Supporting Information

Frontier Orbital Consistent Effective Potential for Bulky Ligand of Transition Metal Complexes

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Table S1. The activation barrier (E_a) and reaction energy (ΔE) of reductive elimination reaction of ethane from $Pt(Me)_2(PMe_3)_2$ calculated by the DFT[B3PW91] method with various parameters of effective potential optimized with the DFT[B3PW91] methods.

C	ζ(B3PW91)	E_a	ΔE
−2.8	1.48334288	52.0	−9.6
−2.9	1.53358358	51.9	−9.6
−3.0	1.58297547	51.9	−9.6
−3.1	1.63155300	51.8	−9.6
−3.2	1.67934821	51.8	−9.6

Table S2. Cartesian coordinates

(a) PMe_3

15	0.000000	0.000000	0.601461
6	0.000000	1.636205	−0.278254
1	0.000000	1.526757	−1.370566
1	−0.884611	2.211871	0.016392
1	0.884611	2.211871	0.016392
6	1.416995	−0.818102	−0.278254
1	1.322210	−0.763378	−1.370566
1	2.357842	−0.339840	0.016392
1	1.473231	−1.872031	0.016392
6	−1.416995	−0.818102	−0.278254
1	−1.322210	−0.763378	−1.370566
1	−1.473231	−1.872031	0.016392
1	−2.357842	−0.339840	0.016392

(b) PEt_3

15	0.000000	0.000000	0.501407
6	−1.136271	1.193562	−0.382903
6	−1.002323	2.637575	0.120375
1	−0.959841	1.145334	−1.468156
1	−2.163372	0.842993	−0.212676
1	−1.718553	3.297198	−0.383980
1	−1.189622	2.697877	1.198370
1	0.000000	3.040351	−0.065425
6	1.601790	0.387259	−0.382903
6	2.785368	−0.450750	0.120375
1	1.471809	0.258580	−1.468156
1	1.811739	1.452039	−0.212676
1	3.714734	−0.160288	−0.383980
1	2.931241	−0.318696	1.198370
1	2.633021	−1.520175	−0.065425
6	−0.465519	−1.580820	−0.382903
6	−1.783045	−2.186825	0.120375
1	−0.511968	−1.403914	−1.468156
1	0.351633	−2.295032	−0.212676
1	−1.996181	−3.136909	−0.383980
1	−1.741619	−2.379181	1.198370
1	−2.633021	−1.520175	−0.065425

(c) P^iPr_3

15	−0.147007	−0.085778	−0.751809
6	0.545542	1.588849	−0.203346
1	−0.096055	2.277453	−0.777566
6	1.980210	1.784001	−0.728029
1	2.276909	2.837252	−0.640927
1	2.698993	1.194169	−0.148288
1	2.070748	1.492636	−1.780453
6	0.446089	1.996579	1.275848
1	0.729010	3.052336	1.390018
1	−0.567650	1.885284	1.674242

1	1.119993	1.408243	1.904894
6	-1.775069	-0.155594	0.195889
1	-1.587823	-0.055516	1.275728
6	-2.486900	-1.498003	-0.051687
1	-3.476369	-1.492776	0.423671
1	-2.631740	-1.672418	-1.125052
1	-1.932079	-2.348247	0.358123
6	-2.682379	1.004483	-0.255439
1	-3.661760	0.933225	0.235029
1	-2.261310	1.984981	-0.010491
1	-2.847256	0.969151	-1.339563
6	0.852000	-1.460277	0.077721
1	0.173957	-2.319451	-0.051742
6	1.179730	-1.350923	1.574460
1	1.573761	-2.307569	1.944755
1	1.947844	-0.592097	1.758410
1	0.301292	-1.099505	2.178351
6	2.116016	-1.783381	-0.743138
1	2.873985	-0.998733	-0.646484
1	2.567152	-2.720827	-0.391926
1	1.882073	-1.895328	-1.807265

(d) P^tBu_3

15	0.000000	0.000000	0.702097
6	0.660189	1.681838	0.000901
6	1.095982	1.723150	-1.477274
1	1.421657	2.742668	-1.731994
1	1.937991	1.056026	-1.681324
1	0.280392	1.457733	-2.155614
6	1.856208	2.092846	0.899766
1	2.165220	3.114762	0.638053
1	1.569999	2.083861	1.957192
1	2.726099	1.446486	0.779357
6	-0.408881	2.778125	0.220348
1	-1.264205	2.676290	-0.451862
1	-0.771845	2.788748	1.253897
1	0.048215	3.757131	0.019365
6	1.126420	-1.412659	0.000901
6	0.944301	-1.810723	-1.477274
1	1.664392	-2.602526	-1.731994
1	-0.054450	-2.206363	-1.681324
1	1.122238	-0.971693	-2.155614
6	0.884354	-2.653946	0.899766
1	1.614853	-3.432517	0.638053
1	1.019679	-2.401590	1.957192
1	-0.110356	-3.084114	0.779357
6	2.610368	-1.034961	0.220348
1	2.949837	-0.243312	-0.451862
1	2.801049	-0.725937	1.253897
1	3.229664	-1.920321	0.019365
6	-1.786609	-0.269178	0.000901
6	-2.040283	0.087573	-1.477274

1	-3.086049	-0.140142	-1.731994
1	-1.883542	1.150337	-1.681324
1	-1.402630	-0.486040	-2.155614
6	-2.740562	0.561099	0.899766
1	-2.615744	1.637628	0.779357
1	-3.780073	0.317755	0.638053
1	-2.589677	0.317728	1.957192
6	-2.201486	-1.743165	0.220348
1	-1.685633	-2.432978	-0.451862
1	-2.029204	-2.062811	1.253897
1	-3.277879	-1.836811	0.019365

(e) $Ni(Me)_2(PH_3)_2$ reactant

28	-0.011670	-0.262255	0.000952
15	-1.628067	1.195528	-0.007271
1	-2.644227	1.016275	-0.975241
1	-2.465395	1.201877	1.133726
1	-1.511541	2.607538	-0.138539
15	1.763276	0.994511	-0.094191
1	2.759557	0.767751	0.884305
1	2.585445	0.819372	-1.232645
1	1.813927	2.416220	-0.066680
6	-1.424311	-1.618285	0.028779
1	-1.146195	-2.420865	0.718024
1	-2.440948	-1.292423	0.296880
1	-1.466806	-2.031034	-0.987230
6	1.235515	-1.770080	0.078083
1	2.281155	-1.583911	-0.211028
1	1.236889	-2.108256	1.122176
1	0.863090	-2.584449	-0.550099

(f) $Ni(Me)_2(PH_3)_2$ TS

28	0.000005	0.173719	-0.000005
15	-1.834970	-1.008627	-0.108453
1	-3.104014	-0.493505	0.287048
1	-2.251075	-1.387252	-1.413072
1	-2.060253	-2.295669	0.459273
15	1.835028	-1.008541	0.108448
1	3.104095	-0.493295	-0.286819
1	2.250994	-1.387323	1.413066
1	2.060450	-2.295491	-0.459432
6	-0.477277	1.819961	0.913313
1	-1.489138	2.181761	0.718651
1	-0.477619	1.115222	1.774233
1	0.173186	2.655955	1.175013
6	0.477151	1.820014	-0.913295
1	1.488996	2.181874	-0.718665
1	0.477507	1.115295	-1.774231
1	-0.173377	2.655969	-1.174959

(g) $Ni(PH_3)_2$

28	0.000000	0.000000	0.000000

15	0.000000	0.000000	2.099886
1	-0.000394	1.219487	2.829939
1	-1.055909	-0.610084	2.829939
1	1.056303	-0.609402	2.829939
15	0.000000	0.000000	-2.099886
1	1.055909	-0.610084	-2.829939
1	-1.056303	-0.609402	-2.829939
1	0.000394	1.219487	-2.829939

(h) $Ni(Me)_2(PMe_3)_2$ reactant

Ni	-0.00000000	0.00000000	-0.85468923
P	0.00129720	1.75485980	0.49364696
C	1.31207524	2.98609447	0.07786914
H	1.25896940	3.24660516	-0.98125521
H	1.20973067	3.89445042	0.68295296
H	2.29454261	2.54110327	0.26905647
C	-1.54478920	2.76324547	0.43450658
H	-1.43421316	3.69762160	0.99715956
H	-1.80066353	2.99435137	-0.60241252
H	-2.36844733	2.18449916	0.86635445
C	0.24735912	1.69764641	2.33193425
H	-0.55923128	1.13699803	2.81263091
H	1.19842317	1.21035023	2.57067709
H	0.26322153	2.71153823	2.74941848
P	-0.00129720	-1.75485980	0.49364696
C	-1.31207524	-2.98609447	0.07786914
H	-1.25896940	-3.24660516	-0.98125521
H	-1.20973067	-3.89445042	0.68295296
H	-2.29454261	-2.54110327	0.26905647
C	1.54478920	-2.76324547	0.43450658
H	1.43421316	-3.69762160	0.99715956
H	1.80066353	-2.99435137	-0.60241252
H	2.36844733	-2.18449916	0.86635445
C	-0.24735912	-1.69764641	2.33193425
H	0.55923128	-1.13699803	2.81263091
H	-1.19842317	-1.21035023	2.57067709
H	-0.26322153	-2.71153823	2.74941848
C	-0.06090563	1.31031631	-2.32095525
H	-0.70074352	0.92460486	-3.12154187
H	-0.40718506	2.33007027	-2.10232444
H	0.95981875	1.39285560	-2.71989945
C	0.06090563	-1.31031631	-2.32095525
H	0.40718506	-2.33007027	-2.10232444
H	-0.95981875	-1.39285560	-2.71989945
H	0.70074352	-0.92460486	-3.12154187

(i) $Ni(Me)_2(PMe_3)_2$ TS

Ni	0.00000000	0.00000000	0.68692436
P	0.01283187	1.88554813	-0.45374274
C	-0.54387603	3.43232794	0.40773175
H	-0.43498529	4.32363926	-0.22265872
H	-1.59541850	3.33132794	0.69900357

H	0.04522052	3.56876490	1.32124056
C	1.71133578	2.40506595	-0.98303204
H	1.70228150	3.36653324	-1.51167293
H	2.35442630	2.48890585	-0.10059113
H	2.13775834	1.63976013	-1.63962269
C	-0.90132045	2.09377145	-2.05631722
H	-0.55532970	1.34164185	-2.77321124
H	-1.97195845	1.93261435	-1.88845823
H	-0.75667507	3.09168402	-2.48992901
P	-0.01283187	-1.88554813	-0.45374274
C	0.54387603	-3.43232794	0.40773175
H	-0.04522052	-3.56876490	1.32124056
H	0.43498529	-4.32363926	-0.22265872
H	1.59541850	-3.33132794	0.69900357
C	-1.71133578	-2.40506595	-0.98303204
H	-1.70228150	-3.36653324	-1.51167293
H	-2.35442630	-2.48890585	-0.10059113
H	-2.13775834	-1.63976013	-1.63962269
C	0.90132045	-2.09377145	-2.05631722
H	0.55532970	-1.34164185	-2.77321124
H	1.97195845	-1.93261435	-1.88845823
H	0.75667507	-3.09168402	-2.48992901
C	-0.93755143	0.39810163	2.34470119
H	-0.83826917	1.41817599	2.72299305
H	-1.78298275	0.33408286	1.62060368
H	-1.16645420	-0.27674285	3.17300102
C	0.93755143	-0.39810163	2.34470119
H	0.83826917	-1.41817599	2.72299305
H	1.78298275	-0.33408286	1.62060368
H	1.16645420	0.27674285	3.17300102

(j) $Ni(PMe_3)_2$

Ni	-0.00000000	-0.00000000	0.00000000
P	0.00000000	0.00000000	2.12457186
C	0.82058644	1.42129741	2.98544489
H	1.86841632	1.47950231	2.67374387
H	0.34707843	2.35784715	2.67374387
H	0.76381822	1.32297196	4.07675589
C	-1.64117288	-0.00000000	2.98544489
H	-2.21549474	0.87834484	2.67374387
H	-2.21549474	-0.87834484	2.67374387
H	-1.52763643	-0.00000000	4.07675589
C	0.82058644	-1.42129741	2.98544489
H	1.86841632	-1.47950231	2.67374387
H	0.76381822	-1.32297196	4.07675589
H	0.34707843	-2.35784715	2.67374387
P	-0.00000000	0.00000000	-2.12457186
C	-0.82058644	1.42129741	-2.98544489
H	-1.86841632	1.47950231	-2.67374387
H	-0.34707843	2.35784715	-2.67374387
H	-0.76381822	1.32297196	-4.07675589
C	1.64117288	-0.00000000	-2.98544489

H	2.21549474	-0.87834484	-2.67374387
H	1.52763643	-0.00000000	-4.07675589
H	2.21549474	0.87834484	-2.67374387
C	-0.82058644	-1.42129741	-2.98544489
H	-1.86841632	-1.47950231	-2.67374387
H	-0.76381822	-1.32297196	-4.07675589
H	-0.34707843	-2.35784715	-2.67374387

(k) $Pd(Me)_2(PH_3)_2$ reactant

Pd	0.00000000	0.00000000	-0.24567266
P	-0.00785233	1.81909831	1.20465434
H	0.98509023	2.80637940	1.00256035
H	-1.12534961	2.68512073	1.14198733
H	0.08652844	1.77524248	2.62077934
P	0.00785233	-1.81909831	1.20465434
H	-0.98509023	-2.80637940	1.00256035
H	1.12534961	-2.68512073	1.14198733
H	-0.08652844	-1.77524248	2.62077934
C	0.02112672	1.38010192	-1.81033966
H	-0.65401054	1.04465827	-2.60142467
H	-0.26896133	2.39732244	-1.51879266
H	1.04365426	1.40935420	-2.20241565
C	-0.02112672	-1.38010192	-1.81033966
H	0.26896133	-2.39732244	-1.51879266
H	-1.04365426	-1.40935420	-2.20241565
H	0.65401054	-1.04465827	-2.60142467

(l) $Pd(Me)_2(PH_3)_2$ TS

Pd	0.00000000	0.00000000	0.14456064
P	0.12984892	1.93640094	-1.17094403
H	-0.19810450	3.23586397	-0.69095703
H	1.41443997	2.30216779	-1.65184633
H	-0.51887945	2.11895055	-2.42317536
P	-0.12984892	-1.93640094	-1.17094403
H	0.19810450	-3.23586397	-0.69095703
H	-1.41443997	-2.30216779	-1.65184633
H	0.51887945	-2.11895055	-2.42317536
C	-0.76446498	0.69229765	2.04962829
H	-0.28941052	1.61465357	2.38343031
H	-1.64279189	0.91819583	1.41963638
H	-1.12389359	0.12120923	2.90440805
C	0.76446498	-0.69229765	2.04962829
H	0.28941052	-1.61465357	2.38343031
H	1.64279189	-0.91819583	1.41963638
H	1.12389359	-0.12120923	2.90440805

(m) $Pd(PH_3)_2$

Pd	0.00000000	-0.00000000	0.00000000
P	-0.00000000	-0.00000000	2.26551500
H	0.00000000	1.22188412	2.98709000
H	-1.05818269	-0.61094206	2.98709000
H	1.05818269	-0.61094206	2.98709000

P	-0.00000000	-0.00000000	-2.26551500
H	-0.00000000	1.22188412	-2.98709000
H	1.05818269	-0.61094206	-2.98709000
H	-1.05818269	-0.61094206	-2.98709000

(n) $Pd(Me)_2(PMe_3)_2$ reactant

Pd	0.00000000	0.00000000	-0.77527737
P	-0.00065362	1.86095292	0.64797100
C	1.31663691	3.08246516	0.23550778
H	1.26427262	3.33458713	-0.82664069
H	1.21844738	3.99700065	0.83222398
H	2.29723664	2.63425480	0.42684581
C	-1.53210416	2.88490654	0.55719186
H	-1.42957483	3.81480312	1.12906096
H	-1.75162867	3.12571242	-0.48664466
H	-2.37644142	2.31207758	0.95489077
C	0.22300159	1.76697960	2.48262285
H	-0.58869283	1.19050145	2.93613422
H	1.17047289	1.27033850	2.71596501
H	0.23377030	2.76873216	2.92869975
P	0.00065362	-1.86095292	0.64797100
C	-1.31663691	-3.08246516	0.23550778
H	-1.26427262	-3.33458713	-0.82664069
H	-1.21844738	-3.99700065	0.83222398
H	-2.29723664	-2.63425480	0.42684581
C	1.53210416	-2.88490654	0.55719186
H	1.42957483	-3.81480312	1.12906096
H	1.75162867	-3.12571242	-0.48664466
H	2.37644142	-2.31207758	0.95489077
C	-0.22300159	-1.76697960	2.48262285
H	0.58869283	-1.19050145	2.93613422
H	-1.17047289	-1.27033850	2.71596501
H	-0.23377030	-2.76873216	2.92869975
C	-0.02656012	1.37321838	-2.35696512
H	-0.67239878	0.99266743	-3.15385227
H	-0.36944378	2.38456853	-2.10578202
H	0.99495349	1.44916836	-2.75040680
C	0.02656012	-1.37321838	-2.35696512
H	0.36944378	-2.38456853	-2.10578202
H	-0.99495349	-1.44916836	-2.75040680
H	0.67239878	-0.99266743	-3.15385227

(o) $Pd(Me)_2(PMe_3)_2$ TS

Pd	0.00000000	0.00000000	0.61741470
P	0.02397738	2.01672102	-0.60284830
C	-0.58749813	3.55428776	0.23272269
H	-0.48789916	4.44174107	-0.40496130
H	-1.64140377	3.43073300	0.50585168
H	-0.01964685	3.71433283	1.15553470
C	1.72059441	2.56903029	-1.09724027
H	1.69885086	3.52455598	-1.63645927
H	2.34244840	2.67709823	-0.20252426

H	2.17986536	1.80765609	-1.73613026
C	-0.85396009	2.18674475	-2.22811331
H	-1.92519422	2.00649205	-2.08676933
H	-0.71687990	3.18318864	-2.66780131
H	-0.47468310	1.43489153	-2.92819330
P	-0.02397738	-2.01672102	-0.60284830
C	0.58749813	-3.55428776	0.23272269
H	0.01964685	-3.71433283	1.15553470
H	0.48789916	-4.44174107	-0.40496130
H	1.64140377	-3.43073300	0.50585168
C	-1.72059441	-2.56903029	-1.09724027
H	-1.69885086	-3.52455598	-1.63645927
H	-2.34244840	-2.67709823	-0.20252426
H	-2.17986536	-1.80765609	-1.73613026
C	0.85396009	-2.18674475	-2.22811331
H	0.47468310	-1.43489153	-2.92819330
H	1.92519422	-2.00649205	-2.08676933
H	0.71687990	-3.18318864	-2.66780131
C	-0.81848801	0.61318370	2.53758469
H	-0.44353082	1.57582207	2.88569970
H	-1.70952308	0.75717517	1.89940668
H	-1.13471811	0.00960253	3.38880969
C	0.81848801	-0.61318370	2.53758469
H	0.44353082	-1.57582207	2.88569970
H	1.70952308	-0.75717517	1.89940668
H	1.13471811	-0.00960253	3.38880969

(p) $Pd(PMe_3)_2$

Pd	-0.00000000	-0.00000000	0.00000000
P	0.00000000	0.00000000	2.28417600
C	0.00000000	1.64482691	3.12680900
H	-0.88487100	2.21162691	2.81998200
H	0.00000000	1.54055991	4.21933000
H	0.88487100	2.21162691	2.81998200
C	1.42446189	-0.82241345	3.12680900
H	2.35776059	-0.33949269	2.81998200
H	1.33416402	-0.77027995	4.21933000
H	1.47288959	-1.87213422	2.81998200
C	-1.42446189	-0.82241345	3.12680900
H	-1.47288959	-1.87213422	2.81998200
H	-1.33416402	-0.77027995	4.21933000
H	-2.35776059	-0.33949269	2.81998200
P	-0.00000000	0.00000000	-2.28417600
C	-0.00000000	1.64482691	-3.12680900
H	0.88487100	2.21162691	-2.81998200
H	-0.00000000	1.54055991	-4.21933000
H	-0.88487100	2.21162691	-2.81998200
C	-1.42446189	-0.82241345	-3.12680900
H	-2.35776059	-0.33949269	-2.81998200
H	-1.33416402	-0.77027995	-4.21933000
H	-1.47288959	-1.87213422	-2.81998200
C	1.42446189	-0.82241345	-3.12680900

H	1.47288959	-1.87213422	-2.81998200
H	1.33416402	-0.77027995	-4.21933000
H	2.35776059	-0.33949269	-2.81998200

(q) $Pt(Me)_2(PH_3)_2$ reactant

Pt	0.00000000	0.00000000	-0.19374826
P	-0.00744968	1.77627415	1.27962474
H	1.00123854	2.75693495	1.12908776
H	-1.11833455	2.65265384	1.24737072
H	0.07622049	1.65005643	2.69014274
P	0.00744968	-1.77627415	1.27962474
H	-1.00123854	-2.75693495	1.12908776
H	1.11833455	-2.65265384	1.24737072
H	-0.07622049	-1.65005643	2.69014274
C	0.01777127	1.39624040	-1.75398226
H	-0.65145246	1.06400647	-2.55345927
H	-0.27830893	2.41444194	-1.47150626
H	1.03735665	1.44131677	-2.15593124
C	-0.01777127	-1.39624040	-1.75398226
H	0.27830893	-2.41444194	-1.47150626
H	-1.03735665	-1.44131677	-2.15593124
H	0.65145246	-1.06400647	-2.55345927

(r) $Pt(Me)_2(PH_3)_2$ TS

Pt	0.00000000	0.00000000	0.06163917
P	0.11601127	1.94785128	-1.12655814
H	-0.29566346	3.21934583	-0.63191580
H	1.39933486	2.37660006	-1.55268120
H	-0.50827485	2.11076006	-2.39215297
P	-0.11601127	-1.94785128	-1.12655814
H	0.29566346	-3.21934583	-0.63191580
H	-1.39933486	-2.37660006	-1.55268120
H	0.50827485	-2.11076006	-2.39215297
C	-0.81403416	0.57802080	2.05863038
H	-0.45994774	1.54843377	2.40326661
H	-1.70417556	0.70003941	1.41333916
H	-1.13153747	-0.03340593	2.90280657
C	0.81403416	-0.57802080	2.05863038
H	0.45994774	-1.54843377	2.40326661
H	1.70417556	-0.70003941	1.41333916
H	1.13153747	0.03340593	2.90280657

(s) $Pt(PH_3)_2$

78	0.000000	0.000000	0.000990
15	0.000000	2.238353	-0.001900
1	-0.000303	2.938229	-1.232175
1	1.064486	2.942219	0.610584
1	-1.063699	2.942630	0.611472
15	0.000000	-2.238353	-0.001900
1	0.000303	-2.938229	-1.232175
1	-1.064486	-2.942219	0.610584
1	1.063699	-2.942630	0.611472

(t) $Pt(Me)_2(PMe_3)_2$ reactant

Pt	0.00000000	0.00000000	-0.63582709
P	-0.00150427	1.83913223	0.78476840
C	1.32130578	3.05390684	0.37672191
H	1.26872635	3.31095488	-0.68407520
H	1.22941230	3.96588300	0.97801911
H	2.29838587	2.59677388	0.56377346
C	-1.53128853	2.86309086	0.69605476
H	-1.43078605	3.78885709	1.27466204
H	-1.74624484	3.11039440	-0.34710441
H	-2.37644344	2.28608570	1.08535858
C	0.22160190	1.73125386	2.61606306
H	1.16320285	1.22306970	2.84677242
H	0.24503691	2.73246954	3.06243059
H	-0.59765334	1.16563171	3.06864692
P	0.00150427	-1.83913223	0.78476840
C	-1.32130578	-3.05390684	0.37672191
H	-1.26872635	-3.31095488	-0.68407520
H	-1.22941230	-3.96588300	0.97801911
H	-2.29838587	-2.59677388	0.56377346
C	1.53128853	-2.86309086	0.69605476
H	1.43078605	-3.78885709	1.27466204
H	1.74624484	-3.11039440	-0.34710441
H	2.37644344	-2.28608570	1.08535858
C	-0.22160190	-1.73125386	2.61606306
H	0.59765334	-1.16563171	3.06864692
H	-1.16320285	-1.22306970	2.84677242
H	-0.24503691	-2.73246954	3.06243059
C	-0.02594719	1.38322858	-2.22131421
H	-0.66579144	1.00442485	-3.02549066
H	-0.37550578	2.39509347	-1.98043570
H	0.99299803	1.47273818	-2.62197973
C	0.02594719	-1.38322858	-2.22131421
H	0.37550578	-2.39509347	-1.98043570
H	-0.99299803	-1.47273818	-2.62197973
H	0.66579144	-1.00442485	-3.02549066

(u) $Pt(Me)_2(PMe_3)_2$ TS

Pt	0.00000000	0.00000000	0.43451246
P	0.02763656	2.02085728	-0.65981455
C	-0.78123444	3.49353953	0.12337746
H	-0.68722058	4.39458103	-0.49581154
H	-1.84469221	3.28448391	0.28430847
H	-0.32470595	3.68423322	1.10054645
C	1.71730381	2.70050074	-0.98031257
H	1.67552747	3.65415614	-1.52147257
H	2.23503993	2.85041763	-0.02754458
H	2.29372116	1.97898321	-1.56750857
C	-0.70535825	2.14098598	-2.35614154
H	-1.76788396	1.87941562	-2.31318953
H	-0.60221297	3.14869795	-2.77921854

H	-0.20622240	1.42217906	-3.01374854
P	-0.02763656	-2.02085728	-0.65981455
C	0.78123444	-3.49353953	0.12337746
H	0.32470595	-3.68423322	1.10054645
H	0.68722058	-4.39458103	-0.49581154
H	1.84469221	-3.28448391	0.28430847
C	-1.71730381	-2.70050074	-0.98031257
H	-1.67552747	-3.65415614	-1.52147257
H	-2.23503993	-2.85041763	-0.02754458
H	-2.29372116	-1.97898321	-1.56750857
C	0.70535825	-2.14098598	-2.35614154
H	1.76788396	-1.87941562	-2.31318953
H	0.60221297	-3.14869795	-2.77921854
H	0.20622240	-1.42217906	-3.01374854
C	-0.84290184	0.53201433	2.44585947
H	-0.54745480	1.51550097	2.80936746
H	-1.73386702	0.61587598	1.79486948
H	-1.13478823	-0.10231758	3.28393747
C	0.84290184	-0.53201433	2.44585947
H	0.54745480	-1.51550097	2.80936746
H	1.73386702	-0.61587598	1.79486948
H	1.13478823	0.10231758	3.28393747

(v) $Pt(PMe_3)_2$

Pt	0.00000000	0.00000000	0.00156200
P	0.00000000	2.26016500	-0.00070900
C	-0.00028700	3.08363500	1.64931600
H	0.88446700	2.76950200	2.21151200
H	-0.00039900	4.17651200	1.55579200
H	-0.88509100	2.76930600	2.21132700
C	-1.42997800	3.08017000	-0.82763000
H	-2.35850300	2.76548300	-0.34149300
H	-1.35014400	4.17328600	-0.78286200
H	-1.47394300	2.76377400	-1.87430500
C	1.43009100	3.08041300	-0.82720900
H	1.35008400	4.17351400	-0.78234800
H	2.35854500	2.76581800	-0.34087500
H	1.47434600	2.76411600	-1.87390000
P	0.00000000	-2.26016500	-0.00070900
C	0.00028700	-3.08363500	1.64931600
H	0.00039900	-4.17651200	1.55579200
H	0.88509100	-2.76930600	2.21132700
H	-0.88446700	-2.76950200	2.21151200
C	1.42997800	-3.08017000	-0.82763000
H	2.35850300	-2.76548300	-0.34149300
H	1.35014400	-4.17328600	-0.78286200
H	1.47394300	-2.76377400	-1.87430500
C	-1.43009100	-3.08041300	-0.82720900
H	-1.47434600	-2.76411600	-1.87390000
H	-1.35008400	-4.17351400	-0.78234800
H	-2.35854500	-2.76581800	-0.34087500

(w) $Pt(Me)_2(PEt_3)_2$ reactant

Pt	0.01937155	-0.00166568	-0.88714485
P	-0.03285299	1.86824607	0.54650955
C	1.05475917	3.30474370	0.02235796
H	1.45316354	3.75285492	0.94314199
H	1.90517847	2.86587278	-0.51301993
C	0.42612463	4.41800274	-0.82908695
H	1.18277928	5.18036420	-1.05173216
H	0.04617464	4.04062756	-1.78045059
H	-0.39499433	4.91790113	-0.30486522
C	-1.69684847	2.67326291	0.72311322
H	-1.59225443	3.59101181	1.31857368
H	-1.99777433	2.97511991	-0.28754600
C	-2.77227725	1.76138565	1.32453836
H	-3.75307292	2.25016330	1.29373021
H	-2.84189019	0.82374182	0.76250421
H	-2.56010340	1.52032988	2.37221118
C	0.51886232	1.74851485	2.32077851
H	0.29576205	2.70627232	2.81343638
H	-0.09443412	0.98719246	2.81299178
C	2.00862795	1.41063648	2.47633519
H	2.64650035	2.23544005	2.14155680
H	2.25525326	1.21134036	3.52584540
H	2.28233320	0.52893704	1.88668946
P	0.05098174	-1.89255716	0.52020264
C	-1.41191927	-3.03920908	0.37378910
H	-1.25293113	-3.85187179	1.09901383
H	-2.27825277	-2.46461376	0.72610083
C	-1.73125950	-3.62504287	-1.00507527
H	-2.61118231	-4.27645882	-0.93683979
H	-1.94609122	-2.83649206	-1.72990987
H	-0.90539068	-4.22709328	-1.39810699
C	1.48521721	-3.02695330	0.19465137
H	1.36679333	-3.92707003	0.81484837
H	1.42565540	-3.34383322	-0.85186469
C	2.84449675	-2.36222111	0.44946922
H	2.94290542	-1.45093671	-0.15066310
H	2.97491121	-2.09278703	1.50398844
H	3.66328010	-3.03898784	0.17896419
C	0.14053512	-1.82997968	2.38781794
H	0.91763443	-1.10579501	2.65291039
H	0.49471025	-2.81201890	2.73325430
C	-1.17254529	-1.48287259	3.10272407
H	-1.89358962	-2.30375509	3.03846302
H	-0.99201181	-1.28990676	4.16691937
H	-1.64861537	-0.59372962	2.67666176
C	-0.08776328	1.40370638	-2.44704748
H	-0.25805295	0.90417933	-3.40503056
H	-0.90545893	2.12304920	-2.31021624
H	0.85040934	1.96702609	-2.53371476
C	0.18850179	-1.32779252	-2.50789072
H	0.35496272	-2.38489579	-2.28575587

H	-0.71504415	-1.26061505	-3.12662227
H	1.03275416	-0.98306345	-3.11769915

(x) $Pt(Me)_2(PEt_3)_2$ TS

Pt	0.00000000	0.00000000	0.54010893
P	0.00245771	2.09550182	-0.43261064
C	-1.41186419	2.57815533	-1.54438850
H	-1.27124308	3.62112005	-1.86586732
H	-1.33639242	1.94999171	-2.44055797
C	-2.79240310	2.39259096	-0.90346121
H	-3.58974457	2.64092193	-1.61414028
H	-2.93115492	1.35426085	-0.58249787
H	-2.92239112	3.03505367	-0.02508401
C	0.01984682	3.57628808	0.70830363
H	-0.01817845	4.49965418	0.11114787
H	-0.90895637	3.53393971	1.29308983
C	1.22349034	3.59857338	1.65771170
H	1.31232292	2.64668182	2.19305337
H	2.16170624	3.76418253	1.11645543
H	1.12543248	4.40043121	2.39925190
C	1.45604401	2.53164139	-1.51547217
H	1.36488811	3.58779184	-1.81090500
H	2.34961917	2.44935912	-0.88344854
C	1.61947834	1.64154252	-2.75125691
H	2.54464432	1.88633399	-3.28683179
H	1.65678397	0.58690592	-2.46143602
H	0.78854607	1.76642267	-3.45452919
P	-0.00245771	-2.09550182	-0.43261064
C	-0.01984682	-3.57628808	0.70830363
H	0.01817845	-4.49965418	0.11114787
H	0.90895637	-3.53393971	1.29308983
C	-1.22349034	-3.59857338	1.65771170
H	-1.12543248	-4.40043121	2.39925190
H	-1.31232292	-2.64668182	2.19305337
H	-2.16170624	-3.76418253	1.11645543
C	-1.45604401	-2.53164139	-1.51547217
H	-1.36488811	-3.58779184	-1.81090500
H	-2.34961917	-2.44935912	-0.88344854
C	-1.61947834	-1.64154252	-2.75125691
H	-1.65678397	-0.58690592	-2.46143602
H	-0.78854607	-1.76642267	-3.45452919
H	-2.54464432	-1.88633399	-3.28683179
C	1.41186419	-2.57815533	-1.54438850
H	1.27124308	-3.62112005	-1.86586732
H	1.33639242	-1.94999171	-2.44055797
C	2.79240310	-2.39259096	-0.90346121
H	3.58974457	-2.64092193	-1.61414028
H	2.93115492	-1.35426085	-0.58249787
H	2.92239112	-3.03505367	-0.02508401
C	-0.94660350	0.40749320	2.53194264
H	-0.75491546	1.39570591	2.95034070
H	-1.83283228	0.43626455	1.87100896

H	-1.17174497	-0.29458291	3.33598654
C	0.94660350	-0.40749320	2.53194264
H	0.75491546	-1.39570591	2.95034070
H	1.83283228	-0.43626455	1.87100896
H	1.17174497	0.29458291	3.33598654

(y) $Pt(PEt_3)_2$

Pt	0.00000000	-0.00000000	0.00000000
P	-0.00000000	0.00000000	2.26574423
C	-0.01994050	1.67490343	3.06989978
H	-0.05026901	1.54594364	4.16176868
H	-0.96185341	2.15245253	2.77201002
C	1.15840942	2.56644366	2.65726768
H	1.05483825	3.56934073	3.08815496
H	1.20386544	2.66051874	1.56688166
H	2.11638754	2.15838153	2.99841870
C	-1.44053867	-0.85472069	3.06989978
H	-1.31369196	-0.81650606	4.16176868
H	-1.38315186	-1.90921575	2.77201002
C	-2.80181012	-0.28000984	2.65726768
H	-3.61855887	-0.87115364	3.08815496
H	-2.90600953	-0.28768132	1.56688166
H	-2.92740700	0.75365461	2.99841870
C	1.46047917	-0.82018274	3.06989978
H	1.36396097	-0.72943758	4.16176868
H	2.34500527	-0.24323678	2.77201002
C	1.64340070	-2.28643382	2.65726768
H	2.56372062	-2.69818709	3.08815496
H	1.70214410	-2.37283742	1.56688166
H	0.81101947	-2.91203614	2.99841870
P	-0.00000000	0.00000000	-2.26574423
C	0.01994050	1.67490343	-3.06989978
H	0.96185341	2.15245253	-2.77201002
H	0.05026901	1.54594364	-4.16176868
C	-1.15840942	2.56644366	-2.65726768
H	-2.11638754	2.15838153	-2.99841870
H	-1.05483825	3.56934073	-3.08815496
H	-1.20386544	2.66051874	-1.56688166
C	1.44053867	-0.85472069	-3.06989978
H	1.31369196	-0.81650606	-4.16176868
H	1.38315186	-1.90921575	-2.77201002
C	2.80181012	-0.28000984	-2.65726768
H	2.92740700	0.75365461	-2.99841870
H	3.61855887	-0.87115364	-3.08815496
H	2.90600953	-0.28768132	-1.56688166
C	-1.46047917	-0.82018274	-3.06989978
H	-1.36396097	-0.72943758	-4.16176868
H	-2.34500527	-0.24323678	-2.77201002
C	-1.64340070	-2.28643382	-2.65726768
H	-0.81101947	-2.91203614	-2.99841870
H	-2.56372062	-2.69818709	-3.08815496
H	-1.70214410	-2.37283742	-1.56688166

(z) $Pt(Me)_2(P^iPr_3)_2$ reactant

Pt	0.00000000	0.00000000	1.09356088
P	0.08702291	1.92857063	-0.31832612
C	-1.11430086	3.26544279	0.25545688
H	-0.69635988	3.54008638	1.23216688
C	-1.19397463	4.55630140	-0.57514512
H	-1.77373439	5.30653892	-0.02119412
H	-0.20939408	4.98981899	-0.77995612
H	-1.70485537	4.39676528	-1.53021212
C	-2.51772022	2.69462569	0.53298388
H	-3.10729504	3.42403047	1.10337588
H	-3.06246902	2.48205533	-0.39229812
H	-2.45493691	1.77044317	1.11606188
C	-0.13904932	1.78640481	-2.19385412
H	0.45672630	0.89482266	-2.42779512
C	0.39862429	2.91638063	-3.09210212
H	-0.11346943	3.86632596	-2.92230512
H	1.47219623	3.08173416	-2.96447412
H	0.23632885	2.64068721	-4.14306812
C	-1.60282325	1.47527129	-2.55197712
H	-1.66960815	1.09880508	-3.58113012
H	-2.03694136	0.72609256	-1.88307412
H	-2.22294290	2.37558767	-2.49485112
C	1.76115627	2.78990803	-0.23449612
H	1.69186557	3.66391488	-0.89775112
C	2.86442566	1.85632883	-0.76494912
H	3.83511825	2.36718406	-0.72778512
H	2.92975138	0.95687785	-0.14231112
H	2.69565073	1.54436661	-1.80074812
C	2.15050597	3.28889547	1.16534088
H	2.23421188	2.45456616	1.86723788
H	3.12569979	3.79038128	1.11006688
H	1.43506136	4.00931898	1.57418188
P	-0.08702291	-1.92857063	-0.31832612
C	1.11430086	-3.26544279	0.25545688
H	0.69635988	-3.54008638	1.23216688
C	2.51772022	-2.69462569	0.53298388
H	3.10729504	-3.42403047	1.10337588
H	3.06246902	-2.48205533	-0.39229812
H	2.45493691	-1.77044317	1.11606188
C	1.19397463	-4.55630140	-0.57514512
H	1.70485537	-4.39676528	-1.53021212
H	1.77373439	-5.30653892	-0.02119412
H	0.20939408	-4.98981899	-0.77995612
C	-1.76115627	-2.78990803	-0.23449612
H	-1.69186557	-3.66391488	-0.89775112
C	-2.86442566	-1.85632883	-0.76494912
H	-2.92975138	-0.95687785	-0.14231112
H	-2.69565073	-1.54436661	-1.80074812
H	-3.83511825	-2.36718406	-0.72778512
C	-2.15050597	-3.28889547	1.16534088

H	-1.43506136	-4.00931898	1.57418188
H	-2.23421188	-2.45456616	1.86723788
H	-3.12569979	-3.79038128	1.11006688
C	0.13904932	-1.78640481	-2.19385412
H	-0.45672630	-0.89482266	-2.42779512
C	1.60282325	-1.47527129	-2.55197712
H	2.22294290	-2.37558767	-2.49485112
H	1.66960815	-1.09880508	-3.58113012
H	2.03694136	-0.72609256	-1.88307412
C	-0.39862429	-2.91638063	-3.09210212
H	-0.23632885	-2.64068721	-4.14306812
H	0.11346943	-3.86632596	-2.92230512
H	-1.47219623	-3.08173416	-2.96447412
C	-0.09781008	1.32841932	2.73011088
H	-1.08145173	1.19119259	3.19721688
H	0.65939272	1.05216198	3.47220788
H	0.02348430	2.39430518	2.53424288
C	0.09781008	-1.32841932	2.73011088
H	1.08145173	-1.19119259	3.19721688
H	-0.65939272	-1.05216198	3.47220788
H	-0.02348430	-2.39430518	2.53424288

(A) $Pt(Me)_2(P^iPr_3)_2$ TS

Pt	0.00000000	-0.00000000	0.74171988
P	0.08069604	2.10169368	-0.26823513
C	-1.15522697	3.35097800	0.42875589
H	-0.93727089	3.26084102	1.50465289
C	-0.99934683	4.83186496	0.04577989
H	-1.64588519	5.44876706	0.68499690
H	0.02550368	5.19691983	0.16723686
H	-1.30243383	5.01280544	-0.99024911
C	-2.61396770	2.89721616	0.23448293
H	-3.27282306	3.44486691	0.92080194
H	-2.96187515	3.09822617	-0.78395807
H	-2.73265550	1.82630312	0.42679793
C	0.00171510	2.15632795	-2.15904713
H	0.77313751	1.41086604	-2.40508214
C	0.37100543	3.46366112	-2.87895414
H	-0.38840479	4.23717947	-2.73100513
H	1.33491996	3.86818337	-2.55448216
H	0.44098569	3.28015514	-3.95998014
C	-1.33130037	1.60367953	-2.69131610
H	-1.22854985	1.32054475	-3.74701010
H	-1.64620005	0.72039692	-2.12545309
H	-2.12840698	2.35237349	-2.63131008
C	1.72411554	2.96138991	0.06136983
H	1.70668273	3.94050749	-0.43870117
C	2.88980801	2.14135607	-0.51722819
H	3.84582712	2.62985008	-0.28765121
H	2.90247532	1.13620479	-0.07989819
H	2.82403730	2.03523780	-1.60533119
C	1.93145327	3.18923908	1.56766783

H	1.86683751	2.23829297	2.10851483
H	2.92389400	3.62151696	1.74998681
H	1.18977693	3.87380536	1.99311484
P	-0.08069604	-2.10169368	-0.26823513
C	1.15522697	-3.35097800	0.42875589
H	0.93727089	-3.26084102	1.50465289
C	2.61396770	-2.89721616	0.23448293
H	3.27282306	-3.44486691	0.92080194
H	2.96187515	-3.09822617	-0.78395807
H	2.73265550	-1.82630312	0.42679793
C	0.99934683	-4.83186496	0.04577989
H	1.30243383	-5.01280544	-0.99024911
H	1.64588519	-5.44876706	0.68499690
H	-0.02550368	-5.19691983	0.16723686
C	-1.72411554	-2.96138991	0.06136983
H	-1.70668273	-3.94050749	-0.43870117
C	-2.88980801	-2.14135607	-0.51722819
H	-2.90247532	-1.13620479	-0.07989819
H	-2.82403730	-2.03523780	-1.60533119
H	-3.84582712	-2.62985008	-0.28765121
C	-1.93145327	-3.18923908	1.56766783
H	-1.18977693	-3.87380536	1.99311484
H	-1.86683751	-2.23829297	2.10851483
H	-2.92389400	-3.62151696	1.74998681
C	-0.00171510	-2.15632795	-2.15904713
H	-0.77313751	-1.41086604	-2.40508214
C	1.33130037	-1.60367953	-2.69131610
H	2.12840698	-2.35237349	-2.63131008
H	1.22854985	-1.32054475	-3.74701010
H	1.64620005	-0.72039692	-2.12545309
C	-0.37100543	-3.46366112	-2.87895414
H	-0.44098569	-3.28015514	-3.95998014
H	0.38840479	-4.23717947	-2.73100513
H	-1.33491996	-3.86818337	-2.55448216
C	-0.88054572	0.47807294	2.75091090
H	-1.77812634	0.52326505	2.10741792
H	-1.13143448	-0.18595385	3.58023291
H	-0.64243290	1.46876760	3.13827889
C	0.88054572	-0.47807294	2.75091090
H	1.77812634	-0.52326505	2.10741792
H	1.13143448	0.18595385	3.58023291
H	0.64243290	-1.46876760	3.13827889

(B) $Pt(P^{i}Pr_3)_2$

Pt	-0.00000000	0.00000000	0.00150704
P	0.11982990	2.27790033	0.01298904
C	-1.00390155	3.05144017	1.30771004
H	-0.53884990	2.67437105	2.23165804
C	-1.04695397	4.58497834	1.38654504
H	-1.57240536	4.89400747	2.29992404
H	-0.04983105	5.03734533	1.41216504
H	-1.59390030	5.01122451	0.53880704

C	-2.42250194	2.45543923	1.25955304
H	-2.96879598	2.71535847	2.17573304
H	-2.99665987	2.84165263	0.41100604
H	-2.37754030	1.36422653	1.17252104
C	-0.20636559	3.03415051	-1.68086896
H	0.46685433	2.42868738	-2.30723096
C	0.15792019	4.51366047	-1.88854996
H	-0.50773422	5.18030566	-1.33224896
H	1.18729178	4.73906696	-1.59213596
H	0.05981125	4.76720751	-2.95261096
C	-1.63886693	2.74367771	-2.16195396
H	-1.72128799	2.95024875	-3.23677396
H	-1.90841784	1.69580406	-1.99097096
H	-2.36963918	3.37889631	-1.64911496
C	1.81449290	2.94967155	0.45606504
H	1.77306390	4.04845613	0.42311804
C	2.85534649	2.46192614	-0.56803496
H	3.85672815	2.80519676	-0.27821596
H	2.86203953	1.36624462	-0.60742996
H	2.65653005	2.83417151	-1.57863496
C	2.22465540	2.51678284	1.87462004
H	2.17506959	1.42559100	1.97015804
H	3.25506112	2.83545879	2.07807204
H	1.58541880	2.95563368	2.64808304
P	-0.11982990	-2.27790033	0.01298904
C	1.00390155	-3.05144017	1.30771004
H	0.53884990	-2.67437105	2.23165804
C	2.42250194	-2.45543923	1.25955304
H	2.96879598	-2.71535847	2.17573304
H	2.99665987	-2.84165263	0.41100604
H	2.37754030	-1.36422653	1.17252104
C	1.04695397	-4.58497834	1.38654504
H	1.59390030	-5.01122451	0.53880704
H	1.57240536	-4.89400747	2.29992404
H	0.04983105	-5.03734533	1.41216504
C	-1.81449290	-2.94967155	0.45606504
H	-1.77306390	-4.04845613	0.42311804
C	-2.85534649	-2.46192614	-0.56803496
H	-2.86203953	-1.36624462	-0.60742996
H	-2.65653005	-2.83417151	-1.57863496
H	-3.85672815	-2.80519676	-0.27821596
C	-2.22465540	-2.51678284	1.87462004
H	-1.58541880	-2.95563368	2.64808304
H	-2.17506959	-1.42559100	1.97015804
H	-3.25506112	-2.83545879	2.07807204
C	0.20636559	-3.03415051	-1.68086896
H	-0.46685433	-2.42868738	-2.30723096
C	1.63886693	-2.74367771	-2.16195396
H	2.36963918	-3.37889631	-1.64911496
H	1.72128799	-2.95024875	-3.23677396
H	1.90841784	-1.69580406	-1.99097096
C	-0.15792019	-4.51366047	-1.88854996

H	-0.05981125	-4.76720751	-2.95261096
H	0.50773422	-5.18030566	-1.33224896
H	-1.18729178	-4.73906696	-1.59213596

(C) $Pt(H)_2(P^tBu_3)_2$ reactant

Pt	0.000000	0.000000	0.854725
P	-1.598500	1.547805	-0.124566
C	-3.314533	1.090332	0.681464
C	-4.559810	1.741948	0.041046
H	-5.445358	1.416340	0.604615
H	-4.530155	2.833861	0.083617
H	-4.714406	1.439388	-0.996295
C	-3.461017	-0.450913	0.612406
H	-4.344020	-0.748197	1.195520
H	-3.596698	-0.822794	-0.404883
H	-2.578132	-0.937137	1.043709
C	-3.347782	1.452267	2.186808
H	-4.286303	1.062811	2.605104
H	-2.521159	0.991826	2.732722
H	-3.336605	2.529694	2.365914
C	-1.910781	1.670577	-2.051217
C	-2.735724	2.861056	-2.586444
H	-3.731626	2.931948	-2.145714
H	-2.223655	3.815837	-2.439278
H	-2.863875	2.731520	-3.671101
C	-2.605146	0.362024	-2.498599
H	-2.551861	0.290098	-3.593372
H	-2.117317	-0.522976	-2.080837
H	-3.661568	0.332705	-2.223198
C	-0.532711	1.712905	-2.751385
H	0.164509	1.014374	-2.288158
H	-0.655619	1.430148	-3.805692
H	-0.082748	2.706350	-2.731540
C	-1.134681	3.342895	0.462191
C	0.000000	3.888049	-0.436561
H	0.419888	4.784203	0.040214
H	0.809571	3.159448	-0.548563
H	-0.352895	4.185464	-1.426478
C	-0.547701	3.308412	1.893944
H	0.364193	2.706839	1.930882
H	-0.304013	4.340474	2.185259
H	-1.237641	2.903329	2.634544
C	-2.298530	4.357977	0.446000
H	-3.063394	4.122667	1.190307
H	-1.897496	5.349943	0.697562
H	-2.782951	4.437239	-0.528715
P	1.598500	-1.547805	-0.124566
C	3.314533	-1.090332	0.681464
C	3.461017	0.450913	0.612406
H	4.344020	0.748197	1.195520
H	3.596698	0.822794	-0.404883
H	2.578132	0.937137	1.043709

C	4.559810	-1.741948	0.041046
H	4.714406	-1.439388	-0.996295
H	5.445358	-1.416340	0.604615
H	4.530155	-2.833861	0.083617
C	3.347782	-1.452267	2.186808
H	4.286303	-1.062811	2.605104
H	2.521159	-0.991826	2.732722
H	3.336605	-2.529694	2.365914
C	1.134681	-3.342895	0.462191
C	0.000000	-3.888049	-0.436561
H	-0.809571	-3.159448	-0.548563
H	0.352895	-4.185464	-1.426478
H	-0.419888	-4.784203	0.040214
C	0.547701	-3.308412	1.893944
H	1.237641	-2.903329	2.634544
H	-0.364193	-2.706839	1.930882
H	0.304013	-4.340474	2.185259
C	2.298530	-4.357977	0.446000
H	3.063394	-4.122667	1.190307
H	1.897496	-5.349943	0.697562
H	2.782951	-4.437239	-0.528715
C	1.910781	-1.670577	-2.051217
C	2.605146	-0.362024	-2.498599
H	3.661568	-0.332705	-2.223198
H	2.551861	-0.290098	-3.593372
H	2.117317	0.522976	-2.080837
C	2.735724	-2.861056	-2.586444
H	2.863875	-2.731520	-3.671101
H	3.731626	-2.931948	-2.145714
H	2.223655	-3.815837	-2.439278
C	0.532711	-1.712905	-2.751385
H	-0.164509	-1.014374	-2.288158
H	0.655619	-1.430148	-3.805692
H	0.082748	-2.706350	-2.731540
H	-0.695515	0.659861	2.110121
H	0.695515	-0.659861	2.110121

(D) $Pt(H)_2(P^tBu_3)_2$ TS

Pt	-0.00000000	0.00000000	0.69772061
P	-2.23958251	0.00230222	-0.09811731
C	-3.13104541	-1.50951844	0.74946636
C	-4.50737640	-1.90350191	0.17393158
H	-4.90613626	-2.73979473	0.76545695
H	-5.23460794	-1.08915425	0.22750326
H	-4.44752970	-2.24446503	-0.86193828
C	-2.17522136	-2.72515475	0.64629385
H	-2.59206733	-3.55449785	1.23528921
H	-2.04147497	-3.07795273	-0.37724601
H	-1.18835070	-2.46904612	1.05018270
C	-3.31732827	-1.24939689	2.26312926
H	-3.66652281	-2.18128108	2.72886067
H	-2.37391486	-0.97047993	2.74110411

H	-4.06427862	-0.48103440	2.47647496
C	-2.59597248	-0.13932176	-2.01361024
C	-4.03317753	0.14637427	-2.50080330
H	-4.78366261	-0.49785571	-2.03771600
H	-4.32414914	1.18783719	-2.33790474
H	-4.07380303	-0.03033987	-3.58563023
C	-2.20325113	-1.56477982	-2.46697465
H	-2.17295925	-1.58885959	-3.56467664
H	-1.21291010	-1.84680896	-2.09713956
H	-2.92285802	-2.32127897	-2.14565830
C	-1.64581047	0.83727559	-2.74526968
H	-0.64888571	0.81149435	-2.30040171
H	-1.56679943	0.54018113	-3.79970656
H	-2.00359847	1.86744595	-2.72184311
C	-3.13127050	1.62100447	0.50265304
C	-2.73619570	2.79535280	-0.42383647
H	-3.04237824	3.73423379	0.05754414
H	-1.65352952	2.83701211	-0.58193753
H	-3.23605934	2.75277904	-1.39421844
C	-2.60117499	2.00503949	1.90539986
H	-1.52079139	2.17233217	1.87716075
H	-3.09439931	2.93650438	2.21789048
H	-2.80065097	1.24821339	2.66455018
C	-4.67250966	1.55399821	0.56913112
H	-5.02423885	0.85227946	1.32943743
H	-5.05319804	2.54725669	0.84679772
H	-5.13122306	1.28337143	-0.38421875
P	2.23958251	-0.00230222	-0.09811731
C	3.13104541	1.50951844	0.74946636
C	2.17522136	2.72515475	0.64629385
H	2.59206733	3.55449785	1.23528921
H	2.04147497	3.07795273	-0.37724601
H	1.18835070	2.46904612	1.05018270
C	4.50737640	1.90350191	0.17393158
H	4.44752970	2.24446503	-0.86193828
H	4.90613626	2.73979473	0.76545695
H	5.23460794	1.08915425	0.22750326
C	3.31732827	1.24939689	2.26312926
H	3.66652281	2.18128108	2.72886067
H	2.37391486	0.97047993	2.74110411
H	4.06427862	0.48103440	2.47647496
C	3.13127050	-1.62100447	0.50265304
C	2.73619570	-2.79535280	-0.42383647
H	1.65352952	-2.83701211	-0.58193753
H	3.23605934	-2.75277904	-1.39421844
H	3.04237824	-3.73423379	0.05754414
C	2.60117499	-2.00503949	1.90539986
H	2.80065097	-1.24821339	2.66455018
H	1.52079139	-2.17233217	1.87716075
H	3.09439931	-2.93650438	2.21789048
C	4.67250966	-1.55399821	0.56913112
H	5.02423885	-0.85227946	1.32943743

H	5.05319804	-2.54725669	0.84679772
H	5.13122306	-1.28337143	-0.38421875
C	2.59597248	0.13932176	-2.01361024
C	2.20325113	1.56477982	-2.46697465
H	2.92285802	2.32127897	-2.14565830
H	2.17295925	1.58885959	-3.56467664
H	1.21291010	1.84680896	-2.09713956
C	4.03317753	-0.14637427	-2.50080330
H	4.07380303	0.03033987	-3.58563023
H	4.78366261	0.49785571	-2.03771600
H	4.32414914	-1.18783719	-2.33790474
C	1.64581047	-0.83727559	-2.74526968
H	0.64888571	-0.81149435	-2.30040171
H	1.56679943	-0.54018113	-3.79970656
H	2.00359847	-1.86744595	-2.72184311
H	-0.53039003	-0.01214445	2.27557464
H	0.53039003	0.01214445	2.27557464

(E) $Pt(P^tBu_3)_2$

Pt	-0.00000000	0.00000000	0.00754580
P	0.00090251	-2.30024613	0.00004987
C	0.11819014	-2.99343789	1.80363693
C	-1.23506779	-2.76513931	2.51652278
H	-1.09952717	-2.96622605	3.58800002
H	-1.56883890	-1.72789015	2.40745734
H	-2.02264665	-3.43266705	2.15853596
C	1.14560456	-2.13256469	2.58139752
H	0.89826724	-1.06921022	2.48691218
H	2.17122813	-2.27111572	2.23844351
H	1.10690808	-2.41552685	3.64302391
C	0.50137703	-4.48114283	1.94321008
H	1.51383378	-4.68497374	1.58377263
H	-0.18956174	-5.14698753	1.41919043
H	0.47662207	-4.75263631	3.00823406
C	1.50596953	-2.98208425	-1.01009251
C	1.66061999	-2.11255311	-2.28292420
H	2.61240528	-2.36950274	-2.76943911
H	0.86420175	-2.27012126	-3.01067099
H	1.67155895	-1.04928933	-2.01741103
C	1.44006469	-4.46691369	-1.42026941
H	1.33256725	-5.13900505	-0.56484779
H	2.37544740	-4.73269404	-1.93295681
H	0.62311960	-4.66693272	-2.11877582
C	2.79830875	-2.75202858	-0.19274335
H	2.86975331	-1.71387786	0.14865617
H	3.66021600	-2.95397589	-0.84332178
H	2.88007777	-3.41707863	0.67016134
C	-1.62457407	-2.98078549	-0.80212793
C	-1.56623177	-2.74471339	-2.32961574
H	-2.56222810	-2.94484288	-2.74797887
H	-1.30566866	-1.70659789	-2.56077087
H	-0.86304779	-3.41009128	-2.83639090

C	-2.80373453	-2.11376621	-0.29275718
H	-3.70167292	-2.36458206	-0.87514007
H	-2.57577320	-1.04974464	-0.42673581
H	-3.03467959	-2.27947824	0.75996208
C	-1.94582919	-4.46811528	-0.54968051
H	-2.13229163	-4.67969704	0.50658724
H	-1.15450447	-5.13649075	-0.89936615
H	-2.86291006	-4.72775177	-1.09750397
P	-0.00090251	2.30024613	0.00004987
C	-0.11819014	2.99343789	1.80363693
C	1.23506779	2.76513931	2.51652278
H	2.02264665	3.43266705	2.15853596
H	1.09952717	2.96622605	3.58800002
H	1.56883890	1.72789015	2.40745734
C	-0.50137703	4.48114283	1.94321008
H	-1.51383378	4.68497374	1.58377263
H	0.18956174	5.14698753	1.41919043
H	-0.47662207	4.75263631	3.00823406
C	-1.14560456	2.13256469	2.58139752
H	-1.10690808	2.41552685	3.64302391
H	-0.89826724	1.06921022	2.48691218
H	-2.17122813	2.27111572	2.23844351
C	-1.50596953	2.98208425	-1.01009251
C	-1.44006469	4.46691369	-1.42026941
H	-2.37544740	4.73269404	-1.93295681
H	-1.33256725	5.13900505	-0.56484779
H	-0.62311960	4.66693272	-2.11877582
C	-1.66061999	2.11255311	-2.28292420
H	-2.61240528	2.36950274	-2.76943911
H	-1.67155895	1.04928933	-2.01741103
H	-0.86420175	2.27012126	-3.01067099
C	-2.79830875	2.75202858	-0.19274335
H	-2.86975331	1.71387786	0.14865617
H	-3.66021600	2.95397589	-0.84332178
H	-2.88007777	3.41707863	0.67016134
C	1.62457407	2.98078549	-0.80212793
C	1.56623177	2.74471339	-2.32961574
H	0.86304779	3.41009128	-2.83639090
H	2.56222810	2.94484288	-2.74797887
H	1.30566866	1.70659789	-2.56077087
C	1.94582919	4.46811528	-0.54968051
H	1.15450447	5.13649075	-0.89936615
H	2.86291006	4.72775177	-1.09750397
H	2.13229163	4.67969704	0.50658724
C	2.80373453	2.11376621	-0.29275718
H	3.70167292	2.36458206	-0.87514007
H	2.57577320	1.04974464	-0.42673581
H	3.03467959	2.27947824	0.75996208

(F) $[Rh(Cl)(P^{i}Pr_3)_2]_2$

Rh	1.928974	0.000000	0.000000
Rh	-1.928974	0.000000	0.000000

Cl	0.000000	1.542046	0.000000
Cl	0.000000	-1.542046	0.000000
P	3.310374	1.731356	0.555509
P	3.310374	-1.731356	-0.555509
P	-3.310374	1.731356	-0.555509
P	-3.310374	-1.731356	0.555509
C	5.197266	1.708492	0.383033
H	5.447560	0.686615	0.689739
C	2.730801	3.347605	-0.231104
H	1.712543	3.424333	0.171604
C	3.139261	2.092865	2.402650
H	3.801296	2.945519	2.611523
C	5.197266	-1.708492	-0.383033
H	5.447560	-0.686615	-0.689739
C	3.139261	-2.092865	-2.402650
H	3.801296	-2.945519	-2.611523
C	2.730801	-3.347605	0.231104
H	1.712543	-3.424333	-0.171604
C	-2.730801	3.347605	0.231104
H	-1.712543	3.424333	-0.171604
C	-5.197266	1.708492	-0.383033
H	-5.447560	0.686615	-0.689739
C	-3.139261	2.092865	-2.402650
H	-3.801296	2.945519	-2.611523
C	-2.730801	-3.347605	-0.231104
H	-1.712543	-3.424333	0.171604
C	-3.139261	-2.092865	2.402650
H	-3.801296	-2.945519	2.611523
C	-5.197266	-1.708492	0.383033
H	-5.447560	-0.686615	0.689739
C	6.020783	2.641682	1.293000
H	5.809109	3.698325	1.112356
H	5.863799	2.439196	2.355947
H	7.088069	2.481532	1.087359
C	5.644278	1.886301	-1.079883
H	5.035714	1.304042	-1.777826
H	5.584991	2.936941	-1.382358
H	6.690773	1.573604	-1.193348
C	1.718008	2.483111	2.835237
H	1.354368	3.381292	2.327182
H	1.007328	1.677934	2.630285
H	1.714045	2.685447	3.914898
C	3.616119	0.883265	3.225122
H	3.520554	1.097408	4.297680
H	3.000285	0.007771	2.989664
H	4.663003	0.624986	3.031109
C	2.574285	3.239815	-1.758574
H	3.540019	3.235291	-2.273601
H	2.028978	2.331067	-2.029374
H	2.005220	4.102435	-2.129613
C	3.483269	4.630467	0.157593
H	3.596644	4.743194	1.240818

H	4.477669	4.674144	-0.298979
H	2.922675	5.502052	-0.206349
C	2.574285	-3.239815	1.758574
H	2.005220	-4.102435	2.129613
H	3.540019	-3.235291	2.273601
H	2.028978	-2.331067	2.029374
C	3.483269	-4.630467	-0.157593
H	2.922675	-5.502052	0.206349
H	3.596644	-4.743194	-1.240818
H	4.477669	-4.674144	0.298979
C	3.616119	-0.883265	-3.225122
H	4.663003	-0.624986	-3.031109
H	3.520554	-1.097408	-4.297680
H	3.000285	-0.007771	-2.989664
C	1.718008	-2.483111	-2.835237
H	1.714045	-2.685447	-3.914898
H	1.354368	-3.381292	-2.327182
H	1.007328	-1.677934	-2.630285
C	5.644278	-1.886301	1.079883
H	6.690773	-1.573604	1.193348
H	5.035714	-1.304042	1.777826
H	5.584991	-2.936941	1.382358
C	6.020783	-2.641682	-1.293000
H	5.809109	-3.698325	-1.112356
H	5.863799	-2.439196	-2.355947
H	7.088069	-2.481532	-1.087359
C	-3.616119	0.883265	-3.225122
H	-3.520554	1.097408	-4.297680
H	-3.000285	0.007771	-2.989664
H	-4.663003	0.624986	-3.031109
C	-1.718008	2.483111	-2.835237
H	-1.007328	1.677934	-2.630285
H	-1.714045	2.685447	-3.914898
H	-1.354368	3.381292	-2.327182
C	-6.020783	2.641682	-1.293000
H	-5.809109	3.698325	-1.112356
H	-5.863799	2.439196	-2.355947
H	-7.088069	2.481532	-1.087359
C	-5.644278	1.886301	1.079883
H	-6.690773	1.573604	1.193348
H	-5.035714	1.304042	1.777826
H	-5.584991	2.936941	1.382358
C	-3.483269	4.630467	-0.157593
H	-2.922675	5.502052	0.206349
H	-3.596644	4.743194	-1.240818
H	-4.477669	4.674144	0.298979
C	-2.574285	3.239815	1.758574
H	-2.005220	4.102435	2.129613
H	-3.540019	3.235291	2.273601
H	-2.028978	2.331067	2.029374
C	-3.616119	-0.883265	3.225122
H	-3.000285	-0.007771	2.989664

H	-4.663003	-0.624986	3.031109
H	-3.520554	-1.097408	4.297680
C	-1.718008	-2.483111	2.835237
H	-1.354368	-3.381292	2.327182
H	-1.007328	-1.677934	2.630285
H	-1.714045	-2.685447	3.914898
C	-5.644278	-1.886301	-1.079883
H	-5.584991	-2.936941	-1.382358
H	-6.690773	-1.573604	-1.193348
H	-5.035714	-1.304042	-1.777826
C	-6.020783	-2.641682	1.293000
H	-7.088069	-2.481532	1.087359
H	-5.809109	-3.698325	1.112356
H	-5.863799	-2.439196	2.355947
C	-2.574285	-3.239815	-1.758574
H	-2.005220	-4.102435	-2.129613
H	-3.540019	-3.235291	-2.273601
H	-2.028978	-2.331067	-2.029374
C	-3.483269	-4.630467	0.157593
H	-4.477669	-4.674144	-0.298979
H	-2.922675	-5.502052	-0.206349
H	-3.596644	-4.743194	1.240818

(G) $Rh(Cl)(P^{i}Pr_3)_2$

Rh	-0.07200234	-0.10181553	-0.01461004
P	0.11690434	2.23220402	0.04130186
P	-0.03161635	-2.38679628	-0.18073066
C	1.09054174	2.87802910	1.51228187
H	1.21103080	3.96413912	1.38706720
C	-1.53099682	3.11552864	0.18106734
H	-1.87807008	2.73087846	1.15164203
C	1.09770493	2.90440610	-1.42665957
H	1.96059410	2.21839928	-1.44897521
C	2.48690026	2.23026935	1.53904860
H	3.05891201	2.60726718	2.39643968
H	2.39598669	1.14221358	1.64033660
H	3.06774532	2.44091818	0.63368971
C	0.35838551	2.61949388	2.83977727
H	0.10462147	1.56031707	2.94989797
H	1.00279546	2.91528122	3.67798646
H	-0.57087700	3.19217617	2.91991345
C	1.65210904	4.33489674	-1.31910500
H	2.25249159	4.56196664	-2.21034493
H	0.85176099	5.07828209	-1.26467570
H	2.29969230	4.46972115	-0.44744789
C	-1.50160144	4.65027295	0.24289738
H	-0.77443342	5.03437392	0.96637120
H	-1.27385598	5.08757829	-0.73570010
H	-2.49028005	5.02330533	0.54098565
C	-2.55131995	2.61700971	-0.85835327
H	-2.56456695	1.52354395	-0.89463358
H	-3.55515794	2.95971226	-0.57670535

H	-2.33935931	3.00145987	-1.86140081
C	0.33631366	2.71794852	-2.75208096
H	1.02453109	2.83113627	-3.59961585
H	-0.13335602	1.73030631	-2.81825095
H	-0.44885192	3.47288415	-2.86447342
C	-1.45199032	-3.37613703	-0.89342833
H	-1.05704260	-4.35233614	-1.21666013
C	0.48533226	-3.34096797	1.34362173
H	-0.39158835	-3.18634990	1.99206256
C	1.29981428	-2.38785637	-1.51160273
H	0.73222716	-2.48219193	-2.44882456
C	-2.04674855	-2.64901306	-2.11283538
H	-2.40174420	-1.65357988	-1.82410572
H	-1.32598370	-2.52625768	-2.92876500
H	-2.89594407	-3.22106908	-2.50720321
C	-2.54701112	-3.59756782	0.16754386
H	-3.40586472	-4.10377421	-0.29062434
H	-2.20537045	-4.21823072	1.00188886
H	-2.88961781	-2.63962023	0.57415085
C	0.70631642	-4.85363685	1.17926926
H	1.61069727	-5.07159717	0.60291220
H	0.82854559	-5.31635950	2.16721136
H	-0.13751039	-5.34879572	0.68766063
C	2.41234720	-3.43937062	-1.52779876
H	3.01959573	-3.40789319	-0.61775026
H	2.00880208	-4.45154050	-1.63362945
H	3.08431573	-3.26042139	-2.37818840
C	1.67357178	-2.66043430	2.04568242
H	1.47936207	-1.59185816	2.18678894
H	1.83541110	-3.11646464	3.03054682
H	2.60328894	-2.77108256	1.47546722
C	1.83834758	-0.94114690	-1.44283262
H	2.46086925	-0.69082106	-2.31354763
H	0.98000312	-0.18644921	-1.56775190
H	2.43542340	-0.76206357	-0.54396009
Cl	-1.79156129	-0.07158034	1.56000826

(H) Rh(Cl)(P^iPr_3)$_2$(CO)

Rh	0.00000000	0.00000000	-0.03532946
P	0.12109631	2.37486210	-0.01685322
P	-0.12109631	-2.37486210	-0.01685322
C	1.90333866	2.95156028	0.03577505
H	1.89555995	4.05086070	0.00845536
C	-0.65687062	3.15846715	1.49634577
H	-0.14080646	2.60748514	2.29466187
C	-0.55047762	3.15476303	-1.59162372
H	0.01644831	2.61559956	-2.36476891
C	2.68502165	2.44094328	-1.18755662
H	3.72701319	2.77871510	-1.12569842
H	2.68343843	1.34553153	-1.21387766
H	2.27528075	2.80550456	-2.13546557
C	2.59395076	2.50299711	1.33596878

H	2.55368896	1.41461151	1.44659854
H	3.64676995	2.81208692	1.31559623
H	2.13467620	2.94089580	2.22742165
C	-0.29163829	4.65642714	-1.79489472
H	-0.57533411	4.93722311	-2.81755177
H	-0.88982581	5.26675570	-1.11217328
H	0.76043276	4.92673010	-1.66223970
C	-0.41457886	4.66167569	1.70532735
H	0.64107854	4.93985407	1.62493776
H	-0.98349328	5.27116007	0.99649157
H	-0.74834553	4.93923906	2.71361272
C	-2.14979613	2.81242445	1.63644692
H	-2.32685868	1.74595393	1.47029198
H	-2.48121150	3.04984592	2.65486165
H	-2.77080161	3.38933828	0.94358882
C	-2.03701958	2.82374089	-1.81933507
H	-2.30115581	3.01551866	-2.86660410
H	-2.26053386	1.77478999	-1.59968684
H	-2.68398109	3.44802292	-1.19553349
C	-1.90333866	-2.95156028	0.03577505
H	-1.89555995	-4.05086070	0.00845536
C	0.65687062	-3.15846715	1.49634577
H	0.14080646	-2.60748514	2.29466187
C	0.55047762	-3.15476303	-1.59162372
H	-0.01644831	-2.61559956	-2.36476891
C	-2.68502165	-2.44094328	-1.18755662
H	-2.68343843	-1.34553153	-1.21387766
H	-2.27528075	-2.80550456	-2.13546557
H	-3.72701319	-2.77871510	-1.12569842
C	-2.59395076	-2.50299711	1.33596878
H	-3.64676995	-2.81208692	1.31559623
H	-2.13467620	-2.94089580	2.22742165
H	-2.55368896	-1.41461151	1.44659854
C	0.41457886	-4.66167569	1.70532735
H	0.98349328	-5.27116007	0.99649157
H	0.74834553	-4.93923906	2.71361272
H	-0.64107854	-4.93985407	1.62493776
C	0.29163829	-4.65642714	-1.79489472
H	0.88982581	-5.26675570	-1.11217328
H	-0.76043276	-4.92673010	-1.66223970
H	0.57533411	-4.93722311	-2.81755177
C	2.14979613	-2.81242445	1.63644692
H	2.32685868	-1.74595393	1.47029198
H	2.48121150	-3.04984592	2.65486165
H	2.77080161	-3.38933828	0.94358882
C	2.03701958	-2.82374089	-1.81933507
H	2.30115581	-3.01551866	-2.86660410
H	2.26053386	-1.77478999	-1.59968684
H	2.68398109	-3.44802292	-1.19553349
Cl	0.00000000	0.00000000	2.36355081
C	0.00000000	0.00000000	-1.83763723
O	0.00000000	0.00000000	-3.00395052

(I) $Rh(H)_2(Cl)(P^iPr_3)_2$

Rh	0.00000000	-0.00000000	-0.02591663
P	0.10403920	2.32859737	-0.14926038
P	-0.10403920	-2.32859737	-0.14926038
C	1.80172144	3.03279478	0.22401371
H	1.75347688	4.11059870	0.01139735
C	-1.01366596	3.17529303	1.09282372
H	-0.55755282	2.84047572	2.03623927
C	-0.23729597	2.96647542	-1.88931445
H	0.34899749	2.26052077	-2.49682502
C	2.85609692	2.39911189	-0.70222666
H	3.83630347	2.85539157	-0.51569584
H	2.93742696	1.32386314	-0.50920402
H	2.62271499	2.53220149	-1.76444709
C	2.20713254	2.85380638	1.69717358
H	2.16076296	1.80373483	2.00140808
H	3.23548270	3.21171737	1.83580160
H	1.56548829	3.42314243	2.37698994
C	0.24419955	4.38987497	-2.22149335
H	0.04690902	4.59855899	-3.28128633
H	-0.28263897	5.14924760	-1.63582870
H	1.31835617	4.52057971	-2.05950447
C	-1.02575078	4.71178718	1.06518047
H	-0.01912492	5.14319318	1.06107578
H	-1.56506181	5.09181815	0.19054655
H	-1.54358785	5.08990700	1.95605176
C	-2.44428640	2.60516294	1.08860528
H	-2.43302667	1.51227894	1.14065006
H	-2.98397256	2.97603011	1.96915472
H	-3.00830656	2.90865580	0.20127524
C	-1.71183822	2.79167051	-2.29361834
H	-1.81565955	2.92177092	-3.37817837
H	-2.09197235	1.79834041	-2.03415711
H	-2.34743092	3.54149028	-1.81066821
C	-1.80172144	-3.03279478	0.22401371
H	-1.75347688	-4.11059870	0.01139735
C	1.01366596	-3.17529303	1.09282372
H	0.55755282	-2.84047572	2.03623927
C	0.23729597	-2.96647542	-1.88931445
H	-0.34899749	-2.26052077	-2.49682502
C	-2.85609692	-2.39911189	-0.70222666
H	-2.93742696	-1.32386314	-0.50920402
H	-2.62271499	-2.53220149	-1.76444709
H	-3.83630347	-2.85539157	-0.51569584
C	-2.20713254	-2.85380638	1.69717358
H	-3.23548270	-3.21171737	1.83580160
H	-1.56548829	-3.42314243	2.37698994
H	-2.16076296	-1.80373483	2.00140808
C	1.02575078	-4.71178718	1.06518047
H	1.56506181	-5.09181815	0.19054655
H	1.54358785	-5.08990700	1.95605176

H	0.01912492	-5.14319318	1.06107578
C	-0.24419955	-4.38987497	-2.22149335
H	0.28263897	-5.14924760	-1.63582870
H	-1.31835617	-4.52057971	-2.05950447
H	-0.04690902	-4.59855899	-3.28128633
C	2.44428640	-2.60516294	1.08860528
H	2.43302667	-1.51227894	1.14065006
H	2.98397256	-2.97603011	1.96915472
H	3.00830656	-2.90865580	0.20127524
C	1.71183822	-2.79167051	-2.29361834
H	1.81565955	-2.92177092	-3.37817837
H	2.09197235	-1.79834041	-2.03415711
H	2.34743092	-3.54149028	-1.81066821
Cl	0.00000000	-0.00000000	2.40667990
H	0.85331837	-0.02098028	-1.29253387
H	-0.85331837	0.02098028	-1.29253387

(J) $Rh(Cl)(P^iPr_3)_2(N_2)$ end-on

Rh	0.00000000	-0.00000000	0.04198482
P	-0.12016607	2.37539641	0.00735046
P	0.12016607	-2.37539641	0.00735046
C	-1.89756561	2.96839462	-0.03017861
H	-1.88176850	4.06731125	0.00591223
C	0.65191074	3.16737341	-1.50460241
H	0.13468575	2.61917633	-2.30413423
C	0.56296547	3.14242322	1.58377070
H	-0.00974780	2.60916964	2.35680105
C	-2.67413289	2.45156693	1.19392424
H	-3.71722324	2.78699553	1.13761267
H	-2.67064254	1.35580342	1.21546036
H	-2.26186932	2.81388860	2.14158463
C	-2.59992174	2.53244967	-1.32844464
H	-2.56710807	1.44424346	-1.44436655
H	-3.65071598	2.84786344	-1.29980626
H	-2.14380698	2.97260697	-2.22043607
C	0.32508308	4.64641270	1.79641352
H	0.61854409	4.91854753	2.81875685
H	0.92727926	5.25209394	1.11302936
H	-0.72392138	4.93215352	1.67163579
C	0.40642687	4.67086293	-1.70911157
H	-0.64993264	4.94654979	-1.62938432
H	0.97251849	5.27956069	-0.99732164
H	0.74117714	4.95291187	-2.71587330
C	2.14527054	2.82519056	-1.64852084
H	2.32542687	1.75943105	-1.48089299
H	2.47457795	3.06331393	-2.66750770
H	2.76539472	3.40482911	-0.95698413
C	2.04521427	2.78934567	1.80670925
H	2.31635557	2.97493650	2.85346832
H	2.25176449	1.73809989	1.58189010
H	2.69917893	3.40527352	1.18198702
C	1.89756561	-2.96839462	-0.03017861

H	1.88176850	-4.06731125	0.00591223
C	-0.65191074	-3.16737341	-1.50460241
H	-0.13468575	-2.61917633	-2.30413423
C	-0.56296547	-3.14242322	1.58377070
H	0.00974780	-2.60916964	2.35680105
C	2.67413289	-2.45156693	1.19392424
H	2.67064254	-1.35580342	1.21546036
H	2.26186932	-2.81388860	2.14158463
H	3.71722324	-2.78699553	1.13761267
C	2.59992174	-2.53244967	-1.32844464
H	3.65071598	-2.84786344	-1.29980626
H	2.14380698	-2.97260697	-2.22043607
H	2.56710807	-1.44424346	-1.44436655
C	-0.40642687	-4.67086293	-1.70911157
H	-0.97251849	-5.27956069	-0.99732164
H	-0.74117714	-4.95291187	-2.71587330
H	0.64993264	-4.94654979	-1.62938432
C	-0.32508308	-4.64641270	1.79641352
H	-0.92727926	-5.25209394	1.11302936
H	0.72392138	-4.93215352	1.67163579
H	-0.61854409	-4.91854753	2.81875685
C	-2.14527054	-2.82519056	-1.64852084
H	-2.32542687	-1.75943105	-1.48089299
H	-2.47457795	-3.06331393	-2.66750770
H	-2.76539472	-3.40482911	-0.95698413
C	-2.04521427	-2.78934567	1.80670925
H	-2.31635557	-2.97493650	2.85346832
H	-2.25176449	-1.73809989	1.58189010
H	-2.69917893	-3.40527352	1.18198702
Cl	0.00000000	-0.00000000	-2.31748518
N	0.00000000	0.00000000	1.91178082
N	0.00000000	0.00000000	3.03747082

(K) Rh(Cl)(P^iPr_3)$_2$(N_2) side-on

Rh	-0.00000000	0.00000000	0.10607385
P	-0.10780523	2.37459812	0.03356285
P	0.10780523	-2.37459812	0.03356285
C	-1.81809740	3.02019113	-0.38923115
H	-1.78750517	4.11102600	-0.25497015
C	1.00529422	3.10795972	-1.28189915
H	0.55146473	2.68517332	-2.18941515
C	0.23254360	3.19696201	1.69651585
H	-0.32494272	2.55663967	2.39588185
C	-2.84906420	2.43120602	0.59179385
H	-3.84524669	2.83461060	0.37115685
H	-2.89021981	1.34088961	0.49173685
H	-2.62018479	2.66127204	1.63813185
C	-2.23902248	2.73222476	-1.83977115
H	-2.22678507	1.65967815	-2.05245615
H	-3.25791309	3.10812817	-2.00016615
H	-1.58693858	3.22227473	-2.56982515
C	-0.28770022	4.63347169	1.88471985

H	-0.05443137	4.96712737	2.90445685
H	0.18470116	5.33704029	1.19329685
H	-1.37191977	4.70797513	1.75926285
C	1.00927900	4.63960844	-1.40258215
H	0.00120938	5.06393544	-1.46107215
H	1.53128489	5.10972953	-0.56187415
H	1.54094837	4.93094083	-2.31783315
C	2.43751542	2.54650402	-1.21998515
H	2.42511009	1.45648082	-1.12712015
H	2.96788772	2.80076543	-2.14633815
H	3.00886853	2.96283678	-0.38491415
C	1.71874670	3.10883357	2.08982685
H	1.83239755	3.34902008	3.15432185
H	2.13392501	2.11023449	1.92444585
H	2.31951029	3.82904686	1.52447085
C	1.81809740	-3.02019113	-0.38923115
H	1.78750517	-4.11102600	-0.25497015
C	-1.00529422	-3.10795972	-1.28189915
H	-0.55146473	-2.68517332	-2.18941515
C	-0.23254360	-3.19696201	1.69651585
H	0.32494272	-2.55663967	2.39588185
C	2.84906420	-2.43120602	0.59179385
H	2.89021981	-1.34088961	0.49173685
H	2.62018479	-2.66127204	1.63813185
H	3.84524669	-2.83461060	0.37115685
C	2.23902248	-2.73222476	-1.83977115
H	3.25791309	-3.10812817	-2.00016615
H	1.58693858	-3.22227473	-2.56982515
H	2.22678507	-1.65967815	-2.05245615
C	-1.00927900	-4.63960844	-1.40258215
H	-1.53128489	-5.10972953	-0.56187415
H	-1.54094837	-4.93094083	-2.31783315
H	-0.00120938	-5.06393544	-1.46107215
C	0.28770022	-4.63347169	1.88471985
H	-0.18470116	-5.33704029	1.19329685
H	1.37191977	-4.70797513	1.75926285
H	0.05443137	-4.96712737	2.90445685
C	-2.43751542	-2.54650402	-1.21998515
H	-2.42511009	-1.45648082	-1.12712015
H	-2.96788772	-2.80076543	-2.14633815
H	-3.00886853	-2.96283678	-0.38491415
C	-1.71874670	-3.10883357	2.08982685
H	-1.83239755	-3.34902008	3.15432185
H	-2.13392501	-2.11023449	1.92444585
H	-2.31951029	-3.82904686	1.52447085
Cl	-0.00000000	0.00000000	-2.24219915
N	-0.57294999	0.03498020	2.15729785
N	0.57294999	-0.03498020	2.15729785

(L) $Rh(Cl)(P^{i}Pr_3)_2(C_2H_4)$

Rh	-0.00000000	0.00000000	0.17577198
P	-0.10618837	2.37603633	0.04695598

P	0.10618837	-2.37603633	0.04695598
C	-1.83126203	3.00088435	-0.37568402
H	-1.80386904	4.09438476	-0.26752702
C	0.95500980	3.08025268	-1.33176102
H	0.48286408	2.61271466	-2.20600402
C	0.29151355	3.32386760	1.63748198
H	-0.11052308	2.67109402	2.42659898
C	-2.86451251	2.43795866	0.61690598
H	-3.85751784	2.84703905	0.39154198
H	-2.91559082	1.34684816	0.53311998
H	-2.63269156	2.68642449	1.65884298
C	-2.26291999	2.67793916	-1.81613802
H	-2.23695464	1.60186140	-2.00831602
H	-3.28873580	3.03720098	-1.97202702
H	-1.62622725	3.16158274	-2.56334302
C	-0.37113111	4.70308994	1.81347698
H	-0.06243063	5.12812226	2.77776398
H	-0.06775696	5.40702257	1.03248898
H	-1.46360411	4.64990846	1.81767298
C	0.91649384	4.60554704	-1.51316402
H	-0.10384076	4.99789658	-1.58113502
H	1.43020002	5.12787023	-0.69879902
H	1.43158021	4.87307478	-2.44520702
C	2.40100823	2.55182699	-1.30532902
H	2.41662371	1.47067709	-1.13809902
H	2.87565246	2.74778876	-2.27510102
H	3.00788120	3.03701676	-0.53518302
C	1.80878250	3.44625088	1.88266398
H	1.98950094	3.74075706	2.92429198
H	2.34474828	2.51065611	1.69819798
H	2.25018502	4.21711478	1.24307798
C	1.83126203	-3.00088435	-0.37568402
H	1.80386904	-4.09438476	-0.26752702
C	-0.95500980	-3.08025268	-1.33176102
H	-0.48286408	-2.61271466	-2.20600402
C	-0.29151355	-3.32386760	1.63748198
H	0.11052308	-2.67109402	2.42659898
C	2.86451251	-2.43795866	0.61690598
H	2.91559082	-1.34684816	0.53311998
H	2.63269156	-2.68642449	1.65884298
H	3.85751784	-2.84703905	0.39154198
C	2.26291999	-2.67793916	-1.81613802
H	3.28873580	-3.03720098	-1.97202702
H	1.62622725	-3.16158274	-2.56334302
H	2.23695464	-1.60186140	-2.00831602
C	-0.91649384	-4.60554704	-1.51316402
H	-1.43020002	-5.12787023	-0.69879902
H	-1.43158021	-4.87307478	-2.44520702
H	0.10384076	-4.99789658	-1.58113502
C	0.37113111	-4.70308994	1.81347698
H	0.06775696	-5.40702257	1.03248898
H	1.46360411	-4.64990846	1.81767298

H	0.06243063	-5.12812226	2.77776398
C	-2.40100823	-2.55182699	-1.30532902
H	-2.41662371	-1.47067709	-1.13809902
H	-2.87565246	-2.74778876	-2.27510102
H	-3.00788120	-3.03701676	-0.53518302
C	-1.80878250	-3.44625088	1.88266398
H	-1.98950094	-3.74075706	2.92429198
H	-2.34474828	-2.51065611	1.69819798
H	-2.25018502	-4.21711478	1.24307798
Cl	-0.00000000	0.00000000	-2.22862502
C	0.70638741	-0.00808611	2.16508598
C	-0.70638741	0.00808611	2.16508598
H	1.24447115	-0.91957729	2.41342698
H	1.26525442	0.88817625	2.41658698
H	-1.24447115	0.91957729	2.41342698
H	-1.26525442	-0.88817625	2.41658698

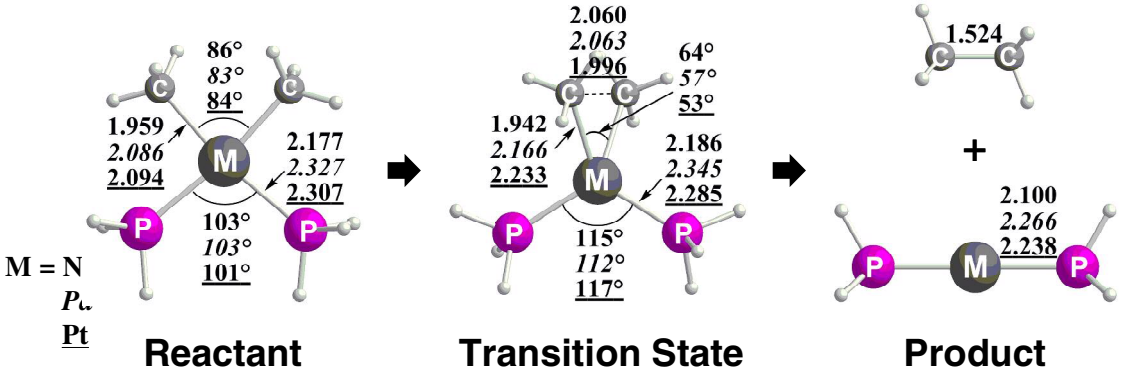

Figure S1. Geometry changes by the reductive elimination of ethane from $M(Me)_2(PH_3)_2$ (M = Ni, Pd, Pt) with DFT[B3PW91] method. Bond lengths are in angstrom and bond angles are in degree. Upper: M = Ni, Middle: M = Pd, Bottom: M = Pt.