Supporting Information

Understanding the Relative Easiness of Oxidative Addition of Aryl and Alkyl Halides to Pd(0)

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Computational Details

Gaussian 03[i] was used to fully optimize all structures at the B3LYP level.[ii] Frequency calculations were carried out at the same level of theory for all the stationary points to characterize the transition states (one imaginary frequency) and the equilibrium structures (no imaginary frequency) and to compute zero-point energy corrections and Gibbs free energies at 298 K. The effective core potentials of Hay and Wadt with double-ζ valance basis sets (LanL2DZ) were chosen to describe Pd, Br and P.[iii] The 6-31G basis set was used for the other atoms. Polarization functions were also added for P(ζ_d = 0.340), C(ζ_d = 0.6), and Br(ζ_d = 0.389).[iv] The partial atomic charges were calculated on the basis of natural bond orbital (NBO) analyses.[v] Analyses on the Laplacian of electron density[vi] of the optimized transition states were carried out with Molden 3.5.[vii]

We carried out single point energy calculations for several selected structures by using a larger basis set; SDDALL for Pd and 6-311G** for all other atoms.[viii] To study the steric effect missed from the small model calculations, we also performed two-layer ONIOM (B3LYP/BSI: HF/Lanl2MB) calculations [ix] on $(PPh_3)_2Pd$ + RBr → $(PPh_3)_2Pd(R)(Br)$ (R = Me, Ph). In the ONIOM calculations, the six phenyl groups on the two phosphine ligands were treated as the second layer while the rest were treated as the first layer.

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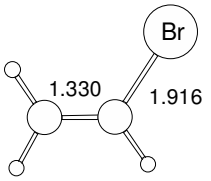
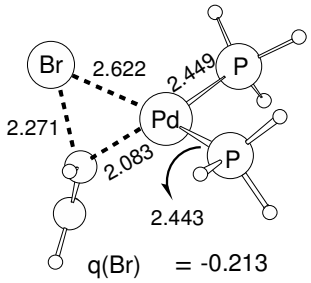


q(Br) = 0.067
q(Vinyl) = -0.067

3



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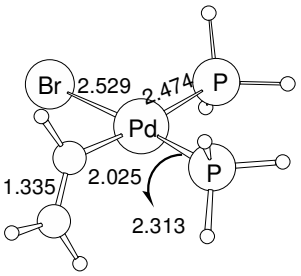
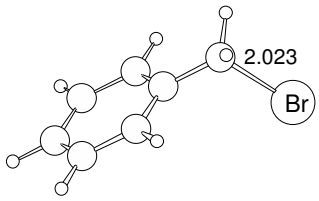
q(Pd) = 0.213

3_TS



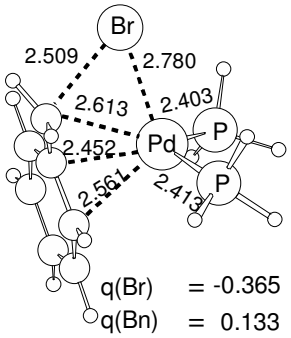
q(Br) = -0.522
q(Vinyl) = -0.196
q(Pd) = 0.228

3_Prod



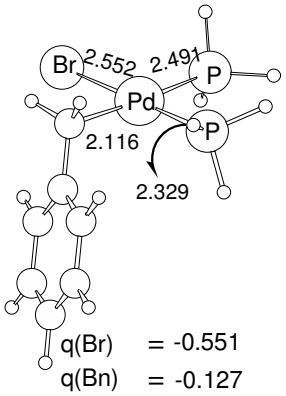
q(Br) = -0.034
q(Bn) = 0.034

4



q(Br) = -0.365
q(Bn) = 0.133
q(Pd) = 0.177

4_TS



q(Br) = -0.551
q(Bn) = -0.127
q(Pd) = 0.288

4_Prod

Figure A. Calculated structures for species involved in the oxidative addition of VinylBr and BnBr.

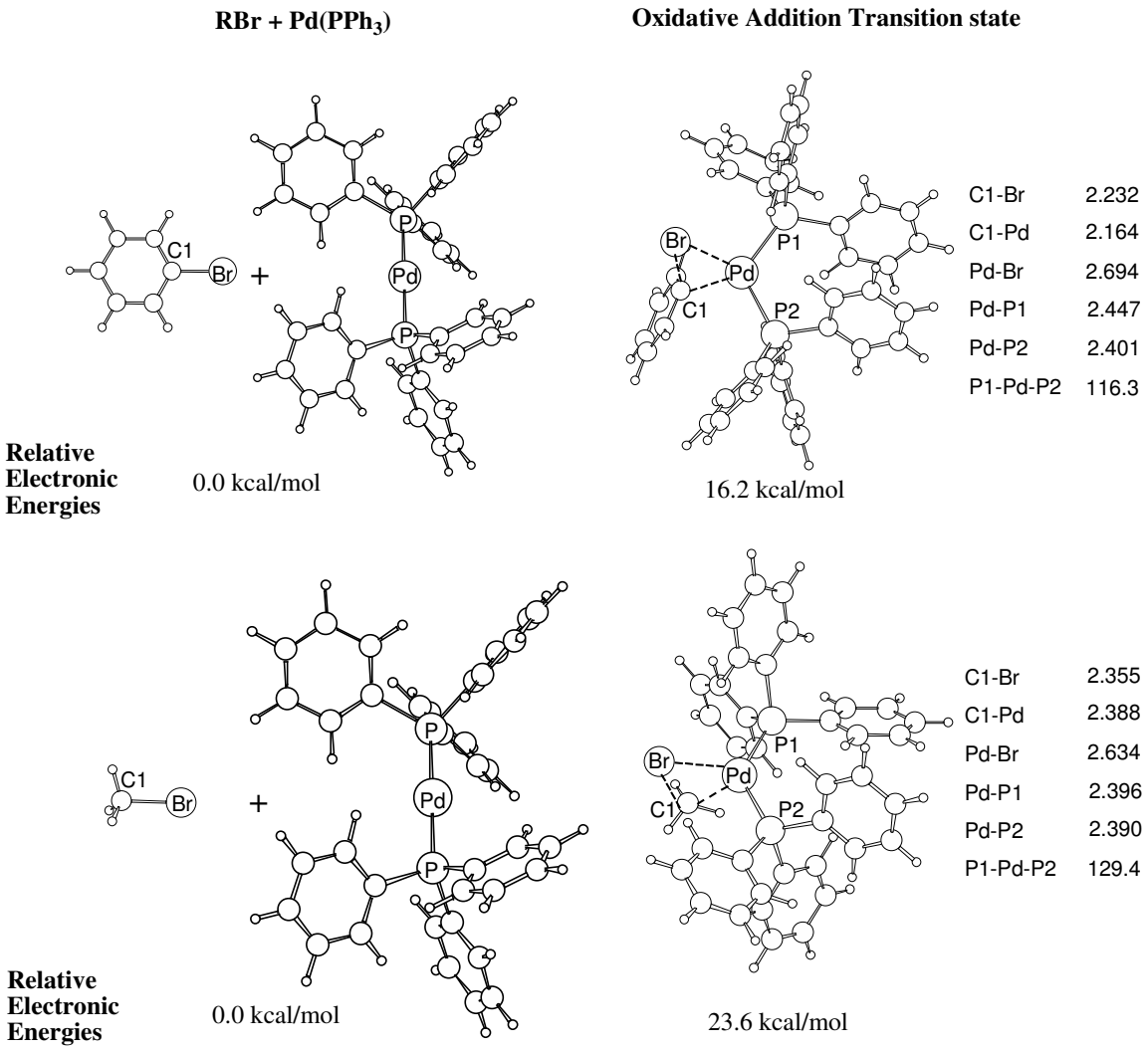


Figure B. ONIOM-calculated structures together with the relative electronic energies for $(PPh_3)_2Pd$ + RBr (R = Me, Ph) and the corresponding oxidative addition transition states. In terms of the electronic energies, the barrier calculated for the oxidative addition of MeBr to $Pd(PH_3)_2$ was calculated to be 24.6 kcal/mol, 1.0 kcal/mol greater than that to $Pd(PPh_3)_2$. The barrier calculated for the oxidative addition of PhBr to $Pd(PH_3)_2$ was calculated to be 14.2 kcal/mol, 2.0 kcal/mol smaller than that to $Pd(PPh_3)_2$.

Tables giving Cartesian coordinates, electronic energies (E), electronic energies corrected by zero point energies (E_0) and Gibbs free energies (G) for all the calculated structures (Page 6)

C_2H_3Br

E = -91.155987 a.u
E_0 = -91.113961 a.u
G = -91.140634 a.u

C	0.45824600	-1.12638300	0.00000000
C	-0.44320500	-2.10381200	0.00000000
H	-0.10878300	-3.14052800	0.00000000
H	-1.51399500	-1.91750000	0.00000000
H	1.53253000	-1.28370700	0.00000000
Br	0.00000000	0.73494000	0.00000000

Pd(vinyl)(Br)(PH_3)$_2$ (transition state)

E = -234.544944 a.u
E_0 = -234.450980 a.u
G = -234.493709 a.u

Pd	-0.45493500	-0.00148700	0.12393900
C	1.05989700	-1.34557800	0.61225200
C	1.22186700	-1.31950200	1.95026300
H	1.28124400	-0.39249900	2.51495300
Br	2.05774600	0.33252600	-0.54840600
P	-1.60125200	2.15675000	0.28892100
H	-0.87459700	3.34436500	-0.03138300
H	-2.76147100	2.49849800	-0.47527900
H	-2.12147100	2.64031700	1.53087800
P	-2.07213400	-1.66425000	-0.64473400
H	-2.99848100	-1.42992000	-1.71086900
H	-1.63672600	-2.94086000	-1.12756200
H	-3.04964800	-2.20059600	0.25299900
H	1.31113900	-2.25299500	2.50805000
H	1.16615400	-2.23333100	-0.00667300

Pd(vinyl)(Br)(PH_3)$_2$

E = -234.580226 a.u
E_0 = -234.483129 a.u
G = -234.523439 a.u

Pd	-0.35086900	0.10994500	-0.05087000
C	-0.94984000	-1.81158900	-0.27343200
C	-1.59063600	-2.55609200	0.63086000
H	-1.88645300	-2.18270400	1.61157200
Br	2.04323100	-0.70509300	-0.05182500
P	0.68614400	2.34172000	0.20717900
H	1.60871600	2.71546400	-0.80819000
H	0.01999200	3.60565700	0.32504300
H	1.55270000	2.48566000	1.32499800
P	-2.62292300	0.53547100	-0.14777300
H	-3.15616900	1.86096800	-0.10458500
H	-3.33168600	0.07084600	-1.28958800
H	-3.43731700	-0.05433200	0.85804300
H	-1.80842500	-3.60950000	0.43707000
H	-0.63989900	-2.22304400	-1.23612800

C_6H_5Br

E = -244.809252 a.u
E_0 = -244.718849 a.u
G = -244.749773 a.u

C	2.88992900	-0.00000500	0.00000200
C	2.18887100	-1.20889700	-0.00001100
C	0.79087000	-1.21785300	0.00000700
C	0.10812500	0.00001800	-0.00001400
C	0.79087800	1.21785900	-0.00001600
C	2.18890300	1.20887800	0.00001300
H	3.97781400	-0.00003300	0.00001100
H	2.72723700	-2.15473600	-0.00000200
H	0.24072000	-2.15449800	0.00001600
H	0.24078000	2.15453400	-0.00001400
H	2.72725100	2.15472700	0.00002600
Br	-1.81883600	0.00000000	0.00000200

Pd(Ph)(Br)(PH_3)$_2$ (transition state)

E = -388.191247 a.u
E_0 = -388.049252 a.u
G = -388.095793 a.u

C	2.70820900	0.27660400	1.87845300
C	3.61300500	0.82921800	0.97236000
C	3.33925700	0.77263800	-0.40337400
C	2.16697800	0.18556000	-0.87444300
C	1.23462000	-0.31626000	0.05356200
C	1.52735000	-0.33169000	1.42797700
Pd	-0.83178300	0.30799900	0.01190800
P	-0.53307600	2.48631100	-1.02391100
P	-3.05556600	0.09827300	1.03171300
H	-3.73198900	-1.16199300	1.04538200
H	-3.26529800	0.37492400	2.42059700
H	0.31708700	3.43733000	-0.37669900
H	0.10742700	2.59983800	-2.29977000
H	0.85620800	-0.82210800	2.12759900
H	2.92499100	0.28626300	2.94552400
H	4.53787400	1.27921700	1.32652900
H	4.04829800	1.18849100	-1.11785600
H	1.96091500	0.12749900	-1.93977200
H	-4.19209500	0.84721200	0.58884900
H	-1.57272000	3.42770100	-1.31910300
Br	0.07327000	-2.08621500	-0.63980800

Pd(Ph)(Br)(PH_3)$_2$

E = -388.231959 a.u
E_0 = -388.086815 a.u
G = -388.132197 a.u

Pd	0.58797900	0.43991000	-0.00011100
C	-1.42083000	0.06914800	-0.00004900
C	-2.11137800	-0.06681400	1.21080600
C	-2.11157900	-0.06659000	-1.21079500
C	-3.48413200	-0.34458200	1.20777200
H	-1.58544000	0.02253800	2.15958600
C	-3.48434800	-0.34438900	-1.20758100
H	-1.58583800	0.02297300	-2.15966800
C	-4.17299900	-0.48292500	0.00013400
H	-4.01095200	-0.45785200	2.15439900
H	-4.01130400	-0.45748800	-2.15415300
H	-5.23959200	-0.70033000	0.00022200
Br	1.02440400	-2.04679600	-0.00003700
P	3.05627500	0.60392900	0.00011600
H	3.71601800	-0.05690300	-1.07206000
H	3.85247000	1.79660400	-0.00052200
H	3.71530600	-0.05521600	1.07377400
P	-0.11832100	2.65034700	0.00005200
H	0.79022800	3.75327300	-0.00059200
H	-0.95061300	3.06852300	-1.07528100
H	-0.94918400	3.06864800	1.07644700

$C_6H_5CH_2Br$

E = -284.125814 a.u
E_0 = -284.006664 a.u
G = -284.040384 a.u

C	-1.30203200	-1.20779900	0.29622000
C	-0.64121500	0.00198500	0.55765300
C	-1.30442900	1.20956200	0.29268200
C	-2.60133700	1.20845600	-0.22281600
C	-3.25146400	-0.00219500	-0.48054000
C	-2.59883800	-1.21084800	-0.21928400
H	-0.79361900	-2.15005700	0.49566600
H	-0.79806600	2.15350700	0.48937300
H	-3.10520500	2.15236200	-0.42159400
H	-4.26320100	-0.00387000	-0.88150700
H	-3.10086300	-2.15629600	-0.41536800
C	0.74123500	0.00414000	1.12553900
H	0.96102700	0.89971900	1.70891000
H	0.96116000	-0.88726800	1.71522300
Br	2.16820700	-0.00079700	-0.30821200

Pd(Bn)(Br)(PH_3)$_2$ (transition state)

E = -427.499398 a.u
E_0 = -427.328932 a.u
G = -427.378439 a.u

C	-0.03258300	-1.55684600	-1.35109700
Pd	-0.29334000	0.59917600	0.10173700
P	-1.56622800	2.27565700	-1.07803600
P	0.46677400	1.00965000	2.34365700
H	-0.04564200	0.25590900	3.44771900
H	1.84273200	0.85654700	2.71619300
H	-1.48357600	3.66807500	-0.74823200
H	-1.59754700	2.51950100	-2.49530000
H	0.31806500	2.27955000	2.99049800
H	-2.98893000	2.20650000	-0.95092600
Br	-2.03038000	-1.56907100	0.16742800
C	1.23966100	-1.01282000	-0.93178400
C	1.71502700	0.23094000	-1.44504600
C	2.07842400	-1.74098000	-0.04017700
C	2.99431100	0.69451100	-1.09173500
H	1.15372900	0.73679000	-2.22586300
C	3.33151700	-1.26379800	0.30313900
H	1.71532400	-2.68318700	0.36601300
C	3.79317200	-0.03956600	-0.22173100
H	3.35708800	1.62956000	-1.51329300
H	3.96497900	-1.83893100	0.97533800
H	4.78291000	0.32492600	0.04634600
H	-0.16115500	-2.62696600	-1.24781600
H	-0.52639300	-1.12114000	-2.21426200

Pd(Bn)(Br)(PH_3)$_2$

E = -427.552509 a.u
E_0 = -427.379005 a.u
G = -427.426328 a.u

Pd	0.73273700	0.48911900	-0.20225600
C	-0.86576200	-0.23418100	-1.38536800
Br	1.80137400	-1.82790800	-0.27002000
P	2.72130000	0.99420900	1.21090400
H	3.97963800	0.75067900	0.59406400
H	3.07040600	2.23754600	1.83779200
H	2.90143700	0.16515800	2.35235500
P	-0.27719800	2.58785400	-0.21676700
H	-1.24071600	2.86776000	0.79510800
H	0.50610000	3.77141300	-0.06747800
H	-1.04989400	3.00996200	-1.33758200
H	-0.45049300	-1.17654300	-1.74275300
H	-1.00213500	0.46342700	-2.21864300
C	-2.07886500	-0.39345700	-0.54530100
C	-2.17893700	-1.44796100	0.38711800
C	-3.16889700	0.49341800	-0.65814900
C	-3.31857400	-1.60024000	1.17486900
H	-1.34430300	-2.13949300	0.48650200
C	-4.31024400	0.34067200	0.13184300
H	-3.13031600	1.29410900	-1.39715800
C	-4.38869800	-0.70496100	1.05582200
H	-3.37450600	-2.42305200	1.88564600
H	-5.14320100	1.03274700	0.01786600
H	-5.27767700	-0.82712600	1.67169600

CH_3Br

E = -53.083298 a.u
E_0 = -53.046002 a.u
G = -53.070927 a.u

C	1.54622900	0.00011800	-0.00016400
H	1.87985700	0.99292600	-0.30494100
H	1.88006400	-0.23214500	1.01219600
H	1.88017300	-0.76126300	-0.70640500
Br	-0.42621300	-0.00000700	0.00000400

Pd(Me)(Br)(PH_3)$_2$ (transition state)

E = -196.448729 a.u
E_0 = -196.360082 a.u
G = -196.402895 a.u

Pd	0.48196400	0.02471200	0.11031100
C	-1.09088300	-1.10281900	1.50060700
Br	-2.06017700	-0.05509700	-0.37335800
P	1.18257400	2.34692100	0.04416500
H	1.40612900	3.06528300	1.26282200
H	2.38398400	2.81367000	-0.58083800
H	0.34651000	3.35114100	-0.53975100
P	2.02456900	-1.75658800	-0.35875600
H	2.25174800	-2.05727100	-1.73846300
H	3.41482100	-1.73552000	-0.01327800
H	1.84034400	-3.12574400	0.03138500
H	-1.14116700	-2.14145800	1.18551100
H	-1.96160100	-0.77660500	2.06075600
H	-0.16674700	-0.83993100	2.04028500

Pd(Me)(Br)(PH_3)$_2$

E = -196.505079 a.u
E_0 = -196.413393 a.u
G = -196.453786 a.u

Pd	0.42602300	-0.13003200	-0.0000230
C	0.55846900	-2.20992800	0.00004100
Br	-2.09447300	-0.38053300	0.00000200
P	-0.10005600	2.28236900	0.00002200
H	-0.91303000	2.74080600	1.07298900
H	0.83286200	3.37197400	0.00000900
H	-0.91303200	2.74077000	-1.07295800
P	2.72930100	-0.15130400	0.00001000
H	3.38733400	-0.81757600	-1.07344100
H	3.51120300	1.04293700	0.00041600
H	3.38737100	-0.81833300	1.07296700
H	0.02318800	-2.52748000	-0.89849200
H	0.02494000	-2.52729300	0.89969600
H	1.57915200	-2.61210100	-0.00091800

Pd (PH_3)$_2$

E = -143.404694 a.u
E_0 = -143.351666 a.u
G = -143.384014 a.u

Pd	-0.00008100	-0.00003700	0.00000000
P	2.31729200	0.00002700	0.00000000
H	3.06098100	-0.61355700	-1.05613300
H	3.06058000	1.22168700	-0.00339800
H	3.06098600	-0.60767500	1.05952500
P	-2.31707900	-0.00001200	0.00000000
H	-3.06044200	0.61335700	1.05650200
H	-3.06044400	0.60887500	-1.05909000
H	-3.06115200	-1.22122000	0.00258700

The following are for the structures calculated with the two-layer ONIOM method

$Pd(PPh_3)_2$

E = -1503.903958 a.u

Pd	-0.000001	0.002615	-0.013398
P	-2.321569	0.001129	-0.004734
P	2.321568	0.000570	-0.004846
C	4.331337	-1.234442	-1.707706
C	4.319106	-3.557188	-2.328081
H	2.699509	-4.725097	-1.541975
C	3.171338	1.549127	-0.746629
C	3.156032	-0.127917	1.714952
C	4.901922	-2.300848	-2.386645
H	4.794276	-0.258398	-1.758474
H	4.766912	-4.388125	-2.858640
C	2.592744	2.131699	-1.868906
C	4.327003	2.098689	-0.205277
C	4.308159	-0.873394	1.932668
C	2.569529	0.557237	2.773416
H	5.806109	-2.147574	-2.961930
C	3.171016	3.250614	-2.448769
H	1.688637	1.706854	-2.288492
C	4.899328	3.221642	-0.784202
H	4.783851	1.655630	0.669113
C	4.869172	-0.930899	3.199856
H	4.771096	-1.412571	1.117485
C	3.136531	0.502557	4.037558
H	1.668163	1.134571	2.605569
C	4.324289	3.797800	-1.906201
H	2.716836	3.696872	-3.324285
H	5.798774	3.645616	-0.356133
C	4.286336	-0.242823	4.252608
H	5.765937	-1.515108	3.362689
H	2.676290	1.041190	4.856097
H	4.773442	4.674136	-2.356507
H	4.726670	-0.288975	5.240763
C	-3.156191	0.011480	1.719754
C	-2.568477	-0.742744	2.729461
C	-3.135500	-0.774698	3.994371
C	-4.286549	-0.047522	4.259304
C	-4.870601	0.709237	3.255496
C	-4.309563	0.738566	1.987354
H	-1.666144	-1.305869	2.522984
H	-2.674304	-1.366713	4.774608
H	-4.726906	-0.069092	5.248290
H	-5.768341	1.279574	3.457437
H	-4.773455	1.330895	1.210505
C	-3.172064	1.483712	-0.870204
C	-2.587284	2.737820	-0.732688
C	-3.165584	3.845327	-1.334016
C	-4.325130	3.704633	-2.082005
C	-4.906379	2.454321	-2.224731
C	-4.333998	1.345368	-1.619469
H	-1.678298	2.845635	-0.152966
H	-2.706527	4.819083	-1.219922
H	-4.774334	4.568824	-2.555153
H	-5.810735	2.338950	-2.808537
H	-4.795716	0.374346	-1.735607
C	-3.168749	-1.494993	-0.849858
C	-4.322908	-2.082562	-0.346560
C	-4.893411	-3.164582	-1.000399
C	-4.318054	-3.661681	-2.159430
C	-3.166276	-3.076399	-2.664102
C	-2.589814	-1.998469	-2.009611
H	-4.779999	-1.701110	0.556285
H	-5.791691	-3.618606	-0.601707
H	-4.765787	-4.506172	-2.668201
H	-2.711855	-3.460960	-3.568297
H	-1.686874	-1.544138	-2.399788
H	1.674470	-2.826679	-0.343885
C	2.583275	-2.681224	-0.915611
C	3.169636	-1.421446	-0.968724
C	3.159785	-3.746454	-1.590526

$Pd(PPh_3)_2(CH_3)Br$ (Transition state)

E = -1556.987256 a.u

Pd	0.024592	-0.885813	-0.074921
C	-0.100931	-2.514871	1.667294
Br	-0.244929	-3.475206	-0.478060
P	2.215807	0.069702	-0.084826
P	-2.109541	0.204404	-0.093336
H	0.731738	-3.160854	1.928337
H	-1.071866	-2.906665	1.954932
H	0.051828	-1.478016	2.003479
C	-2.290225	2.093846	0.230617
C	-3.334924	2.632359	0.973433
C	-1.341464	2.940496	-0.328907
C	-3.423471	4.004035	1.157395
H	-4.081163	1.987117	1.416017
C	-1.436022	4.312277	-0.149169
H	-0.526097	2.525158	-0.906734
C	-2.475981	4.846265	0.596389
H	-4.238505	4.414541	1.739902
H	-0.692795	4.963683	-0.591212
H	-2.548013	5.916948	0.740745
C	-3.232173	-0.534065	1.281451
C	-4.271663	-1.404170	0.980754
C	-2.938424	-0.250327	2.612459
C	-5.020648	-1.972485	2.001979
H	-4.501336	-1.642753	-0.048966
C	-3.691308	-0.815479	3.628647
H	-2.125308	0.421966	2.855366
C	-4.735000	-1.678291	3.325318
H	-5.830280	-2.648834	1.758056
H	-3.460899	-0.582579	4.660602
H	-5.321150	-2.122083	4.119954
C	-3.209643	0.010714	-1.655735
C	-2.814596	-0.888259	-2.636611
C	-4.378884	0.746865	-1.823120
C	-3.587298	-1.054197	-3.778714
H	-1.905031	-1.462530	-2.508063
C	-5.145167	0.580603	-2.964593
H	-4.693597	1.452509	-1.066625
C	-4.750616	-0.320673	-3.943942
H	-3.274272	-1.758911	-4.538522
H	-6.053366	1.156116	-3.089968
H	-5.351876	-0.448587	-4.835519
C	2.521476	1.719507	-1.026362
C	1.988380	1.835071	-2.304821
C	3.269613	2.764063	-0.497033
C	2.203408	2.985504	-3.048459
H	1.403581	1.022327	-2.718086
C	3.476824	3.916312	-1.240874
H	3.689268	2.689334	0.496644
C	2.946355	4.028838	-2.516542
H	1.786692	3.066537	-4.044416
H	4.057719	4.727473	-0.820504
H	3.111029	4.929020	-3.095256
C	2.632550	0.537533	1.730887
C	3.551971	-0.190140	2.475563
C	1.931583	1.578483	2.334734
C	3.781788	0.132052	3.805758
H	4.094605	-1.008205	2.021750
C	2.167536	1.899600	3.661810
H	1.206098	2.144087	1.764193
C	3.094102	1.177406	4.400331
H	4.502727	-0.438997	4.377156
H	1.624168	2.716118	4.120410

H	3.276091	1.427812	5.437727
C	3.796264	-0.883365	-0.631401
C	3.660615	-2.167127	-1.138241
C	5.059744	-0.302563	-0.552499
C	4.782377	-2.871810	-1.557684
H	2.679326	-2.619457	-1.210521
C	6.175318	-1.007289	-0.970710
H	5.176333	0.700495	-0.165170
C	6.037998	-2.294493	-1.473723
H	4.667889	-3.873517	-1.952021
H	7.154845	-0.551132	-0.905579
H	6.912131	-2.843469	-1.801254

$Pd(PPh_3)_2(Ph)Br$ (Transition state)

E = -1748.687340 a.u

Pd	0.039428	-0.851674	-0.249303
C	0.879377	-2.834709	-0.033355
C	2.234916	-3.140666	-0.249657
C	2.956638	-3.766160	0.763739
C	2.336944	-4.131722	1.968924
C	0.975596	-3.886437	2.143724
C	0.224831	-3.273606	1.130472
H	2.708592	-2.870782	-1.188308
H	4.014410	-3.974566	0.610715
H	2.908965	-4.631120	2.747585
H	0.474314	-4.200109	3.058049
H	-0.848280	-3.151326	1.237250
P	1.953249	0.592901	-0.117783
P	-2.140873	0.199715	0.106553
Br	-0.381278	-2.960526	-1.871413
C	1.522300	2.420324	-0.552586
C	2.819732	0.741443	1.585522
C	3.482141	0.292386	-1.265223
C	1.963049	3.501358	0.200121
C	1.609632	4.792501	-0.163796
C	0.818134	5.013348	-1.279736
C	0.372243	3.935871	-2.030228
C	0.717347	2.643907	-1.664893
H	2.578175	3.346491	1.074736
H	1.956782	5.628621	0.429975
H	0.545484	6.022548	-1.561661
H	-0.249529	4.098483	-2.901495
H	0.359089	1.805245	-2.248079
C	4.063566	1.352783	1.726632
C	4.659379	1.440106	2.974129
C	4.020271	0.918852	4.090428
C	2.784429	0.308062	3.954146
C	2.186192	0.218503	2.704493
H	4.572988	1.756949	0.862183
H	5.626306	1.916461	3.074498
H	4.488592	0.987491	5.064472
H	2.281730	-0.103917	4.819874
H	1.222927	-0.265049	2.601135
C	3.559089	0.881452	-2.520633
C	4.637454	0.613127	-3.350447
C	5.641175	-0.248155	-2.936085
C	5.562002	-0.842557	-1.685968
C	4.485548	-0.577677	-0.853941
H	2.783371	1.554695	-2.856890
H	4.690177	1.080241	-4.325807
H	6.481580	-0.457157	-3.585701
H	6.340577	-1.518133	-1.354820
H	4.432739	-1.047092	0.118553
C	-2.210147	1.972226	0.848093
C	-3.313029	0.323790	-1.403100
C	-3.271815	-0.788131	1.317200
C	-3.010055	2.975016	0.316091
C	-3.005067	4.242349	0.881011
C	-2.206134	4.514871	1.979773
C	-1.403930	3.515935	2.511619
C	-1.400662	2.251684	1.944356
H	-3.638064	2.776075	-0.540894
H	-3.630989	5.018239	0.458591
H	-2.205623	5.504239	2.419560
H	-0.774995	3.721436	3.368518
H	-0.767457	1.477203	2.357199
C	-4.693305	0.414936	-1.245053
C	-5.515318	0.494136	-2.356982
C	-4.966441	0.482502	-3.631782
C	-3.593438	0.389499	-3.791632
C	-2.766578	0.308301	-2.679157
H	-5.128929	0.420940	-0.254828
H	-6.587786	0.564080	-2.227614
H	-5.611565	0.542355	-4.499550
H	-3.159815	0.374105	-4.783392
H	-1.694985	0.222711	-2.807190
C	-3.730884	-0.262105	2.516044
C	-4.529180	-1.032461	3.350590
C	-4.872661	-2.325062	2.991181
C	-4.414752	-2.851106	1.790975
C	-3.613648	-2.088575	0.957000
H	-3.473604	0.747077	2.805481
H	-4.884150	-0.615280	4.284503
H	-5.496138	-2.923151	3.643622
H	-4.680499	-3.860297	1.502388
H	-3.258620	-2.502346	0.021157