

Supporting Information

Theoretical Study of Oxidative Addition of H₂ and MeCN to Nickel(0) Complex: Significantly Large Correlation Effects and Characteristic Features of the Reaction

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Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Montgomery, Jr., J. A.; Vreven, T.; Kudin, K. N.; Burant, J. C.; Millam, J. M.; Iyengar, S. S.; Tomasi, J.; Barone, V.; Mennucci, B.; Cossi, M.; Scalmani, G.; Rega, N.; Petersson, G. A.; Nakatsuji, H.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Klene, M.; Li, X.; Knox, J. E.; Hratchian, H. P.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Ayala, P. Y.; Morokuma, K.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Zakrzewski, V. G.; Dapprich, S.; Daniels, A. D.; Strain, M. C.; Farkas, O.; Malick, D. K.; Rabuck, A. D.; Raghavachari, K.; Foresman, J. B.; Ortiz, J. V.; Cui, Q.; Baboul, A. G.; Clifford, S.; Cioslowski, J.; Stefanov, B. B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I.; Martin, R. L.; Fox, D. J.; Keith, T.; Al-Laham, M. A.; Peng, C. Y.; Nanayakkara, A.; Challacombe, M.; Gill, P. M. W.; Johnson, B.; Chen, W.; Wong, M. W.; Gonzalez, C.; and Pople, J. A.; Gaussian, Inc., Wallingford CT, 2004.

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Table S1. $\langle S^2 \rangle$ values of broken symmetry Hartree Fock wavefunction.

RC	-2.14	-1.52	-1.04	-0.49	-0.30	-0.10
$\langle S^2 \rangle$	0.5943	0.5981	0.5998	0.6064	0.5919	0.5704
RC	0	+0.10	+0.40	+0.60	+1.19	+1.78
$\langle S^2 \rangle$	0.5435	0.5034	0.4333	0.3720	0.3243	0.3207

Table S2. IRC-calculated Cartesian coordinates of the oxidative

addition of H ₂ to Ni(PH ₃) ₂									
(A) Ni(H ₂)(PH ₃) ₂ RC = -2.14080									
28	0.000000	0.000000	0.000000	0.000000	0.000000	-0.330733	1.843053	-2.505430	
15	0.000000	-1.808416	-1.105401	-1.105401	-1.105401	-0.783343	2.929134	-0.768086	
1	-1.253479	-2.413626	-1.393801	-1.393801	-1.393801	0.000000	-0.464317	1.472006	
1	0.503140	-1.911034	-2.431449	-2.431449	-2.431449	0.000000	0.464317	1.472006	
1	0.619331	-3.002878	-0.645211	-0.645211	-0.645211				
15	0.000000	1.808416	-1.105401	-1.105401	-1.105401				
1	1.253479	2.413626	-1.393801	-1.393801	-1.393801				
1	-0.503140	1.911034	-2.431449	-2.431449	-2.431449				
1	-0.619331	3.002878	-0.645211	-0.645211	-0.645211				
1	0.000000	-0.461146	1.474784	1.474784	1.474784				
1	0.000000	0.461146	1.474784	1.474784	1.474784				
(B) Ni(H ₂)(PH ₃) ₂ RC = -1.52172									
28	0.000000	0.000000	0.000000	0.000000	0.000000	-0.330733	1.843053	-2.505430	
15	0.000000	-1.796881	-1.123300	-1.123300	-1.123300	-0.783343	2.929134	-0.768086	
1	-1.218677	-2.516040	-1.255386	-1.255386	-1.255386	0.000000	-0.464317	1.472006	
1	0.330733	-1.843053	-2.505430	-2.505430	-2.505430	0.000000	0.464317	1.472006	
1	0.783343	-2.929134	-0.768086	-0.768086	-0.768086				
15	0.000000	1.796881	-1.123300	-1.123300	-1.123300				
1	1.218677	2.516040	-1.255386	-1.255386	-1.255386				
(C) Ni(H ₂)(PH ₃) ₂ RC = -1.04395									
28	0.000000	0.000000	0.000000	0.000000	0.000000	-0.330733	1.843053	-2.505430	
15	0.000000	-1.781685	-1.147065	-1.147065	-1.147065	-0.783343	2.929134	-0.768086	
1	-1.169788	-2.587924	-1.184287	-1.184287	-1.184287	0.000000	-0.464317	1.472006	
1	0.206521	-1.782637	-2.554089	-2.554089	-2.554089	0.000000	0.464317	1.472006	
1	0.893661	-2.856639	-0.885890	-0.885890	-0.885890				
15	0.000000	1.781685	-1.147065	-1.147065	-1.147065				
1	1.169788	2.587924	-1.184287	-1.184287	-1.184287				
1	-0.206521	1.782637	-2.554089	-2.554089	-2.554089				
1	-0.893661	2.856639	-0.885890	-0.885890	-0.885890				
1	0.000000	-0.465457	1.469443	1.469443	1.469443				
1	0.000000	0.465457	1.469443	1.469443	1.469443				
(D) Ni(H ₂)(PH ₃) ₂ RC = -0.49153									
28	0.000000	0.000000	0.000000	0.000000	0.000000	-0.330733	1.843053	-2.505430	
15	0.000000	-1.766596	-1.184058	-1.184058	-1.184058	-0.783343	2.929134	-0.768086	
1	-1.114527	-2.647262	-1.145344	-1.145344	-1.145344	0.000000	-0.464317	1.472006	
1	0.088379	-1.724929	-2.602797	-2.602797	-2.602797	0.000000	0.464317	1.472006	

1	0.980232	-2.784143	-1.022466	15	0.000000	-1.767031	-1.201108
15	0.000000	1.766596	-1.184058	1	-1.112863	-2.644610	-1.126815
1	1.114527	2.647262	-1.145344	1	0.049841	-1.717168	-2.620258
1	-0.088379	1.724929	-2.602797	1	0.989652	-2.776958	-1.061129
1	-0.980232	2.784143	-1.022466	15	0.000000	1.767031	-1.201108
1	0.000000	-0.471284	1.462228	1	1.112863	2.644610	-1.126815
1	0.000000	0.471284	1.462228	1	-0.049841	1.717168	-2.620258
(E) Ni(H ₂)(PH ₃) ₂ RC = -0.29894				1	-0.989652	2.776958	-1.061129
28	0.000000	0.000000	0.000000	1	0.000000	-0.557544	1.382832
15	0.000000	-1.766608	-1.196745	1	0.000000	0.557544	1.382832
1	-1.112112	-2.647577	-1.132959	(G) Ni(H ₂)(PH ₃) ₂ RC = 0.0000			
1	0.059071	-1.719985	-2.616251	28	0.000000	0.000000	0.000000
1	0.987561	-2.778908	-1.053092	15	0.000000	-1.767332	-1.205109
15	0.000000	1.766608	-1.196745	1	-1.114531	-2.640584	-1.124225
1	1.112112	2.647577	-1.132959	1	0.045082	-1.713978	-2.623590
1	-0.059071	1.719985	-2.616251	1	0.990157	-2.775927	-1.066207
1	-0.987561	2.778908	-1.053092	15	0.000000	1.767332	-1.205109
1	0.000000	-0.500332	1.427349	1	1.114531	2.640584	-1.124225
1	0.000000	0.500332	1.427349	1	-0.045082	1.713978	-2.623590
(F) Ni(H ₂)(PH ₃) ₂ RC = -0.09998				1	-0.990157	2.775927	-1.066207
28	0.000000	0.000000	0.000000	1	0.000000	-0.633546	1.335772

1	0.000000	0.633546	1.335772				
(H) Ni(H ₂)(PH ₃) ₂ RC = +0.09889							
28	0.000000	0.000000	0.000000	0.000000			
15	0.000000	-1.767317	-1.209740				
1	-1.116060	-2.636569	-1.122843				
1	0.040491	-1.710103	-2.627709				
1	0.990815	-2.774766	-1.072335				
15	0.000000	1.767317	-1.209740				
1	1.116060	2.636569	-1.122843				
1	-0.040491	1.710103	-2.627709				
1	-0.990815	2.774766	-1.072335				
1	0.000000	-0.709322	1.289596				
1	0.000000	0.709322	1.289596				
(I) Ni(H ₂)(PH ₃) ₂ RC = +0.39875							
28	0.000000	0.000000	0.000000				
15	0.000000	-1.766014	-1.218697				
1	-1.116076	-2.632674	-1.121415				
1	0.029586	-1.701973	-2.636142				
1	0.994153	-2.770352	-1.087953				
15	0.000000	1.766014	-1.218697				
1	1.116076	2.632674	-1.121415				
(J) Ni(H ₂)(PH ₃) ₂ RC = +0.59822							
28	0.000000	0.000000	0.000000				
15	0.000000	-1.763966	-1.227272				
1	-1.114412	-2.630770	-1.119986				
1	0.017272	-1.694024	-2.644442				
1	0.998396	-2.764905	-1.105257				
15	0.000000	1.763966	-1.227272				
1	1.114412	2.630770	-1.119986				
1	-0.017272	1.694024	-2.644442				
1	-0.998396	2.764905	-1.105257				
1	0.000000	-0.858121	1.196245				
1	0.000000	0.858121	1.196245				
(K) Ni(H ₂)(PH ₃) ₂ RC = +1.18021							
28	0.000000	0.000000	0.000000				
15	0.000000	-1.742020	-1.266409				
1	-1.081264	-2.645997	-1.135835				

Table S3. DFT(B3LYP)-optimized Cartesian coordinates of transition state of oxidative addition of MeCN to Ni(PH₃)₂

1	-0.039780	-1.637633	-2.681005
1	1.035351	-2.710457	-1.205272
15	0.000000	1.742020	-1.266409
1	1.081264	2.645997	-1.135835
1	0.039780	1.637633	-2.681005
1	-1.035351	2.710457	-1.205272
1	0.000000	-0.894409	1.170494
1	0.000000	0.894409	1.170494
(L) Ni(H ₂)(PH ₃) ₂	RC = +1.77984		
28	0.000000	0.000000	0.000000
15	0.000000	-1.715506	-1.300942
1	-1.064241	-2.641508	-1.185760
1	-0.052194	-1.574537	-2.711856
1	1.053183	-2.665919	-1.272689
15	0.000000	1.715506	-1.300942
1	1.064241	2.641508	-1.185760
1	0.052194	1.574537	-2.711856
1	-1.053183	2.665919	-1.272689
1	0.000000	-0.898180	1.167477
1	0.000000	0.898180	1.167477

(A) cc-pVTZ for Ni

28	-0.053929	-0.098062	-0.142447
15	-2.264129	-0.168360	0.273919
1	-3.221158	0.699461	-0.314281
1	-3.042609	-1.349505	0.134250
1	-2.630290	0.099384	1.616805
15	0.695409	1.979665	-0.146827
1	-0.028389	3.156398	-0.479268
1	1.216632	2.446653	1.083083
1	1.837988	2.264668	-0.932398
6	1.531032	-0.898133	0.272328
7	2.551658	-1.031096	0.850033
6	0.460759	-2.030645	-0.665873
1	1.336242	-2.497436	-1.108318
1	-0.048231	-2.734719	-0.008057
1	-0.191726	-1.718394	-1.498640

(B) SDB for Ni

28	0.132581	0.028574	0.127565
15	0.534417	2.203331	-0.242331
1	0.040864	3.266985	0.558365

1	1.846302	2.731568	-0.388116	0.532569	-1.648407	-0.427340
1	0.028840	2.695392	-1.471426	0.296251	-2.658141	-0.994368
15	-1.979962	-0.356454	0.607925	1.995609	-0.853247	0.125489
1	-2.877100	0.509688	1.289530	2.388077	-1.751716	0.595376
1	-2.816207	-0.629575	-0.500474	2.611995	-0.585199	-0.732470
1	-2.284424	-1.525576	1.345569	2.051559	-0.059125	0.887618
6	0.498962	-1.615327	-0.548007			
7	0.293528	-2.582261	-1.193461			
6	1.996767	-0.872595	0.149032			
1	2.362441	-1.852929	0.441559			
1	2.624601	-0.453648	-0.636842			
1	2.016515	-0.241761	1.054186			
(C) Wa-TZ(f) for Ni						
28	0.137304	0.031045	0.105279	0.126062	-0.067954	-0.000011
15	0.493932	2.187464	-0.244016	-0.134960	2.042695	-0.000001
1	0.107620	3.192627	0.681350	0.940134	2.973430	-0.000513
1	1.789334	2.717688	-0.495512	-0.855058	2.666623	-1.053532
1	-0.128567	2.776337	-1.373093	-0.854098	2.666662	1.054162
15	-1.956999	-0.326251	0.536942	2.219401	-0.682923	0.000002
1	-2.789960	0.466902	1.373098	3.352211	0.174562	-0.000248
1	-2.834079	-0.347556	-0.575670	2.664335	-1.517131	1.056505
1	-2.337302	-1.580504	1.069290	2.664222	-1.517612	-1.056167
				-1.558279	-0.909936	0.000001
				-0.716792	-1.793668	0.000005

Table S4. DFT(B3PW91)-optimized Cartesian coordinates of oxidative addition of MeCN to Ni(PH₃)₂, where SDB and 6-31G(d,p) basis sets were employed for Ni and the other atoms, respectively.

(A) Ni(PH₃)₂(MeCN) **1a**

28	0.126062	-0.067954	-0.000011
15	-0.134960	2.042695	-0.000001
1	0.940134	2.973430	-0.000513
1	-0.855058	2.666623	-1.053532
1	-0.854098	2.666662	1.054162
15	2.219401	-0.682923	0.000002
1	3.352211	0.174562	-0.000248
1	2.664335	-1.517131	1.056505
1	2.664222	-1.517612	-1.056167
6	-1.558279	-0.909936	0.000001
7	-0.716792	-1.793668	0.000005

6	-3.024049	-0.681487	0.000004		28	0.000016	-0.144195	-0.085457
1	-3.568594	-1.630822	-0.000149		15	1.927803	-1.036802	0.039295
1	-3.314008	-0.102820	0.881821		1	2.119436	-2.425117	-0.194186
1	-3.313982	-0.102543	-0.881638		1	3.056036	-0.631442	-0.730926
					1	2.603410	-1.009338	1.288536
					15	-1.927705	-1.036975	0.039279
					1	-2.119462	-2.425085	-0.195312
					1	-2.602599	-1.010584	1.288923
					1	-3.056383	-0.630956	-0.729955
					6	-0.000136	1.846147	0.306350
					7	-0.000101	2.052868	1.465904
					6	-0.000093	1.974159	-1.161540
					1	-0.895632	2.507370	-1.490530
					1	0.895385	2.507506	-1.490470
					1	-0.000010	0.969849	-1.662094
(D) Ni(CN)(Me)(PH ₃) ₂ TS ₁₋₂								
					28	-0.062289	-0.103285	-0.152343
					15	-2.236683	-0.144949	0.274437
					1	-3.187919	0.724954	-0.319560
					1	-3.036251	-1.316275	0.177181
					1	-2.573486	0.162075	1.616073
					15	0.700253	1.935434	-0.146837
(B) Ni(PH ₃) ₂ (MeCN) 1b								
28	0.007254	-0.329103	0.000000					
15	0.028965	-1.469923	1.790547					
1	-1.006290	-2.415796	2.041294					
1	1.088581	-2.390455	2.033799					
1	0.027737	-0.964500	3.128472					
15	0.028965	-1.469923	-1.790547					
1	-1.006290	-2.415796	-2.041293					
1	0.027737	-0.964500	-3.128472					
1	1.088581	-2.390455	-2.033799					
6	-0.052011	2.672456	0.000000					
7	-0.029517	1.507642	0.000000					
6	-0.081923	4.124267	0.000000					
1	0.418090	4.521882	-0.889136					
1	-1.118082	4.476484	0.000000					
1	0.418090	4.521882	0.889136					
(C) Ni(PH ₃) ₂ (MeCN) 1c								

1	0.004813	3.120375	-0.509690	-0.333276	-2.531937	0.888906
1	1.180614	2.396088	1.101326	-1.831006	-2.174824	-0.000313
1	1.875123	2.196175	-0.890879	-0.332697	-2.532264	-0.888407
6	1.512254	-0.874333	0.267832			
7	2.541563	-0.991130	0.834246			
6	0.438264	-2.019775	-0.629548			
1	1.316291	-2.493207	-1.062062			
1	-0.066272	-2.712499	0.044599			
1	-0.216418	-1.740426	-1.474801			

Table S5. DFT(B3LYP)-optimized Cartesian coordinates of oxidative addition of MeCN to Ni(PH₃)₂, where SDB and 6-31G(d,p) basis sets were employed for Ni and the other atoms, respectively.

(A) Ni(PH₃)₂(MeCN) 1a						
28	0.123562	-0.061326	-0.000090			
15	-0.129554	2.072121	-0.000010			
1	0.953069	2.994337	-0.004059			
1	-0.848968	2.698223	-1.052611			
1	-0.841351	2.698451	1.057623			
15	2.236508	-0.705195	-0.000004			
1	3.382774	0.134967	-0.002998			
1	2.666564	-1.543679	1.059489			
1	2.665046	-1.549356	-1.055571			
6	-1.571009	-0.918661	0.000024			
7	-0.727544	-1.799231	0.000058			
6	-3.043864	-0.701229	0.000016			
1	-3.580705	-1.655252	-0.001657			
1	-3.339391	-0.126743	0.882898			
(E) Ni(CN)(Me)(PH₃)₂ 2						
28	-0.059979	-0.210742	-0.000012			
15	-2.136230	0.388770	-0.000004			
1	-2.922609	-0.092251	-1.069483			
1	-2.922686	-0.092533	1.069289			
1	-2.600869	1.729254	0.000152			
15	1.038467	1.725468	0.000012			
1	1.936297	1.910226	1.070796			
1	1.936265	1.910271	-1.070791			
1	0.451961	3.018393	0.000047			
6	1.646489	-0.938773	-0.000009			
7	2.760802	-1.295738	-0.000009			
6	-0.740011	-2.042388	0.000024			

1	-3.339050	-0.123769	-0.881024	1	2.951269	-0.079503	-1.069333
(B) Ni(PH₃)₂(MeCN) 1b							
28	-0.000166	0.335540	0.000000	1	2.611660	1.740400	0.000117
15	-0.000039	1.474481	1.813881	15	-1.038996	1.759569	0.000056
1	1.048225	2.404557	2.071566	1	-1.935328	1.952994	-1.070711
1	-1.049708	2.402693	2.072517	1	-1.935340	1.952852	1.070837
1	0.001070	0.948948	3.144103	1	-0.440366	3.047413	0.000145
15	-0.000039	1.474481	-1.813881	6	-1.666806	-0.945794	-0.000059
1	1.048225	2.404557	-2.071566	7	-2.785577	-1.287373	-0.000094
1	0.001070	0.948948	-3.144103	6	0.731304	-2.073604	0.000132
1	-1.049708	2.402693	-2.072517	1	0.324430	-2.561970	-0.888639
6	-0.000815	-2.683432	0.000000	1	1.822384	-2.198332	-0.000372
7	-0.000039	-1.518561	0.000000	1	0.325305	-2.561284	0.889694
6	-0.000092	-4.140318	0.000000	Table S6. DFT(B3PW91)-optimized Cartesian coordinates of			
1	-0.508115	-4.527759	-0.888949	oxidative addition of ethane to Ni(PH ₃) ₂ , where SDB and			
1	1.028573	-4.514020	0.000000	6-31G(d,p) basis sets were employed for Ni and the other atoms,			
1	-0.508115	-4.527759	0.888949	respectively.			
(A) Ni(Me)₂(PH₃)₂ TS₃₋₄							
28	0.000005	0.173719	-0.000005	28	0.000005	0.173719	-0.000005
15	-1.834970	-1.008627	-0.108453	15	-1.834970	-1.008627	-0.108453
1	-3.104014	-0.493505	0.287048	1	-3.104014	-0.493505	0.287048
1	-2.251075	-1.387252	-1.413072	1	-2.251075	-1.387252	-1.413072
1	-2.060253	-2.295669	0.459273	1	-2.060253	-2.295669	0.459273
(C) Ni(CN)(Me)(PH₃)₂ 2							
28	0.057430	-0.229047	-0.000021	28	0.057430	-0.229047	-0.000021
15	2.160901	0.395669	-0.000050	15	2.160901	0.395669	-0.000050
1	2.951415	-0.079827	1.068979	1	2.951415	-0.079827	1.068979

15	1. 835028	-1. 008541	0. 108448	6	-1. 424311	-1. 618285	0. 028779
1	3. 104095	-0. 493295	-0. 286819	1	-1. 146195	-2. 420865	0. 718024
1	2. 250994	-1. 387323	1. 413066	1	-2. 440948	-1. 292423	0. 296880
1	2. 060450	-2. 295491	-0. 459432	1	-1. 466806	-2. 031034	-0. 987230
6	-0. 477277	1. 819961	0. 913313	6	1. 235515	-1. 770080	0. 078083
1	-1. 489138	2. 181761	0. 718651	1	2. 281155	-1. 583911	-0. 211028
1	-0. 477619	1. 115222	1. 774233	1	1. 236889	-2. 108256	1. 122176
1	0. 173186	2. 655955	1. 175013	1	0. 863090	-2. 584449	-0. 550099
6	0. 477151	1. 820014	-0. 913295				
1	1. 488996	2. 181874	-0. 718665				
1	0. 477507	1. 115295	-1. 774231				
1	-0. 173377	2. 655969	-1. 174959				
(B) Ni(Me)₂(Me)(PH₃)₂ 4							
28	-0. 011670	-0. 262255	0. 000952				
15	-1. 628067	1. 195528	-0. 007271				
1	-2. 644227	1. 016275	-0. 975241				
1	-2. 465395	1. 201877	1. 133726				
1	-1. 511541	2. 607538	-0. 138539				
15	1. 763276	0. 994511	-0. 094191				
1	2. 759557	0. 767751	0. 884305				
1	2. 585445	0. 819372	-1. 232645				
1	1. 813927	2. 416220	-0. 066680				

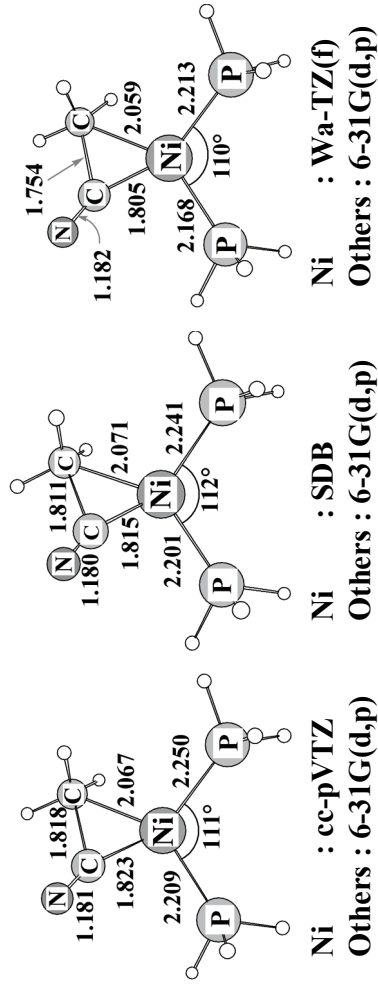


Figure S1. The transition state geometries of oxidative addition of MeCN to Ni(PH₃)₂ optimized by the DFT(B3LYP) method, where cc-pVTZ, SDB, and Wa-TZ(f) basis sets were employed for Ni and 6-31G(d,p) basis sets were employed for the other atoms. Bond lengths are in angstrom and bond angles are in degree.

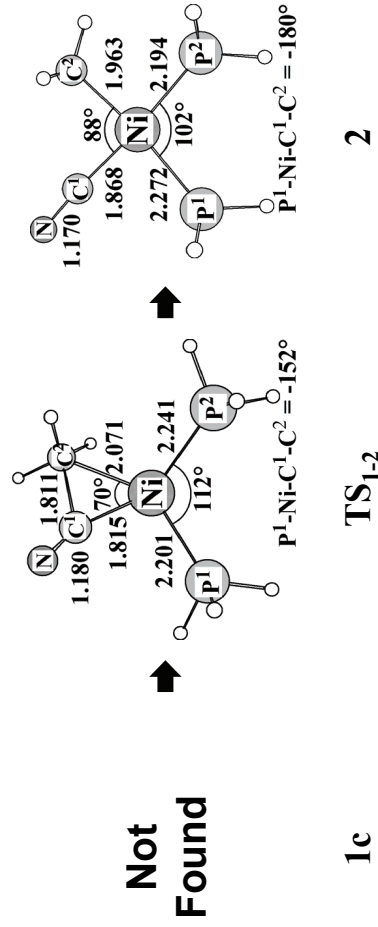


Figure S2. Geometry change in oxidative addition of MeCN to Ni(PH₃)₂ optimized by the DFT(B3LYP) method, where SDB and 6-31G(d,p) basis sets were employed for Ni and the other atoms, respectively. Bond lengths are in angstrom and bond angles are in degree.

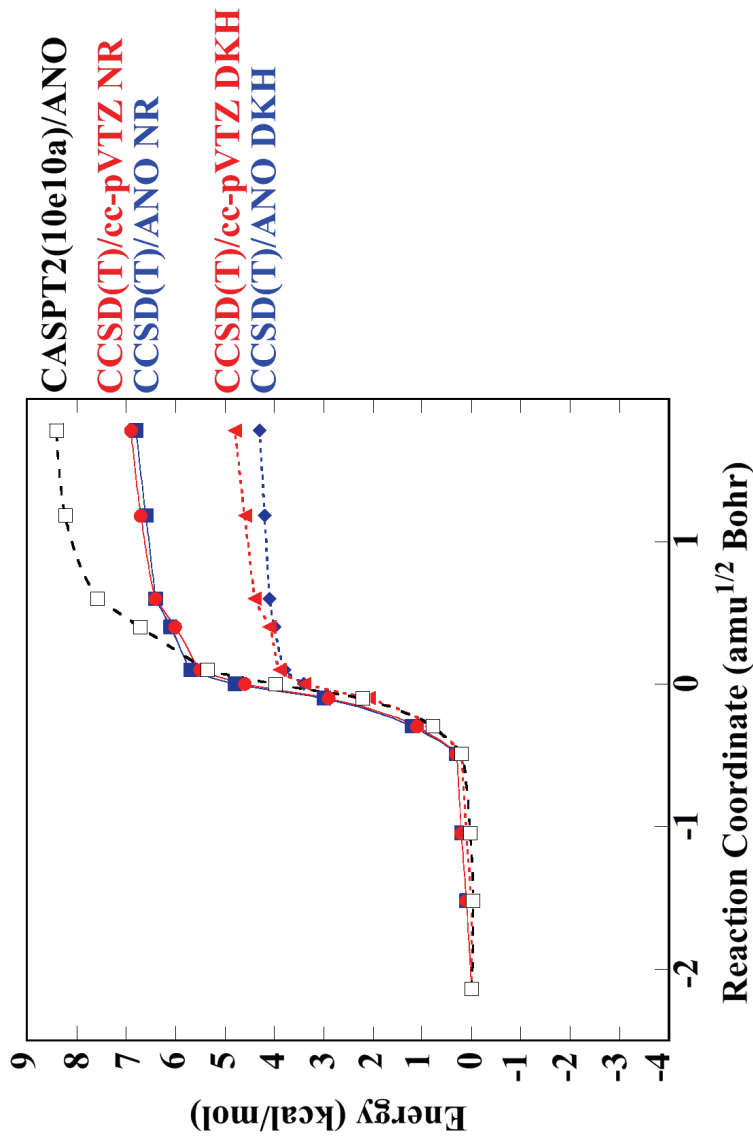


Figure S3. Potential energy curves of the oxidative addition of H_2 to $\text{Ni}(\text{PH}_3)_2$ calculated by the non-relativistic (NR) and relativistic (DKH) CCSD(T) methods^{a)}

a) In the relativistic calculations, the ANO-RCC^{b)} and cc-pVTZ-DK^{c)} basis sets were employed for Ni.

b) Roos, B. O.; Lindh, R.; Malmqvist, P.-Å.; Veryazov, V.; Widmark, P.-O. *J. Phys. Chem. A* **2005**, *109*, 6575-6579.

c) Balabanov, N. B.; Peterson, K. A. *J. Chem. Phys.* **2005**, *123*, 064107.