Supplementary Material (ESI) for Dalton Transactions

Supporting Information for

Steric Nature of the Bite Angle. A Closer and a Broader Look

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Contents

Movies

Table S1. Energy ΔE relative to reactants (in kcal mol^{-1}) and C–X bond distance (in Å) of stationary points in oxidative insertion (OxIn) reactions of [Pd] complexes into the C–X bond of CH_3X with X = H, CH_3 and Cl.[a]

		RC		TS		P	
[Pd]	CH_3X	ΔE	C–X	ΔE	C–X	ΔE	C–X
Pd	CH_4	–6.7	1.123	3.9	1.616	–3.4	2.479
Pd[P2P]	CH_4	–1.3	1.108	18.6	1.704	12.6	2.473
Pd[P3P]	CH_4	–0.5	1.102	22.3	1.691	15.7	2.479
Pd[P4P]	CH_4	–0.5	1.097	25.7	1.701	19.6	2.453
Pd[P5P]	CH_4	–0.1	1.096	29.2	1.697	23.1	2.437
Pd[P6P]	CH_4	-	-	32.1	1.705	26.4	2.423
$Pd(PH_3)_2$	CH_4	-	-	32.2	1.725	27.1	2.432
Pd	C_2H_6	–6.8	1.540	18.3	1.945	–9.3	3.025
Pd[P2P]	C_2H_6	–1.7	1.539	38.4	2.073	11.3	2.861
Pd[P3P]	C_2H_6	-	-	43.1	2.078	14.3	2.857
Pd[P4P]	C_2H_6	-	-	46.3	2.090	18.7	2.838
Pd[P5P]	C_2H_6	-	-	49.5	2.094	22.4	2.825
Pd[P6P]	C_2H_6	-	-	51.5	2.107	26.0	2.829
$Pd(PH_3)_2$	C_2H_6	-	-	51.3	2.107	26.4	2.836
Pd	CH_3Cl	–12.9	1.862	–0.6	2.054	–33.1	3.221
Pd[P2P]	CH_3Cl	–6.4	1.856	14.3	2.206	–27.1	3.175
Pd[P3P]	CH_3Cl	–3.3	1.849	18.5	2.217	–25.1	3.183
Pd[P4P]	CH_3Cl	–1.3	1.839	21.7	2.227	–20.3	3.174
Pd[P5P]	CH_3Cl	–0.9	1.828	25.1	2.249	–17.9	3.191
Pd[P6P]	CH_3Cl	–1.1	1.829	26.2	2.240	–13.3	3.151
$Pd(PH_3)_2$	CH_3Cl	–0.5	1.828	27.1	2.250	–11.6	3.148

[a] Computed at ZORA-BLYP/TZ2P. RC = reactant complex, TS = transition state, P = product, Pd[PnP] = $Pd[PH_2(CH_2)_nPH_2]$.

Table S2. Entropy effects at 298 K on activation barriers (relative to the reactants) for the oxidative insertion of [Pd] complexes into the C–X bond of CH_3X with X = H, CH_3 and Cl. Values in parenthesis include water solvent effects as obtained by the COSMO method.[a]

[Pd]	CH_3X	$\Delta H^{\neq}$		$\Delta S^{\neq}$		$-T\Delta S^{\neq}$		$\Delta G^{\neq}$	
Pd	CH_4	0.0	(–3.9)	–17.4	(–19.0)	5.2	(5.7)	5.2	(1.8)
Pd[P2P]	CH_4	16.2	(12.3)	–27.7	(–28.7)	8.3	(8.5)	24.5	(20.9)
Pd[P3P]	CH_4	19.8	(15.7)	–29.2	(–35.0)	8.7	(10.4)	28.5	(26.1)
Pd[P4P]	CH_4	22.2	(21.5)	–30.9	(–25.5)	9.2	(7.6)	31.4	(29.0)
Pd[P5P]	CH_4	25.4	(24.9)	–29.1	(–31.9)	8.7	(9.5)	34.1	(34.4)
Pd[P6P]	CH_4	28.0	(28.4)	–28.0	(–34.8)	8.4	(10.4)	36.4	(38.8)
$Pd(PH_3)_2$	CH_4	28.9	(27.2)	–25.8	(–41.0)	7.7	(12.2)	36.6	(39.4)
Pd	C_2H_6	14.8	(12.5)	–22.9	(–23.0)	6.8	(6.9)	21.6	(19.4)
Pd[P2P]	C_2H_6	36.2	(34.8)	–32.2	(–31.4)	9.6	(9.4)	45.8	(44.1)
Pd[P3P]	C_2H_6	40.8	(39.6)	–31.9	(–30.9)	9.5	(9.2)	50.3	(48.8)
Pd[P4P]	C_2H_6	43.0	(44.5)	–34.6	(–28.2)	10.3	(8.4)	53.3	(52.9)
Pd[P5P]	C_2H_6	45.8	(47.8)	–33.1	(–31.8)	9.9	(9.5)	55.7	(57.2)
Pd[P6P]	C_2H_6	47.6	(50.0)	–31.4	(–38.2)	9.4	(11.4)	56.9	(61.3)
$Pd(PH_3)_2$	C_2H_6	48.1	(50.0)	–28.8	(–34.4)	8.6	(10.3)	56.6	(60.3)
Pd	CH_3Cl	–2.3	(–4.5)	–20.5	(–21.5)	6.1	(6.4)	3.8	(1.9)
Pd[P2P]	CH_3Cl	13.5	(11.1)	–29.8	(–30.0)	8.9	(8.9)	22.4	(20.1)
Pd[P3P]	CH_3Cl	17.6	(15.0)	–31.1	(–29.0)	9.3	(8.6)	26.9	(23.6)
Pd[P4P]	CH_3Cl	19.7	(19.3)	–33.0	(–31.8)	9.8	(9.5)	29.5	(28.8)
Pd[P5P]	CH_3Cl	22.8	(22.4)	–30.4	(–35.3)	9.0	(10.5)	31.9	(33.0)
Pd[P6P]	CH_3Cl	23.5	(24.0)	–29.7	(–28.5)	8.8	(8.5)	32.4	(32.5)
$Pd(PH_3)_2$	CH_3Cl	25.3	(25.8)	–27.2	(–27.8)	8.1	(8.3)	33.4	(34.1)

In kcal mol^{-1} (for $\otimes S^{\neq}$ in cal mol^{-1} K^{-1}); computed at ZORA-BLYP/TZ2P.

Table S3. Cartesian coordinates (in Å) of stationary points in oxidative insertion (OxIn) reactions of [Pd] complexes into the C–X bond of CH_3X with X = H, CH_3 and Cl.[a] Each entry contains the ADF total energy in kcal mol^{-1}.

Substrate: CH_4			-534.79
C	0.000000	0.000000	0.000000
H	0.631964	0.631964	-0.631964
H	-0.631964	0.631964	0.631964
H	0.631964	-0.631964	0.631964
H	-0.631964	-0.631964	-0.631964
Substrate: C_2H_6			-895.92
C	0.000000	0.000000	-0.770216
C	0.000000	0.000000	0.770216
H	0.885535	-0.511264	1.168886
H	0.000000	1.022527	1.168886
H	-0.885535	-0.511264	1.168886
H	-0.885535	0.511264	-1.168886
H	0.885535	0.511264	-1.168886
H	0.000000	-1.022527	-1.168886
Substrate: CH_3Cl			-491.27
C	0.000000	0.000000	0.000000
Cl	0.000000	1.825482	0.000000
H	1.037497	-0.336024	0.000000
H	-0.518749	-0.336024	0.898498
H	-0.518748	-0.336024	-0.898499
Catalyst: $Pd(PH_3)_2$			-754.32
Pd	0.000000	0.000000	0.000000
P	0.000000	0.000000	-2.286816
P	0.000000	0.000000	2.286816
H	0.609528	-1.055733	3.025917
H	0.609528	1.055733	3.025917
H	-1.219055	0.000000	3.025917
H	-1.219055	0.000000	-3.025917
H	0.609528	-1.055733	-3.025917
H	0.609528	1.055733	-3.025917
Catalyst: Pd[P2P]			-1297.80
Pd	0.000000	0.000000	0.000005
C	-0.708303	0.315633	-3.077827
C	0.708303	-0.315633	-3.077827
P	-1.712083	-0.063777	-1.499400
P	1.712083	0.063777	-1.499400
H	0.632219	-1.410505	-3.118912
H	1.266401	0.008827	-3.964374
H	-1.266401	-0.008827	-3.964374
H	-0.632219	1.410505	-3.118912
H	2.851753	-0.748208	-1.820542
H	2.334696	1.285990	-1.914336
H	-2.334696	-1.285990	-1.914336
H	-2.851753	0.748208	-1.820542
Catalyst: Pd[P3P]			-1664.06
Pd	0.009907	-0.013160	0.000000
P	1.229704	0.036740	1.905132
P	1.229704	0.036740	-1.905132
C	3.444257	0.312615	0.000000
C	2.996709	-0.358935	1.330691
C	2.996709	-0.358935	-1.330691
H	1.245857	-0.755187	-3.104114
H	3.047899	-1.452089	-1.232938
H	4.543666	0.308080	0.000000
H	3.047899	-1.452089	1.232938
H	1.245857	-0.755187	3.104114
H	1.491525	1.266655	-2.591503
H	3.688973	-0.073795	-2.132346
H	3.151424	1.372919	0.000000
H	3.688973	-0.073795	2.132346
H	1.491525	1.266655	2.591503
Catalyst: Pd[P4P]			-2027.29
Pd	0.002859	-0.495750	-0.074638
P	-2.235176	-0.306048	0.317155
P	1.209081	-0.249214	-1.996308
H	1.697470	1.047775	-2.346003
H	2.386504	-0.921138	-2.464087
H	-3.148651	-1.122790	1.062014
H	-2.734736	0.922167	0.854238
C	-3.162347	-0.297554	-1.347470
C	-2.255829	0.128089	-2.534169
H	-1.630078	0.972556	-2.214103
H	-2.891655	0.509867	-3.345559
H	-3.550350	-1.311678	-1.507720
H	-4.026888	0.369479	-1.253312
C	0.076908	-0.600918	-3.497139
H	0.550763	-1.409306	-4.066528
H	0.064018	0.284996	-4.143618
C	-1.356999	-1.019082	-3.086140
H	-1.852693	-1.473293	-3.956707
H	-1.271754	-1.810099	-2.328829
Catalyst: Pd[P5P]			-2391.93
Pd	-0.004306	-0.209971	-0.063659
P	-2.268268	0.091021	0.147329
P	1.791917	-0.204234	-1.489817
H	2.546489	1.001305	-1.636491
H	2.944097	-1.054515	-1.453408
H	-2.757034	1.386820	0.502621
H	-3.169915	-0.610271	1.011653
C	-3.222332	-0.140944	-1.478645
C	-2.449880	0.398781	-2.712384
H	-3.406451	-1.218261	-1.586216
H	-4.197611	0.349061	-1.377628
H	-3.158578	0.521683	-3.543547
H	-2.074041	1.405922	-2.482761
C	1.319904	-0.471989	-3.310079
C	-1.267602	-0.514241	-3.141424
H	1.242368	-1.557131	-3.460217
H	2.145654	-0.113449	-3.935428
H	-1.618426	-1.252137	-3.877842
H	-0.951504	-1.083033	-2.254707
C	-0.015013	0.221165	-3.694319
H	-0.068635	0.295971	-4.789636
H	0.001449	1.254621	-3.320130
Catalyst: Pd[P6P]			-2754.68
Pd	-0.015100	0.017641	-0.010470
P	0.014767	-0.042464	2.283236
P	0.877773	-0.010644	-2.129131
C	2.714148	-0.476364	-2.202086
C	3.547518	0.194653	-1.078224
C	3.318296	-0.435470	0.319603
C	3.516913	0.539755	1.502881
C	2.927180	0.042336	2.856103
H	-0.974642	0.572656	3.114832
H	-0.099757	-1.327236	2.900508
H	0.924495	1.184213	-2.912995
H	0.408651	-0.835297	-3.199383
H	2.765918	-1.569895	-2.115012
H	3.098191	-0.206847	-3.192756
H	4.611676	0.139993	-1.349279
H	3.298878	1.265628	-1.043377
H	2.913893	-1.057438	2.875906
H	3.602973	0.345743	3.667903
H	3.973784	-1.311414	0.443708
H	2.281778	-0.805665	0.358828
H	4.589685	0.744697	1.631586
H	3.051066	1.503408	1.249130
C	1.525522	0.592814	3.240765
H	1.515589	1.684976	3.121723
H	1.333269	0.383056	4.300526
Catalyst: Pd[P2P]^{Me}			-2769.12
Pd	0.086582	0.030356	-1.516126
P	-1.332662	1.047394	-2.992969
P	1.331136	-1.208281	-2.981381
C	0.659915	-0.386238	-4.566209
C	-0.845654	-0.007831	-4.505160
H	1.267375	0.519253	-4.707598
H	0.851640	-1.039965	-5.431063
H	-1.143832	0.510993	-5.429281
H	-1.457425	-0.918904	-4.437122
C	-3.200708	1.035158	-3.209595
H	-3.499265	1.309627	-4.231356
H	-3.589021	0.036988	-2.975892
H	-3.645285	1.747681	-2.504337
C	-0.969798	2.780425	-3.616251
H	-1.437408	2.968436	-4.593043
H	-1.353092	3.506569	-2.888926
H	0.113636	2.924746	-3.697907
C	0.912918	-3.011548	-3.292360
H	1.384734	-3.624541	-2.514668
H	-0.171380	-3.156581	-3.224408
H	1.264687	-3.347359	-4.278056
C	3.160462	-1.244645	-3.415980
H	3.564775	-0.226319	-3.380263
H	3.691349	-1.848623	-2.670253
H	3.338969	-1.670204	-4.413728
Catalyst: Pd[P3P]^{Me}			-3136.22
Pd	0.054750	0.006927	0.007749
P	1.247629	0.057302	1.943479
P	1.216932	0.038209	-1.947049
C	3.439872	0.309413	-0.020681
C	2.992204	-0.350842	1.317487
C	2.970799	-0.364904	-1.344388
H	3.011580	-1.458451	-1.233850
H	4.539809	0.294052	-0.029356
H	3.032761	-1.445496	1.218450
H	3.670494	-0.100265	-2.153045
H	3.159564	1.373144	-0.023947
H	3.704087	-0.076432	2.112165
C	1.553525	1.683162	2.828237
C	1.510119	1.655545	-2.851472
C	1.188362	-1.086617	3.432660
C	1.133842	-1.119758	-3.424211
H	2.388138	1.606247	3.539486
H	0.644515	1.970376	3.370531
H	1.772046	2.468766	2.095981
H	1.740679	2.447378	-2.129611
H	0.593163	1.939080	-3.382167
H	2.333671	1.571049	-3.574604
H	2.083040	-0.985899	4.063610
H	1.101325	-2.125157	3.092760
H	0.300812	-0.848017	4.031340
H	2.017915	-1.024194	-4.070721
H	0.236284	-0.887354	-4.010235
H	1.053358	-2.155138	-3.073261
Catalyst: Pd[P4P]^{Me}			-3499.70
Pd	-0.024149	-0.290316	-0.106664
P	-2.268082	-0.411360	0.353521
P	1.269343	-0.222548	-1.999930
C	-3.138916	-0.610307	-1.321565
C	-2.383559	0.060000	-2.504530
H	-1.911752	0.984298	-2.145253
H	-3.118823	0.365480	-3.262757
H	-3.250441	-1.688195	-1.504676
H	-4.154008	-0.197994	-1.222635
C	0.059971	-0.134442	-3.460447
H	0.559586	-0.574040	-4.336434
H	-0.100419	0.928973	-3.686788
C	-1.301124	-0.837236	-3.190500
H	-1.702702	-1.203960	-4.146044
H	-1.123848	-1.726579	-2.571100
C	-3.133451	1.114596	1.018153
H	-4.226183	0.998805	1.003854
H	-2.803326	1.294004	2.048546
H	-2.853435	1.986911	0.416284
C	-3.159390	-1.726046	1.351210
H	-4.250273	-1.649392	1.242334
H	-2.832804	-2.719404	1.022054
H	-2.897902	-1.613430	2.410423
C	2.264767	-1.743961	-2.461943
H	3.089933	-1.862874	-1.749346
H	1.628077	-2.633682	-2.394069
H	2.673880	-1.666587	-3.478938
C	2.494328	1.106800	-2.500314
H	2.033686	2.093981	-2.377660
H	3.371214	1.054446	-1.843535
H	2.821136	0.987160	-3.542742
Catalyst: $Pd(PMe_3)_2$			-2962.85
Pd	0.000000	0.000000	0.000000
P	0.000000	0.000000	-2.310895
P	0.000000	0.000000	2.310895
C	0.828681	-1.435317	-3.174546
C	-1.657361	0.000000	-3.174546
C	0.828681	1.435317	-3.174546
C	0.828681	-1.435317	3.174546
C	-1.657361	0.000000	3.174546
C	0.828681	1.435317	3.174546
H	1.880921	-1.482827	-2.871085
H	-2.224626	-0.887511	-2.871085
H	0.343706	2.370339	-2.871085
H	1.880921	1.482827	-2.871085
H	0.343706	-2.370339	-2.871085
H	-2.224626	0.887511	-2.871085
H	1.880921	-1.482827	2.871085
H	-2.224626	-0.887511	2.871085
H	0.343706	2.370339	2.871085
H	1.880921	1.482827	2.871085
H	0.343706	-2.370339	2.871085
H	-2.224626	0.887511	2.871085
H	0.769911	-1.333525	-4.267151
H	-1.539821	0.000000	-4.267151
H	0.769911	1.333525	-4.267151
H	0.769911	-1.333525	4.267151
H	-1.539821	0.000000	4.267151
H	0.769911	1.333525	4.267151

Catalyst: Pd[P2P^{Ph}] -7295.80

Pd	0.110428	0.021594	-1.869224
P	-1.388359	0.943329	-3.342977
P	1.305406	-1.250024	-3.351168
C	0.480510	-0.574784	-4.936141
C	-1.031030	-0.267392	-4.768010
H	1.016569	0.344057	-5.199453
H	0.629335	-1.284438	-5.759922
H	-1.434979	0.127406	-5.710145
H	-1.573278	-1.191551	-4.530846
C	3.111746	-1.118304	-3.785915
C	3.632975	0.090155	-4.294439
C	5.008079	0.256559	-4.486557
C	5.897602	-0.775083	-4.162201
C	5.395531	-1.973772	-3.641357
C	4.020098	-2.143199	-3.452551
H	2.968233	0.916919	-4.533295
H	5.383667	1.196114	-4.886794
H	6.967580	-0.644498	-4.308979
H	6.075133	-2.782297	-3.379708
H	3.653031	-3.080694	-3.042630
C	0.967624	-3.081213	-3.488691
C	1.310534	-3.843978	-4.621416
C	1.017236	-5.210165	-4.676682
C	0.375131	-5.836677	-3.599952
C	0.028843	-5.090250	-2.468927
C	0.324554	-3.721844	-2.415161
H	1.822281	-3.375147	-5.459215
H	1.292057	-5.787129	-5.557293
H	0.148895	-6.900097	-3.644756
H	-0.469547	-5.569291	-1.628926
H	0.054496	-3.137855	-1.536421
C	-0.900704	2.579737	-4.103652
C	-1.621075	3.179385	-5.153645
C	-1.206449	4.400833	-5.695160
C	-0.063853	5.041264	-5.197972
C	0.661066	4.454975	-4.154377
C	0.242141	3.234905	-3.609265
H	-2.517478	2.700053	-5.541774
H	-1.778334	4.854772	-6.501879
H	0.254197	5.993566	-5.617485
H	1.545636	4.949208	-3.757959
H	0.796796	2.781128	-2.788352
C	-3.249710	1.052449	-3.363298
C	-3.847393	1.985839	-2.490290
C	-5.235436	2.081768	-2.379535
C	-6.062965	1.228873	-3.124686
C	-5.485356	0.290481	-3.984530
C	-4.091212	0.204994	-4.107328
H	-3.215518	2.638431	-1.889642
H	-5.673191	2.814600	-1.704847
H	-7.144812	1.294399	-3.030303
H	-6.116742	-0.377946	-4.566438
H	-3.672207	-0.529180	-4.789128

Catalyst: Pd[P3P^{Ph}] -7662.20

Pd	-0.177917	-0.397209	-1.941378
P	-2.333324	-0.975030	-2.403446
P	1.153458	0.174160	-3.689541
C	-2.238253	-1.279188	-4.274811
C	-1.430569	-0.219826	-5.085611
H	-1.673679	0.788311	-4.725188
H	-1.804459	-0.265407	-6.118913
H	-1.783437	-2.269676	-4.409621
H	-3.261614	-1.328473	-4.671042
C	0.114674	-0.412233	-5.166967
H	0.350481	-1.480925	-5.259109
H	0.500193	0.065950	-6.078056
H	2.132465	5.816677	-4.438698
H	3.252841	4.534345	-2.613405
H	2.810985	2.117961	-2.339260
C	-3.648030	0.350287	-2.305662
C	-5.006070	0.095606	-2.572884
C	-5.952595	1.122249	-2.491514
C	-5.555804	2.420408	-2.145024
C	-4.208112	2.685896	-1.877991
C	-3.261558	1.656347	-1.952993
H	-5.331746	-0.910422	-2.829502
H	-7.000197	0.907227	-2.692367
H	-6.294594	3.216608	-2.077720
H	-3.892424	3.690275	-1.603832
H	-2.214038	1.857561	-1.732562
C	-3.259871	-2.475174	-1.790443
C	-3.458117	-2.571648	-0.397367
C	-4.091793	-3.681443	0.164883
C	-4.524163	-4.734704	-0.653691
C	-4.324765	-4.658750	-2.035049
C	-3.702400	-3.536276	-2.600277
H	-3.103018	-1.770357	0.249377
H	-4.238506	-3.731289	1.241865
H	-5.005733	-5.606633	-0.215997
H	-4.653569	-5.471923	-2.679006
H	-3.567105	-3.501703	-3.677527
C	2.796150	-0.606024	-4.121861
C	3.196670	-1.741510	-3.393619
C	4.407154	-2.384236	-3.678933
C	5.240259	-1.892030	-4.690478
C	4.853970	-0.759398	-5.418201
C	3.639813	-0.122327	-5.138112
H	2.556651	-2.112265	-2.593734
H	4.703355	-3.259516	-3.104543
H	6.187400	-2.382531	-4.905789
H	5.499924	-0.368066	-6.201512
H	3.357700	0.762600	-5.704408
C	1.473820	1.977443	-4.036700
C	0.852262	2.711803	-5.061978
C	1.086219	4.087187	-5.203669
C	1.951550	4.749502	-4.328615
C	2.579464	4.028701	-3.302410
C	2.334139	2.662528	-3.152824
H	0.175941	2.223831	-5.758368
H	0.589156	4.636889	-6.000284

Catalyst: Pd[P4P^{Ph}] -8025.39

Pd	-0.302251	-0.043717	-1.952194
P	-2.336134	-0.962970	-2.486468
P	1.509437	0.724572	-3.132909
C	-2.284429	-1.282027	-4.355436
C	-1.491632	-0.185875	-5.127630
H	-1.633266	0.779788	-4.626183
H	-1.942838	-0.076726	-6.123523
H	-1.816799	-2.263057	-4.507387
H	-3.314685	-1.345637	-4.727723
C	0.977683	0.724652	-4.953498
H	1.877927	0.701824	-5.580497
H	0.465373	1.675986	-5.145062
C	0.038879	-0.468324	-5.302508
H	0.224375	-0.753650	-6.347250
H	0.324522	-1.338543	-4.698249
C	-3.831946	0.152934	-2.343308
C	-5.141148	-0.286826	-2.612904
C	-6.225428	0.588751	-2.495865
C	-6.017762	1.919041	-2.108113
C	-4.720829	2.367869	-1.836863
C	-3.635704	1.489243	-1.949984
H	-5.321958	-1.321004	-2.899120
H	-7.232555	0.230801	-2.699787
H	-6.863116	2.597566	-2.012284
H	-4.551888	3.398014	-1.530377
H	-2.625449	1.832149	-1.729048
C	-2.989389	-2.571214	-1.801814
C	-2.934305	-2.740446	-0.403754
C	-3.383287	-3.919677	0.196582
C	-3.881174	-4.965002	-0.592808
C	-3.932848	-4.815536	-1.982222
C	-3.495132	-3.626705	-2.581871
H	-2.526123	-1.941888	0.214283
H	-3.334495	-4.027864	1.278095
H	-4.219705	-5.888835	-0.128335
H	-4.314420	-5.622963	-2.603860
H	-3.551199	-3.534596	-3.663016
C	3.014511	-0.386705	-3.187401
C	2.951127	-1.633223	-2.538484
C	4.046929	-2.505640	-2.557545
C	5.223766	-2.138984	-3.219127
C	5.299748	-0.897716	-3.864605
C	4.203674	-0.029147	-3.849321
H	2.036789	-1.910529	-2.014940
H	3.981694	-3.465710	-2.049912
H	6.079339	-2.811393	-3.227415
H	6.215065	-0.602571	-4.373639
H	4.285269	0.937875	-4.341605
C	2.283998	2.408744	-2.919512
C	2.548074	3.307266	-3.968887
C	3.101452	4.568823	-3.710411
C	3.408792	4.948917	-2.400252
C	3.154439	4.061764	-1.345709
C	2.589742	2.809902	-1.603506
H	2.323947	3.034915	-4.996542
H	3.291915	5.252094	-4.535554
H	3.837042	5.928930	-2.200355
H	3.385638	4.349743	-0.322298
H	2.372620	2.135336	-0.776402

Catalyst: Pd[PPh_3)$_2$] -9750.57

Pd	-0.013990	-0.018278	0.000820
P	-0.001877	-0.005386	2.319868
P	0.011629	-0.018940	-2.318118
C	-2.623599	-0.992549	2.518941
C	-1.179006	-1.733418	4.315880
C	-1.357750	-0.989729	3.136556
C	-3.688128	-1.706271	3.077996
C	-3.499928	-2.442892	4.254676
C	-2.243160	-2.457033	4.868895
C	2.109954	-0.164767	4.285958
C	2.178489	-1.770120	2.474066
C	1.544327	-0.684475	3.108744
C	3.278135	-0.722604	4.820504
C	3.893106	-1.809230	4.189661
C	3.338816	-2.333136	3.014538
C	-0.333704	4.275207	4.186952
C	0.453227	2.761875	2.462375
C	0.378897	4.049561	3.002159
C	-0.967422	3.205516	4.828125
C	-0.884138	1.913097	4.294384
C	-0.169042	1.675589	3.107710
H	1.646440	0.681886	4.785817
H	0.983592	2.592582	1.526561
H	-1.530593	3.373624	5.743769
C	-1.150570	-2.570099	-2.504664
C	-1.749291	-1.103380	-4.336404
C	-1.046583	-1.316223	-3.137650
C	-1.922873	-3.591013	-3.067588
C	-2.617137	-3.369346	-4.264013
C	-2.531029	-2.123112	-4.893672
C	0.003779	2.092574	-4.291774
C	-1.629208	2.252327	-2.510549
C	-0.566951	1.559442	-3.123117
C	-0.481814	3.286580	-4.839876
C	-1.546023	3.960232	-4.231110
C	-2.120280	3.438460	-3.064667
C	4.285334	-0.630704	-4.129389
C	2.801695	0.270864	-2.435500
C	4.088984	0.110842	-2.957180
C	3.186878	-1.206543	-4.776437
C	1.895369	-1.037124	-4.261093
C	1.687449	-0.293201	-3.086706
H	-2.764087	-0.443578	1.589082
H	-0.207528	-1.758138	4.802833
H	-4.659508	-1.698088	2.588341
H	-4.324434	-3.008695	4.683773
H	-2.085443	-3.033298	5.778167
H	1.764555	-2.159936	1.545397
H	3.706605	-0.303640	5.728571
H	4.802410	-2.238930	4.605208
H	3.816604	-3.171063	2.511538
H	-0.401840	5.278911	4.601672
H	0.865628	4.877601	2.491481
H	-1.384669	1.092844	4.802645
H	-0.634139	-2.734424	-1.560169
H	-1.696232	-0.139232	-4.835578
H	-1.992962	-4.553667	-2.565807
H	-3.227893	-4.159020	-4.697089
H	-3.073976	-1.939219	-5.818413
H	0.833502	1.582787	-4.774729
H	-2.058217	1.862812	-1.588632
H	-0.024269	3.688689	-5.741361
H	-1.919720	4.889423	-4.656558
H	-2.941509	3.961269	-2.579232
H	5.288097	-0.766090	-4.529633
H	2.653592	0.822849	-1.508652
H	4.938804	0.553089	-2.441838
H	3.331603	-1.791718	-5.682216
H	1.052554	-1.494067	-4.773418

Catalyst: Pd[P2P]^{tBu} -7082.52

Pd	0.107258	0.004660	-1.705434
P	-1.282244	1.134198	-3.150093
P	1.302649	-1.336785	-3.142499
C	0.620004	-0.529942	-4.753033
C	-0.813305	0.093995	-4.702149
H	1.342573	0.258014	-4.989837
H	0.661387	-1.246639	-5.586713
H	-0.972959	0.681604	-5.618453
H	-1.553261	-0.712927	-4.722451
C	-3.241554	0.904677	-3.157960
C	-0.842988	2.981693	-3.667613
C	0.817217	-3.235766	-3.321702
C	3.240934	-1.129328	-3.445263
C	3.741334	-1.404767	-4.886114
H	4.821555	-1.194959	-4.940358
H	3.595686	-2.444562	-5.192539
H	3.251101	-0.760223	-5.625048
C	4.011701	-2.030109	-2.448377
H	3.649675	-1.894615	-1.420930
H	3.936307	-3.092875	-2.703105
H	5.079688	-1.764668	-2.465395
C	3.556533	0.348902	-3.091507
H	3.086331	1.050860	-3.789517
H	3.215263	0.600689	-2.080002
H	4.643985	0.511711	-3.142839
C	1.515664	-4.014769	-4.460346
H	2.590260	-4.133980	-4.285074
H	1.084669	-5.026448	-4.528527
H	1.376605	-3.536062	-5.437994
C	-0.714127	-3.278979	-3.560181
H	-0.988636	-2.898349	-4.551188
H	-1.062007	-4.321479	-3.500060
H	-1.251549	-2.698117	-2.801707
C	1.099725	-3.929900	-1.962513
H	0.604551	-3.399818	-1.139288
H	0.711317	-4.959742	-1.989624
H	2.168699	-3.985350	-1.732841
C	0.642434	2.974155	-4.111646
H	0.985240	4.010712	-4.251231
H	1.281632	2.504804	-3.354924
H	0.786049	2.450242	-5.064119
C	-0.948425	3.869690	-2.399002
H	-0.576924	4.880547	-2.627769
H	-1.977731	3.968926	-2.039556
H	-0.342928	3.460524	-1.580565
C	-1.694299	3.593156	-4.804476
H	-1.682331	2.975467	-5.711450
H	-2.736945	3.747533	-4.506753
H	-1.285895	4.579628	-5.076481
C	-3.880958	1.949273	-2.209672
H	-3.850129	2.962627	-2.624642
H	-4.939152	1.695209	-2.045318
H	-3.383973	1.961518	-1.230950
C	-3.493094	-0.502728	-2.553137
H	-3.017657	-0.607488	-1.570300
H	-4.576088	-0.660214	-2.434745
H	-3.113488	-1.303877	-3.197437
C	-3.932277	0.971772	-4.543858
H	-5.008140	0.767883	-4.422260
H	-3.838172	1.953935	-5.015833
H	-3.539296	0.220883	-5.239205

Catalyst: Pd[P3P]^{tBu} -7448.22

Pd	1.057719	0.160880	-4.739658
P	2.604241	-1.321267	-5.558877
P	-0.247785	1.385462	-6.170369
C	1.896823	0.300561	-7.962225
C	2.262144	-1.124494	-7.436183
C	0.406941	0.757904	-7.860980
H	-0.234431	-0.090152	-8.134614
H	2.142546	0.304374	-9.036403
H	1.431867	-1.802625	-7.664716
H	0.227192	1.533737	-8.619646
H	2.549434	1.049698	-7.504689
H	3.126187	-1.496292	-8.002717
H	5.394438	-2.611575	-6.613326
H	2.169408	2.993468	-5.903636
H	3.207904	-3.994074	-7.150183
H	-2.506573	1.552302	-4.260055
C	-2.163069	0.969864	-6.356328
C	-2.796353	1.275605	-7.737445
H	-3.845299	0.939238	-7.735893
H	-2.797019	2.343423	-7.974759
H	-2.289909	0.745985	-8.552937
C	-2.276613	-0.556531	-6.091706
H	-1.746262	-1.149947	-6.846427
H	-3.336284	-0.853391	-6.121984
H	-1.867934	-0.822437	-5.109773
C	-2.958561	1.705216	-5.248734
H	-3.028163	2.783136	-5.433206
H	-3.986286	1.312465	-5.212693
C	2.269775	-3.245870	-5.296183
C	2.350402	-3.549586	-3.775625
H	2.017667	-4.582978	-3.593001
H	3.365077	-3.455364	-3.377917
H	1.698099	-2.876662	-3.204638
C	0.800775	-3.504987	-5.731364
H	0.118378	-2.766222	-5.293141
H	0.494550	-4.503043	-5.384165
H	0.674731	-3.488064	-6.819866
C	3.200365	-4.205785	-6.073392
H	4.232654	-4.166924	-5.708089
H	2.850865	-5.242781	-5.945608
C	0.023486	3.331546	-6.272417
C	-0.823193	4.085794	-7.323578
H	-0.501749	5.138686	-7.365266
H	-0.703630	3.670422	-8.332469
H	-1.890096	4.084327	-7.074998
C	-0.247381	3.922928	-4.863182
H	-1.300198	3.848136	-4.571620
H	0.025162	4.989680	-4.854980
H	0.351661	3.411144	-4.099563
C	1.525702	3.552514	-6.593676
H	1.777832	3.258806	-7.619408
H	1.763352	4.622114	-6.489611
C	4.540906	-0.946919	-5.424428
C	4.669520	0.601433	-5.438804
H	5.719453	0.880027	-5.258396
H	4.376312	1.030429	-6.403737
H	4.048858	1.062913	-4.661451
C	5.067475	-1.450110	-4.056685
H	4.419298	-1.130311	-3.230550
H	6.069911	-1.032483	-3.876888
H	5.159189	-2.541334	-4.022832
C	5.430025	-1.519129	-6.555657
H	5.160341	-1.115586	-7.539101
H	6.477708	-1.234024	-6.369726

Catalyst: Pd[P4P]^{tBu} -7814.61

Pd	0.190893	0.344105	-2.337963
P	-1.852174	1.148744	-3.076652
P	1.982336	-0.856650	-3.184218
C	-1.933650	0.640475	-4.924295
C	-0.549948	0.300872	-5.552986
H	0.192199	1.018312	-5.186869
H	-0.615457	0.447276	-6.642527
H	-2.591147	-0.234338	-4.998909
H	-2.424103	1.442954	-5.491193
C	1.484068	-1.261033	-4.991671
H	1.844878	-2.267556	-5.241920
H	2.025680	-0.568680	-5.647782
C	-0.043736	-1.148231	-5.271489
H	-0.288434	-1.782896	-6.137602
H	-0.592493	-1.561264	-4.418373
H	0.112284	3.178381	-3.785786
H	-2.899265	0.868297	-0.324122
H	5.008982	-1.613479	-4.154875
H	3.362479	-3.574428	-4.058823
C	2.239184	-2.637434	-2.399370
C	2.416297	-2.467173	-0.866537
H	2.418378	-3.457891	-0.386029
H	3.357374	-1.971446	-0.605548
H	1.593836	-1.880180	-0.438369
C	0.912171	-3.409256	-2.635825
H	0.049173	-2.836234	-2.274998
H	0.946236	-4.360609	-2.083747
H	0.750430	-3.648580	-3.693561
C	3.410151	-3.473096	-2.966912
H	4.385636	-3.049545	-2.703184
H	3.373097	-4.489273	-2.543417
C	3.711248	0.033697	-3.442901
C	3.358555	1.462276	-3.942302
H	4.284169	2.047643	-4.052920
H	2.858863	1.448825	-4.919028
H	2.699878	1.980090	-3.235077
C	4.431614	0.168149	-2.077535
H	3.764064	0.579127	-1.309025
H	5.288243	0.851785	-2.180054
H	4.821552	-0.791318	-1.718989
C	4.668378	-0.622832	-4.469876
H	4.211236	-0.719851	-5.461789
H	5.562332	0.010069	-4.586107
C	-3.511317	0.366970	-2.380278
C	-4.771825	0.545669	-3.264021
H	-5.611863	-0.003272	-2.809903
H	-5.077458	1.592026	-3.355304
H	-4.632284	0.142735	-4.274199
C	-3.215939	-1.152698	-2.246083
H	-3.025350	-1.625749	-3.217558
H	-4.088043	-1.654610	-1.799793
H	-2.343482	-1.333945	-1.607233
C	-3.790206	0.927423	-0.962762
H	-4.127830	1.969784	-0.988816
H	-4.586964	0.337220	-0.484727
C	-1.998408	3.104427	-3.160795
C	-3.341534	3.668782	-3.679583
H	-3.256794	4.760226	-3.801674
H	-3.621631	3.253567	-4.656285
H	-4.164294	3.485867	-2.979487
C	-1.708437	3.670393	-1.744629
H	-2.494009	3.419739	-1.023838
H	-1.642529	4.768328	-1.795657
H	-0.756494	3.287507	-1.355359
C	-0.857697	3.582843	-4.100218
H	-1.028989	3.297420	-5.144940
H	-0.798553	4.681103	-4.063667

Catalyst: Pd(P(*t*-Bu)$_3$)$_2$ -9416.63

Pd	-0.171228	-0.253685	-0.020007
P	-0.221439	-0.040948	-2.364309
P	-0.077670	-0.454706	2.324372
H	2.702882	-0.493419	-3.604996
H	-2.807889	0.473838	-1.052737
H	1.652081	1.779731	-1.005039
H	2.267493	-1.532763	0.905331
H	-1.193974	-2.501886	4.637370
H	2.547230	0.984773	3.478590
C	0.369804	1.290557	3.172734
C	-0.445858	2.389682	2.431217
H	-0.088180	3.377592	2.760919
H	-0.307428	2.311788	1.345674
H	-1.517381	2.342009	2.638414
C	0.113317	1.410828	4.696204
H	-0.947428	1.316697	4.950478
H	0.437482	2.407794	5.034998
H	0.671613	0.670893	5.278968
C	1.864016	1.609635	2.896122
H	2.108198	1.502882	1.832644
H	2.056576	2.655077	3.180831
C	-1.818131	-1.065137	3.074435
C	-2.836287	0.103992	2.987662
H	-3.840163	-0.290225	3.206582
H	-2.635421	0.897654	3.713099
H	-2.861661	0.542276	1.982981
C	-2.364303	-2.177375	2.132192
H	-2.364968	-1.838559	1.088701
H	-3.399416	-2.411848	2.425813
H	-1.789532	-3.104870	2.184754
C	-1.800835	-1.597013	4.529841
H	-1.437052	-0.854211	5.247316
H	-2.828481	-1.862614	4.825112
C	1.313384	-1.770129	2.873022
C	1.758793	-1.734801	4.356833
H	2.497841	-2.534039	4.526617
H	2.242890	-0.790270	4.625596
H	0.929836	-1.904077	5.051796
C	0.804872	-3.199698	2.543065
H	0.012219	-3.535658	3.217831
H	1.644404	-3.902848	2.651912
H	0.442597	-3.269814	1.510631
C	2.555576	-1.538852	1.963858
H	3.074869	-0.601633	2.176757
H	3.271289	-2.359361	2.128599
C	0.615923	1.671384	-2.942365
C	1.001935	1.787800	-4.438581
H	1.416426	2.791795	-4.623004
H	1.772532	1.066247	-4.728845
H	0.144906	1.660735	-5.108023
C	-0.342952	2.839680	-2.586426
H	-1.222659	2.880849	-3.235188
H	0.199953	3.788401	-2.713977
H	-0.676112	2.783480	-1.543391
C	1.888454	1.883515	-2.071281
H	2.692225	1.182493	-2.307723
H	2.272344	2.900247	-2.248813
C	-2.087061	-0.068130	-3.059395
C	-2.296833	0.433953	-4.510370
H	-3.361333	0.328804	-4.774153
H	-2.042022	1.492223	-4.627795
H	-1.720876	-0.139742	-5.243861
C	-2.638181	-1.515875	-2.952921
H	-2.198300	-2.193767	-3.690127
H	-3.722403	-1.491354	-3.139905
H	-2.481648	-1.933851	-1.951458
C	-2.954158	0.790491	-2.092931
H	-2.734610	1.858887	-2.153699
H	-4.014962	0.654633	-2.355422
C	0.773197	-1.527995	-3.238783
C	0.407313	-2.838688	-2.482826
H	1.072239	-3.644428	-2.831043
H	0.543479	-2.715539	-1.401195
H	-0.621204	-3.162380	-2.658126
C	0.528719	-1.732919	-4.755211
H	-0.506705	-2.010134	-4.978260
H	1.165877	-2.558282	-5.111036
H	0.780870	-0.847480	-5.347855
C	2.293575	-1.313306	-3.007706
H	2.517574	-1.125989	-1.950947
H	2.825115	-2.229718	-3.305589

Catalyst: Pd[P2P]^{Cl} -1224.09

C	-0.690255	0.350890	-3.037085
C	0.690255	-0.350890	-3.037085
P	-1.676383	-0.022176	-1.468638
P	1.676383	0.022176	-1.468638
H	0.574050	-1.442454	-3.047944
H	1.275798	-0.062114	-3.917043
H	-1.275798	0.062114	-3.917043
H	-0.574050	1.442454	-3.047944
Cl	3.321427	-1.300966	-1.834173
Cl	2.495418	1.916386	-2.010936
Cl	-2.495418	-1.916386	-2.010936
Cl	-3.321427	1.300966	-1.834173
Pd	0.000000	0.000000	0.043644

Catalyst: Pd[P3P]^{Cl} -1590.99

Pd	-0.021428	-0.080481	0.000000
P	1.249162	-0.002354	1.846446
P	1.249162	-0.002354	-1.846446
C	3.484809	0.224748	0.000000
C	3.002996	-0.427994	1.324872
C	3.002996	-0.427994	-1.324872
Cl	1.166546	-1.231621	-3.606151
H	3.018540	-1.524145	-1.248877
H	4.581059	0.148715	0.000000
H	3.018540	-1.524145	1.248877
Cl	1.166546	-1.231621	3.606151
Cl	1.591363	1.925850	-2.683426
H	3.662827	-0.143406	-2.151975
H	3.264739	1.300830	0.000000
H	3.662827	-0.143406	2.151975
Cl	1.591363	1.925850	2.683426

Catalyst: Pd[P4P]^{Cl} -1952.24

Pd	0.039552	-0.222430	0.003110
P	-2.181179	-0.459733	0.228947
P	1.121508	-0.078467	-1.958762
Cl	2.588862	1.401379	-2.439725
Cl	2.059144	-1.856120	-2.669954
Cl	-3.134546	-1.898705	1.491974
Cl	-3.294808	1.302930	0.673630
C	-3.011298	-0.942302	-1.379371
C	-2.566809	-0.122418	-2.624719
H	-2.427334	0.931029	-2.347054
H	-3.423912	-0.128910	-3.309785
H	-2.788553	-2.010022	-1.508854
H	-4.090489	-0.848339	-1.213699
C	-0.042644	0.241279	-3.390973
H	0.544699	0.106141	-4.306246
H	-0.301763	1.306209	-3.318831
C	-1.320629	-0.645754	-3.415091
H	-1.606402	-0.731384	-4.471027
H	-1.070851	-1.667818	-3.099974

Catalyst: Pd(PCl$_3$)$_2$ -622.01

Pd	0.000000	0.000000	-2.573014
P	-1.892174	1.094427	-3.188065
P	1.892174	-1.094427	-3.188065
Cl	2.108924	-3.095941	-2.574373
Cl	-2.214019	1.280896	-5.249135
Cl	2.214019	-1.280896	-5.249135
Cl	3.734885	-0.282720	-2.575000
Cl	-3.734885	0.282720	-2.575000
Cl	-2.108924	3.095941	-2.574373

Catalyst: Pd(PH$_3$)$_2$Cl$^-$ -855.37

Pd	-0.024481	0.014441	0.000000
P	-0.981559	0.009276	2.063940
P	-0.981559	0.009276	-2.063940
H	-0.752429	-1.039936	3.029192
H	-0.752429	-1.039936	-3.029192
H	-2.397382	0.020655	2.358441
H	-2.397382	0.020655	-2.358441
H	-0.732152	1.034310	3.050417
H	-0.732152	1.034310	-3.050417
Cl	2.524842	0.024202	0.000000

Catalyst: Pd(PH$_3$)$_2$Br$^-$ -848.23

Pd	-0.068372	0.011681	0.000000
P	-1.021219	0.012942	2.068515
P	-1.021219	0.012942	-2.068515
H	-0.780537	-1.021312	3.045640
H	-0.780537	-1.021312	-3.045640
H	-2.437910	0.009540	2.355499
H	-2.437910	0.009540	-2.355499
H	-0.786490	1.054503	3.039178
H	-0.786490	1.054503	-3.039178
Br	2.627177	0.011900	0.000000

Catalyst: Pd(PH$_3$)$_2$I$^-$ -840.72

Pd	-0.176411	0.011260	0.000000
P	-1.019810	0.010570	2.123349
P	-1.019810	0.010570	-2.123349
H	-0.693400	-1.034052	3.058786
H	-0.693400	-1.034052	-3.058786
H	-2.404976	0.016106	2.539105
H	-2.404976	0.016106	-2.539105
H	-0.683664	1.046462	3.064972
H	-0.683664	1.046462	-3.064972
I	2.680637	0.009855	0.000000

Catalyst: Pd[P2P]Cl$^-$ -1409.87

Pd	0.000000	0.000000	-2.270370
C	0.302484	0.709777	-5.505365
C	-0.302484	-0.709777	-5.505365
P	-0.041154	1.632694	-3.852577
P	0.041154	-1.632694	-3.852577
H	-1.397847	-0.651049	-5.585697
H	0.063405	-1.295863	-6.358386
H	-0.063405	1.295863	-6.358386
H	1.397847	0.651049	-5.585697
H	-0.731444	-2.804718	-4.239552
H	1.274061	-2.262616	-4.273575
H	-1.274061	2.262616	-4.273575
H	0.731444	2.804718	-4.239552
Cl	0.000000	0.000000	0.236528

Catalyst: Pd[C2C] -2329.29

C	-1.576633	0.382722	1.060549
C	1.576633	-0.382722	1.060549
H	3.379480	0.459618	-1.420588
C	1.307559	0.489956	-1.106424
Pd	0.000000	0.000000	-2.641861
N	0.683638	0.114632	0.103059
C	2.813901	-0.271399	0.509644
H	3.783648	-0.497184	0.928844
N	2.632040	0.241799	-0.777904
C	-1.307559	-0.489956	-1.106424
H	1.259936	-0.751109	2.024005
C	-2.813901	0.271399	0.509644
H	-3.783648	0.497184	0.928844
N	-2.632040	-0.241799	-0.777904
N	-0.683638	-0.114632	0.103059
H	-1.259936	0.751109	2.024005
H	-3.379480	-0.459618	-1.420588

Catalyst: Pd[C3C] -2722.63

C	-0.179397	2.033360	-1.139437
C	-0.180594	-2.040792	-1.133433
H	-1.121976	-3.230538	1.656155
C	0.101657	-1.613988	1.138136
Pd	0.174390	0.002285	2.397356
N	0.441456	-1.238125	-0.170980
C	-0.903116	-2.975996	-0.460585
H	-1.511823	-3.790071	-0.825355
N	-0.711400	-2.704106	0.898529
C	0.104995	1.614780	1.133445
H	-0.047888	-1.896166	-2.195932
C	-0.900635	2.971472	-0.469262
H	-1.509481	3.784353	-0.836408
N	-0.707493	2.704673	0.890673
N	0.443365	1.233956	-0.174705
H	-0.048077	1.884539	-2.201523
H	-1.116960	3.234143	1.646781
C	1.191383	-0.003008	-0.443184
H	2.068364	-0.002683	0.204773
H	1.493012	-0.004907	-1.494189

Catalyst: Pd[C4C] -3093.61

C	0.037649	3.009640	-0.773513
C	-0.037649	-3.009640	-0.773513
H	0.315862	-3.529886	2.337105
C	-0.168332	-1.830983	1.218419
Pd	0.000000	0.000000	2.084553
N	-0.291963	-1.773311	-0.171959
C	0.246536	-3.889313	0.225471
H	0.489183	-4.940599	0.190326
N	0.158482	-3.156762	1.411916
C	0.168332	1.830983	1.218419
H	-0.087690	-3.162202	-1.841590
C	-0.246536	3.889313	0.225471
H	-0.489183	4.940599	0.190326
N	-0.158482	3.156762	1.411916
N	0.291963	1.773311	-0.171959
H	0.087690	3.162202	-1.841590
H	-0.315862	3.529886	2.337105
C	0.578939	0.529749	-0.911929
H	1.475989	0.075804	-0.484565
H	0.795494	0.826998	-1.945151
C	-0.578939	-0.529749	-0.911929
H	-1.475989	-0.075804	-0.484565
H	-0.795494	-0.826998	-1.945151

Catalyst: Pd[C5C] -3462.33

H	5.099242	-0.001692	-1.584010
C	5.242257	1.248161	0.212771
C	5.482850	-0.091041	-0.563380
C	4.511861	2.361746	-0.612122
Pd	2.264353	0.058402	-0.318355
C	4.639929	-3.214851	1.113866
C	3.033077	4.072847	0.554649
H	5.151027	3.248313	-0.695391
H	4.659419	1.035328	1.111688
H	6.556655	-0.302230	-0.625226
H	4.307519	1.999251	-1.623886
H	6.216237	1.640243	0.538767
C	1.735996	4.117555	0.967053
H	1.181893	4.895358	1.470061
N	1.179110	2.892859	0.595967
N	3.227904	2.830256	-0.053336
H	3.815649	4.812955	0.634508
H	0.227339	2.607042	0.775815
C	2.074465	2.053502	-0.031498
C	5.560373	-2.308808	0.682185
H	6.636293	-2.309283	0.776694
N	4.860079	-1.291765	0.028825
H	2.508903	-3.154103	0.891542
H	4.761667	-4.143102	1.651038
N	3.400779	-2.717203	0.708291
C	3.487371	-1.514845	0.039801

Catalyst: PdNHC$_2$ -2570.81

C	-2.553369	-3.416279	0.487052
C	2.553369	3.416279	0.487052
H	0.061533	2.928370	-1.424982
C	1.021929	1.747779	0.003243
Pd	0.000000	0.000000	0.002168
N	2.111211	2.120497	0.758670
C	1.724004	3.901876	-0.476599
H	1.706657	4.858733	-0.974940
N	0.812383	2.880961	-0.750501
H	2.520591	1.488610	1.432523
H	3.395084	3.870152	0.986784
C	-1.724004	-3.901876	-0.476599
H	-1.706657	-4.858733	-0.974940
N	-0.812383	-2.880961	-0.750501
H	-2.520591	-1.488610	1.432523
H	-3.395084	-3.870152	0.986784
H	-0.061533	-2.928370	-1.424982
C	-1.021929	-1.747779	0.003243
N	-2.111211	-2.120497	0.758670

RC: Pd + CH$_4$ -541.51

C	0.000000	0.000000	0.090500
Pd	0.000000	0.000000	-2.301700
H	0.000000	0.902200	0.706100
H	0.000000	-0.902200	0.706100
H	0.945700	0.000000	-0.515900
H	-0.945700	0.000000	-0.515900

TS: Pd + CH$_4$ -530.91

C	0.133482	0.101995	0.000000
Pd	-1.221860	-1.519552	0.000000
H	0.163100	0.719768	-0.900024
H	0.163100	0.719768	0.900024
H	0.978119	-0.603905	0.000000
H	-1.480417	0.021291	0.000000

P: Pd + CH$_4$ -538.19

C	-0.019200	0.013100	0.000000
Pd	1.557300	-1.252000	0.000000
H	2.459700	-0.006000	0.000000
H	-0.002900	0.627900	-0.903700
H	-0.002900	0.627900	0.903700
H	-0.877200	-0.676200	0.000000

RC: Pd[P2P] + CH_4 -1833.89

C	-0.798031	-0.763448	0.019280
Pd	2.350853	0.176841	-0.005157
H	-1.135714	-1.803997	0.046924
H	-1.179530	-0.270450	-0.879085
H	-1.145502	-0.233910	0.910539
H	0.309882	-0.760263	-0.003018
C	5.119191	1.782298	0.269925
C	5.532085	0.427764	-0.358851
P	3.306285	2.256032	-0.087703
P	4.314391	-0.987203	0.035909
H	5.542897	0.509245	-1.454183
H	6.544717	0.153994	-0.039281
H	5.790929	2.579419	-0.070359
H	5.198425	1.729145	1.364193
H	4.951219	-1.989503	-0.771285
H	4.903184	-1.451205	1.257559
H	3.499949	2.957260	-1.322529
H	3.283491	3.452272	0.706311

TS: Pd[P2P] + CH_4 -1813.98

C	0.000421	0.000436	0.000064
Pd	2.211628	-0.000029	-0.000066
H	-0.651082	-0.875174	0.038227
H	-0.209412	0.552279	-0.921797
H	-0.195755	0.620265	0.881002
H	1.184886	-1.224179	-0.000520
C	5.073599	1.951471	0.260557
C	5.587803	0.631733	-0.359252
P	3.218912	2.193015	-0.081596
P	4.402078	-0.799491	0.029251
H	5.615993	0.713854	-1.454133
H	6.603959	0.406816	-0.017183
H	5.651173	2.807757	-0.103570
H	5.177377	1.921510	1.353591
H	4.983698	-1.801549	-0.805110
H	4.995738	-1.279329	1.238290
H	3.307412	2.898975	-1.322961
H	3.017611	3.368627	0.709571

P: Pd[P2P] + CH_4 -1819.98

C	0.132426	0.418005	0.008290
Pd	2.209107	-0.060507	-0.000700
H	-0.514402	-0.458495	0.064622
H	-0.083579	0.970422	-0.914553
H	-0.053621	1.064883	0.874408
H	1.630096	-1.549984	0.035463
C	4.972692	2.024401	0.263722
C	5.565521	0.731409	-0.343495
P	3.112909	2.142728	-0.087371
P	4.439200	-0.749305	0.023681
H	5.613181	0.813004	-1.437483
H	6.583464	0.554639	0.020563
H	5.497016	2.911742	-0.106670
H	5.073317	2.011047	1.357107
H	5.024085	-1.727879	-0.831638
H	5.027393	-1.237344	1.229427
H	3.128274	2.867504	-1.318384
H	2.780977	3.263347	0.732382

RC: Pd[P3P] + CH_4 -2183.14

C	-1.022763	-0.772380	0.011432
C	5.722327	1.335071	0.118457
C	5.697783	-0.077110	-0.534409
C	4.817724	2.432839	-0.512158
Pd	2.442538	0.184762	-0.003943
P	4.243455	-1.191922	-0.035106
P	2.989159	2.386751	-0.002485
H	-1.169985	-1.856621	-0.010517
H	-1.462347	-0.321568	-0.883633
H	-1.495302	-0.353183	0.905139
H	0.056943	-0.551762	0.035911
H	2.559566	3.524717	-0.767972
H	4.832546	2.344949	-1.607297
H	6.757249	1.698674	0.044497
H	5.649328	0.018164	-1.627958
H	4.616614	-2.336406	-0.820402
H	3.087922	3.121424	1.223482
H	5.219229	3.422510	-0.262350
H	5.513009	1.252140	1.195292
H	6.630660	-0.603153	-0.297403
H	4.785964	-1.722453	1.180101

TS: Pd[P3P] + CH_4 -2176.59

C	0.000318	0.000215	-0.000573
C	5.825353	1.495789	0.059061
C	5.804316	0.067913	-0.550266
C	4.822029	2.510995	-0.553611
Pd	2.220700	0.000002	0.000041
P	4.330446	-0.982934	-0.003752
P	3.033011	2.260504	0.005303
H	-0.653195	-0.875185	-0.005287
H	-0.206727	0.591821	-0.898166
H	-0.205584	0.580190	0.905099
H	1.178921	-1.212388	-0.000443
H	2.447955	3.362860	-0.699320
H	4.825777	2.423016	-1.649056
H	6.836181	1.902905	-0.083120
H	5.757585	0.132041	-1.646418
H	4.645618	-2.166353	-0.740926
H	3.108309	2.952344	1.255732
H	5.133837	3.533094	-0.310443
H	5.679009	1.438397	1.148828
H	6.732747	-0.457393	-0.296783
H	4.862759	-1.466549	1.232593

P: Pd[P3P] + CH_4 -2183.14

C	0.141714	0.464111	0.008720
C	5.783701	1.546589	0.067242
C	5.808857	0.114676	-0.533118
C	4.738348	2.518221	-0.547440
Pd	2.209619	-0.068099	-0.002363
P	4.356020	-0.968490	-0.009481
P	2.964489	2.178417	-0.011930
H	-0.525419	-0.398895	-0.008525
H	-0.051661	1.087384	-0.873492
H	-0.052135	1.049275	0.916909
H	1.592585	-1.545905	0.017891
H	2.294347	3.193933	-0.759056
H	4.758385	2.442275	-1.643502
H	6.777375	1.989234	-0.086415
H	5.781570	0.170594	-1.630288
H	4.653502	-2.129958	-0.779114
H	2.954958	2.885540	1.229128
H	4.995864	3.551854	-0.290012
H	5.647147	1.492343	1.158246
H	6.743942	-0.387149	-0.258344
H	4.870993	-1.475292	1.222050

RC: Pd[P4P] + CH_4 -2562.57

C	0.427020	1.575523	0.675323
H	0.942105	1.921949	-0.226556
H	-0.311970	2.322518	0.982875
H	1.156360	1.431835	1.479254
H	-0.078196	0.624785	0.466980
PD	-1.385218	-2.012700	-0.274290
P	-3.577436	-2.176227	0.332497
P	0.365907	-3.467935	-0.142891
H	1.205617	-3.990427	-1.179596
H	1.452532	-3.215061	0.753703
H	-4.351437	-1.362723	1.222640
H	-4.600134	-2.238886	-0.667012
C	-3.876286	-3.865530	1.157057
C	-2.855668	-4.941848	0.695494
H	-2.658295	-4.803518	-0.376144
H	-3.321995	-5.932090	0.794505
H	-3.812719	-3.714184	2.242137
H	-4.903062	-4.177477	0.933652
C	-0.239402	-5.115198	0.594119
H	0.583824	-5.554475	1.169257
H	-0.445414	-5.791977	-0.244811
C	-1.504574	-4.941481	1.478660
H	-1.526064	-5.750386	2.222319
H	-1.410877	-4.006441	2.047398

TS: Pd[P4P] + CH_4 -2536.39

C	0.133700	0.102300	0.000000
H	0.594800	-0.010300	-0.986700
H	-0.113300	1.156100	0.147900
H	0.825600	-0.205300	0.791000
H	-1.550900	-0.037900	0.193000
PD	-1.288300	-1.599000	0.000000
P	-3.462800	-2.458200	0.107600
P	0.056700	-3.571900	-0.367300
H	-0.071700	-4.237900	-1.625900
H	1.487700	-3.549800	-0.412400
H	-4.531100	-1.716500	0.697000
H	-4.112500	-2.614200	-1.156400
C	-3.889100	-4.158500	0.840200
C	-2.763100	-5.193100	0.592400
H	-2.453100	-5.137900	-0.461800
H	-3.174500	-6.202900	0.724500
H	-4.044300	-4.020400	1.918400
H	-4.840600	-4.498800	0.415700
C	-0.154600	-5.044400	0.816900
H	0.647100	-4.959600	1.561300
H	0.000800	-5.986600	0.278000
C	-1.527200	-5.010000	1.526400
H	-1.542900	-5.786000	2.304500
H	-1.608600	-4.047400	2.049300

P: Pd[P4P] + CH_4 -2542.48

C	0.382625	-0.270558	-0.085493
H	0.856999	-0.415280	-1.064848
H	0.141872	0.785453	0.043735
H	1.078790	-0.581929	0.704182
H	-2.049154	-0.140606	0.205352
Pd	-1.321276	-1.548680	0.012322
P	-3.463795	-2.505244	0.096957
P	0.022192	-3.492388	-0.340458
H	-0.076266	-4.131469	-1.613548
H	1.442614	-3.360742	-0.371804
H	-4.520030	-1.759468	0.691407
H	-4.091581	-2.644069	-1.178004
C	-3.873394	-4.212284	0.813457
C	-2.732774	-5.234962	0.582501
H	-2.417945	-5.190957	-0.470878
H	-3.136141	-6.246372	0.724277
H	-4.047582	-4.079278	1.889314
H	-4.814299	-4.561329	0.372534
C	-0.129461	-4.985106	0.817970
H	0.664895	-4.877648	1.567188
H	0.071253	-5.908373	0.261233
C	-1.504189	-5.029568	1.523664
H	-1.485140	-5.831055	2.274805
H	-1.625864	-4.090361	2.080281

RC: Pd[P5P] + CH_4 -2926.81

C	0.422158	1.700240	0.638137
H	0.976827	2.003983	-0.255720
H	-0.319198	2.467346	0.884725
H	1.117631	1.583807	1.475938
H	-0.084570	0.747164	0.448360
Pd	-1.340159	-2.102767	-0.196178
P	-3.605625	-2.246905	0.140100
P	0.678085	-3.183238	-0.046095
H	1.154276	-3.910869	-1.181056
H	1.953042	-2.609842	0.265018
H	-4.444268	-2.612373	-0.958715
H	-4.485530	-1.222350	0.616816
C	-4.105323	-3.620102	1.355009
C	-3.188922	-4.869182	1.256361
H	-4.052376	-3.187330	2.362849
H	-5.152972	-3.881058	1.166237
H	-3.705527	-5.723514	1.716458
H	-3.055623	-5.128766	0.196592
C	0.702919	-4.590797	1.227983
C	-1.799335	-4.658696	1.918199
H	0.877218	-4.125664	2.207550
H	1.564532	-5.233522	1.013036
H	-1.855275	-4.925530	2.983804
H	-1.574253	-3.583139	1.876970
C	-0.614215	-5.412366	1.250080
H	-0.423742	-6.361002	1.771324
H	-0.881070	-5.682668	0.218545

TS: Pd[P5P] + CH_4 -2897.50

C	0.133700	0.102300	0.000000
H	0.633700	-0.045600	-0.963100
H	-0.118400	1.160800	0.098300
H	0.796700	-0.170200	0.828400
H	-1.552200	-0.036300	0.135900
PD	-1.289600	-1.600700	0.000000
P	-3.476700	-2.435500	0.036500
P	0.274500	-3.443900	-0.201100
H	0.222300	-4.448200	-1.222400
H	1.614800	-3.046700	-0.508500
H	-4.037500	-2.741000	-1.243000
H	-4.568600	-1.611300	0.445100
C	-3.986500	-4.024400	0.943300
C	-2.850500	-5.074900	0.918800
H	-4.232300	-3.749100	1.977300
H	-4.902300	-4.412100	0.483400
H	-3.279400	-6.082300	1.019400
H	-2.362200	-5.054700	-0.067000
C	0.699800	-4.559500	1.273600
C	-1.792300	-4.862400	2.032600
H	0.949300	-3.867500	2.090400
H	1.609200	-5.124500	1.037400
H	-2.202600	-5.253200	2.974200
H	-1.642400	-3.784300	2.188000
C	-0.416800	-5.528100	1.740800
H	-0.048000	-6.026800	2.647500
H	-0.544600	-6.323100	0.991700

P: Pd[P5P] + CH_4 -2903.59

C	0.371005	-0.237893	-0.005305
H	0.842601	-0.327217	-0.992762
H	0.112043	0.806612	0.174345
H	1.081477	-0.566738	0.765395
H	-2.057481	-0.150010	0.175683
Pd	-1.313355	-1.547510	0.017153
P	-3.463021	-2.495196	-0.001012
P	0.204051	-3.405124	-0.216968
H	0.073219	-4.419805	-1.217746
H	1.515391	-2.998490	-0.602646
H	-3.970059	-2.825170	-1.295360
H	-4.557735	-1.663581	0.365441
C	-3.966932	-4.072738	0.918576
C	-2.819013	-5.110137	0.926174
H	-4.233550	-3.786523	1.944277
H	-4.870473	-4.474788	0.446985
H	-3.238884	-6.120054	1.036503
H	-2.320168	-5.103137	-0.054609
C	0.691498	-4.488150	1.256185
C	-1.777374	-4.869992	2.051577
H	0.942896	-3.778545	2.056968
H	1.611279	-5.026766	0.998685
H	-2.181119	-5.283271	2.985987
H	-1.663459	-3.789382	2.220044
C	-0.379757	-5.487205	1.764107
H	0.018787	-5.942321	2.680855
H	-0.482878	-6.308931	1.040425

TS: Pd[P6P] + CH_4 -3257.39

C	0.133700	0.102300	0.000000
H	0.580500	0.003700	-0.994700
H	-0.115000	1.153000	0.165100
H	0.836400	-0.213200	0.778200
H	-1.552500	-0.045900	0.204700
PD	-1.288600	-1.599400	0.000000
P	-3.588900	-2.128700	0.204700
P	0.312800	-3.380900	-0.418700
C	0.215900	-4.700300	-1.779900
C	-1.031800	-5.604100	-1.634100
C	-2.358400	-4.860200	-1.915700
C	-3.614700	-5.531800	-1.312400
C	-4.794000	-4.563500	-1.045400
H	-4.171900	-1.532200	1.363300
H	-4.391200	-1.393000	-0.721500
H	0.740000	-4.232600	0.649700
H	1.627300	-2.899300	-0.713700
H	0.193500	-4.163700	-2.738400
H	1.135900	-5.295400	-1.757700
H	-0.928800	-6.470400	-2.303900
H	-1.054500	-6.013600	-0.612500
H	-4.954400	-3.917300	-1.921900
H	-5.711000	-5.161800	-0.944000
H	-2.488300	-4.737200	-3.001800
H	-2.269300	-3.848200	-1.505900
H	-3.957900	-6.338000	-1.976800
H	-3.348100	-6.017800	-0.360800
C	-4.682700	-3.698300	0.241300
H	-4.314100	-4.315400	1.073000
H	-5.684300	-3.350400	0.522700

P: Pd[P6P] + CH_4 -3263.07

C	0.366192	-0.210219	-0.061787
H	0.809390	-0.276632	-1.063813
H	0.097194	0.826204	0.145185
H	1.094851	-0.550933	0.685001
H	-2.036852	-0.144610	0.242240
Pd	-1.300426	-1.535697	-0.004874
P	-3.586387	-2.187632	0.213603
P	0.251620	-3.342485	-0.378480
C	0.199991	-4.643532	-1.753061
C	-1.025788	-5.580531	-1.644764
C	-2.365648	-4.865637	-1.938400
C	-3.614354	-5.567847	-1.352598
C	-4.794383	-4.615552	-1.040778
H	-4.136205	-1.605424	1.391276
H	-4.400140	-1.451678	-0.697190
H	0.576170	-4.208230	0.712248
H	1.581852	-2.873272	-0.586599
H	0.188066	-4.097376	-2.706299
H	1.134291	-5.215536	-1.713561
H	-0.888243	-6.431899	-2.327109
H	-1.054910	-6.007910	-0.630902
H	-4.981509	-3.954499	-1.900703
H	-5.703958	-5.222482	-0.926579
H	-2.484953	-4.739347	-3.024907
H	-2.303524	-3.852821	-1.525633
H	-3.958672	-6.350504	-2.043511
H	-3.339492	-6.086817	-0.421239
C	-4.651995	-3.773335	0.257262
H	-4.253647	-4.399893	1.067796
H	-5.646648	-3.437167	0.575103

TS: Pd(PH_3)$_2$ + CH_4 -1256.89

C	-0.000000	-0.000000	0.000000
H	-1.075777	0.186324	0.000000
H	0.255761	-0.564451	-0.902600
H	0.255761	-0.564451	0.902600
H	-0.000000	1.724737	0.000000
Pd	1.581735	1.543543	0.000000
P	3.604587	0.235894	0.000000
P	2.179811	3.806451	0.000000
H	4.569912	0.316152	-1.050600
H	3.495030	4.372361	0.000000
H	1.697291	4.640061	-1.052300
H	1.697291	4.640061	1.052300
H	3.548880	-1.192879	0.000000
H	4.569912	0.316152	1.050600

P: Pd(PH_3)$_2$ + CH_4 -1262.04

C	-2.132600	-0.012500	0.000000
Pd	-0.002700	-0.003100	0.000000
H	-0.269800	-1.575400	0.000000
H	-2.464300	0.526000	0.896800
H	-2.563200	-1.014100	0.000000
H	-2.464300	0.526000	-0.896800
P	2.259600	-0.628300	0.000000
H	0.632900	3.132500	1.055900
H	0.632900	3.132500	-1.055900
H	-1.205300	3.086300	0.000000
P	0.034000	2.382600	0.000000
H	3.419800	0.209100	0.000000
H	2.699800	-1.472700	1.057900
H	2.699800	-1.472700	-1.057900

TS: Pd[P2P]^{Me} + CH_4 -3287.19

C	0.006657	-0.013415	0.010437
Pd	2.237809	0.016781	-0.006492
H	-0.653428	-0.884812	0.032697
H	-0.214781	0.560881	-0.895585
H	-0.188134	0.586846	0.905829
H	1.166122	-1.177870	-0.011234
C	5.071153	1.946172	0.274151
C	5.587688	0.622969	-0.338891
P	3.230434	2.223577	-0.090924
P	4.420273	-0.824001	0.035447
H	5.629167	0.706456	-1.434562
H	6.606392	0.396554	0.007729
H	5.664243	2.803216	-0.075672
H	5.162110	1.914491	1.369617
H	4.876618	-1.859938	-2.153967
H	6.178775	-1.646239	1.606432
H	3.640063	2.369332	-2.522704
H	3.620971	4.509091	0.855684
C	2.891734	3.702146	1.010650
H	1.886760	4.084742	0.794654
H	2.917209	3.389439	2.061244
C	3.305497	3.078720	-1.756693
H	2.296955	3.413936	-2.028249
H	3.980844	3.945117	-1.742749
C	5.099841	-1.446897	1.665188
H	4.908488	-0.709558	2.453526
H	4.575857	-2.371429	1.935741
C	5.108213	-2.127814	-1.116572
H	6.195275	-2.241673	-1.004492
H	4.623021	-3.086181	-0.896716

TS: Pd[P3P]^{Me} + CH_4 -3649.72

C	-0.190207	0.653160	-0.443614
H	0.497667	1.674825	0.636753
H	-0.174992	-0.428818	-0.271816
H	-0.197865	0.873318	-1.516561
H	-1.111259	1.051835	-0.009092
Pd	1.922511	1.188067	0.078695
P	3.527989	2.365428	1.299541
P	3.424769	-0.070099	-1.319991
C	5.774503	1.033955	0.000528
C	5.261681	2.392646	0.552555
C	5.187520	0.601051	-1.371534
H	5.176549	1.464747	-2.053103
H	6.865764	1.108263	-0.111561
H	5.242895	3.134001	-0.260388
H	5.837222	-0.159304	-1.830463
H	5.608769	0.240455	0.745598
H	5.961053	2.771592	1.313356
C	3.901347	1.768101	3.035353
C	3.740816	-1.858570	-0.857182
C	3.308618	4.192778	1.639718
C	3.109991	-0.272722	-3.156109
H	4.690768	2.368101	3.509129
H	2.985999	1.836241	3.635040
H	4.210369	0.716618	3.012311
H	4.094698	-1.919596	0.178633
H	2.796567	-2.412888	-0.921837
H	4.479912	-2.327723	-1.521192
H	3.166882	4.726473	0.692707
H	2.405652	4.332548	2.245938
H	4.171273	4.618798	2.171022
H	3.916770	-0.826545	-3.655761
H	2.165214	-0.811655	-3.298905
H	3.009556	0.715630	-3.620177

TS: Pd[P4P]^{Me} + CH_4 -4008.22

Pd	0.165073	0.001639	-1.835890
H	0.228735	0.536719	-0.328298
C	0.921370	-0.909465	0.069497
H	2.925258	-2.038955	-3.691193
H	2.331683	-3.076852	-2.378980
H	2.113885	-3.585409	-4.078073
H	0.313620	-1.818727	0.132369
H	1.951160	-1.150955	-0.215253
H	0.944474	-0.451587	1.062333
P	-0.725718	1.893606	-2.897462
P	0.486986	-1.810634	-3.402728
C	-1.311433	1.842871	-4.697772
C	-0.455723	0.911492	-5.596623
H	0.596388	0.977136	-5.284615
H	-0.485351	1.292643	-6.626381
H	-2.358749	1.509006	-4.695959
H	-1.307335	2.872080	-5.086022
C	0.226128	-1.600973	-5.264650
H	0.007493	-2.588179	-5.697178
H	1.178833	-1.266839	-5.699275
C	-0.898345	-0.588093	-5.604183
H	-1.303385	-0.833028	-6.595502
H	-1.731173	-0.725421	-4.899954
C	0.483509	3.321964	-2.993292
H	1.357856	3.028828	-3.586226
H	0.022208	4.211257	-3.444618
H	0.827742	3.563687	-1.981101
C	-2.184881	2.768796	-2.117635
H	-2.479903	3.659199	-2.690018
H	-3.036357	2.080748	-2.057759
H	-1.916503	3.067231	-1.097500
C	-0.676456	-3.240667	-3.065389
H	-0.556346	-3.560000	-2.023080
H	-1.714137	-2.912735	-3.199212
H	-0.477421	-4.092572	-3.729797
C	2.121629	-2.724219	-3.396253

TS: Pd(PMe_3)$_2$ + CH_4 -3463.61

C	-0.904500	2.583700	-0.862000
Pd	0.057000	0.647200	-0.259800
H	0.659500	2.081500	-0.622900
H	-0.400400	3.516600	-1.128900
H	-1.496300	2.263600	-1.726200
H	-1.551300	2.784000	-0.001300
P	-1.945300	-0.698100	-0.030400
C	-3.256500	0.078900	1.056100
H	-3.451900	1.101000	0.709900
H	-4.194100	-0.492900	1.037200
H	-2.889000	0.134500	2.087900
C	-2.910400	-0.893400	-1.622200
H	-3.093300	0.096900	-2.056400
H	-2.318500	-1.474500	-2.339500
H	-3.872500	-1.396700	-1.456300
C	-2.011200	-2.461400	0.604800
H	-1.606000	-2.495200	1.623500
H	-1.388600	-3.101600	-0.031900
H	-3.037100	-2.854400	0.614600
P	2.101000	-0.424300	0.174000
C	2.248300	-2.250500	0.577000
H	1.839000	-2.838800	-0.253400
H	3.292400	-2.548800	0.746600
H	1.661300	-2.473500	1.476300
C	3.368000	-0.307000	-1.197900
H	3.536200	0.749000	-1.438800
H	4.320900	-0.772600	-0.910500
H	2.981600	-0.802700	-2.096500
C	3.088700	0.290900	1.593100
H	3.243100	1.361700	1.416900
H	4.063200	-0.205800	1.698000
H	2.524500	0.177700	2.526500

TS: Pd[P2P]^{Ph} + CH_4 -7813.52

C	-0.061102	0.135392	0.141183
H	-1.129530	0.351845	0.219426
H	0.105820	-0.449099	-0.769481
H	0.241215	-0.431200	1.028476
H	0.032965	1.782432	0.071978
C	0.634438	6.382477	-2.218290
C	1.606923	7.060594	-2.964959
C	2.954688	6.718544	-2.815848
C	3.331420	5.709034	-1.920259
H	0.247272	4.822998	-0.778502
H	-0.417058	6.637173	-2.332490
H	1.315068	7.843832	-3.661475
H	3.716809	7.235496	-3.395185
H	4.385503	5.465039	-1.820547
Pd	1.625190	1.582995	0.046653
P	2.747272	3.645218	0.027053
P	3.816369	0.550988	-0.004325
C	5.006069	1.970023	0.389492
C	4.568093	3.264832	-0.333457
H	4.967572	2.121815	1.476011
H	6.036091	1.707299	0.118719
H	5.214155	4.101012	-0.039368
H	4.653609	3.134608	-1.420088
C	4.386642	-0.812403	1.122036
C	5.429768	-0.693038	2.057739
C	5.740286	-1.751403	2.922580
C	5.018422	-2.947074	2.861910
C	3.978115	-3.079739	1.931807
C	3.661149	-2.021191	1.077718
H	6.009475	0.223272	2.124006
H	6.548134	-1.637264	3.642338
H	5.259023	-3.767090	3.535172
H	3.407327	-4.004351	1.879298
H	2.838676	-2.128246	0.372670
C	4.432298	-0.017980	-1.671465
C	5.659633	-0.684404	-1.846930
C	6.077031	-1.081015	-3.121410
C	5.275148	-0.816047	-4.239578
C	4.052561	-0.155633	-4.076967
C	3.631221	0.236857	-2.800137
H	6.285623	-0.909049	-0.985703
H	7.024575	-1.602298	-3.240965
H	5.599985	-1.129268	-5.229770
H	3.421997	0.048133	-4.939732
H	2.672813	0.737988	-2.669722
C	2.861224	4.547019	1.659576
C	3.475084	5.806250	1.793535
C	3.544774	6.434354	3.041053
C	3.001202	5.813204	4.173333
C	2.385397	4.563059	4.051167
C	2.311985	3.935443	2.800955
H	3.885736	6.309944	0.920782
H	4.015598	7.411425	3.128016
H	3.051505	6.306198	5.142133
H	1.954434	4.078295	4.924579
H	1.818319	2.969857	2.698186
C	2.364114	5.019839	-1.166837
C	1.008997	5.366089	-1.335271

TS: Pd[P3P]^{Ph} + CH_4 -8175.07

C	-0.039077	0.057715	-0.088753
H	-1.110015	0.251176	0.012843
H	0.128823	-0.453765	-1.042284
H	0.279167	-0.568281	0.751271
H	0.024481	1.714921	-0.106713
C	2.930115	-3.442692	1.400160
C	3.685786	-3.560533	2.574913
C	4.501744	-2.499088	2.976732
C	4.566785	-1.326504	2.211246
H	2.385108	-2.189216	-0.260372
H	2.289010	-4.260914	1.078950
H	3.634379	-4.469232	3.170964
H	5.091596	-2.578811	3.887501
H	5.211178	-0.519536	2.548466
Pd	1.618992	1.550988	-0.065832
P	2.472472	3.729618	-0.035769
P	3.712719	0.361202	0.015233
C	5.243370	2.808286	0.032751
C	4.251140	3.874718	0.574924
C	5.135630	1.400794	0.684767
H	4.975414	1.513834	1.765331
H	6.260702	3.179455	0.221333
H	4.180539	3.794441	1.668433
H	6.077005	0.854190	0.545949
H	5.154989	2.721319	-1.058902
H	4.629782	4.883879	0.367315
C	2.484783	4.615041	-1.677943
C	1.266300	4.656869	-2.387946
C	1.182880	5.283109	-3.633528
C	2.321899	5.863280	-4.208878
C	3.539162	5.815786	-3.523660
C	3.619214	5.200434	-2.266389
H	0.382354	4.188309	-1.958609
H	0.231029	5.311476	-4.159819
H	2.259948	6.342203	-5.183867
H	4.431079	6.257193	-3.963365
H	4.578927	5.182725	-1.756921
C	4.399901	-0.201978	-1.625890
C	3.784021	0.256621	-2.804555
C	4.266799	-0.134434	-4.060247
C	5.366301	-0.994158	-4.151796
C	5.984363	-1.460853	-2.983682
C	5.505045	-1.067606	-1.730424
H	2.920030	0.915542	-2.731976
H	3.779174	0.228619	-4.962316
H	5.737868	-1.305073	-5.126211
H	6.834906	-2.136233	-3.049107
H	5.983997	-1.450470	-0.831225
C	1.652481	4.986683	1.077428
C	0.729248	4.533021	2.035574
C	0.109435	5.433681	2.911161
C	0.399444	6.800199	2.833285
C	1.313707	7.263096	1.878071
C	1.936551	6.362805	1.007319
H	0.489613	3.471592	2.078348
H	-0.605543	5.067980	3.645208
H	-0.088797	7.502306	3.506251
H	1.536030	8.325710	1.805613
H	2.631927	6.739504	0.259974
C	3.813167	-1.194461	1.030776
C	2.988090	-2.271617	0.641677

TS: Pd[P4P]^{Ph} + CH_4 -8532.78

C	-0.465259	1.877458	-0.769169
H	-1.378721	1.605307	-0.234755
H	-0.597159	2.881111	-1.186023
H	-0.297244	1.144544	-1.564344
H	0.176599	1.753961	0.784580
C	2.490389	4.189291	5.435648
C	1.212631	3.799591	5.844702
C	0.507355	2.852130	5.089709
C	1.074967	2.309903	3.934875
H	4.063306	3.952742	3.998086
H	3.045944	4.928281	6.009345
H	0.766129	4.232159	6.737713
H	-0.490665	2.544584	5.395275
H	0.506872	1.599467	3.337316
Pd	1.592822	1.995839	0.083929
P	2.952142	2.359269	-1.865305
P	3.020646	1.904918	1.944018
C	4.815254	2.065303	-1.805104
C	5.565429	2.820952	-0.672666
H	5.143606	3.827837	-0.546346
H	6.590413	2.977981	-1.034043
H	4.969528	0.985842	-1.685678
H	5.233470	2.341776	-2.781060
C	4.759960	2.632833	1.862241
H	5.255171	2.437612	2.822003
H	4.643143	3.721579	1.775057
C	5.665585	2.107363	0.713195
H	6.699956	2.222826	1.063846
H	5.520472	1.025196	0.587512
C	2.876897	4.092079	-2.555018
C	3.445268	4.448565	-3.792573
C	3.360364	5.762055	-4.263923
C	2.706378	6.741795	-3.504257
C	2.138453	6.400779	-2.272626
C	2.221978	5.083438	-1.802179
H	3.941081	3.695274	-4.401618
H	3.798300	6.020257	-5.225842
H	2.637118	7.762589	-3.874846
H	1.625035	7.154498	-1.679476
H	1.769567	4.812199	-0.849093
C	2.452236	1.321088	-3.328778
C	1.349980	1.713358	-4.117000
C	0.860861	0.885930	-5.132498
C	1.455910	-0.356898	-5.381084
C	2.543276	-0.764586	-4.600958
C	3.033594	0.062951	-3.583678
H	0.871346	2.673186	-3.938590
H	0.011163	1.213274	-5.728017
H	1.074206	-1.000811	-6.170582
H	3.012718	-1.729592	-4.780570
H	3.871942	-0.287661	-2.987545
C	3.386539	0.161506	2.518790
C	2.966883	-0.913380	1.715004
C	3.215538	-2.236476	2.103179
C	3.883067	-2.500888	3.303573
C	4.300066	-1.437672	4.115602
C	4.052617	-0.117381	3.726469
H	2.430200	-0.702796	0.790476
H	2.879497	-3.056781	1.472294
H	4.070728	-3.527854	3.610819
H	4.808968	-1.637294	5.056394
H	4.364393	0.696083	4.379160
C	2.368895	2.682022	3.517175
C	3.066457	3.631495	4.284831

TS: Pd(PPh_3)$_2$ + CH_4 -10248.81

C	0.626147	0.515037	-2.381505
H	-0.050748	0.948377	-3.121191
H	1.402864	-0.051463	-2.903469
H	0.049723	-0.138113	-1.719365
H	0.693600	2.183063	-1.896240
C	0.127952	5.880271	0.323624
C	-1.121655	6.321630	0.776790
C	-1.983549	5.440274	1.438443
C	-1.593002	4.110394	1.639508
C	-0.350739	3.666349	1.175085
H	0.785117	6.577255	-0.190351
H	-1.420017	7.354192	0.608006
H	-2.955812	5.783528	1.786202
H	-2.260632	3.415028	2.143761
Pd	1.860593	1.675155	-0.947320
P	2.166277	3.867657	-0.067917
H	-0.066008	2.623381	1.303765
P	3.349335	-0.062445	-0.104833
H	3.928945	6.347466	-0.102827
H	4.705555	1.449936	-2.157336
H	1.886076	5.477154	2.510390
H	4.922666	-1.810151	-2.035437
H	2.617184	1.460941	2.252914
C	3.278882	-0.519832	1.701583
C	3.592067	-1.802806	2.189530
C	3.498450	-2.087806	3.556094
C	3.091316	-1.095726	4.456560
C	2.779833	0.183796	3.983370
C	2.869690	0.467782	2.615895
H	3.895821	-2.586928	1.500990
H	3.738501	-3.086504	3.914866
H	3.011988	-1.320879	5.518288
H	2.459898	0.960491	4.674178
C	3.069128	-1.719910	-0.918248
C	1.843424	-2.376399	-0.684670
C	1.543154	-3.582196	-1.323387
C	2.454196	-4.149070	-2.224442
C	3.665549	-3.498971	-2.477270
C	3.972087	-2.294683	-1.829213
H	1.121672	-1.944961	0.005958
H	0.594623	-4.075768	-1.122874
H	2.218166	-5.085023	-2.726566
H	4.380283	-3.927002	-3.177000
C	3.299529	4.315438	1.351329
C	4.619397	3.823992	1.318063
C	5.517166	4.112513	2.349809
C	5.106477	4.882213	3.446056
C	3.794574	5.363643	3.497678
C	2.898450	5.086678	2.456883
H	4.946361	3.209105	0.482162
H	6.532669	3.726563	2.302223
H	5.801845	5.098580	4.254506
H	3.463232	5.960064	4.345272
C	5.163186	0.234766	-0.429216
C	6.198213	-0.280316	0.369936
C	7.537116	-0.016083	0.057809
C	7.861320	0.760998	-1.060276
C	6.838525	1.281142	-1.862560
C	5.499845	1.026084	-1.544652
H	5.964280	-0.883849	1.242793
H	8.325699	-0.418913	0.689958
H	8.902748	0.964500	-1.301036
H	7.079992	1.892786	-2.728937
C	2.685885	5.106109	-1.370210
C	2.202910	4.936175	-2.683009
C	2.552672	5.834674	-3.695749
C	3.404876	6.911467	-3.420148
C	3.897389	7.085318	-2.122811
C	3.538072	6.192990	-1.104612
H	1.557009	4.090387	-2.907080
H	2.166046	5.688095	-4.702165
H	3.685352	7.604821	-4.210535
H	4.562412	7.916159	-1.896806
C	0.528996	4.547460	0.517974

TS: Pd[P2P]^{tBu} + CH_4			-7599.82
C	-0.114606	0.150443	0.014640
H	0.174814	4.847756	-1.106396
H	-1.182672	0.387416	0.024346
H	0.094904	-0.435173	-0.886934
H	0.109740	-0.435239	0.912723
H	0.028568	1.773470	0.005765
C	2.191637	3.906683	-2.805176
H	1.448009	3.121014	-2.626063
H	1.876566	4.493789	-3.681105
H	3.143067	3.426426	-3.060402
C	3.417107	5.904859	-1.897661
H	3.137056	6.444849	-2.815660
H	3.533190	6.648777	-1.104734
H	4.396273	5.446421	-2.080947
Pd	1.619934	1.573876	0.000727
P	2.690195	3.684479	-0.040420
P	3.815915	0.497283	0.037706
C	5.035257	1.952087	0.282668
C	4.554050	3.319890	-0.281489
H	5.166890	2.034799	1.366683
H	6.022923	1.708914	-0.132313
H	5.170653	4.128179	0.135453
H	4.710190	3.338440	-1.365370
C	2.325431	4.850716	-1.579877
C	2.620969	4.756478	1.603863
C	4.441974	-0.376741	-1.605233
C	4.264337	-0.636758	1.577516
C	5.773921	-0.789597	1.893838
H	5.890056	-1.376815	2.818381
H	6.322045	-1.311616	1.104835
H	6.261101	0.177966	2.064314
C	3.630209	-2.037467	1.381156
H	2.567671	-1.967093	1.117474
H	4.140228	-2.620757	0.607193
H	3.705306	-2.605336	2.320781
C	3.578318	0.025706	2.803334
H	4.033463	0.989343	3.058229
H	2.508626	0.190377	2.628120
H	3.690841	-0.630753	3.679470
C	5.820680	-1.072992	-1.526770
H	5.806397	-1.952342	-0.874517
H	6.109558	-1.419749	-2.531511
H	6.610603	-0.396308	-1.176798
C	4.510244	0.721550	-2.697645
H	5.312059	1.445856	-2.509867
H	4.715872	0.250159	-3.670548
H	3.561025	1.261093	-2.781596
C	3.362202	-1.402773	-2.044569
H	2.377570	-0.928080	-2.129788
H	3.630643	-1.813381	-3.030121
H	3.272670	-2.243888	-1.350044
C	3.345242	3.934410	2.701069
H	3.213402	4.434950	3.672076
H	2.926423	2.926144	2.784322
H	4.423815	3.855134	2.518546
C	1.136255	4.900730	2.034840
H	1.092769	5.371266	3.029224
H	0.558022	5.526491	1.347877
H	0.645403	3.922047	2.093172
C	3.278475	6.154722	1.527613
H	4.320605	6.109347	1.186257
H	2.729869	6.837466	0.870550
H	3.284099	6.607050	2.531766
C	0.962534	5.560544	-1.380095
H	1.007878	6.340451	-0.612484
H	0.665937	6.046347	-2.321875

TS: Pd[P3P]^{tBu} + CH_4			-7960.19
C	-0.175947	0.204445	-0.262670
H	5.031012	0.665822	2.854543
H	-1.223942	0.497710	-0.377392
H	0.103762	-0.388020	-1.140201
H	-0.091914	-0.397639	0.647419
H	0.039841	1.840917	-0.226803
H	3.263192	0.875006	2.908310
C	2.603283	-1.642394	1.906768
H	1.734129	-0.977953	1.966268
H	2.680709	-2.190129	2.858665
H	2.413580	-2.376577	1.117598
C	5.115923	-1.803324	1.662741
H	6.063179	-1.291245	1.450802
H	5.214618	-2.272156	2.654480
Pd	1.606018	1.576323	-0.068023
P	3.674655	0.269240	0.064113
P	2.479224	3.781793	-0.028851
C	5.121536	2.744399	0.790323
C	5.230655	1.367612	0.073023
C	4.381093	3.877127	0.022951
H	4.719574	3.870691	-1.021625
H	6.151126	3.096189	0.962491
H	5.491649	1.541588	-0.979193
H	4.687679	4.847527	0.436974
H	4.682374	2.616269	1.783383
H	6.069321	0.805715	0.505877
H	4.991222	-2.612075	0.934927
H	2.407205	3.141520	2.833296
H	6.197359	-0.452479	-1.771251
H	-0.025443	4.332244	-1.523787
C	2.121710	4.795128	-1.676026
C	2.994430	6.058054	-1.893229
H	2.746645	6.498826	-2.871444
H	2.821834	6.828297	-1.136180
H	4.066367	5.827982	-1.907253
C	2.402426	3.803120	-2.837625
H	3.452919	3.488362	-2.870889
H	2.175495	4.293452	-3.796586
H	1.781883	2.904212	-2.749915
C	0.624718	5.189269	-1.738808
H	0.379631	5.996559	-1.039582
H	0.386320	5.550526	-2.750766
C	4.028720	-0.822227	-1.531885
C	3.089962	-2.055543	-1.539666
H	3.136097	-2.541523	-2.526218
H	3.383187	-2.803954	-0.795204
H	2.046718	-1.773696	-1.354561
C	3.643844	0.078823	-2.737499
H	2.604547	0.418994	-2.667727
H	3.762612	-0.492858	-3.670588
H	4.284337	0.966239	-2.813328
C	5.493186	-1.291600	-1.725489
H	5.827306	-1.973479	-0.938373
H	5.571901	-1.831252	-2.682294
C	1.937485	4.855381	1.528847
C	2.321591	6.353363	1.478507
H	2.086937	6.820297	2.447897
H	3.392606	6.508807	1.295553
H	1.758531	6.898924	0.713885
C	0.402479	4.724861	1.717559
H	-0.161881	5.205281	0.912042
H	0.113408	5.211108	2.662154
H	0.096985	3.673030	1.760755
C	2.614354	4.216468	2.771620
H	3.700296	4.365668	2.778809
H	2.212637	4.688718	3.680655
C	3.908912	-0.836100	1.674430
C	4.071997	0.135468	2.874374
H	4.036517	-0.442682	3.810083

TS: Pd[P4P]^{tBu} + CH_4			-8317.90
C	-0.211063	0.244578	0.337233
H	2.643619	6.756417	1.175881
H	-1.241791	0.548286	0.130328
H	0.017546	-0.618710	-0.291851
H	-0.145373	-0.023383	1.397085
H	0.057958	1.907324	0.046398
C	-0.002340	4.527182	1.714676
H	-0.652219	4.884279	0.909019
H	-0.339930	5.002813	2.648630
H	0.948555	6.858198	0.652953
H	-0.143426	3.445133	1.807619
C	2.291260	4.373572	2.707228
H	3.345469	4.672876	2.675934
H	1.856108	4.801221	3.622886
Pd	1.600524	1.566485	0.053343
P	2.193980	3.900596	-0.075283
P	3.549446	0.018558	0.056296
C	4.033325	4.421836	-0.012875
C	4.939655	3.304126	0.560676
H	4.426322	2.819398	1.399438
H	5.853500	3.752912	0.978049
H	4.356778	4.664430	-1.031802
H	4.133684	5.344747	0.570559
C	5.302243	0.778669	0.063077
H	5.982350	0.129479	-0.501502
H	5.665075	0.779217	1.097390
C	5.332511	2.225752	-0.488618
H	6.339281	2.446850	-0.873627
H	4.655910	2.299440	-1.347249
H	2.242400	3.280950	2.789058
H	-0.390318	3.827406	-1.548922
H	5.200830	-2.594258	1.107804
H	5.669460	-1.913714	-1.265748
C	3.636488	-1.085915	-1.569906
C	2.229139	-1.658943	-1.880394
H	2.268224	-2.216313	-2.829126
H	1.874143	-2.348184	-1.107309
H	1.490512	-0.857314	-1.986802
C	4.015035	-0.131877	-2.736516
H	3.334515	0.725804	-2.792571
H	3.939863	-0.682871	-3.686054
H	5.041929	0.243060	-2.657308
C	4.658350	-2.247210	-1.530554
H	4.360739	-3.033754	-0.828682
H	4.719007	-2.709009	-2.528468
C	3.634989	-1.123622	1.649550
C	3.390101	-0.156319	2.841538
H	3.372174	-0.730773	3.780263
H	4.184281	0.596151	2.932292
H	2.434483	0.371200	2.738660
C	2.485792	-2.163208	1.623148
H	1.516248	-1.696940	1.418892
H	2.421233	-2.657386	2.604756
H	2.657683	-2.947187	0.876773
C	4.976866	-1.862209	1.889099
H	5.827362	-1.175057	1.966207
H	4.916481	-2.408884	2.843176
C	1.600374	4.751634	-1.741774
C	2.159434	6.172140	-2.012168
H	1.815651	6.508293	-3.002851
H	1.812731	6.907570	-1.280414
H	3.255319	6.197349	-2.027041
C	2.097256	3.805017	-2.869481
H	3.192225	3.733500	-2.897968
H	1.767044	4.193918	-3.844743
H	1.692480	2.793829	-2.743046
C	0.052726	4.798617	-1.799904
H	-0.361480	5.554948	-1.123463
H	-0.264232	5.064260	-2.819982
C	1.488235	4.885157	1.478455
C	1.622095	6.425853	1.400924
H	1.346797	6.861503	2.373980

TS: Pd(P(*t*-Bu)$_3$)$_2$ + CH$_4$ -9897.53

C	0.359912	0.781764	-2.112328
H	0.073296	1.454021	-2.927072
H	0.901337	-0.060252	-2.544405
H	-0.551862	0.428331	-1.620222
H	0.650102	2.398920	-1.272513
H	4.314499	-0.431284	-2.854549
H	4.168763	1.190028	-2.159934
C	5.820010	0.803289	0.017691
H	5.255782	1.734467	0.118431
H	6.732406	1.028170	-0.555086
H	6.136308	0.473153	1.011634
C	5.882041	-1.554464	-0.829822
H	5.438377	-2.330013	-1.460322
H	6.852465	-1.291342	-1.280040
Pd	1.766338	1.566292	-0.587907
P	1.989732	4.107501	0.139192
P	3.207464	-0.447700	0.083384
H	4.591649	5.673652	-0.958079
H	3.271606	4.623834	3.781599
H	3.919587	6.758496	0.806984
H	2.321562	3.343604	3.015033
H	3.944210	6.642854	2.566109
H	2.420033	6.964389	1.730337
H	6.087063	-1.988584	0.153926
C	2.535080	4.416744	2.990050
H	1.621115	4.955034	3.252217
C	4.525193	4.185510	1.523399
H	5.097259	4.514798	0.653843
H	5.113739	4.438813	2.418959
H	4.434228	3.099240	1.480939
H	-0.343208	2.562443	1.109480
H	4.526455	-2.640004	2.118758
H	4.144941	-3.557544	-0.115059
C	2.454503	-2.188731	-0.568579
C	0.926409	-2.193404	-0.274283
H	0.473749	-3.053940	-0.790760
H	0.702416	-2.299971	0.789317
H	0.438697	-1.286217	-0.635871
C	2.619821	-2.283122	-2.111158
H	2.265426	-1.388204	-2.628073
H	2.019287	-3.131651	-2.471903
H	3.654197	-2.469833	-2.412715
C	3.064702	-3.479830	0.039671
H	2.861548	-3.578577	1.109906
H	2.600183	-4.348112	-0.454036
C	3.461431	-0.692842	2.049467
C	3.694064	0.709463	2.663204
H	3.666276	0.630815	3.760738
H	4.661154	1.136982	2.391627
H	2.910978	1.405258	2.347754
C	2.134323	-1.209243	2.669563
H	1.273938	-0.612318	2.343785
H	2.204148	-1.121985	3.764427
H	1.936841	-2.259682	2.442440
C	4.619402	-1.619795	2.499802
H	5.599602	-1.232090	2.203894
H	4.617003	-1.678835	3.599995
C	0.110159	4.650718	0.588245
C	-0.063745	6.046869	1.242632
H	-1.137047	6.216989	1.421188
H	0.435968	6.133411	2.210422
H	0.290166	6.858535	0.598845
C	-0.804430	4.628302	-0.667324
H	-0.569998	5.425369	-1.378674
H	-1.842083	4.784314	-0.335142
H	-0.767529	3.668002	-1.190183
C	-0.437297	3.561127	1.554014
H	0.073196	3.553999	2.520695
H	-1.504333	3.754924	1.744085
C	3.133439	4.862515	1.628294
C	3.351977	6.396683	1.669677
C	2.514005	5.118366	-1.505741
C	1.914700	4.406966	-2.751173
H	2.261673	4.938630	-3.651217
H	2.244497	3.365113	-2.815717
H	0.822308	4.412156	-2.765080
C	2.090806	6.610426	-1.551759
H	1.003898	6.734583	-1.574904
H	2.484157	7.058659	-2.478116
H	2.483519	7.194062	-0.715225
C	4.056040	5.041685	-1.671900
H	4.426264	4.013933	-1.580395
H	4.317260	5.398863	-2.679329
C	5.010460	-0.275143	-0.747444
C	4.790443	0.286316	-2.182390
H	5.768544	0.548133	-2.615156

TS: Pd[P2P]^{Cl} + CH$_4$ -1734.05

C	0.065349	0.134893	0.013454
Pd	2.249287	0.017196	0.000061
H	-0.599950	-0.726840	0.048623
H	-0.109973	0.696292	-0.909073
H	-0.091341	0.755893	0.900723
H	1.258834	-1.241719	0.037979
C	5.091559	1.944021	0.281702
C	5.604914	0.647429	-0.384535
P	3.255060	2.162496	-0.081123
P	4.422421	-0.764610	0.013711
H	5.599030	0.740069	-1.478413
H	6.622243	0.400801	-0.062874
H	5.651969	2.822355	-0.054916
H	5.170463	1.881034	1.375052
Cl	5.176765	-2.237133	-1.291466
Cl	5.215746	-1.388680	1.875361
Cl	3.375915	3.082620	-1.987623
Cl	2.851789	3.807117	1.189837

TS: Pd[P3P]^{Cl} + CH$_4$ -2098.66

C	0.113306	0.188461	-0.682755
C	5.825936	1.494301	-0.244116
C	5.702647	0.028493	-0.735757
C	4.713337	2.474913	-0.699922
Pd	2.216694	0.000839	-0.115286
P	4.312412	-0.945019	0.057865
P	3.047833	2.198620	0.110758
H	-0.503403	-0.635618	-1.040092
H	0.169487	0.963805	-1.451492
H	-0.304135	0.578854	0.251151
H	1.281243	-1.198488	-0.599665
Cl	1.994919	3.809785	-0.797131
H	4.526102	2.380810	-1.779429
H	6.773639	1.883614	-0.640933
H	5.498658	-0.007669	-1.815604
Cl	4.677954	-2.809364	-0.877349
Cl	3.446968	2.992213	2.037004
H	5.012693	3.509906	-0.502691
H	5.925677	1.518220	0.848985
H	6.636570	-0.514356	-0.554210
Cl	5.161692	-1.280526	1.976185

TS: Pd[P4P]^{Cl} + CH$_4$ -2456.18

C	0.435984	0.177830	1.132583
H	0.930339	0.405662	0.182819
H	0.216130	1.106533	1.658994
H	1.062551	-0.458618	1.762918
H	-1.358353	0.083751	1.291959
Pd	-1.091330	-1.211246	0.404301
P	-3.229908	-2.087431	0.208950
P	0.202946	-3.008006	-0.447811
Cl	-0.155413	-3.759380	-2.404375
Cl	2.317528	-2.774495	-0.529031
Cl	-4.832562	-1.034060	1.109379
Cl	-4.005895	-2.371211	-1.748260
C	-3.590220	-3.783673	0.932665
C	-2.516590	-4.842343	0.572838
H	-2.315758	-4.809923	-0.506010
H	-2.960322	-5.829252	0.755916
H	-3.647707	-3.637018	2.019755
H	-4.584836	-4.079771	0.582040
C	0.118288	-4.594611	0.571205
H	0.976263	-4.544728	1.252412
H	0.273464	-5.446106	-0.100816
C	-1.190003	-4.716351	1.390779
H	-1.080228	-5.595746	2.039299
H	-1.253409	-3.853317	2.067277

TS: Pd(PCl$_3$)$_2$ + CH$_4$ -1127.65

C	0.353234	2.140018	0.000000
Pd	-0.011297	-0.005379	0.000000
H	1.354613	2.568150	0.000000
H	-0.179466	2.441605	-0.906155
H	-0.179466	2.441605	0.906155
H	1.443229	0.633529	0.000000
P	-2.392801	-0.072755	0.000000
P	0.726093	-2.209058	0.000000
Cl	-3.319807	-1.015718	-1.626801
Cl	-0.559096	-3.890908	0.000000
Cl	1.966483	-2.687537	-1.621826
Cl	1.966483	-2.687537	1.621826
Cl	-3.394600	1.776066	0.000000
Cl	-3.319807	-1.015718	1.626801

TS: Pd(PH$_3$)$_2$Cl$^-$ + CH$_4$ -1356.60

C	-0.062947	0.120544	0.600327
H	-0.076696	-0.567344	1.453451
H	-0.674603	0.992391	0.855482
H	-0.499573	-0.355455	-0.285085
H	1.112335	1.235482	0.446283
Cl	6.445664	-1.952985	-1.249558
Pd	2.115615	0.047353	0.063838
H	2.642328	-3.274630	0.643212
H	5.337183	0.228089	-0.709206
H	4.854170	1.803056	0.698942
H	4.143814	-2.541236	-0.745545
H	2.127540	-3.046768	-1.380999
H	4.354737	2.059201	-1.325978
P	2.776478	-2.268855	-0.368000
P	4.212051	1.042435	-0.329158

TS: Pd(PH$_3$)$_2$Br$^-$ + CH$_4$ -1349.48

C	-0.108687	0.133928	0.618428
H	-0.119754	-0.548931	1.475444
H	-0.721673	1.005857	0.868936
H	-0.544628	-0.347769	-0.264079
H	1.066041	1.258409	0.463651
Br	6.582985	-2.013416	-1.289763
Pd	2.066464	0.069597	0.079062
H	2.542522	-3.249887	0.665107
H	5.295648	0.308409	-0.691079
H	4.779537	1.855279	0.719965
H	4.046338	-2.572716	-0.728534
H	2.028463	-3.016845	-1.358738
H	4.278790	2.108375	-1.305510
P	2.695698	-2.250716	-0.349308
P	4.150525	1.088328	-0.310809

TS: Pd(PH$_3$)$_2$I$^-$ + CH$_4$ -1341.15

C	-0.260394	0.185996	0.560503
H	-0.306194	-0.481665	1.428151
H	-0.886017	1.059647	0.768758
H	-0.655184	-0.312495	-0.331812
H	0.917170	1.323141	0.439295
I	6.738381	-2.084830	-1.355618
Pd	1.932542	0.129951	0.117182
H	2.522187	-3.118313	0.856019
H	5.166403	0.450794	-0.654595
H	4.642898	1.861965	0.867784
H	3.849146	-2.565762	-0.728070
H	1.785118	-3.039185	-1.110051
H	4.128073	2.267870	-1.129360
P	2.551235	-2.198587	-0.239328
P	4.010638	1.174874	-0.214830

TS: Pd[P2P]Cl$^-$ + CH$_4$ -1913.72

C	-0.131610	0.356309	-0.522378
Pd	2.055697	0.071919	-0.127444
H	-0.898899	-0.406678	-0.689060
H	-0.103263	1.010663	-1.401162
H	-0.405023	0.924769	0.374141
H	0.852550	-0.937958	-0.453884
C	5.121604	1.469921	0.723652
C	5.515824	0.133594	0.059898
P	3.409627	2.048136	0.151023
P	4.088434	-1.098320	0.188233
H	5.755633	0.276399	-1.003186
H	6.366363	-0.307905	0.597626
H	5.874439	2.245013	0.538391
H	5.059151	1.315687	1.809803
H	4.565254	-2.111280	-0.698518
H	4.501355	-1.715432	1.418610
H	3.790493	2.780862	-1.023414
H	3.294537	3.228911	0.964259
Cl	6.555270	-1.566285	2.964465

TS: Pd[C2C] + CH$_4$ -2856.23

C	-0.000000	-0.000000	0.000000
H	-1.089687	0.099425	-0.043862
H	0.319393	-0.574392	-0.877795
H	0.245603	-0.539108	0.922671
H	-0.000000	1.526486	0.000000
H	4.097158	-1.023048	1.203711
C	5.719199	1.712071	1.200929
C	4.821942	4.266602	-0.411942
H	1.769929	4.965325	-0.994913
C	2.710301	3.295599	-0.172235
Pd	1.612663	1.532150	0.000000
N	4.075684	3.173450	0.029259
C	3.902293	5.155229	-0.884631
H	4.040205	6.144255	-1.295204
N	2.653570	4.550810	-0.732718
C	3.697642	0.859286	0.395071
H	5.897364	4.324881	-0.353733
C	5.647131	0.403514	1.575354
H	6.349515	-0.201296	2.129633
N	4.431960	-0.076813	1.083969
N	4.551449	1.945268	0.472992
H	6.473823	2.460484	1.384510

TS: Pd[C3C] + CH$_4$ -3244.18

C	-0.000000	-0.000000	0.000000
H	-1.088211	0.092217	-0.084358
H	0.350301	-0.588069	-0.856032
H	0.215431	-0.525431	0.938332
H	-0.000000	1.519610	0.000000
H	5.557293	3.151253	-1.252155
C	5.913034	1.235288	0.563261
C	4.088353	5.090298	-0.197725
H	1.083574	4.825200	0.802211
C	2.426544	3.481099	-0.051733
Pd	1.619466	1.560062	0.000000
N	3.724928	3.760277	-0.442995
C	2.998541	5.688431	0.356192
H	2.848262	6.703991	0.690095
N	2.015565	4.699893	0.431400
C	3.655896	0.805138	0.228103
H	5.061086	5.492399	-0.441242
C	5.580288	0.191612	1.369670
H	6.180855	-0.385601	2.056716
N	4.222299	-0.048312	1.143806
N	4.746443	1.579823	-0.133262
H	6.859980	1.734534	0.417239
H	3.674973	-0.757600	1.612134
C	4.579126	2.720703	-1.028180
H	4.108665	2.365072	-1.947718

TS: Pd[C4C] + CH$_4$ -3607.80

C	-0.000000	-0.000000	0.000000
H	-1.093978	0.065477	-0.021741
H	0.302832	-0.566884	-0.890776
H	0.267883	-0.542403	0.915786
H	-0.000000	1.486640	0.000000
H	6.338170	1.988053	0.700283
C	3.860266	5.271080	0.189139
C	5.573616	-0.451920	0.487669
H	2.630529	-1.544455	0.034681
C	3.445676	0.371273	0.115455
Pd	1.628217	1.570187	0.000000
N	4.770993	0.688392	0.334827
C	4.746422	-1.526672	0.371220
H	4.951681	-2.584937	0.432951
N	3.477026	-1.000214	0.148107
C	2.387283	3.494243	-0.005226
H	6.638093	-0.402810	0.664872
C	2.795780	5.715979	-0.532587
H	2.591376	6.685815	-0.960184
N	1.925856	4.631016	-0.632592
N	3.600326	3.930499	0.504995
H	4.753570	5.787238	0.509133
H	1.027350	4.635992	-1.094942
C	4.524833	3.058719	1.236696
H	3.957792	2.505762	1.989798
H	5.240753	3.709982	1.748615
C	5.307063	2.060318	0.339510
H	5.335595	2.444179	-0.686647

TS: Pd[C5C] + CH_4 -3971.18

C	-0.000000	-0.000000	0.000000
H	-1.090275	0.106304	0.005285
H	0.276016	-0.557044	-0.903117
H	0.284754	-0.565823	0.893946
H	-0.000000	1.540914	0.000000
C	2.330268	3.525900	-0.005482
H	2.345192	3.097709	2.577031
C	4.504078	2.766628	2.579887
C	3.255700	3.654683	2.329925
C	4.364864	1.251283	2.276417
Pd	1.614765	1.574847	0.000000
C	3.189386	5.536199	-0.776664
C	5.854560	0.490281	0.370714
H	5.085297	0.704183	2.896586
H	5.375076	3.180267	2.054103
H	3.311743	4.526996	2.992482
H	3.359293	0.909595	2.543264
H	4.723751	2.843002	3.655132
C	5.661082	0.134517	-0.927845
H	6.358320	-0.208454	-1.677442
N	4.291836	0.275374	-1.156945
N	4.597546	0.835814	0.886914
H	6.758484	0.511345	0.962095
H	3.826932	0.087523	-2.034049
C	3.593106	0.716791	-0.055105
C	3.602875	5.385878	0.510107
H	4.202466	6.034764	1.131819
N	3.077207	4.168590	0.966468
H	1.954312	4.223311	-1.938384
H	3.359854	6.333534	-1.484173
N	2.424388	4.405065	-1.063251

TS: Pd(NHC)$_2$ + CH_4 -3065.22

C	-0.000000	-0.000000	0.000000
H	-1.091924	0.086671	0.003639
H	0.272749	-0.556462	-0.906634
H	0.278099	-0.559751	0.903039
H	-0.000000	1.548011	0.000000
Pd	1.616320	1.578102	0.000000
C	5.376610	-0.805620	-0.005869
C	2.822243	5.686990	-0.677907
C	2.823219	5.685907	0.681597
H	3.045052	6.472652	1.386312
N	2.461778	4.391404	1.067772
H	2.338709	4.085053	-2.019632
H	3.043151	6.474878	-1.381656
H	2.341927	4.081670	2.021397
C	2.213075	3.546138	0.000543
N	2.460266	4.393099	-1.065676
C	4.441595	-1.796220	-0.004288
H	4.552394	-2.870169	-0.004800
N	3.204320	-1.153694	-0.001638
H	5.067147	1.317993	-0.004547
H	6.454972	-0.854109	-0.008017
H	2.303352	-1.618041	-0.000249
C	3.296478	0.214470	-0.001420
N	4.658700	0.393187	-0.004125

RC: Pd + C_2H_6 -902.67

Pd	0.066074	0.011102	-0.789205
C	-0.786404	0.025808	2.678372
C	0.318915	-0.103508	1.613166
H	-1.761634	0.218625	2.217619
H	0.112691	-0.992628	0.952315
H	-0.570014	0.851867	3.367917
H	-0.869424	-0.894646	3.270353
H	1.306638	-0.282102	2.050722
H	0.408380	0.854469	1.031596

TS: Pd + C_2H_6 -877.66

C	0.283100	0.930500	-0.470800
C	-0.283100	-0.930500	-0.470800
H	0.278000	1.735100	0.312100
H	1.285200	0.860500	-0.892200
H	-0.444200	1.227900	-1.225100
H	-0.278000	-1.735100	0.312100
H	-1.285200	-0.860500	-0.892200
H	0.444200	-1.227900	-1.225100
Pd	0.000000	0.000000	1.465500

P: Pd + C_2H_6 -905.17

Pd	-0.000203	0.000000	-0.446909
C	-1.511753	-0.009970	0.901417
C	1.513271	0.009982	0.899034
H	-2.410017	0.034706	0.266716
H	2.410628	-0.034170	0.262960
H	-1.447100	0.868966	1.548886
H	-1.485955	-0.937907	1.479948
H	1.449950	-0.869199	1.546335
H	1.488148	0.937705	1.477981

RC: Pd[P2P] + C_2H_6 2195.47

C	-0.001810	0.024256	-0.043702
Pd	0.918315	3.154699	-0.011093
C	-1.419376	-0.539102	0.159822
H	0.406941	-0.251150	-1.022821
H	0.691219	-0.334338	0.725874
H	-0.014485	1.136346	0.008914
C	2.556897	5.909156	0.287742
C	1.187550	6.348663	-0.287821
P	3.001289	4.101400	-0.130298
P	-0.222979	5.129399	0.117604
H	1.235772	6.389013	-1.384468
H	0.930980	7.353907	0.067442
H	3.349457	6.582182	-0.060661
H	2.538595	5.961515	1.384776
H	-1.245094	5.795392	-0.639885
H	-0.643895	5.688163	1.368673
H	3.667552	4.322641	-1.379989
H	4.221092	4.048868	0.625858
H	-1.416454	-1.635872	0.105629
H	-2.110389	-0.169858	-0.608086
H	-1.825396	-0.255778	1.138816

TS: Pd[P2P] + C_2H_6 -2155.35

Pd	0.000000	0.000000	-0.000254
C	-0.610551	0.837564	2.001327
C	0.610551	-0.837564	2.001327
H	-0.698253	1.718406	1.341858
H	0.698253	-1.718406	1.341858
H	-1.593878	0.468741	2.294256
H	1.593878	-0.468741	2.294256
H	-0.029869	1.133435	2.874745
H	0.029869	-1.133435	2.874745
C	-0.665529	0.391440	-3.354787
C	0.665529	-0.391440	-3.354787
P	-1.626976	0.151745	-1.727834
P	1.626976	-0.151745	-1.727834
H	0.469683	-1.469722	-3.432224
H	-0.469683	1.469722	-3.432224
H	1.283613	-0.105483	-4.212935
H	-1.283613	0.105483	-4.212935
H	2.724936	-1.019624	-2.053850
H	-2.724936	1.019624	-2.053850
H	2.334050	1.042751	-2.080791
H	-2.334050	-1.042751	-2.080791

P: Pd[P2P] + C_2H_6 -2182.42

Pd	-0.000081	-0.000080	0.047486
C	-1.356099	0.455233	1.632597
C	1.356674	-0.454248	1.632314
H	-2.173754	1.103963	1.300031
H	2.175855	-1.100796	1.299328
H	-1.767966	-0.496443	1.989759
H	1.766302	0.497897	1.990772
H	-0.811834	0.941525	2.447462
H	0.813151	-0.942683	2.446415
C	-0.570804	0.521827	-3.342279
C	0.571235	-0.521377	-3.342405
P	-1.507206	0.470860	-1.695963
P	1.507090	-0.471361	-1.695750
H	0.158989	-1.535475	-3.426922
H	-0.158540	1.536018	-3.426071
H	1.249729	-0.367261	-4.188323
H	-1.249027	0.368215	-4.188491
H	2.316826	-1.639379	-1.831163
H	-2.317215	1.638720	-1.831233
H	2.545488	0.457352	-2.013812
H	-2.545202	-0.458030	-2.014877

TS: Pd[P3P] + C_2H_6 -2516.92

Pd	2.254780	0.000337	0.000252
C	0.000628	-0.001101	-0.001578
C	0.951159	-1.849447	-0.000647
H	0.233018	0.980890	0.446358
H	-0.396463	0.111584	-1.010979
H	-0.723539	-0.496246	0.645584
H	1.888423	-2.229768	-0.440887
H	0.807895	-2.232870	1.010155
H	0.130509	-2.153012	-0.650795
P	4.193480	-0.318112	1.326532
P	3.086410	1.771826	-1.339477
C	5.649275	1.830683	0.016449
C	5.799761	0.412707	0.629648
C	4.975797	1.904400	-1.380846
H	2.866156	1.956091	-2.747280
H	5.335896	1.079860	-2.011862
H	6.658317	2.256359	-0.079263
H	6.157548	-0.287135	-0.138888
H	4.777518	-1.524322	1.851350
H	2.811148	3.145065	-1.025943
H	5.257924	2.839010	-1.879215
H	5.116950	2.486921	0.722451
H	6.555698	0.433941	1.423359
H	4.216241	0.357320	2.589566

P: Pd[P3P] + C_2H_6 -2545.63

Pd	2.194964	-0.038947	-0.000757
C	0.269957	0.235720	-0.891538
C	1.281350	-1.752721	0.893692
H	0.112835	1.258781	-1.254637
H	0.203087	-0.458658	-1.738014
H	-0.507646	-0.010562	-0.162271
H	2.015938	-2.475664	1.268372
H	0.664572	-1.398487	1.728689
H	0.638142	-2.243384	0.156686
P	4.231367	-0.470856	1.069242
P	3.016773	1.877430	-1.061794
C	5.683407	1.812980	0.048362
C	5.817218	0.310200	0.414988
C	4.876553	2.119915	-1.242189
H	2.609990	2.186285	-2.394240
H	5.204893	1.455280	-2.053407
H	6.697303	2.213177	-0.089453
H	6.108994	-0.264952	-0.474743
H	4.691103	-1.809983	1.249798
H	2.666223	3.148238	-0.509958
H	5.071841	3.148363	-1.567130
H	5.256119	2.368333	0.897278
H	6.610668	0.179152	1.159774
H	4.339782	-0.097982	2.444388

TS: Pd[P4P] + C_2H_6 -2876.88

C	0.283000	0.425200	-0.504200
C	-1.610200	-0.454900	-0.596000
H	1.189900	0.256600	0.101500
H	0.536400	0.622600	-1.546300
H	-0.254600	1.268400	-0.070200
H	-1.988300	-1.446800	-0.897000
H	-2.112000	-0.098300	0.304300
H	-1.769300	0.231600	-1.427800
PD	0.141100	-1.785800	-0.094700
P	2.062100	-2.774800	-1.097100
P	-0.540400	-3.320600	1.600900
H	0.390000	-3.489000	2.674300
H	-1.672800	-3.251800	2.484000
H	2.635600	-2.414400	-2.364000
H	3.291600	-2.578100	-0.388300
C	2.206000	-4.660700	-1.297800
C	1.539400	-5.417600	-0.121200
H	1.843800	-4.946100	0.824700
H	1.942200	-6.439100	-0.083800
H	1.718000	-4.928400	-2.244400
H	3.264400	-4.928200	-1.390400
C	-0.769400	-5.144300	1.093100
H	-1.847500	-5.282000	0.939300
H	-0.472100	-5.808500	1.913800
C	-0.016000	-5.478200	-0.214000
H	-0.318200	-6.479500	-0.552600
H	-0.358400	-4.774900	-0.985100

P: Pd[P4P] + C_2H_6 -2904.48

C	0.540962	-0.044303	-1.385132
C	-1.651605	-0.555000	0.342118
H	1.605650	0.010578	-1.642522
H	-0.044593	-0.169555	-2.304663
H	0.241038	0.885254	-0.892843
H	-2.491819	-1.196462	0.634623
H	-1.394751	0.106689	1.179618
H	-1.942273	0.052481	-0.519323
Pd	0.089199	-1.702714	-0.115802
P	2.119558	-2.729640	-0.758455
P	-0.579205	-3.371993	1.414401
H	0.250634	-3.581178	2.558430
H	-1.783560	-3.193389	2.157553
H	2.805416	-2.193049	-1.887782
H	3.206776	-2.566650	0.155239
C	2.339578	-4.571820	-1.130867
C	1.575553	-5.490526	-0.143345
H	1.800686	-5.182219	0.888545
H	1.983512	-6.505363	-0.238690
H	1.975890	-4.738183	-2.153683
H	3.411928	-4.799722	-1.126468
C	-0.838293	-5.162767	0.851521
H	-1.899221	-5.247883	0.584070
H	-0.659996	-5.842497	1.693959
C	0.030407	-5.533391	-0.372477
H	-0.256923	-6.540737	-0.703081
H	-0.234744	-4.853994	-1.193739

TS: Pd[P5P] + C_2H_6 -3238.36

C	-1.037500	-3.228500	3.643800
C	-0.119900	-1.369800	3.347900
H	-0.916100	-4.236200	3.210200
H	-0.527300	-3.209900	4.607100
H	-2.092200	-2.975400	3.757600
H	-0.050300	-0.661400	2.503700
H	-0.886100	-1.003700	4.031700
H	0.839200	-1.468100	3.858400
PD	-0.267900	-2.751100	1.581700
P	-1.978400	-3.363200	0.045200
P	1.928500	-2.650100	0.639000
H	2.249500	-1.817300	-0.485100
H	3.002900	-2.124700	1.434300
H	-2.477200	-2.245300	-0.694900
H	-3.289300	-3.850300	0.376300
C	-1.666700	-4.519800	-1.437000
C	-0.196300	-4.437300	-1.912200
H	-1.907600	-5.541200	-1.113500
H	-2.362900	-4.262000	-2.242400
H	-0.134100	-4.726100	-2.971700
H	0.139800	-3.391000	-1.863700
C	2.844900	-4.213800	0.061100
C	0.764500	-5.330200	-1.086200
H	2.818100	-4.900000	0.919300
H	3.895700	-3.956700	-0.117000
H	0.636300	-6.370500	-1.417500
H	0.458900	-5.303100	-0.031000
C	2.263600	-4.924200	-1.187800
H	2.877100	-5.819100	-1.361700
H	2.412300	-4.283800	-2.069600

P: Pd[P5P] + C_2H_6 -3265.48

C	-1.777057	-3.119970	3.146937
C	0.935438	-2.365112	3.371752
H	-2.585793	-3.763641	2.780634
H	-1.318841	-3.579367	4.027457
H	-2.193656	-2.143551	3.425760
H	1.856833	-1.820525	3.130576
H	0.357372	-1.779773	4.093733
H	1.193748	-3.330553	3.824526
Pd	-0.290245	-2.751158	1.660309
P	-1.855274	-3.251798	-0.032550
P	1.617797	-2.330481	0.306245
H	1.606128	-1.756563	-1.006631
H	2.551703	-1.402273	0.851629
H	-2.150684	-2.265823	-1.025546
H	-3.210108	-3.485380	0.348662
C	-1.596143	-4.724805	-1.186331
C	-0.152366	-4.750032	-1.747974
H	-1.803904	-5.636892	-0.611547
H	-2.335975	-4.669360	-1.992905
H	-0.145719	-5.302440	-2.698270
H	0.149809	-3.723985	-2.005727
C	2.808448	-3.769262	0.006187
C	0.892443	-5.385209	-0.787956
H	2.952904	-4.217715	0.998746
H	3.775681	-3.362417	-0.312325
H	0.871248	-6.474392	-0.927627
H	0.592169	-5.203396	0.254206
C	2.341062	-4.858273	-0.996820
H	3.051957	-5.691444	-0.913971
H	2.445822	-4.474670	-2.022169

TS: Pd[P6P] + C_2H_6 -3599.08

C	0.264500	0.217700	0.886100
C	-1.231300	-0.075800	-0.569200
H	1.278900	-0.185500	1.059100
H	0.361700	1.208400	0.441600
H	-0.304000	0.264900	1.816100
H	-1.825200	-0.936200	-0.922200
H	-1.853600	0.520700	0.098500
H	-0.873500	0.524700	-1.406100
PD	0.141100	-1.785800	-0.094700
P	-0.106500	-3.164600	1.876700
P	0.889400	-2.521900	-2.241200
C	1.031600	-4.308700	-2.887600
C	1.718900	-5.245600	-1.864100
C	0.805300	-5.605500	-0.669800
C	1.557400	-6.116300	0.580200
C	0.740800	-6.036200	1.895800
H	-0.161400	-2.430100	3.108700
H	-1.438500	-3.675400	2.009100
H	2.216500	-2.110000	-2.586000
H	0.298700	-1.968300	-3.425600
H	0.010900	-4.656300	-3.099000
H	1.576400	-4.295400	-3.838500
H	2.055800	-6.160000	-2.374500
H	2.630900	-4.756500	-1.488300
H	-0.304100	-6.323000	1.702800
H	1.133300	-6.789100	2.595100
H	0.064600	-6.355900	-0.987600
H	0.239900	-4.707200	-0.398700
H	1.872000	-7.157300	0.415700
H	2.484700	-5.537000	0.709000
C	0.782500	-4.679400	2.648100
H	1.828500	-4.371700	2.789800
H	0.351400	-4.816300	3.647200

P: Pd[P6P] + C_2H_6 -3624.55

C	0.012414	-0.336287	1.602389
C	0.389293	0.112559	-1.164864
H	0.535747	-0.748514	2.475511
H	0.457391	0.627199	1.342587
H	-1.046300	-0.191950	1.855490
H	0.343524	-0.019771	-2.253458
H	-0.387907	0.821708	-0.864382
H	1.372178	0.517271	-0.898229
Pd	0.104741	-1.689289	-0.048545
P	-0.404278	-3.370275	1.574138
P	0.372574	-2.714339	-2.190024
C	0.606386	-4.494134	-2.806307
C	1.618891	-5.276060	-1.934476
C	1.003476	-5.695347	-0.576824
C	1.991980	-5.773318	0.607293
C	1.294761	-5.782737	1.990025
H	-1.064425	-2.783669	2.692298
H	-1.389957	-4.384065	1.354186
H	1.504472	-2.146892	-2.843890
H	-0.578686	-2.279063	-3.159732
H	-0.373201	-4.990376	-2.792159
H	0.932631	-4.442770	-3.851810
H	1.973510	-6.158462	-2.484673
H	2.506713	-4.649348	-1.762564
H	0.421855	-6.451917	1.956418
H	1.981570	-6.217921	2.730094
H	0.486029	-6.660031	-0.688918
H	0.223374	-4.966491	-0.332754
H	2.612055	-6.676080	0.509073
H	2.684167	-4.918825	0.563445
C	0.862923	-4.402591	2.552542
H	1.743632	-3.755721	2.667523
H	0.438879	-4.549269	3.552986

TS: Pd(PH_3)$_2$ + C_2H_6 -1598.98

Pd	0.000000	0.000000	-1.980900
C	-0.000400	1.053300	0.000400
C	0.000400	-1.053300	0.000400
H	0.409900	1.834700	-0.662600
H	-1.009300	1.304800	0.328800
H	0.670400	0.943500	0.852100
H	-0.409900	-1.834700	-0.662600
H	1.009300	-1.304800	0.328800
H	-0.670400	-0.943500	0.852100
P	-1.641700	1.101700	-3.296600
P	1.641700	-1.101700	-3.296600
H	2.419600	-2.231200	-2.874300
H	-1.418400	1.641400	-4.604500
H	1.418400	-1.641400	-4.604500
H	2.781700	-0.341200	-3.704200
H	-2.781700	0.341200	-3.704200
H	-2.419600	2.231200	-2.874300

P: Pd(PH_3)$_2$ + C_2H_6 -1623.86

Pd	0.000000	0.000000	0.003400
C	-0.999200	1.006400	1.604800
C	0.999200	-1.006400	1.604800
H	-1.524600	1.915200	1.286500
H	-1.723700	0.300800	2.027000
H	-0.260800	1.270600	2.367400
H	1.524600	-1.915200	1.286500
H	1.723700	-0.300800	2.027000
H	0.260800	-1.270600	2.367400
P	-1.280800	1.297300	-1.481300
P	1.280800	-1.297300	-1.481300
H	1.242400	-2.714900	-1.342300
H	-1.205300	1.287400	-2.908400
H	1.205300	-1.287400	-2.908400
H	2.699900	-1.184200	-1.411600
H	-2.699900	1.184200	-1.411600
H	-1.242400	2.714900	-1.342300

TS: Pd[P2P]^{Me} + C_2H_6 -3625.54

Pd	-0.012910	-0.022916	-1.851556
C	-0.065189	1.100012	0.113885
C	0.205987	-0.931442	0.210880
H	0.262610	1.871207	-0.605854
H	-1.090967	1.279170	0.439418
H	0.619074	1.135036	0.962739
H	-0.176926	-1.773130	-0.393380
H	1.255902	-1.079782	0.467776
H	-0.405633	-0.873132	1.112302
P	-1.349000	0.967295	-3.576549
P	1.180318	-1.199342	-3.564924
C	0.596601	-0.394498	-5.181441
C	-0.900366	-0.012297	-5.138828
H	1.211544	0.507982	-5.311251
H	0.810428	-1.056427	-6.033520
H	-1.188490	0.553479	-6.037047
H	-1.519900	-0.920679	-5.116653
C	-3.219096	0.994895	-3.768378
H	-3.526319	1.320280	-4.772552
H	-3.620900	-0.006909	-3.575905
H	-3.646163	1.680587	-3.026595
C	-0.967872	2.718533	-4.140129
H	-1.462080	2.962995	-5.090977
H	-1.307950	3.421711	-3.369477
H	0.115647	2.843369	-4.252767
C	0.763188	-3.000267	-3.900021
H	1.169924	-3.616210	-3.088094
H	-0.325263	-3.132609	-3.907825
H	1.177982	-3.349081	-4.856259
C	3.027870	-1.254426	-3.908933
H	3.438890	-0.239113	-3.861014
H	3.519387	-1.856846	-3.135438
H	3.251629	-1.688322	-4.893970

TS: Pd[P3P]^{Me} + C_2H_6 -3987.97

C	0.434687	1.193384	-2.450743
C	0.416008	-0.865913	-2.452423
H	1.035592	1.948590	-2.989330
H	-0.611480	1.497058	-2.386766
H	0.862275	1.087999	-1.452316
H	0.132091	-1.623833	-3.203303
H	1.321798	-1.161223	-1.920568
H	-0.419029	-0.761901	-1.757798
Pd	0.893951	0.171023	-4.416081
P	2.534354	-1.069320	-5.616577
P	-0.076025	1.405997	-6.209901
C	1.779709	0.220325	-8.129125
C	2.203221	-1.124220	-7.477254
C	0.305182	0.650871	-7.899463
H	-0.352543	-0.224578	-8.007390
H	1.934159	0.126670	-9.213962
H	1.411207	-1.871885	-7.634674
H	0.005313	1.372097	-8.675323
H	2.459099	1.023630	-7.804712
H	3.106997	-1.507060	-7.976444
C	4.288704	-0.398689	-5.617707
C	0.477012	3.177198	-6.504423
C	2.917416	-2.891144	-5.350735
C	-1.929227	1.643055	-6.420458
H	4.939378	-0.961848	-6.301865
H	4.694756	-0.462945	-4.600967
H	4.284670	0.657542	-5.911038
H	1.569412	3.218339	-6.588518
H	0.184371	3.788041	-5.641221
H	0.027770	3.602671	-7.413077
H	1.992926	-3.475424	-5.433884
H	3.317336	-3.030901	-4.338797
H	3.648303	-3.270948	-6.078929
H	-2.176674	2.143338	-7.367986
H	-2.311769	2.246732	-5.588213
H	-2.427155	0.666662	-6.388456

TS: Pd[P4P]^{Me} + C_2H_6 -4346.54

Pd	-0.028112	-0.042018	-1.801392
C	-0.300972	0.792842	0.276292
C	0.017905	-1.253677	0.108504
H	0.041216	1.678047	-0.289739
H	-1.352529	0.884403	0.553229
H	0.321294	0.711036	1.168911
H	-0.242028	-2.014768	-0.648108
H	1.033179	-1.399546	0.480390
H	-0.703782	-1.331317	0.923112
P	-1.667273	1.107813	-3.131354
P	1.771267	-0.869034	-3.162447
C	-1.840478	0.635511	-4.963374
C	-0.510257	0.125951	-5.571155
H	0.308770	0.771530	-5.225184
H	-0.538981	0.239730	-6.664181
H	-2.607252	-0.149096	-5.032530
H	-2.223817	1.507222	-5.513276
C	1.264172	-1.654990	-4.825295
H	1.395001	-2.739876	-4.709557
H	1.961630	-1.332039	-5.612462
C	-0.202387	-1.358205	-5.211409
H	-0.492126	-2.000409	-6.056376
H	-0.834340	-1.656365	-4.364031
C	-1.370971	2.954311	-3.309121
H	-0.394984	3.128656	-3.777452
H	-2.152266	3.437675	-3.912001
H	-1.352509	3.412099	-2.312299
C	-3.487638	1.151587	-2.662758
H	-4.085141	1.727820	-3.383605
H	-3.875142	0.126828	-2.614006
H	-3.596209	1.604287	-1.669370
C	2.979768	-2.188779	-2.576493
H	3.522550	-1.816788	-1.698492
H	2.426306	-3.088011	-2.279306
H	3.705916	-2.457851	-3.356540
C	3.031366	0.410502	-3.716732
H	2.527837	1.235972	-4.232418
H	3.534545	0.819155	-2.831862
H	3.784271	-0.026296	-4.387122

TS: Pd(PMe_3)$_2$ + C_2H_6 -3802.73

C	0.467900	2.569600	-0.815500
C	-0.681700	2.483300	0.929000
H	0.591500	1.919000	-1.699500
H	-0.196700	3.390100	-1.090700
H	1.429100	2.954700	-0.472300
H	-0.736000	1.798900	1.793800
H	-0.102900	3.358400	1.228900
H	-1.678000	2.782900	0.600000
PD	-0.004200	0.528800	0.023400
P	2.106100	-0.601200	-0.027700
C	3.686900	0.402500	-0.195300
H	3.757700	1.109900	0.640300
H	4.581500	-0.236100	-0.201500
H	3.656300	0.981000	-1.127200
C	2.555800	-1.611800	1.486200
H	2.565600	-0.959000	2.367400
H	1.797100	-2.387000	1.645400
H	3.541100	-2.086800	1.380000
C	2.435000	-1.874600	-1.366900
H	2.354600	-1.393700	-2.349600
H	1.676400	-2.664600	-1.312100
H	3.433400	-2.324100	-1.269100
P	-2.043500	-0.727800	0.029900
C	-2.063100	-2.604700	-0.037600
H	-1.541400	-3.004700	0.840600
H	-3.086000	-3.007100	-0.061500
H	-1.526400	-2.938300	-0.934200
C	-3.223100	-0.472400	1.467200
H	-3.449000	0.596300	1.568400
H	-4.162100	-1.026200	1.329400
H	-2.743500	-0.806400	2.395400
C	-3.209200	-0.372300	-1.397700
H	-3.454600	0.696700	-1.408400
H	-4.138100	-0.954900	-1.320900
H	-2.710500	-0.615200	-2.343800

TS: Pd[P2P]^{Ph} + C_2H_6			-8151.80
C	0.088167	1.282533	0.188760
C	0.612395	-0.690097	0.359426
H	0.279375	2.056339	-0.572916
H	-0.936081	1.345527	0.558415
H	0.800669	1.442672	0.998368
H	0.296353	-1.608251	-0.162599
H	1.689420	-0.691968	0.531795
H	0.070858	-0.653004	1.305009
Pd	0.154849	0.070929	-1.731975
P	-1.319028	0.900755	-3.432259
P	1.295844	-1.148517	-3.454412
C	0.597076	-0.418521	-5.057730
C	-0.924108	-0.183594	-4.935658
H	1.105016	0.539734	-5.223884
H	0.820429	-1.073415	-5.908974
H	-1.320567	0.269570	-5.852640
H	-1.433292	-1.143510	-4.783542
C	3.128145	-1.164364	-3.779163
C	3.749254	-0.519207	-4.865036
C	5.146029	-0.490888	-4.980934
C	5.947791	-1.113723	-4.020299
C	5.342276	-1.764583	-2.935310
C	3.951840	-1.780229	-2.812437
H	3.153960	-0.034344	-5.633047
H	5.603166	0.016900	-5.827838
H	7.031644	-1.091353	-4.111428
H	5.955520	-2.252184	-2.180351
H	3.496188	-2.274041	-1.955884
C	0.846382	-2.951320	-3.667309
C	1.557166	-3.831725	-4.505696
C	1.160614	-5.166542	-4.637949
C	0.044218	-5.644370	-3.939052
C	-0.671819	-4.779695	-3.103963
C	-0.269780	-3.445224	-2.964828
H	2.429587	-3.477841	-5.050581
H	1.724957	-5.833948	-5.286168
H	-0.260578	-6.683935	-4.041506
H	-1.537218	-5.142943	-2.553588
H	-0.819955	-2.777863	-2.303429
C	-0.958462	2.600243	-4.124489
C	-1.834349	3.284320	-4.989381
C	-1.500191	4.546792	-5.490354
C	-0.283140	5.146208	-5.140163
C	0.596821	4.476685	-4.282760
C	0.258565	3.216146	-3.774351
H	-2.785628	2.835126	-5.266083
H	-2.191603	5.063039	-6.153335
H	-0.026696	6.129644	-5.529025
H	1.541964	4.936369	-4.001405
H	0.938521	2.703122	-3.096143
C	-3.179590	0.883471	-3.395986
C	-3.816694	1.717865	-2.452487
C	-5.204242	1.704887	-2.300181
C	-5.991432	0.840589	-3.075291
C	-5.374529	0.001291	-4.007267
C	-3.982376	0.024858	-4.170220
H	-3.216738	2.381116	-1.831758
H	-5.672467	2.362222	-1.570489
H	-7.071923	0.821571	-2.949836
H	-5.973762	-0.673454	-4.615281
H	-3.534324	-0.632456	-4.909473

TS: Pd[P3P]^{Ph} + C_2H_6			-8513.59
C	-0.705164	0.917872	0.249142
C	-0.397098	-1.110015	0.473173
H	-0.276306	1.684342	-0.419553
H	-1.777739	1.067275	0.379568
H	-0.187816	0.995031	1.206169
H	-0.626497	-1.995680	-0.141104
H	0.596141	-1.194471	0.915336
H	-1.161370	-1.038953	1.247409
Pd	-0.306274	-0.266738	-1.637544
P	1.265465	-1.511862	-2.913071
P	-1.636615	0.631788	-3.400359
C	-0.074211	-0.755186	-5.403626
C	0.630798	-1.913482	-4.647251
C	-1.527540	-0.440620	-4.951386
H	-2.049027	-1.382045	-4.733241
H	-0.116398	-1.037362	-6.465359
H	-0.071632	-2.746045	-4.504908
H	-2.071781	0.055924	-5.765057
H	0.538091	0.156174	-5.363428
H	1.453981	-2.314823	-5.252050
C	2.894243	-0.650374	-3.223475
C	3.476925	0.025267	-2.131661
C	4.690877	0.704956	-2.268393
C	5.338866	0.743301	-3.509772
C	4.766964	0.088808	-4.605502
C	3.559163	-0.606711	-4.461671
H	2.965148	0.019813	-1.170567
H	5.125243	1.212630	-1.409637
H	6.277203	1.282491	-3.622275
H	5.259793	0.115727	-5.575149
H	3.145070	-1.114361	-5.328635
C	-1.178726	2.303028	-4.105195
C	0.062044	2.863227	-3.750636
C	0.461190	4.104213	-4.264352
C	-0.379829	4.805881	-5.134225
C	-1.619905	4.259780	-5.492372
C	-2.015057	3.018631	-4.983647
H	0.714493	2.322110	-3.067690
H	1.425101	4.520911	-3.980251
H	-0.075218	5.773343	-5.528630
H	-2.280931	4.802203	-6.165390
H	-2.985457	2.612427	-5.261794
C	1.794168	-3.228986	-2.400333
C	0.779294	-4.132617	-2.019139
C	1.091466	-5.424691	-1.586516
C	2.428593	-5.836034	-1.506518
C	3.445065	-4.945355	-1.868146
C	3.132376	-3.654617	-2.313674
H	-0.263053	-3.818456	-2.052447
H	0.292509	-6.105932	-1.301012
H	2.674123	-6.837878	-1.160344
H	4.487166	-5.253074	-1.807621
H	3.937344	-2.980018	-2.593542
C	-3.476302	0.815736	-3.172274
C	-3.934257	1.823664	-2.294951
C	-5.288730	1.944395	-1.979596
C	-6.223608	1.050409	-2.522124
C	-5.785820	0.043323	-3.386984
C	-4.426891	-0.072284	-3.711089
H	-3.221362	2.520260	-1.857494
H	-5.616246	2.733591	-1.305726
H	-7.278331	1.139141	-2.270549
H	-6.500526	-0.656338	-3.815765
H	-4.120003	-0.864157	-4.388537

TS: Pd[P4P]^{Ph} + C_2H_6			-8873.29
C	0.732265	0.281382	0.557876
C	0.040905	-1.674205	0.437780
H	0.457427	1.234782	0.076432
H	0.281504	0.267951	1.550603
H	1.815973	0.180894	0.626557
H	0.060266	-2.445003	-0.352022
H	0.854907	-1.888830	1.130552
H	-0.919013	-1.674595	0.955012
Pd	-0.066407	-0.421088	-1.441074
P	-2.100904	-1.074879	-2.490205
P	1.289952	0.605488	-3.093479
C	-1.997091	-1.759875	-4.253527
C	-1.518349	-0.796796	-5.372687
H	-2.095618	0.137617	-5.333410
H	-1.805095	-1.279441	-6.317957
H	-1.319471	-2.623203	-4.206920
H	-2.989542	-2.146758	-4.520843
C	0.500969	0.839959	-4.792397
H	1.226370	1.344954	-5.442952
H	-0.342322	1.528636	-4.657287
C	0.002001	-0.471347	-5.472727
H	0.236931	-0.375882	-6.540836
H	0.587584	-1.332972	-5.122420
C	-3.394561	0.260487	-2.697037
C	-4.666157	0.010760	-3.247069
C	-5.595071	1.045229	-3.397530
C	-5.269148	2.348346	-2.997649
C	-4.010915	2.609463	-2.445371
C	-3.081058	1.571448	-2.296725
H	-4.940721	-0.998370	-3.547586
H	-6.574730	0.834743	-3.821744
H	-5.994564	3.151370	-3.112636
H	-3.752133	3.616705	-2.125275
H	-2.103293	1.770986	-1.860252
C	-3.080194	-2.428736	-1.662502
C	-3.908335	-2.114937	-0.563621
C	-4.546761	-3.119267	0.168551
C	-4.363611	-4.467413	-0.168635
C	-3.533095	-4.796151	-1.244607
C	-2.896628	-3.789297	-1.982124
H	-4.059224	-1.074683	-0.281915
H	-5.188353	-2.848514	1.004819
H	-4.859040	-5.249373	0.402959
H	-3.377836	-5.838623	-1.515407
H	-2.255371	-4.078321	-2.810820
C	2.865772	-0.290075	-3.563457
C	3.107061	-1.562963	-3.017400
C	4.266485	-2.277778	-3.347267
C	5.204008	-1.724113	-4.225184
C	4.977019	-0.454193	-4.772965
C	3.817325	0.255516	-4.445881
H	2.380802	-1.985828	-2.324232
H	4.437303	-3.261204	-2.914027
H	6.108165	-2.273854	-4.479244
H	5.705808	-0.015551	-5.451559
H	3.662036	1.245683	-4.869737
C	1.921707	2.320252	-2.734355
C	1.290675	3.485425	-3.213784
C	1.713439	4.755841	-2.800830
C	2.773630	4.890319	-1.898816
C	3.407278	3.740119	-1.408471
C	2.982703	2.473199	-1.815721
H	0.463594	3.414810	-3.914907
H	1.212324	5.640201	-3.189477
H	3.102060	5.877048	-1.579248
H	4.233020	3.829913	-0.705458
H	3.483792	1.591710	-1.420641

TS: $Pd(PPh_3)_2 + C_2H_6$ -10589.53

C	0.450743	2.216881	-1.385753
C	-0.521975	2.480962	0.491061
H	0.446360	1.436218	-2.165749
H	-0.204813	3.025930	-1.709936
H	1.457933	2.586666	-1.194148
H	-0.584735	1.936159	1.447835
H	0.164242	3.320177	0.607997
H	-1.507595	2.829280	0.181980
Pd	-0.009021	0.399422	-0.164736
P	2.140138	-0.700826	-0.032137
H	2.642703	1.739317	1.435637
P	-2.090784	-0.802589	0.024403
H	3.136261	-3.571683	-0.322350
H	-0.587913	-2.795265	-1.444820
H	4.623326	-1.416761	1.571539
H	-4.177612	-2.445609	-1.475874
H	-1.413624	-0.496441	2.829044
C	-3.127568	-0.356430	1.512456
C	-4.498566	-0.050821	1.450916
C	-5.202884	0.311214	2.606566
C	-4.551418	0.366266	3.843042
C	-3.185319	0.064071	3.917723
C	-2.479096	-0.283901	2.762262
H	-5.023065	-0.093029	0.499933
H	-6.262505	0.548308	2.536141
H	-5.100062	0.648190	4.739419
H	-2.667240	0.109667	4.873326
C	-3.262146	-0.484285	-1.402170
C	-3.245084	0.791055	-1.999195
C	-4.096993	1.095887	-3.065987
C	-4.972166	0.123925	-3.566488
C	-4.992425	-1.149591	-2.987643
C	-4.147442	-1.450893	-1.912283
H	-2.550812	1.542122	-1.630498
H	-4.069115	2.087503	-3.513067
H	-5.626888	0.355380	-4.404275
H	-5.664710	-1.913842	-3.372000
C	2.488801	-1.770849	1.461487
C	1.409188	-2.439196	2.067463
C	1.606860	-3.246373	3.193695
C	2.887796	-3.388928	3.739724
C	3.969393	-2.726266	3.147566
C	3.772631	-1.925861	2.016551
H	0.410840	-2.326179	1.652461
H	0.759419	-3.757254	3.645203
H	3.041722	-4.007679	4.621691
H	4.968657	-2.828474	3.565808
C	-2.107536	-2.672571	0.091178
C	-2.913488	-3.423160	0.965762
C	-2.849326	-4.822926	0.971584
C	-1.990231	-5.493573	0.094901
C	-1.186767	-4.755973	-0.784689
C	-1.237400	-3.359231	-0.777976
H	-3.594105	-2.919110	1.646934
H	-3.475536	-5.385684	1.660977
H	-1.941009	-6.580598	0.100634
H	-0.509795	-5.265819	-1.466206
C	2.554105	-1.827040	-1.463683
C	2.356331	-1.328241	-2.768176
C	2.590320	-2.130949	-3.887480
C	3.010028	-3.458721	-3.726160
C	3.200354	-3.968065	-2.437859
C	2.979125	-3.158710	-1.315081
H	2.013783	-0.304946	-2.907858
H	2.436103	-1.723777	-4.884520
H	3.182557	-4.088162	-4.596718
H	3.525079	-4.997447	-2.299948
C	3.620313	0.445690	0.003288
C	4.785676	0.261425	-0.761437
C	5.846054	1.174008	-0.680653
C	5.763547	2.279264	0.172269
C	4.608081	2.472959	0.941121
C	3.544316	1.570615	0.849047
H	4.872919	-0.596900	-1.422553
H	6.737696	1.014609	-1.283593
H	6.588314	2.986189	0.235029
H	4.532483	3.331105	1.605769

TS: $Pd[P2P]^{tBu} + C_2H_6$ -7937.26

C	0.295268	1.139397	0.397736
C	0.111482	-0.889896	0.537581
H	0.767442	1.807269	-0.344621
H	-0.660047	1.545875	0.733416
H	0.985781	1.046271	1.238060
H	-0.439616	-1.641884	-0.054689
H	1.101890	-1.258956	0.808698
H	-0.477261	-0.685913	1.433930
Pd	0.087613	-0.003956	-1.545471
P	-1.216388	1.109116	-3.263234
P	1.202235	-1.336557	-3.240582
C	0.617837	-0.523349	-4.871880
C	-0.809558	0.090241	-4.831870
H	1.345458	0.268649	-5.076729
H	0.688391	-1.232850	-5.708051
H	-0.977224	0.687600	-5.738844
H	-1.549600	-0.716345	-4.852204
C	-3.172472	0.871191	-3.178915
C	-0.832927	2.959402	-3.834135
C	0.771886	-3.241886	-3.525066
C	3.153923	-1.103073	-3.402553
C	3.755299	-1.334643	-4.812350
H	4.832422	-1.104845	-4.786386
H	3.650908	-2.368022	-5.153978
H	3.305750	-0.679170	-5.567622
C	3.866283	-2.024735	-2.380640
H	3.436368	-1.920661	-1.376352
H	3.819605	-3.080433	-2.668911
H	4.930207	-1.749605	-2.320042
C	3.438196	0.367016	-2.993016
H	3.022246	1.082178	-3.711888
H	3.019986	0.596829	-2.005716
H	4.526162	0.530901	-2.958956
C	1.556420	-3.968042	-4.642807
H	2.617283	-4.084707	-4.397490
H	1.143216	-4.980267	-4.780566
H	1.480812	-3.452709	-5.608701
C	-0.738952	-3.308500	-3.867976
H	-0.958106	-2.893803	-4.859066
H	-1.063056	-4.360337	-3.874527
H	-1.343829	-2.776916	-3.125019
C	0.978104	-3.986941	-2.179563
H	0.414384	-3.510455	-1.368621
H	0.619590	-5.023432	-2.277483
H	2.029705	-4.029005	-1.879292
C	0.630851	2.970930	-4.345867
H	0.944886	4.010992	-4.522319
H	1.317043	2.534501	-3.611636
H	0.743251	2.431321	-5.293742
C	-0.895940	3.871703	-2.580458
H	-0.556279	4.884282	-2.848337
H	-1.908880	3.960273	-2.175629
H	-0.244599	3.497998	-1.781354
C	-1.739990	3.542316	-4.943008
H	-1.766486	2.907442	-5.837695
H	-2.768574	3.696572	-4.600321
H	-1.351572	4.525838	-5.253079
C	-3.775113	1.921905	-2.212449
H	-3.767878	2.931264	-2.637782
H	-4.824006	1.664396	-2.000754
H	-3.237064	1.945133	-1.256303
C	-3.400057	-0.531826	-2.554890
H	-2.875353	-0.635395	-1.597565
H	-4.476683	-0.682340	-2.381907
H	-3.059620	-1.336566	-3.216526
C	-3.926217	0.923838	-4.532418
H	-4.992674	0.708639	-4.359100
H	-3.865779	1.903469	-5.014256
H	-3.558600	0.172411	-5.241197

TS: $Pd[P3P]^{tBu} + C_2H_6$ -8297.12

C	0.964992	1.331465	-2.505442
C	0.663008	-0.705505	-2.378309
H	1.568187	1.973567	-3.170183
H	-0.009945	1.777975	-2.304991
H	1.522824	1.204318	-1.575686
H	0.197090	-1.461957	-3.033173
H	1.580074	-1.090010	-1.929445
H	-0.061319	-0.452270	-1.601691
Pd	0.992670	0.160290	-4.443032
P	2.500534	-1.300348	-5.674359
P	-0.167417	1.338378	-6.227484
C	1.997232	0.426112	-8.021760
C	2.415554	-0.996617	-7.555741
C	0.481444	0.766730	-7.927914
H	-0.095707	-0.127787	-8.195894
H	2.282581	0.510972	-9.082339
H	1.692881	-1.719158	-7.956798
H	0.236270	1.524319	-8.684332
H	2.586288	1.180802	-7.493307
H	3.383590	-1.251353	-8.008772
H	5.381829	-2.900449	-5.536844
H	2.142379	3.098987	-5.916128
H	2.640806	-3.738000	-7.762798
H	-2.443387	1.423272	-4.322354
C	-2.066902	0.836339	-6.412474
C	-2.711999	1.107665	-7.795682
H	-3.743566	0.721247	-7.791802
H	-2.764552	2.172881	-8.037226
H	-2.182188	0.599560	-8.609972
C	-2.119293	-0.692437	-6.147813
H	-1.566106	-1.263608	-6.902950
H	-3.166165	-1.031529	-6.179338
H	-1.702215	-0.941204	-5.165363
C	-2.902649	1.537758	-5.312506
H	-3.035198	2.606927	-5.511960
H	-3.906069	1.086825	-5.271981
C	2.196955	-3.251405	-5.649488
C	2.585195	-3.818452	-4.260945
H	2.217826	-4.852491	-4.171325
H	3.670807	-3.846007	-4.115631
H	2.142527	-3.235288	-3.444307
C	0.664219	-3.426196	-5.828324
H	0.102445	-2.896567	-5.052175
H	0.410059	-4.495621	-5.770248
H	0.316455	-3.060232	-6.802197
C	2.905659	-4.076377	-6.754156
H	3.995268	-4.055556	-6.664423
H	2.590265	-5.129006	-6.674102
C	-0.007248	3.304070	-6.377055
C	-0.842903	3.982856	-7.487786
H	-0.559975	5.045435	-7.558310
H	-0.674165	3.537399	-8.476333
H	-1.916670	3.949919	-7.274185
C	-0.376169	3.935259	-5.008852
H	-1.434896	3.810286	-4.761260
H	-0.170070	5.016562	-5.041323
H	0.215149	3.505452	-4.193376
C	1.493176	3.603674	-6.641868
H	1.804087	3.306746	-7.650053
H	1.666053	4.686877	-6.551170
C	4.400933	-0.939787	-5.281492
C	4.689747	0.509258	-5.758554
H	5.687435	0.811999	-5.406030
H	4.689470	0.594936	-6.851378
H	3.959186	1.219337	-5.352176
C	4.595766	-0.972381	-3.742416
H	3.891277	-0.297378	-3.242044
H	5.618355	-0.645735	-3.497460
H	4.460695	-1.975157	-3.323717
C	5.427201	-1.886127	-5.947581
H	5.298317	-1.948314	-7.035708
H	6.445087	-1.507356	-5.762897

TS: Pd[P4P]^{tBu} + C_2H_6 -8654.57

C	0.573970	1.634610	-0.174253
C	0.133108	-0.408013	0.205754
H	0.926723	2.255400	-1.015655
H	-0.292102	2.089339	0.306198
H	1.388908	1.518128	0.542024
H	-0.355783	-1.252017	-0.310355
H	1.089711	-0.714267	0.628582
H	-0.531196	-0.044528	0.991470
Pd	0.160594	0.296237	-1.913059
P	-1.832924	1.132381	-3.177930
P	1.893518	-0.959446	-3.210526
C	-1.835164	0.758450	-5.059276
C	-0.416079	0.447031	-5.593891
H	0.306332	1.098173	-5.087972
H	-0.359174	0.695653	-6.664671
H	-2.492035	-0.099550	-5.243583
H	-2.276004	1.604309	-5.598738
C	1.515227	-1.202174	-5.075367
H	1.869545	-2.188941	-5.394058
H	2.094821	-0.468164	-5.647127
C	0.009532	-1.031643	-5.392497
H	-0.248078	-1.606787	-6.294966
H	-0.578283	-1.463506	-4.574102
H	0.068511	3.309425	-3.530295
H	-2.964143	0.556337	-0.504568
H	5.041633	-1.494235	-4.021178
H	3.260711	-3.492965	-4.548785
C	2.217290	-2.842059	-2.699109
C	2.506935	-2.932254	-1.179574
H	2.558376	-3.991721	-0.883239
H	3.462798	-2.470860	-0.909821
H	1.719251	-2.457213	-0.588001
C	0.873975	-3.575553	-2.970522
H	0.033219	-3.075607	-2.474800
H	0.936716	-4.601628	-2.577703
H	0.646216	-3.648628	-4.040461
C	3.345580	-3.581233	-3.458919
H	4.338316	-3.225844	-3.163260
H	3.301672	-4.654804	-3.215924
C	3.597658	0.020747	-3.302713
C	3.213557	1.465447	-3.727711
H	4.115943	2.095601	-3.729603
H	2.786423	1.501703	-4.737622
H	2.486522	1.906074	-3.036143
C	4.234204	0.089351	-1.891349
H	3.504359	0.402832	-1.134662
H	5.055726	0.822150	-1.893828
H	4.658371	-0.873345	-1.584523
C	4.645626	-0.516483	-4.309813
H	4.246675	-0.598028	-5.327976
H	5.496701	0.181764	-4.350651
C	-3.490350	0.230082	-2.619324
C	-4.730799	0.453112	-3.520787
H	-5.551823	-0.191824	-3.169339
H	-5.092202	1.484852	-3.489052
H	-4.541243	0.191057	-4.568605
C	-3.150803	-1.286487	-2.628749
H	-2.926147	-1.655756	-3.637153
H	-4.016396	-1.854872	-2.255787
H	-2.290332	-1.507912	-1.987230
C	-3.837237	0.635073	-1.164120
H	-4.225023	1.658210	-1.103612
H	-4.618940	-0.034000	-0.772742
C	-2.108969	3.089642	-3.237543
C	-3.387041	3.586522	-3.956244
H	-3.329597	4.679506	-4.081159
H	-3.515421	3.153424	-4.955606
H	-4.290781	3.377363	-3.374167
C	-2.097829	3.666051	-1.799259
H	-2.966836	3.345025	-1.215239
H	-2.124284	4.765889	-1.850054
H	-1.194502	3.377918	-1.254156
C	-0.868170	3.654035	-3.984667
H	-0.856629	3.376398	-5.045208
H	-0.884633	4.753214	-3.933536

TS: Pd(P(*t*-Bu)$_3$)$_2$ + C_2H_6 -10240.51

C	0.216900	0.205600	-0.024300
C	-1.062200	-1.391500	-0.587300
H	0.587900	1.146600	-0.467000
H	-0.516000	0.449000	0.746800
H	1.034800	-0.371700	0.404400
H	-1.267400	-2.002200	-1.484500
H	-0.540000	-2.006100	0.147700
H	-1.990200	-1.013700	-0.159800
Pd	-0.137200	-0.153400	-2.202100
P	-2.110500	1.226300	-3.268400
P	2.129100	-1.026800	-3.128700
H	-2.056400	1.442900	-6.503800
H	-0.753300	4.851000	-3.008400
H	-2.719100	3.290600	-5.777900
H	-0.610800	3.435700	-1.950700
H	-2.140000	4.795300	-5.061700
H	-3.537000	3.969600	-4.360200
H	4.316700	-1.773800	-5.484000
C	-1.269100	3.940200	-2.668100
H	-2.175100	4.259000	-2.145700
C	-0.223300	2.896900	-4.658600
H	-0.326700	2.374100	-5.611700
H	0.181000	3.898100	-4.874700
H	0.507100	2.358000	-4.050200
H	-2.234600	1.198300	-0.274500
H	5.383700	-0.901000	-3.404400
H	4.488300	-3.245300	-3.512200
C	2.696700	-2.763300	-2.288000
C	2.396500	-2.694600	-0.765800
H	2.635600	-3.672300	-0.318700
H	2.989700	-1.943000	-0.241000
H	1.340400	-2.489400	-0.581200
C	1.802800	-3.904800	-2.844000
H	0.738000	-3.645300	-2.808500
H	1.946600	-4.799200	-2.218700
H	2.061100	-4.184900	-3.869000
C	4.182000	-3.175400	-2.465300
H	4.867300	-2.492600	-1.953100
H	4.326900	-4.170400	-2.014200
C	3.615400	0.270100	-2.757800
C	3.064300	1.693700	-3.043300
H	3.819600	2.436000	-2.741500
H	2.843100	1.862000	-4.099700
H	2.151000	1.885800	-2.469700
C	3.969100	0.242900	-1.246600
H	3.081900	0.349000	-0.613600
H	4.632400	1.094400	-1.029800
H	4.504600	-0.663900	-0.952500
C	4.927900	0.081000	-3.561000
H	4.787200	0.225700	-4.636500
H	5.657400	0.837500	-3.229200
C	-3.608400	1.542600	-1.961300
C	-4.655300	2.627400	-2.327700
H	-5.440300	2.632100	-1.554100
H	-4.224200	3.633200	-2.346400
H	-5.146400	2.446000	-3.287700
C	-4.363900	0.204800	-1.729700
H	-4.998300	-0.075100	-2.575300
H	-5.024000	0.322700	-0.856600
H	-3.682500	-0.624700	-1.517800
C	-2.977400	1.930800	-0.595200
H	-2.499000	2.912700	-0.608200
H	-3.775100	1.965300	0.163400
C	-1.569400	3.049400	-3.903500
C	-2.561400	3.804900	-4.824700
C	-2.962300	0.306700	-4.833200
C	-3.024500	-1.206900	-4.480700
H	-3.329600	-1.771100	-5.375700
H	-2.046700	-1.581900	-4.159100
H	-3.745100	-1.429300	-3.690000
C	-4.376900	0.774100	-5.263400
H	-5.135300	0.592200	-4.496900
H	-4.680600	0.203000	-6.155600
H	-4.407100	1.834800	-5.531500
C	-2.031500	0.440400	-6.066800
H	-0.994800	0.188900	-5.829300
H	-2.372600	-0.260500	-6.843800
C	2.165100	-1.379000	-5.108300
C	0.834200	-2.099200	-5.457800
H	0.691200	-2.084200	-6.549200
H	0.819900	-3.144200	-5.140900
H	-0.019000	-1.594300	-4.995900
C	2.135200	-0.013700	-5.843400
H	1.348500	0.638300	-5.453300
H	1.925800	-0.189200	-6.909700
H	3.088500	0.519500	-5.785900
C	3.335900	-2.213600	-5.687200
H	3.337700	-3.243900	-5.318800
H	3.222800	-2.267400	-6.782200

TS: Pd[P2P]^{Cl} + C_2H_6 -2081.23

Pd	0.000000	0.000000	-0.059572
C	-0.766173	0.743877	1.925650
C	0.766173	-0.743877	1.925650
H	-1.004659	1.609548	1.287475
H	1.004659	-1.609548	1.287475
H	-1.664583	0.191349	2.197933
H	1.664583	-0.191349	2.197933
H	-0.232115	1.102426	2.802152
H	0.232115	-1.102426	2.802152
C	-0.657743	0.404161	-3.369906
C	0.657743	-0.404161	-3.369906
P	-1.592235	0.129964	-1.754835
P	1.592235	-0.129964	-1.754835
H	0.453990	-1.482321	-3.408791
H	-0.453990	1.482321	-3.408791
H	1.291685	-0.143127	-4.223966
H	-1.291685	0.143127	-4.223966
Cl	3.159921	-1.559381	-2.077418
Cl	-3.159921	1.559381	-2.077418
Cl	2.558387	1.709694	-2.239968
Cl	-2.558387	-1.709694	-2.239968

TS: Pd[P3P]^{Cl} + C_2H_6 -2444.90

Pd	2.281991	0.003942	0.005725
C	0.096920	-0.254511	-0.439073
C	1.272432	-2.015041	-0.173022
H	0.096275	0.747114	0.023264
H	-0.065687	-0.198103	-1.514576
H	-0.664597	-0.855729	0.052160
H	2.306726	-2.313499	-0.397246
H	0.966724	-2.362530	0.813181
H	0.625549	-2.403906	-0.956204
P	4.157668	-0.217175	1.344411
P	3.085099	1.783990	-1.255969
C	5.749208	1.693254	-0.136151
C	5.776633	0.303968	0.550937
C	4.951052	1.790484	-1.462345
Cl	2.584252	1.983753	-3.342227
H	5.174038	0.936175	-2.117491
H	6.791215	1.949747	-0.372925
H	6.004598	-0.486451	-0.178792
Cl	4.838761	-2.121516	2.095474
Cl	2.829355	3.799709	-0.571603
H	5.219217	2.703481	-2.004239
H	5.406221	2.460287	0.570834
H	6.551416	0.274178	1.324600
Cl	4.239984	0.986493	3.098825

TS: Pd[P4P]^{Cl} + C_2H_6 -2801.65

C	0.816275	0.339091	-0.632994
C	-1.280231	-0.090040	-0.827928
H	1.617732	0.013926	0.050538
H	1.161904	0.378628	-1.664910
H	0.443324	1.302554	-0.293217
H	-1.882889	-0.962394	-1.123522
H	-1.715000	0.418939	0.031376
H	-1.189048	0.571295	-1.686755
Pd	0.100984	-1.726647	-0.127195
P	1.727229	-3.163557	-0.992744
P	-1.118302	-3.008482	1.387077
Cl	-0.039772	-3.651948	3.105442
Cl	-2.896851	-2.243688	2.343979
Cl	2.776675	-2.676918	-2.811076
Cl	3.369253	-3.624059	0.296234
C	1.243492	-4.921604	-1.466076
C	0.315464	-5.587696	-0.419453
H	0.707055	-5.402174	0.589212
H	0.380530	-6.674215	-0.560859
H	0.745909	-4.846338	-2.442173
H	2.171908	-5.484631	-1.607387
C	-1.841046	-4.654237	0.783842
H	-2.905179	-4.456192	0.610612
H	-1.764774	-5.388451	1.593651
C	-1.178320	-5.143169	-0.524858
H	-1.779857	-5.980356	-0.904088
H	-1.272275	-4.347011	-1.276198

TS: Pd(PCl_3)$_2$ + C_2H_6 -1475.95

Pd	0.000000	0.000000	-1.913038
C	-0.003053	1.078643	0.038435
C	0.003053	-1.078643	0.038435
H	0.404472	1.868253	-0.614404
H	-1.020967	1.304795	0.351156
H	0.665397	0.946950	0.885799
H	-0.404472	-1.868253	-0.614404
H	1.020967	-1.304795	0.351156
H	-0.665397	-0.946950	0.885799
P	-1.581898	1.097094	-3.245808
P	1.581898	-1.097094	-3.245808
Cl	2.707970	-2.692198	-2.388722
Cl	-1.039998	1.996301	-5.085978
Cl	1.039998	-1.996301	-5.085978
Cl	3.138921	0.180827	-3.872105
Cl	-3.138921	-0.180827	-3.872105
Cl	-2.707970	2.692198	-2.388722

TS: Pd(PH_3)$_2$$Cl^-$ + C_2H_6 -1694.90

Pd	0.000000	0.000000	1.629758
C	-0.059103	1.016020	3.653554
C	0.059103	-1.016020	3.653554
H	0.333510	1.795414	2.975186
H	-1.082169	1.246041	3.959097
H	0.598207	0.976707	4.525951
H	-0.333510	-1.795414	2.975186
H	1.082169	-1.246041	3.959097
H	-0.598207	-0.976707	4.525951
P	-1.472091	1.106598	0.076476
P	1.472091	-1.106598	0.076476
H	1.814925	-2.503688	0.068200
H	-1.151371	0.987528	-1.324650
H	1.151371	-0.987528	-1.324650
H	2.834604	-0.676016	-0.034006
H	-2.834604	0.676016	-0.034006
H	-1.814925	2.503688	0.068200
Cl	0.000000	0.000000	-3.299386

TS: Pd(PH_3)$_2$$Br^-$ + C_2H_6 -1688.03

Pd	0.000000	0.000000	1.683691
C	-0.047424	1.019177	3.704471
C	0.047424	-1.019177	3.704471
H	0.351561	1.796395	3.027634
H	-1.067736	1.257767	4.012050
H	0.610876	0.969788	4.575225
H	-0.351561	-1.796395	3.027634
H	1.067736	-1.257767	4.012050
H	-0.610876	-0.969788	4.575225
P	-1.487259	1.117327	0.160965
P	1.487259	-1.117327	0.160965
H	1.878316	-2.501005	0.203145
H	-1.182918	1.068674	-1.243349
H	1.182918	-1.068674	-1.243349
H	2.832787	-0.642894	0.034602
H	-2.832787	0.642894	0.034602
H	-1.878316	2.501005	0.203145
Br	0.000000	0.000000	-3.464792

TS: $Pd(PH_3)_2I^-$ + C_2H_6 -1680.02

Pd	0.000000	0.000000	1.827237
C	-0.027548	1.023481	3.842985
C	0.027548	-1.023481	3.842985
H	0.382335	1.796307	3.167986
H	-1.042938	1.277089	4.153996
H	0.632296	0.958110	4.711009
H	-0.382335	-1.796307	3.167986
H	1.042938	-1.277089	4.153996
H	-0.632296	-0.958110	4.711009
P	-1.507472	1.130134	0.344939
P	1.507472	-1.130134	0.344939
H	2.015357	-2.468090	0.492525
H	-1.200203	1.233735	-1.050584
H	1.200203	-1.233735	-1.050584
H	2.802699	-0.555568	0.147613
H	-2.802699	0.555568	0.147613
H	-2.015357	2.468090	0.492525
I	0.000000	0.000000	-3.654133

TS: $Pd[P2P]Cl^-$ + C_2H_6 -2252.26

Pd	1.984859	1.025483	-0.011539
C	0.002274	-0.054550	-0.116013
C	-0.085963	1.954281	0.134252
H	0.710005	-0.714259	-0.652695
H	0.562251	2.672087	0.666679
H	-0.275068	-0.484104	0.848956
H	-0.396672	2.356825	-0.831623
H	-0.879801	0.059467	-0.749822
H	-0.955728	1.761821	0.767234
C	5.372398	0.492789	0.288727
C	5.307340	1.981223	-0.110332
P	3.770014	-0.098339	1.122548
P	3.701955	2.358919	-1.042842
H	5.349134	2.627571	0.778082
H	5.498314	-0.109383	-0.621843
H	6.133728	2.210980	-0.796362
H	6.233941	0.298577	0.938679
H	3.811419	3.788087	-1.070674
H	4.199720	-1.452524	1.389793
H	4.231999	2.125188	-2.359606
H	4.057444	0.336668	2.462300
Cl	6.519023	1.586234	-3.437604

TS: Pd[C2C] + C_2H_6 -3192.47

C	0.000000	-0.000000	0.000000
C	0.000000	1.980410	0.000000
H	0.680282	-0.725614	-0.487442
H	-0.264522	-0.330988	1.006450
H	-0.891085	0.051246	-0.629084
H	0.680282	2.706025	0.487442
H	-0.264522	2.311399	-1.006450
H	-0.891085	1.929164	0.629084
H	3.418291	4.352939	-0.479570
C	5.941731	2.566983	0.264873
C	5.941731	-0.586573	-0.264873
H	3.418291	-2.372528	0.479570
C	3.718041	-0.300365	0.421173
Pd	2.029660	0.990205	0.000000
N	4.929564	0.306183	0.099677
C	5.394168	-1.825247	-0.123954
H	5.837150	-2.800648	-0.264177
N	4.071766	-1.628941	0.277670
C	3.718041	2.280775	-0.421173
H	6.925588	-0.276526	-0.581196
C	5.394168	3.805658	0.123954
H	5.837150	4.781058	0.264177
N	4.071766	3.609352	-0.277670
N	4.929564	1.674227	-0.099677
H	6.925588	2.256937	0.581196

TS: Pd[C3C] + C_2H_6 -3579.24

C	-0.000000	1.979389	0.000000
C	-0.000000	0.000000	0.000000
H	0.653761	2.705924	0.522742
H	-0.236723	2.322692	-1.010396
H	-0.918946	1.916008	0.588930
H	0.700490	-0.743427	-0.424076
H	-0.319350	-0.303659	0.999356
H	-0.859903	0.043312	-0.672527
H	6.197501	0.213390	-1.196417
C	5.652561	2.773877	-1.653763
C	5.954167	0.073459	1.466855
H	3.210492	-0.110823	3.054816
C	3.667549	0.026802	1.018314
Pd	2.050246	1.002855	0.000000
N	4.954993	0.068056	0.482090
C	5.315312	-0.020346	2.663117
H	5.710095	-0.076121	3.666862
N	3.948960	-0.057569	2.367707
C	3.481657	2.201254	-1.070310
H	7.009636	0.115133	1.238460
C	4.902371	3.905129	-1.753416
H	5.178461	4.909728	-2.038711
N	3.603374	3.531859	-1.398368
N	4.778937	1.755973	-1.253708
H	6.704438	2.612726	-1.842061
H	2.811034	4.159021	-1.370169
C	5.150070	0.369967	-0.928735
H	4.508637	-0.296154	-1.508213

TS: Pd[C4C] + C_2H_6 -3082.33

C	0.000000	0.000000	0.000000
C	0.000000	1.975858	0.000000
H	0.667512	-0.721485	0.509872
H	-0.259398	-0.340024	-1.006798
H	-0.904356	0.052284	0.613010
H	0.667512	2.697343	-0.509872
H	-0.259398	2.315881	1.006798
H	-0.904356	1.923574	-0.613010
H	6.569259	1.441507	1.061656
C	5.282537	-1.696176	-1.312263
C	5.282537	3.672034	1.312263
H	2.148619	4.126461	1.143047
C	3.362682	2.444059	0.880780
Pd	2.074240	0.987929	0.000000
N	4.743498	2.415985	1.000431
C	4.232547	4.532974	1.406940
H	4.205126	5.587954	1.636207
N	3.095440	3.770286	1.145978
C	3.362682	-0.468202	-0.880780
H	6.341495	3.842278	1.443192
C	4.232547	-2.557117	-1.406940
H	4.205126	-3.612096	-1.636207
N	3.095440	-1.794428	-1.145978
N	4.743498	-0.440128	-1.000431
H	6.341495	-1.866420	-1.443192
H	2.148619	-2.150603	-1.143047
C	5.545577	0.760796	-0.746384
H	5.166233	1.575865	-1.368493
H	6.569259	0.534350	-1.061656
C	5.545577	1.215062	0.746384
H	5.166233	0.399993	1.368493

TS: Pd[C5C] + C_2H_6 -4306.49

C	-0.000000	2.003402	0.000000
C	-0.000000	-0.000000	0.000000
H	0.678810	2.753469	-0.442601
H	-0.300292	2.305026	1.005529
H	-0.873306	1.935942	-0.652853
H	0.656687	-0.746217	0.487941
H	-0.264922	-0.319687	-1.010061
H	-0.898624	0.075116	0.617501
C	3.409134	-0.258568	-1.065519
H	3.443330	1.762981	-2.697537
C	5.317184	2.550580	-1.899987
C	4.482860	1.436942	-2.585634
C	4.625881	3.359506	-0.771423
Pd	2.053862	0.987685	0.000000
C	5.025616	-1.913092	-1.296937
C	5.690010	2.828398	1.462513
H	5.131909	4.329595	-0.681224
H	6.271268	2.140837	-1.541159
H	4.895289	1.262311	-3.587736
H	3.580419	3.546063	-1.035611
H	5.567573	3.276440	-2.688169
C	5.307465	2.170098	2.589306
H	5.827423	2.009412	3.521952
N	4.013298	1.712086	2.340318
N	4.618183	2.748894	0.561865
H	6.610087	3.348416	1.237159
H	3.450380	1.180680	2.988169
C	3.542312	2.037070	1.079609
C	5.423002	-0.850779	-2.047785
H	6.298704	-0.724588	-2.668397
N	4.441534	0.139058	-1.903430
H	3.262769	-2.111052	-0.099243
H	5.486290	-2.877132	-1.139611
N	3.812480	-1.534752	-0.720510

TS: $Pd(NHC)_2$ + C_2H_6 -3401.93

C	-0.000000	-0.000000	0.000000
C	-0.000000	2.057502	0.000000
H	0.657958	-0.763505	0.453711
H	-0.296983	-0.286078	-1.011023
H	-0.876961	0.094565	0.645082
H	0.657958	2.821007	-0.453711
H	-0.296983	2.343580	1.011023
H	-0.876961	1.962937	-0.645082
H	2.578603	-2.183696	-0.773878
C	4.261190	-0.989843	-3.187517
C	4.261190	3.047346	3.187517
H	2.578603	4.241198	0.773878
C	3.005116	2.280320	1.384358
PD	2.042115	1.028751	0.000000
N	3.767348	1.943270	2.488638
C	3.810366	4.145121	2.522804
H	3.959376	5.196484	2.717038
N	3.060372	3.661472	1.446434
C	3.005116	-0.222818	-1.384358
H	4.874502	2.963175	4.071891
C	3.810366	-2.087618	-2.522804
H	3.959376	-3.138981	-2.717038
N	3.060372	-1.603969	-1.446434
N	3.767348	0.114232	-2.488638
H	4.874502	-0.905673	-4.071891
H	3.943085	0.978482	2.728992
H	3.943085	1.079020	-2.728992

RC: Pd + CH_3Cl -504.14

C	-0.042900	-0.019900	0.000000
Cl	1.818800	-0.022400	0.000000
H	-0.363500	0.499400	-0.902100
H	-0.350200	-1.066800	0.000000
H	-0.363500	0.499400	0.902100
Pd	2.766400	2.111400	0.000000

TS: Pd + CH_3Cl -491.84

Pd	-0.028000	-0.023200	0.000000
Cl	2.336700	0.003300	0.000000
C	1.584600	1.914800	0.000000
H	2.046100	2.278100	-0.912100
H	0.493200	2.067900	0.000000
H	2.046100	2.278100	0.912100

P: Pd + CH_3Cl -524.32

C	-0.052800	-0.012200	0.000000
Cl	3.168500	0.004400	0.000000
H	0.020500	0.592200	0.906500
H	0.020500	0.592200	-0.906500
H	-0.938400	-0.669200	0.000000
Pd	1.400100	-1.396400	0.000000

RC: Pd[P2P] + CH_3Cl -1795.46

C	-0.862295	-0.892740	-0.571726
Pd	2.767018	-0.005029	0.041648
Cl	0.703211	-1.475026	0.236620
H	-1.149790	0.036897	-0.081317
H	-0.641254	-0.737737	-1.627343
H	-1.609580	-1.674228	-0.425276
C	5.149590	2.268247	-0.049167
C	5.908996	0.973426	0.321836
P	3.523316	1.911407	-0.978062
P	4.770256	-0.327714	1.124020
H	6.310226	0.499489	-0.584467
H	6.756298	1.197593	0.980284
H	5.788487	2.935270	-0.639627
H	4.857817	2.809036	0.861655
H	5.739492	-1.385004	1.192198
H	4.941168	0.051336	2.495904
H	4.044254	1.875745	-2.313617
H	3.088190	3.277353	-1.079858

TS: Pd[P2P] + CH_3Cl -1774.75

C	-0.078172	-0.061306	-0.668911
Pd	2.392452	-0.082484	0.055010
Cl	0.773707	-1.967470	0.044610
H	0.219770	0.883107	-0.209306
H	0.040685	-0.105386	-1.745897
H	-1.037108	-0.409402	-0.305251
C	4.912692	2.157047	0.158696
C	5.433151	1.031947	1.081534
P	3.606225	1.518801	-1.064130
P	4.015443	0.006761	1.829772
H	6.045310	0.323459	0.507095
H	6.064988	1.446466	1.874405
H	5.740359	2.633379	-0.378671
H	4.413367	2.933341	0.754321
H	4.838300	-0.924104	2.551524
H	3.748213	0.821657	2.978063
H	4.469925	1.140668	-2.141101
H	3.245461	2.782621	-1.636786

P: Pd[P2P] + CH_3Cl -1816.16

C	0.496106	0.495798	-0.904045
Pd	2.394911	0.038822	-0.067223
Cl	1.561277	-2.104214	0.574871
H	-0.142918	0.745780	-0.051400
H	0.502198	1.312423	-1.632182
H	0.170823	-0.437422	-1.367497
C	4.856544	2.368093	0.170158
C	5.671325	1.055399	0.272903
P	3.188496	2.053246	-0.655202
P	4.557753	-0.360028	0.852567
H	6.046188	0.762564	-0.716468
H	6.536935	1.180813	0.931792
H	5.412212	3.144420	-0.367764
H	4.628154	2.755478	1.171749
H	5.374918	-1.493083	0.581609
H	4.761025	-0.332352	2.263214
H	3.470788	2.319145	-2.026961
H	2.493256	3.264542	-0.382295

RC: Pd[P3P] + CH_3Cl -2158.65

C	-0.918010	-1.161626	-0.568974
Pd	2.735340	0.027852	0.004138
Cl	0.654896	-1.541243	0.325028
H	-1.334045	-0.258047	-0.123267
H	-0.666855	-1.009337	-1.618426
H	-1.583224	-2.016000	-0.434772
P	4.584700	-0.354254	1.292170
P	3.189391	1.844092	-1.301687
C	5.714499	2.068578	0.133455
C	6.056014	0.629608	0.610943
C	5.052312	2.199361	-1.266674
H	2.998823	2.088860	-2.706939
H	5.517978	1.491177	-1.966397
H	6.657686	2.632486	0.101125
H	6.460527	0.045653	-0.227654
H	5.312852	-1.554397	1.605140
H	2.733229	3.149079	-0.919414
H	5.225533	3.207013	-1.663590
H	5.091922	2.573119	0.888249
H	6.836485	0.672901	1.380336
H	4.625465	0.133242	2.639746

TS: Pd[P3P] + CH_3Cl -2136.85

C	0.000199	-0.002246	-0.004085
Pd	2.541057	0.000707	0.000809
Cl	1.004738	-1.978175	-0.000465
H	0.423662	0.855458	0.526384
H	-0.228075	0.168883	-1.050305
H	-0.795321	-0.474076	0.559339
P	4.464245	-0.248635	1.371764
P	3.172122	1.806594	-1.290901
C	5.714938	2.042862	0.092638
C	5.990028	0.629370	0.672725
C	5.040620	2.092700	-1.305323
H	2.946247	1.993111	-2.697680
H	5.470286	1.318184	-1.955631
H	6.683519	2.555331	0.007464
H	6.393369	-0.023167	-0.114234
H	5.129982	-1.439772	1.821200
H	2.764490	3.137530	-0.946779
H	5.241992	3.060398	-1.779462
H	5.128553	2.634780	0.812098
H	6.751857	0.695934	1.457788
H	4.457676	0.364069	2.666551

P: Pd[P3P] + CH_3Cl -2180.38

C	0.476371	0.463135	-0.973146
Pd	2.377242	0.022032	-0.131023
Cl	1.463611	-1.997452	0.787341
H	0.282830	-0.356125	-1.671575
H	-0.219125	0.416426	-0.131215
H	0.392476	1.427229	-1.486187
P	4.415535	-0.578754	0.921365
P	3.120846	1.950229	-0.991440
C	5.697078	1.936921	0.340247
C	5.964461	0.419999	0.540752
C	4.961730	2.314080	-0.975033
H	2.805006	2.278475	-2.339926
H	5.400394	1.766707	-1.820671
H	6.667922	2.450292	0.334006
H	6.399518	-0.003776	-0.374925
H	4.902826	-1.905696	0.779966
H	2.605420	3.139460	-0.399109
H	5.089437	3.383702	-1.180674
H	5.149832	2.340824	1.205407
H	6.695907	0.273031	1.343454
H	4.405523	-0.537541	2.343481

RC: Pd[P4P] + CH_3Cl -2519.92

C	3.156585	0.690713	-1.533498
Cl	2.269933	0.760971	0.076666
H	3.210719	-0.356626	-1.831213
H	2.581557	1.276507	-2.250682
H	4.151099	1.112168	-1.380159
Pd	-0.347399	0.047675	0.109583
P	-1.229072	-0.085112	2.222718
P	-1.667076	-0.502481	-1.686540
H	-2.717315	0.426924	-1.968797
H	-1.401035	-0.736183	-3.082097
H	-0.612227	-0.306326	3.502041
H	-1.949182	1.069397	2.667260
C	-2.628573	-1.361232	2.413979
C	-3.399735	-1.589341	1.088550
H	-3.588227	-0.614617	0.616613
H	-4.389568	-2.007262	1.320147
H	-2.167640	-2.299101	2.751374
H	-3.301541	-1.024831	3.211162
C	-2.691494	-2.084288	-1.389016
H	-2.240386	-2.862818	-2.017298
H	-3.717032	-1.932555	-1.747808
C	-2.662259	-2.531634	0.090446
H	-3.090400	-3.542091	0.165038
H	-1.608139	-2.615643	0.388142

TS: Pd[P4P] + CH_3Cl -2496.82

C	2.109100	-0.354500	-1.109400
CL	1.924600	1.443900	0.191000
H	1.564200	-1.287300	-0.927100
H	1.981300	0.068200	-2.099800
H	3.136100	-0.412100	-0.770500
PD	-0.099200	-0.015700	0.012200
P	-1.084900	-0.239500	2.177600
P	-1.650800	-0.502500	-1.660500
H	-2.625300	0.524900	-1.849300
H	-1.441200	-0.697600	-3.068900
H	-0.404500	-0.567300	3.396300
H	-1.634100	0.976600	2.691600
C	-2.616500	-1.341400	2.413900
C	-3.430700	-1.475000	1.101800
H	-3.534200	-0.480300	0.644500
H	-4.452500	-1.796500	1.345700
H	-2.266000	-2.328100	2.743700
H	-3.230800	-0.928300	3.221300
C	-2.799700	-1.998600	-1.388500
H	-2.416500	-2.800900	-2.032200
H	-3.810900	-1.758100	-1.739200
C	-2.802200	-2.471500	0.082200
H	-3.329300	-3.434200	0.146400
H	-1.760300	-2.670000	0.368700

P: Pd[P4P] + CH_3Cl -2538.81

C	1.271164	0.051554	-1.916301
Cl	1.833529	0.957553	1.073368
H	1.432102	-0.978653	-2.254060
H	0.812250	0.645325	-2.714614
H	2.205756	0.503409	-1.583001
Pd	0.026771	0.026669	-0.198531
P	-1.205725	0.184155	1.876839
P	-1.620198	-0.733266	-1.548147
H	-2.681672	0.189959	-1.778748
H	-1.326488	-0.987845	-2.917054
H	-0.408849	0.216037	3.049444
H	-1.828266	1.454096	2.049531
C	-2.618323	-0.947744	2.426950
C	-3.435767	-1.507822	1.236056
H	-3.759702	-0.675394	0.593704
H	-4.360863	-1.949294	1.628942
H	-2.164454	-1.774498	2.989074
H	-3.261232	-0.396909	3.122991
C	-2.576494	-2.301652	-1.120772
H	-2.040819	-3.124098	-1.612016
H	-3.570643	-2.238002	-1.581730
C	-2.666462	-2.577459	0.396758
H	-3.141329	-3.557890	0.534781
H	-1.642806	-2.678582	0.782035

RC: Pd[P5P] + CH_3Cl -2884.10

C	3.570313	0.323940	0.248656
Cl	4.302062	1.999097	0.267854
H	2.480648	0.422389	0.189826
H	3.961041	-0.199966	-0.624479
H	3.865907	-0.179188	1.170065
Pd	-0.197860	-0.113468	0.047671
P	-1.056946	0.037541	2.173250
P	-0.542583	-0.852256	-2.098691
H	-1.129163	0.047877	-3.041018
H	0.429530	-1.363744	-3.017293
H	-1.802190	1.205608	2.522842
H	-0.343315	-0.020939	3.412932
C	-2.373378	-1.276352	2.554625
C	-3.286979	-1.586261	1.338180
H	-1.835478	-2.181301	2.867358
H	-2.962018	-0.932871	3.413056
H	-4.190641	-2.096140	1.700590
H	-3.629309	-0.637678	0.900836
C	-1.802059	-2.267724	-2.220878
C	-2.586173	-2.442414	0.246250
H	-1.252778	-3.197807	-2.022647
H	-2.164542	-2.315930	-3.254161
H	-2.759850	-3.510021	0.445545
H	-1.502762	-2.279463	0.342515
C	-2.979977	-2.114317	-1.221216
H	-3.803866	-2.763609	-1.549149
H	-3.363183	-1.085729	-1.279678

TS: Pd[P5P] + CH_3Cl -2858.08

C	2.770400	-0.524300	0.081400
CL	2.248000	1.655800	0.257200
H	2.118900	-1.393900	0.246000
H	3.204200	-0.465900	-0.910200
H	3.471900	-0.372300	0.892600
PD	0.398800	-0.015500	0.063800
P	-0.853000	0.067900	2.113300
P	-0.314400	-0.858700	-2.018400
H	-0.828000	0.137200	-2.906500
H	0.563600	-1.436000	-2.995600
H	-1.572700	1.278400	2.364400
H	-0.195800	0.070400	3.386000
C	-2.245800	-1.149600	2.555600
C	-3.199800	-1.404100	1.361200
H	-1.766700	-2.088300	2.865700
H	-2.792600	-0.760000	3.421700
H	-4.115900	-1.883500	1.733000
H	-3.516100	-0.435200	0.947900
C	-1.734300	-2.112600	-2.205800
C	-2.553300	-2.265400	0.239400
H	-1.313700	-3.111700	-2.027600
H	-2.087200	-2.086800	-3.242800
H	-2.828900	-3.321100	0.375800
H	-1.464600	-2.213400	0.360100
C	-2.887600	-1.827200	-1.211500
H	-3.801100	-2.327900	-1.562100
H	-3.110400	-0.750100	-1.226200

P: Pd[P5P] + CH_3Cl -2901.14

C	2.413502	-0.596005	-1.051605
Cl	1.767273	0.781996	1.753273
H	2.411632	-1.681399	-1.204894
H	2.566962	-0.079820	-2.005979
H	3.174951	-0.309734	-0.325140
Pd	0.577681	0.034358	-0.199184
P	-1.347760	0.813321	1.061001
P	-0.437555	-0.838443	-2.015304
H	-1.265260	0.027298	-2.789915
H	0.367620	-1.322790	-3.084631
H	-2.609585	1.229638	0.525475
H	-1.080277	1.982591	1.816821
C	-1.922659	-0.356972	2.417232
C	-2.701673	-1.615813	1.947550
H	-0.994277	-0.652125	2.924348
H	-2.525964	0.208628	3.137219
H	-2.800629	-2.269602	2.824172
H	-3.726050	-1.329524	1.667751
C	-1.620190	-2.282703	-1.789403
C	-2.050828	-2.412478	0.781293
H	-1.013233	-3.180276	-1.612671
H	-2.147613	-2.424476	-2.740484
H	-2.198034	-3.488426	0.944760
H	-0.964110	-2.246679	0.798482
C	-2.615656	-2.053607	-0.623209
H	-3.517637	-2.653333	-0.808103
H	-2.955070	-1.007859	-0.640827

RC: Pd[P6P] + CH_3Cl -3247.05

C	2.394829	2.619636	0.009629
Cl	1.874411	4.372674	-0.030867
H	1.497405	1.991308	-0.012471
H	3.019891	2.438465	-0.865748
H	2.959078	2.462122	0.929730
Pd	-0.318775	-0.097138	0.004176
P	-0.867978	-0.143649	2.235873
P	-0.623256	-0.472722	-2.247387
C	-2.356323	-1.089753	-2.704510
C	-2.903486	-2.140296	-1.702054
C	-3.352934	-1.525665	-0.352814
C	-3.292914	-2.496831	0.848922
C	-3.334024	-1.804743	2.243050
H	0.090793	-0.147905	3.298078
H	-1.599125	0.975352	2.741401
H	0.151644	-1.459804	-2.931977
H	-0.474486	0.523019	-3.261951
H	-3.008986	-0.206932	-2.727112
H	-2.317941	-1.496281	-3.721650
H	-3.740883	-2.674114	-2.174011
H	-2.126120	-2.896999	-1.519510
H	-3.910995	-0.870325	2.179553
H	-3.889581	-2.450158	2.937717
H	-4.370678	-1.117686	-0.452545
H	-2.690836	-0.673102	-0.133548
H	-4.124524	-3.213085	0.781024
H	-2.371533	-3.094049	0.780175
C	-1.962463	-1.533311	2.923096
H	-1.347788	-2.443164	2.884980
H	-2.126636	-1.300449	3.982688

TS: Pd[P6P] + CH_3Cl -3219.79

C	2.161500	1.360300	0.068600
CL	0.540400	2.901600	-0.041100
H	2.107100	0.259000	0.096700
H	2.628400	1.742200	-0.831700
H	2.543000	1.790800	0.987100
PD	-0.029400	0.420400	-0.018500
P	-0.717700	-0.105800	2.206500
P	-0.437100	-0.416800	-2.203900
C	-2.193600	-0.966200	-2.672200
C	-2.799600	-1.963100	-1.653000
C	-3.205800	-1.304200	-0.314500
C	-3.369500	-2.295400	0.861200
C	-3.257600	-1.660400	2.273400
H	0.294000	-0.241400	3.210600
H	-1.391700	0.962500	2.879800
H	0.265900	-1.560600	-2.701300
H	-0.178300	0.377200	-3.368300
H	-2.803300	-0.054300	-2.727200
H	-2.164000	-1.402300	-3.677000
H	-3.669300	-2.457100	-2.110900
H	-2.067700	-2.761500	-1.456900
H	-3.766000	-0.684500	2.287100
H	-3.812500	-2.294800	2.979300
H	-4.136800	-0.732900	-0.452000
H	-2.431400	-0.571300	-0.052200
H	-4.342100	-2.801800	0.776100
H	-2.609400	-3.087300	0.777400
C	-1.820700	-1.521700	2.851600
H	-1.261300	-2.450400	2.671500
H	-1.884500	-1.391200	3.938700

P: Pd[P6P] + CH_3Cl -3259.24

C	1.103826	1.590856	-1.837902
Cl	0.621831	2.611165	1.104200
H	2.051789	1.067650	-2.005121
H	0.488410	1.565131	-2.744701
H	1.276810	2.617736	-1.515433
Pd	0.115038	0.666330	-0.210519
P	-0.900426	0.053692	1.963641
P	-0.172702	-1.075133	-1.641809
C	-1.810481	-1.434784	-2.512847
C	-2.832912	-2.162481	-1.608948
C	-3.287594	-1.331414	-0.381493
C	-3.673515	-2.173102	0.861259
C	-3.438053	-1.462513	2.216003
H	0.097419	0.089770	2.973806
H	-1.673103	1.146318	2.436880
H	0.131972	-2.393198	-1.186282
H	0.697626	-1.071773	-2.766518
H	-2.203912	-0.472377	-2.865802
H	-1.579494	-2.043318	-3.395834
H	-3.699098	-2.451230	-2.220886
H	-2.378776	-3.103536	-1.265098
H	-3.894136	-0.461114	2.201031
H	-3.974541	-2.024460	2.993315
H	-4.124966	-0.677809	-0.664926
H	-2.470733	-0.653929	-0.108889
H	-4.728643	-2.473410	0.794255
H	-3.093184	-3.108845	0.863396
C	-1.954228	-1.362191	2.672715
H	-1.429913	-2.305784	2.465476
H	-1.925701	-1.217406	3.759586

RC: Pd(PH_3)$_2$ + CH_3Cl -1246.06

C	2.853000	1.002100	0.090500
Cl	3.052300	2.811200	-0.080400
Pd	-1.030200	-0.393700	0.005300
H	1.783900	0.773100	0.080000
H	3.362800	0.530500	-0.750700
H	3.309100	0.704600	1.035700
P	-0.797600	-0.684200	-2.252300
P	-1.363000	-0.070500	2.246800
H	-0.890000	1.101600	2.905000
H	-1.193600	-1.898900	-2.884000
H	-2.683500	-0.009000	2.778500
H	-0.863900	-0.987200	3.217900
H	-1.471600	0.177300	-3.165300
H	0.471500	-0.602000	-2.896600

TS: Pd(PH_3)$_2$ + CH_3Cl -1218.54

C	2.307600	-0.129100	-0.173800
Cl	1.452700	1.919200	0.197800
Pd	-0.099200	-0.015700	0.012200
H	1.833900	-1.103100	0.015900
H	2.618100	0.032500	-1.199900
H	3.057700	0.112600	0.569100
P	-0.804400	-0.950700	-2.013100
P	-1.320800	-0.219500	2.049600
H	-1.195500	0.682100	3.154300
H	-1.615800	-2.124200	-2.104100
H	-2.749400	-0.212400	2.071200
H	-1.209900	-1.396900	2.851600
H	-1.658300	-0.162600	-2.843000
H	0.058900	-1.350500	-3.085500

P: Pd(PH_3)$_2$ + CH_3Cl -1257.17

C	-0.109600	2.095000	0.000000
Cl	2.381400	0.171000	0.000000
H	0.435700	2.391600	0.899400
H	-1.115100	2.529100	0.000000
H	0.435700	2.391600	-0.899400
Pd	-0.005200	-0.024000	0.000000
P	-2.251800	0.043800	0.000000
H	-3.053400	-1.132600	0.000000
H	-2.908000	0.716600	1.066600
H	-2.908000	0.716600	-1.066600
P	0.513300	-2.374700	0.000000
H	-0.412500	-3.464500	0.000000
H	1.326000	-2.831000	-1.069300
H	1.326000	-2.831000	1.069300

TS: Pd[P2P]^{Cl} + CH_3Cl -1699.89

C	0.098648	0.004097	-0.915923
Pd	2.432806	-0.076705	0.053660
Cl	0.775964	-1.868867	0.173440
H	0.348813	1.003786	-0.557962
H	0.355550	-0.203319	-1.948858
H	-0.894758	-0.304190	-0.619490
C	4.927942	2.165409	0.181218
C	5.458475	1.014917	1.064691
P	3.645761	1.501036	-1.019899
P	4.034466	0.018744	1.807327
H	6.037767	0.296341	0.469994
H	6.102146	1.393101	1.865672
H	5.736616	2.666065	-0.361946
H	4.402718	2.913544	0.788992
Cl	5.222069	-1.480453	2.776867
Cl	3.525484	1.329461	3.416181
Cl	4.924296	0.870775	-2.600451
Cl	2.882618	3.345457	-1.770557

TS: Pd[P3P]^{Cl} + CH_3Cl -2063.52

C	0.086093	-0.121001	-0.472633
Pd	2.535647	0.000928	0.006199
Cl	1.204900	-2.061735	-0.068438
H	0.283395	0.797879	0.085129
H	0.116659	-0.032921	-1.553102
H	-0.765820	-0.659768	-0.080453
P	4.428635	-0.177854	1.375115
P	3.192267	1.803829	-1.202858
C	5.841238	1.909085	-0.058304
C	5.983430	0.498911	0.569373
C	5.045163	1.995934	-1.386327
Cl	2.665975	2.031220	-3.278410
H	5.348665	1.197571	-2.078580
H	6.858171	2.262331	-0.278152
H	6.256072	-0.243622	-0.194363
Cl	5.247655	-2.037327	2.048415
Cl	2.708411	3.741635	-0.449957
H	5.228862	2.954842	-1.882621
H	5.432795	2.614277	0.677628
H	6.771996	0.497588	1.329368
Cl	4.439437	0.989510	3.158893

TS: Pd[P4P]^{Cl} + CH_3Cl -2419.10

C	2.286221	0.547471	-0.834896
Cl	1.351288	2.296145	0.323691
H	2.068682	-0.511201	-0.670250
H	2.163256	0.895639	-1.853743
H	3.196451	0.862808	-0.343160
Pd	-0.041761	0.308236	-0.043249
P	-1.273718	-0.124357	1.922097
P	-0.902476	-0.836074	-1.822867
Cl	-2.026633	0.424163	-3.127472
Cl	0.433718	-1.785192	-3.220933
Cl	-0.467958	-1.775608	3.011999
Cl	-1.493072	1.310921	3.488115
C	-3.087638	-0.660451	1.776487
C	-3.442818	-1.121831	0.345113
H	-3.285780	-0.275815	-0.336706
H	-4.521666	-1.325790	0.311789
H	-3.273873	-1.436984	2.526676
H	-3.678892	0.221199	2.049095
C	-2.138037	-2.264341	-1.608452
H	-1.600286	-3.176079	-1.890286
H	-2.950141	-2.113578	-2.327970
C	-2.652183	-2.368512	-0.155805
H	-3.284334	-3.264215	-0.085568
H	-1.796073	-2.564090	0.501665

TS: Pd(PCl_3)$_2$ + CH_3Cl -1092.63

C	2.342805	0.042776	1.020427
Cl	1.984525	1.388520	-0.799954
H	1.845761	-0.910573	1.224588
H	3.329700	-0.091136	0.597800
H	2.266910	0.786176	1.805226
Pd	0.132320	0.046062	-0.027397
P	-0.868197	-0.939771	-1.966869
P	-1.235840	-0.142685	1.795322
Cl	-0.336005	-0.269996	3.724557
Cl	-0.702353	-3.044716	-2.012933
Cl	-2.536112	1.487229	2.061614
Cl	-2.593806	-1.748755	1.936723
Cl	-2.942746	-0.683966	-2.255555
Cl	-0.137427	-0.434822	-3.886262

TS: Pd(PH_3)$_2$$Cl^-$ + CH_3Cl -1317.09

Pd	0.171942	0.389946	1.465981
C	-1.044163	0.841469	3.750272
Cl	1.052571	1.428692	3.669435
H	-1.607770	1.720325	3.454826
H	-1.335650	-0.081278	3.243843
H	-0.941416	0.714389	4.822252
H	-2.915008	0.528151	0.146962
H	-1.695603	1.994715	-0.747228
Cl	-0.358196	-1.555944	-2.860822
P	-1.514222	0.723703	-0.110082
P	1.711043	-1.080163	0.378564
H	1.992184	-2.396448	0.873750
H	-1.396300	-0.085160	-1.304405
H	1.309567	-1.467281	-0.947105
H	3.086452	-0.786910	0.087209

TS: Pd(PH_3)$_2$$Br^-$ + CH_3Cl -1310.01

Pd	0.177384	0.407195	1.512844
C	-1.022137	0.810362	3.784535
Cl	1.056808	1.472111	3.694415
H	-1.611944	1.681742	3.520047
H	-1.302638	-0.109363	3.264737
H	-0.896062	0.661333	4.851005
H	-2.927062	0.627600	0.232721
H	-1.671301	2.050835	-0.680189
Br	-0.374344	-1.621054	-3.005425
P	-1.523557	0.778338	-0.038975
P	1.726825	-1.068005	0.454215
H	1.942948	-2.395948	0.947594
H	-1.465237	-0.022711	-1.234889
H	1.390515	-1.442953	-0.889539
H	3.122474	-0.813000	0.232350

TS: Pd(PH_3)$_2$$I^-$ + CH_3Cl -1301.78

Pd	0.196228	0.450879	1.633353
C	-1.010244	0.765671	3.875293
Cl	1.035300	1.541715	3.801818
H	-1.634419	1.627061	3.662335
H	-1.271013	-0.140824	3.320526
H	-0.859263	0.571432	4.931074
H	-2.909525	0.786508	0.367311
H	-1.596446	2.153471	-0.550035
I	-0.401219	-1.686336	-3.174542
P	-1.502722	0.875482	0.088208
P	1.785407	-1.017909	0.633812
H	1.926245	-2.360572	1.110420
H	-1.506154	0.087140	-1.112065
H	1.568805	-1.369343	-0.735812
H	3.200203	-0.795523	0.531412

TS: Pd[P2P]Cl^- + CH_3Cl -1874.78

Pd	2.139844	0.945603	0.011414
Cl	-0.362434	0.468403	0.261568
C	0.004906	1.379604	-1.683303
H	4.004812	0.144426	2.628697
H	0.102574	2.448162	-1.525130
H	4.481935	2.166824	-2.166921
H	0.821524	0.927710	-2.239751
Cl	6.086056	2.170985	-3.665889
H	-0.977342	1.058843	-2.011473
C	5.357035	0.066470	0.482387
C	5.463921	1.560600	0.107958
P	3.695435	-0.350180	1.312097
P	3.921194	2.168063	-0.813492
H	5.578756	2.168992	1.015110
H	5.400154	-0.548847	-0.426781
H	6.321758	1.736206	-0.553014
H	6.188865	-0.236147	1.129757
H	4.054661	3.568588	-0.555348
H	4.045055	-1.713352	1.672772

[a] Computed at ZORA-BLYP/TZ2P. RC = reactant complex, TS = transition state, P = product, Pd[PnP] = Pd[$PH_2(CH_2)_nPH_2$]. All species labeled "TS" have one imaginary frequency, all others have none.