

Supplementary Information

A Comparison of β -Phenyl Elimination in Nickel and Palladium Alkyl Complexes: A Potentially Relevant Process in the Mizoroki–Heck Reaction

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SUPPLEMENTARY INFORMATION

Detail of Computational Results: Energy Components and Molecular Structures (Ball and Spoke Molecular views and Fractional Coordinates) for optimized stationary point geometries.

CONTENTS	Page
1. Effect of the steric bulk of diphosphine ligands on the π-arene interaction in cationic diphosphine neophyl-nickel and Palladium complexes.	
Figure S1. Tube molecular views and distances in nickel and palladium σ,π -complexes	3
Table S1. Fractional coordinates for the DiPPE and DtBPE Ni complexes.....	3
2. Conformational isomers of the neophyl-nickel DMPE triflate species [Ni(CH₂CMe₂Ph)(DMPE)OTf]	
Table S2. Energies and relative stability of DMPE-stabilized neophylnickel-triflate conformational isomers.....	4
3. Energy Components, and Optimized Geometries for all stationary points involved in β-Ph Elimination and Hydrolyses Reactions.	
Table S3. SCF, ZPE, and G° Energies for species involved in β -Ph eliminations and hydrolysis reactions.....	7
Table S4. Molecular structures and fractional coordinates of the species involved in β -Ph elimination and hydrolysis.....	9

1. Effect of the steric bulk of diphosphine ligands on the π -arene interaction in cationic diphosphine neophyl-nickel and Palladium complexes.

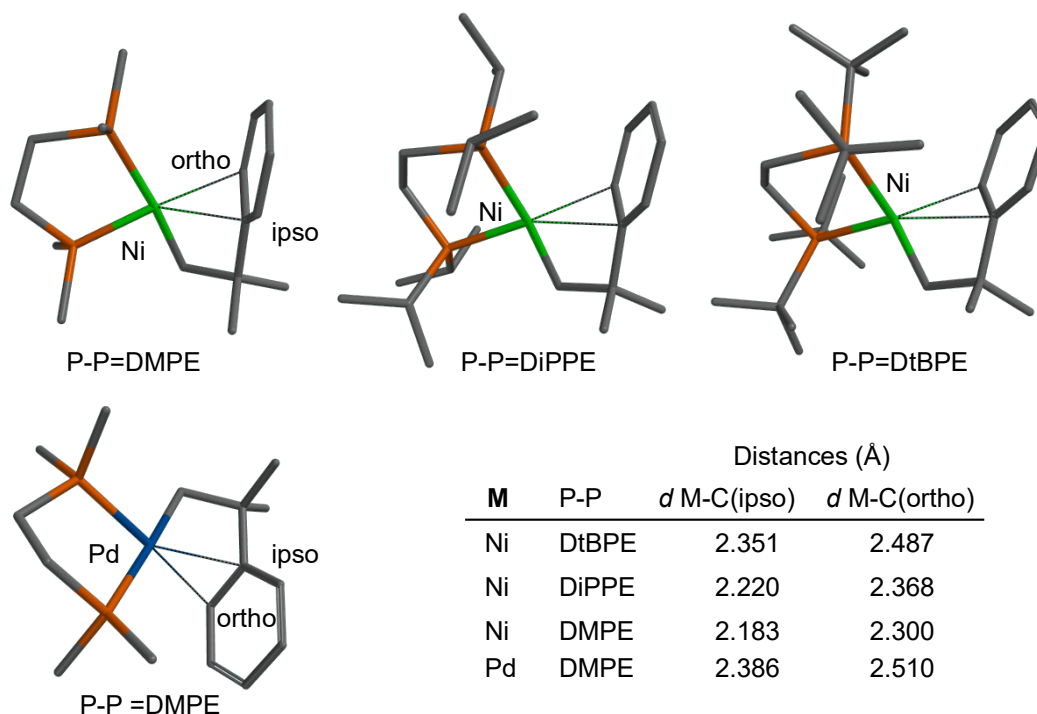


Figure S1. Tube molecular views and distances in nickel and palladium σ,π -complexes (H-atoms omitted for clarity).

Table S1. Fractional coordinates for the DiPPE and DtBPE Ni complexes (for DMPE derivatives, see Table S3)

[Ni(CH₂CMe₂Ph)(DiPPE)]				C	-1.018500	4.071156	-1.495154
				C	2.682241	-1.830312	-0.918244
				C	3.193487	-2.462044	-2.205309
				C	1.047221	0.136313	-2.346260
				C	-0.312484	3.156048	-0.507868
				C	3.622762	-0.738134	-0.420875
				C	-3.362289	2.084276	0.299187
				C	-3.163911	-0.055834	-0.984269
				C	-0.253965	0.918657	-2.363698
				C	1.202648	3.267700	-0.616133
				H	0.943588	-2.644688	1.403243
				H	-0.677907	5.105488	-1.351762
				H	-2.107968	4.068026	-1.373908
				H	-0.793264	3.803995	-2.536558
				H	4.233684	-2.785147	-2.066846
				H	3.186853	-1.749684	-3.041295
				H	1.890914	0.789910	-2.086541
				H	-1.014874	-3.229586	2.676118
				H	0.886512	-2.798343	4.333042
				H	-0.130398	-3.740534	0.095966
				H	-0.694232	-4.533434	-1.374517
				H	0.793613	-2.892333	-3.598874
				H	-0.899437	-3.383623	-3.490505
				H	-0.187083	-2.465014	-1.683587
				H	-0.185653	-2.601669	-3.200395
				H	0.025335	-3.801716	-0.986107
				H	2.618101	-3.345205	-2.503262
				H	-0.257631	-0.052475	-1.079159
				C	-2.645213	1.366897	-0.832108

H	1.278107	-0.304688	-3.325423	C	0.324196	-2.907208	-1.593856
H	-0.495576	-1.681195	-3.708197	C	-1.142945	-2.931382	-1.163119
H	4.595387	-1.171158	-0.156196	C	0.370447	-3.052561	-3.115834
H	3.234150	-0.218331	0.464895	C	1.046369	-4.099953	-0.969095
H	3.807044	0.015458	-1.198384	H	-1.576411	-3.906659	-1.425506
H	-4.417726	2.231361	0.035261	H	-1.275017	-2.787477	-0.083935
H	-2.939251	3.069849	0.530454	H	3.318891	-2.913899	-2.416186
H	-3.338611	1.487210	1.218390	H	0.000392	-4.053234	-3.377925
H	-2.913433	-0.662276	-0.100928	H	1.379800	-2.960234	-3.531856
H	-2.765749	-0.564868	-1.870696	H	0.501429	-5.012594	-1.247216
H	-1.055591	0.319420	-2.816583	H	1.077895	-4.066536	0.124582
H	-0.167210	1.824266	-2.978434	H	2.069913	-4.214219	-1.341329
H	1.534241	4.280383	-0.353164	H	3.056410	-3.164165	0.278526
H	1.540082	3.076063	-1.644665	H	-1.920255	-2.757691	2.497685
H	1.722686	2.560458	0.045518	H	-0.074243	-2.999106	4.250362
Ni	0.234756	-0.152849	0.726798	C	-2.816818	1.333317	-0.629349
P	0.966783	-1.150320	-1.035394	C	-0.351481	3.603673	-2.295087
P	-0.795247	1.366762	-0.644085	C	2.963581	-1.317541	-0.948407
C	0.998412	-1.619920	1.782535	C	3.526718	-1.848647	-2.266436
C	0.882665	1.023779	2.677560	C	0.774822	-0.094461	-2.456836
C	-0.217372	0.152287	2.878728	C	-0.203141	3.019801	-0.892221
C	0.721278	2.412983	2.753146	C	3.472863	0.107981	-0.719019
C	0.038613	-1.362921	2.938611	C	-3.349179	-0.080092	-0.878686
C	-1.245886	-2.158407	2.721626	C	3.478183	-2.158113	0.219245
C	-0.528129	2.957470	3.021728	C	-0.858808	3.949964	0.124884
C	0.649677	-1.726356	4.295163	C	-3.425132	2.269636	-1.669152
C	-1.480172	0.733732	3.105525	C	-0.619778	0.501872	-2.387366
C	-1.628935	2.112803	3.191580	C	-3.259942	1.729139	0.777710
H	2.046061	-1.399685	2.028662	C	1.289085	2.935230	-0.568939
H	1.890486	0.619292	2.581051	H	0.203991	-2.801114	1.414923
H	1.587049	3.062341	2.616274	H	0.021630	4.637673	-2.284411
H	-1.741412	-1.883652	1.778385	H	-1.386376	3.636435	-2.650120
H	-1.966960	-2.015810	3.536070	H	0.249110	3.060755	-3.035043
H	-0.651671	4.039170	3.092395	H	-1.734092	-2.171759	-1.684423
H	1.577377	-1.169040	4.475942	H	4.619691	-1.734347	-2.253180
H	-0.048279	-1.502935	5.114979	H	3.155611	-1.296733	-3.139039
H	-2.352179	0.093434	3.243351	H	1.532607	0.694382	-2.404537
H	-2.614857	2.537338	3.384893	H	0.946808	-0.607460	-3.410287
H	-2.826258	1.912517	-1.773603	H	-0.281177	-2.331604	-3.623243
H	2.614443	-2.610948	-0.144346	H	4.547850	0.060676	-0.498756
H	-1.178699	-2.090134	-1.383386	H	2.981895	0.586837	0.140168
H	-0.611905	3.443185	0.511263	H	3.358834	0.755079	-1.594776
[Ni(CH₂CMe₂Ph)(DtBPE)]				H	-4.417072	-0.104190	-0.622841
84				H	-2.848715	-0.829580	-0.252472
				H	-3.266728	-0.394546	-1.924851
				H	4.565632	-2.267088	0.106682
				H	3.309071	-1.655844	1.177259
H	-4.518756	2.157569	-1.649987	H	-0.307171	4.900519	0.141290

H	-0.829050	3.539637	1.140605	C	1.389607	2.109495	2.914562
H	-1.898362	4.186607	-0.124853	C	-0.367736	-1.310128	2.908369
H	-3.093924	2.031858	-2.688351	C	-1.820958	-1.669902	2.598545
H	-3.210487	3.325315	-1.472472	C	0.389777	2.953371	3.379367
H	-1.368213	-0.284872	-2.532069	C	0.025713	-1.905535	4.267039
H	-0.785211	1.225697	-3.194425	C	-1.151232	1.091430	3.431368
H	-4.358073	1.762746	0.806291	C	-0.885122	2.437825	3.638282
H	-2.894830	2.706458	1.104657	H	1.578630	-1.925746	2.120376
H	-2.937872	0.983612	1.513907	H	1.955558	0.094445	2.443448
H	1.712271	3.949891	-0.554363	H	2.391425	2.496427	2.722861
H	1.848047	2.370660	-1.321820	H	-2.160866	-1.221756	1.652668
H	1.476124	2.480274	0.409899	H	-2.513236	-1.350813	3.386706
Ni	0.119078	-0.281565	0.682555	H	0.597240	4.011624	3.545057
P	1.068365	-1.239310	-1.027769	H	1.064878	-1.662226	4.520818
P	-0.919242	1.258679	-0.723211	H	-0.622815	-1.515109	5.064421
C	0.537669	-1.832636	1.798765	H	-2.144092	0.705206	3.661288
C	1.126462	0.749947	2.708996	H	-1.675021	3.094590	4.006182
C	-0.154989	0.213306	2.964308				

2. Conformational isomers of the neophyl-nickel DMPE triflate species $[\text{Ni}(\text{CH}_2\text{CMe}_2\text{Ph})(\text{DMPE})\text{OTf}]$

Table S2. Energies and relative stability of DMPE-stabilized neophylnickel-triflate conformational isomers.

Conformer No.	M06-L/SPVD/CPCM (dichloromethane)			Single point M06-L/SVPD (g) E(SCF,g)	Corrections ^a		Single point M06/TZVPPD E(SCF,g)	G° estim ^b	ΔG°
	E(SCF)	G°	ZPE		TC	SC			
Ni-M0001	-2370894,423	-2370651,774	275,656	-2370879,625	242,649	-14,798	-2371688,892	-2371461,041	0,00
Ni-M0005	-2370894,56	-2370650,548	276,682	-2370876,623	244,012	-17,937	-2371686,656	-2371460,581	0,46
Ni-M0008	-2370893,627	-2370649,716	276,578	-2370876,553	243,911	-17,074	-2371686,900	-2371460,063	0,98
Ni-M0003	-2370894,381	-2370651,660	275,728	-2370879,424	242,721	-14,957	-2371687,803	-2371460,039	1,00
Ni-M0004	-2370892,849	-2370649,101	276,498	-2370876,288	243,748	-16,561	-2371686,570	-2371459,383	1,66
Ni-M0006	-2370892,628	-2370647,405	277,709	-2370875,93	245,223	-16,698	-2371686,174	-2371457,649	3,39
Ni-M0007	-2370888,91	-2370644,250	277,250	-2370869,696	244,66	-19,214	-2371679,504	-2371454,058	6,98

(a): Corrections (@ M06-L/SVPD): TC (Thermal Correction) = $G(\text{solv}) - E(\text{SCF, solv})$; SC (solvent correction) = $E(\text{SCF, solv}) - E(\text{SCF, g})$. (b) G° estim. = $E(\text{SCF, g, M06/TZVPPD}) + \text{TC} + \text{SC}$

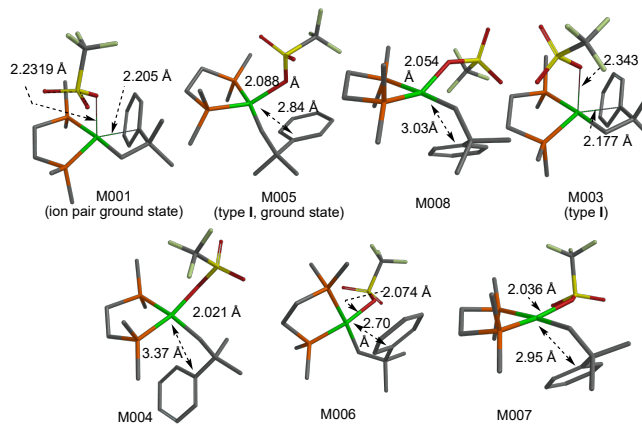


Figure S2. Geometries of seven neophylnickel-triflate conformational isomers. H atoms omitted for clarity, in order of increasing energy..

3. Energy Components and Optimized Geometries for all stationary points involved in β -Ph Elimination and Hydrolyses Reactions.

Table S3. SCF, ZPE, and G° Energies for species involved in c β -Ph eliminations and hydrolysis reactions

Species	M06-L/SPVD				Single point M06-L/SVPD (g) E(SCF,g)	Corrections ^a		Single point M06/TZVPPD E(SCF,g)	G° estim ^b E(SCF)+TC+SC
	i-Frq (cm ⁻¹)	E(SCF)	G°	ZPE		TC	SC		
triflate(-)		-603054,637	-603057,713	16,770	-603004,932	-3,076	-49,705	-603424,817	-603477,598
CH ₂ =CMe ₂		-98576,776	-98526,846	67,043	-98575,437	49,93	-1,339	-98614,31	-98565,719
H ₂ O		-47925,175	-47922,811	13,440	-47919,859	2,364	-5,316	-47959,482	-47962,434
C ₆ H ₆		-145617,925	-145572,49	62,678	-145615,918	45,435	-2,007	-145671,535	-145628,107
PMe ₃		-289213,296	-289161,854	69,861	-289210,791	51,442	-2,505	-289306,023	-289257,086
6'		-1767823,669	-1767593,483	258,930	-1767786,38	230,186	-37,289	-1768182,057	-1767989,160
TS1-Ni	261	-1767803,054	-1767574,863	257,269	-1767765,741	228,191	-37,313	-1768161,811	-1767970,933
[Ni(Ph)(CH ₂ =CMe ₂)(DMPE)] ⁺		-1767812,271	-1767584,524	257,149	-1767773,174	227,747	-39,097	-1768169,047	-1767980,397
TS2-Ni	9	-1767810,454	-1767582,197	257,518	-1767771,788	228,257	-38,666	-1768167,791	-1767978,200
[Ni(Ph)(CH ₂ =CMe ₂ ⊥)(DMPE)] ⁺		-1767810,577	-1767582,232	257,581	-1767771,955	228,345	-38,622	-1768167,447	-1767977,724
[Ni(Ph)(DMPE)](+)		-1669207,019	-1669045,493	188,221	-1669167,165	161,526	-39,864	-1669528,647	-1669406,975
[Ni(Ph)(H ₂ O)(DMPE)](+)		-1717155,662	-1716978,895	204,489	-1717111,89	176,767	-43,772	-1717511,141	-1717378,146
TS3-Ni	1588	-1717134,673	-1716960,96	201,372	-1717091,355	173,713	-43,318	-1717489,647	-1717359,252
[Ni(OH)(Ph-H)(DMPE)](+)		-1717155,290	-1716978,543	204,401	-1717111,969	176,747	-43,321	-1717508,64	-1717375,214
cis-5a'		-3143106,992	-3142854,133	285,219	-3142976,648	252,859	-130,344	-3143659,709	-3143537,194
trans-5a'		-3143102,310	-3142850,783	284,211	-3142977,868	251,527	-124,442	-3143663,911	-3143536,826

Table S3 (cont).

[Ni(CH ₂ CMe ₂ Ph)(PMe ₃)(DMPE)] ⁺ (c)		-2057062,072	-2056761,611	332,327	-2057024,568	300,461	-37,504	-2057511,458	-2057248,501
IV'		-2057057,207	-2056757,714	331,583	-2057020,034	299,493	-37,173	-2057505,827	-2057243,507
TS4	219	-2057027,841	-2056730,218	329,976	-2056991,268	297,623	-36,573	-2057477,077	-2057216,027
13'		-2057037,706	-2056740,930	329,612	-2057000,207	296,776	-37,499	-2057486,692	-2057227,415
TS5	39	-2057037,180	-2056740,255	329,670	-2056999,873	296,925	-37,307	-2057486,295	-2057226,677
[Ni(Ph)(PMe ₃)(DMPE)] ⁺		-1958467,339	-1958237,426	260,426	-1958428,968	229,913	-38,371	-1958883,597	-1958692,055
1'		-901778,726	-901549,236	258,602	-901741,65	229,49	-37,076	-902002,587	-901810,173
TS1-Pd	319	-901752,681	-901524,987	257,106	-901716,339	227,694	-36,342	-901977,634	-901786,282
[Pd(Ph)(CH ₂ =CMe ₂ -II)(DMPE)] ⁺		-901767,748	-901540,368	257,103	-901729,549	227,38	-38,199	-901991,607	-901802,426
TS2-Pd	39	-901767,678	-901540,656	256,802	-901729,273	227,022	-38,405	-901991,179	-901802,562
[Pd(Ph)(CH ₂ =CMe ₂ -I)(DMPE)] ⁺		-901767,882	-901540,833	256,845	-901729,379	227,049	-38,503	-901991,087	-901802,541
[Pd(Ph)(DMPE)] ⁺		-803165,648	-803004,830	187,89	-803125,806	160,818	-39,842	-803349,498	-803228,522
[Pd(Ph)(H ₂ O)(DMPE)] ⁺		-851109,237	-850933,664	203,688	-851066,32	175,573	-42,917	-851328,606	-851195,95
TS3-Pd	1659	-851085,166	-850912,460	200,757	-851042,190	172,706	-42,976	-851302,623	-851172,893
[Pd(OH)(η ² -Ph-H)(DMPE)] ⁺		-851108,676	-850932,625	204,062	-851063,854	176,051	-44,822	-851323,82	-851192,591
<i>cis</i> -[Pd(μ-OH)(DMPE)] ₂ ²⁺		-1411001,355	-1410750,471	283,926	-1410879,234	250,884	-122,121	-1411286,985	-1411158,222
<i>trans</i> -[Pd(μ-OH)(DMPE)] ₂ ²⁺		-1411001,480	-1410750,360	284,053	-1410879,972	251,12	-121,508	-1411288,853	-1411159,241
[Pd(CH ₂ CMe ₂ Ph)(PMe ₃)(DMPE)] ⁺ (a)		-1191019,973	-1190720,88	331,544	-1190982,547	299,093	-37,426	-1191335,303	-1191073,636
[Pd(Ph)(PMe ₃)(DMPE)] ⁺		-1092422,922	-1092193,758	259,919	-1092384,63	229,164	-38,292	-1092703,712	-1092512,840

(a): Corrections (@ M06-L/SVPD): TC (Thermal Correction) = G(solv)-E(SCF, solv); SC (solvent correction) = E(SCF, solv)-E(SCF, g). (b) G° estim. = E(SCF, g, M06/TZVPPD)+TC+SC. (c): Only the most stable conformer shown.

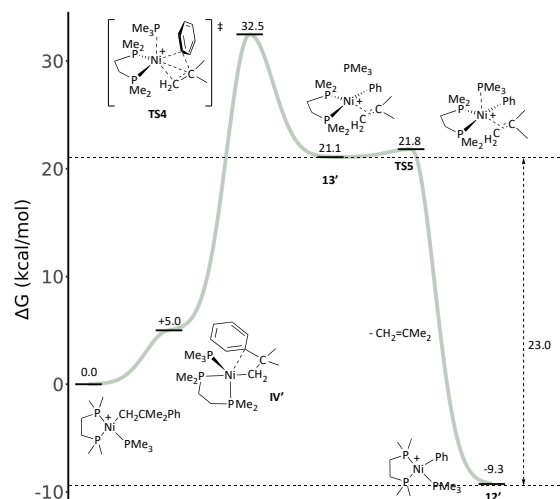



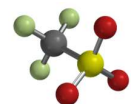
Figure S3. Free energy diagram corresponding to Scheme 8. All free energies in Kcal/mol.

Table S4. Structure and coordinates of the species involved in β -Ph elimination and hydrolysis

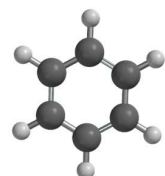
Water

3			
	O	0.000000	0.000000
	H	0.000000	-0.757387
8	H	0.000000	0.757387

Triflate Anion

8			
	C	0.412837	0.702019
	F	-0.154696	1.833775
12	F	1.697625	0.715721
	F	0.371385	0.702958
	S	-0.465655	-0.791363
	O	0.293531	-1.919462
	O	-0.310056	-0.615552
	O	-1.844970	-0.628096

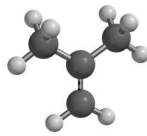
Benzene

12			
	C	0.412837	0.702019
	F	-0.154696	1.833775
	F	1.697625	0.715721
	F	0.371385	0.702958
	S	-0.465655	-0.791363

12

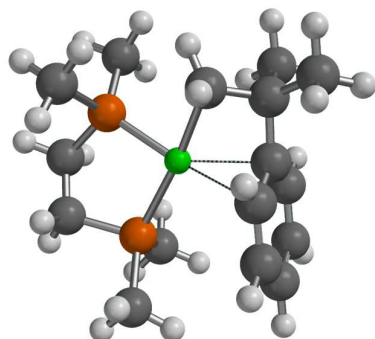
6	-0.365716	-1.330453	0.211711
6	0.365716	1.330453	-0.211712
6	0.812552	-0.832975	0.770979
6	-1.178255	-0.497409	-0.559355
6	-0.812553	0.832975	-0.770979
6	1.178255	0.497408	0.559356
1	1.448010	-1.484669	1.374011
1	-1.448012	1.484668	-1.374012
1	2.099985	0.886313	0.996760
1	0.651807	2.371054	-0.377227
1	-0.651806	-2.371053	0.377227
1	-2.099984	-0.886314	-0.996758

Isobutene

12			
	C	0.190855	1.450692
	H	1.184164	1.891629
	H	-0.662804	2.071133
	C	0.026411	0.200858
	C	1.182896	-0.662570
12	H	2.146204	-0.157168
	H	1.100889	-0.977936
	H	1.195744	-1.592112
	C	-1.325149	-0.418822
	C	0.532448	-0.080917

H	-1.406345	-1.339401	0.517427
H	-1.499927	-0.724886	-1.123897
H	-2.132938	0.258583	0.218768

[Ni(CH₂CMe₂Ph)(DMPE)]⁺, 6'

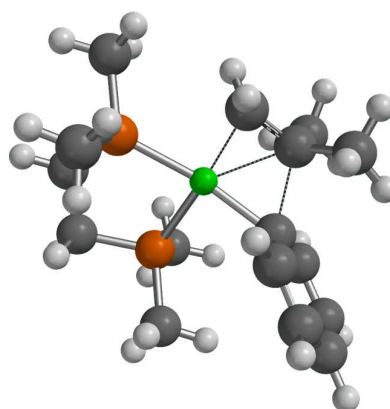


48

Ni	-0.032031	0.391586	-0.200987
P	-2.110095	0.730352	0.241889
P	0.414350	0.604725	2.020948
C	-2.328355	0.830411	2.070165
H	-2.486668	-0.197462	2.428099
H	-3.240523	1.395088	2.308350
C	-1.087075	1.436236	2.698742
H	-1.102070	1.363048	3.795173
H	-1.003127	2.504413	2.448708
C	-2.757281	2.302436	-0.399658
H	-2.177757	3.138494	0.008679
H	-3.810487	2.422299	-0.114345
H	-2.675939	2.323012	-1.492280
C	-3.319007	-0.520801	-0.277140
H	-3.020655	-1.504616	0.102857
H	-3.385175	-0.568811	-1.369174
H	-4.306951	-0.265928	0.127424
C	1.772275	1.602448	2.715734
H	2.728580	1.081586	2.600581
H	1.597095	1.781060	3.784535
H	1.835502	2.565910	2.196533
C	0.493560	-0.945852	2.980579
H	1.427909	-1.474540	2.759316
H	-0.340223	-1.603189	2.705645
H	0.448425	-0.738198	4.057767
C	-0.570608	0.346015	-2.079980
H	-0.212519	1.319066	-2.453143
H	-1.611908	0.213092	-2.395130
C	0.335378	-0.820111	-2.473032
C	1.718081	-1.916963	-0.565280
C	3.124828	0.463041	-0.162410
C	2.744558	-1.854381	0.369138

C	1.388017	-0.796546	-1.357203
C	2.083372	0.414411	-1.104143
C	3.462316	-0.668486	0.565892
H	2.993237	-2.742655	0.952209
H	4.271408	-0.631669	1.296776
H	3.665123	1.398708	-0.009967
C	0.994159	-0.620393	-3.838625
H	1.569499	0.313088	-3.877398
H	0.230078	-0.574674	-4.626566
H	1.675702	-1.449928	-4.076101
C	-0.460875	-2.117892	-2.471982
H	0.165731	-2.987268	-2.710152
H	-1.252692	-2.067027	-3.229344
H	-0.941058	-2.300791	-1.500837
H	1.187110	-2.857358	-0.712177
H	1.906783	1.285014	-1.738682

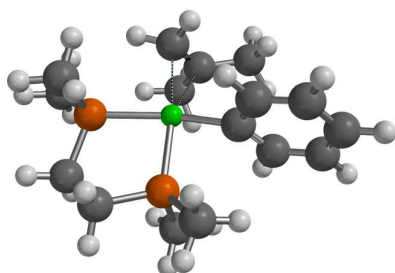
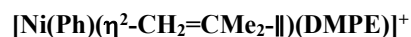
TS1-Ni



48

Ni	-0.464605	0.019020	-0.298265
P	-2.347074	0.975981	0.239607
P	0.048879	0.098325	1.865265
C	-2.597419	0.814822	2.055010
H	-2.977484	-0.201550	2.234418
H	-3.372694	1.514798	2.396697
C	-1.267864	1.032363	2.757591
H	-1.302595	0.739754	3.815698
H	-0.982272	2.093737	2.728888
C	-2.236874	2.768445	-0.056881
H	-1.347964	3.181939	0.434435
H	-3.130160	3.278847	0.326527
H	-2.150478	2.956672	-1.133498
C	-3.927882	0.487153	-0.502396
H	-4.086837	-0.589662	-0.372972
H	-3.922402	0.714090	-1.574727
H	-4.753747	1.032621	-0.029427
C	1.605789	0.860651	2.402350

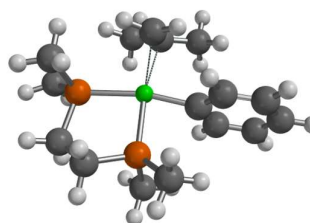
H	2.455712	0.309001	1.983448
H	1.680587	0.857823	3.497106
H	1.650942	1.894757	2.040761
C	0.043936	-1.549455	2.640782
H	0.808672	-2.184900	2.179169
H	-0.933588	-2.025040	2.496638
H	0.249514	-1.470367	3.716072
C	-1.107269	-0.250772	-2.112465
H	-1.116034	0.646153	-2.741356
H	-2.062703	-0.780994	-2.087002
C	0.096089	-1.056843	-2.113846
C	2.236584	-1.420076	-0.232088
C	3.377145	1.048451	-0.854303
C	3.601883	-1.209731	-0.035582
C	1.423850	-0.403738	-0.754294
C	2.021431	0.828396	-1.081162
C	4.177619	0.024597	-0.339292
H	4.217190	-2.015899	0.368688
H	1.417012	1.625071	-1.526180
H	5.244949	0.187379	-0.182699
H	3.816219	2.018183	-1.097119
C	1.027470	-0.839985	-3.288133
H	1.165211	0.221050	-3.518740
H	0.559798	-1.310404	-4.166016
H	2.011014	-1.302030	-3.137952
C	-0.113420	-2.518600	-1.791339
H	0.828469	-3.076306	-1.759226
H	-0.729095	-2.964363	-2.584658
H	-0.642899	-2.672147	-0.841475
H	1.807394	-2.387217	0.033944



48

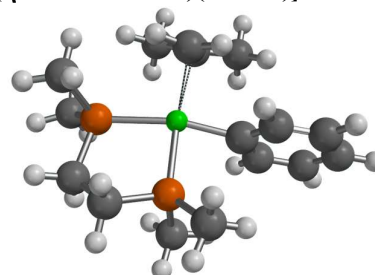
Ni	-0.228190	0.114194	-0.317903
P	-2.318913	0.777904	0.267861
P	0.198981	0.172778	1.832268
C	-2.495727	0.653972	2.093952
H	-2.772191	-0.384758	2.325302
H	-3.317184	1.292569	2.446246
C	-1.168804	1.019236	2.731115
H	-1.124799	0.756443	3.797266

H	-0.978696	2.099876	2.659623
C	-2.446744	2.565263	-0.068040
H	-1.597921	3.096031	0.379478
H	-3.380742	2.971897	0.340917
H	-2.424726	2.741316	-1.150149
C	-3.878551	0.101560	-0.381088
H	-3.977801	-0.952357	-0.096163
H	-3.910678	0.172771	-1.474882
H	-4.728211	0.661890	0.028510
C	1.701972	0.932603	2.502879
H	2.587275	0.369424	2.188583
H	1.647142	0.945340	3.598736
H	1.792129	1.961307	2.135019
C	0.180282	-1.522852	2.488889
H	1.006312	-2.101984	2.062132
H	-0.763263	-2.016446	2.227616
H	0.287236	-1.503053	3.581274
C	-0.789148	0.281139	-2.364062
H	-0.131712	1.025795	-2.820967
H	-1.850902	0.524222	-2.354267
C	-0.368609	-1.031685	-2.279793
C	2.466611	-1.173476	-0.225241
C	3.722607	1.180057	-1.019114
C	3.853109	-1.143701	-0.392551
C	1.684951	-0.035100	-0.459395
C	2.337125	1.145987	-0.844851
C	4.486899	0.034233	-0.789864
H	4.440336	-2.046672	-0.210500
H	1.760611	2.060204	-1.021929
H	5.570409	0.060722	-0.919166
H	4.207730	2.107707	-1.331929
C	0.900312	-1.488545	-2.916594
H	1.612595	-0.676357	-3.090912
H	0.631119	-1.916271	-3.895089
H	1.393221	-2.288872	-2.352173
C	-1.282787	-2.124400	-1.827988
H	-0.817177	-2.713634	-1.022284
H	-1.456209	-2.834665	-2.650700
H	-2.253331	-1.756939	-1.481704
H	1.994052	-2.114673	0.071629



48

Ni	-0.150643	0.134915	-0.261119
P	-2.366429	0.481955	0.323706
P	0.299333	0.380157	1.870481
C	-2.408561	0.624032	2.163004
H	-2.538064	-0.393365	2.560202
H	-3.292611	1.198557	2.471336
C	-1.118583	1.237382	2.666933
H	-1.020048	1.176524	3.760038
H	-1.048668	2.300586	2.394413
C	-2.991294	2.101072	-0.239981
H	-2.269945	2.891376	0.000578
H	-3.951603	2.331451	0.238306
H	-3.135829	2.088206	-1.327298
C	-3.774610	-0.635970	0.010866
H	-3.497558	-1.672429	0.235183
H	-4.102698	-0.576989	-1.031626
H	-4.614919	-0.344904	0.654172
C	1.755324	1.311879	2.417032
H	2.667243	0.744263	2.201434
H	1.685208	1.491760	3.497205
H	1.809385	2.273386	1.893839
C	0.420754	-1.204641	2.753925
H	1.320306	-1.740901	2.432614
H	-0.452714	-1.833555	2.547347
H	0.485272	-1.019012	3.833879
C	-0.321758	0.771893	-2.297199
H	0.606338	1.321233	-2.465736
H	-1.241570	1.357779	-2.277046
C	-0.364479	-0.584428	-2.515892
C	2.304591	-1.379637	-0.132403
C	3.984025	0.704240	-0.891860
C	3.670720	-1.613691	-0.309142
C	1.753201	-0.109449	-0.351016
C	2.618315	0.932237	-0.715276
C	4.516109	-0.571171	-0.689855
H	4.074437	-2.615610	-0.146444
H	2.227374	1.941730	-0.873108
H	5.584533	-0.749600	-0.824019
H	4.637534	1.528450	-1.187009
C	0.829040	-1.355528	-2.968579
H	1.757724	-0.779742	-2.923015
H	0.659705	-1.657420	-4.013223
H	0.957390	-2.286875	-2.399671
C	-1.655388	-1.334029	-2.545750
H	-1.694881	-2.107987	-1.763649
H	-1.752768	-1.869564	-3.500912
H	-2.519427	-0.672681	-2.434512
H	1.661189	-2.215884	0.158846

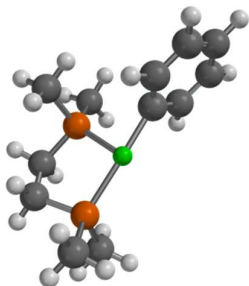


48

Ni	-0.124498	0.164331	-0.243528
P	-2.347766	0.398939	0.350669
P	0.329548	0.457836	1.877188
C	-2.377962	0.663818	2.179059
H	-2.481988	-0.327625	2.643161
H	-3.272025	1.237115	2.458737
C	-1.097714	1.333762	2.634733
H	-0.991095	1.340631	3.728842
H	-1.051687	2.379611	2.297585
C	-3.168622	1.887480	-0.311312
H	-2.551019	2.772703	-0.116083
H	-4.151839	2.024032	0.155647
H	-3.304050	1.795955	-1.395973
C	-3.606773	-0.907380	0.154366
H	-3.203794	-1.870912	0.488051
H	-3.926001	-1.003263	-0.887727
H	-4.484086	-0.659906	0.765719
C	1.780184	1.413813	2.394748
H	2.694099	0.841630	2.200827
H	1.707435	1.630380	3.467970
H	1.832707	2.357077	1.839252
C	0.457797	-1.098233	2.808466
H	1.359274	-1.638827	2.499488
H	-0.412425	-1.737457	2.619735
H	0.522762	-0.882713	3.882765
C	-0.241506	0.929836	-2.234176
H	0.724233	1.421033	-2.362005
H	-1.117006	1.578371	-2.168599
C	-0.382673	-0.401530	-2.543779
C	2.224394	-1.440419	-0.123765
C	4.054147	0.512659	-0.881976
C	3.566463	-1.779133	-0.315592
C	1.771632	-0.129994	-0.331730
C	2.711366	0.845030	-0.693288
C	4.486576	-0.802140	-0.696415
H	3.892604	-2.810369	-0.162851
H	2.399160	1.883017	-0.839919
H	5.536680	-1.061691	-0.841959
H	4.767380	1.286455	-1.175093

C	0.762889	-1.236799	-3.009101
H	1.727489	-0.728165	-2.926509
H	0.595422	-1.494573	-4.065581
H	0.817829	-2.192438	-2.468574
C	-1.725601	-1.042092	-2.666966
H	-1.833124	-1.901261	-1.988010
H	-1.846801	-1.446974	-3.682226
H	-2.542967	-0.336443	-2.487333
H	1.520955	-2.225177	0.173061

[Ni(Ph)(DMPE)]⁺

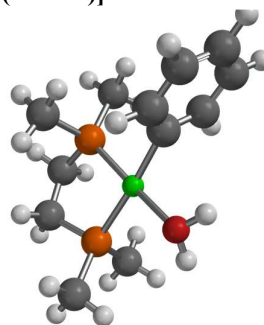


36

Ni	-0.218416	-0.212965	-0.823579
P	-2.418431	0.167074	-0.553331
P	0.178709	0.290379	1.186674
C	-2.590724	0.298675	1.275917
H	-2.660842	-0.725961	1.669102
H	-3.527329	0.808972	1.539158
C	-1.379893	1.017313	1.848002
H	-1.353584	0.986275	2.946873
H	-1.377078	2.078133	1.557981
C	-3.003425	1.776973	-1.173018
H	-2.353935	2.581050	-0.807293
H	-4.032134	1.966865	-0.839896
H	-2.975664	1.788267	-2.268861
C	-3.710596	-1.002918	-1.065880
H	-3.490857	-2.001986	-0.673004
H	-3.747024	-1.059503	-2.159937
H	-4.691481	-0.677553	-0.695803
C	1.471459	1.489270	1.590265
H	2.458273	1.049273	1.410235
H	1.385583	1.771988	2.647390
H	1.362235	2.385175	0.968677
C	0.518710	-1.165495	2.212106
H	1.477477	-1.608514	1.920376
H	-0.269751	-1.915826	2.083486
H	0.564060	-0.867685	3.267819
C	2.132695	-1.798218	-0.909375
C	3.704854	0.218795	-2.032469
C	3.400482	-2.098356	-1.413026
C	1.623554	-0.492001	-0.997244

C	2.438874	0.521078	-1.528671
C	4.186196	-1.090798	-1.974665
H	3.778289	-3.121513	-1.359020
H	2.083053	1.554910	-1.565216
H	5.181044	-1.324011	-2.358270
H	4.321699	1.010409	-2.462976
H	1.533916	-2.597575	-0.462528

[Ni(Ph)(H₂O)(DMPE)]⁺

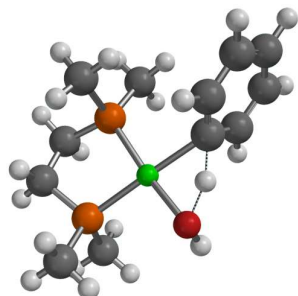


39

Ni	-0.254402	-0.112793	-0.701729
P	-2.418381	0.284936	-0.226533
P	0.190693	0.202596	1.357452
C	-2.550316	0.288604	1.608450
H	-2.643436	-0.759154	1.929234
H	-3.461794	0.807928	1.934209
C	-1.293896	0.920862	2.182969
H	-1.215781	0.789477	3.271415
H	-1.273562	2.003184	1.987909
C	-3.003157	1.937900	-0.723616
H	-2.348102	2.710435	-0.303719
H	-4.029835	2.109381	-0.374257
H	-2.979582	2.029398	-1.816297
C	-3.721960	-0.839038	-0.810567
H	-3.501916	-1.863884	-0.490436
H	-3.760746	-0.820877	-1.906681
H	-4.703036	-0.540302	-0.419206
C	1.561907	1.277239	1.858385
H	2.516681	0.807427	1.597160
H	1.523157	1.441588	2.942782
H	1.493368	2.243427	1.345519
C	0.490336	-1.361863	2.232557
H	1.405078	-1.829918	1.851083
H	-0.346186	-2.052701	2.075551
H	0.604524	-1.173621	3.308025
C	2.180417	-1.673905	-0.893286
C	3.797297	0.452939	-1.677009
C	3.513753	-1.902302	-1.246090
C	1.629886	-0.383296	-0.930623
C	2.465338	0.676013	-1.319599

C	4.326760	-0.838171	-1.637957
H	3.918086	-2.916698	-1.213311
H	2.078282	1.699606	-1.344134
H	5.369303	-1.013581	-1.909840
H	4.426168	1.292864	-1.981571
H	1.563164	-2.525470	-0.589728
O	-0.544078	-0.596118	-2.629908
H	0.246748	-0.574707	-3.184026
H	-1.250781	-0.197404	-3.152580

TS3-Ni

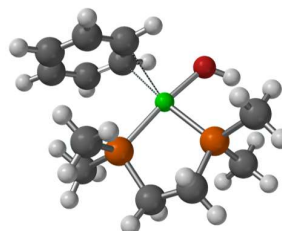


39

Ni	-0.420152	-0.161478	-0.811024
P	-2.469501	0.292551	-0.152937
P	0.175263	0.122283	1.255363
C	-2.517845	0.350807	1.680323
H	-2.654792	-0.679966	2.036428
H	-3.382544	0.930515	2.029294
C	-1.198516	0.926237	2.172217
H	-1.060338	0.796229	3.254157
H	-1.138175	2.004429	1.966328
C	-2.992778	1.940377	-0.709673
H	-2.305881	2.702882	-0.324574
H	-4.008648	2.156708	-0.354049
H	-2.980098	1.983576	-1.805046
C	-3.771590	-0.840714	-0.695906
H	-3.558830	-1.853350	-0.335808
H	-3.804147	-0.857628	-1.791187
H	-4.747640	-0.515621	-0.313582
C	1.667440	1.078370	1.623560
H	2.546007	0.549724	1.236284
H	1.771807	1.201697	2.708987
H	1.610692	2.064512	1.149396
C	0.422492	-1.477237	2.078357
H	1.263768	-2.004729	1.614442
H	-0.474859	-2.098762	1.980908
H	0.640230	-1.320123	3.142664
C	2.142113	-1.676345	-1.085197
C	3.717052	0.571504	-1.590338
C	3.526539	-1.758017	-0.952776

C	1.513772	-0.469280	-1.452141
C	2.331466	0.649222	-1.710252
C	4.313774	-0.630922	-1.202619
H	3.996086	-2.699062	-0.661769
H	1.874563	1.594672	-2.015631
H	5.398587	-0.691648	-1.100649
H	4.335176	1.446518	-1.798325
H	1.535796	-2.567039	-0.898327
O	-0.782477	-0.635965	-2.678720
H	0.449424	-0.579824	-2.284457
H	-0.963237	0.154897	-3.203722

[Ni(OH)(Ph-H)(DMPE)]⁺

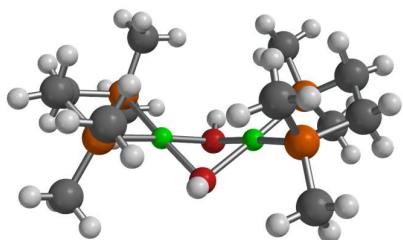


39

Ni	-0.231162	0.125187	-0.969899
P	-2.249095	0.445908	-0.253384
P	0.411373	0.200644	1.160614
C	-2.291941	0.318195	1.572065
H	-2.380661	-0.747654	1.825708
H	-3.186484	0.821786	1.963088
C	-1.001534	0.907025	2.106015
H	-0.863408	0.716158	3.178938
H	-0.975961	1.997373	1.965644
C	-2.862926	2.108932	-0.635856
H	-2.220187	2.862638	-0.166968
H	-3.885948	2.217653	-0.251865
H	-2.867554	2.281095	-1.717951
C	-3.489214	-0.709158	-0.884345
H	-3.183638	-1.738269	-0.665138
H	-3.599208	-0.596608	-1.968076
H	-4.454473	-0.507066	-0.401395
C	1.809720	1.231181	1.695266
H	2.765048	0.763146	1.442276
H	1.757048	1.361391	2.784044
H	1.758251	2.214268	1.213515
C	0.682154	-1.410131	1.962812
H	1.586103	-1.886758	1.571110
H	-0.167997	-2.075131	1.769892
H	0.792229	-1.270144	3.045996
C	2.108642	-2.182849	-1.202698
C	3.035787	0.453474	-1.379513
C	3.264306	-1.801076	-0.533206

C	1.408364	-1.251079	-1.984119
C	1.872012	0.077883	-2.070032
C	3.730468	-0.482545	-0.624864
H	3.815339	-2.530310	0.063092
H	1.392176	0.777112	-2.754767
H	4.641621	-0.191678	-0.099433
H	3.400864	1.478845	-1.455622
H	1.753425	-3.212660	-1.143377
O	-0.897537	0.191536	-2.704241
H	0.570038	-1.574527	-2.600295
H	-1.746040	0.616214	-2.853032

Cis-5a'

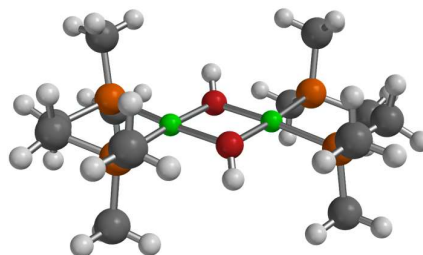


54

Ni	-0.005464	0.796250	1.324025
P	-1.497596	0.073199	2.726462
P	1.489903	0.091320	2.729216
C	-0.675707	-0.918513	4.034238
H	-0.568792	-1.940944	3.644713
H	-1.313772	-0.977691	4.926107
C	0.680919	-0.300872	4.326785
H	1.321522	-0.955758	4.932455
H	0.574895	0.646333	4.874772
C	-2.343373	1.433972	3.576722
H	-1.618729	2.042919	4.129198
H	-3.089140	1.034742	4.276574
H	-2.844982	2.073686	2.841097
C	-2.814808	-0.974383	2.054403
H	-2.379199	-1.834270	1.533184
H	-3.435989	-0.406120	1.352471
H	-3.453091	-1.333322	2.872181
C	2.858845	1.216513	3.097735
H	3.441281	1.412068	2.190201
H	3.518111	0.766319	3.851234
H	2.469241	2.166832	3.479050
C	2.261061	-1.449193	2.158742
H	2.797029	-1.265178	1.220624
H	1.494106	-2.210929	1.976218
H	2.970794	-1.820675	2.909353
O	-1.221644	1.475150	-0.004123
H	-2.133653	1.168450	-0.010183
O	1.219881	1.475766	0.003792

H	2.132082	1.169639	0.009979
Ni	0.004108	0.795771	-1.324133
P	-1.490163	0.090683	-2.730405
P	1.497310	0.072550	-2.725365
C	2.812390	-0.976876	-2.051978
H	3.452233	-1.335141	-2.868836
H	2.374978	-1.837186	-1.532953
H	3.432394	-0.410100	-1.347796
C	2.345683	1.433160	-3.573270
H	3.092133	1.033754	-4.272294
H	2.846766	2.071861	-2.836408
H	1.622419	2.043162	-4.126386
C	0.676308	-0.917366	-4.035061
H	1.315102	-0.975618	-4.926464
H	0.568817	-1.940240	-3.646859
C	-2.260067	-1.451370	-2.162422
H	-1.492402	-2.212390	-1.979901
H	-2.968524	-1.822867	-2.914229
H	-2.797303	-1.269071	-1.224716
C	-0.679952	-0.299068	-4.327933
H	-0.573317	0.648944	-4.874401
H	-1.320120	-0.952991	-4.935108
C	-2.859976	1.214990	-3.098353
H	-3.518472	0.765012	-3.852651
H	-2.471065	2.166086	-3.478436
H	-3.443009	1.409000	-2.190871

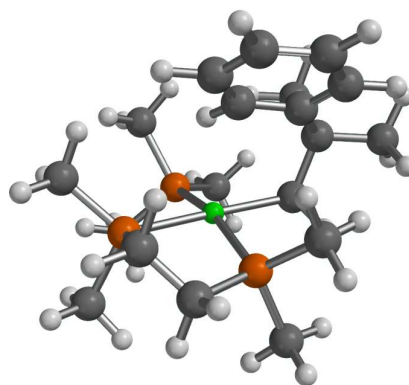
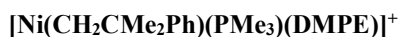
Trans-5a'



54

H	1.901327	3.373530	1.094023
H	-1.941848	3.363304	1.054483
H	-0.004802	2.048810	-0.405584
O	-0.005922	1.260136	0.146203
C	4.637696	-0.651033	-0.331114
C	4.629389	0.687116	0.390084
C	2.815220	2.805869	1.302535
C	3.201322	2.354112	-1.526089
C	3.204547	-2.324451	1.575315
C	2.850356	-2.786981	-1.255652
H	4.727037	-0.513846	-1.418182

H	5.469803	-1.294874	-0.016135
H	4.710414	0.550583	1.477890
H	5.459137	1.337442	0.082338
H	4.006913	3.097634	-1.464810
H	4.016602	-3.061674	1.523996
Ni	1.450233	0.005707	0.012573
P	3.017180	1.501204	0.065383
P	3.029246	-1.477355	-0.020247
C	-4.638195	0.651030	0.329163
C	-4.628863	-0.687214	-0.391846
C	-2.812916	-2.805339	-1.302307
C	-3.203437	-2.354712	1.525889
C	-3.202390	2.323334	-1.576193
C	-2.852697	2.787924	1.254984
H	-4.728920	0.513994	1.416135
H	-5.469932	1.294780	0.013015
H	-4.708505	-0.550824	-1.479771
H	-5.458964	-1.337553	-0.085090
H	-4.008833	-3.098319	1.463091
H	-4.014567	3.060544	-1.526618
Ni	-1.450249	-0.005584	-0.008932
P	-3.017003	-1.501175	-0.064982
P	-3.029414	1.477385	0.020229
H	-1.899160	-3.372789	-1.092640
H	1.939593	-3.362163	-1.054207
H	0.004760	-2.047093	0.415504
O	0.005882	-1.260506	-0.139253
H	-2.778451	2.348851	2.256074
H	-3.717908	3.462256	1.216639
H	-3.440076	-1.632354	2.315584
H	-2.267732	-2.862329	1.788360
H	3.426216	-1.597860	2.365464
H	2.270038	-2.838839	1.828710
H	3.715408	-3.461610	-1.219015
H	2.774814	-2.347185	-2.256329
H	3.436641	1.631423	-2.315875
H	2.265273	2.861736	-1.787319
H	3.674547	3.488236	1.275812
H	2.734165	2.362720	2.301306
H	-2.267522	2.837580	-1.828549
H	-3.422818	1.596176	-2.366168
H	-2.730534	-2.361811	-2.300803
H	-3.672100	-3.487942	-1.277071

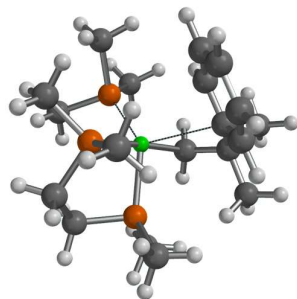


61

Ni	-0.078611	-0.676721	0.290054
P	2.130653	-0.614505	0.384853
P	0.015884	-0.132083	2.475232
C	2.697505	-0.051361	2.054579
H	3.644670	0.496036	1.965731
H	2.899980	-0.940761	2.667239
C	1.596730	0.791324	2.674793
H	1.491329	1.750586	2.146418
H	1.782482	1.014540	3.734959
C	2.905539	-2.244483	0.153566
H	2.486373	-2.961686	0.868876
H	3.991120	-2.179256	0.303242
H	2.710232	-2.611097	-0.860917
C	3.061158	0.469262	-0.741063
H	2.817325	1.516667	-0.526684
H	2.811846	0.259627	-1.786828
H	4.137073	0.312793	-0.592043
C	0.243817	-1.502961	3.663083
H	-0.700931	-2.024676	3.842541
H	0.616235	-1.115506	4.620434
H	0.960766	-2.232912	3.269461
C	-1.221945	0.931498	3.285644
H	-1.410309	1.823996	2.677598
H	-0.863783	1.242735	4.275131
H	-2.167988	0.392708	3.414426
C	0.135096	-0.968349	-1.693913
H	-0.500310	-1.805371	-2.018943
H	1.160119	-1.295818	-1.924066
C	-0.179635	0.258638	-2.592113
C	0.248382	1.574640	-1.940363
C	0.989533	3.977868	-0.640645
C	-0.275368	1.920842	-0.684026
C	1.118607	2.486755	-2.545090
C	1.488266	3.672824	-1.904814

C	0.092437	3.096135	-0.034326
H	-1.023409	1.267203	-0.216777
H	2.179343	4.357568	-2.399852
H	-0.330743	3.330656	0.944121
H	1.282718	4.899878	-0.136448
C	-1.683125	0.355401	-2.871118
H	-2.271276	0.435078	-1.949920
H	-2.031565	-0.527816	-3.422838
H	-1.913096	1.239567	-3.480624
C	0.519088	0.040372	-3.935719
H	0.210457	-0.923523	-4.359495
H	1.612344	0.019676	-3.833090
H	0.262020	0.819086	-4.667695
H	1.539945	2.270646	-3.527139
P	-2.199670	-1.400767	0.338939
C	-2.557300	-2.467269	1.781758
H	-3.546534	-2.929346	1.670149
H	-2.563396	-1.872116	2.701862
H	-1.803906	-3.257535	1.878440
C	-2.808250	-2.456480	-1.018892
H	-3.827878	-2.794863	-0.796103
H	-2.813663	-1.916881	-1.970230
H	-2.158774	-3.333761	-1.124690
C	-3.519819	-0.144761	0.500621
H	-3.567472	0.495133	-0.386979
H	-3.326750	0.496553	1.368026
H	-4.493566	-0.633628	0.631670

IV'



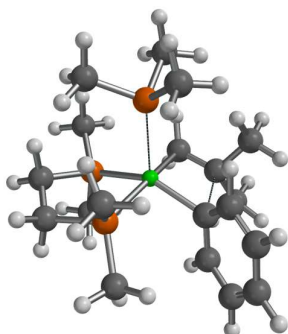
61

Ni	-0.058517	-0.446326	0.046757
P	2.108273	-0.940403	-0.042220
P	0.486914	0.390046	2.093241
C	2.352672	-1.648458	1.641280
H	3.398089	-1.960000	1.779766
H	1.735881	-2.556424	1.686856
C	1.910608	-0.645498	2.699361
H	2.731568	0.031080	2.973429
H	1.604847	-1.152272	3.623584
C	2.649426	-2.285332	-1.143278

H	1.959024	-3.132412	-1.054653
H	3.660761	-2.612842	-0.871870
H	2.654384	-1.953210	-2.187765
C	3.496949	0.250970	-0.139219
H	3.448574	0.958158	0.696433
H	3.474666	0.827942	-1.069710
H	4.451564	-0.287735	-0.079862
C	-0.588302	0.523505	3.567030
H	-1.348336	1.296235	3.400976
H	0.020353	0.821142	4.430431
H	-1.089492	-0.421210	3.802922
C	1.152765	2.090694	2.055775
H	1.806745	2.250674	1.193085
H	1.707796	2.298530	2.979709
H	0.321407	2.799379	1.977212
C	-0.347015	-0.982307	-1.850602
H	-1.374175	-1.333944	-1.985779
H	0.310447	-1.786009	-2.206714
C	-0.139080	0.315561	-2.656649
C	-0.419055	1.503623	-1.730693
C	-1.123383	3.724742	-0.130366
C	-1.654892	1.558105	-1.056767
C	0.457732	2.585954	-1.568872
C	0.107276	3.685515	-0.785300
C	-2.002854	2.650606	-0.263106
H	0.806870	4.517226	-0.682657
H	-2.972485	2.669782	0.238054
H	-1.394966	4.586321	0.481787
C	-1.144694	0.358480	-3.817328
H	-2.180384	0.316097	-3.456487
H	-0.989677	-0.498931	-4.487009
H	-1.029427	1.276545	-4.411447
C	1.260204	0.369718	-3.253761
H	1.427303	-0.507344	-3.891103
H	2.045537	0.382949	-2.490743
H	1.402460	1.260693	-3.879422
H	1.425487	2.582873	-2.072007
P	-1.946367	-1.436489	0.710675
C	-1.543819	-2.723238	1.946994
H	-2.455917	-3.183053	2.349788
H	-0.956669	-2.314517	2.776828
H	-0.940877	-3.501897	1.463990
C	-2.947326	-2.393718	-0.478753
H	-3.765747	-2.898748	0.049258
H	-3.379806	-1.729624	-1.237426
H	-2.332164	-3.145715	-0.986117
C	-3.257856	-0.446489	1.511856
H	-3.739838	0.184375	0.755199
H	-2.857939	0.207841	2.290610
H	-4.019091	-1.103712	1.952059

H	-2.376431	0.752498	-1.207259
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TS4

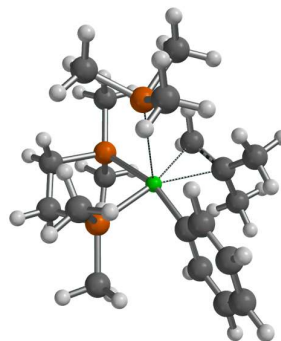


61

Ni	0.350220	-0.116466	-0.290616
P	2.006440	-1.471328	0.154235
P	0.728185	0.734539	1.753633
C	2.157065	-1.650834	1.980062
H	3.109353	-2.133941	2.241479
H	1.355172	-2.330153	2.298501
C	2.009194	-0.285705	2.626973
H	2.950331	0.276113	2.545526
H	1.776872	-0.352537	3.698266
C	2.026304	-3.180530	-0.468228
H	1.121048	-3.712020	-0.152511
H	2.904426	-3.717786	-0.088171
H	2.062361	-3.180187	-1.563790
C	3.624746	-0.812245	-0.368969
H	3.786803	0.176193	0.078093
H	3.640820	-0.696308	-1.459520
H	4.442322	-1.481892	-0.070284
C	-0.714642	0.788709	2.870973
H	-1.504890	1.386124	2.398349
H	-0.443910	1.254739	3.826977
H	-1.106153	-0.213979	3.066859
C	1.382273	2.421203	1.973426
H	2.237142	2.597927	1.310448
H	1.702806	2.548088	3.015655
H	0.605329	3.159723	1.748251
C	0.405717	-0.880762	-2.109367
H	-0.183676	-1.799215	-2.141860
H	1.409376	-1.001124	-2.527233
C	-0.257011	0.362205	-2.418744
C	-0.356736	1.709970	-0.853678
C	-1.033047	4.419416	-0.380345
C	-1.651358	2.080491	-0.452308
C	0.584008	2.741089	-1.021127
C	0.254915	4.075161	-0.793751
C	-1.983299	3.411840	-0.202877

H	1.013022	4.849305	-0.930866
H	-2.994825	3.662492	0.123672
H	-1.296206	5.463500	-0.203016
C	-1.728339	0.265777	-2.736260
H	-2.298644	-0.237474	-1.949215
H	-1.845449	-0.322145	-3.658064
H	-2.179783	1.249906	-2.904771
C	0.497288	1.226056	-3.401022
H	0.432041	0.733857	-4.382649
H	1.561036	1.309048	-3.152994
H	0.074268	2.231861	-3.500518
H	1.602852	2.497133	-1.331376
P	-1.652130	-1.621653	0.409233
C	-1.330002	-2.758059	1.821664
H	-2.216013	-3.369724	2.038959
H	-1.049165	-2.219591	2.733842
H	-0.505155	-3.434355	1.564831
C	-2.111573	-2.895419	-0.835890
H	-2.899459	-3.552772	-0.445245
H	-2.470971	-2.437608	-1.765189
H	-1.237087	-3.511600	-1.080226
C	-3.323305	-0.995288	0.854878
H	-3.785360	-0.512641	-0.016138
H	-3.258870	-0.249367	1.656225
H	-3.979552	-1.812474	1.183850
H	-2.417128	1.314721	-0.318041

13'



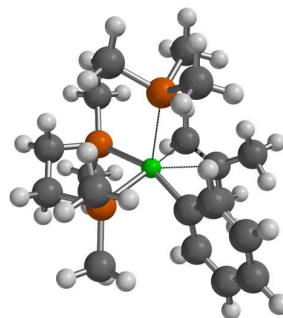
61

Ni	0.588196	0.160095	-0.376808
P	1.990150	-1.505725	0.152133
P	0.981609	0.883989	1.656426
C	2.190095	-1.559724	1.977181
H	3.060283	-2.169671	2.256120
H	1.297341	-2.053711	2.388322
C	2.296377	-0.130066	2.466704
H	3.265343	0.310522	2.192721
H	2.202477	-0.043525	3.557914

C	1.718324	-3.237598	-0.329217
H	0.745705	-3.587087	0.034460
H	2.503253	-3.872695	0.099710
H	1.741434	-3.342850	-1.419549
C	3.671928	-1.153946	-0.458359
H	3.989451	-0.154985	-0.137322
H	3.684092	-1.175475	-1.554622
H	4.386952	-1.897603	-0.083039
C	-0.441625	0.656754	2.769157
H	-1.343348	1.107078	2.340497
H	-0.227781	1.128811	3.736632
H	-0.619696	-0.411579	2.930793
C	1.513492	2.588120	1.997470
H	2.311600	2.890425	1.310208
H	1.887274	2.640542	3.027892
H	0.671806	3.279288	1.883595
C	0.546934	-0.930907	-2.205798
H	-0.119217	-1.768603	-1.995393
H	1.569405	-1.189716	-2.485912
C	0.028724	0.274390	-2.634880
C	-0.310148	1.898466	-0.459983
C	-1.586441	4.424491	-0.587038
C	-1.656215	2.055101	-0.098087
C	0.384208	3.048887	-0.864123
C	-0.242224	4.293315	-0.940753
C	-2.290717	3.297927	-0.160635
H	0.325830	5.167124	-1.268444
H	-3.342523	3.382933	0.121819
H	-2.079062	5.397183	-0.639255
C	-1.444947	0.455426	-2.814241
H	-2.028214	-0.117316	-2.083340
H	-1.721338	0.098173	-3.818540
H	-1.745888	1.507341	-2.752084
C	0.907606	1.235964	-3.367750
H	0.840376	1.016152	-4.444927
H	1.961346	1.146325	-3.077425
H	0.588851	2.276304	-3.241287
H	1.444240	2.978275	-1.125150
P	-1.758120	-1.744125	0.478217
C	-1.585151	-2.927457	1.881912
H	-2.454380	-3.596537	1.949475
H	-1.494768	-2.388247	2.833188
H	-0.684581	-3.542824	1.763010
C	-2.214990	-2.932377	-0.854068
H	-3.050588	-3.576814	-0.548533
H	-2.508161	-2.392036	-1.763509
H	-1.360887	-3.572962	-1.109643
C	-3.426320	-1.065571	0.860353
H	-3.802815	-0.494066	0.001806
H	-3.374575	-0.385251	1.720478

H	-4.145300	-1.864515	1.088267
H	-2.234679	1.186160	0.223251

TS5

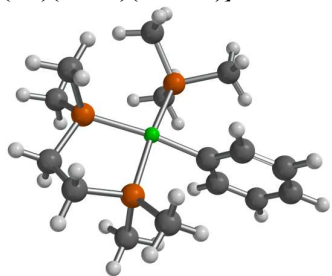


61

Ni	0.423242	0.054439	-0.210237
P	1.964903	-1.521003	0.199591
P	1.020585	0.881732	1.713971
C	2.229197	-1.593859	2.014782
H	3.123418	-2.183923	2.258571
H	1.365634	-2.108429	2.458499
C	2.326404	-0.164180	2.510538
H	3.295174	0.275251	2.235156
H	2.241623	-0.085214	3.602750
C	1.845327	-3.257902	-0.337050
H	0.960391	-3.740630	0.090976
H	2.736236	-3.814427	-0.020284
H	1.772756	-3.310373	-1.429527
C	3.603653	-1.024447	-0.435190
H	3.839040	-0.000236	-0.123476
H	3.607552	-1.050650	-1.530988
H	4.385519	-1.702121	-0.067796
C	-0.346560	0.851059	2.916959
H	-1.171147	1.478914	2.561522
H	0.001173	1.229272	3.886798
H	-0.715468	-0.171103	3.048661
C	1.701325	2.555383	1.931548
H	2.493675	2.748089	1.199162
H	2.123331	2.635569	2.941531
H	0.916264	3.308370	1.809446
C	0.552949	-0.863370	-2.308017
H	-0.112389	-1.704959	-2.130688
H	1.605862	-1.098295	-2.464287
C	0.072237	0.324354	-2.781340
C	-0.420640	1.825736	-0.323642
C	-1.581872	4.395444	-0.658438
C	-1.755886	2.078243	0.023493
C	0.325171	2.914333	-0.805644
C	-0.243616	4.175566	-0.989191
C	-2.334020	3.339640	-0.141898

H	0.366941	4.993276	-1.378807
H	-3.379252	3.495243	0.134089
H	-2.029635	5.381987	-0.791268
C	-1.387472	0.574142	-2.957613
H	-2.002073	-0.044211	-2.293554
H	-1.666552	0.338902	-3.996508
H	-1.645342	1.627700	-2.795145
C	0.996285	1.309683	-3.413104
H	0.987066	1.140625	-4.501317
H	2.030831	1.195522	-3.069838
H	0.674381	2.345716	-3.262635
H	1.384246	2.778568	-1.041284
P	-1.625780	-1.556229	0.331425
C	-1.383791	-2.681238	1.767833
H	-2.228645	-3.377074	1.859514
H	-1.304440	-2.116842	2.703709
H	-0.467717	-3.271552	1.654312
C	-2.009453	-2.816850	-0.951900
H	-2.799538	-3.494954	-0.603652
H	-2.348773	-2.337626	-1.878782
H	-1.121224	-3.416323	-1.187225
C	-3.332503	-0.982670	0.703051
H	-3.738904	-0.412394	-0.141407
H	-3.335388	-0.332903	1.587212
H	-3.994018	-1.837372	0.898340
H	-2.372650	1.277330	0.427006

[Ni(Ph)(PMe₃)(DMPE)]⁺

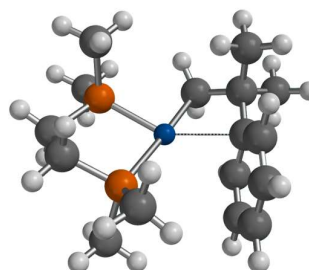


49

Ni	-0.124489	0.001258	-0.121940
P	-2.250233	0.529668	-0.582396
P	0.337834	2.127193	-0.409819
C	-2.374632	2.372068	-0.632986
H	-2.521026	2.711533	0.402931
H	-3.268007	2.674348	-1.196706
C	-1.098508	2.952350	-1.214961
H	-1.037473	4.042362	-1.089442
H	-1.027207	2.746789	-2.293089
C	-2.788495	0.027299	-2.250836
H	-2.090994	0.424001	-2.998269
H	-3.795229	0.410477	-2.462616

H	-2.796042	-1.064613	-2.340190
C	-3.638521	0.062544	0.500219
H	-3.432421	0.394689	1.524552
H	-3.784949	-1.022851	0.513322
H	-4.565499	0.535695	0.151881
C	1.791003	2.650904	-1.360962
H	2.702883	2.363555	-0.824692
H	1.779623	3.739798	-1.495794
H	1.796864	2.165752	-2.343771
C	0.515222	2.988825	1.183367
H	1.392161	2.600721	1.714594
H	-0.369247	2.821389	1.809224
H	0.643018	4.066934	1.021498
C	2.228174	-0.089401	1.575158
C	4.028526	-0.751238	-0.437257
C	3.576470	-0.292097	1.883611
C	1.749994	-0.220445	0.261464
C	2.680494	-0.549124	-0.737913
C	4.483508	-0.626339	0.877308
H	3.917981	-0.188845	2.916316
H	2.352145	-0.655078	-1.776772
H	5.537108	-0.785645	1.114299
H	4.729225	-1.009256	-1.235093
H	1.538208	0.170398	2.384751
P	-0.412113	-2.154969	0.361635
C	1.024177	-3.265184	0.209818
H	1.397939	-3.260645	-0.821003
H	0.734411	-4.288191	0.481535
H	1.833640	-2.930956	0.868413
C	-1.697467	-3.096987	-0.528030
H	-1.461356	-3.128768	-1.598469
H	-2.683509	-2.636563	-0.405270
H	-1.744121	-4.125501	-0.147745
C	-0.882349	-2.334187	2.113557
H	-0.104095	-1.895032	2.749437
H	-0.996005	-3.394586	2.374881
H	-1.826618	-1.814049	2.312254

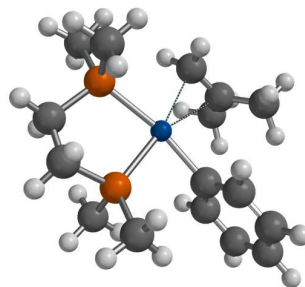
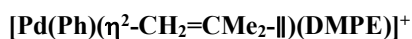
6'



48

Pd	-0.262932	0.295476	-0.124545
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P	-1.517762	0.968774	1.621674
P	-1.230249	-1.879080	0.214666
C	-2.718109	-0.369127	2.013046
H	-3.564343	-0.246634	1.321040
H	-3.113143	-0.217948	3.027872
C	-2.076538	-1.737498	1.850450
H	-2.816050	-2.542477	1.965390
H	-1.307857	-1.900574	2.620451
C	-0.297209	-3.436204	0.354285
H	0.098174	-3.723949	-0.626450
H	-0.948431	-4.241034	0.720235
H	0.545520	-3.311099	1.044178
C	-2.581558	-2.297776	-0.936289
H	-2.172084	-2.462435	-1.940356
H	-3.298793	-1.470304	-0.994010
H	-3.107177	-3.205689	-0.611767
C	-0.532723	1.197706	3.129892
H	0.193920	2.004164	2.976608
H	0.015139	0.278742	3.367962
H	-1.186869	1.457182	3.972803
C	-2.498951	2.483409	1.469928
H	-3.169773	2.411992	0.606665
H	-1.833792	3.343032	1.329785
H	-3.093923	2.638469	2.379571
C	0.550284	2.204712	-0.347266
H	0.559360	2.840424	0.546131
H	-0.031811	2.699727	-1.138656
C	0.771485	0.190409	-2.409149
C	2.306345	-1.993270	-1.625097
C	0.578675	-1.057684	-3.017334
C	1.751223	0.370815	-1.401596
C	2.495982	-0.760511	-1.009238
C	1.350886	-2.147600	-2.633610
H	-0.173328	-1.161501	-3.800953
H	3.247404	-0.668360	-0.225275
H	1.205886	-3.119041	-3.108478
H	2.907460	-2.847693	-1.309668
C	1.951211	1.775842	-0.800002
C	2.885526	1.740530	0.403626
H	2.507387	1.074514	1.192206
H	2.972718	2.746333	0.831964
H	3.897130	1.410467	0.134137
C	2.520976	2.717916	-1.862446
H	3.513693	2.383817	-2.196904
H	2.625219	3.732918	-1.455677
H	1.868314	2.776595	-2.742580
H	0.213489	1.053523	-2.777214

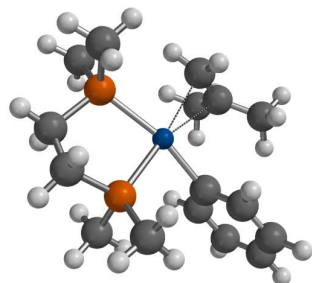


48

Pd	-0.034650	0.385579	0.229374
P	-1.603512	0.985798	1.928894
P	-1.188724	-1.583093	0.151685
C	-2.926596	-0.293625	1.882089
H	-3.629116	-0.006206	1.086366
H	-3.490891	-0.286432	2.825003
C	-2.317189	-1.654665	1.603803
H	-3.083163	-2.422081	1.423002
H	-1.715163	-2.000580	2.456764
C	-0.326441	-3.175815	0.157618
H	0.201640	-3.317337	-0.791921
H	-1.058559	-3.982795	0.289837
H	0.402459	-3.211045	0.975227
C	-2.280387	-1.653511	-1.296384
H	-1.678710	-1.659879	-2.212380
H	-2.943594	-0.781336	-1.319022
H	-2.886377	-2.568283	-1.260254
C	-0.893196	0.827271	3.598052
H	-0.109691	1.580430	3.742435
H	-0.440584	-0.163403	3.723217
H	-1.668048	0.967505	4.363159
C	-2.494390	2.568644	1.980834
H	-2.978569	2.764425	1.017233
H	-1.793930	3.384783	2.193128
H	-3.256929	2.549652	2.769887
C	0.765254	2.531824	0.589261
H	1.221862	2.452672	1.578535
H	-0.144600	3.128140	0.514918
C	0.957723	-0.670255	-2.485981
C	3.170033	-2.004451	-1.448565
C	1.819677	-1.366137	-3.340260
C	1.196202	-0.620028	-1.108313
C	2.304870	-1.311349	-0.600497
C	2.929611	-2.034173	-2.823944
H	1.617613	-1.386964	-4.413613
H	2.509868	-1.308378	0.474264
H	3.601742	-2.579923	-3.488645
H	4.033632	-2.528019	-1.032032
C	1.501790	2.275525	-0.541430

C	2.934402	1.863339	-0.466899
H	3.186991	1.377102	0.481647
H	3.554796	2.768635	-0.555245
H	3.220268	1.204397	-1.295557
C	1.008957	2.686458	-1.888830
H	1.206158	1.914974	-2.644617
H	1.564779	3.579418	-2.214352
H	-0.059058	2.930585	-1.892692
H	0.091740	-0.157394	-2.914801

TS2-Pd

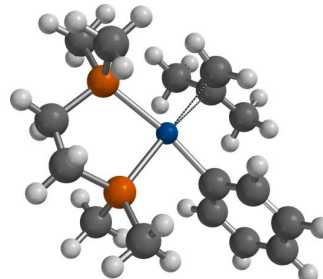


48

Pd	0.092293	0.258550	0.298533
P	-1.506441	0.942365	1.946864
P	-1.116599	-1.668287	0.203104
C	-2.836157	-0.333191	1.913606
H	-3.529192	-0.054807	1.106233
H	-3.411014	-0.307274	2.849680
C	-2.236283	-1.705051	1.662457
H	-3.008510	-2.471366	1.504130
H	-1.630438	-2.034689	2.519255
C	-0.258618	-3.262936	0.218973
H	0.283752	-3.399363	-0.723622
H	-0.989920	-4.072701	0.337714
H	0.459707	-3.298322	1.045822
C	-2.217120	-1.745891	-1.237783
H	-1.622120	-1.775644	-2.157461
H	-2.869355	-0.865817	-1.270784
H	-2.834318	-2.652160	-1.182655
C	-0.872170	0.887320	3.653314
H	-0.084527	1.639465	3.782120
H	-0.439023	-0.098306	3.860846
H	-1.675979	1.085311	4.374472
C	-2.397759	2.526059	1.859663
H	-2.882434	2.630139	0.881897
H	-1.699329	3.361024	1.992038
H	-3.160432	2.581149	2.647086
C	1.326913	2.200173	0.847182
H	2.191892	1.816832	1.393361
H	0.579976	2.738691	1.428590
C	0.985551	-0.726660	-2.442796

C	3.329890	-1.944198	-1.564991
C	1.840016	-1.342223	-3.362374
C	1.295955	-0.700747	-1.077623
C	2.471304	-1.331058	-0.649266
C	3.016095	-1.952462	-2.925578
H	1.583568	-1.343725	-4.424263
H	2.736212	-1.341861	0.412369
H	3.683784	-2.435957	-3.641054
H	4.247512	-2.421227	-1.212735
C	1.373016	2.332355	-0.515508
C	2.611442	2.028364	-1.288396
H	3.317621	1.406337	-0.729931
H	3.106204	2.986733	-1.509590
H	2.400004	1.556023	-2.255490
C	0.274210	3.002251	-1.273777
H	-0.045708	2.384416	-2.125735
H	0.640673	3.944312	-1.708692
H	-0.597615	3.224591	-0.648759
H	0.073471	-0.246544	-2.810446

[Pd(Ph)(η^2 -CH₂=CMe₂-1)(DMPE)]⁺

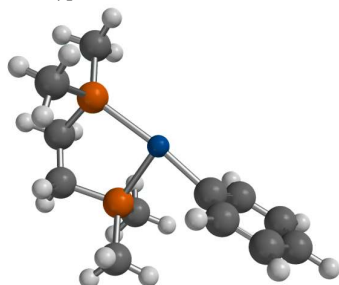


48

Pd	0.115795	0.230183	0.247284
P	-1.574199	1.033225	1.763272
P	-1.190633	-1.630259	0.079782
C	-2.976298	-0.152265	1.598465
H	-3.565433	0.162252	0.724504
H	-3.638351	-0.077420	2.472502
C	-2.451925	-1.565631	1.417505
H	-3.256781	-2.277847	1.186243
H	-1.963010	-1.926169	2.334308
C	-0.427748	-3.267218	0.214265
H	0.212034	-3.446869	-0.657510
H	-1.208516	-4.037462	0.257057
H	0.187697	-3.323641	1.119237
C	-2.142988	-1.680854	-1.464093
H	-1.462666	-1.772681	-2.318153
H	-2.729862	-0.762772	-1.580960
H	-2.819968	-2.545157	-1.453585
C	-1.053439	0.845908	3.500523
H	-0.246052	1.553104	3.725085

H	-0.673311	-0.167475	3.675908
H	-1.892678	1.037108	4.182229
C	-2.372310	2.668787	1.738276
H	-2.771491	2.882802	0.740044
H	-1.641309	3.444162	1.997788
H	-3.191080	2.703737	2.468543
C	1.587653	1.977303	0.822784
H	2.498743	1.439180	1.093485
H	1.019867	2.431483	1.635339
C	1.285453	-0.939826	-2.313797
C	3.499241	-2.102187	-1.089955
C	2.236689	-1.613744	-3.084886
C	1.433343	-0.827209	-0.926191
C	2.544187	-1.430727	-0.322069
C	3.347662	-2.196658	-2.474526
H	2.107020	-1.682652	-4.167354
H	2.682463	-1.375599	0.761829
H	4.090734	-2.725351	-3.074350
H	4.365118	-2.556193	-0.602364
C	1.368941	2.351217	-0.476034
C	2.354287	2.066957	-1.557868
H	3.116881	1.339221	-1.264145
H	2.858191	3.012008	-1.811921
H	1.865682	1.722596	-2.478719
C	0.228525	3.234895	-0.861376
H	-0.377045	2.773772	-1.655692
H	0.613590	4.173151	-1.287073
H	-0.422010	3.480432	-0.017162
H	0.429308	-0.479617	-2.816475

[Pd(Ph)(DiPPE)]

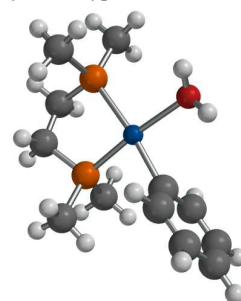


36

Pd	-0.555061	-0.879091	0.085420
P	1.072327	-1.854711	1.556709
P	0.729103	0.940082	-0.048025
C	2.495262	-0.697355	1.358033
H	3.031783	-0.997260	0.446040
H	3.198362	-0.815495	2.194274
C	2.010534	0.738746	1.253166
H	2.831943	1.436803	1.034428
H	1.552573	1.073203	2.195605

C	-0.012015	2.562549	0.234121
H	-0.653641	2.830392	-0.612237
H	0.788213	3.307568	0.335624
H	-0.613469	2.551377	1.149865
C	1.608971	1.051484	-1.624359
H	0.894318	1.220807	-2.437411
H	2.158094	0.124078	-1.821949
H	2.316453	1.890458	-1.584134
C	0.686565	-1.766447	3.334862
H	-0.126981	-2.460505	3.576254
H	0.360207	-0.754187	3.601408
H	1.568754	-2.028229	3.933989
C	1.805508	-3.504924	1.347095
H	2.149014	-3.636244	0.314776
H	1.056080	-4.274581	1.564831
H	2.655695	-3.636356	2.029359
C	-1.731549	-0.045918	-2.539634
C	-3.938013	1.269300	-1.446925
C	-2.756685	0.412924	-3.371903
C	-1.816175	0.127689	-1.151839
C	-2.913568	0.813693	-0.613433
C	-3.859759	1.070381	-2.826363
H	-2.687867	0.259818	-4.451001
H	-2.983649	0.994689	0.462998
H	-4.655170	1.436813	-3.477738
H	-4.796385	1.788878	-1.015709
H	-0.869776	-0.550428	-2.986195

[Pd((Ph)(H₂O)(DMPE)]⁺

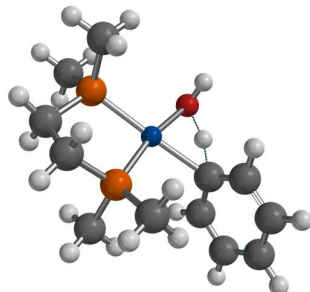


39

Pd	0.400883	0.691174	0.115159
P	-1.261429	1.584900	1.582981
P	-0.929630	-1.088503	-0.098227
C	-2.716804	0.481765	1.331288
H	-3.234802	0.831810	0.426393
H	-3.424712	0.586325	2.165298
C	-2.257769	-0.957664	1.169354
H	-3.084693	-1.627163	0.892468
H	-1.836795	-1.344662	2.109067
C	-0.219603	-2.740275	0.111361

H	0.453756	-2.959894	-0.724923
H	-1.023637	-3.487354	0.134348
H	0.350140	-2.792671	1.045967
C	-1.786205	-1.141556	-1.695613
H	-1.053994	-1.255451	-2.503206
H	-2.346047	-0.213598	-1.858789
H	-2.480729	-1.991689	-1.717330
C	-0.900018	1.434127	3.362576
H	-0.061301	2.087536	3.630756
H	-0.617206	0.402488	3.603394
H	-1.776106	1.714899	3.962222
C	-1.919949	3.270510	1.409678
H	-2.248969	3.440405	0.378188
H	-1.135343	3.999101	1.646650
H	-2.767006	3.430834	2.089701
C	1.622866	-0.115377	-2.536372
C	3.778451	-1.512433	-1.457338
C	2.605445	-0.646542	-3.378072
C	1.707686	-0.269068	-1.145948
C	2.793977	-0.982044	-0.618612
C	3.684919	-1.347741	-2.840134
H	2.523824	-0.512566	-4.459203
H	2.882841	-1.134430	0.461218
H	4.450009	-1.766647	-3.496405
H	4.619710	-2.060960	-1.027212
H	0.783784	0.427707	-2.981483
O	1.798819	2.442138	0.134675
H	1.946235	2.905361	0.968453
H	2.679398	2.217209	-0.192328

TS3-Pd

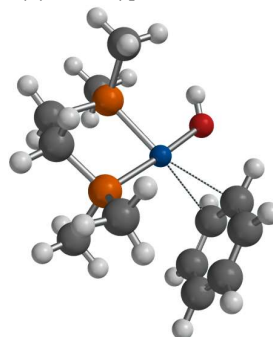


39

Pd	0.366496	0.873215	0.209174
P	-1.355495	1.520783	1.592670
P	-0.871657	-0.986149	-0.111851
C	-2.748067	0.339289	1.386279
H	-3.330516	0.674480	0.516139
H	-3.415970	0.384580	2.257141
C	-2.190589	-1.056573	1.163877
H	-2.966908	-1.770925	0.856742

H	-1.732039	-1.452848	2.081393
C	0.002314	-2.568090	-0.066519
H	0.710239	-2.615771	-0.902505
H	-0.717936	-3.391798	-0.156690
H	0.556337	-2.669624	0.873300
C	-1.730583	-0.953125	-1.708241
H	-0.996880	-0.952298	-2.522569
H	-2.349053	-0.052480	-1.793135
H	-2.369682	-1.841341	-1.801643
C	-0.899121	1.449202	3.346928
H	-0.067353	2.135894	3.542691
H	-0.584453	0.434444	3.615940
H	-1.757100	1.738406	3.968461
C	-2.020190	3.182183	1.327628
H	-2.387443	3.279920	0.300049
H	-1.228237	3.922476	1.491214
H	-2.842461	3.377385	2.028713
C	1.822349	0.198101	-2.448863
C	3.594756	-1.637947	-1.318549
C	2.428421	-0.764055	-3.254103
C	2.082874	0.262113	-1.065757
C	2.978529	-0.678137	-0.518840
C	3.313400	-1.684067	-2.686381
H	2.215625	-0.799813	-4.324285
H	3.203917	-0.650878	0.551309
H	3.788403	-2.440277	-3.314276
H	4.291814	-2.354668	-0.880163
H	1.135637	0.917983	-2.903667
O	1.729523	2.555980	0.168935
H	2.091041	1.501620	-0.482912
H	2.250059	2.572810	0.982366

[Pd(OH)(Ph-H)(DMPE)]⁺

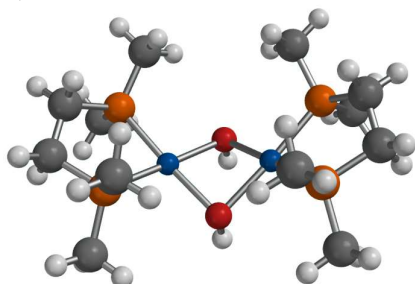


39

Pd	0.588491	0.770188	0.283956
P	-1.124407	1.366117	1.621037
P	-0.719568	-1.042750	-0.268951
C	-2.573100	0.309106	1.251450
H	-3.082901	0.755489	0.385758

H	-3.275518	0.345477	2.095637
C	-2.099814	-1.097678	0.947224
H	-2.908323	-1.731467	0.558046
H	-1.712432	-1.589640	1.851088
C	-0.057044	-2.731343	-0.238048
H	0.593231	-2.908859	-1.099662
H	-0.895091	-3.439897	-0.278147
H	0.514872	-2.898682	0.681423
C	-1.540984	-0.891949	-1.882827
H	-0.797972	-0.917042	-2.687579
H	-2.085055	0.057746	-1.943105
H	-2.246113	-1.722305	-2.020536
C	-0.731585	1.125660	3.371573
H	0.141692	1.728675	3.645214
H	-0.506798	0.071638	3.569064
H	-1.589667	1.435448	3.983178
C	-1.661301	3.081399	1.450457
H	-1.924943	3.291278	0.408309
H	-0.858155	3.759679	1.757869
H	-2.538334	3.249310	2.089952
C	1.828952	0.265192	-2.818015
C	3.142285	-1.223296	-0.839983
C	2.083280	-1.087534	-3.012408
C	2.245867	0.892977	-1.634258
C	2.901409	0.144134	-0.638679
C	2.746640	-1.829165	-2.026598
H	1.771094	-1.573291	-3.938512
H	3.283812	0.649521	0.248858
H	2.947489	-2.889371	-2.189823
H	3.661164	-1.800436	-0.073302
H	1.324755	0.847529	-3.590715
O	1.649070	2.435748	0.829427
H	1.369873	2.821031	1.664710
H	2.135128	1.971360	-1.513081

Cis-[Pd(μ -OH)(DMPE)]₂²⁺

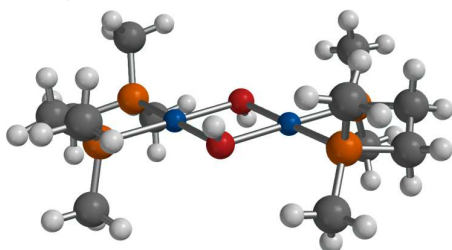


54

H	1.450035	3.397978	0.378502
H	-1.474633	3.383357	0.353295
H	0.012105	1.508250	-2.373101
O	0.004807	1.454465	-1.409355

C	4.497126	-0.662427	0.452164
C	4.157807	0.684830	1.067136
C	2.148537	2.832099	1.004939
C	3.845182	2.386371	-1.294556
C	2.305708	-2.339067	1.440761
C	3.386754	-2.828986	-1.192304
H	5.096141	-0.540844	-0.461841
H	5.076782	-1.298139	1.134946
H	3.701422	0.562789	2.059894
H	5.045062	1.319425	1.195882
H	4.524281	3.125012	-0.848451
H	3.036148	-3.073342	1.805091
Pd	1.478629	0.014507	-0.805090
P	2.921579	1.537058	0.010277
P	2.945238	-1.511847	-0.037883
C	-4.165941	0.649004	1.022236
C	-4.493825	-0.697829	0.400114
C	-3.364895	-2.840464	-1.261419
C	-2.300234	-2.377987	1.382752
C	-3.855616	2.356201	-1.335565
C	-2.175944	2.814551	0.973835
H	-3.711832	0.525493	2.015811
H	-5.057956	1.276877	1.150814
H	-5.090709	-0.576145	-0.515305
H	-5.071580	-1.340535	1.077986
H	-3.030091	-3.118802	1.734835
H	-4.543651	3.088283	-0.892334
Pd	-1.468582	0.004126	-0.829412
P	-2.935053	-1.535320	-0.089051
P	-2.931657	1.513761	-0.026526
H	-2.462807	-3.402389	-1.528387
H	2.488111	-3.397161	-1.457784
H	0.024048	-1.465478	-2.420774
O	0.015064	-1.416076	-1.457153
H	-1.631429	2.371481	1.815118
H	-2.950711	3.491506	1.356748
H	-2.103654	-1.654208	2.181832
H	-1.363438	-2.888270	1.131383
H	2.103637	-1.606279	2.230246
H	1.371381	-2.855221	1.192359
H	4.112794	-3.505870	-0.723096
H	3.822708	-2.403729	-2.102791
H	4.427858	1.665755	-1.879326
H	3.145732	2.899441	-1.964794
H	2.915645	3.512898	1.396251
H	1.598357	2.384936	1.840346
H	-3.157173	2.876258	-2.001387
H	-4.428753	1.631262	-1.924449
H	-3.797438	-2.406201	-2.169287
H	-4.091077	-3.525358	-0.804131

Trans-[Pd(μ -OH)(DMPE)]₂²⁺

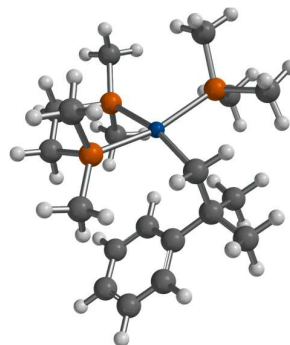


54

Pd	0.000032	-0.003626	1.603087
P	-1.520934	0.010286	3.262624
P	1.520377	-0.008582	3.263410
C	-0.680057	-0.338533	4.855942
H	-0.577254	-1.430381	4.932954
H	-1.310736	-0.012638	5.694085
C	0.678438	0.340803	4.856190
H	1.308750	0.014698	5.694618
H	0.575895	1.432682	4.933290
C	-2.290680	1.640890	3.432591
H	-1.530524	2.398892	3.652664
H	-3.029435	1.621933	4.244749
H	-2.792118	1.909183	2.495556
C	-2.884846	-1.165519	3.104613
H	-2.497934	-2.187305	3.025220
H	-3.470156	-0.932820	2.207583
H	-3.539707	-1.092174	3.982857
C	2.881285	1.170470	3.103817
H	3.467586	0.937975	2.207412
H	3.536009	1.100220	3.982428
H	2.491720	2.191161	3.022597
C	2.294119	-1.636952	3.436311
H	2.796073	-1.905804	2.499706
H	1.535713	-2.396300	3.657896
H	3.032865	-1.614731	4.248376
O	-1.407895	0.030507	-0.001128
H	-1.986804	-0.739912	-0.004183
O	1.407747	-0.050587	-0.000859
H	1.995147	0.713363	-0.004695
Pd	0.000321	-0.004956	-1.606216
P	-1.522534	-0.031257	-3.263973
P	1.522484	0.029755	-3.264484
C	2.875782	-1.154066	-3.086222
H	3.541587	-1.092327	-3.957017
H	2.477859	-2.171248	-3.003743
H	3.447990	-0.922219	-2.180878
C	2.303257	1.654071	-3.452813
H	3.037386	1.621296	-4.268825

H	2.814201	1.930637	-2.523057
H	1.547320	2.415069	-3.676847
C	0.682278	-0.329396	-4.856321
H	1.308018	0.002348	-5.695966
H	0.590953	-1.422386	-4.932191
C	-2.303208	-1.654780	-3.459155
H	-1.547331	-2.414743	-3.687012
H	-3.037935	-1.618527	-4.274534
H	-2.813490	-1.935443	-2.530283
C	-0.683087	0.335581	-4.854461
H	-0.591657	1.428914	-4.924882
H	-1.309195	0.008153	-5.695451
C	-2.875889	1.151419	-3.079150
H	-3.542586	1.093309	-3.949498
H	-2.478247	2.168380	-2.992464
H	-3.446953	0.915217	-2.174267

[Pd(CH₂CMe₂Ph)(PMe₃)(DMPE)]⁺

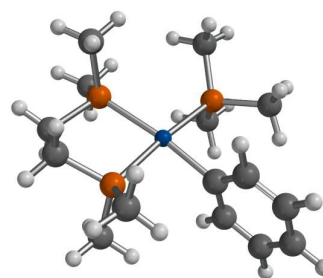


61

Pd	0.514373	-0.622437	0.290415
P	-1.593158	-1.600320	0.080663
P	-0.102971	-0.473137	2.599515
C	-2.582597	-1.222042	1.585268
H	-3.458372	-1.884786	1.632448
H	-2.963128	-0.195803	1.471445
C	-1.713598	-1.350545	2.824656
H	-1.480215	-2.405613	3.028463
H	-2.219760	-0.960963	3.719212
C	-2.755108	-1.418264	-1.300638
H	-3.173804	-0.406725	-1.318330
H	-3.570780	-2.144489	-1.191528
H	-2.243814	-1.601841	-2.252909
C	-1.333372	-3.402929	0.172192
H	-0.831241	-3.744581	-0.740796
H	-2.292200	-3.929687	0.269603
H	-0.693309	-3.656217	1.025336
C	-0.538741	1.267481	2.943667
H	0.335562	1.913503	2.799218

H	-0.900428	1.379582	3.974061
H	-1.326052	1.602139	2.258446
C	0.831078	-0.954185	4.089475
H	1.124707	-2.008882	4.033953
H	0.214566	-0.802938	4.985183
H	1.735034	-0.340668	4.182639
C	0.674508	-0.429898	-1.821068
H	-0.017919	-1.124880	-2.319817
H	1.686247	-0.729135	-2.129718
C	0.405609	0.999668	-2.343340
C	-1.046112	1.413183	-2.087938
C	-3.717064	2.202113	-1.559647
C	-1.462154	1.781616	-0.797683
C	-2.007049	1.459069	-3.105363
C	-3.324133	1.847697	-2.848323
C	-2.773519	2.166321	-0.530748
H	-0.739093	1.772196	0.020452
H	-4.046081	1.872270	-3.666698
H	-3.059496	2.446487	0.485274
H	-4.743999	2.510024	-1.357378
C	0.725250	0.995811	-3.843022
H	0.161359	0.226624	-4.385656
H	1.791514	0.783771	-3.992988
H	0.509090	1.967200	-4.310233
C	1.333865	2.027803	-1.684683
H	2.384542	1.782708	-1.881491
H	1.204498	2.076989	-0.596469
H	1.153203	3.033552	-2.087577
H	-1.735468	1.190131	-4.126010
P	2.832621	-0.285729	0.586914
C	3.378758	1.256411	1.391954
H	4.462167	1.234205	1.568324
H	2.865758	1.376425	2.353805
H	3.140921	2.121873	0.762777
C	3.953208	-0.438029	-0.844985
H	4.994019	-0.346951	-0.508966
H	3.818796	-1.421144	-1.312260
H	3.758371	0.328716	-1.601128
C	3.508440	-1.578830	1.683711
H	3.303071	-2.569259	1.261014
H	3.048945	-1.526086	2.675268
H	4.594653	-1.458575	1.792037

[Pd(Ph)(PMe₃)(DMPE)]⁺



49

Pd	-0.104085	0.098972	-0.008303
P	-2.351894	0.610997	0.577428
P	0.339301	0.441923	2.247131
C	-2.410099	0.614007	2.424178
H	-2.516745	-0.434824	2.738753
H	-3.311241	1.141293	2.767738
C	-1.145691	1.222828	3.006458
H	-1.107777	1.118777	4.100092
H	-1.089521	2.299029	2.785706
C	-2.914189	2.285170	0.126758
H	-2.202477	3.031155	0.500101
H	-3.904196	2.489552	0.555562
H	-2.970598	2.384999	-0.963237
C	-3.747986	-0.462946	0.117443
H	-3.531027	-1.497621	0.407623
H	-3.911490	-0.434949	-0.965853
H	-4.667869	-0.135561	0.619273
C	1.747651	1.467032	2.750917
H	2.679355	0.973939	2.448938
H	1.750874	1.605605	3.839677
H	1.697482	2.446233	2.261099
C	0.565804	-1.115877	3.156491
H	1.452850	-1.635478	2.775002
H	-0.303516	-1.768571	3.014596
H	0.698155	-0.919682	4.228589
C	2.361657	-1.652113	-0.139975
C	4.181664	0.346713	-0.795860
C	3.706280	-1.972753	-0.351447
C	1.902089	-0.332870	-0.261108
C	2.836468	0.661188	-0.585080
C	4.621712	-0.973371	-0.683446
H	4.037918	-3.009626	-0.257784
H	2.517986	1.703454	-0.682692
H	5.671720	-1.220741	-0.850694
H	4.890035	1.138668	-1.051157
H	1.663308	-2.455101	0.116237
P	-0.425520	-0.398298	-2.292208
C	1.027253	-0.269994	-3.381127
H	1.419379	0.753890	-3.365973
H	0.751980	-0.534104	-4.410459

H	1.818691	-0.944128	-3.033362
C	-1.683606	0.571392	-3.185644
H	-1.413490	1.634085	-3.175344
H	-2.664369	0.459451	-2.709766
H	-1.758477	0.234752	-4.227992
C	-0.968353	-2.122059	-2.515361
H	-0.216944	-2.803112	-2.097680
H	-1.100970	-2.350772	-3.581332
H	-1.917482	-2.290549	-1.992909