

Supporting Information

DFT Studies on the Effect of the Nature of the Aryl Halide, Y-C₆H₄-X, on the Mechanism of its Oxidative Addition to Pd(0)L versus Pd(0)L₂

King Chung Lam,^a Todd B. Marder*^b and Zhenyang Lin*^a

^a*Department of Chemistry, The Hong Kong University of Science and Technology, Clear Water Bay, Kowloon, Hong Kong*

^b*Department of Chemistry, Durham University, South Road, Durham DH1 3LE, UK*

Author Email Addresses: todd.marder@durham.ac.uk and chzlin@ust.hk

Computational Details

Geometry optimizations have been performed using the B3LYP functionalⁱ with the Gaussian 03 software package.ⁱⁱ The effective core potentials (ECPs) of Hay and Wadt with a double- ζ valence basis set (LanL2DZ)ⁱⁱⁱ were used in describing Pd, P and halides (Cl, Br, I), whereas the 6-31G basis set was used for all other atoms.^{iv} Polarisation functions were added for Pd ($\zeta_f = 1.472$),^v P ($\zeta_d = 0.340$), I ($\zeta_d = 0.266$), Br ($\zeta_d = 0.389$), Cl ($\zeta_d = 0.514$), and the carbon atoms bonded directly to the metal center ($\zeta_d = 0.600$).^{vi} Frequency calculations were carried out to confirm the characteristics of all of the optimized structures as minima or transition states, and to provide free energies at 298.15 K which include entropic contributions by taking into account the vibrational, rotational and translational motions of the species under consideration.

- (i). (a) Becke, A. D. *J. Chem. Phys.* **1993**, 98, 5648. (b) Miehlich, B.; Savin, A.; Stoll, H.; Preuss, H. *Chem. Phys. Lett.* **1989**, 157, 200. (c) Lee, C.; Yang, W.; Parr, G. *Phys. Rev.* **1988**, B37, 785. (d) Becke, A. D. *J. Chem. Phys.* 1993, 98, 5648.
- (ii) Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Montgomery, J. A.; Vreven, T., Jr.; Kudin, K. N.; Burant, J. C.;

Millam, J. M.; Iyengar, S. S.; Tomasi, J.; Barone, V.; Mennucci, B.; Cossi, M.; Scalmani, G.; Rega, N.; Petersson, G. A.; Nakatsuji, H.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Klene, M.; Li, X.; Knox, J. E.; Hratchian, H. P.; Cross, J. B.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Ayala, P. Y.; Morokuma, K.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Zakrzewski, V. G.; Dapprich, S.; Daniels, A. D.; Strain, M. C.; Farkas, O.; Malick, D. K.; Rabuck, A. D.; Raghavachari, K.; Foresman, J. B.; Ortiz, J. V.; Cui, Q.; Baboul, A. G.; Clifford, S.; Cioslowski, J.; Stefanov, B. B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I.; Martin, R. L.; Fox, D. J.; Keith, T.; Al-Laham, M. A.; Peng, C. Y.; Nanayakkara, A.; Challacombe, M.; Gill, P. M. W.; Johnson, B.; Chen, W.; Wong, M. W.; Gonzalez, C.; Pople, J. A. *Gaussian 03*, revision B05; Gaussian, Inc.: Pittsburgh, PA, 2003.

- (iii) Hay, P. J.; Wadt, W. R. *J. Chem. Phys.* **1985**, *82*, 299.
- (iv) Hariharan, P. C.; Pople, J. A. *Theor. Chim. Acta* **1973**, *28*, 213.
- (v) Ehlers, A. W.; Bohme, M.; Dapprich, S.; Gobbi, A.; Hollwarth, A.; Jonas, V.; Kohler, K. F.; Stegmann, R.; Veldkamp, A.; Frenking, G. *Chem. Phys. Lett.* **1993**, *208*, 111.
- (vi) Huzinaga, S. *Gaussian Basis Sets for Molecular Calculations*; Elsevier Science: Amsterdam, 1984.

Cartesian coordinates for all the complexes calculated in this study:

1			H	3.615595	0.662445	2.287702
E = -379.288134 a.u.			H	2.729749	-0.466977	3.328164
P	2.326038	0.002027	-0.002022	H	4.725781	-1.555953
Pd	0.000062	-0.005954	-0.002940	H	3.466348	-1.530106
P	-2.325871	0.000779	-0.002008	H	4.079175	-0.004041
C	-3.186182	-0.820919	1.439825	H	3.375157	-3.277934
C	-3.175845	1.665695	-0.004356	H	1.708730	-3.026243
C	-3.191721	-0.829294	-1.435659	H	1.984770	-3.419075
C	3.187317	-0.820133	1.438960	N	-2.261312	-2.333990
C	3.192814	-0.825650	-1.436492			
C	3.174047	1.667947	-0.002731			
H	4.266442	1.566872	0.001818			
H	2.865842	2.228315	-0.891094			
H	2.859168	2.231613	0.881140			
H	4.283896	-0.764438	-1.340317			
H	2.891963	-1.877186	-1.480629			
H	2.883832	-0.343875	-2.369577			
H	4.278842	-0.754150	1.349923			
H	2.870214	-0.338188	2.369202			
H	2.890598	-1.872874	1.482814			
H	-4.277790	-0.756404	1.350710			
H	-2.888132	-1.873237	1.484781			
H	-2.869690	-0.337606	2.369565			
H	-4.268108	1.563242	0.000382			
H	-2.861614	2.230651	0.878921			
H	-2.868418	2.225551	-0.893314			
H	-4.282876	-0.769432	-1.339446			
H	-2.883449	-0.347951	-2.369202			
H	-2.889474	-1.880466	-1.478867			
2						
E = -253.004311 a.u.						
Pd	0.000021	0.000156	0.067360			
P	0.000289	0.000009	2.296514			
C	1.661740	0.000104	3.150323			
C	-0.830832	1.439095	3.150026			
C	-0.830886	-1.439117	3.150021			
H	1.551488	0.000380	4.241936			
H	2.225398	-0.885988	2.842379			
H	2.225306	0.886105	2.842413			
H	-0.775757	-1.343864	4.241909			
H	-1.880423	-1.484075	2.842441			
H	-0.345452	-2.370259	2.842263			
H	-0.775820	1.343815	4.241906			
H	-0.345335	2.370217	2.842328			
H	-1.880007	1.484161	2.842362			
3 (NC-Ar-Br)						
E = -590.015974429 a.u.						
C	-2.294055	-1.154403	-1.129232			
C	-1.817896	-0.791759	-2.406777			
C	-1.077904	0.399546	-2.561078			
C	-0.851160	1.246243	-1.471146			
C	-1.372334	0.901586	-0.190774			
C	-2.079932	-0.323724	-0.024374			
Pd	0.464318	-0.016567	0.377697			
P	2.472404	-1.057035	0.958209			
C	3.826664	-1.040046	-0.325318			
Br	-1.554313	2.294767	1.166269			
C	2.386747	-2.875879	1.365882			
C	3.377204	-0.393614	2.448714			
C	-2.062188	-1.637131	-3.531716			
H	-2.519148	-0.567829	0.935279			
H	-2.846649	-2.079127	-1.005910			
H	-0.695194	0.669765	-3.538930			
H	-0.353741	2.197955	-1.613461			
H	4.303991	-0.949119	2.634771			
3 (NC-Ar-Cl)						
E = -591.801468028 a.u.						
C	-2.468012	-0.854367	-0.952249			
C	-1.993441	-0.490329	-2.230165			
C	-1.253750	0.701457	-2.384067			
C	-1.031803	1.550895	-1.294612			
C	-1.558759	1.206366	-0.018162			
C	-2.258815	-0.021053	0.152325			
Pd	0.284839	0.220314	0.482112			
P	2.292684	-0.798216	1.085489			
C	3.672431	-0.777595	-0.170348			
Cl	-1.722148	2.473311	1.219381			
C	2.233771	-2.611616	1.520637			
C	3.156116	-0.094723	2.583083			
C	-2.237261	-1.335519	-3.355156			
H	-2.701068	-0.258351	1.112214			
H	-3.018334	-1.780178	-0.828454			
H	-0.870242	0.971884	-3.361355			
H	-0.541473	2.506785	-1.432956			
H	4.088965	-0.630460	2.795833			
H	3.378661	0.962784	2.409725			
H	2.492858	-0.166186	3.450768			
H	4.573181	-1.269828	0.215505			
H	3.340539	-1.290726	-1.078260			
H	3.910403	0.258455	-0.430789			
H	3.224520	-2.989133	1.800680			
H	1.540893	-2.762243	2.354358			
H	1.861354	-3.176349	0.660324			
N	-2.437068	-2.032151	-4.280609			
3 (NC-Ar-I)						
E = -588.232753594 a.u.						
C	-2.681543	-1.340009	-0.875454			
C	-1.831953	-0.267885	-1.152748			
C	-1.356019	0.548555	-0.089491			
C	-1.760932	0.271300	1.245802			
C	-2.611000	-0.805730	1.502141			
C	-3.087403	-1.612876	0.447926			
Pd	0.623764	-0.133178	0.012876			
P	2.766278	-1.071759	0.177220			
C	4.207814	0.109048	0.269237			
I	-0.562845	2.548007	-0.562345			
C	3.305771	-2.191469	-1.214326			
C	3.091121	-2.155212	1.660996			
H	-1.443553	0.916637	2.056121			
H	-2.916905	-1.020603	2.520182			
C	-3.966757	-2.705439	0.719759			
H	-3.041612	-1.965816	-1.684745			
H	-1.567681	-0.035955	-2.177578			
H	5.161339	-0.426453	0.347628			
H	4.217937	0.736595	-0.627517			
H	4.087077	0.760955	1.140164			
H	4.316668	-2.581074	-1.045178			
H	2.605538	-3.028464	-1.297721			
H	3.287306	-1.634584	-2.156472			
H	4.114491	-2.548992	1.655169			

H	2.934092	-1.574104	2.575220
H	2.382572	-2.989314	1.660474
N	-4.687273	-3.606528	0.944278

3 (Ph-Br)

E = -497.803282684 a.u.

C	-2.202710	-1.012017	-2.576119
C	-1.405382	0.106037	-2.849670
C	-1.056702	1.006596	-1.829989
C	-1.526532	0.775188	-0.508516
C	-2.295427	-0.385453	-0.221550
C	-2.625205	-1.265267	-1.265418
Pd	0.304447	-0.211912	0.050825
Br	-1.544152	2.264576	0.767225
H	-2.484212	-1.687199	-3.377249
P	2.279814	-1.239070	0.687501
C	2.245423	-3.085644	0.966522
C	3.040918	-0.660154	2.292032
C	3.743629	-3.318690	-0.463098
H	-2.691714	-0.537799	0.775361
H	-3.229078	-2.140178	-1.045920
H	-1.061282	0.296818	-3.861356
H	-0.509462	1.913745	-2.057363
H	3.974073	-1.193859	2.509805
H	3.244647	0.413438	2.229035
H	2.331098	-0.824594	3.108850
H	4.627303	-1.598231	-0.060826
H	3.485688	-1.521159	-1.434459
H	3.975480	-0.028391	-0.612671
H	3.226455	-3.465145	1.277764
H	1.505987	-3.318690	1.739213
H	1.940485	-3.584626	0.041323

3 (Ph-Cl)

E = -499.588638840 a.u.

C	-2.256382	-0.591862	-2.562716
C	-1.506667	0.580807	-2.718138
C	-1.246886	1.418512	-1.620885
C	-1.758772	1.064698	-0.344445
C	-2.472805	-0.150855	-0.173832
C	-2.714173	-0.965084	-1.293043
Pd	0.105112	0.050110	0.144584
Cl	-1.874719	2.320535	0.918936
H	-2.471605	-1.216742	-3.422898
P	2.097584	-0.937244	0.769969
C	2.064641	-2.749768	1.221300
C	2.944162	-0.221503	2.273374
C	3.502173	-0.915089	-0.461567
H	-2.901780	-0.390591	0.791826
H	-3.279429	-1.882605	-1.164316
H	-1.133380	0.864465	-3.696975
H	-0.744390	2.369326	-1.752981
H	3.879413	-0.749347	2.496582
H	3.159323	0.837215	2.097766
H	2.273293	-0.293972	3.135171
H	4.400420	-1.398482	-0.057826
H	3.190040	-1.434437	-1.373094
H	3.736034	0.121710	-0.723115
H	3.058600	-3.111150	1.512804
H	1.366846	-2.902172	2.050701
H	1.706203	-3.327858	0.363764

3 (Ph-I)

E = -496.020272503 a.u.

C	0.050660	-2.262021	0.772671
C	-0.445996	-1.527733	-0.336802
C	-1.846658	-1.420460	-0.545345
C	-2.724786	-2.049230	0.348840
C	-2.234322	-2.785566	1.434247

C	-0.853793	-2.879072	1.648793
Pd	-0.081429	0.424911	0.390461
I	0.911187	-1.110160	-2.025538
P	0.214894	2.538027	1.319374
C	0.565605	2.622486	3.151785
C	-1.212522	3.734241	1.178483
C	1.611057	3.581538	0.649101
H	-2.229347	-0.898355	-1.414556
H	-3.795018	-1.968112	0.184671
H	-2.923585	-3.281125	2.109954
H	-0.470819	-3.442494	2.494254
H	1.118627	-2.383923	0.911016
H	1.663682	4.555080	1.151253
H	2.557884	3.050499	0.789331
H	1.463505	3.735651	-0.424532
H	0.684224	3.658171	3.492843
H	-0.258190	2.152929	3.698429
H	1.481531	2.063963	3.369547
H	-0.977224	4.698927	1.644412
H	-1.447090	3.892216	0.121018
H	-2.094246	3.303627	1.663398

3 (MeO-Ar-Br)

E = -612.285784430 a.u.

C	-2.770507	-1.334506	0.273846
C	-2.353819	-0.898377	-0.987285
C	-1.590672	0.279978	-1.107346
C	-1.252307	1.025631	0.051107
C	-1.657410	0.550010	1.330804
C	-2.407952	-0.619725	1.429385
Pd	0.689559	0.072682	0.018718
Br	-0.740107	2.909834	-0.135475
O	-3.540674	-2.471686	0.497395
C	-3.972676	-3.257155	-0.643652
P	2.778679	-0.917215	0.003471
C	3.379597	-1.690541	1.594468
C	4.228630	0.183800	-0.414954
C	3.054963	-2.325883	-1.192242
H	-1.429567	1.130246	2.216865
H	-2.732217	-0.994557	2.392981
H	-2.613458	-1.443449	-1.886258
H	-1.355288	0.669577	-2.090485
H	5.174397	-0.371573	-0.401016
H	4.078340	0.617619	-1.408556
H	4.279587	1.002671	0.309647
H	4.076375	-2.720262	-1.123887
H	2.341828	-3.127006	-0.974116
H	2.870983	-1.973386	-2.212070
H	4.380328	-2.124871	1.479455
H	3.405171	-0.927539	2.378951
H	2.678527	-2.472554	1.902615
H	-4.558190	-4.073726	-0.222865
H	-4.598446	-2.663850	-1.321168
H	-3.116212	-3.662572	-1.195524

3 (MeO-Ar-Cl)

E = -614.070970342 a.u.

C	-2.472347	-0.221934	1.427820
C	-2.819161	-0.958090	0.280055
C	-2.399641	-0.535895	-0.984309
C	-1.651063	0.652358	-1.118209
C	-1.332956	1.415952	0.032426
C	-1.736770	0.955455	1.316280
O	-3.576351	-2.101859	0.515992
C	-3.989792	-2.909258	-0.616465
Pd	0.590143	0.365179	-0.017492
P	2.685602	-0.598761	-0.015392
C	3.007390	-1.980125	-1.231565
Cl	-0.862495	3.128130	-0.153982
C	3.274950	-1.392011	1.570422
C	4.122468	0.534920	-0.389320

H	-1.520164	1.556231	2.191476
H	-2.798011	-0.586772	2.394610
H	-2.647166	-1.096689	-1.876823
H	-1.422873	1.040136	-2.103809
H	5.077734	-0.003793	-0.367402
H	3.981767	0.982429	-1.378210
H	4.145711	1.342439	0.349231
H	4.034932	-2.356449	-1.153348
H	2.306434	-2.798563	-1.039635
H	2.833360	-1.612365	-2.247688
H	4.284787	-1.807161	1.463557
H	3.274807	-0.643883	2.369492
H	2.582734	-2.191614	1.852371
H	-4.567175	-3.727689	-0.188121
H	-4.618768	-2.334118	-1.306648
H	-3.123946	-3.310493	-1.156587

3 (MeO-Ar-I)

E = -610.503148460 a.u.

C	-0.583371	-2.655851	1.301669
C	0.321816	-1.978255	0.469191
C	-0.148875	-1.260030	-0.657552
C	-1.543857	-1.236219	-0.935974
C	-2.429413	-1.912504	-0.098587
C	-1.952705	-2.628305	1.012025
Pd	0.141150	0.696616	0.103024
P	0.353723	2.796861	1.074704
C	1.563623	3.987815	0.296096
I	1.266353	-0.790800	-2.286752
C	0.907860	2.852079	2.857932
C	-1.179508	3.860749	1.153260
H	-1.913572	-0.724592	-1.816746
H	-3.496143	-1.905297	-0.290309
O	-2.926609	-3.276091	1.765263
H	-0.201356	-2.3198529	2.157742
H	1.385449	-0.052691	0.662154
H	1.591927	4.944657	0.831384
H	2.562798	3.540864	0.300991
H	1.274997	4.164078	-0.744990
H	0.975235	3.882320	3.228236
H	0.196652	2.291951	3.473122
H	1.887812	2.372193	2.946056
H	-0.975945	4.825550	1.633600
H	-1.550948	4.034462	0.138351
H	-1.956669	3.333513	1.715484
C	-2.514204	-4.053745	2.919135
H	-3.435982	-4.460534	3.333248
H	-1.845917	-4.873091	2.628299
H	-2.018850	-3.423953	3.667673

4 (NC-Ar-Br)

E = -590.020302949 a.u.

C	-3.987606	-1.189541	0.517733
C	-3.364894	-1.782308	-0.599413
C	-1.994549	-1.553921	-0.838424
C	-1.254576	-0.752671	0.035379
C	-1.869575	-0.208107	1.175232
C	-3.246209	-0.388561	1.390560
Pd	-0.741600	0.450380	2.655241
P	0.682250	1.175487	4.551824
C	2.233524	2.034145	3.996742
Br	-1.008075	2.696254	1.665345
C	1.319672	-0.041211	5.812672
C	-0.135241	2.465108	5.610329
C	-4.124450	-2.598460	-1.496391
H	-3.741720	0.089827	2.229552
H	-5.047007	-1.349394	0.687546
H	-1.522653	-1.993717	-1.710555
H	-0.207920	-0.556249	-0.174987
H	0.560156	2.869016	6.354422
H	-0.490999	3.271015	4.961855

H	-0.998378	2.027719	6.122029
H	2.775248	2.466039	4.845498
H	2.882805	1.321634	3.478174
H	1.958754	2.825354	3.293132
H	1.928887	0.459920	6.573199
H	0.476475	-0.538996	6.302433
H	1.927557	-0.803130	5.314084
N	-4.747293	-3.271335	-2.230885

4 (NC-Ar-Cl)

E = -591.796458300 a.u.

C	-3.995185	-1.177324	0.503517
C	-3.378742	-1.745835	-0.629533
C	-2.002153	-1.540871	-0.853183
C	-1.249938	-0.786463	0.051466
C	-1.860517	-0.266655	1.204441
C	-3.241382	-0.423207	1.407082
Pd	-0.732788	0.369563	2.690077
P	0.690638	1.146300	4.571957
C	2.208707	2.026009	3.962036
Cl	-0.939984	2.526046	1.812810
C	1.371302	0.002804	5.877132
C	-0.159964	2.457566	5.575659
C	-4.150850	-2.513454	-1.558249
H	-3.731154	0.037024	2.259696
H	-5.058899	-1.318979	0.662123
H	-1.534655	-1.961828	-1.736895
H	-0.197429	-0.607590	-0.145762
H	0.527586	2.922771	6.290698
H	-0.548269	3.214570	4.888072
H	-1.002799	2.017714	6.118249
H	2.741788	2.519278	4.782360
H	2.878364	1.310607	3.474171
H	1.897624	2.769053	3.221940
H	1.971177	0.552964	6.610611
H	0.546488	-0.497605	6.394748
H	1.997426	-0.762152	5.406524
N	-4.783808	-3.146009	-2.319421

4 (NC-Ar-I)

E = -588.244463289 a.u.

C	-3.330177	-1.846987	-0.536312
C	-1.979765	-1.593761	-0.791429
C	-1.256315	-0.730465	0.050342
C	-1.911965	-0.049795	1.091499
C	-3.262319	-0.301922	1.347923
C	-3.979055	-1.206766	0.538880
Pd	0.719456	-0.847647	0.073037
P	3.169760	-1.133558	0.216236
C	4.063689	0.379198	0.821216
I	0.648478	1.190111	-1.582406
C	3.981691	-1.450595	-1.425050
C	3.885919	-2.481022	1.287838
H	-1.378147	0.673037	1.700211
H	-3.769025	0.205591	2.161815
C	-5.363237	-1.461249	0.797405
H	-3.889016	-2.526868	-1.170531
H	-1.498504	-2.066976	-1.641433
H	5.150064	0.246693	0.770203
H	3.767669	1.231351	0.202299
H	3.772885	0.588417	1.855494
H	5.073295	-1.466956	-1.332675
H	3.638029	-2.409533	-1.825539
H	3.683296	-0.661121	-2.121138
H	4.981040	-2.480286	1.247629
H	3.567329	-2.334077	2.324929
H	3.517566	-3.454775	0.949053
N	-6.498664	-1.673144	1.012120

4 (Ph-Br)

E = -497.808231782 a.u.
C -3.340819 -1.810832 -0.562225
C -1.984619 -1.569686 -0.813828
C -1.245655 -0.734402 0.037269
C -1.868455 -0.181344 1.166893
C -3.239481 -0.374926 1.396266
C -3.967425 -1.212216 0.537652
Pd -0.743706 0.478793 2.643349
Br -0.996323 2.739480 1.667209
H -3.912069 -2.445770 -1.232371
P 0.681051 1.179707 4.549664
C 1.316346 -0.039773 5.810499
C -0.128138 2.469186 5.616934
C 2.238714 2.037372 4.006786
H -3.736994 0.116841 2.227010
H -5.024529 -1.381257 0.721146
H -1.503146 -2.016138 -1.679033
H -0.203640 -0.520182 -0.181302
H 0.568819 2.865235 6.364133
H -0.479160 3.280133 4.971962
H -0.994426 2.033830 6.125235
H 2.779800 2.462300 4.859764
H 2.886831 1.325612 3.485531
H 1.968228 2.833258 3.306610
H 1.925948 0.457642 6.573329
H 0.471484 -0.537479 6.297663
H 1.922735 -0.802054 5.310444

4 (Ph-Cl)

E = -499.584433665 a.u.
C -3.362161 -1.750819 -0.608869
C -1.997813 -1.538141 -0.841405
C -1.243819 -0.754640 0.045174
C -1.861635 -0.225817 1.188411
C -3.238567 -0.390234 1.401378
C -3.981730 -1.175701 0.507439
Pd -0.736518 0.399406 2.674575
Cl -0.918174 2.578809 1.826545
H -3.944685 -2.345217 -1.305948
P 0.690025 1.141191 4.572708
C 1.372557 -0.001921 5.879541
C -0.153941 2.452060 5.584579
C 2.212341 2.023303 3.973577
H -3.729446 0.083744 2.246499
H -5.044465 -1.322648 0.676854
H -1.521284 -1.966266 -1.718520
H -0.194126 -0.562088 -0.157149
H 0.534737 2.911586 6.302438
H -0.538453 3.213011 4.899183
H -0.999428 2.013347 6.124118
H 2.745052 2.511101 4.797615
H 2.881645 1.310101 3.481851
H 1.902337 2.770703 3.237404
H 1.972000 0.548433 6.613439
H 0.547927 -0.503442 6.396541
H 1.998993 -0.766532 5.408612

4 (Ph-I)

E = -496.032396038 a.u.
C -0.152580 -2.407067 0.626691
C -1.059538 -1.350358 0.443426
C -2.441330 -1.596840 0.391108
C -2.917799 -2.895456 0.624041
C -2.020768 -3.944272 0.860571
C -0.641801 -3.701166 0.858283
Pd -0.441397 0.495924 0.777619
I -0.117231 0.647150 -1.829313
P 0.295927 2.769161 1.407441
C 0.297046 3.296988 3.197196

C -0.683549 4.127223 0.598636
C 2.033564 3.168976 0.879647
H -3.138349 -0.793755 0.171291
H -3.986755 -3.086938 0.603776
H -2.393864 -4.950457 1.024845
H 0.055659 -4.517981 1.019843
H 0.918025 -2.229697 0.588903
H 2.281448 4.216836 1.083029
H 2.736392 2.520774 1.412672
H 2.127902 2.969524 -0.191862
H 0.649522 4.328739 3.308123
H -0.717329 3.220761 3.602217
H 0.948717 2.633036 3.774511
H -0.258680 5.112627 0.820638
H -0.683732 3.961432 -0.482729
H -1.719149 4.091775 0.951516

4 (MeO-Ar-Br)

E = -612.291375598 a.u.
C -1.734774 -3.724357 1.022508
C -0.341778 -3.572489 1.003162
C 0.211977 -2.320770 0.691360
C -0.622830 -1.220225 0.455285
C -2.019319 -1.395296 0.412877
C -2.572642 -2.638460 0.721480
Pd 0.113809 0.601946 0.578833
Br 0.455283 0.507115 -1.870603
O -2.388695 -4.919230 1.309061
C -1.595082 -6.101273 1.588797
P 1.012545 2.893846 0.861792
C 0.101522 4.152313 -0.159313
C 2.754920 3.064288 0.236325
C 1.103487 3.725190 2.529796
H -2.672242 -0.569694 0.146363
H -3.645118 -2.796980 0.720078
H 0.316399 -4.408462 1.207947
H 1.291474 -2.216478 0.636810
H 3.080925 4.110448 0.236004
H 3.429804 2.475262 0.865594
H 2.795498 2.663699 -0.780827
H 1.531930 4.730855 2.451169
H 0.098179 3.798048 2.957500
H 1.721998 3.125307 3.205375
H 0.603926 5.125832 -0.137943
H 0.047932 3.786248 -1.188776
H -0.919210 4.263765 0.220265
H -2.319298 -6.893827 1.773742
H -0.963866 -6.369109 0.733217
H -0.967795 -5.959302 2.477105

4 (MeO-Ar-Cl)

E = -614.067511521 a.u.
C -1.737870 -3.735419 1.017016
C -0.345023 -3.580656 1.004113
C 0.206979 -2.318220 0.735450
C -0.629615 -1.212764 0.534845
C -2.025544 -1.387698 0.486316
C -2.577480 -2.641431 0.752676
Pd 0.099963 0.607286 0.669062
Cl 0.491128 0.574382 -1.641937
O -2.389729 -4.940676 1.262275
C -1.593574 -6.130557 1.498293
P 1.008837 2.907254 0.891901
C 0.098579 4.109205 -0.195167
C 2.746025 3.023982 0.241355
C 1.119487 3.827980 2.510417
H -2.680063 -0.554398 0.248134
H -3.649705 -2.801467 0.745510
H 0.314189 -4.422041 1.181645

H	1.286429	-2.209873	0.686573
H	3.080166	4.065199	0.170095
H	3.423365	2.471133	0.900179
H	2.768365	2.557464	-0.747831
H	1.555477	4.823935	2.372841
H	0.118540	3.933349	2.941574
H	1.738774	3.261450	3.213542
H	0.604560	5.080440	-0.233437
H	0.041569	3.679496	-1.199606
H	-0.920413	4.246851	0.180556
H	-2.316050	-6.930755	1.654956
H	-0.962596	-6.365709	0.633002
H	-0.965809	-6.019532	2.390634

4 (MeO-Ar-I)

E = -610.515589963 a.u.

C	-0.337096	-3.563878	0.987287
C	0.218481	-2.326553	0.625717
C	-0.612730	-1.226877	0.367706
C	-2.011559	-1.396207	0.356094
C	-2.566631	-2.625076	0.714081
C	-1.730331	-3.706326	1.035343
Pd	0.132268	0.598702	0.489129
P	1.016106	2.877037	0.832889
C	2.767280	3.101688	0.248573
I	0.427150	0.442953	-2.120502
C	1.072432	3.620311	2.543494
C	0.108547	4.182358	-0.131826
H	-2.664475	-0.575774	0.074820
H	-3.639923	-2.776459	0.736432
O	-2.386152	-4.886992	1.371438
H	0.319730	-4.396913	1.207879
H	1.297466	-2.231706	0.550088
H	3.082401	4.148859	0.319564
H	3.436878	2.480447	0.851919
H	2.832826	2.766822	-0.790962
H	1.486447	4.634955	2.524420
H	0.060687	3.655670	2.960566
H	1.691067	2.994484	3.194984
H	0.595232	5.159691	-0.038591
H	0.081931	3.882288	-1.183591
H	-0.921959	4.255530	0.230117
C	-1.594875	-6.064202	1.677173
H	-2.320553	-6.845552	1.900137
H	-0.979526	-6.364196	0.820722
H	-0.952158	-5.896874	2.549883

5 (NC-Ar-Br)

E = -716.308948904 a.u.

C	3.971969	-1.706358	0.062601
C	3.312298	-1.457764	-1.156784
C	2.034441	-0.891360	-1.161299
C	1.379111	-0.560294	0.039618
C	2.040622	-0.826953	1.253209
C	3.318622	-1.391535	1.270915
Pd	-0.523464	0.186547	0.001655
P	-2.949394	0.701259	-0.102994
C	-3.862408	0.128024	1.410207
P	0.512153	2.286386	-0.119922
C	-0.527094	3.829854	-0.063488
Br	-1.268507	-2.238736	0.240433
C	1.730123	2.634715	1.238297
C	1.514011	2.572492	-1.657277
C	-3.696169	2.398137	-0.349688
C	-3.777717	-0.236420	-1.477457
H	1.549007	-0.616754	2.198269
H	3.812911	-1.597863	2.214780
C	5.286081	-2.270503	0.073961
H	3.801025	-1.714769	-2.091099
H	1.538133	-0.731135	-2.114129

H	2.196416	3.615012	1.090961
H	1.213704	2.622344	2.203345
H	2.498229	1.858731	1.248541
H	0.114660	4.717044	-0.104198
H	-1.217324	3.850114	-0.910315
H	-1.107105	3.852205	0.863559
H	2.016771	3.544915	-1.613676
H	2.259592	1.779594	-1.754050
H	0.858685	2.544457	-2.533486
H	-4.946148	0.207395	1.269194
H	-3.585132	-0.911573	1.602098
H	-3.564765	0.735130	2.271502
H	-4.866312	-0.119852	-1.430202
H	-3.416076	0.133474	-2.442597
H	-3.508043	-1.291041	-1.384630
H	-4.789108	2.325917	-0.382661
H	-3.412369	3.064561	0.469923
H	-3.346068	2.830458	-1.292412
N	6.370238	-2.724380	0.082405

5 (NC-Ar-Cl)

E = -718.090771784 a.u.

C	3.818611	-1.992286	0.119442
C	3.176609	-1.753395	-1.111611
C	1.921161	-1.140134	-1.142013
C	1.271872	-0.751433	0.044551
C	1.916034	-1.005100	1.269836
C	3.171451	-1.617620	1.313408
Pd	-0.619664	0.012996	-0.002214
P	-3.055568	0.497017	-0.033976
C	-3.885779	-0.224645	-1.462532
P	0.408104	2.096864	-0.116643
C	-0.655893	3.620582	-0.204820
Cl	-1.373968	-2.268771	0.123926
C	1.512335	2.506457	1.318318
C	1.519746	2.343893	-1.582738
C	-3.874777	2.174761	-0.129313
C	-3.880466	-0.387212	-1.443681
H	1.428021	-0.747100	2.205220
H	3.652217	-1.814652	2.266225
C	5.109084	-2.607740	0.156689
H	3.661358	-2.055436	-2.034438
H	1.437196	-0.988254	-2.102417
H	1.991409	3.480324	1.169023
H	0.920785	2.533138	2.238772
H	2.277023	1.733015	1.420157
H	-0.028450	4.517672	-0.253679
H	-1.290910	3.580653	-1.093942
H	-1.295236	3.680315	0.680077
H	1.997971	3.328662	-1.540944
H	2.284994	1.564403	-1.593445
H	0.932977	2.266978	-2.503428
H	-4.976501	-0.195277	1.361760
H	-3.543888	-1.257105	1.566368
H	-3.589928	0.336588	2.355043
H	-4.971540	-0.347167	-1.350687
H	-3.581401	0.071174	-2.392114
H	-3.538279	-1.424699	-1.430588
H	-4.964798	2.061988	-0.125055
H	-3.582946	2.789579	0.727647
H	-3.579601	2.690305	-1.048349
N	6.173365	-3.105542	0.187081

5 (NC-Ar-I)

E = -714.526602577 a.u.

C	4.251816	-0.169334	0.226625
C	3.588506	-0.153768	-1.016652
C	2.198203	-0.026343	-1.070641
C	1.429698	0.088167	0.103929

C	2.101313	0.058231	1.341051	H	-3.170006	0.420497	2.347399
C	3.491645	-0.068770	1.408111	H	-4.572343	-0.185295	-1.358506
Pd	-0.612361	0.236253	0.011483	H	-3.157433	0.151101	-2.396742
P	-3.090587	0.058741	-0.096611	H	-3.206886	-1.346083	-1.440613
C	-3.817853	-0.864105	1.344253	H	-4.469447	2.183602	-0.135936
C	5.675665	-0.287693	0.287053	H	-3.065555	2.863975	0.719698
P	-0.225710	2.569182	0.015842	H	-3.060821	2.763123	-1.055643
C	-1.633286	3.766760	-0.217094				
I	-0.560098	-2.483619	0.070945				
C	0.522790	3.200055	1.594282				
C	0.959943	3.181740	-1.276717				
C	-4.255692	1.520503	-0.171477				
C	-3.683957	-0.912889	-1.566326				
H	1.536823	0.105285	2.267706				
H	3.992721	-0.099171	2.370300				
H	4.165174	-0.249393	-1.931057				
H	1.710458	-0.040235	-2.040759				
H	0.734202	4.272273	1.518100				
H	-0.169630	3.026664	2.424069				
H	1.449781	2.657989	1.794511				
H	-1.254906	4.794904	-0.195210				
H	-2.121585	3.588280	-1.179007				
H	-2.370000	3.642247	0.580110				
H	1.124888	4.258706	-1.161809				
H	1.909970	2.651585	-1.185347				
H	0.547906	2.984702	-2.271543				
H	-4.891763	-1.027424	1.199838				
H	-3.304484	-1.823322	1.442712				
H	-3.660209	-0.288769	2.262526				
H	-4.767090	-1.071399	-1.516589				
H	-3.439832	-0.370261	-2.485501				
H	-3.166588	-1.874935	-1.582954				
H	-5.292264	1.169006	-0.225457				
H	-4.144374	2.140980	0.722751				
H	-4.046712	2.132008	-1.053792				
N	6.846260	-0.381034	0.336858				

5 (Ph-Br)

E = -624.093699391 a.u.

C	3.685146	-1.611311	-1.108740
C	2.398096	-1.052663	-1.144003
C	1.737648	-0.694415	0.043830
C	2.391716	-0.916577	1.267888
C	3.678767	-1.475258	1.302475
C	4.331930	-1.820121	0.114206
Pd	-0.175744	0.035708	-0.002501
P	0.865380	2.127166	-0.117895
C	1.972701	2.531483	1.317247
Br	-0.929043	-2.401917	0.133605
P	-2.613983	0.550892	-0.038266
C	-3.375890	2.258229	-0.137258
C	-3.485143	-0.289490	-1.449301
C	-3.492824	-0.124629	1.454211
C	1.980107	2.367764	-1.583757
C	-0.177436	3.667308	-0.207438
H	1.893708	-0.679383	2.204378
H	4.163292	-1.648534	2.259809
H	5.326293	-2.255486	0.141402
H	4.174659	-1.891033	-2.037939
H	1.905109	-0.922465	-2.103847
H	2.461764	3.500309	1.166473
H	1.379016	2.565786	2.236334
H	2.726551	1.747947	1.421012
H	0.462570	4.555468	-0.255871
H	-0.812387	3.635875	-1.096867
H	-0.816945	3.735876	0.676627
H	2.468704	3.347527	-1.540445
H	2.734233	1.577725	-1.594864
H	1.391123	2.298294	-2.503884
H	-4.579504	-0.031749	1.346475
H	-3.214808	-1.175322	1.566657

5 (Ph-Cl)

E = -625.875465338 a.u.

C	3.559402	-1.875899	-1.122501
C	2.293027	-1.270422	-1.137040
C	1.646261	-0.928826	0.062943
C	2.292691	-1.211742	1.278269
C	3.559163	-1.815760	1.292187
C	4.198593	-2.146177	0.092015
Pd	-0.254865	-0.180428	0.027134
P	0.782648	1.894970	-0.093069
C	1.976783	2.257675	1.282095
Cl	-1.026276	-2.454079	0.247319
P	-2.694080	0.310375	-0.067003
C	-3.499238	1.983657	-0.299957
C	-3.495260	-0.657002	-1.436623
C	-3.575444	-0.307357	1.447469
C	1.804363	2.184166	-1.616039
C	-0.274240	3.427887	-0.060255
H	1.803571	-0.986380	2.222176
H	4.038579	-2.036227	2.242367
H	5.176799	-2.617429	0.103829
H	4.038374	-2.142768	-2.060955
H	1.804328	-1.091206	-2.091490
H	2.447642	3.236236	1.136238
H	1.441827	2.252748	2.237129
H	2.740641	1.477575	1.310960
H	0.354100	4.324874	-0.099217
H	-0.953915	3.429831	-0.916337
H	-0.867940	3.447677	0.858241
H	2.300744	3.159804	-1.570305
H	2.552914	1.392431	-1.696214
H	1.161174	2.146774	-2.500885
H	-4.662652	-0.280272	1.312632
H	-3.243498	-1.332975	1.627711
H	-3.302805	0.309027	2.310555
H	-4.587929	-0.597383	-1.376717
H	-3.164040	-0.267005	-2.404853
H	-3.166383	-1.694866	-1.344754
H	-4.590433	1.882447	-0.317894
H	-3.221813	2.656567	0.516997
H	-3.173942	2.428195	-1.246078

5 (Ph-I)

E = -622.311674734 a.u.

C	2.198844	-0.182816	-1.148666
C	1.530347	0.159101	0.039896
C	2.192552	-0.046815	1.262822
C	3.493034	-0.573430	1.295609
C	4.152887	-0.902734	0.106616
C	3.499317	-0.709421	-1.115277
Pd	-0.394109	0.871553	-0.005413
I	-1.128787	-1.751358	0.141333
P	-2.829907	1.403441	-0.042197
P	0.648001	2.984358	-0.122191
C	1.766168	3.223730	-1.586642
C	-0.379125	4.537251	-0.212437
C	1.759066	3.387498	1.311416
C	-3.727460	0.595330	-1.457303
C	-3.735526	0.760079	1.450156
C	-3.548354	3.129303	-0.142026
H	1.689622	0.174433	2.200504
H	3.982140	-0.735928	2.252484
H	5.156889	-1.315378	0.132507

H	3.993338	-0.978351	-2.045256	C	3.497844	-0.648390	-0.976064
H	1.700865	-0.068559	-2.107886	C	2.109765	-0.430755	-1.042755
H	2.246850	4.356633	1.158685	C	1.333065	-0.302023	0.116227
H	1.168626	3.421917	2.232592	C	1.982317	-0.404168	1.361673
H	2.513959	2.604791	1.412453	C	3.360922	-0.619030	1.443067
H	0.273274	5.416535	-0.260430	Pd	-0.703457	-0.150227	0.011341
H	-1.013354	4.515925	-1.102623	P	-3.177472	-0.406098	-0.107106
H	-1.017810	4.616050	0.671313	C	-3.800400	-1.430517	1.312484
H	2.253481	4.204029	-1.541695	O	5.491487	-0.946972	0.460093
H	2.521327	2.434829	-1.595154	C	6.321931	-1.164767	-0.706128
H	1.180243	3.153984	-2.508705	P	-0.323626	2.138468	0.023347
H	-4.817780	0.891384	1.337639	C	-1.788984	3.286894	-0.022846
H	-3.498088	-0.299462	1.573329	Cl	-0.761368	-2.562553	-0.010963
H	-3.396598	1.299082	2.341203	C	0.598735	2.795652	1.494903
H	-4.810275	0.738236	-1.366374	C	0.675421	2.771961	-1.407740
H	-3.383377	1.030277	-2.401649	C	-4.459268	0.956385	-0.152983
H	-3.489739	-0.471281	-1.458635	C	-3.669987	-1.408524	-1.592101
H	-4.643126	3.080013	-0.142243	H	1.409817	-0.341038	2.283163
H	-3.223868	3.726004	0.715625	H	3.863837	-0.710179	2.399757
H	-3.218991	3.625323	-1.059849	H	4.063038	-0.755099	-1.894949
				H	1.641405	-0.392093	-2.022774
				H	0.764995	3.874014	1.394006
				H	0.019504	2.603654	2.403581
				H	1.557710	2.279637	1.579634
				H	-1.455352	4.330806	-0.014887
				H	-2.373849	3.105616	-0.928719
				H	-2.427753	3.109829	0.846931
				H	0.846358	3.850051	-1.313018
				H	1.632610	2.246440	-1.435047
				H	0.141810	2.571270	-2.342131
				H	-4.847141	-1.719435	1.164536
				H	-3.168352	-2.319220	1.380166
				H	-3.710206	-0.861788	2.243999
				H	-4.725014	-1.700630	-1.541719
				H	-3.499022	-0.825709	-2.503365
				H	-3.032254	-2.295485	-1.616256
				H	-5.466920	0.528274	-0.204216
				H	-4.386429	1.574646	0.747192
				H	-4.304125	1.593802	-1.029097
				H	7.325709	-1.334953	-0.317018
				H	5.992206	-2.043501	-1.274015
				H	6.327664	-0.287825	-1.366012

5 (MeO-Ar-Br)

E = -738.576067091 a.u.

C	4.191323	-0.445829	0.229554
C	3.547911	-0.388936	-1.010938
C	2.152605	-0.219320	-1.060241
C	1.387243	-0.105046	0.108060
C	2.056087	-0.176997	1.345149
C	3.442479	-0.343773	1.409357
Pd	-0.654380	0.038735	0.015429
P	-3.131960	-0.166092	-0.107049
C	-3.827381	-1.120164	1.328960
O	5.570433	-0.601936	0.399558
C	6.393804	-0.785846	-0.777605
P	-0.256343	2.342880	0.022109
C	-1.695875	3.519685	-0.101341
Br	-0.673042	-2.516085	0.048610
C	0.594685	2.985107	1.543146
C	0.827658	2.970334	-1.349718
C	-4.352236	1.249987	-0.204368
C	-3.666181	-1.176073	-1.574131
H	1.493656	-0.128894	2.273575
H	3.960619	-0.410440	2.359906
H	4.103716	-0.484806	-1.936704
H	1.669974	-0.203020	-2.033874
H	0.784422	4.060401	1.451738
H	-0.035869	2.803476	2.419257
H	1.539615	2.453972	1.678157
H	-1.340756	4.556342	-0.084245
H	-2.241436	3.345049	-1.032717
H	-2.378011	3.363175	0.738534
H	0.996318	4.047646	-1.242792
H	1.782238	2.440751	-1.324229
H	0.347460	2.773800	-2.313613
H	-4.887482	-1.350359	1.173181
H	-3.253375	-2.044511	1.432030
H	-3.716071	-0.534092	2.247301
H	-4.739050	-1.395883	-1.531703
H	-3.445510	-0.628021	-2.496201
H	-3.091393	-2.105408	-1.573763
H	-5.375761	0.863047	-0.265810
H	-4.269368	1.883936	0.683875
H	-4.154224	1.861161	-1.090285
H	7.409141	-0.911634	-0.401917
H	6.095048	-1.679036	-1.339991
H	6.352414	0.089437	-1.438454

5 (MeO-Ar-Cl)

E = -740.357813228 a.u.

C	4.121404	-0.738888	0.272361
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5 (MeO-Ar-I)

E = -736.793853867 a.u.

C	3.594089	-0.134186	-1.022158
C	2.194809	-0.002282	-1.070282
C	1.428117	0.106375	0.098142
C	2.102069	0.066585	1.334205
C	3.492649	-0.062406	1.397282
C	4.241740	-0.159588	0.217335
Pd	-0.620136	0.234360	0.007542
P	-0.218186	2.558628	0.015421
C	0.592675	3.192458	1.562267
I	-0.577222	-2.492642	0.050377
P	-3.103198	0.058959	-0.102543
C	-4.272229	1.518826	-0.183789
C	-3.696549	-0.916537	-1.571085
C	-3.836823	-0.865108	1.335434
C	0.914742	3.175584	-1.321992
C	-1.631678	3.762729	-0.155444
H	1.540999	0.107748	2.263757
H	4.013731	-0.105154	2.347586
O	5.624372	-0.279685	0.385791
H	4.149849	-0.227514	-1.948186
H	1.710438	-0.011767	-2.043032
H	0.799465	4.264932	1.475394
H	-0.066622	3.020538	2.419042
H	1.526166	2.649580	1.725936
H	-1.253076	4.790962	-0.134230

H	-2.153782	3.595578	-1.101555	C	-2.885558	-0.920439	-0.000482
H	-2.340730	3.628095	0.665305	C	-3.360008	0.397112	-0.000575
H	1.091381	4.250866	-1.207287	Br	1.283881	-0.424214	0.001362
H	1.862202	2.635336	-1.271141	H	-1.135684	-2.181513	0.000221
H	0.459595	2.986866	-2.299607	H	-3.566735	-1.762301	-0.000908
H	-4.907718	-1.041093	1.182554	O	-4.704753	0.747925	-0.001338
H	-3.312811	-1.818062	1.441276	H	-2.849220	2.479912	-0.000437
H	-3.693565	-0.284586	2.252873	H	-0.385409	2.060688	0.000650
H	-4.780103	-1.073846	-1.524705	C	-5.702787	-0.306690	-0.002074
H	-3.447995	-0.377630	-2.491439	H	-6.662088	0.209134	-0.003359
H	-3.179045	-1.878730	-1.581891	H	-5.618197	-0.933300	-0.897819
H	-5.309555	1.167975	-0.228123	H	-5.620293	-0.932616	0.894340
H	-4.153525	2.148974	0.702740				
H	-4.067386	2.121460	-1.073468				
C	6.448961	-0.465214	-0.790456				
H	7.467434	-0.563936	-0.415232				
H	6.167488	-1.373307	-1.337640				
H	6.388141	0.398351	-1.465044				

Ph-Br

E = -244.775300672 a.u.

C	0.025002	0.000003	0.014435
C	0.008089	0.000005	1.412738
C	1.225614	0.000006	2.105009
C	2.439244	0.000005	1.408298
C	2.435799	0.000003	0.008908
C	1.227512	0.000002	-0.699364
H	-0.933505	0.000005	1.949117
H	1.219832	0.000008	3.190376
H	3.378730	0.000006	1.950711
H	3.372863	0.000003	-0.538782
H	1.221232	0.000001	-1.782998
Br	-1.643626	0.000001	-0.948948

Ph-Cl

E = -246.562709643 a.u.

C	0.015454	0.000003	0.008922
C	-0.003469	0.000005	1.406623
C	1.213544	0.000006	2.098622
C	2.427133	0.000005	1.401306
C	2.424232	0.000004	0.001649
C	1.216437	0.000002	-0.706316
H	-0.948023	0.000005	1.937762
H	1.208669	0.000007	3.183881
H	3.366579	0.000006	1.943695
H	3.361657	0.000003	-0.545202
H	1.204139	0.000001	-1.789893
Cl	-1.509566	0.000001	-0.871549

Ph-I

E = -242.989133104 a.u.

C	-1.252027	1.219016	0.000502
C	-0.563312	-0.000065	0.000402
C	-1.252114	-1.219073	0.000500
C	-2.652956	-1.209944	0.000119
C	-3.355350	0.000052	-0.000674
C	-2.652876	1.210000	0.000117
I	1.558803	0.000000	-0.000108
H	-0.711835	-2.158677	0.001218
H	-3.190538	-2.152976	-0.000531
H	-4.440274	0.000069	-0.001431
H	-3.190381	2.153076	-0.000535
H	-0.711697	2.158586	0.001218

MeO-Ar-Br

E = -359.258072480 a.u.

C	-2.455763	1.470354	-0.000247
C	-1.082948	1.231661	0.000350
C	-0.613522	-0.089402	0.000562
C	-1.504551	-1.162605	0.000128

MeO-Ar-Cl

E = -361.045237968 a.u.

C	-2.442496	1.467488	-0.000349
C	-1.070568	1.225978	0.000445
C	-0.606058	-0.095980	0.000654
C	-1.497353	-1.167849	0.000107
C	-2.877607	-0.922691	-0.000692
C	-3.349294	0.396089	-0.000927
Cl	1.127357	-0.405332	0.001644
H	-1.124751	-2.185572	0.000287
H	-3.560583	-1.762976	-0.001107
O	-4.693468	0.750322	-0.001623
H	-2.834509	2.477633	-0.000520
H	-0.366963	2.049949	0.000885
C	-5.692963	-0.301525	-0.002023
H	-6.651764	0.215389	-0.002599
H	-5.610815	-0.928718	-0.897789
H	-5.611799	-0.928499	0.893984

MeO-Ar-I

E = -357.472223117 a.u.

C	-2.470040	1.473949	0.000494
C	-1.096386	1.237346	0.000854
C	-0.621118	-0.083466	0.000314
C	-1.514879	-1.156350	-0.000593
C	-2.896298	-0.916704	-0.000953
C	-3.372896	0.399788	-0.000351
I	1.466474	-0.455491	0.000860
H	-1.151437	-2.177191	-0.001033
H	-3.575675	-1.760104	-0.001674
O	-4.718111	0.747215	-0.000790
H	-2.864739	2.483165	0.000857
H	-0.405650	2.072471	0.001520
C	-5.713329	-0.310521	-0.002029
H	-6.674056	0.202514	-0.003516
H	-5.626505	-0.936621	-0.897855
H	-5.628992	-0.936295	0.894271

NC-Ar-Br

E = -336.984947850 a.u.

C	1.245786	0.000002	-0.689221
C	0.040700	0.000003	0.023667
C	0.028768	0.000005	1.423752
C	1.239089	0.000006	2.117976
C	2.461615	0.000005	1.418070
C	2.453606	0.000004	0.009302
Br	-1.621691	0.000001	-0.933827
H	-0.910475	0.000005	1.963453
H	1.241388	0.000007	3.202024
C	3.701709	0.000007	2.131683
H	3.392477	0.000003	-0.532615
H	1.241313	0.000001	-1.772474
N	4.721113	0.000008	2.714753

NC-Ar-Cl

E = -338.772476395 a.u.

C	1.235243	0.000002	-0.696275
C	0.032873	0.000003	0.019210

C	0.017958	0.000005	1.418267
C	1.228346	0.000006	2.111729
C	2.450720	0.000006	1.411100
C	2.442748	0.000004	0.002174
Cl	-1.485521	0.000001	-0.854891
H	-0.924309	0.000005	1.952498
H	1.231922	0.000007	3.195710
C	3.690791	0.000007	2.124908
H	3.381941	0.000003	-0.539067
H	1.224027	0.000001	-1.779393
N	4.708660	0.000008	2.710572

NC-Ar-I

E = -335.198726288 a.u.

C	-2.638281	1.179473	0.000141
C	-1.230144	1.186948	0.000078
C	-0.518124	-0.013804	0.000181
C	-1.215167	-1.229685	0.000388
C	-2.616497	-1.253332	0.000524
C	-3.324501	-0.050232	0.000420
I	-0.140019	-3.049867	0.000590
C	-3.366345	2.411243	0.000032
N	-3.965737	3.420969	-0.000071
H	-3.152468	-2.194735	0.000695
H	-4.408586	-0.060301	0.000521
H	-0.698064	2.131533	-0.000087
H	0.565056	0.001258	0.000086

TS1-5 (NC-Ar-Br)

E = -716.254877197 a.u.

C	-2.331109	-0.359046	-1.077316
C	-3.515735	-0.204734	-0.373692
C	-3.638654	-0.679673	0.958564
C	-2.547626	-1.349115	1.546078
C	-1.354767	-1.527288	0.841669
C	-1.204564	-0.950758	-0.446004
Br	0.097412	-2.022694	-1.741276
Pd	0.657016	0.098336	-0.118837
P	-0.075200	2.396643	-0.272086
C	1.233490	3.716203	-0.071085
P	2.905793	-0.306761	0.814720
C	3.077843	-1.811871	1.911027
C	4.234659	-0.648867	-0.450959
C	3.751690	0.978891	1.876441
C	-0.926379	3.007401	-1.820031
C	-1.303620	2.920974	1.031913
H	-2.252950	-0.016073	-2.102337
H	-4.365674	0.278337	-0.844636
C	-4.859245	-0.509376	1.675511
H	-2.647750	-1.757063	2.546492
H	-0.553544	-2.116722	1.272097
H	-1.228183	4.057344	-1.725569
H	-0.248748	2.902326	-2.673506
H	-1.814631	2.397022	-2.007428
H	-1.590751	3.973151	0.917905
H	-2.196263	2.292800	0.957607
H	-0.864134	2.773289	2.023535
H	0.799342	4.723050	-0.088867
H	1.752835	3.566790	0.880850
H	1.964933	3.627583	-0.881241
H	4.734061	0.634794	2.221516
H	3.878459	1.901671	1.301003
H	3.123528	1.199717	2.745761
H	5.191085	-0.900073	0.022695
H	3.914829	-1.480983	-1.086260
H	4.367765	0.232489	-1.086593
H	4.115934	-1.960786	2.232113
H	2.442980	-1.693511	2.795290
H	2.740838	-2.696652	1.361399
N	-5.864417	-0.358907	2.268164

TS1-5 (NC-Ar-Cl)

E = -718.034323998 a.u.

C	-2.225771	-0.662793	-1.327229
C	-3.485444	-0.394402	-0.816056
C	-3.796091	-0.660352	0.543956
C	-2.805488	-1.245111	1.362332
C	-1.539846	-1.535496	0.858631
C	-1.204981	-1.159663	-0.470031
Cl	0.054576	-2.389245	-1.344612
Pd	0.703312	-0.151321	-0.215009
P	-0.066193	2.118505	-0.305477
C	1.194747	3.466245	-0.013924
P	3.056721	-0.444746	0.521640
C	3.373593	-1.921927	1.621551
C	4.258894	-0.782176	-0.866966
C	3.969998	0.886321	1.464055
C	-0.858803	2.727865	-1.882642
C	-1.370135	2.568444	0.949545
H	-2.005118	-0.483336	-2.373144
H	-4.253544	0.016639	-1.463250
C	-5.092480	-0.374955	1.059942
H	-3.044803	-1.495317	2.390750
H	-0.810209	-2.047627	1.475510
H	-1.211692	3.760892	-1.780927
H	-0.132358	2.673412	-2.699938
H	-1.706956	2.082606	-2.129221
H	-1.682291	3.614482	0.846945
H	-2.238025	1.916422	0.815139
H	-0.975204	2.407613	1.957748
H	0.736120	4.461934	-0.039249
H	1.667199	3.313858	0.961773
H	1.969806	3.410731	-0.785678
H	4.995906	0.580621	1.701497
H	3.999505	1.802052	0.864887
H	3.436330	1.101931	2.395664
H	5.267384	-0.988531	-0.489273
H	3.905115	-1.643617	-1.442524
H	4.295272	0.082743	-1.537227
H	4.442666	-2.050173	1.829492
H	2.837096	-1.793028	2.567340
H	2.990356	-2.822209	1.130613
N	-6.161401	-0.128936	1.487210

TS1-5 (NC-Ar-I)

E = -714.475905166 a.u.

C	0.599456	-2.269959	0.958826
C	1.150216	-3.320559	0.240188
C	0.712647	-3.603287	-1.079815
C	-0.314105	-2.824887	-1.641874
C	-0.890938	-1.773273	-0.919639
C	-0.380273	-1.433930	0.360077
I	-1.849396	-0.406829	1.771321
Pd	0.059407	0.639190	-0.141722
P	2.401660	0.890762	0.449484
C	3.166494	2.572453	0.154347
P	-1.040314	2.434172	-1.392810
C	-0.114467	3.331267	-2.747082
C	-2.627039	2.019535	-2.292395
C	-1.609863	3.872699	-0.346779
C	2.936117	0.601747	2.218630
C	3.617374	-0.197478	-0.459826
H	0.926348	-2.074524	1.973507
H	1.920677	-3.939296	0.688361
C	1.289495	-4.683206	-1.813050
H	-0.684505	-3.063267	-2.633387
H	-1.745002	-1.246703	-1.327504
H	4.012722	0.767410	2.346291
H	2.385365	1.279350	2.178899
H	2.698064	-0.426095	2.509177
H	4.644978	-0.035709	-0.112828

H	3.343706	-1.246152	-0.308233
H	3.561569	0.015970	-1.532199
H	4.229673	2.588561	0.423449
H	3.060928	2.834932	-0.903470
H	2.634890	3.321684	0.750451
H	-2.135159	4.626655	-0.945256
H	-2.278462	3.501757	0.436562
H	-0.743653	4.335641	0.136814
H	-3.072620	2.907089	-2.757779
H	-2.420548	1.274810	-3.068235
H	-3.339866	1.588536	-1.581953
H	-0.724212	4.123593	-3.197809
H	0.797159	3.772820	-2.331601
H	0.175419	2.615906	-3.523707
N	1.772413	-5.569208	-2.417162

TS1-5 (Ph-Br)

E = -624.039050071 a.u

C	-3.498908	-0.459660	-1.598757
C	-4.165300	-0.293499	-0.370283
C	-3.484346	-0.555233	0.820792
C	-2.142205	-0.971411	0.804291
C	-1.457957	-1.044329	-0.428124
C	-2.161906	-0.854746	-1.639467
Br	0.101709	-2.546674	-0.505171
Pd	0.326505	0.093346	0.099666
P	1.993028	0.182746	1.904884
P	0.053275	2.038899	-1.306851
C	3.367552	-1.069274	1.728685
C	2.984930	1.733688	2.239583
C	1.398364	-0.204106	3.636798
C	-0.000770	1.847085	-3.167500
C	-1.521638	3.002788	-1.019856
C	1.320705	3.407926	-1.161385
H	-1.656624	-1.007164	-2.586417
H	-4.030630	-2.288314	-2.530687
H	-5.209173	0.001885	-0.351738
H	-3.999845	-0.471179	1.773331
H	-1.643611	-1.251529	1.725396
H	-0.168049	2.808324	-3.668670
H	0.944900	1.418697	-3.515417
H	-0.808666	1.159280	-3.434600
H	-1.599508	3.864475	-1.694212
H	-2.377751	2.339298	-1.175131
H	-1.546250	3.352948	0.017253
H	1.072983	4.263094	-1.802201
H	1.370935	3.742309	-0.120004
H	2.305230	3.021282	-1.445617
H	3.707342	1.585232	3.051413
H	3.521605	2.023998	1.330505
H	2.304155	2.547481	2.510784
H	4.045685	-1.055118	2.590406
H	2.927454	-2.066191	1.625790
H	3.936380	-0.856214	0.817733
H	2.224460	-0.206980	4.358660
H	0.656949	0.541609	3.942148
H	0.917293	-1.187580	3.638478

TS1-5 (Ph-Cl)

E = -625.817260771 a.u

C	1.128390	-3.729604	0.683232
C	1.534291	-3.928473	-0.649490
C	0.942919	-3.169441	-1.664421
C	-0.033628	-2.206800	-1.366855
C	-0.357843	-1.948283	-0.017442
C	0.170890	-2.768115	1.006262
Cl	-2.300518	-1.424517	0.265653
Pd	-0.323491	0.222143	0.059602
P	-1.327045	2.223336	-1.001780
P	1.781955	0.526102	1.169774
C	-2.743547	2.972024	-0.041831

C	-0.330316	3.754898	-1.402492
C	-2.154582	1.915226	-2.650347
C	2.042137	-0.202651	2.871563
C	3.245558	-0.194858	0.261314
C	2.376484	2.274955	1.464306
H	-0.160751	-2.633614	2.029657
H	1.555960	-4.338171	1.475481
H	2.269378	-4.689384	-0.889561
H	1.214780	-3.342160	-2.702027
H	-0.541430	-1.671226	-2.161394
H	3.066471	-0.040143	3.228219
H	1.338048	0.254112	3.574772
H	1.842069	-1.277252	2.830897
H	4.180568	-0.041164	0.813720
H	3.079371	-1.266672	0.115454
H	3.327494	0.275099	-0.724081
H	3.374067	2.295824	1.919769
H	2.406501	2.809497	0.509268
H	1.671061	2.790197	2.125011
H	-0.947484	4.531258	-1.870703
H	0.107287	4.153072	-0.481050
H	0.485915	3.487781	-2.082032
H	-3.227608	3.785868	-0.594920
H	-3.479017	2.189409	0.170480
H	-2.371845	3.356685	0.913582
H	-2.673165	2.807898	-3.021032
H	-1.401281	1.607585	-3.383192
H	-2.875167	1.098862	-2.536836

TS1-5 (Ph-I)

E = -622.261192673 a.u

C	0.985732	-3.891291	0.830967
C	0.480743	-4.213797	-0.442185
C	-0.525771	-3.427438	-1.003332
C	-1.034578	-2.312502	-0.311900
C	-0.466058	-1.948184	0.928800
C	0.507806	-2.781471	1.527465
I	-1.877258	-0.799740	2.376051
Pd	-0.011278	0.127344	0.401820
P	-1.121986	1.893689	-0.867444
P	2.361587	0.346237	0.885014
C	-2.464619	1.395270	-2.073563
C	-2.054841	3.128971	0.178464
C	-0.125852	3.048590	-1.951974
C	2.997231	0.008566	2.613165
C	3.513748	-0.736765	-0.112212
C	3.138203	2.022916	0.587244
C	0.884433	-2.548513	2.517130
H	1.751684	-4.514585	1.283957
H	0.852481	-5.086164	-0.969782
H	-0.950508	-3.690490	-1.967885
H	-1.876120	-1.760869	-0.713864
H	4.082885	0.150985	2.681147
H	2.499518	0.681167	3.319236
H	2.754165	-1.020727	2.894478
H	4.563346	-0.585293	0.168347
H	3.241612	-1.784911	0.046548
H	3.388244	-0.510785	-1.176204
H	4.213686	2.021072	0.803706
H	2.982198	2.308823	-0.458053
H	2.645535	2.765572	1.223852
H	-2.578271	3.871117	-0.436382
H	-2.779789	2.592471	0.798848
H	-1.353578	3.641634	0.844902
H	-2.931585	2.268679	-2.545493
H	-2.035705	0.753730	-2.850522
H	-3.230658	0.823774	-1.539324
H	-0.760377	3.799790	-2.438009
H	0.627455	3.556817	-1.341059
H	0.392461	2.465121	-2.720238

TS1-5 (MeO-Ar-Br)

E = -738.520229796 a.u.

C	-0.559207	-1.343987	0.351654
C	0.282517	-2.221833	1.062354
C	0.811267	-3.351542	0.430843
C	0.462014	-3.640501	-0.900295
C	-0.434669	-2.811554	-1.583306
C	-0.977647	-1.686577	-0.953437
O	0.933048	-4.744293	-1.614619
C	1.805884	-5.685181	-0.942268
Br	-2.098908	-0.360768	1.560026
Pd	-0.117454	0.768443	0.095287
P	-1.193525	2.703502	-0.981937
C	-2.093885	3.838081	0.196937
P	2.264479	0.823422	0.492351
C	3.283309	-0.202055	-0.692093
C	3.132097	2.475001	0.343645
C	2.963040	0.239447	2.127646
C	-0.205543	3.947274	-1.972129
C	-2.563706	2.327204	-2.199723
H	0.528257	-2.015246	2.097750
H	1.479852	-3.999181	0.986070
H	-0.722656	-3.078686	-2.593838
H	-1.726510	-1.090176	-1.461570
H	4.058892	0.286121	2.141339
H	2.565297	0.862834	2.935132
H	2.646592	-0.793222	2.303689
H	4.355335	-0.139826	-0.467896
H	2.958108	-1.245030	-0.628502
H	3.107854	0.147326	-1.714697
H	4.216808	2.381262	0.477800
H	2.927806	2.899230	-0.644831
H	2.735330	3.160171	1.100345
H	-2.638081	4.628731	-0.333566
H	-2.797963	3.244328	0.788552
H	-1.373388	4.294171	0.883761
H	-3.041611	3.242480	-2.570224
H	-2.153575	1.768269	-3.047414
H	-3.316129	1.702642	-1.707324
H	-0.838273	4.755221	-2.359432
H	0.575112	4.377698	-1.336166
H	0.278729	3.437954	-2.812039
H	2.022553	-6.454955	-1.682471
H	2.741292	-5.207990	-0.624061
H	1.313516	-6.137816	-0.072738

TS1-5 (MeO-Ar-Cl)

E = -740.297707197 a.u.

C	-0.682012	-1.320257	0.679627
C	0.201470	-2.124235	1.426881
C	0.645978	-3.344440	0.907948
C	0.170373	-3.796450	-0.335439
C	-0.770713	-3.035932	-1.039922
C	-1.231013	-1.822118	-0.521748
O	0.551086	-5.000940	-0.935379
C	1.459228	-5.872870	-0.219752
Cl	-2.031798	-0.281926	1.818214
Pd	-0.316030	0.765851	0.203886
P	-1.390231	2.797893	-0.709049
C	-3.236629	2.916233	-0.444613
P	2.080271	0.705619	0.034954
C	2.737027	-0.533291	-1.197897
C	2.977788	2.254241	-0.509311
C	3.089324	0.256697	1.544506
C	-0.842212	4.432913	0.014777
C	-1.278803	3.179321	-2.536615
H	0.543068	-1.789644	2.399813
H	1.348282	-3.934848	1.485128
H	-1.157069	-3.425023	-1.975337
H	-2.011633	-1.272161	-1.035456
H	4.160319	0.200679	1.314307

H	2.926830	1.006819	2.325388
H	2.752773	-0.713114	1.922774
H	3.833629	-0.550147	-1.213267
H	2.359712	-1.526370	-0.935053
H	2.366333	-0.282425	-2.196964
H	4.059638	2.094032	-0.593668
H	2.586447	2.573231	-1.481104
H	2.790438	3.053135	0.216202
H	-3.641002	3.873444	-0.795648
H	-3.730062	2.097938	-0.979118
H	-3.451988	2.798131	0.622057
H	-1.810004	4.104152	-2.792274
H	-0.226668	3.278926	-2.823107
H	-1.709406	2.349300	-3.106320
H	-1.415052	5.272614	-0.397295
H	-0.975689	4.404930	1.101187
H	0.221495	4.586366	-0.194882
H	1.589805	-6.742726	-0.863118
H	2.431027	-5.391025	-0.052542
H	1.038592	-6.186631	0.743733

TS1-5 (MeO-Ar-I)

E = -736.743467879 a.u.

C	0.440534	-2.708716	1.209626
C	0.810995	-3.761576	0.361602
C	0.090938	-3.988608	-0.820586
C	-1.006339	-3.179163	-1.146976
C	-1.385132	-2.130806	-2.305383
C	-0.617630	-1.855625	0.847067
I	-1.674977	-0.730694	2.585506
Pd	0.235854	0.171876	0.368672
P	2.553692	0.325691	0.976802
C	3.405498	1.973708	0.717215
P	-1.133195	1.721563	-0.890732
C	-0.233153	2.868813	-2.064694
C	-2.529106	1.164763	-2.011148
C	-2.047751	2.965951	0.162712
C	3.107316	-0.030500	2.731058
C	3.719775	-0.788503	0.027681
H	0.966642	-2.555864	2.144006
H	1.644102	-4.395024	0.641786
O	0.372710	-5.008661	-1.726204
H	-1.561753	-3.397970	-2.051632
H	-2.264610	-1.542980	-0.533226
H	4.193028	0.080041	2.843858
H	2.601589	0.658595	3.415231
H	2.821312	-1.050965	3.006665
H	4.757599	-0.677181	0.365459
H	3.403845	-1.828950	0.154035
H	3.659340	-0.543721	-1.037949
H	4.471075	1.930128	0.975914
H	3.301067	2.268592	-0.332126
H	2.916669	2.733052	1.336683
H	-2.631068	3.668094	-0.445645
H	-2.716659	2.430239	0.843818
H	-1.326162	3.523900	0.768078
H	-3.019291	2.015950	-2.499678
H	-2.134885	0.488941	-2.777252
H	-3.272326	0.620024	-1.418960
H	-0.913170	3.587479	-2.539150
H	0.538031	3.413250	-1.509990
H	0.260216	2.273857	-2.840514
C	1.463265	-5.919281	-1.435392
H	1.482457	-6.618282	-2.270853
H	2.421754	-5.389303	-1.376217
H	1.289001	-6.465849	-0.500652

TS3-4 (NC-Ar-Br)

E = -590.008096091 a.u.

C	-2.066761	-3.138776	0.579295
C	-0.750262	-3.091421	1.085797

C	0.173225	-2.180236	0.573255
C	-0.234876	-1.274409	-0.430858
C	-1.535902	-1.340829	-0.976963
C	-2.448645	-2.257294	-0.454684
Pd	0.259072	0.624228	0.052601
Br	1.392261	-0.676902	-1.901312
P	0.616557	2.853429	0.864834
C	-0.845857	4.009168	0.815711
C	1.913696	3.852177	-0.024175
C	1.163503	3.022745	2.639369
H	-1.818561	-0.692617	-1.798229
H	-3.457823	-2.302614	-0.849600
C	-3.005076	-4.080246	1.103999
H	-0.455974	-3.776912	1.873167
H	1.194817	-2.172584	0.934979
H	2.013855	4.854630	0.407878
H	2.874483	3.332010	0.038248
H	1.641423	3.937462	-1.080667
H	1.310608	4.074037	2.912620
H	0.407540	2.582164	3.297018
H	2.102328	2.478938	2.783969
H	-0.581440	5.003046	1.194933
H	-1.202435	4.100817	-0.215056
H	-1.657066	3.595998	1.423433
N	-3.777829	-4.852001	1.538090

TS3-4 (NC-Ar-Cl)

E = -591.782599446 a.u.

C	-1.776308	-3.348764	0.394366
C	-0.415285	-3.263733	0.758786
C	0.394665	-2.253594	0.239158
C	-0.179433	-1.291417	-0.615283
C	-1.521020	-1.391576	-1.034293
C	-2.318689	-2.407259	-0.506762
Pd	0.374133	0.579588	-0.175039
Cl	1.184405	-0.591219	-2.196246
P	0.837603	2.800175	0.654908
C	-0.503355	4.075022	0.428540
C	2.305439	3.660511	-0.103041
C	1.203415	2.962164	2.476190
H	-1.923608	-0.693085	-1.758533
H	-3.360990	-2.484261	-0.796651
C	-2.597847	-4.390905	0.924672
H	0.002325	-3.997532	1.439596
H	1.449604	-2.211076	0.483703
H	2.446482	4.660886	0.322192
H	3.205242	3.062275	0.070500
H	2.154866	3.742446	-1.183862
H	1.406205	4.003970	2.750079
H	0.348197	2.597986	3.054232
H	2.073761	2.348221	2.728504
H	-0.195533	5.049530	0.824796
H	-0.731934	4.175638	-0.637107
H	-1.411260	3.747262	0.944632
N	-3.274557	-5.245415	1.364043

TS3-4 (NC-Ar-I)

E = -588.232613799 a.u.

C	-2.754741	-1.438838	-1.088408
C	-1.768355	-0.485936	-1.342460
C	-1.212876	0.254651	-0.267151
C	-1.699320	0.058354	1.051261
C	-2.686203	-0.898497	1.288405
C	-3.225639	-1.652213	0.224549
Pd	0.780364	-0.282967	-0.198434
P	2.978281	-1.147100	-0.051991
C	4.361968	0.099890	0.028266
I	-0.259162	2.287096	-0.756969
C	3.546228	-2.234578	-1.456948
C	3.366052	-2.220893	1.423122
H	-1.320468	0.661786	1.867760

H	-3.049916	-1.062024	2.297079
C	-4.241691	-2.625031	0.475061
H	-3.171117	-2.017620	-1.905774
H	-1.442026	-0.299595	-2.358897
H	5.340884	-0.389655	0.091385
H	4.329216	0.731694	-0.864810
H	4.220803	0.740933	0.904088
H	4.575200	-2.580650	-1.303674
H	2.882701	-3.101378	-1.536839
H	3.491075	-1.673337	-2.395042
H	4.406167	-2.567007	1.404413
H	3.193174	-1.651341	2.341731
H	2.697547	-3.087544	1.427008
N	-5.075157	-3.427545	0.681641

TS3-4 (Ph-Br)

E = -497.795693359 a.u.

C	-1.074748	-3.377841	1.218897
C	-0.114034	-2.493238	0.711142
C	-0.482403	-1.615820	-0.329418
C	-1.765237	-1.672336	-0.911978
C	-2.706231	-2.566782	-0.384825
C	-2.365005	-3.418117	0.674287
Pd	0.000035	0.296169	0.146453
P	0.335937	2.520041	0.936671
C	1.582119	3.548651	0.006580
Br	1.202016	-1.051508	-1.757348
C	0.944405	2.708860	2.690602
C	-1.144170	3.656787	0.943797
H	-2.010148	-1.043761	-1.760656
H	-3.702938	-2.605107	-0.814205
H	-3.096376	-4.118595	1.064063
H	-0.806704	-4.044890	2.032818
H	0.898517	-2.489787	1.098544
H	1.680770	4.551797	0.438020
H	2.553390	3.044850	0.031838
H	1.270650	3.631821	-1.039312
H	1.081666	3.763967	2.955327
H	0.221643	2.255968	3.376703
H	1.897891	2.182851	2.801508
H	-0.882292	4.653543	1.317913
H	-1.537726	3.746171	-0.073746
H	-1.927744	3.228544	1.576952

TS3-4 (Ph-Cl)

E = -499.570226959 a.u.

C	-0.960758	-3.562662	0.955087
C	-0.010776	-2.625429	0.527142
C	-0.371364	-1.723453	-0.490062
C	-1.611187	-1.807178	-1.148854
C	-2.541970	-2.754270	-0.700738
C	-2.221090	-3.628666	0.346146
Pd	0.153248	0.167430	-0.068631
P	0.507710	2.414168	0.697593
C	1.720585	3.439451	-0.278430
Cl	1.306731	-1.166598	-1.819873
C	1.168442	2.615694	2.430697
C	-0.976206	3.544912	0.740619
H	-1.832904	-1.158738	-1.988877
H	-3.512865	-2.815969	-1.183168
H	-2.942809	-4.369885	0.673479
H	-0.706445	-4.250742	1.755749
H	0.982843	-2.598312	0.959880
H	1.825250	4.446949	0.141071
H	2.694881	2.941004	-0.276340
H	1.378573	3.511168	-1.315582
H	1.307536	3.672994	2.685018
H	0.469872	2.162965	3.141524
H	2.127942	2.095741	2.515210
H	-0.706449	4.545178	1.099447
H	-1.399289	3.625831	-0.265709

H	-1.739650	3.119297	1.399632	C	-0.600094	-3.572896	0.639687
TS3-4 (Ph-I)				Pd	-0.003044	0.822392	-0.154549
E = -496.020064369 a.u.				P	1.332765	2.782291	0.177093
C	0.919503	-3.069814	-0.745441	C	2.445478	2.824239	1.675550
C	0.406952	-2.255291	-1.785365	Cl	-2.141686	0.501611	-1.392289
C	-0.984771	-2.229424	-2.050057	C	0.402884	4.387191	0.369104
C	-1.847479	-2.994929	-1.254623	C	2.534959	3.218063	-1.180814
C	-1.344165	-3.795961	-0.221773	H	-2.125316	-0.652473	1.531659
C	0.032634	-3.824749	0.033472	H	-1.747048	-2.990214	2.356446
Pd	0.831995	-0.315155	-1.151171	O	-0.477268	-4.846332	1.187852
I	1.823828	-1.675232	-3.480068	H	0.484558	-3.894728	-1.212172
P	1.164202	1.824370	-0.248527	H	0.113586	-1.591457	-2.042645
C	1.524217	1.935501	1.580304	H	3.004364	3.765698	1.734550
C	-0.245085	3.038184	-0.408830	H	1.839738	2.707990	2.579953
C	2.574583	2.826500	-0.948074	H	3.150824	1.988430	1.627734
H	-1.372091	-1.646193	-2.877556	H	1.085137	5.234925	0.503390
H	-2.914771	-2.970222	-1.453237	H	-0.212445	4.552732	-0.520711
H	-2.020203	-4.396214	0.378303	H	-0.263324	4.318258	1.234839
H	0.424727	-4.444182	0.834556	H	3.088765	4.134379	-0.945392
H	1.988368	-3.129430	-0.575495	H	3.242500	2.394416	-1.319220
H	2.641789	3.814139	-0.476185	H	1.985658	3.358314	-2.117074
H	3.513274	2.285719	-0.791475	C	0.239234	-5.863250	0.441249
H	2.428541	2.948246	-2.025968	H	0.203690	-6.754436	1.066769
H	1.669152	2.974400	1.900109	H	-0.245578	-6.067398	-0.520924
H	0.691847	1.497433	2.140105	H	1.282913	-5.572061	0.271792
H	2.427600	1.359833	1.805833	TS3-4 (MeO-Ar-I)			
H	0.008704	4.008949	0.033733	E = -610.503048978 a.u.			
H	-0.483344	3.176243	-1.468246	C	0.170579	-3.778929	0.026158
H	-1.130702	2.633492	0.091136	C	1.057864	-2.996556	-0.727433
TS3-4 (MeO-Ar-Br)				C	0.574049	-2.202671	-1.792671
E = -612.278281219 a.u.				C	-0.808387	-2.233230	-2.116120
C	0.042608	-3.166846	0.689200	C	-1.678907	-3.013872	-1.358721
C	0.448135	-2.090044	-0.112718	C	-1.193296	-3.789277	-0.292876
C	-0.484225	-1.097791	-0.469056	Pd	0.956298	-0.249204	-1.166488
C	-1.843067	-1.227411	-0.101156	P	1.217967	1.900394	-0.273350
C	-2.234218	-2.301652	0.695499	C	2.443525	3.031647	-1.110879
C	-1.295926	-3.269289	1.092001	I	2.039087	-1.625263	-3.448715
Pd	0.232109	0.752535	-0.035966	C	1.783070	2.020193	1.502703
P	1.030935	2.839724	0.780469	C	-0.298944	2.988615	-0.234578
C	2.881562	3.028672	0.923873	H	-1.182055	-1.668836	-2.962522
Br	-0.127695	-0.113616	-2.491242	H	-2.739617	-3.045445	-1.579674
C	0.480991	3.370011	2.484263	O	-2.150905	-4.538980	0.382378
C	0.591091	4.347748	-0.225019	H	0.559424	-4.372951	0.844331
H	-2.573385	-0.502338	-0.441147	H	2.119156	-3.028127	-0.509468
H	-3.263608	-2.418977	1.014202	H	2.491595	4.011733	-0.621271
O	-1.802028	-4.300760	1.876968	H	3.434362	2.566965	-1.089591
H	0.772931	-3.913408	0.976995	H	2.152946	3.163241	-2.157976
H	1.471503	-2.031470	-0.465645	H	1.869895	3.063962	1.827953
H	3.154542	4.022435	1.297838	H	1.066424	1.499580	2.145730
H	3.273616	2.266784	1.605036	H	2.755565	1.528415	1.606597
H	3.336885	2.875183	-0.059553	H	-0.078017	3.970725	0.200556
H	0.905507	4.343171	2.758366	H	-0.674016	3.122400	-1.254217
H	-0.611559	3.434178	2.508691	H	-1.080516	2.499497	0.355319
H	0.794932	2.619759	3.216965	C	-1.727634	-5.390152	1.478993
H	1.010914	5.260858	0.213353	H	-2.637929	-5.872126	1.833555
H	0.973699	4.223628	-1.242846	H	-1.014159	-6.150693	1.139938
H	-0.498118	4.440838	-0.280413	H	-1.280519	-4.802874	2.289911
C	-0.904669	-5.354858	2.311585	TS3-4 (MeO-Ar-Cl)			
H	-1.523255	-6.031035	2.900543	E = -614.052600545 a.u.			
H	-0.478714	-5.893621	1.456732	C	-0.064487	-3.191066	-0.598286
H	-0.095053	-4.957047	2.935199	C	-0.253713	-1.881769	-1.064859
TS3-4 (MeO-Ar-Cl)				C	-0.932644	-0.955815	-0.256659
E = -614.052600545 a.u.				C	-1.525763	-1.351618	0.960261
C	-0.064487	-3.191066	-0.598286	C	-1.331301	-2.655330	1.413093
C	-0.253713	-1.881769	-1.064859				
C	-0.932644	-0.955815	-0.256659				
C	-1.525763	-1.351618	0.960261				
C	-1.331301	-2.655330	1.413093				