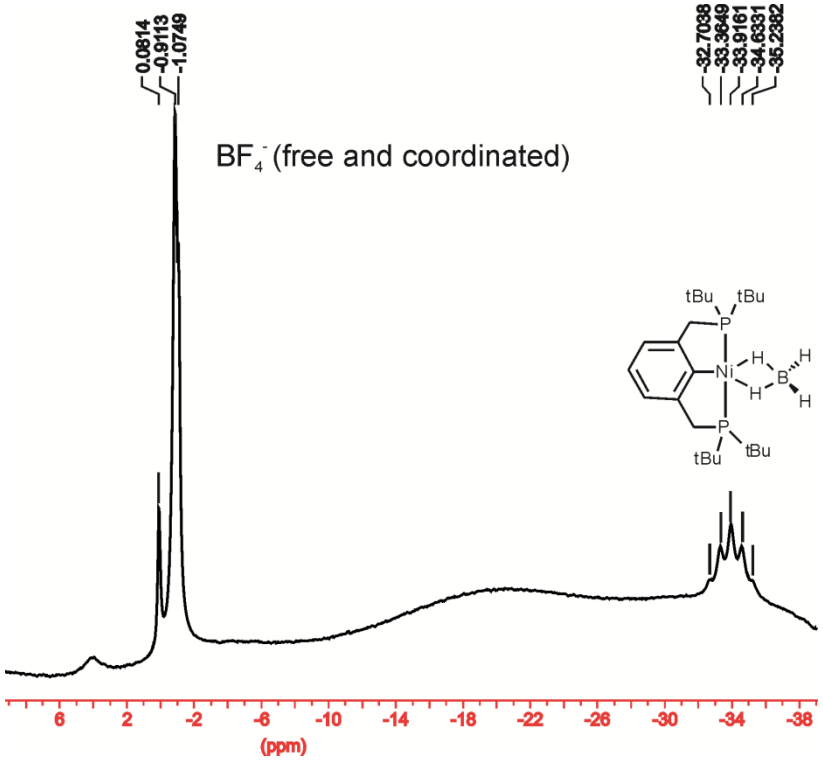
(a)


-146.0438
-151.5377
-152.3794
-155.9864
-158.6457
-177.7899
Mixed species
(tBuPCP)Ni(BFxH4-x)
-148
-152
-156
-160
-164
-168
-172
-176
(ppm)

(b)

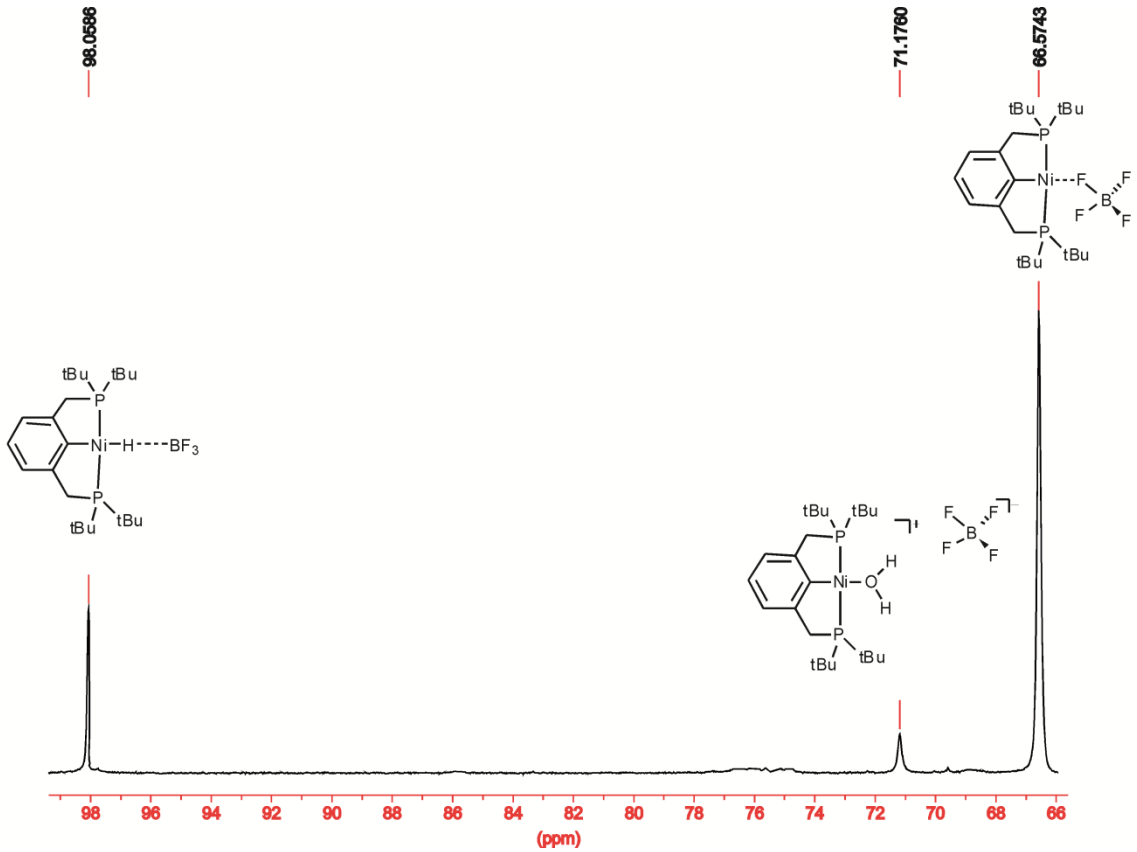


(c)

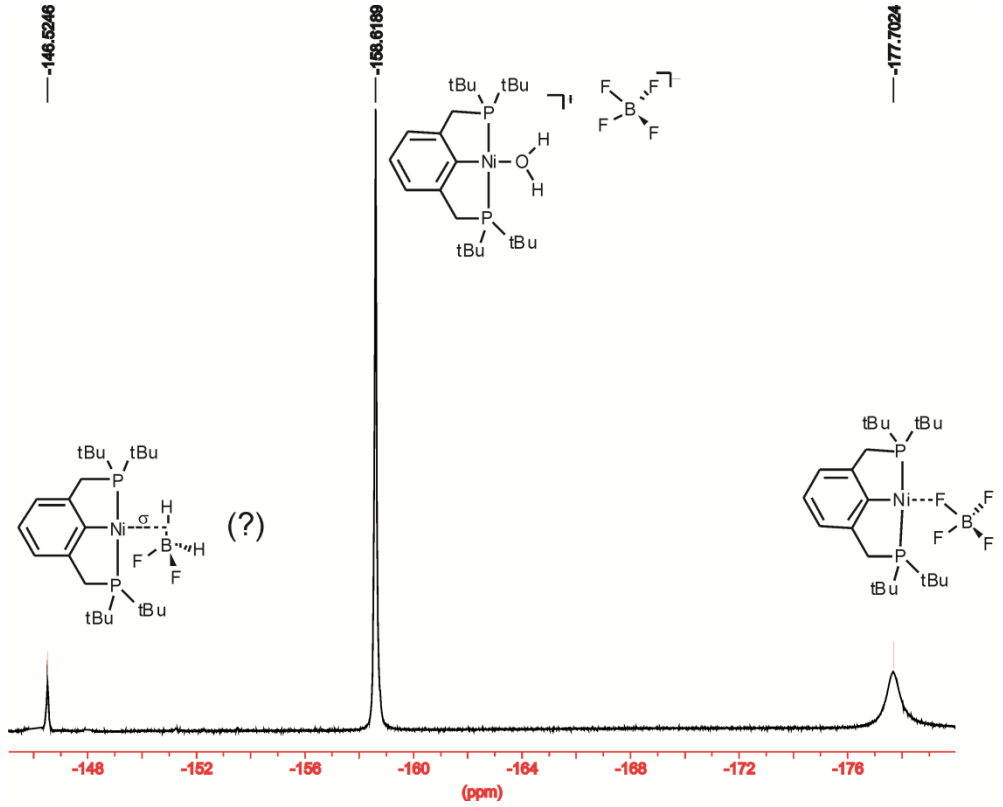


(d)

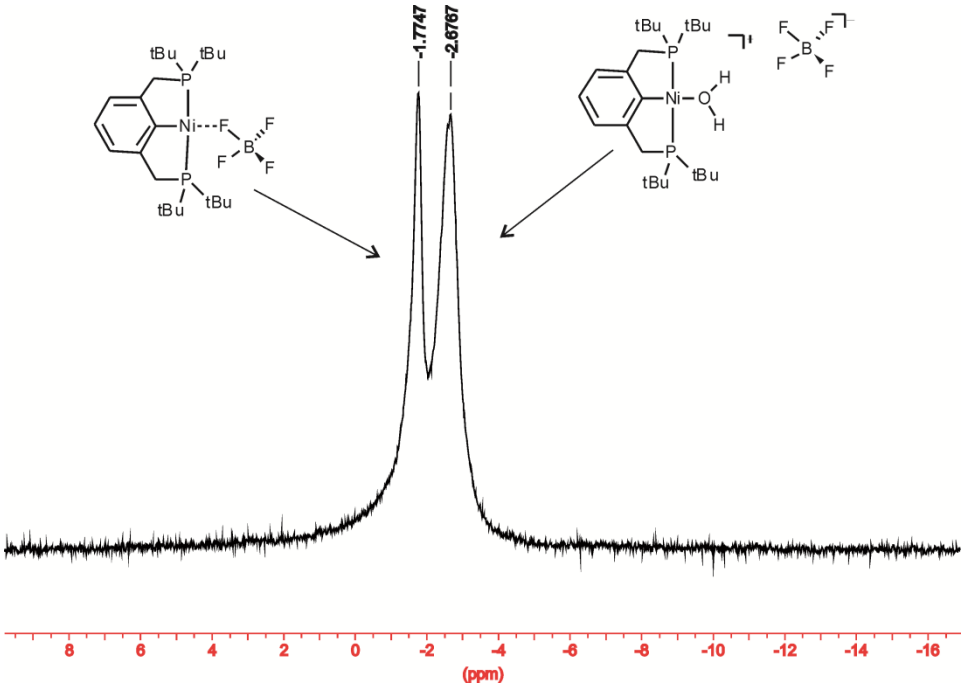
Figure S2. (a) $^{31}P\{^{1}H\}$, (b) $^{19}F\{^{1}H\}$, (c) ^{1}H and (d) ^{11}B NMR spectra of the **2** + BH_3 • thf mixture at ambient temperature, after reaching the equilibrium.


98.0586
71.1760
66.5743
98
96
94
92
90
88
86
84
82
80
78
76
74
72
70
68
66
(ppm)

(a)


-146.5246
-158.6189
-177.7024
(?)
-148
-152
-156
-160
-164
-168
-172
-176
(ppm)

(b)



(c)

Figure S3. (a) $^{31}P\{^{1}H\}$, (b) $^{19}F\{^{1}H\}$ and (c) ^{11}B NMR spectra of the **1** + $BF_3 \bullet Et_2O$ mixture at ambient temperature.

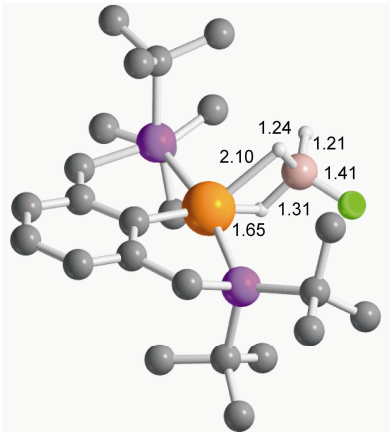


Figure S4. Optimized geometry of (^{tBu}PCP)Ni(η^1-κ,*H*-BH_3F). H atoms on the pincer ligand omitted for clarity. Selected bond lengths (Å) reported. Atom color code: orange, Ni; white, H; pink, B; gray, C; magenta, P; green, F.

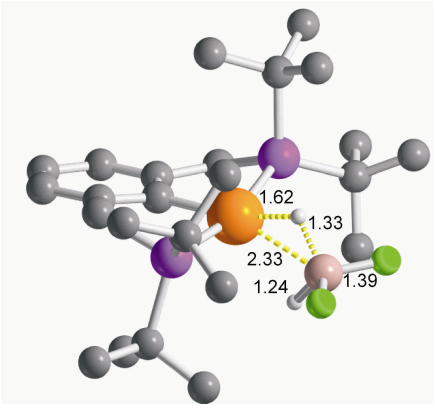


Figure S5. Optimized geometry of (^{tBu}PCP)Ni(σ-BH-BH_2F_2). H atoms on the pincer ligand omitted for clarity. Selected bond lengths (Å) reported. Atom color code: see Figure S4.

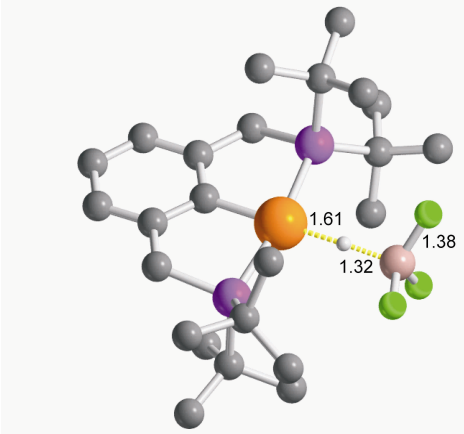


Figure S6. Optimized geometry of (^{tBu}PCP)Ni(η^1-κ,*H*-BHF_3). H atoms on the pincer ligand omitted for clarity. Selected bond lengths (Å) reported. Atom color code: see Figure S4.

Optimised geometries (Cartesian coordinates) and related absolute internal energy (gas-phase).

(^{tBu}PCP)Ni(η^1-BH_4) (3a)

E(gas) = –1149.295711 ha.

Ni	0.021800	-0.418864	-0.224500
P	-2.202637	-0.232227	0.070793
C	0.033377	1.520855	-0.075479
C	-1.099012	2.228644	0.375809
C	-1.117022	3.623339	0.421306
H	-2.016668	4.138344	0.763198
C	0.004455	4.354697	0.049745
H	-0.011203	5.442979	0.085243
C	-2.279472	1.448125	0.867269
H	-3.238155	1.966442	0.716717
H	-2.181209	1.282686	1.951859
C	-3.050886	-1.348608	1.368860
C	-1.968739	-1.661708	2.406542
H	-2.420654	-2.211832	3.246344
H	-1.502244	-0.754183	2.819952
H	-1.176576	-2.286152	1.975212
C	-4.221007	-0.655151	2.071477
H	-4.651893	-1.357236	2.801840
H	-5.024049	-0.370410	1.381539
H	-3.914948	0.239323	2.628357
C	-3.545153	-2.666715	0.774908
H	-2.761603	-3.182047	0.205711
H	-4.420353	-2.527827	0.126149
H	-3.856712	-3.328118	1.598348
C	-3.259980	-0.041138	-1.502693
C	-4.717360	0.297784	-1.198387
H	-4.827398	1.181315	-0.555000
H	-5.249226	-0.540792	-0.730557
H	-5.233747	0.520244	-2.144933
C	-3.207556	-1.304873	-2.361184
H	-3.670584	-2.169338	-1.872191
H	-2.179164	-1.580335	-2.619059
H	-3.760882	-1.113854	-3.293640
C	-2.633113	1.101636	-2.307382
H	-3.176795	1.197752	-3.259726
H	-1.578124	0.901528	-2.537665
H	-2.688636	2.069469	-1.791699
H	0.096982	-2.064465	0.134598
P	2.239074	-0.171163	-0.135229
C	1.171806	2.285442	-0.400323
C	1.153075	3.680567	-0.343773
H	2.052509	4.240993	-0.605335
C	2.442319	1.570441	-0.750156
H	3.334699	2.075595	-0.349169
H	2.580829	1.508381	-1.840699
C	3.475320	-1.144814	-1.215453

C	2.832133	-1.284655	-2.599465
H	3.559823	-1.756166	-3.277782
H	2.561630	-0.313220	-3.038114
H	1.932307	-1.907376	-2.569688
C	4.804828	-0.403431	-1.383485
H	5.452526	-1.003704	-2.040804
H	5.345000	-0.256787	-0.442178
H	4.681642	0.576012	-1.863620
C	3.737529	-2.542457	-0.655086
H	2.804562	-3.089730	-0.469128
H	4.332339	-2.521638	0.268452
H	4.314139	-3.116627	-1.396476
C	2.780415	-0.170830	1.695285
C	4.281347	0.013387	1.902848
H	4.661969	0.934373	1.440175
H	4.864191	-0.834133	1.523015
H	4.483322	0.086124	2.982736
C	2.334275	-1.494487	2.320707
H	2.808985	-2.366180	1.854830
H	1.247402	-1.624796	2.241752
H	2.602455	-1.497229	3.388548
C	2.052482	0.964258	2.421164
H	2.318929	0.917203	3.488460
H	0.961417	0.875793	2.335936
H	2.336368	1.958165	2.049122
H	-0.134475	-1.633281	-1.883974
B	-0.105591	-2.546124	-1.046071
H	0.847048	-3.274250	-1.232541
H	-1.159163	-3.143219	-1.009522

(^{tBu}PCP)Ni(η^2-BH_4) (3b)

E(gas) = –1149.293799 ha.

C	0.002550	1.532234	-0.005387
C	-1.149583	2.272666	0.330596
C	-1.150931	3.668545	0.325386
H	-2.065311	4.204751	0.586825
C	-0.000037	4.373935	0.000632
H	-0.001340	5.462813	0.002757
C	-2.394562	1.535741	0.717201
H	-3.316070	2.036139	0.382809
H	-2.463296	1.465190	1.813538
C	-3.016054	-0.184669	-1.651735
C	-2.831095	-1.543551	-2.328545
H	-3.384727	-2.346021	-1.828409
H	-1.776147	-1.840422	-2.365043
H	-3.205074	-1.475226	-3.361661
C	-2.251442	0.860347	-2.470976
H	-2.643518	0.852440	-3.499820
H	-1.176639	0.634136	-2.513199
H	-2.364979	1.879765	-2.077127

C	-4.498263	0.177933	-1.640749
H	-4.697942	1.135737	-1.141489
H	-5.112032	-0.597585	-1.165869
H	-4.848779	0.276055	-2.679949
C	-3.304009	-1.177660	1.333851
C	-2.416587	-1.413685	2.560922
H	-1.954470	-0.486688	2.934906
H	-1.611422	-2.123754	2.341254
H	-3.032485	-1.826533	3.374554
C	-3.768527	-2.529733	0.795722
H	-2.936061	-3.126523	0.405406
H	-4.531657	-2.426857	0.012800
H	-4.229577	-3.094831	1.620724
C	-4.537561	-0.379262	1.767106
H	-5.128190	-1.005387	2.453474
H	-5.192226	-0.110327	0.929108
H	-4.283592	0.538895	2.311310
P	-2.229942	-0.203241	0.083858
Ni	-0.000875	-0.419853	-0.021271
C	1.152952	2.274516	-0.337605
C	1.152309	3.670960	-0.326378
H	2.065979	4.209353	-0.584846
C	2.398613	1.538672	-0.721142
H	3.319062	2.039144	-0.383800
H	2.470967	1.467021	-1.817282
C	2.984571	-0.181836	1.659901
C	2.782621	-1.538783	2.335836
H	3.338252	-2.345239	1.844958
H	1.725407	-1.828995	2.359209
H	3.142327	-1.471364	3.373710
C	2.214480	0.866118	2.468516
H	2.593062	0.855507	3.501986
H	1.138788	0.644819	2.497030
H	2.338173	1.884923	2.077356
C	4.468681	0.174223	1.673452
H	4.680430	1.132724	1.180437
H	5.088448	-0.602430	1.207473
H	4.801937	0.268377	2.718381
C	3.333181	-1.172953	-1.316759
C	2.472875	-1.417802	-2.560409
H	2.021927	-0.492910	-2.952288
H	1.661856	-2.124843	-2.352789
H	3.105885	-1.838428	-3.356728
C	3.792124	-2.521289	-0.763572
H	2.954538	-3.121302	-0.390631
H	4.536800	-2.410152	0.035966
H	4.274254	-3.086630	-1.576539
C	4.572147	-0.370582	-1.729123
H	5.178461	-0.996757	-2.401749
H	5.210082	-0.094690	-0.880791
H	4.323725	0.544083	-2.282261
P	2.230140	-0.201505	-0.090592
B	-0.004823	-2.671151	-0.039577

H	-1.020887	-3.331418	-0.010850
H	0.037218	-1.952436	0.991317
H	1.006140	-3.338458	-0.080703
H	-0.042391	-1.937325	-1.059437

(^{tBu}PCP)Ni(η^2-κ,*H*:κ,*H*-BH_3F)

E(gas) = -1248.574062 ha.

C	-0.068477	1.619562	-0.181573
C	1.068026	2.376925	-0.527229
C	1.027650	3.771605	-0.580898
H	1.928610	4.323901	-0.854013
C	-0.144255	4.455869	-0.286640
H	-0.176402	5.543110	-0.338349
C	2.353921	1.663154	-0.803062
H	3.233165	2.210129	-0.429453
H	2.505260	1.531768	-1.885350
C	2.757977	0.108831	1.743108
C	2.449618	-1.218501	2.440611
H	3.020601	-2.059718	2.031135
H	1.383085	-1.469893	2.362076
H	2.701234	-1.130898	3.508892
C	1.921516	1.201639	2.414557
H	2.192148	1.237641	3.481323
H	0.844647	0.999016	2.341583
H	2.101522	2.198343	1.989993
C	4.233105	0.462297	1.915342
H	4.497412	1.402227	1.409750
H	4.902369	-0.327735	1.553986
H	4.443548	0.601895	2.986990
C	3.511997	-1.001451	-1.101375
C	2.841213	-1.359722	-2.431010
H	2.398124	-0.485218	-2.930251
H	2.057834	-2.110192	-2.292143
H	3.602672	-1.772984	-3.110131
C	3.981670	-2.284640	-0.417350
H	3.145174	-2.930638	-0.134125
H	4.605219	-2.081631	0.463881
H	4.605684	-2.847172	-1.128883
C	4.739855	-0.133148	-1.402972
H	5.459227	-0.749321	-1.963444
H	5.251848	0.226317	-0.503017
H	4.504895	0.733138	-2.033528
P	2.208603	-0.041017	-0.075329
Ni	-0.027514	-0.324866	-0.125227
C	-1.228412	2.342624	0.163350
C	-1.269216	3.736277	0.094241
H	-2.190039	4.260118	0.357217
C	-2.422341	1.592779	0.668467
H	-3.379578	2.050608	0.377965
H	-2.409961	1.575485	1.769223

C	-3.263402	-0.224540	-1.520832
C	-3.129057	-1.582528	-2.210910
H	-3.570111	-2.401447	-1.630337
H	-2.082965	-1.841382	-2.411208
H	-3.660928	-1.534972	-3.173808
C	-2.650098	0.837446	-2.439034
H	-3.153850	0.787624	-3.416359
H	-1.578068	0.662486	-2.600018
H	-2.772052	1.858024	-2.052323
C	-4.744995	0.086167	-1.312940
H	-4.917244	1.026713	-0.771438
H	-5.269950	-0.720772	-0.784663
H	-5.223539	0.188651	-2.299085
C	-3.094705	-1.150816	1.499117
C	-2.052497	-1.255151	2.616761
H	-1.671734	-0.272957	2.934111
H	-1.194923	-1.867305	2.311528
H	-2.514894	-1.729106	3.496128
C	-3.478652	-2.559861	1.054161
H	-2.643578	-3.083301	0.571546
H	-4.333657	-2.553210	0.365215
H	-3.778593	-3.142428	1.938845
C	-4.336282	-0.447887	2.054048
H	-4.761029	-1.073424	2.853982
H	-5.119440	-0.306666	1.300635
H	-4.109351	0.530139	2.497167
P	-2.255886	-0.166575	0.096284
B	-0.057681	-2.544498	-0.714202
F	1.121117	-3.320595	-0.682471
H	-0.082134	-1.884164	0.412617
H	-1.060114	-3.228901	-0.689513
H	-0.077099	-1.745528	-1.666713

(^{tBu}PCP)Ni(σ-*BH*-BH_2F_2)

E(gas) = -1347.864444 ha.

C	0.062076	1.684359	-0.265546
C	1.206254	2.389145	-0.685651
C	1.197837	3.779462	-0.816403
H	2.102456	4.292454	-1.147508
C	0.055015	4.508460	-0.515848
H	0.047107	5.591661	-0.627136
C	2.473604	1.627974	-0.917354
H	3.364560	2.177677	-0.577745
H	2.624280	1.410667	-1.985632
C	2.770930	0.240630	1.763859
C	2.340205	-1.007373	2.539758
H	2.861408	-1.914406	2.211898
H	1.261396	-1.186388	2.438880
H	2.563532	-0.860954	3.607855
C	2.000298	1.436774	2.330102

H	2.256235	1.537392	3.396259
H	0.913248	1.301518	2.250478
H	2.256204	2.383002	1.834316
C	4.262792	0.488905	1.971666
H	4.623747	1.370093	1.422735
H	4.876093	-0.374907	1.688351
H	4.444964	0.678565	3.040719
C	3.543792	-1.096872	-0.979571
C	2.921219	-1.466222	-2.329946
H	2.595112	-0.585404	-2.901588
H	2.066884	-2.137258	-2.213986
H	3.681425	-1.983421	-2.934960
C	3.869009	-2.376083	-0.210561
H	2.968925	-2.942651	0.052857
H	4.451422	-2.175115	0.698847
H	4.485426	-3.024092	-0.852202
C	4.842501	-0.331034	-1.255170
H	5.526899	-1.005504	-1.792000
H	5.359127	-0.000716	-0.347666
H	4.685804	0.543191	-1.899391
P	2.267842	-0.009434	-0.060644
Ni	0.037569	-0.250086	-0.111597
C	-1.058798	2.454139	0.101286
C	-1.068033	3.842273	-0.041013
H	-1.959982	4.405258	0.239441
C	-2.226178	1.758601	0.726842
H	-3.185833	2.264792	0.547565
H	-2.086210	1.731359	1.818883
C	-3.252426	0.022610	-1.444745
C	-3.263282	-1.345897	-2.126648
H	-3.778783	-2.112713	-1.538613
H	-2.250762	-1.711790	-2.331032
H	-3.792960	-1.247645	-3.086913
C	-2.585071	1.019049	-2.397205
H	-3.141554	1.018173	-3.346877
H	-1.545403	0.739807	-2.613493
H	-2.584693	2.046580	-2.010846
C	-4.689302	0.471086	-1.182929
H	-4.748131	1.455217	-0.698147
H	-5.251413	-0.249415	-0.575019
H	-5.212355	0.556936	-2.147826
C	-3.103275	-0.935407	1.562489
C	-2.014296	-1.305637	2.573268
H	-1.411128	-0.437372	2.882176
H	-1.332783	-2.063372	2.165313
H	-2.483825	-1.719882	3.478787
C	-3.795460	-2.215132	1.095211
H	-3.131579	-2.863320	0.514675
H	-4.694684	-2.002320	0.501712
H	-4.124568	-2.774703	1.984545
C	-4.142940	-0.047168	2.252040
H	-4.670330	-0.650069	3.006908
H	-4.898500	0.339581	1.557102

H	-3.695866	0.804542	2.779306
P	-2.201837	-0.009512	0.148280
B	-0.115687	-2.487368	-0.752948
H	-0.123837	-1.740173	-1.740157
H	0.079956	-1.794593	0.365186
F	-1.328434	-3.147741	-0.562201
F	0.935832	-3.401890	-0.774325

(^{tBu}PCP)Ni(η^1-κ,*H*-BHF_3)

E(gas) = -1447.161576 ha.

C	-0.000848	1.897390	-0.006970
C	-1.170300	2.631131	0.276816
C	-1.186572	4.025385	0.217734
H	-2.112572	4.560456	0.435046
C	-0.033262	4.730719	-0.100445
H	-0.046857	5.818776	-0.140480
C	-2.407819	1.894049	0.681945
H	-3.334682	2.376231	0.336468
H	-2.468099	1.858060	1.779558
C	-2.968312	0.089998	-1.642987
C	-2.699145	-1.291450	-2.242992
H	-3.218572	-2.096090	-1.710218
H	-1.626893	-1.533192	-2.244122
H	-3.046895	-1.301695	-3.287422
C	-2.224157	1.130702	-2.484608
H	-2.609013	1.084574	-3.514909
H	-1.143555	0.933014	-2.517821
H	-2.366362	2.156561	-2.118360
C	-4.461007	0.406562	-1.674047
H	-4.687532	1.392829	-1.244905
H	-5.063289	-0.345106	-1.149692
H	-4.801829	0.423486	-2.720610
C	-3.293219	-0.830158	1.368857
C	-2.331257	-1.138864	2.521063
H	-1.830243	-0.235387	2.903591
H	-1.559892	-1.855486	2.209366
H	-2.892038	-1.584689	3.356815
C	-3.865820	-2.142752	0.834002
H	-3.100729	-2.807621	0.425550
H	-4.644763	-1.978509	0.078478
H	-4.342353	-2.671064	1.674156
C	-4.463527	0.012976	1.885328
H	-5.058282	-0.606978	2.572974
H	-5.135635	0.340257	1.081297
H	-4.147078	0.898481	2.448961
P	-2.233381	0.136863	0.103319
Ni	0.000958	-0.036425	0.030481
C	1.155907	2.637107	-0.323797
C	1.137660	4.032902	-0.362336
H	2.052899	4.573692	-0.609365
C	2.423795	1.908550	-0.644263

H	3.317872	2.398428	-0.228907
H	2.573863	1.871115	-1.733126
C	2.967966	0.132058	1.693465
C	2.617751	-1.198393	2.360205
H	3.050523	-2.065658	1.848613
H	1.531581	-1.356487	2.399726
H	2.998217	-1.189149	3.393373
C	2.291219	1.253374	2.487559
H	2.668118	1.223765	3.521296
H	1.200136	1.126937	2.521498
H	2.500144	2.253475	2.084370
C	4.478200	0.348120	1.713281
H	4.779714	1.273897	1.202982
H	5.024183	-0.490311	1.263240
H	4.813770	0.428758	2.758554
C	3.251017	-0.818247	-1.326014
C	2.361880	-0.891190	-2.573209
H	2.074014	0.103384	-2.945753
H	1.450781	-1.472596	-2.385869
H	2.918083	-1.391972	-3.380211
C	3.572077	-2.235001	-0.855939
H	2.682132	-2.804093	-0.570057
H	4.275885	-2.239784	-0.012722
H	4.056596	-2.774944	-1.683777
C	4.560573	-0.109993	-1.681893
H	5.074048	-0.704302	-2.453029
H	5.243361	-0.027233	-0.828227
H	4.409749	0.893226	-2.099648
P	2.225591	0.158460	-0.052826
B	0.059777	-2.957875	-0.062961
H	-0.009886	-1.645774	0.101216
F	0.384127	-3.177672	-1.386401
F	1.028960	-3.396614	0.812740
F	-1.183564	-3.457015	0.258274

(^{tBu}PCP)Ni(η^1-BF_4) (4)

E(gas) = -1546.454102 ha.

C	-0.056798	2.040180	-0.105147
C	1.126217	2.775753	-0.331580
C	1.103136	4.168165	-0.433110
H	2.039063	4.702548	-0.605075
C	-0.090092	4.868861	-0.333869
H	-0.102763	5.953728	-0.424986
C	2.435872	2.069773	-0.510381
H	3.257304	2.556351	0.037427
H	2.725153	2.093482	-1.570420
C	2.937226	0.154777	1.728852
C	2.594051	-1.223576	2.297112
H	3.085496	-2.042259	1.759020
H	1.514943	-1.422745	2.271623
H	2.924593	-1.267089	3.346456

C	2.222024	1.216398	2.570220
H	2.557851	1.125006	3.614293
H	1.130820	1.082358	2.553505
H	2.438770	2.241573	2.240005
C	4.443618	0.386693	1.791902
H	4.744851	1.343673	1.341859
H	5.004867	-0.418944	1.301479
H	4.760460	0.407022	2.845961
C	3.237843	-0.636945	-1.327208
C	2.353243	-0.638895	-2.579081
H	2.078533	0.376394	-2.903215
H	1.434877	-1.216844	-2.417964
H	2.904216	-1.109416	-3.407503
C	3.524291	-2.076602	-0.906634
H	2.626957	-2.626814	-0.605591
H	4.259531	-2.125400	-0.091891
H	3.958331	-2.610783	-1.765557
C	4.566336	0.054101	-1.643155
H	5.083052	-0.533719	-2.417108
H	5.234517	0.106378	-0.775247
H	4.444566	1.068316	-2.043524
P	2.220540	0.293932	-0.018565
Ni	-0.029232	0.131346	0.056917
C	-1.256434	2.777809	0.013832
C	-1.266802	4.167719	-0.113250
H	-2.214232	4.701883	-0.023354
C	-2.543973	2.076068	0.328742
H	-3.393586	2.454210	-0.259847
H	-2.808299	2.239734	1.383517
C	-2.983162	-0.167267	-1.605376
C	-2.527940	-1.576206	-1.987486
H	-2.907816	-2.350114	-1.310560
H	-1.433140	-1.666244	-1.997353
H	-2.893655	-1.806052	-2.999845
C	-2.378750	0.822151	-2.605643
H	-2.715460	0.547170	-3.616469
H	-1.280199	0.789769	-2.597963
H	-2.689334	1.860209	-2.424213
C	-4.504893	-0.069656	-1.650313
H	-4.876622	0.912181	-1.323490
H	-4.986112	-0.844077	-1.039524
H	-4.843013	-0.219014	-2.687207
C	-3.171147	-0.547393	1.537259
C	-2.247356	-0.337966	2.743202
H	-2.000867	0.721528	2.911630
H	-1.306113	-0.892327	2.627432
H	-2.747884	-0.707550	3.651029
C	-3.373651	-2.045111	1.323256
H	-2.447571	-2.567318	1.061403
H	-4.120335	-2.255162	0.545637
H	-3.753306	-2.483085	2.259191
C	-4.526904	0.107339	1.809388
H	-4.992821	-0.398637	2.668751

H	-5.217623	0.012746	0.962111
H	-4.447742	1.170886	2.067885
P	-2.256847	0.262714	0.085031
B	0.097873	-3.217690	-0.139943
F	-0.125089	-1.860596	0.439256
F	1.099620	-3.792813	0.607210
F	-1.097169	-3.891563	-0.043919
F	0.472388	-3.014973	-1.458373